The EM Algorithm is Adaptively-Optimal for Unbalanced Symmetric Gaussian Mixtures

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Abstract

This paper studies the problem of estimating the means $\pm \theta_* \in \mathbb{R}^d$ of a symmetric twocomponent Gaussian mixture $\delta_* \cdot N(\theta_*, I) + (1 - \delta_*) \cdot N(-\theta_*, I)$, where the weights δ_* and $1 - \delta_*$ are unequal. Assuming that δ_* is known, we show that the population version of the EM algorithm globally converges if the initial estimate has non-negative inner product with the mean of the larger weight component. This can be achieved by the trivial initialization $\theta_0 = 0$. For the empirical iteration based on n samples, we show that when initialized at $\theta_0 = 0$, the EM algorithm adaptively achieves the minimax error rate $\tilde{O}\left(\min\left\{\frac{1}{(1-2\delta_*)}\sqrt{\frac{d}{n}}, \frac{1}{\|\theta_*\|}\sqrt{\frac{d}{n}}, \left(\frac{d}{n}\right)^{1/4}\right\}\right)$ in no more than $O\left(\frac{1}{\|\theta_*\|}\sqrt{\frac{d}{n}}\right)$ iterations (with high probability). We also consider the EM iteration for estimating the weight δ_* , assuming a fixed mean θ (which is possibly mismatched to θ_*). For the empirical iteration of nsamples, we show that the minimax error rate $\tilde{O}\left(\frac{1}{\|\theta_*\|}\sqrt{\frac{d}{n}}\right)$ is achieved in no more than $O\left(\frac{1}{\|\theta_*\|^2}\right)$ iterations. These results robustify and complement recent results of Wu and Zhou (2019) obtained for the equal weights case $\delta_* = 1/2$.

Keywords: expectation-maximization, finite-sample guarantees, Gaussian mixtures, global convergence, parameter estimation

1. Introduction

The expectation-maximization (EM) algorithm developed by Dempster et al. (1977) is a heuristic formulated to approximate the maximum likelihood estimator (MLE) in parametric models $(X, S) \sim P_{\theta}(x, s)$ when X is observed, but S is latent. Remarkably, despite its simplicity, widespread use, and rich history (McLachlan and Krishnan, 2007; Gupta and Chen, 2011), no theoretical guarantees on its performance for finite number of iterations and samples were established until recently. Recently, Balakrishnan et al. (2017) obtained the first such explicit guarantees, and proved general bounds on the statistical precision, the convergence rate, and the basin of attraction (the distance of the initial estimate from the ground truth sufficient to obtain a statistically accurate solution). These bounds ap-

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ply to any latent variables model, yet require verifying several conditions for each concrete model. As a canonical example, these conditions were explicitly verified for the symmetric two-component Gaussian mixture (2-GM). The resulting guarantees are not sharp, however, both in the strong conditions required for their validity, as well as their distance from the accuracy guarantees of optimal algorithms. Consequently, a dedicated analysis of EM for 2-GM was conducted by various authors (Klusowski and Brinda, 2016; Wu et al., 2016; Xu et al., 2016; Daskalakis et al., 2017; Wu and Zhou, 2019; Dwivedi et al., 2020a, 2018, 2020b). The performance of EM for 2-GM with *balanced* components, i.e., when both weights equal 1/2, was by and large recently settled by Wu and Zhou (2019).

In this paper, we proceed in the direction of Wu and Zhou (2019), and sharply analyze a slight variation of the balanced 2-GM model—namely, the unbalanced symmetric 2-GM model. Some of the key arguments made by Wu and Zhou (2019) strongly depend on the symmetry properties of the EM iteration, which are a direct result of the symmetry in the model. It seems challenging to adapt these arguments to the unbalanced model, where symmetry breaks down due to the unequal weights. Our analysis therefore uses *indirect* arguments, which are based on *comparisons* between the EM iterations of unbalanced models for different weights. In particular, we compare the iterations for unbalanced models with the iterations for the *balanced* model, since the latter is already known to globally converge (Wu and Zhou, 2019). For the population iteration, we prove that increasing the larger of the two weights, that is, enhancing the model imbalance, makes the corresponding EM iteration converge faster. By contrast, this increase also increases our empirical error bound, i.e., the bound on the difference between the empirical iteration and the population iteration. As we prove, however, this does not result in deterioration of the statistical accuracy of the estimate because this increased error is compensated for by the improved convergence of the population iteration. Hence, the overall statistical accuracy actually improves when the model is more unbalanced.

1.1 EM for Two-Component Gaussian Mixture

The symmetric two-component Gaussian mixture (2-GM) model in $d \ge 1$ dimensions is given by

$$P_{\theta,\rho} = \frac{1+\rho}{2} \cdot N(\theta, I_d) + \frac{1-\rho}{2} \cdot N(-\theta, I_d).$$
(1)

The goal is to estimate the parameter $\theta_* \in \mathbb{R}^d$ from n samples $(X_1, \ldots, X_n) \stackrel{\text{i.i.d.}}{\sim} P_{\theta_*, \rho_*}$ under the ℓ_2 loss function $\ell(\theta, \theta_*) = \|\theta - \theta_*\|$ when $\rho_* \neq 0$ (unbalanced model), or under $\ell_0(\theta, \theta_*) = \min(\|\theta - \theta_*\|, \|\theta + \theta_*\|)$ when $\rho_* = 0$ (balanced model). The dimension d is allowed to be high, and both d and ρ_* may scale with the number of samples n. Based on the n samples and the value of ρ_* , the EM algorithm defines a mapping $f_n(\theta)$ which is iteratively applied to produce a sequence of estimates $\theta_t = f_n(\theta_{t-1})$ for all $t \geq 1$, given an initial guess θ_0 . This mapping f_n is described in detail later in the introduction. We will refer to $f_n(\theta)$ as the *empirical iteration*, and to the idealized operator $f(\theta)$ obtained by replacing empirical averages with expected values as the *population iteration*.

Balanced GM. The general results of Balakrishnan et al. (2017) specialized to the balanced 2-GM (1) ($\rho_* = 0$) require that the separation between the means is lower bounded as $\|\theta_*\| = \Omega(1)$, and that the initial estimate θ_0 is at most $\|\theta_*\|/4$ in ℓ_2 distance from θ_* .

When these two conditions hold, Balakrishnan et al. (2017) state that EM converges to a neighborhood of θ_* of radius $O(\sqrt{d/n})$ (i.e., parametric error rate), after no more than $O(1/||\theta_*||^2)$ iterations. The qualifying conditions above are problematic for several reasons: (1) Without knowing θ^* one has no way of knowing when the separation condition holds; (2) EM can be slow and inaccurate when there is no separation between the components (Redner and Walker, 1984) and in this case no guarantees are provided by Balakrishnan et al. (2017); (3) One of the main challenges in utilizing EM is the choice of initial guess. A common method is attempting multiple random guesses followed by a choice of the optimal converged solution (Karlis and Xekalaki, 2003). For a high-dimensional parameter vector, the guarantee of Balakrishnan et al. (2017) on the volume of the basin of attraction that ensures good convergence is negligible compared to the volume of the feasible set of parameter vectors, and hence randomly initializing is not proved to succeed.

These drawbacks have led to various attempts to sharpen the above results (Klusowski and Brinda, 2016; Wu et al., 2016; Xu et al., 2016; Daskalakis et al., 2017; Wu and Zhou, 2019), which will be discussed in more detail in Section 1.5. For the population iteration, various authors (Xu et al., 2016; Daskalakis et al., 2017; Wu and Zhou, 2019) proved global convergence to $\pm \theta_*$ at a geometric rate, unless the initial guess θ_0 is orthogonal to θ_* (in which case EM converges to the saddle point $\theta = 0$). For the empirical iteration, sharp high-probability guarantees were obtained by Wu and Zhou (2019) as follows: In the worst case, without any separation condition, the EM algorithm applied to (1) achieves an error rate of $\tilde{O}((d/n)^{1/4})$ in at most $O(\sqrt{n})$ iterations. If, however, a separation of $\|\theta_*\| = \Omega((\frac{\log^3 n \cdot d}{n})^{1/4})$ holds, then an error rate of $O(\frac{1}{\|\theta_*\|}\sqrt{\frac{\log^3 n \cdot d}{n}})$ is achieved by EM after no more than $O(\frac{\log n}{\|\theta_*\|^2})$ iterations, and in addition, the EM iteration converges to the MLE. Evidently, for $\|\theta_*\| = \Omega(1)$, this implies a parametric error rate in the number of samples, and geometric rate in the number of iterations. Hence, the EM algorithm *adapts* to the actual separation between the two means (as captured by $\|\theta_*\|$), to achieve error rate of $\tilde{O}(\min\{\frac{1}{\|\theta_*\|}\sqrt{d/n}, (d/n)^{1/4}\})$. Moreover, no other estimation technique can perform significantly better since, up to logarithmic factors, this error rate matches the *local* minimax rate (Wu and Zhou, 2019, Appendix B). Remarkably, it was also shown by Wu and Zhou (2019) that these guarantees are achieved by a random initialization of the EM algorithm, in which θ_0 is an isotropic random d-dimensional vector scaled to have appropriately low norm.

Unbalanced GM and preview of results. In this work, we study the model (1) for $\rho_* \in (0,1)$. The value of ρ_* may be fixed, or, more interestingly, $\rho_* \equiv \rho_{*,n} \to 0$ as $n \to \infty$ at some arbitrary rate. Note that the samples from the model (1) are equal in distribution to

$$X = S\theta + Z, \qquad (2)$$

where $S \in \{\pm 1\}$ is such that $\mathbb{P}[S = 1] = (1 + \rho_*)/2$ and $Z \sim N(0, I_d)$, with S and Z independent. Intuitively, moving ρ_* away from 0 reduces uncertainty in the signs $\{S_i\}$, and one might expect that this would lead to better error rates for estimating θ_* . The problem is indeed trivial for the extreme case $\rho_* = 1$ in which case (1) coincides with the Gaussian location model. More generally, it seems helpful that for $\rho_* \neq 0$ the expectation $\mathbb{E}[X] = \rho_* \theta_*$ is a vector in the direction of θ_* . While estimation seems easier for $\rho_* \neq 0$, in this case the model (1) is no longer balanced, and this makes a direct analysis of the EM iteration difficult. Nonetheless, we prove a global convergence property for the population iteration, which shows that any initial guess θ_0 with $\langle \theta_0, \theta_* \rangle \geq 0$ converges to θ_* (including the trivial initialization $\theta_0 = 0$). We also show that the EM iteration might have a spurious (stable) fixed point $\theta_- \neq -\theta_*$ which satisfies $\langle \theta_-, \theta_* \rangle < 0$ whose existence depends on the value of (ρ_*, θ_*) . This phenomenon does not occur in the balanced case.

For the empirical iteration, we first note that a method-of-moments estimator $\frac{1}{\rho_*}\mathbb{E}_n[X] := \frac{1}{\rho_*n}\sum_{i=1}^n X_i$ achieves an error rate of $O(\frac{1}{\rho_*}\sqrt{d/n})$. In addition, an estimator can always ignore the reduced uncertainty in the signs, formally, by multiplying each sample with a random sign $R_i \in \{\pm 1\}$ such that $\mathbb{P}[R_i = 1] = 1/2$ for each $i \in [n]$. This reduces the $\rho_* \neq 0$ case to the $\rho_* = 0$ case, and then an error rate of $\tilde{O}(\min\{\frac{1}{\|\theta_*\|}\sqrt{d/n}, (d/n)^{1/4}\})$ can be achieved, using the balanced EM iteration.¹ The main result of this paper is analysis of the unbalanced EM iteration for the estimation of θ_* , which shows that the EM iteration adaptively achieves the minimum of both error rates, i.e., $\tilde{O}(\min\{\frac{1}{\rho_*}\sqrt{d/n}, \frac{1}{\|\theta_*\|}\sqrt{d/n}, (d/n)^{1/4}\})$. As for the balanced case, this error rate obtained by the EM algorithm coincides with the local minimax rate for any ρ_* , up to logarithmic terms.

1.2 Main Result

It will be convenient throughout to use the weight parameter $\delta := (1 - \rho)/2$ interchangeably with ρ according to convenience.² We denote the corresponding *inverse-temperature parameter* by

$$\beta_{\rho} := \frac{1}{2} \log \frac{1+\rho}{1-\rho} = \tanh^{-1}(\rho)$$
(3)

and let ρ_{β} denote the inverse relation. With a slight abuse of notation from (3), we also denote $\beta_{\delta} := \frac{1}{2} \log \frac{1-\delta}{\delta}$ (and sometimes just β). Let $\theta_* \in \mathbb{R}^d$ and $\rho_* \in [0,1]$ (or $\delta_* \in [0,1/2]$) denote the ground truth of the model (1). Given *n* independent and identically distributed (i.i.d.) samples $\underline{X} = (X_1, \ldots, X_n) \stackrel{\text{i.i.d.}}{\sim} P_{\theta_*, \rho_*}$, the goal is to estimate the parameter θ_* under the ℓ_2 loss function, up to the identifiability of the model. For $\rho_* > 0$ this amounts to the standard loss function $\ell(\theta, \theta_*) = \|\theta - \theta_*\|$ and when $\rho_* = 0$ then the loss function is $\ell_0(\theta, \theta_*) = \min \{\|\theta - \theta_*\|, \|\theta + \theta_*\|\}.$

Assumptions. Our results will depend on the following global assumptions:

- 1. Norm assumption: There exists $C_{\theta} > 0$ such that $\|\theta_*\| \leq C_{\theta}$.
- 2. Unbalancedness assumption: There exists $\mathsf{C}_{\rho} \in (0,1)$ such that $|\rho_*| \leq \mathsf{C}_{\rho}$.

Because $\rho \mapsto \frac{1}{2} \log \frac{1+2a}{1-2a}$ is convex and increasing in [0, 1/2), an immediate consequence of the unbalancedness assumption is that $|\beta_{\rho_*}| \leq C_{\beta}$ holds for $C_{\beta} := \frac{1}{2} \log \frac{1+C_{\rho}}{1-C_{\rho}}$, and that there exist $(\underline{C}_{\beta}, \overline{C}_{\beta})$ such that $\underline{C}_{\beta}\rho_* \leq |\beta_{\rho_*}| \leq \overline{C}_{\beta}\rho_*$. These assumptions are based on the fact that the interesting regime is in which $\|\theta_*\|$ and ρ_* are close to zero.

^{1.} In the latter case, this error is actually only with respect to (w.r.t.) the sign-ambiguous loss function ℓ_0 (see Proposition 11).

^{2.} The notation used in this section is standard. See Section 1.6 for notational conventions.

EM iteration. While we focus on estimating θ_* for a given ρ_* , we will also consider the opposite case of estimating ρ_* , and briefly discuss the joint estimation problem. Thus, we will next consider the more general *joint* iteration. The evolution of the iterates $\{(\theta_t, \rho_t)\}_{t=1}^{\infty}$ of the EM algorithm can be brought to a simple closed form we describe next. To start, the density function of observed samples X from (1) is given by

$$p_{\theta,\rho}(x) = \left(\frac{1+\rho}{2}\right)\varphi(x-\theta) + \left(\frac{1-\rho}{2}\right)\varphi(x+\theta)$$
$$= e^{-\|x\|^2/2} \cdot \varphi(x) \cdot \left[\left(\frac{1+\rho}{2}\right)e^{-\langle\theta,X\rangle} + \left(\frac{1-\rho}{2}\right)e^{\langle\theta,X\rangle}\right]$$
$$= e^{-\|x\|^2/2} \cdot \varphi(x) \cdot \cosh\left(\langle\theta,X\rangle + \beta_\rho\right), \tag{4}$$

where $\varphi(x) := \frac{1}{\sqrt{2\pi}} e^{-\|x\|^2/2}$ is the standard normal density in \mathbb{R}^d . Similarly, the full observation, which also includes the latent sign s (2) is given by a standard Gaussian density

$$p_{\theta,\rho}(s,x) = \left(\frac{1+s\rho}{2}\right)\varphi(x-s\theta).$$

Assume that $\underline{X} = \underline{x}$ is given and the EM algorithm has ran up to its *t*th iteration, and so (θ_t, ρ_t) is given. The next iteration of the EM algorithm is the pair $(\theta_{t+1}, \rho_{t+1})$ which maximizes the following *Q*-function:

$$Q(\theta, \rho \mid \theta_t, \rho_t) := \sum_{\underline{s} \in \{\pm 1\}^n} p_{\theta_t, \rho_t}(\underline{s} \mid \underline{X}) \log p_{\theta, \rho}(\underline{s}, \underline{X}) \,.$$

Using the i.i.d. property of \underline{X} , and the expression (4) for the density, this is equivalent to

$$(\theta_{t+1}, \rho_{t+1}) \in \underset{\rho}{\operatorname{argmin}} \sum_{i=1}^{n} \mathbb{E}_{\theta_{t}, \rho_{t}} \left[\log \left(\frac{1+S_{i}\rho}{2} \right) \mid X_{i} = x_{i} \right]$$
$$+ \underset{\theta}{\operatorname{argmin}} \left\{ n \|\theta\|^{2} - \left\langle \theta, \sum_{i=1}^{n} x_{i} \mathbb{E}_{\theta_{t}, \rho_{t}} \left[S_{i} \mid X_{i} = x_{i} \right] \right\rangle \right\}$$

where $S_i \in \{\pm 1\}$ for $i \in [n]$ with $\mathbb{P}[S_i = 1] = (1 + \rho_t)/2$, and are i.i.d.. Hence, given (θ_t, ρ_t) , the optimization over (θ, ρ) is decoupled, and its solution is given by the pair

$$\theta_{t+1} = \frac{1}{n} \sum_{i=1}^{n} x_i \cdot \mathbb{E}_{\theta_t, \rho_t} \left[S_i \mid X_i = x_i \right], \qquad \rho_{t+1} = \frac{1}{n} \sum_{i=1}^{n} \mathbb{E}_{\theta_t, \rho_t} \left[S_i \mid X_i = x_i \right],$$

where

$$\mathbb{E}_{\theta_t,\rho_t}\left[S \mid X=x\right] = \frac{(1+\rho) \cdot e^{\langle \theta, x \rangle} - (1-\rho) \cdot e^{-\langle \theta, x \rangle}}{(1+\rho) \cdot e^{\langle \theta, x \rangle} + (1-\rho) \cdot e^{-\langle \theta, x \rangle}} = \tanh(\langle \theta, x \rangle + \beta_\rho).$$
(5)

Hence the EM iteration $\{\theta_{t}, \rho_{t}\}_{t=1}^{\infty}$ of the symmetric 2-GM model evolves according to

$$\theta_{t+1} = f_n(\theta_t, \rho_t \mid \theta_*, \rho_*) \tag{6}$$

,

$$\rho_{t+1} = h_n(\rho_t, \theta_t \mid \theta_*, \rho_*), \qquad (7)$$

where the sample mean EM iteration is

$$f_n(\theta, \rho \mid \theta_*, \rho_*) = \mathbb{E}_n \left[X \cdot \frac{(1+\rho) \cdot e^{\langle \theta, X \rangle} - (1-\rho) \cdot e^{-\langle \theta, X \rangle}}{(1+\rho) \cdot e^{\langle \theta, X \rangle} + (1-\rho) \cdot e^{-\langle \theta, X \rangle}} \right] = \mathbb{E}_n \left[X \cdot \tanh\left(\langle \theta, X \rangle + \beta_\rho\right) \right],$$
(8)

and the sample weight EM iteration is

$$h_n(\rho,\theta \mid \theta_*,\rho_*) = \mathbb{E}_n\left[\frac{(1+\rho)e^{\langle \theta,X\rangle} - (1-\rho)e^{-\langle \theta,X\rangle}}{(1+\rho)e^{\langle \theta,X\rangle} + (1-\rho)e^{-\langle \theta,X\rangle}}\right] = \mathbb{E}_n\left[\tanh\left(\langle \theta,X\rangle + \beta_\rho\right)\right].$$
(9)

In the limit of $n \to \infty$, the iterations (8) and (9) tend, respectively, to the population mean and population weight EM iterations

$$f(\theta, \rho \mid \theta_*, \rho_*) = \mathbb{E} \left[X \cdot \tanh\left(\langle \theta, X \rangle + \beta_\rho\right) \right], \quad X \sim P_{\theta_*, \rho_*}$$

and

$$h(\rho, \theta \mid \theta_*, \rho_*) = \mathbb{E} \left[\tanh\left(\langle \theta, X \rangle + \beta_\rho\right) \right], \quad X \sim P_{\theta_*, \rho_*}$$

We will usually omit (θ_*, ρ_*) from the notation for the iteration, except when it is required to avoid confusion.

Statement of Results. The balanced case $\rho_* = 0$ was analyzed by Wu and Zhou (2019):

Theorem 1 (Wu and Zhou, 2019, Theorems 1 and 2) Assume that $\|\theta_*\| \leq C_{\theta}$ and that $n \gtrsim d \log^3 d$, and consider the balanced EM iteration $\theta_{t+1} = f_n(\theta_t, 0 \mid \theta_*, 0)$. There exists $C_0 > 0$ such that if \hat{u} is drawn uniformly from the unit sphere \mathbb{S}^{d-1} , and the iteration is initialized with $\theta_0 = C_0 \left(\frac{d \log n}{n}\right)^{1/4} \cdot \hat{u}$ then with probability $1 - o_n(1)$

$$\ell_0(\theta_*, \theta_t) \lesssim \left(\frac{d\log^3 n}{n}\right)^{1/4} \tag{10}$$

holds for all $t \gtrsim \sqrt{n}$. Furthermore, if $\|\theta_*\| \gtrsim \left(\frac{d \log^3 n}{n}\right)^{1/4}$ then with probability $1 - o_n(1)$

$$\ell_0(\theta_*, \theta_t) \lesssim \frac{1}{\|\theta_*\|} \sqrt{\frac{d\log n}{n}}$$

holds for all $t \gtrsim \frac{\log n}{\|\theta_*\|^2}$. The constants involved in the asymptotic inequalities depend only on C_{θ} .

Our main result complements Theorem 1 in the unbalanced case, $\rho_* \neq 0$:

Theorem 2 (Simplified version of Theorem 10) Assume that $\|\theta_*\| \leq C_{\theta}$ and that $|\rho_*| \leq C_{\rho}$, as well as $n \gtrsim d \log n$.

If $\rho_* \gtrsim \left(\frac{d\log n}{n}\right)^{1/4}$ then the unbalanced EM iteration $\theta_{t+1} = f_n(\theta_t, \rho_* \mid \theta_*, \rho_*)$ initialized with either $\theta_0 = 0$ or $\theta_0 = \frac{1}{\rho_*} \mathbb{E}_n(X)$ satisfies that with probability $1 - o_n(1)$

$$\ell(\theta_*, \theta_t) \lesssim \frac{1}{\max\left\{\rho_*, \|\theta_*\|\right\}} \sqrt{\frac{d\log n}{n}}$$

	$\ heta_*\ \lesssim rac{1}{ ho_*} \sqrt{rac{d\log n}{n}}$	$rac{1}{ ho_*}\sqrt{rac{d\log n}{n}}\lesssim \ heta_*\ \lesssim ho_*$	$ ho_* \lesssim \ heta_*\ $
$\theta_0 = 0$	$T\lesssim 1$	$T\lesssimrac{1}{ ho_*^2}$	$T \lesssim \frac{1}{\rho_* \ \theta_*\ }$
$\theta_0 = \frac{1}{\rho_*} \mathbb{E}_n(X)$	$T \lesssim 1$	$T\lesssim 1$	$T \lesssim \frac{1}{\ \theta_*\ ^2}$

Table 1: T: Number of iterations until convergence of unbalanced EM algorithm.

hold for all $t \ge T$, where upper bounds on T are specified in Table 1. The constants involved in the asymptotic inequalities depend only on (C_{θ}, C_{ρ}) .

If $\rho_* \lesssim \left(\frac{d\log n}{n}\right)^{1/4}$ the balanced EM iteration as in Theorem 1 guarantees (10). If, in addition

$$\|\theta_*\| \gtrsim \left(\frac{d\log n}{n}\right)^{1/4} \gtrsim \rho_* \gtrsim \frac{1}{\|\theta_*\|} \sqrt{\frac{d\log n}{n}}$$
(11)

holds, then by setting $s_t = \operatorname{sign} \langle \theta_t, \mathbb{E}_n[X] \rangle$ it holds that

$$\ell(\theta_*, s_t \cdot \theta_t) \lesssim \frac{1}{\|\theta_*\|} \sqrt{\frac{d\log n}{n}}$$

for all $t \gtrsim \frac{\log n}{\|\theta_*\|^2}$.

Interpretation of results. Note that in comparison to the balanced case $\rho_* = 0$, the case $\rho_* > 0$ simplifies the analysis of the EM iteration in the sense that the algorithm may be initialized at $\theta_0 = 0$ or at $\theta_0 = \frac{1}{\rho_*} \mathbb{E}_n[X]$, and no random initialization is required—the expected value $\mathbb{E}[X]$ is proportional to θ_* and steers the iteration in the right direction. Nonetheless, an isotropic random initialization in a ball is not advised for the $\rho_* > 0$ case, since there is a probability of 1/2 that the random initialization θ_0 is negatively correlated with θ_* (the mean of the component with the larger weight $1-\delta_*$), which leads to convergence to a spurious fixed point (even for the population version).

The convergence times specified in Table 1 in case $\rho_* \gtrsim \left(\frac{d \log n}{n}\right)^{1/4}$ can be interpreted as follows. While the EM iteration is *d*-dimensional, it can be decomposed into movements in the signal direction (the direction of θ_*), and in its orthogonal direction (Daskalakis et al., 2017; Wu and Zhou, 2019). The factor dominating the number of iterations until convergence is the time it takes the projected one-dimensional EM iteration in the direction of θ_* to converge:

- When $\|\theta_*\| \lesssim \frac{1}{\rho_*} \sqrt{\frac{d \log n}{n}}$ the signal is very low, and the EM estimate remains around θ_* for all iterations (for both types of initialization).
- When $\frac{1}{\rho_*}\sqrt{\frac{d\log n}{n}} \lesssim \|\theta_*\| \lesssim \rho_*$, an error rate of $O(\frac{1}{\rho_*}\sqrt{\frac{d\log n}{n}})$ is achieved by $\theta_0 = \frac{1}{\rho_*}\mathbb{E}_n(X)$ starting from the first iteration (and the EM iterations remain at this area of low statistical error). When $\theta_0 = 0$ the one-dimensional EM iteration in direction of θ_* is contracting with slope bounded by $1 c\rho_*^2$ for some c > 0 and the convergence time is $O(1/\rho_*^2)$.

• When $\rho_* \lesssim \|\theta_*\|$, an error rate of $O(\frac{1}{\|\theta_*\|}\sqrt{\frac{d\log n}{n}})$ is achieved. For $\theta_0 = \frac{1}{\rho_*}\mathbb{E}_n(X)$, it is shown that the empirical iteration converges faster than the corresponding balanced iteration starting from the first iteration. For $\theta_0 = 0$ the same effect occurs, but after an initial phase of additive increase in θ_t , and this early phase dominates the convergence time.

Evidently, the worst convergence time of the balanced iteration is also similar to the worst case convergence time of the unbalanced iteration and given by $\tilde{O}(\sqrt{n})$, which is achieved when $\rho_* \asymp \left(\frac{d\log n}{n}\right)^{1/4}$. We also remark that as was shown by Daskalakis et al. (2017) and Wu and Zhou (2019), the analysis of the EM iteration in high dimension is possible when it is initialized with a low norm, but not zero. For the unbalanced model, initializing at $\theta_0 = 0$ leads to global convergence, yet represents the longest convergence time (worst-case scenario). It should be noted that the bounds on the convergence times for $\theta_0 = \frac{1}{\rho_*}\mathbb{E}_n(X)$ exhibit a discontinuity at $\|\theta_*\| = \rho_*$. This is because T does not capture the time required for convergence to a fixed point but rather to a neighborhood around θ_* within the statistical error rate.³

The information-theoretic lower bounds obtained by Wu and Zhou (2019) for $\rho_* = 0$ are generalized in Theorem 20 (Appendix B) and show that the error rate achieved by EM in Theorem 2 equals the minimax error rates (up to logarithmic factors) whenever $\rho_* \gtrsim \left(\frac{d\log n}{n}\right)^{1/4}$. It switches from the minimax error rate $O(\frac{1}{\rho_*}\sqrt{d/n})$ assured for any signal strength to the local minimax error rates for stronger signals $O(\frac{1}{\|\theta_*\|}\sqrt{d/n})$ at $\|\theta_*\| \approx \rho_*$. In the balanced case $\rho_* = 0$, a similar switch occurs at $\|\theta_*\| \approx (d/n)^{1/4}$, improving from error rate of $O((d/n)^{1/4})$ to $O(\frac{1}{\|\theta_*\|}\sqrt{d/n})$. This observation along with expected monotonicity of the error rates in ρ_* elucidates the condition $\rho_* \gtrsim \left(\frac{d\log n}{n}\right)^{1/4}$ in Theorem 2 (see the rigorous statement in Theorem 20).

We complete the picture by discussing the case $\rho_* \leq \left(\frac{d\log n}{n}\right)^{1/4}$. In this case, the minimax error rate analysis (Theorem 20) suggests that the error rates cannot be improved due to the unbalancedness of the samples. However, the error rate of the balanced case can be achieved for the ℓ_0 loss function (which allows for sign ambiguity), and when condition (11) holds, it can be achieved without sign ambiguity. The idea is simply to use the balanced iteration which is insensitive to the actual signs generating the samples \underline{X} , and upon convergence, evaluate the angle between θ_t and $\mathbb{E}_n[X]$. With high probability, this detects the correct sign required to estimate θ_* when $\rho_* \gtrsim \frac{1}{\|\theta_*\|} \sqrt{\frac{d\log n}{n}}$. If this condition fails then no correct decoding of the sign is possible, as the signal is too low compared to the unbalancedness of the iteration (cf. the minimax error rates of estimating ρ when θ_* is known and d is fixed of Theorem 22 in Appendix B).

^{3.} For illustration, consider one-dimensional convergence, let the required statistical accuracy be ω , and suppose that $\theta_0 = 0$. If $\theta_* \leq \omega$ then statistical accuracy is achieved already in the first iteration, and then it is only need to be proved (and also possible, as we shall show throughout) that the iteration remains at this accuracy for all subsequent iterations. If, however, the order of θ_* is increased, say $\theta_* = 2\omega$, then the iteration should increase, say, from $\theta_0 = 0$ to $\theta_t \geq \omega$ to achieve statistical accuracy, and the required number of iteration for this increase depends on ω .

We note in passing that we also analyze an EM iteration for estimating ρ_* given any fixed value of θ (perhaps mismatched to θ_*). As we will discuss in Section 2.5, this shows that the given EM algorithm can be used for joint estimation of (θ_*, ρ_*) if sufficient separation holds. Characterizing the minimal separation required for *joint* estimation remains an open problem.

Significance of the unbalanced model:

1. The likelihood-based EM has method-of-moments alternatives (Anandkumar et al., 2014; Heinrich and Kahn, 2015; Wu and Yang, 2020) which may achieve the same error rates as the EM algorithm, perhaps at a higher computational cost. Specifically, for the balanced 2-GM model, the optimal error rate⁴ is achieved by a *spectral* algorithm (Wu and Zhou, 2019). Such an algorithm estimates θ_* by $\theta_{\rm SP} = \sqrt{\max{\{\lambda_{\rm max} - 1, 0\}}} \cdot \hat{\theta}_{\rm sp}$ where $\lambda_{\rm max}$ and $\hat{\theta}_{\rm sp}$ are, respectively, the maximal eigenvalue and the corresponding normalized maximal eigenvector $\hat{\theta}_{\rm sp}$, of the empirical covariance matrix $\mathbb{E}_n[XX^T]$. The spectral algorithm can be interpreted as eliminating the sign ambiguity by "squaring" the samples, since the covariance matrix

$$\mathbb{E}[XX^T] = \theta_* \theta_*^T + I_d \,,$$

does not depend on the unknown sign S (cf. the model in Equation 1). Hence, while EM attempts to *learn* the latent signs, spectral algorithms attempt to *eliminate* them. Despite this conceptual difference, it was observed by Daskalakis et al. (2017) that whenever $\|\theta_t\|$ has sufficiently low norm, the EM iteration behaves as a power iteration on the empirical covariance matrix, and in this regime the operation of EM is not fundamentally different from a spectral algorithm. Nonetheless, sign elimination can only be optimal for sufficiently small values of ρ_* , since the distribution of the statistic $\mathbb{E}_n[XX^T]$ is insensitive to the value of ρ_* , so it cannot lower its error in case $\rho_* > 0$. Our results thus demonstrate that EM is nearly optimal in a regime in which the estimator must learn the latent signs.

- 2. The worst case error over $\|\theta\|^*$ is given by $\max\{(d/n)^{1/4}, \frac{1}{\rho_*}\sqrt{d/n}\}$ and improves as ρ_* is increased. In practice, ρ_* may be increased, e.g., by collecting additional information on the latent signs generating $\lceil \frac{1}{2}\rho_*n \rceil$ of the samples, and then align the signs of those samples by proper multiplication by $\{\pm 1\}$. As another example, consider a communication system in which $(S_1, \ldots, S_n) \in \{\pm 1\}^n$ are the input bits to a noisy channel whose output at time *i* is given by $X_i = \theta_*S_i + Z$, as in (2). In order to decode the bits, a typical decoder will estimate θ_* as a preliminary step, and assume that the samples are i.i.d..⁵ The input distribution $\mathbb{P}[S_i = 1] = (1 - \rho_*)/2$ then trades-off between estimation and data rate, with best estimation and zero data rate for $\rho_* = 1$ versus maximal data rate and worst estimation for $\rho_* = 0$.
- 3. The proofs of global convergence for the balanced 2-GM model ($\rho_* = 0$) (Xu et al., 2016; Daskalakis et al., 2017; Wu and Zhou, 2019) rely heavily on global symmetry

^{4.} In fact, unlike EM, method-of-moments do not have "spurious" logarithmic terms.

^{5.} Typically, the data bits are encoded using an error correcting code before being sent over the channel, and so the bits $\{S_i\}$ are not i.i.d.. Nonetheless, the receiver may ignore these dependencies for the purpose of estimation.

properties of the population iteration (see next, Section 1.3). This lack of symmetry is challenging for proving global convergence. For example, we show that a stable spurious fixed point is possible at some $\theta \in (-\theta_*, 0)$. Nonetheless, we show that (essentially) global convergence to θ_* is not restricted to $\rho_* = 0$.

1.3 Discussion of Proof Ideas

In order to give context for the proof ideas, we first consider the balanced case $\rho_* = 0$ and describe the ideas behind the results of Xu et al. (2016); Daskalakis et al. (2017); Wu and Zhou (2019), and how they compare with the general analysis of Balakrishnan et al. (2017). There are two main ideas—one pertains to the population iteration and the other to the empirical error.

For the population iteration, Balakrishnan et al. (2017) prove a guarantee on the convergence radius using a fixed-point theorem whose conditions require *contractivity* of the iterative iteration. The guarantee on the size of the basin of attraction is obtained from a guarantee on the contractivity of $f(\theta)$ in this region. However, global convergence cannot be established by such an argument since the EM iteration for (1) with $\rho_* = 0$ is in fact *not* globally contractive. Nonetheless, contractivity is only a sufficient, but not necessary condition for convergence, and other global properties of the iteration has two stable fixed points $\theta = \pm \theta_*$, due to the well known consistency property of EM (both which are acceptable solutions with $\ell_0(\theta, \theta_*) = 0$), and a single unstable fixed point $\theta = 0$. The fact that any other fixed point is impossible follows from the observation that $f(\theta)$ is an odd function, which is concave for $\theta \in \mathbb{R}_+$ (Wu and Zhou, 2019). By contrast, in the unbalanced case $(\rho_* > 0)$, neither concavity (say, for all $\theta \in \mathbb{R}_+$) nor global contractivity hold for unbalanced iterations. It is also seems to be difficult to analytically characterize the required distance of θ from θ_* for these properties to hold.

For the empirical iteration, the error guarantee made by Balakrishnan et al. (2017) is obtained from the following high probability uniform error bound on the empirical error

$$\sup_{\theta:\|\theta_0-\theta_*\|\leq \frac{1}{4}\|\theta_*\|} \|f_n(\theta) - f(\theta)\| = \tilde{O}\left(\sqrt{\frac{d}{n}}\right).$$
(12)

However, it was observed by Dwivedi et al. (2020a) and Wu and Zhou (2019) that a stronger bound on the error can be obtained which allows arbitrarily small $\|\theta_*\|$ and $\|\theta\|$ by "localizing" the error as follows:

$$\sup_{\theta: \|\theta\| \le \mathsf{C}_{\theta}} \|f_n(\theta) - f(\theta)\| = \|\theta\| \cdot \tilde{O}\left(\sqrt{\frac{d}{n}}\right) \,. \tag{13}$$

So, while the empirical iteration analyzed using (12) requires strong separation $\|\theta_*\| = \Omega(1)$, no such condition is required when the bound (13) is used, leading to the sharp results obtained by Wu and Zhou (2019).

The analysis of the unbalanced case $\rho_* \neq 0$ in this paper is based on the following intuitive idea of ρ -ordering of iterations, which allows a comparison with the $\rho_* = 0$ case. If $\rho_* = 1$, the model (1) is the Gaussian location model, for which it can be easily verified

(see Section 1.2) that the EM iteration converges in a single iteration to the sample mean (which is also the MLE). Extrapolating from this extreme case, we might expect that if $\rho_1 > \rho_0$ then the iteration for ρ_1 will converge faster since the model more closely resembles the Gaussian location model. We state global comparison results (Theorem 4 for d = 1and Proposition 9 for d > 1) establishing this property for any arbitrary pair $\rho_0, \rho_1 \in [0, 1]$. Combining this property with the known global convergence rate of the balanced case $\rho_* = 0$ yields the global convergence proof of the population iteration for unbalanced $\rho_* \neq 0$.

For the empirical iteration, it turns out that increasing ρ has an *opposite* effect. We generalize the localized error bound developed by Wu and Zhou (2019) in (13) from $\rho_* = 0$ to a general $\rho_* \in [0, 1]$ and obtain that

$$\sup_{\theta: \|\theta\| \le C} \|f_n(\theta) - f(\theta)\| = \max\left\{\|\theta\|, \rho_*\right\} \cdot \tilde{O}\left(\sqrt{\frac{d}{n}}\right), \tag{14}$$

indicating that the empirical error increases with ρ_* . The main challenge of the analysis of the empirical iteration is to prove that the increased empirical error for larger ρ_* is compensated by the improved convergence rate of the population iteration. It should be noted, however, that the empirical error may break key properties of the population iteration. For example, for d = 1, the convergence of the population iteration for $\theta_0 = 0$ towards θ_* is based on the fact that f(0) > 0, assuming without loss of generality (w.l.o.g.) that $\theta_* > 0$. Clearly, the empirical error (14) might result in $f_n(0) < 0$ which would steer the iteration towards a spurious fixed point in \mathbb{R}_- . Our analysis shows that with high probability this occurs only if $\|\theta_*\|$ is low, so that this bad convergence does not dominate the error rate.

It is reasonable to expect that an argument that hinges on "ordering-of-iterations" and error localization would be beneficial in analyzing more complicated models. These include, e.g., a hidden-Markov 2-GM model, which is similar to the model studied here, except that S_0 is uniform, and the the unknown signs $\{S_i\}_{i>1}$ evolve according to a stationary symmetric binary Markov chain with flip probability $\zeta \in (0, 1/2)$. As ζ approaches 0, this model also tends to essentially a Gaussian location model (except for a sign-ambiguity). So it expected that the population EM iteration will converge better for ζ compared to models with larger flip probability. We envision that with some additional innovation, similar ideas could be used for unbalanced 2-GM model with zero mean (unlike the non-zero mean in our model), or a model with unknown covariance matrix.

1.4 General Background on the EM Algorithm

In this section, we briefly outline relevant background on the EM algorithm. It is well known that it is typically computationally complex to compute the MLE

$$\theta_{\mathrm{MLE}} = \operatorname*{argmax}_{\theta} \mathbb{E}_n \left[\log P_{\theta}(X) \right]$$

in parametric models $(X, S) \sim P_{\theta}(x, s)$ for which only X is observed but S is latent. For one thing, exact marginalization over the latent variables S to obtain the likelihood $P_{\theta}(x)$ (or its gradient) is computationally heavy due the need to sum over all possible configurations of the latent variable. Moreover, in most interesting cases, the likelihood $P_{\theta}(x)$ is not a concave function of θ , and so standard optimization techniques do not have strong guarantees. Various authors (Baum et al., 1970; Beale and Little, 1975; Hartley, 1958; Healy and Westmacott, 1956; Sundberg, 1974; Woodbury, 1970; Hasselblad, 1966, 1969) have independently proposed several heuristics akin to the EM algorithm for this problem, and the EM algorithm was later on formulated in its well known form in the seminal paper of Dempster et al. (1977), which also proposed a wide range of statistical applications.

The EM is an iterative procedure, which determines an empirical operator f_n based on n samples from the data $X \sim P_{\theta}$. Given an initial guess θ_0 , the algorithm produces a sequence of iterations $\theta_t = f_n(\theta_{t-1})$ for all $t \ge 1$. Owing to its name, the empirical operator is determined by solving two steps. The first step computes a posterior probability $P_{\theta_t}(S \mid X)$ on the latent variable S based on the current estimate θ_t , and then averages the log-likelihood with this posterior ("expectation") to obtain the Q-function

$$Q(\theta \mid \theta_t) = \int p_{\theta_t}(s \mid X) \cdot \log p_{\theta}(X, s) \cdot \mathrm{d}s.$$

The second step then sets $\theta_{t+1} = f_n(\theta_t) := \operatorname{argmax}_{\theta} Q(\theta \mid \theta_t)$ ("maximization"). In many practical cases, the last maximization step can be solved analytically and an explicit expression of the operator $f_n(\cdot)$ is available. A different interpretation of EM as a minorization-maximization algorithm is obtained from the fact that the bound

$$\log P_{\theta}(x) - \log P_{\theta_t}(x) \ge Q(\theta \mid \theta_t) - Q(\theta_t \mid \theta_t)$$

holds for any θ , which immediately implies a strong general property: The EM algorithm produces increasing likelihoods $P_{\theta_t}(x)$ as t increases. This elegant property, along with its typically low computational complexity has contributed to its widespread application in numerous applications (Gupta and Chen, 2011).

Despite the above appealing properties, not long after its formulation by Dempster et al. (1977), it was recognized that the EM algorithm may actually fail to compute the MLE. Wu (1983) clarified that in the general case, the EM algorithm may converge to *local* maxima of the likelihood, or even get trapped in a saddle point. Clearly, such local maxima may be far from the required MLE, and in high dimension their number could be exponentially large. Consequently, except in favorable cases in which the likelihood is unimodal, the convergence of the EM algorithm heavily depends on the initial guess. In practice, this necessitates complicated initialization algorithms such as multiple restarts with random initial estimates (Karlis and Xekalaki, 2003), or using a pilot estimator to obtain an initial guess. Both options are typically costly. In the more restricted case of mixtures of exponential families, Redner and Walker (1984) showed that EM converges at a geometric rate to the MLE, under positivity conditions of the Fisher information matrix and the mixing weights, and more importantly, assuming local initialization. However, the dependence of the guarantees on the convergence radius and rate are only qualitative and do not specify their dependence on the parameters of the model. Furthermore, it was empirically observed by Redner and Walker (1984) that the EM iterations can become painfully slow to converge whenever the separation between the components is low.

Later works (Hero and Fessler, 1995; Meng and Rubin, 1994; Chrétien and Hero, 2008) displayed similar guarantees, albeit to a local maxima of the likelihood, which, naturally, might be far from the true likelihood. Xu and Jordan (1996) have cast the EM algorithm for Gaussian mixtures as a gradient ascent algorithm, where in each step the gradient is pre-multiplied by a positive-definite matrix, and exemplified slow convergence akin to firstorder optimization methods. These drawbacks of EM were then addressed by a multitude of ad hoc methods and variants, comprehensively summarized by McLachlan and Krishnan (2007). The bottom line however, that even if the MLE is known to have good statistical properties, it is not clear whether they can be computationally achieved by the EM algorithm.

The apparent discrepancy between the wide practicality of the EM algorithm versus its relatively weak theoretical guarantees mentioned above, along with the growth in size and dimension of modern data sets, resulted in two paradigm shifts in the anticipated goals expected from its analysis. The first one, most notably made by Balakrishnan et al. (2017), is the explicit characterization of the statistical precision, convergence rate, and the distance of the initialization from the ground truth required to obtain that statistically accurate solution (basin of attraction). The characterization made by Balakrishnan et al. (2017) is based on general smoothness and stability properties of the auxiliary function $Q(\theta \mid \theta')$, which need to be verified independently for any given problem. As concrete examples, these conditions were applied by Balakrishnan et al. (2017) to canonical models such as the balanced 2-GM, symmetric mixture of two regressions, and linear regression with missing covariates. Nonetheless, as discussed in Section 1.1, this approach, even when combined with further refinements (Klusowski and Brinda, 2016; Wu et al., 2016), did not lead to sharp results for the basic balanced 2-GM model. As discussed in Section 1.2, the local convergence result of the 2-GM model was then improved to global convergence guarantees by various authors. For the idealized population version, it was shown by various authors (Xu et al., 2016; Daskalakis et al., 2017) that EM converges at a geometric rate to $\pm \theta_*$, unless the initial guess θ_0 is orthogonal to θ_* . A finite sample analysis was made by Daskalakis et al. (2017), but was based on sample-splitting—EM was assumed to run on a fresh batch of samples at each iteration. Optimality of EM in terms of statistical error and convergence time was ultimately established by Wu and Zhou (2019).

1.5 Other Known Results

The unbalanced 2-GM model studied in this paper was mostly explored in relation to misspecification or overspecification, i.e., cases in which the true model does not belong to the set of fitted models, or belongs to a simpler set of models. An extreme case of 2-GM mixture model was considered by Dwivedi et al. (2020a), in which the components are not separated at all, thus reduced to a zero-mean Gaussian $\theta_* = 0$. The EM algorithm was designed to operate on the unbalanced model (1) with $\rho_* \neq 0$ that over-fits the true model. For this case, it was shown that the population iteration is globally contracting at a rate $\|\theta_{t+1}\| \approx \|\theta_t\| (1 - \frac{\rho_*^2}{2})$ and thus globally converging at a geometric rate, and has a statistical error of $O(\frac{1}{\rho_*^2}\sqrt{\frac{d}{n}})$, which is parametric for fixed ρ , but in general, worse than the minimax rate $(\frac{1}{\rho_*}\sqrt{\frac{d}{n}})$, and from our Theorem 2. This behavior was contrasted with the same setting, except for which $\rho_* = 0$, where it was shown that convergence of the population EM is much slower, and behaves as $\|\theta_{t+1}\| \approx \|\theta_t\| (1 - \|\theta_t\|^2)$, and the error rate for the sample-based EM is $O((d/n)^{1/4})$. This error rate was achieved by partitioning the

EM iterations to multi-epochs, where in the *l*th epoch, $\|\theta_t\| \in [\left(\frac{d}{n}\right)^{\alpha_{l+1}}, \left(\frac{d}{n}\right)^{\alpha_l}]$ for judiciously chosen powers α_l . With this approach, the guarantees on the empirical error in the iterations of the *l*th epoch improve as $l \uparrow \infty$, which allows the "localization" of the empirical error discussed in Section 1.3. Dwivedi et al. (2020b) also considered the EM for 2-GM mixture model with $\theta_* = 0$, but in which the algorithm is also allowed to fit the variance of the samples. The obtained behavior is distinctively different in one and multiple dimensions. For $d \geq 2$, the number of required iterations is $O(\sqrt{d/n})$, and the error rate for estimating the mean is $O((d/n)^{1/4})$, whereas for d = 1 the number of required iterations is even larger $O(n^{3/4})$, and so is the error rate $O((1/n)^{1/8})$. Other misspecified models were considered by Dwivedi et al. (2018), and one of them is an unbalanced 2-GM one-dimensional mixture to a balanced 2-GM one-dimensional mixture, albeit with a smaller, unknown variance. The paper bounded the distance between the true parameter and the parameter corresponding to the KL projection of the true model onto the set of allowed models. Based on this bound, the population EM operator was shown be contractive w.r.t. the projected parameter, and geometric convergence with statistical error rate $O(1/\sqrt{n})$ of the samples-based EM iteration was established.

Following the general analysis made by Balakrishnan et al. (2017), various latent models were explored. A high-dimensional setting with $d \geq n$ and sparsity assumptions was studied by various authors (Wang et al., 2014; Yi and Caramanis, 2015), which proposed truncation and regularization approaches for modifying EM to that setting, and provided results comparable to that of Balakrishnan et al. (2017). The problem of estimating mixtures of linear regressions was considered by Klusowski et al. (2019), which enlarged the contraction region assured by Balakrishnan et al. (2017) for this case, and showed that any initial guess with sufficiently large angle with the target parameter vector, rather than the small distance requirement of Balakrishnan et al. (2017), will converge to θ_* . It also showed that a sample-splitting version of the EM algorithm converges with high probability. Global convergence of the sample EM iteration was later established by Kwon et al. (2019) by controlling both the empirical error and empirical angle between the population and empirical iterations. Results of this nature were then generalized to the k mixture of linear regression by Klusowski et al. (2019). The k-GM for a general $k \ge 2$ was studied by Yan et al. (2017); Zhao et al. (2018), which provided results comparable to Balakrishnan et al. (2017) for gradient EM under minimal separation condition between the means, and closeness of the initial guess to the true means. Beyond the i.i.d. setting, estimation problems in hidden Markov models using EM were studied by Yang et al. (2015); Aiylam (2018).

1.6 Notational Conventions

Constant values which are used to state results or used in more than a single place in the paper are denoted by sans-serif letters and are summarized in Table 2.⁶ Constants which are used only locally are denoted by c, C, c_0, \ldots . Those constants are either universal or depend only on the parameters of the global assumptions C_{θ} and C_{ρ} . Asymptotic relations such as \leq, \approx are within these constant factors. Standard Bachmann—Landau asymptotic notation

^{6.} In principle, these constants can be upper bounded by functions of the global constants C_{θ} and C_{ρ} . Since, this will lead to rather cumbersome statements of the results described in this paper, and since obtaining tight bounds for these constants is an onerous task, we opt to leave them unspecified.

EM Algorithm is Adaptively-Optimal

Constant	Description
C _θ	Global assumption (Section 1.2): Maximal norm of θ_*
C _ρ	Global assumption (Section 1.2): Maximal absolute value of ρ_*
Cβ	Global assumption (Section 1.2): Maximal absolute value of β_{ρ_*}
$(\underline{C}_{\beta},\overline{C}_{\beta})$	Global assumption (Section 1.2): $\underline{C}_{\beta}\rho \leq \beta_{\rho} \leq \overline{C}_{\beta}\rho$.
Cω	Concentration (Section 2.1): Constant for empirical iteration error (w.h.p.)
$\{C_{i}^{(1)}\}$	Result for $d = 1$ mean iteration (Section 2.1): Constants in Theorem 6
T ⁽¹⁾	Result for $d = 1$ mean iteration (Section 2.1): Convergence time in Theorem 6
c‴	Proof of $d = 1$ mean iteration (Lemma 15): A constant for a bound on $f''(\theta)$
$\{C_i^{(d)}\}$	Result for $d > 1$ mean iteration (Section 2.3): Constants in Theorem 10
$T_{\theta_0}^{(d)}, T_G^{(d)}$	Result for $d > 1$ mean iteration (Section 2.3): Convergence times in Theorem 10
$C_{F,0},C_F^{\prime\prime},C_F^{\prime\prime\prime}$	Proof of $d > 1$ mean iteration (Lemma 17): Constants for bounds on $F(a, b)$ and its derivatives
$C_{G,\rho}^{(d)},C_{G,\eta}^{(d)}$	Proof of $d > 1$ mean iteration (Proposition 9): Constants for bounds on $G(a, b)$ and its derivatives
$C^{(d)}_\eta$	Proof of $d > 1$ mean iteration (Proposition 11): A constant for a condition on $\eta = \ \theta_*\ $
$\{C_i^{(\rho)}\}$	Result for weight iteration (Section 2.4): Constants in Theorem 12
Τ ^(ρ)	Result for weight iteration (Section 2.4): Convergence time in Theorem 12
C_h''	Proof for weight iteration (Lemma 18): A constant for a bound on the second derivative of $h(\rho)$

Table 2: Summary of global constants.

will be used, where in specific, the notation $a_n = O(b_n)$ for a pair of positive sequences $\{a_n\}_{n\in\mathbb{N}}, \{b_n\}_{K\in\mathbb{N}}$ implies that there exists $k\in\mathbb{N}_+$ so that $\limsup_{n\to\infty}\frac{a_n}{b_n(\log n)^k} < \infty$ (i.e., $a_n = O(b_n \cdot (\log n)^k)$).

The expectation of a random variable U is denoted by $\mathbb{E}[U]$, and the empirical mean of n i.i.d. samples (U_1, \ldots, U_n) of U is denoted by $\mathbb{E}_n[(U)] := \frac{1}{n} \sum_{i=1}^n U_i$. The distribution (law) of a random variable U will be denoted by $\mathcal{L}(U)$. The 1-Wasserstein distance between probability measures μ and ν is given by (Villani, 2003) $W_1(V,U) = \inf \mathbb{E}|V - U|$ where the infimum is over all couplings of μ and ν , i.e., a pair of random variables (V,U) such that $\mathcal{L}(V) = \mu$ and $\mathcal{L}(U) = \nu$. The Euclidean norm is denoted by $\|\cdot\|$, and the Euclidean ball of radius r in dimension d is denoted by $\mathbb{B}^d(r)$, where for d = 1 we omit the superscript. A unit vector in the direction of a vector θ is denoted by $\hat{\theta}$. For a given Orlicz function ψ , the Orlicz norm of a random variable U is denoted by $\|U\|_{\psi} = \inf_{t>0} \{\mathbb{E}[\psi(|U|/t)] \le 1\}$, where Uis called σ^2 -sub-gaussian (resp. σ -sub-exponential) if $\|U\|_{\psi_2} \le \sigma$ where $\psi_2(t) = \exp(t^2) - 1 =$ (resp. $\|U\|_{\psi_1} \le \sigma$ where $\psi_1(t) = \exp(t) - 1$). The set $\{1, \ldots, n\}$ is denoted by [n], equivalence (usually local simplification of notation) is denoted by \equiv , and equality in distribution by \underline{d} .

1.7 Organization

Section 2 contains detailed statements of the results, along with discussions, and proof outlines. Proofs appear in later sections according to order. Specifically:

• In Section 2.1 we generalize the uniform error concentration bounds of Wu and Zhou (2019) to the unbalanced case, and also states such a bound for the weight iteration.

The proof is not fundamentally different from Wu and Zhou (2019) and is provided in Appendix A for completeness.

- In Section 2.2 we analyze the mean population and empirical EM iterations assuming the true weight ρ_* is known for d = 1.
- In Section 2.3 we extend the analysis of the previous section to d > 1, and prove the main result of the paper.
- In Section 2.4 we analyze the population and empirical EM iterations for the weight assuming a fixed mean θ (possibly mismatched to θ_*).
- In Section 2.5 we briefly discuss the problem in which both ρ_* and θ_* are unknown, and the estimator is required to jointly estimate both.

In Appendix B we analyze minimax rates, and in Appendix C we provide miscellaneous results used in the paper.

2. Detailed Results

In this section we describe our results in detail.

2.1 Concentration of the Empirical EM Iteration

We first establish the concentration properties of the empirical iterations to their population versions. The following theorem is a generalization of the result of Wu and Zhou (2019, Theorem 4) from the $\rho = 0$ case to $\rho \neq 0$ case, and is proved in Appendix A.

Theorem 3 Assume that $\|\theta_*\| \leq C_{\theta}$ and that $|\rho_*| \leq C_{\rho}$, and consider the event

$$\mathcal{E} := \{ \|f_n(\theta, \rho) - f(\theta, \rho)\| \le \max\{\|\theta\|, \rho\} \cdot \omega_d \} \cap \{ |h_n(\rho, \theta) - h(\rho, \theta)| \le \|\theta\| \cdot \omega_1 \}$$
(15)

where

$$\omega_d := \sqrt{\mathsf{C}_\omega \frac{d\log n}{n}} \,.$$

Then, there exist a constant C_{ω} which depends on (C_{θ}, C_{ρ}) such that $\mathbb{P}[\mathcal{E}] \geq 1 - \frac{1}{n^{cd}}$ for all $n \geq Cd \log n$.

We assume in the rest of the paper that the high probability event (15) holds, and often denote ω_d by ω for brevity. Note that in general, the error bound depends on the iteration values (θ, ρ) and is uniform in the ground truth parameters (θ_*, ρ_*) (as long as they satisfy the global assumptions). For the mean iteration, it is interesting to contrast the balanced iteration of $\rho = 0$ with $\rho \neq 0$. For the balanced iteration, $f_n(\theta, 0) = \mathbb{E}_n[X \cdot \tanh(\theta, X)]$ and so $f_n(0,0) = f(0,0) = 0 \in \mathbb{R}^d$ with probability 1. Hence, a valid upper bound on the empirical error may tend to zero as $\|\theta\| \to 0$, and, indeed, Wu and Zhou (2019, Theorem 4) have obtained an empirical error bound of order $O_P(\|\theta\|\omega)$. Similar intuition was used by Dwivedi et al. (2020a,b) to "localize" the error around $\|\theta\| \approx 0$, although in a more granular way. When the iteration is unbalanced, i.e., $\rho \neq 0$, the iteration $f_n(0,\rho) = \rho \cdot \mathbb{E}_n[X]$ is a nondegenerate random variable, whose population version is $f(0,\rho) = \rho \cdot \mathbb{E}[X] = \rho^2 \cdot \theta_*$. In fact,

in one-dimension, $f_n(0, \rho)$ might even be negative (i.e., have opposite sign to its population version). Hence, one cannot expect the empirical error to behave as in the balanced case, and an additional term is required, which depends on ρ , as given in (15). Evidently, as ρ increases, so does the error bound. Intuition again may arise from the extreme case, this time when $\rho = 1$. In this case the iteration is simply $\lim_{\rho \to 1} f_n(\theta, \rho) = \mathbb{E}_n[X]$, i.e., the iteration provides the empirical mean at a single step, which clearly must have an empirical error of $O_P(\sqrt{\frac{d}{n}})$, even with $\|\theta\|$ being arbitrarily small. Figuratively speaking, the more the iteration is "aggressive" in assuming prior knowledge regarding the signs $\{S_i\}$ generating the samples, the larger is the empirical error in the iteration. On the other hand, as we shall see, such (correct) prior knowledge improves the convergence properties of the population iteration. So, the convergence properties of the empirical iteration for $\rho > 0$ are obtained from a balance between improved population convergence compared to $\rho = 0$ which compensate for the larger empirical error. The error in the weight iteration is proportional to $O_P(\|\theta\|\cdot\omega_1)$, which agrees with the observations that $h_n(\theta,\rho) \to \rho$ as $\|\theta\| \to 0$, and ρ is unidentifiable, along with the observation that the weight iteration is effectively one-dimensional, and so the error is proportional to ω_1 rather than to ω_d .

2.2 The Mean Iteration for Known Weight at d = 1

In this section we consider the mean iteration in one dimension. While the model for d = 1 is simple, its analysis already captures some of the complication of the analysis, and also serves as a building block for the analysis of the d > 1 case. We assume that $\delta_* = (1 - \rho_*)/2 \equiv \delta$ is known and fixed, and this true parameter is used in the EM iteration. Hence the model can be written as

$$P_{\eta,\delta} = (1-\delta) \cdot N(\eta, 1) + \delta \cdot N(-\eta, 1),$$

where $\eta := \|\theta_*\| > 0$ is assumed w.l.o.g.. The population version of the EM iteration for this case can be written as

$$f(\theta \mid \eta, \delta) := \mathbb{E}\left[X \cdot \frac{(1-\delta) \cdot e^{X\theta} - \delta \cdot e^{-X\theta}}{(1-\delta) \cdot e^{X\theta} + \delta \cdot e^{-X\theta}}\right] = \mathbb{E}\left[X \cdot \tanh(X\theta + \beta)\right],$$

with $X \sim (1 - \delta)N(\eta, 1) + \delta N(-\eta, 1)$ and where we abbreviate to $f(\theta \mid \eta)$ or $f(\theta)$ when possible. Similarly, the empirical iteration will be denoted by $f_n(\theta \mid \eta, \delta)$, and abbreviated to $f_n(\theta)$. Figure 1 illustrates several EM iterations (based on single runs of $n = 10^4$ samples).

We begin with the population iteration.

Theorem 4 (Population mean iteration, known weight, d = 1) The following holds:

- 1. The unique fixed point of $\theta \mapsto f(\theta \mid \eta, \delta)$ in \mathbb{R}_+ is $\theta = \eta$, and its fixed points in \mathbb{R}_- are confined to the interval $(-\eta, 0)$.
- 2. If $\theta_0 \geq 0$ then the iteration $\theta_{t+1} = f(\theta_t \mid \eta, \delta)$ converges to η .
- 3. Let $\delta \leq \tilde{\delta} < 1/2$ and $\theta_0 \geq 0$. Consider the iteration $\tilde{\theta}_t = f(\tilde{\theta}_{t-1} \mid \eta, \tilde{\delta})$ such that $\theta_0 = \tilde{\theta}_0 \geq 0$. Then $|\eta \tilde{\theta}_t| > |\eta \theta_t|$ for all $t \geq 1$, i.e., the convergence is faster as δ is lower. The same holds for $\tilde{\delta} = 1/2$ if $\theta_0 > 0$.



Figure 1: Illustration of $f(\theta, \delta \mid \eta, \delta)$ for $\eta = 2$ and $\eta = 0.4$.

Though not crucial for the analysis or later derivations, we conjecture from exhaustive numerical evidence that there are only two spurious fixed points of $f(\theta)$ in \mathbb{R}_- , and furthermore, there exists $\delta_{\rm cr} \in (0, 1/2)$ such that the number of fixed points of $f(\theta)$ in $\mathbb{R}_$ is

$$\begin{cases} 2, \quad \delta \in (\delta_{\rm cr}, \frac{1}{2}) \\ 1, \quad \delta = \delta_{\rm cr} \\ 0, \quad \delta \in [0, \delta_{\rm cr}) \end{cases}$$

Theorem 4 establishes global convergence properties for the unbalanced one-dimensional EM population iteration, when initializing either with the correct sign of the larger weight component, or with a neutral sign ($\theta = 0$). Nonetheless, the illustration in Figure 1 also demonstrates that initializing with the strictly wrong sign may lead to convergence to a spurious stable fixed point which is at a non-zero distance from $-\eta$, even when $n \to \infty$. Thus, a correct initialization of this iteration is both simple and crucial.

To describe the proof idea of Theorem 4, we briefly recall the properties of the balanced iteration $f(\theta \mid \eta, \frac{1}{2})$ and why this iteration globally converges. As evident from Figure 1 and proved by Wu and Zhou (2019, Section 2), $\theta \mapsto f(\theta \mid \eta, \frac{1}{2})$ is an odd increasing function which is concave on \mathbb{R}_+ . It is not difficult to show (see also Proposition 23 in Appendix C) that in this case that the iteration must converge to one of the three unique fixed points $\theta = 0, \pm \tilde{\theta}$. The general consistency property of EM⁷ then implies that $\tilde{\theta} = \eta$. Thus, for the balanced iteration, the concavity property provides a global property on the iteration which is used to establish global convergence.

The reduced uncertainty in the $\delta < 1/2$ case hints that the iteration should converge faster and more accurately than for the $\delta = 1/2$ case. However, at the same time, the change from $\delta = 1/2$ to $\delta < 1/2$ breaks the symmetry in the iteration, and hence the concavity property of the iteration in \mathbb{R}_+ . For example, the yellow iteration in Figure 1 corresponding to $\delta = 0.01$ is non-concave around $\theta \approx 0.6$. While the second-derivative of the iteration at $\theta \approx 0.6$ can be numerically shown have a small magnitude (and as evident from the figure, the iteration is rather flat there), no general concavity statement can be made, and hence a different global property is required. The consistency property assures at $\theta = \eta$ the iteration is insensitive to δ , and specifically that $f(\eta \mid \eta, \delta) = \eta$ for all δ . As evident from Figure 1, and as is true in general, for $\theta < \eta$ and $\theta > \eta$ a change in δ bares an opposite, yet consistent effect. The next proposition summarizes this property, along with another global property related to "oddness dominance" that will be used in the analysis of the empirical iteration.

Proposition 5 Assume that $\eta > 0$ and $\delta \in [0, \frac{1}{2}]$.

- 1. $f(\theta \mid \eta, \delta) \ge -f(-\theta \mid \eta, \delta)$ for all $\theta > 0$.
- 2. $\delta \mapsto f(\theta \mid \eta, \delta)$ is non-increasing (resp. constant, resp. non-decreasing) for $\theta < \eta$ (resp. for $\eta = \theta$, resp. $\theta > \eta$).

The second property can be described as $\theta = \eta$ being a "pivot-point" for the iteration as δ is varied (see Figure 1). Given the second property of Proposition 5, along with the known convergence for the case $\delta = 1/2$, global convergence can be easily established for $\theta_0 \ge 0$.

^{7.} Consistency can also be proved directly for the Gaussian mixture model—see proof of Lemma 15 below.

In order to prove property 2 in Proposition 5, one may assume an arbitrary and fixed true parameter $\eta > 0$, and attempt to establish this property for all $\theta \in \mathbb{R}$. It turns out that if $\theta < 0$, this property can be proved by a direct reasoning on $\frac{\partial}{\partial \delta} f(\theta \mid \eta, \delta)$. However, similar strategy seems daunting for $\theta > 0$, and our proof is built on an indirect argument. More explicitly, for $\theta > 0$ it is required to be proved that:

$$\frac{\partial f(\theta \mid \eta, \delta)}{\partial \delta} \begin{cases} > 0, & 0 < \eta < \theta \\ = 0, & \eta = \theta \\ < 0, & \eta > \theta \end{cases}$$
(16)

The proof of (16) is based on the following ideas:

- Analyzing $\frac{\partial}{\partial \delta} f(\theta \mid \eta, \delta)$ as a function of η , rather than as a function of θ directly. For this to be useful, we will need to analyze $\eta \in \mathbb{R}$ and not just $\eta \in \mathbb{R}_+$.
- Expressing $\frac{\partial}{\partial \delta} f(\theta \mid \eta, \delta)$ as a convolution of some function with a Gaussian kernel. We then exploit a variation diminishing property of Gaussian kernels which implies that if a function $h(\theta)$ has k zero-crossings in \mathbb{R} , its convolution with a Gaussian kernel may only reduce the number of zero-crossings. See Proposition 25 in Appendix C.3 for a formal statement. This allows us to prove that $\eta \mapsto \frac{\partial}{\partial \delta} f(\theta \mid \eta, \delta)$ has a single crossing point for some θ_0 .
- Then, utilizing the consistency property, which states that $f(\theta \mid \eta, \delta) = \theta$ for $\theta = \eta$ and any δ , establishes that $\theta_0 = \theta$, and this results (16).

The idea of analyzing the iteration w.r.t. the true parameter η , rather than w.r.t. θ was previously used by Daskalakis et al. (2017), which used it in order to prove one-dimensional global convergence (as well as convergence rates) for the balanced iteration. While such an argument is not essential for this case given the direct analysis of Wu and Zhou (2019), an idea in that spirit is useful here for proving a different global property.

We now turn to the empirical iteration. As we show next, the improved convergence in the unbalanced case compared to the balanced case stated in Theorem 4 compensates for the larger empirical error.

Theorem 6 Assume that $|\eta| \leq C_{\theta}$, $|\rho_*| \leq C_{\rho}$ and that the high probability event (15) holds. Consider the empirical mean EM iteration $\theta_t = f_n(\theta_{t-1}) \equiv f_n(\theta_{t-1}, \delta \mid \eta, \delta)$. There exists $n_0(C_{\theta}, C_{\rho})$ and constants $\{C_i^{(1)}(C_{\theta}, C_{\rho})\}$ such that if $\rho_* > C_1^{(1)}\sqrt{\omega_1}$ and $n \geq n_0$ then

$$\ell(\theta_t, \eta) \le \mathsf{C}_2^{(1)} \cdot \min\left\{\frac{\omega_1}{\rho}, \frac{\omega_1}{\eta}\right\}$$

holds for all $t \geq \mathsf{T}_{\theta_0=0}^{(1)}$ where

$$\mathsf{T}_{\theta_{0}=0}^{(1)} := \begin{cases} 1, & \eta \leq \frac{\omega_{1}}{\rho} \\ \mathsf{C}_{3}^{(1)} \cdot \frac{1}{\rho^{2}} \log \left(\frac{\omega_{1}}{\mathsf{C}_{5}^{(1)}\rho}\right), & \frac{\omega_{1}}{\rho} \leq \eta \leq \mathsf{C}_{4}^{(1)}\rho \\ \mathsf{C}_{3}^{(1)} \cdot \left(\frac{1}{\rho\eta} + \frac{1}{\eta^{2}} \log \left(\frac{1}{\mathsf{C}_{6}^{(1)}\rho\omega_{1}}\right)\right), & \mathsf{C}_{4}^{(1)}\rho < \eta \leq \mathsf{C}_{\theta} \end{cases}$$

in case the iteration was initialized by $\theta_0 = 0$, and for all $t \ge \mathsf{T}_{\theta_0 = \frac{1}{\rho}\mathbb{E}_n[X]}^{(1)}$ where

$$\mathsf{T}_{\theta_{0}=\frac{1}{\rho}\mathbb{E}_{n}[X]}^{(1)} := \begin{cases} 1, & \eta \leq \mathsf{C}_{4}^{(1)}\rho \\ \mathsf{C}_{3}^{(1)}\frac{1}{\eta^{2}}\log\left(\frac{1}{\mathsf{C}_{6}^{(1)}\rho\omega_{1}}\right), & \mathsf{C}_{4}^{(1)}\rho < \eta \leq \mathsf{C}_{\theta} \end{cases}$$

in case the iteration was initialized by $\theta_0 = \frac{1}{\rho} \mathbb{E}_n[X]$.

The proof uses a "sandwiching" argument developed by Wu and Zhou (2019) that bounds the empirical iteration $f_{-}(\theta) \leq f_{n}(\theta) \leq f_{+}(\theta)$ by the envelopes $f_{\pm}(\theta) = f(\theta) \pm \max\{|\theta|, \rho\} \cdot \omega_{1}$ (which holds with high probability), and the resulting iterations $\theta_{t}^{\pm} = f_{\pm}(\theta_{t-1})$ obtained when initializing those iterations and the empirical iteration with the same initial guess $\theta_{0}^{\pm} = \theta_{0}$. We consider both $\theta_{0} = 0$ or $\theta_{0} = \frac{1}{\rho} \mathbb{E}_{n}[X]$. First, it is proved that all three iterations $\{\theta_{t}\}, \{\theta_{t}^{\pm}\}$ converge to fixed points, η_{n}, η_{\pm} respectively. Then, the analysis is split into three regimes. For initialization at $\theta_{0} = 0$:

- 1. If $\frac{\omega_1}{\rho} \leq \eta \leq \rho$ then the envelopes converge to fixed points $0 < \eta_- \leq \eta_n \leq \eta_+$, and the envelopes are approximated as $f_{\pm}(\theta) \approx 1 c\rho^2$ for some c > 0. Thus, the envelopes are contractions whose convergence times is on the order of $\tilde{O}(\frac{1}{\rho^2})$.
- 2. If $\rho \lesssim \eta$ then convergence has two phases. At the first phase, θ_t is low, and the iteration increases additively each step from $\theta_0 = 0$ by $\Omega(\rho^2 \eta)$ at each iteration. Thus, after $T_1 = O(\frac{1}{\rho\eta})$ iterations, $\theta_t = \Omega(\rho)$. At this point, the empirical error is $\omega_1 \cdot \max\{\theta, \rho\} \lesssim \omega_1 \theta$, to wit, the same empirical error as for the balanced iteration. Since the population iteration converges faster in the unbalanced case than in the balanced case (Theorem 4), and the empirical error in this case is of the same order, then the convergence of the unbalanced empirical iteration is only faster than that of the empirical balanced iteration. The latter was analyzed by Wu and Zhou (2019, Theorem 3), and its result is used here.
- 3. If $\eta \lesssim \frac{\omega_1}{\rho}$ then analysis similar to the previous cases shows that the upper envelope θ_t^+ will increase, and will remain within the required statistical error, i.e., $0 \leq \theta_t^+ \lesssim \frac{\omega_1}{\rho}$, for all $t \geq 1$. On the other hand, for the lower envelope, it is not guaranteed that $f_-(0) > 0$, and so it is also not guaranteed that θ_t^- will increase and converge to a positive fixed point. If it does converge to a positive fixed point $\eta_- > 0$, then $\eta_- < \eta_+$ must also hold, and, as for the upper envelope, $0 \leq \theta_t^- \lesssim \frac{\omega_1}{\rho}$, for all $t \geq 1$. If, however, this is not the case and $f_-(0) < 0$, then θ_t^- will decrease and converge to a negative fixed point $\eta_- < 0$. In that event, the oddness domination property of the population iteration (Proposition 5, item 1) assures that $|\eta_-| \leq \eta_+$, and so the same statistical error $O(\frac{\omega_1}{\rho})$ is again assured.

For initialization at $\theta_0 = \frac{1}{\rho} \mathbb{E}_n[X]$, the error in the first iteration is already within the statistical accuracy in Cases 1 and 3. For Case 2, it can be shown that the first phase of convergence does not occur, and the convergence is as in the balanced case.

2.3 The Mean Iteration for Known Weight at d > 1

We now consider the general d > 1 case. Recall that the *n* i.i.d. samples are given by $X \sim (1 - \delta) \cdot N(\theta_*, I_d) + \delta \cdot N(-\theta_*, I_d)$ where $\theta_* \in \mathbb{R}^d$ and $\delta \in (0, 1/2)$ is known. For the population mean EM iteration we show that:

Theorem 7 (Population iteration, known weight, d > 1) Consider the population mean EM iteration $\theta_t = f(\theta_{t-1}, \delta \mid \theta_*, \delta)$. If $\langle \theta_0, \theta_* \rangle \ge 0$ then $\lim_{t\to\infty} \theta_t = \theta_*$. Specifically, this holds for $\theta_0 = 0$.

As in the one-dimensional case, the idealized population iteration does not converge to a spurious fixed point, whenever the iteration is not initialized in a direction which has an obtuse angle with θ_* (which is the mean of the larger weight component, $1-\delta$). Furthermore, such initialization can be achieved by setting $\theta_0 = 0$, since $f(0, \delta \mid \theta_*, \delta) = (1 - 2\delta)^2 \cdot \theta_*$ which already points to the desired direction. Evidently, in this case, $\theta_t \propto \hat{\theta}_*$ for all $t \ge 1$. A slightly more general property holds for any initialization, and this is the basic ingredient of the proof which we describe next.

The proof of Theorem 7 is based on an observation made by Xu et al. (2016); Daskalakis et al. (2017) that the population mean EM iteration is "trapped" to the two-dimensional space spanned by the true vector θ_* and the initial guess θ_0 . Wu and Zhou (2019) formulated this observation in the following way. Let us denote $\eta := \|\theta_*\|$ for brevity, let $V \sim (1 - \delta) \cdot$ $N(\eta, 1) + \delta \cdot N(-\eta, 1)$ and $W \sim N(0, 1)$ be such that $V \perp W$, and define:

$$F((a,b),\delta \mid \eta,\delta) = \mathbb{E}\left[V \tanh(aV + bW + \beta)\right],$$

and

$$G((a, b), \delta \mid \eta, \delta) = \mathbb{E} \left[W \tanh(aV + bW + \beta) \right]$$

where we omit the dependence in (η, δ) whenever it is inessential and simply write $F(a, b \mid \eta, \delta)$, $G(a, b \mid \eta, \delta)$, or even just, F(a, b), G(a, b). The following was proved by Wu and Zhou (2019, Lemma 4) for the balanced case,⁸ but the proof is similar for any $\delta \in [0, 1]$ and thus omitted.

Lemma 8 Consider the population mean iteration $\theta_{t+1} = f(\theta_t, \delta \mid \theta_*, \delta)$, and define

 $\theta_t = a_t \cdot \hat{\theta}_* + b_t \cdot \xi_t$

where $\eta = \|\theta_*\|$, $\hat{\theta}_* = \theta_*/\eta$, $\xi_t \perp \eta$ and $\|\xi_t\| = 1$ such that $\operatorname{span}\{\theta_*, \xi_t\} = \operatorname{span}\{\theta_*, \theta_t\}$ and $b_t \geq 0$. Then, $\theta_t \in \operatorname{span}\{\theta_0, \theta_*\}$ (i.e., $\xi_t = \xi_0$) for all t, and

$$a_{t+1} = F(a_t, b_t)$$
$$b_{t+1} = G(a_t, b_t).$$

We refer to $F(\cdot)$ as the signal iteration and to $G(\cdot)$ as the orthogonal iteration. Lemma 8 thus implies that to analyze the iteration $\theta_{t+1} = f(\theta_t, \delta \mid \theta_*, \delta)$ it suffices to analyze the evolution of $\{a_t, b_t\}$, and that $\theta_t \to \theta_*$ is equivalent to $a_t \to \eta$ and $b_t \to 0$.

In the balanced case, the population mean EM iteration was shown to globally converge to $\pm \theta_*$ by showing that the orthogonal error goes to zero unconditionally of the

^{8.} A similar, but not identical, claim was previously made by Daskalakis et al. (2017).

signal iteration, i.e., $b_t \to 0$ is always satisfied. Then, the problem is reduced to the onedimensional iteration studied in the previous section. Essentially, this global property holds due to the fact that for $G(a, b \mid \eta, \frac{1}{2})$ is a concave increasing function with G(a, 0) = 0, and $\frac{\partial}{\partial b}G(a, b)|_{b=0} < 1$ (Wu and Zhou, 2019, Lemma 5). As in the one-dimensional case, in the unbalanced case, the lack of symmetry in case of $\delta < 1/2$ breaks down the concavity property of $G(a, b \mid \eta, \delta)$, and so a different global property is required. This is achieved in the following proposition, which states properties of $G(a, b \mid \eta, \delta)$ w.r.t. the true parameters (η, δ) , and specifically states that $G(a, b \mid \eta, \delta)$ is dominated by $G(a, b \mid \eta, 1/2)$, and so the orthogonal iteration in case of $\delta < 1/2$ converges faster than in the case of $\delta = 1/2$.

Proposition 9

- 1. Monotonicity w.r.t. δ : If $a \ge 0$ then $\delta \mapsto G(a, b \mid \eta, \delta)$ is an increasing function on [0, 1/2].
- 2. Dominance w.r.t. δ : Let $C_f > 0$ be given. There exists $\mathsf{C}_{G,\rho}^{(d)}(\mathsf{C}_{\theta},\mathsf{C}_{\beta},C_f) > 0$ and $n_0(\mathsf{C}_{\theta},\mathsf{C}_{\beta},C_f)$ such that for any $n \ge n_0$

$$G(a,b \mid \eta, \delta) \le G(a,b \mid \eta, \frac{1}{2}) - \mathsf{C}_{G,\rho}^{(d)} \rho^2 b \le b \left(1 - \frac{a^2 + b^2}{2 + 4(a^2 + b^2)} - \mathsf{C}_{G,\rho}^{(d)} \rho^2 \right)$$

for all $(a, b, \eta) \in [0, C_f]^2 \times [0, \mathsf{C}_{\theta}].$

- 3. Monotonicity w.r.t. η : For $a \ge 0$, $\eta \mapsto G(a, b \mid \eta, \delta)$ is a decreasing function in $\eta \in [0, a + \frac{b^2}{a}]$.
- 4. Dominance w.r.t. η : Let $C_{G,\eta}^{(d)} = 3C_{\theta}$. Then,

$$G(a, b \mid \eta, \delta) \le G(a, b \mid 0, \delta) + \mathsf{C}_{G, n}^{(d)} b \eta^2$$

for all $(a, b, \eta) \in \mathbb{R} \times \mathbb{R}_+ \times [0, \mathsf{C}_\theta].$

Given items 1 and 2 of Proposition 9, it is evident that unconditional convergence of the orthogonal part of the iteration to zero is assured in the unbalanced case (and the convergence is only faster compared to the balanced case). After such convergence, the problem is almost precisely reduced to the one-dimensional setting in the signal iteration $\{a_t\}$, except for a small residual additive error resulting from orthogonal iteration. However, as was shown in the one-dimensional analysis, the unbalanced mean EM iteration may tolerate small additive term (therein, this was due to the term $\omega_1 \rho$ which, unlike the error term $\omega_1 \theta$ does not vanishes when $\|\theta\| \to 0$), and so this additive term does not prevent convergence.

We now turn to the empirical iteration:

Theorem 10 Assume that $\|\theta_*\| \leq C_{\theta}$ and that $|\rho_*| \leq C_{\rho}$, and that the high probability event (15) holds. Consider the empirical mean EM iteration $\theta_t = f_n(\theta_{t-1}, \delta \mid \theta_*, \delta)$. There exists n_0 and constants $\{C_i^{(d)}\}$ which depend on (C_{θ}, C_{ρ}) such that if $\rho_* > C_1^{(d)} \sqrt{\omega}$ and $n \geq n_0$ then

$$\ell(\theta_t, \theta_*) \le \mathsf{C}_2^{(d)} \min\left\{\frac{\omega}{\rho}, \frac{\omega}{\eta}\right\}$$

holds for all $t \geq \mathsf{T}_{\theta_0}^{(d)} = \mathsf{T}_{\theta_0}^{(1)} + \mathsf{T}_G^{(d)}$ where either $\theta_0 = 0$ or $\theta_0 = \frac{1}{\rho} \mathbb{E}_n[X]$, $\mathsf{T}_{\theta_0}^{(1)}$ is determined as in Theorem 6 by replacing⁹ $\omega_1 \to \omega = \sqrt{\mathsf{C}_{\omega} \frac{d \log n}{n}}$ and where

$$\mathsf{T}_{G}^{(d)} := \begin{cases} 1, & \eta \leq \rho \\ \frac{C_{3}^{(d)}}{\eta^{2}} \cdot \log\left(C_{4}^{(d)}\frac{\omega}{\eta}\right), & \eta \geq \rho \end{cases}$$

The proof of this theorem is based on splitting the analysis into three regimes $0 < \eta \lesssim \frac{\omega}{\rho}$ $\frac{\omega}{\rho} \lesssim \eta \lesssim \rho$ and $\eta \gtrsim \rho$. First, it is shown that when initializing at either $\theta_0 = 0$ or $\dot{\theta}_0 = \frac{1}{\rho} \mathbb{E}_n[X]$, the orthogonal iteration satisfies $b_t = O(\frac{\omega}{\rho})$, and remains so for all iterations. In the $\eta \lesssim \frac{\omega}{\rho}$ regime, this is shown by the local behavior of $G(a, b \mid \eta, \delta)$ around $\eta \approx 0$ (Proposition 9, item 4). In the $\eta \gtrsim \frac{\omega}{\rho}$ this is proved by the dominance relation to the balanced orthogonal iteration (Proposition 9, items 1 and 2), along with a verification that a_t remains positive for all iterations (so that these dominance relations are in fact valid). Given that $b_t = O(\frac{\omega}{\rho})$, the effect of the orthogonal iteration on the signal iteration is negligible, and it is essentially reduced to the one-dimensional iteration. The convergence time for this is $T_{\theta_0}^{(1)}$ (when setting the specific initialization for $\theta_0^{(10)}$), and the resulting error for the signal iteration is $|a_t - \eta| = O(\min\{\frac{\omega}{\rho}, \frac{\omega}{\eta}\})$. If $\eta < \rho$ then this is also the error rate for θ_* as $|\theta - \theta_*| = O(|a_t - \eta| + b_t)$. If $\eta > \rho$, then the orthogonal iteration can be shown to decrease to $O(\frac{\omega}{n})$ after additional $\mathsf{T}_{G}^{(d)}$ iterations.

We next consider the case of ρ_* which is too small to satisfy the condition of Theorem 10.

Proposition 11 (Empirical iteration, known weight, d > 1, small ρ_*) Assume that $\|\theta_*\| \leq 1$ C_{θ} and that the high probability event (15) holds. Further assume that the balanced EM weight iteration is run $\theta_t = f_n(\theta_{t-1}, \delta = \frac{1}{2} \mid \theta_*, \delta = \frac{1}{2})$ with random initialization as in Theorem 1. Let $\tilde{\theta}_t = s_t \theta_t$ where $s_t = \operatorname{sign} \langle \mathbb{E}_n[X], \theta_t \rangle$. Then, there exists $\mathsf{C}_{\rho}^{(d)}(\mathsf{C}_{\theta}) > 0$ such that if

$$\frac{\omega}{\eta} \le \rho_* \le \mathsf{C}_1^{(d)} \sqrt{\omega} \le \mathsf{C}_\eta^{(d)} \eta \,,$$

then

$$\ell(\theta_t,\theta_*) \leq \mathsf{C}_2^{(d)} \frac{\omega}{\eta}$$

holds for all $t \geq \frac{\log n}{\|\theta_*\|^2}$.

Theorem 10 and Proposition 11 together imply Theorem 2, which is the main result of the paper.

2.4 The Weight Iteration for a Fixed Mean

In previous sections, we have considered the mean iteration assuming a known weight. In this section, we study the opposite extreme case, and study the weight iteration assuming a

^{9.} The constants determining $\mathsf{T}_{\theta_0}^{(1)}$ might also be different than for d = 1. 10. In fact, Theorem 10 is valid for any θ_0 for which $b_t = O(\frac{\omega}{\rho})$.

fixed mean θ , and specifically, the case in which $\theta = \theta_*$ holds. In this case, the log-likelihood is given by

$$\rho_{\text{MLE}} = \underset{\rho \in [0,1]}{\operatorname{argmax}} \sum_{i=1}^{n} \log \left(\frac{1+\rho}{2} e^{-\langle X_i, \theta_* \rangle} + \frac{1-\rho}{2} e^{+\langle X_i, \theta_* \rangle} \right).$$

As apparent and also well-known, the log-likelihood is a concave function of the unknown parameter ρ , and so, the EM algorithm is assured to converge to the MLE (Wu, 1983). Alternatively, a simple method-of-moments estimator $\rho_{\text{MoM}} = \frac{1}{\|\theta\|} \langle \hat{\theta}, \mathbb{E}_n[X] \rangle$ can be readily shown to achieve the minimax error rate for this problem, given roughly by min $\{\frac{1}{\|\theta_*\|\sqrt{n}}, 1\}$ (see Theorem 22 in Appendix B). Nonetheless, in this section we directly analyze the EM iteration and provide statistical and computational guarantees similar to the previous sections. Despite the favorable behavior mentioned above, the analysis of the EM iteration is delicate, especially in the mismatched case $\theta \neq \theta_*$. Understanding the EM iteration in this setting may then further illuminate its basic features.

We thus assume in this section the model

$$P_{\rho} = \frac{1+\rho}{2} \cdot N(\theta_{*}, 1) + \frac{1-\rho}{2} \cdot N(-\theta_{*}, 1)$$

where $\delta = \frac{1-\rho}{2}$. As in Section 2.3, the weight iteration can be written as

$$h(\rho, \theta \mid \theta_*, \rho_*) = \mathbb{E}\left[\frac{(1+\rho)e^{\|\theta\|V} - (1-\rho)e^{-\|\theta\|V}}{(1+\rho)e^{\|\theta\|V} + (1-\rho)e^{-\|\theta\|V}}\right]$$

where $V \sim (\frac{1+\rho_*}{2}) \cdot N(\langle \hat{\theta}, \theta_* \rangle, 1) + (\frac{1-\rho_*}{2}) \cdot N(-\langle \hat{\theta}, \theta_* \rangle, 1)$ and $\hat{\theta} = \theta/||\theta||$. Similarly, the empirical iteration will be denoted by $h_n(\rho, \theta)$. In addition, since $|\rho_*| \leq C_{\rho}$ is assumed, we may also consider truncated iterations given by $[h(\rho, \theta \mid \theta_*, \rho_*)]_{C_{\rho}}$ where

$$[t]_{\mathsf{C}_{\rho}} = \begin{cases} -\mathsf{C}_{\rho}, & t < -\mathsf{C}_{\rho} \\ t, & -\mathsf{C}_{\rho} < t < \mathsf{C}_{\rho} \\ \mathsf{C}_{\rho}, & t > \mathsf{C}_{\rho} \end{cases} .$$

Figure 2 illustrates EM iteration (based on single runs of $n = 10^6$ samples).

As expected, for a given fixed θ , the iteration is essentially one-dimensional and does not depend on d. Note also that if $\langle \theta, \theta_* \rangle = 0$ then ρ_* is not identifiable, and, in accordance, the population iteration is useless; indeed $h(\rho) = \rho$ for this case. Regarding the population iteration, we have the following theorem:

Theorem 12 (Population weight iteration, fixed mean) Assume that $\rho_* > 0$ and that $\langle \theta, \theta_* \rangle \neq 0$. The following holds:

1. The iteration $h(\rho, \theta)$ has either two or three fixed points in [-1, 1]. The boundaries $\rho = \pm 1$ are always fixed points. There exists a third fixed point $\rho_{\#} \in (-1, 1)$ if and only if

$$\frac{\mathrm{d}}{\mathrm{d}\rho}h(\rho,\theta)\Big|_{\rho=1} = e^{2\|\theta\|^2} \left[\left(\frac{1+\rho_*}{2}\right) e^{-2\langle\theta,\theta_*\rangle} + \left(\frac{1-\rho_*}{2}\right) \cdot e^{2\langle\theta,\theta_*\rangle} \right] > 1 \quad (17)$$



Figure 2: Illustration of $h(\rho, \eta \mid \eta, \rho_*)$ for $\rho_* = 0.6$.

and if it exists, it satisfies $\rho_{\#} \in (0,1)$ if $\langle \theta, \theta_* \rangle > 0$ and $\rho_{\#} \in (-1,0)$ if $\langle \theta, \theta_* \rangle < 0$. Specifically, condition (17) holds if $\|\theta\| > |\langle \hat{\theta}, \theta_* \rangle|$, and, furthermore, if $\theta = \theta_*$ then $\rho_{\#} = \rho_*$.

2. If $\rho_{\#} > 0$ exists then the iteration $\rho_{t+1} = h(\rho_t, \theta)$ converges monotonically upwards (resp. downwards) to $\rho_{\#}$ if $\rho_0 \in (-1, \rho_{\#}]$ (resp. $\rho_0 \in [\rho_{\#}, 1)$).

The proof mainly uses the following properties of $\rho \mapsto h(\rho, \theta)$: It increases monotonically from $h(-1, \theta) = -1$ to $h(1, \theta) = 1$, and in case there is a fixed point $\rho_{\#} \in (-1, 1)$, its uniqueness follows from the fact that $h(\rho, \theta)$ changes its curvature only once as ρ traverse from -1 to 1 (from concave to convex).

A rough characterization of the influence of mismatched θ can be derived as follows. Note that for the method-of-moments estimator, a mismatch in the knowledge of θ_* when assuming the true vector is $\theta \neq \theta_*$ results in bias in estimation, such that, on the population level

$$\rho_{\mathrm{MoM}} = \frac{1}{\|\theta\|} \langle \hat{\theta}, \mathbb{E}[X] \rangle = \frac{1}{\|\theta\|} \langle \hat{\theta}, \theta_* \rangle \cdot \rho_* \,.$$

Thus, $\rho_{\text{MoM}} < \rho_*$ if and only if $\langle \hat{\theta}, \theta_* \rangle < \|\theta\|$. The next proposition shows the same effect for the EM iteration:

Proposition 13 Assume that $\rho_* > 0$ and that $\langle \hat{\theta}, \theta_* \rangle > 0$. Let $\rho_{\#}$ be the fixed point of $\rho \mapsto h(\rho, \theta)$ which satisfies $\rho_{\#} \in (-1, 1)$ (if such exists). Then, $\rho_{\#} < \rho_*$ if and only if $\langle \hat{\theta}, \theta_* \rangle < \|\theta\|$.

The proof of the global property in Proposition 13 is again based on the variation diminishing property of the Gaussian kernel, on consistency, and on exploring the location of the fixed point as a function of the true parameter θ_* for a fixed θ .

The empirical weight iteration satisfies the following theorem:

Theorem 14 (Empirical weight iteration, known mean) Assume that $\|\theta_*\| \leq C_{\theta}$ and that $|\rho_*| \leq C_{\rho}$, and that the high probability event (15) holds. Consider the truncated empirical weight iteration $\rho_t = [h_n(\rho_{t-1}, \theta_* \mid \theta_*, \rho_*)]_{C_{\rho}}$ when initialized with $\rho_0 = 0$. There exists $n_0(C_{\theta}, C_{\rho})$ and constants $\{C_i^{(\rho)}\}$ which depend on (C_{θ}, C_{ρ}) such that if $\|\theta_*\| > C_1^{(\rho)} \frac{\omega_1}{\rho_*}$ and $n \geq n_0$ then

$$\ell(\rho_t, \rho_*) \le \mathsf{C}_2^{(\rho)} \frac{\omega_1}{\|\theta_*\|}$$

holds for all $t \ge \mathsf{T}^{(\rho)} = \frac{\mathsf{C}_3^{(\rho)}}{\|\theta_*\|^2}.$

The proof is based on bounding the empirical iteration with envelopes of absolute error $\omega_1 \|\theta_*\|$, and analyzing their convergence. As might be expected, both the error bound and convergence time diverge when $\|\theta_*\| \rightarrow 0$; In the extreme case $\|\theta_*\| = 0$, ρ_* is not identifiable at all. The error bound of the EM iteration (and thus, also the MLE) matches that of the method-of-moments estimator, and also the minimax error rate (Theorem 22 in Appendix B).

2.5 An Open Problem: Joint Mean and Weight Estimation

We have analyzed the EM algorithm for the model $P_{\theta,\delta}$ in case one of the parameters is known and the other is required to be estimated. We next briefly discuss the more challenging scenario in which both δ_* and θ_* are required to be jointly estimated. In this case, each of the parameters serves as a nuisance parameter for estimating the other one, and the exact statistical and computational rates of EM remains an open problem. We nonetheless briefly discuss several aspects of this problem.

For the idealized population version, it is straightforward to ensure convergence, even far from the solution by a proper "scheduling", i.e., not necessarily running both (6)-(7) at each iteration. Specifically, a simple possible scheduling is "freezing" $\theta_t = \theta_0$ and running the weight iteration for T_0 steps until convergence, then freezing $\rho_t = \rho_{T_0}$ and running the mean iteration until convergence, and so on. The initialization and scheduling order will then affect convergence. If we set $\rho_0 = 0$ and run the balanced mean iteration $\theta_{t+1} =$ $f(\theta_t, \frac{1}{2}|\eta, \delta)$ it will converge to θ_* . If we after this convergence we will run the weight iteration $\rho_{t+1} = h(\rho_t, \theta_*)$ it will converge to ρ_* . Thus, this scheduling globally converges to (θ_*, ρ_*) . By contrast, while we have empirically observed that initializing with a frozen θ_0 also globally converges, it is more challenging to establish via our methods. To see this, suppose for simplicity that d = 1. Note that Proposition 13 hints the importance of assuring that $\theta_0 > \theta_* \equiv \eta$ so that the weight iteration $\rho_{t+1} = h(\rho_t, \theta_0)$ will have a fixed point $\rho_{\#} < \rho_*$. If this condition does not hold, then the weight iteration might not have a fixed point $\rho_{\#}$ in (-1,1), and the iteration will converge to the spurious fixed point of $\rho = 1$. Thus, we would like to initialize with a frozen θ_0 such that $|\theta_0| > \eta$. By our assumptions, this could be achieved, by setting $\|\theta_0\| = C_{\theta}$. Next, we freeze ρ_t at the obtained fixed point $\rho_{\#}$, and run the mean iteration. The following property can be proved: Let $X \sim (1 - \delta_*) \cdot N(\eta, 1) + \delta_* \cdot N(-\eta, 1)$ with $\eta > 0$ and assume that $\theta > 0$. Then $f(\theta, \delta \mid \eta, \delta_*) < f(\theta, \delta \mid \eta, \delta)$ if and only if $\delta_* > \delta$. Due to consistency and the convergence properties of $f(\theta, \delta \mid \eta, \delta)$ (Theorem 4), it can also be assured that $f(\theta, \delta \mid \eta, \delta_*)$ has no fixed points in (η, ∞) , and has at least a single fixed point in $(0, \eta]$ (which might not be unique). Upon convergence to such a fixed point $\eta_0 \leq \eta$, we may freeze it and run the weight iteration $h(\rho, \eta_0)$. At this phase, since $\eta_0 < \eta$ it is not clear that the weight iteration will have a non-trivial fixed point $\rho_{\#} \in (-1, 1)$. A more delicate argument is required to assure global convergence for a scheduling that begins with a phase of frozen θ_t . For the population iteration, we can always choose to begin with $\rho = 0$ that is provably globally converges, but it is not clear if this scheduling is better in terms of the empirical iteration.

For the empirical iteration, the result of running the balanced mean EM iteration (or a spectral algorithm) can clearly be used to obtain with high probability an initial guess θ_0 with $\|\theta_0 - \theta_*\| = \tilde{O}(\sqrt{\omega})$ if $\|\theta_*\| \lesssim \sqrt{\omega}$ and $\|\theta_0 - \theta_*\| = \tilde{O}(\frac{\omega}{\|\theta_*\|})$ otherwise. In the former case, θ_0 is not informative regarding the direction of θ_* , and so this initial guess is not expected to be better than $\theta_0 = 0$. When $\|\theta_*\| \gtrsim \sqrt{\omega}$, the initial guess has non-trivial angle with θ_* , and so it seems beneficial to initialize with that θ_0 . Furthermore, the only possible case case in which EM algorithm can improve the error rate is $\rho_* > \|\theta_*\| \gtrsim \sqrt{\omega}$. A possible direction to prove such a result, is to learn the stability of the mean iteration w.r.t. error in the weight and vice-versa. Specifically, using θ with $\|\theta - \theta_*\| \lesssim \frac{\omega}{\|\theta_*\|}$ in the iteration $\rho_{t+1} = h(\rho_t, \theta \mid \theta_*, \rho_*)$ shifts the population fixed point by at most $O(\frac{\omega}{\|\theta_*\|^2})$, but this is larger than the shift due to the empirical error which is $O(\frac{\omega}{\|\theta_*\|})$. If, however, one can use ρ with $|\rho - \rho_*| \lesssim \frac{\omega}{\|\theta_*\|}$ in the empirical mean iteration $\theta_{t+1} = f_n(\theta_t, \rho_t \mid \theta_*, \rho_*)$ then this mismatch can be shown to be negligible compared to the empirical error. Thus, with this scheduling, the key point is how to finely estimate θ_* so that its effect on the weight iteration will be negligible. Nonetheless, if non trivial separation holds and $\theta_* = \Omega(1)$ then running the balanced EM mean iteration followed by the weight iteration leads to (nearly) optimal error rates.

3. Proofs for Section 2.2

In this section we prove the results of Section 2.2.

3.1 Population Iteration

The following lemma summarizes simple properties of the mean population iteration for d = 1.

Lemma 15 Assume that $\eta \ge 0$. The following properties hold for $f(\theta) \equiv f(\theta, \delta \mid \eta, \delta)$:

- 1. Iteration: $f(0) = (1 2\delta)^2 \cdot \eta > 0$, $f(\eta) = \eta$ (consistency) and $\lim_{\theta \to \infty} f(\theta) \le \eta + 1 < C_{\theta} + 1$.
- 2. First order derivative: $f(\theta)$ is increasing on \mathbb{R} and

$$f'(\theta) = \mathbb{E}\left[\frac{X^2}{\cosh^2(X\theta + \beta)}\right] = 4\delta(1 - \delta) \cdot \mathbb{E}\left[\frac{X^2}{\left((1 - \delta) \cdot e^{X\theta} + \delta \cdot e^{-X\theta}\right)^2}\right] > 0.$$

 $At \; \theta = 0$

$$f'(0) = 4\delta(1-\delta) \cdot [\eta^2 + 1]$$
,

and furthermore, if $\theta \geq \eta$ then

$$f'(\theta) \le 2\sqrt{\delta(1-\delta)}e^{-\frac{1}{2}\eta^2} \le 1 - \frac{1}{4} \cdot \max\{\min\{\eta^2, 1\}, \rho^2\}.$$

3. Second order derivative:

$$f''(\theta) = -2\mathbb{E}_X \left[\frac{X^3 \tanh(X\theta + \beta)}{\cosh^2(X\theta + \beta)} \right] = -8 \cdot \delta(1 - \delta) \cdot \mathbb{E} \left[X^3 \frac{\left((1 - \delta) \cdot e^{X\theta} - \delta \cdot e^{-X\theta}\right)}{\left((1 - \delta) \cdot e^{X\theta} + \delta \cdot e^{-X\theta}\right)^3} \right]$$

Furthermore, there exists $C''(C_{\theta}, C_{\rho})$ such that for all $\theta \in \mathbb{R}$

$$|f''(\theta)| \leq \mathsf{C}'' \cdot \max\{\theta, \rho\}.$$

Proof We only explicitly prove non-trivial properties, or ones which are non-trivial extensions of the results of Wu and Zhou (2019, Lemma 3). Let $Z \sim N(0, 1)$.

1. The consistency property is well-known, but can also be proved explicitly:

$$\begin{split} f(\eta) &\stackrel{(a)}{=} e^{-\eta^2/2} \cdot \mathbb{E} \left[Z \cdot \left((1-\delta) \cdot e^{Z\eta} - \delta \cdot e^{-Z\eta} \right) \right] \\ &= e^{-\eta^2/2} \cdot \mathbb{E} \left[Z e^{Z\eta} \right] - \delta e^{-\eta^2/2} \cdot \mathbb{E} \left[Z \cdot \left(e^{Z\eta} + e^{-Z\eta} \right) \right] \\ &\stackrel{(b)}{=} e^{-\eta^2/2} \cdot \mathbb{E} \left[Z e^{Z\eta} \right] \stackrel{(c)}{=} e^{-\eta^2/2} \cdot \mathbb{E} \left[\eta e^{Z\eta} \right] = \eta \,, \end{split}$$

where (a) is by change of measure (see Equation 52 in Appendix C.1), (b) is by oddness of the argument in the second expectation, (c) is by Stein's identity (see Equation 55 in Appendix C.1).

2. The bound on $f'(\theta)$ for $\theta > \eta$ holds since

$$f'(\theta) \stackrel{(a)}{=} e^{-\frac{1}{2}\eta^{2}} \cdot \mathbb{E}\left[Z^{2} \cdot \frac{4\delta(1-\delta)}{((1-\delta) \cdot e^{Z\theta} + \delta \cdot e^{-Z\theta})^{2}} \cdot \left((1-\delta) \cdot e^{Z\eta} + \delta \cdot e^{-Z\eta}\right)\right]$$

$$\stackrel{(b)}{\leq} e^{-\frac{1}{2}\eta^{2}} \cdot \mathbb{E}\left[Z^{2} \cdot 2\sqrt{\delta(1-\delta)} \cdot \frac{(1-\delta) \cdot e^{Z\eta} + \delta \cdot e^{-Z\eta}}{(1-\delta) \cdot e^{Z\theta} + \delta \cdot e^{-Z\theta}}\right]$$

$$\stackrel{(c)}{=} 2\sqrt{\delta(1-\delta)}e^{-\frac{1}{2}\eta^{2}} \times$$

$$\mathbb{E}\left[\frac{1}{2}Z^{2} \cdot \frac{(1-\delta) \cdot e^{Z\eta} + \delta \cdot e^{-Z\eta}}{(1-\delta) \cdot e^{Z\theta} + \delta \cdot e^{-Z\theta}} + \frac{1}{2}Z^{2} \cdot \frac{(1-\delta) \cdot e^{-Z\eta} + \delta \cdot e^{Z\eta}}{(1-\delta) \cdot e^{-Z\theta} + \delta \cdot e^{Z\theta}}\right]$$

$$\stackrel{(d)}{\leq} e^{-\frac{1}{2}\eta^{2}} \cdot 2\sqrt{\delta(1-\delta)} \cdot \mathbb{E}\left[Z^{2}\right] \tag{18}$$

where: (a) is proved again by a change of measure; (b) holds since by the inequality of arithmetic and geometric means, for any $a \ge 0$

$$\frac{4\delta(1-\delta)}{(1-\delta)\cdot a+\delta\cdot a^{-1}} \le 2\sqrt{\delta(1-\delta)},$$

(c) follows since $Z \stackrel{d}{=} -Z$; (d) holds since

$$\max_{\delta \in [0,\frac{1}{2}], \ a > b > 1} \frac{1}{2} \cdot \frac{(1-\delta) \cdot b + \delta \cdot b^{-1}}{(1-\delta) \cdot a + \delta \cdot a^{-1}} + \frac{1}{2} \cdot \frac{(1-\delta) \cdot b^{-1} + \delta \cdot b}{(1-\delta) \cdot a^{-1} + \delta \cdot a} = 1.$$
(19)

To show that (19) holds, note that objective function on the left-hand side (l.h.s.) is a convex function of b for a given (a, δ) , hence it is maximized for either b = a or b = 1. At b = a the value of the objective is 1. At b = 1 we maximize over a > 1:

$$\begin{aligned} \max_{a>1} \frac{1}{2} \cdot \frac{1}{(1-\delta) \cdot a + \delta \cdot a^{-1}} + \frac{1}{2} \cdot \frac{1}{(1-\delta) \cdot a^{-1} + \delta \cdot a} \\ &= \max_{a>1} \frac{1}{2} \cdot \frac{a + a^{-1}}{(1-\delta)^2 + \delta^2 + \delta(1-\delta) \cdot (a + a^{-1})} \\ &= \max_{c>2} \frac{1}{2} \cdot \frac{c}{(1-2\delta)^2 + \delta(1-\delta) \cdot c} = 1 \,, \end{aligned}$$

where $c = a + a^{-1}$ was used, and the fact that the function to be maximized has a single maximum in \mathbb{R}_+ at $c = \frac{1-2\delta}{\sqrt{\delta(1-\delta)}} \leq 2$. Using $\delta = \frac{1-\rho}{2}$, we thus have $f'(\theta) = \sqrt{1-\rho^2} \cdot e^{-\frac{1}{2}\eta^2}$. The final bound is obtained from $\sqrt{1-\rho^2} \leq 1-\frac{\rho^2}{2}$ and $e^{-\frac{1}{2}\eta^2} \leq \max\{e^{-1}, 1-\frac{\eta^2}{4}\}$.

3. The bound on the second derivative follows from $|\tanh(t)| \le t$ and $\cosh(t) > 1$.

We next turn to prove Proposition 5. To this end, we need the following technical lemma: Lemma 16 Let $\beta > 0$ be given, and let

$$s(u) := -\tanh(u+\beta) + \tanh(u-\beta) - \frac{1}{2\delta\cosh^2(u+\beta)} + \frac{1}{2(1-\delta)\cosh^2(u-\beta)}.$$
 (20)

Then, $\frac{d}{du}s(u) = 0$ has a unique solution, this solution is negative, and s(u) < 0 for all $u \in \mathbb{R}$.

Proof For u < 0 the claim that s(u) < 0 holds since both $tanh(u - \beta) < tanh(u + \beta)$ and $(1 - \delta) \cosh^2(u - \beta) > \delta \cosh^2(u + \beta)$ hold when $\beta > 0$. For $u \ge 0$, we begin by analyzing $\frac{d}{du}s(u)$ and show that the real solution of $\frac{d}{du}s(u) = 0$ is negative and unique. Using the double-argument identities $1 + \cosh(2t) = 2\cosh^2(t)$, $\sinh(2t) = 2\sinh(t)\cosh(t)$, the half-argument identity $tanh(\frac{t}{2}) = \frac{\sinh(t)}{\cosh(t)+1}$ we obtain that the derivative is

$$\frac{\mathrm{d}s(u)}{\mathrm{d}u} = -\frac{1 - \frac{1}{\delta}\tanh(u+\beta)}{\cosh^2(u+\beta)} + \frac{1 - \frac{1}{1-\delta}\tanh(u-\beta)}{\cosh^2(u-\beta)},\tag{21}$$

and thus get that $\frac{\mathrm{d}}{\mathrm{d}u}s(u)=0$ is equivalent to

$$\left[\frac{1+\cosh(2u-2\beta)}{1+\cosh(2u+2\beta)}\right]^2 = \frac{1+\cosh(2u-2\beta) - \frac{1}{1-\delta}\sinh(2u-2\beta)}{1+\cosh(2u+2\beta) - \frac{1}{\delta}\sinh(2u+2\beta)}$$

or, by using $\exp(2\beta) = \frac{1-\delta}{\delta}$ and denoting $\psi := e^{2u}$, equivalent to

$$\frac{\left[2+\frac{1-\delta}{\delta}\psi^{-1}+\frac{\delta}{(1-\delta)}\psi\right]^2}{\left[2+\frac{\delta}{1-\delta}\psi^{-1}+\frac{1-\delta}{\delta}\psi\right]^2} = \frac{2+\frac{2-\delta}{\delta}\psi^{-1}-\frac{\delta^2}{(1-\delta)^2}\psi}{2+\frac{1+\delta}{1-\delta}\psi^{-1}-\frac{(1-\delta)^2}{\delta^2}\psi}.$$

After further algebraic manipulations, the last display can be shown to be equivalent to

$$(2\delta - 1) \cdot [\delta\psi + 1 - \delta] \cdot [(1 - \delta)\psi + \delta] \cdot [2\delta(1 - \delta)\psi^3 + 3\delta(1 - \delta)\psi^2 + (1 - 2\delta)^2\psi - \delta(1 - \delta)] = 0.$$

As $\delta \in (0, \frac{1}{2})$ and $\psi > 0$, the only real solution to this equation is the solution to

$$2\delta(1-\delta)\psi^3 + 3\delta(1-\delta)\psi^2 + (1-2\delta)^2\psi - \delta(1-\delta) = 0.$$

The l.h.s. of the last display is an increasing function of $\psi \in \mathbb{R}_+$ with value $-\delta(1-\delta)$ at $\psi = 0$ and a strictly positive value at $\psi = 1$. Thus, the above equation has a single real solution which belongs to (0, 1). Hence, $\frac{d}{du}s(u) = 0$ has a unique solution, and this solution is negative.

We next use this property $\frac{d}{du}s(u)$ to show that s(u) < 0 for all $u \ge 0$. As $s(0) = 4(2\delta - 1) < 0$ and $\lim_{u\to\infty} s(u) = 0$, the mean value theorem implies that $\frac{d}{du}s(u)$ must be strictly positive for some u > 0. Since $\frac{d}{du}s(u) \ne 0$ for u > 0, s(u) must be increasing for all u > 0. Since $\lim_{u\to\infty} s(u) = 0$ holds, $s(u) \ge 0$ is impossible for u > 0.

Proof (of Proposition 5) Let $U \sim N(\eta, 1)$. To prove the first property, we write

$$f(\theta \mid \eta, \delta) + f(-\theta \mid \eta, \delta)$$

= $\mathbb{E} [X \cdot \tanh(X\theta + \beta) - X \cdot \tanh(X\theta - \beta)]$
= $(1 - 2\delta) \cdot \mathbb{E} [U \cdot \tanh(U\theta + \beta) - U \cdot \tanh(U\theta - \beta)]$
 ≥ 0

which holds since $u \mapsto u \cdot \tanh(u\theta + \beta) - u \cdot \tanh(u\theta - \beta)$ is an odd function, that is positive on \mathbb{R}_+ .

To prove the second property, we write the iteration as

$$f(\theta \mid \eta, \delta) = \mathbb{E}\left[(1 - \delta) \cdot U \tanh(U\theta + \beta) + \delta \cdot U \tanh(U\theta - \beta)\right],$$

and then analyze its derivative w.r.t. δ

$$\frac{\partial f(\theta \mid \eta, \delta)}{\partial \delta} = \mathbb{E} \left[-U \tanh(U\theta + \beta) + U \tanh(U\theta - \beta) \right] \\ - \frac{1}{2\delta(1 - \delta)} \mathbb{E} \left[\frac{(1 - \delta)U}{\cosh^2(U\theta + \beta)} - \frac{\delta U}{\cosh^2(U\theta - \beta)} \right].$$

To prove the required property, we will show that

$$\frac{\partial f(\theta \mid \eta, \delta)}{\partial \delta} \quad \begin{cases} < 0, \quad \theta < \eta \\ = 0, \quad \eta = \theta \\ > 0, \quad \theta > \eta \end{cases}$$

and to this end we split the analysis to the cases $\theta = 0$, $\theta < 0$ and $\theta \ge 0$.

 $\begin{array}{l} \underline{Case \ \theta = 0:} \\ \delta \in \underline{(0, \frac{1}{2})}. \\ \underline{Case \ \theta < 0:} \\ \underline{Let} \end{array} \text{ In this case, trivially, } \begin{array}{l} \frac{\partial f(\theta | \eta, \delta)}{\partial \delta} \Big|_{\theta = 0} = -4(1 - 2\delta)\eta < 0 \text{ for } \eta > 0 \text{ and} \\ \end{array}$

$$q_1(u) := -u \tanh(u\theta + \beta) + u \tanh(u\theta - \beta)$$

and note that since tanh is monotonically increasing and negative for t < 0, it holds that $q_1(u)$ is an odd function, and $q_1(u) < 0$ for all u > 0. Thus $\mathbb{E}[q_1(U)] < 0$. Also let

$$q_2(u) := \frac{(1-\delta)u}{\cosh^2(u\theta+\beta)} - \frac{\delta u}{\cosh^2(u\theta-\beta)}.$$

Since \cosh is an even function with a unique minimum at t = 0, it holds that

$$q_2(u) = u \left[\frac{(1-\delta)}{\cosh^2(u\theta+\beta)} - \frac{\delta}{\cosh^2(u\theta-\beta)} \right] > 0,$$

and

$$q_2(u) + q_2(-u) = \frac{(1-\delta)u}{\cosh^2(u\theta+\beta)} - \frac{\delta u}{\cosh^2(u\theta-\beta)} - \frac{(1-\delta)u}{\cosh^2(u\theta-\beta)} + \frac{\delta u}{\cosh^2(u\theta+\beta)}$$
$$= u\left(\frac{1}{\cosh^2(u\theta+\beta)} - \frac{1}{\cosh^2(u\theta-\beta)}\right) > 0$$

for any u > 0. Thus $q_2(u) > -q_2(-u)$ for u > 0, and $\mathbb{E}[q_2(U)] > 0$ (see Appendix C.1). The required property then follows since $\frac{\partial f(\theta|\eta,\delta)}{\partial \delta} = \mathbb{E}[q_1(U)] - \frac{1}{2\delta(1-\delta)}\mathbb{E}[q_2(U)] < 0$.

<u>Case $\theta > 0$ </u>: We follow the ideas outlined in the discussion following the statement of the proposition. We note that $\frac{\partial f(\theta|\eta,\delta)}{\partial \delta} = \mathbb{E}\left[U \cdot s(U)\right]$ where s(u) is as defined in (20), and so

$$\frac{\partial f(\theta \mid \eta, \delta)}{\partial \delta} = [\eta \cdot s(\theta \eta)] * \varphi(\eta)$$
(22)

where $\varphi(\eta) := \frac{1}{\sqrt{2\pi}} \cdot e^{-\eta^2/2}$ is the Gaussian kernel, and the convolution is w.r.t. η .

We begin by proving that $\eta \mapsto \frac{\partial f(\theta|\eta, \delta)}{\partial \delta}$ has at least a single zero-crossing in \mathbb{R}_+ by showing that for $\eta = 0$ and as $\eta \to \infty$:

$$\left.\frac{\partial f(\theta\mid\eta,\delta)}{\partial\delta}\right|_{\eta=0}>0, \ \, \frac{\partial f(\theta\mid\eta,\delta)}{\partial\delta}\uparrow 0 \ \text{as} \ \eta\to\infty.$$

At $\eta = 0$, using the definitions of $q_1(u)$ and $q_2(u)$, and recalling that $Z \sim N(0, 1)$

$$\begin{aligned} \frac{\partial f(\theta \mid \eta, \delta)}{\partial \delta} \bigg|_{\eta=0} &= \mathbb{E}\left[q_1(Z)\right] - \frac{1}{2\delta(1-\delta)} \mathbb{E}\left[q_2(Z)\right] \\ &\stackrel{(a)}{=} -\frac{1}{2\delta(1-\delta)} \mathbb{E}\left[q_2(Z)\right] \\ &= -\frac{1}{2\delta(1-\delta)} \mathbb{E}\left[q_2(Z) + q_2(-Z)\right] \\ &= -\frac{1}{2\delta(1-\delta)} \mathbb{E}\left[Z\left(\frac{1}{\cosh^2(Z\theta+\beta)} - \frac{1}{\cosh^2(Z\theta-\beta)}\right)\right] \\ &\stackrel{(b)}{>} 0 \end{aligned}$$

where (a) is since $q_1(u)$ is an odd function, and (b) is since for $\theta > 0$ and any $u \in \mathbb{R}$

$$u\left(\frac{1}{\cosh^2(u\theta+\beta)} - \frac{1}{\cosh^2(u\theta-\beta)}\right) < 0$$

For $\eta \to \infty$, we note that the first term in the limit of $\frac{\partial f(\theta|\eta,\delta)}{\partial \delta}$ is

$$\lim_{\eta \to \infty} \mathbb{E} \left[-(Z+\eta) \tanh\left((Z+\eta)\theta + \beta\right) + (Z+\eta) \tanh\left((Z+\eta)\theta - \beta\right) \right]$$
$$= \mathbb{E} \left[\lim_{\eta \to \infty} \left(-(Z+\eta) \left[\tanh\left((Z+\eta)\theta + \beta\right) - \tanh\left((Z+\eta)\theta - \beta\right) \right] \right) \right]$$

by dominated convergence theorem. Then, by L'H $\ddot{i}_{L}^{\frac{1}{2}}$ pital

$$\begin{split} &\lim_{\eta \to \infty} (z+\eta) \left[\tanh\left((z+\eta)\theta + \beta\right) - \tanh\left((z+\eta)\theta - \beta\right) \right] \\ &= \lim_{\eta \to \infty} \frac{\left[\tanh\left((z+\eta)\theta + \beta\right) - \tanh\left((z+\eta)\theta - \beta\right) \right]}{(z+\eta)^{-1}} \\ &= \lim_{\eta \to \infty} \theta \frac{\left[\frac{1}{\cosh^2((z+\eta)\theta + \beta)} - \frac{1}{\cosh^2((z+\eta)\theta - \beta)} \right]}{-(z+\eta)^{-2}} = 0 \end{split}$$

since $\cosh(t) > e^t/2$ for t > 0. The second term in the limit of $\frac{\partial f(\theta|\eta,\delta)}{\partial \delta}$ can be analyzed similarly and also equals zero. The fact that the limit of $\frac{\partial f(\theta|\eta,\delta)}{\partial \delta}$ to 0 is from below, can be deduced from $\eta \cdot s(\theta\eta) < 0$ for all $\eta > 0$ (Lemma 16) and the convolution relation (22).

Next, we prove that the zero-crossing of $\eta \mapsto \frac{\partial f(\theta|\eta,\delta)}{\partial \delta}$ in \mathbb{R}_+ is unique. The function $\eta \mapsto \eta \cdot s(\theta\eta)$ has a unique zero-crossing at $\eta = 0$ since Lemma 16 implies that $s(\theta\eta) < 0$ for all $\eta > 0$. Furthermore, for any given θ , $\eta \mapsto \eta \cdot s(\theta\eta)$ is a bounded function. Indeed, $\eta \cdot s(\theta\eta)$ is clearly bounded for $|\eta| \leq 1$. For $|\eta| > 1$, note that using $\tanh(t) = 1 - \frac{e^{-t}}{\cosh(t)}$, it holds that for any $\eta > 0$

$$\begin{split} |\tanh(\theta\eta+\beta) - \tanh(\theta\eta-\beta)| \\ &= e^{-\theta\eta} \left| \frac{e^{-\beta}}{\cosh(\theta\eta+\beta)} - \frac{e^{\beta}}{\cosh(\theta\eta-\beta)} \right| \\ &\leq e^{-\theta\eta} \cdot 2e^{\beta}, \end{split}$$

and analogous result holds for $\eta < 0$. Also, using $\cosh(t) \ge 1 + \frac{t^2}{2}$, it holds that

$$\left| \left(\frac{1}{2\delta \cosh^2(\theta\eta + \beta)} - \frac{1}{2(1 - \delta) \cosh^2(\theta\eta - \beta)} \right) \right| \le \frac{1}{2\delta \left(1 + \frac{\theta\eta + \beta}{2} \right)^2} + \frac{1}{2(1 - \delta) \left(1 + \frac{\theta\eta - \beta}{2} \right)^2}.$$

Hence, $|\eta \cdot s(\theta \eta)| \le |\eta| \cdot [e^{-\theta|\eta|} \cdot 2e^{\beta} + \frac{1}{\delta \theta^2 \eta^2}]$ which is bounded for all $|\eta| > 1$.

The variation diminishing property of the Gaussian kernel (Proposition 25, Appendix C.3), and the convolution relation (22) imply that $\frac{\partial f(\theta|\eta,\delta)}{\partial \delta}$ has at most a single zero-crossing as a function of η . From all the above, $\frac{\partial f(\theta|\eta,\delta)}{\partial \delta}$ has exactly a single zero-crossing for some $\eta > 0$. The consistency property implies that $\frac{\partial f(\theta|\eta,\delta)}{\partial \delta}\Big|_{\theta=\eta} = 0$, and so this zero-crossing must occur at $\eta = \theta$. From this, (16) follows.

Proof (of theorem 4) Recall that $\pm \eta$ and 0 are the only fixed points of the balanced iteration $f(\theta, \frac{1}{2} \mid \eta, \frac{1}{2})$, and that $f(|\theta|, \frac{1}{2} \mid \eta, \frac{1}{2}) > |\theta|$ for $0 < |\theta| < \eta$, and $f(|\theta|, \frac{1}{2} \mid \eta, \frac{1}{2}) < |\theta|$ for $|\theta| > \eta$. The claim then follows from Proposition 5, item 2. The last two claims follow from Proposition 23, items 4 and 5.

3.2 Empirical Iteration

Proof (of Theorem 6) We analyze the empirical iteration $f_n(\theta) \equiv f_n(\theta, \delta \mid \eta, \delta)$. From Lemma 15 and assuming the high probability event (15), it holds that

$$|f_n(\theta)| \leq \mathsf{C}_{\theta} + 1 + \omega \leq \mathsf{C}_{\theta} + 2$$

for all n sufficiently large, and that

$$f_n(\theta) \ge f_-(\theta) := f(\theta) - \max\{|\theta|, \rho\} \cdot \omega, \qquad (23)$$

and

$$f_n(\theta) \le f_+(\theta) := f(\theta) + \max\{|\theta|, \rho\} \cdot \omega, \qquad (24)$$

where we abbreviate here $\omega \equiv \omega_1 = \sqrt{C_{\omega} \frac{\log n}{n}}$ and $f_{\pm}(\theta)$ will be referred to as the lower (-) and upper (+) envelopes. We consider the empirical iteration $\theta_{t+1} = f_n(\theta_t)$ as well as the lower and upper envelopes iterations $\theta_{t+1}^{\pm} = f_{\pm}(\theta_t^{\pm})$, all which are initialized at the same point, to wit, $\theta_0 = \theta_0^{\pm}$. We begin by thoroughly analyzing the initialization $\theta_0 = 0$ and then briefly discuss the initialization $\theta_0 = \frac{1}{\rho} \mathbb{E}_n[X]$ (which is similar and simpler). In the first step of the proof, we show that $\{\theta_t\}$ and $\{\theta_t^{\pm}\}$ all converge monotonically to fixed points. In the second step, we analyze the convergence time and the distance between the fixed points. We split the analysis into three different regimes for η .

<u>Fixed points</u>: We show that $\{\theta_t\}$ and $\{\theta_t^{\pm}\}$ converge monotonically to fixed points, which we denote, respectively, by η_n and η_{\pm} . We use several intuitive properties of convergence of one-dimensional iterations, which are formally stated and proved in Proposition 23, items 1 and 4.

For the empirical iteration $f_n(\theta)$, since

$$f'_n(\theta) = \mathbb{E}_n\left[\frac{X^2}{\cosh^2(X\theta + \beta)}\right] > 0$$

and $f_n(\theta)$ is bounded by assumption, $\{\theta_t\}$ converges monotonically to a fixed point η_n , and is either increasing or decreasing according to the sign of $f_n(0)$.

For the upper envelope $f_+(\theta)$, recall from Lemma 15 that $f(\theta)$ is increasing and bounded. So $\lim_{\theta\to\infty} f'(\theta) = 0$. Hence, $f_+(\theta)$ is increasing, and for $n > n_0(\mathsf{C}_\omega)$ it holds that $\lim_{\theta\to\infty} f'_+(\theta) < 1$. Thus $\{\theta_t^+\}$ is increasing and converges to a fixed point η_+ .

For the lower envelope $f_{-}(\theta)$, first note that there exists $n_1(\mathsf{C}_{\theta},\mathsf{C}_{\rho})$ such that $f_{-}(\theta)$ is increasing for all $\theta \in [-\mathsf{C}_{\theta},\mathsf{C}_{\theta}]$ since

$$f'_{-}(\theta) \ge f'(\theta) - \omega \ge \min_{0 \le \eta \le \mathsf{C}_{\theta}} \mathbb{E}\left[\frac{X^2}{\cosh^2(|X|\mathsf{C}_{\theta} + \beta)}\right] - \omega > 0.$$
(25)

If $f_{-}(0) > 0$ then since $f(\theta)$ has a unique fixed point η in $[0,\infty)$, $f_{-}(\theta)$ must have a fixed point in $[0,\eta]$, and no fixed points in $[\eta,\infty)$, and $\{\theta_t^-\}$ is increasing to one of the fixed points in $[0,\eta)$. If $f_{-}(0) < 0$ then as the negative fixed points of $f(\theta)$ are confined to $[-\eta,0]$ (Theorem 4) similar reasoning as for the upper envelope leads to the conclusion that $\{\theta_t^-\}$ is decreasing and converges to some fixed point $\eta_- < 0$. Furthermore, since the negative fixed points of $f(\theta)$ are confined to $[-\eta,0]$ (Theorem 4) and since $f(\theta) \ge -f(-\theta)$ for all $\theta > 0$ (Proposition 5, item 1) the minimal negative fixed point $\underline{\eta}_- < 0$ satisfies $|\underline{\eta}_-| \le |\eta_+|$.

<u>Stochastic error and convergence time</u>: We now prove bounds on the stochastic error and on the required number of iterations for convergence. We will use constants $C_1, C_2, C_3 > 0$ which satisfy relations that will be specified throughout the proof. Assume that $\rho \geq C_1 \sqrt{\omega}$. We split the analysis to three regimes for η given by $[0, \frac{\omega}{\rho}], [\frac{\omega}{\rho}, C_2\rho]$ and $[C_2\rho, C_{\theta}]$ where $C_1 \geq \sqrt{1/C_2}$ is assumed so that these are three non-empty intervals. For simplicity, we assume that $C_2 \leq 1$ (its value will eventually be chosen to be sufficiently small).

<u>Case 1:</u> Assume $\eta \in [\frac{\omega}{\rho}, C_2\rho]$. For $\theta \ge \eta$, Lemma 15 implies that

$$f_+'(\theta) \le 1 - \frac{\rho^2}{4} + \omega$$

Thus, assuming $C_1 \ge \sqrt{12}$ then $f'_+(\theta) \le 1 - \frac{\rho^2}{6}$. For $0 \le \theta < \eta$, we have

$$|f''(\theta)| \le \mathsf{C}'' \cdot \max\{\eta, \rho\} \le \mathsf{C}''\rho$$
,

and using $f'_{+}(\theta) = f'_{+}(\eta) - \int_{\theta}^{\eta} f''(\tilde{\theta}) d\tilde{\theta}$, it holds that

$$\begin{split} f'_{+}(\theta) &\leq 1 - \frac{\rho^2}{4} + \mathsf{C}''\rho(\eta - \theta) + \omega \\ &\leq 1 - \frac{\rho^2}{4} + \mathsf{C}''\eta\rho + \omega \\ &\leq 1 - \frac{\rho^2}{4} + \mathsf{C}''C_2\rho^2 + \omega \,. \end{split}$$

Assuming that $C_1 \ge \sqrt{12}$ and $C_2 \le \frac{1}{12 \cdot C'}$ we get that $f'_+(\theta) \le 1 - \frac{\rho^2}{12}$. Thus, $f_+(\theta)$ is a contraction for $\theta \in [0, \infty)$. Hence, so is $f_-(\theta)$ (as $0 \le f'_-(\theta) \le f'_+(\theta)$). Furthermore, it holds that $f_+(0) > f_-(0) = f(0) - \rho\omega > 0$ for all $n \ge n_2(\mathsf{C}_\theta, \mathsf{C}_\rho)$. Thus both θ_t^{\pm} are increasing and converge to fixed points $\eta_{\pm} > 0$ where $\eta_+ \ge \eta \ge \eta_-$ and satisfy $\eta_{\pm} - \theta_t^{\pm} \le \eta_{\pm}(1 - \frac{\rho^2}{12})^t$ (Proposition 23, item 6). We next analyze the errors $\epsilon_- = \eta - \eta_- > 0$ and $\epsilon_+ = \eta_+ - \eta > 0$. For the error of the lower envelope, let $\theta \in [\eta_-, \eta]$ and recall that $\eta_- \le \eta \le C_2\rho$. Then, $f''(\theta) \ge -\mathsf{C}''\rho$ and so

$$f'(\eta) \ge f'(\theta) - \mathsf{C}''\rho(\eta - \theta),$$

as well as $f_{-}(\theta) > f(\theta) - \rho \omega$. Hence

$$\begin{split} \eta - \rho \omega &= f_{-}(\eta) \\ &= f_{-}(\eta_{-}) + \int_{\eta_{-}}^{\eta} f_{-}'(\theta) \cdot \mathrm{d}\theta \\ &\leq \eta_{-} + \int_{\eta_{-}}^{\eta} f'(\theta) \cdot \mathrm{d}\theta \\ &\leq \eta_{-} + f'(\eta)\epsilon_{-} + \mathsf{C}''\rho \left(\eta\epsilon_{-} - \frac{\eta^{2} - \eta_{-}^{2}}{2}\right) \\ &\leq \eta_{-} + f'(\eta)\epsilon_{-} + \mathsf{C}''C_{2}\rho^{2}\epsilon_{-} \,. \end{split}$$

The above implies $\epsilon_{-}(1 - f'(\eta) - C_{2}\rho^{2}) \leq \rho\omega$ and since $f'(\eta) \leq 1 - \frac{\rho^{2}}{4}$ then if $C_{2} \leq \frac{1}{8}$ we obtain $\eta - \eta_{-} \leq 8\frac{\omega}{\rho}$. Since $\eta_{-} - \theta_{t}^{-} \leq \eta_{-}(1 - \frac{\rho^{2}}{12})^{t} \leq C_{\theta}(1 - \frac{\rho^{2}}{12})^{t}$ it holds that $\eta_{-} - \theta_{t}^{-} \leq 8\frac{\omega}{\rho}$ for all $t \geq \frac{12}{\rho^{2}} \log\left(\frac{C_{\theta}}{8} \cdot \frac{\rho}{\omega}\right)$ (Proposition 23, item 6) and so also $\eta - \theta_{t}^{-} \leq 16\frac{\omega}{\rho}$. The analysis for η_{+} is similar:

$$\eta_{+} = f_{+}(\eta_{+})$$
$$= f_{+}(\eta) + \int_{\eta}^{\eta_{+}} f'_{+}(\theta) \cdot d\theta$$
$$= \eta + \rho\omega + \epsilon_{+} \left(f'(\eta) + \omega \right)$$

Then, since $\eta \leq C_2 \rho$ and $f'(\theta) \leq 1 - \frac{\rho^2}{4}$ it holds that $\epsilon_+(\frac{\rho^2}{4} - \omega) \leq \rho \omega$ for all $\theta > \eta$. Since $\rho \geq C_1 \sqrt{\omega}$, assuming $C_1 \geq \sqrt{8}$ we get $\eta_+ - \eta \leq 8\frac{\omega}{\rho}$. Furthermore, for all $n \geq n_3(\mathsf{C}_\omega)$, $\eta_+ \leq 2\eta$ and so for all $t \geq \frac{12}{\rho^2} \log\left(\frac{\mathsf{C}_\theta}{4}\frac{\rho}{\omega}\right)$ it holds that $|\eta - \theta_t^+| \leq 16\frac{\omega}{\rho}$.

<u>Case 2</u>: Assume $\eta \in [C_2\rho, C_{\theta}]$. The convergence has two phases. The time spent in phase 1 (resp. phase 2) until the required convergence is assured will be denoted by T_1 (resp. T_2).

1. We show that there exists $C_3 \leq \frac{1}{2}$ sufficiently small and C_1 sufficiently large such that $f_-(\theta) > \theta + \frac{1}{6}\rho^2\eta$ holds for all $\theta \in [0, C_3\rho]$ (note that $\rho > 2\theta$ is assured). In turn, this inequality is satisfied if

$$f(\theta) > \theta + \omega(\theta + \rho) + \frac{1}{6}\rho^2\eta$$
(26)
holds. Since

$$f'(\theta) = f'(0) + \int_0^{\theta} f''(\tilde{\theta}) \cdot d\tilde{\theta}$$

$$\geq (1 - \rho^2)(1 + \eta^2) - \frac{\mathsf{C}''}{2}\theta^2 - \mathsf{C}''\rho\theta,$$

and as $f(0) = \rho^2 \eta$, we get that

$$f(\theta) = f(0) + \int_0^{\theta} f'(\tilde{\theta}) \cdot d\tilde{\theta}$$

$$\geq \rho^2 \eta + (1 - \rho^2)(1 + \eta^2)\theta - \frac{\mathsf{C}''}{6}\theta^3 - \frac{\mathsf{C}''}{2}\rho\theta^2.$$

Thus, (26) is satisfied if the following inequality holds:

$$\frac{5}{6}\rho^2\eta + (1-\rho^2)\eta^2\theta > \rho^2\theta + \frac{\mathsf{C}''}{6}\theta^3 + \frac{\mathsf{C}''}{2}\rho\theta^2 + \omega\theta + \omega\rho.$$
(27)

Since clearly $(1 - \rho^2)\eta^2 \theta > 0$, this inequality can be assured to hold for all $n > n_4(\mathsf{C}_{\omega}, C_1)$ large enough, by proper choice of constants. Specifically, by "allocating" $\frac{1}{6}\rho^2\eta$ for each of the five additive terms on the right-hand side (r.h.s.) of (27), and using the assumption $\rho > C_1\sqrt{\omega}$, the inequality (27) is satisfied for $C_3 \leq \min\left\{\frac{C_2}{6}, \frac{4C_2}{C''}, \frac{2C_2}{3C''}\right\}$ (for the first three terms) and $C_1 \geq \max\left\{\sqrt{\frac{6C_3}{C_2}}, \sqrt{\frac{6}{C_2}}\right\}$ (for the fourth and fifth terms). Therefore, as long as $\theta_t \leq C_3\rho$, it holds that $\theta_{t+1} - \theta_t \geq \frac{1}{6}\rho^2\eta$. So, initializing from $\theta_0 = 0$, it holds that $\theta_t^- \geq C_3\rho$ for all $t \geq T_1 = \frac{6C_3}{\rho\eta}$ where $T_1 \leq \frac{1}{\omega}$. Naturally, this holds for θ_t^+ too.

2. At this phase, the convergence behaves similarly to the balanced case. Specifically, as $C_3 \leq 1$ and since $\theta > C_3 \rho$ then

$$f_+(\theta) \le f(\theta) + \frac{1}{C_3} \theta \omega$$

and

$$f_{-}(\theta) \ge f(\theta) + \frac{1}{C_3} \theta \omega$$
.

Using Theorem 4, the convergence of the envelopes with $f(\theta) \pm \frac{1}{C_3} \theta \omega$ is faster than the convergence of the envelopes of the balanced iterations $f(\theta, \frac{1}{2} \mid \eta, \frac{1}{2}) \pm \frac{1}{C_3} \theta \omega$. Thus, the one-dimensional analysis and result of Wu and Zhou (2019, Theorem 3) holds. Specifically, Wu and Zhou (2019, Theorem 3) demonstrated the existence of constants $\{c_i\}$ such that if the balanced EM is initialized at $\theta_0 = C_3 \rho$, assuming that $\eta > c_4 \sqrt{\omega}$ it holds that $|\eta_{\pm} - \eta| \le c_2 \frac{\omega}{\eta}$ for all $t \ge T_2 = \frac{c_3}{\eta^2} \log \left(\frac{1}{C_3 \rho \omega}\right)$. The condition $\eta > c_4 \sqrt{\omega}$ is satisfied by requiring that $C_1 > \frac{c_4}{C_2}$. <u>Case 3:</u> Assume $\eta \in [0, \frac{\omega}{\rho}]$. For the upper envelope, as in case 2, $f_+(\theta)$ is increasing and satisfies $f_+(0) > 0$ and thus θ_t^+ is increasing and converges to a fixed point $\eta_+ > 0$. In addition, similar analysis shows that $\eta_+ - \eta \leq 8\frac{\omega}{\rho}$. Thus, for all t > 1

$$|\theta_t^+ - \eta| \le |\theta_t^+| + |\eta| \le |\eta_+| + |\eta| \le 10 \frac{\omega}{\rho}.$$

So, the error is $O(\frac{\omega}{\rho})$ for all iterations. For the lower envelope, by the assumption on $n > n_1$ in (25), $f_-(\theta)$ is increasing for $\theta \in \mathbb{B}(\mathsf{C}_{\theta})$. If $f_-(0) > 0$ then θ_t^- will converge to a fixed point $0 < \eta_- \le \eta_+$ and similar analysis as for the upper envelope implies that $|\theta_t^- - \eta| \le 10\frac{\omega}{\rho}$ for all t > 1. Otherwise, if $f_-(0) < 0$, $\{\theta_t^-\}$ is decreasing and converges to a fixed point η_- . As was shown in the analysis of the fixed points, it must hold that $|\eta_-| \le |\eta_+|$ and so the last bound on $|\theta_t^- - \eta|$ is valid in this case too.

The result for $\theta_0 = 0$ then follows from summarizing all three cases, and determining the constants in the following order: C_2 to be sufficiently small, then C_3 sufficiently small, and finally C_1 sufficiently large.

We now discuss the case $\theta_0 = \frac{1}{\rho} \mathbb{E}_n[X]$. Since $f(0) = \rho^2 \eta$ and $f_n(0) = \rho \mathbb{E}_n[X]$, and under the high probability event $|f_n(0) - f(0)| \le \omega \rho$ we have that $|\theta_0 - \eta| \le \frac{\omega}{\rho}$ which is in fact already within the error rate obtained in Cases 1 and 3 above. By repeating the same arguments in those cases, the error is $O(\frac{\omega}{\rho})$ for all subsequent iterations. In Case 2, the first phase is unnecessary since in this case $\eta > C_2\rho$ and so $\eta - \frac{\omega}{\rho} > C_3\rho$ as long as $C_3 < \frac{C_2}{2}$ and $C_1 \ge \sqrt{\frac{1}{C_2}}$. Thus, if $\theta_0 \le \eta$ only the second phase in the analysis above occurs. If $\theta_0 > \eta$ then the analysis of the balanced iteration (Wu and Zhou, 2019, Theorem 3) is similarly intact.

4. Proofs for Section 2.3

In this section we prove the results of Section 2.3.

4.1 Population Iteration

The next lemma summarizes basic properties of $F(\cdot)$ and $G(\cdot)$ which are useful for the unbalanced iteration analysis.

Lemma 17 (Properties of F and G as functions of (a, b)) Assume that $b \ge 0$ and $\delta \in [0, \frac{1}{2})$. Then:

- 1. Monotonicity: $a \mapsto F(a, b)$ and $b \mapsto G(a, b)$ are monotonically increasing functions.
- 2. Positivity: F(a,b) > 0 for $a \ge 0$, and $G(a,b) \ge 0 = G(a,0)$.
- 3. Strict positivity of F(0,b): For any $C_f > 0$ there exists $C_{F,0} > 0$ which depends on (C_f, C_β) such that $\min_{b \in [0, C_f]} F(0, b) \ge C_{F,0} \rho^2 \eta$.
- 4. Boundedness: $|F(a,b)| \le \eta + 1$ and $G(a,b) \le \eta + 1$.

5. Upper bounded first derivatives:

$$\left|\frac{\partial F(a,b)}{\partial a}\right| \le 1 + \eta^2, \ \left|\frac{\partial F(a,b)}{\partial b}\right| \le \sqrt{1 + \eta^2}, \ \left|\frac{\partial G(a,b)}{\partial a}\right| \le \sqrt{1 + \eta^2}, \ \left|\frac{\partial G(a,b)}{\partial b}\right| \le 1.$$

6. Lower bounded first derivative: Let $C_f > 0$ be given. There exists $C''_F(C_{\theta}, C_f, C_{\beta}) > 0$ such that $\partial F(a, b)$

$$\min_{a,b\in[0,C_f]^2}\frac{\partial F(a,b)}{\partial a}\geq \mathsf{C}''_F.$$

7. Derivative at b = 0: For $a \in [0, \eta]$

$$\left. \frac{\partial G(a,b)}{\partial b} \right|_{b=0} \le 4\delta(1-\delta)$$

and for $a \geq \eta$

$$\frac{\partial G(a,b)}{\partial b}\Big|_{b=0} \le 2\sqrt{\delta(1-\delta)}e^{-\frac{1}{2}\eta^2} \le 1 - \frac{1}{4} \cdot \max\{\min\{\eta^2,1\},\rho^2\}.$$

8. Crossed derivative at b = 0:

$$\left. \frac{\partial F(a,b)}{\partial b} \right|_{b=0} = 0.$$

9. Upper bounded crossed second order derivatives at b = 0:

$$\left| \frac{\partial^2 F(a,b)}{\partial b^2} \right|_{b=0} \right| \le a(1+\eta^2) + \rho \overline{\mathsf{C}}_{\beta}(1+\eta)$$

and the same bound holds for $\frac{\partial^2 G(a,b)}{\partial b \partial a} = \frac{\partial^2 F(a,b)}{\partial b^2}$.

10. Upper bounded crossed third order derivatives: There exists $C_F''(C_{\theta}) > 0$ such that

$$\left|\frac{\partial^3 F(a,b)}{\partial b^3}\right| \le \mathsf{C}_F'''\,.$$

Proof

1. We have

$$\frac{\partial F(a,b)}{\partial a} = \mathbb{E}\left[\frac{V^2}{\cosh^2(aV + bW + \beta)}\right] > 0,$$

and similarly,

$$\frac{\partial G(a,b)}{\partial b} = \mathbb{E}\left[\frac{W^2}{\cosh^2(aV + bW + \beta)}\right] > 0.$$

2. $F(a,b) \ge 0$ for $a \ge 0$ since $a \mapsto F(a,b)$ is increasing and

$$F(0,b) = \mathbb{E}[V] \cdot \mathbb{E}[\tanh(bW + \beta)] > 0$$
(28)

where the inequality is because $\mathbb{E}[V] = (1 - 2\delta)\eta > 0$ and since \tanh is odd and increasing and W is symmetric. Similarly, $G(a, b) \ge 0 = G(a, 0) = \mathbb{E}[W] \cdot \mathbb{E}[\tanh(aV + \beta)] = 0$ because $b \mapsto G(a, b)$ is increasing.

3. The minimal value of $\min_{b \in [0, C_f]} \mathbb{E} [\tanh(bW + \beta)]$ is obtained for $b = C_f$ as

$$\frac{\partial \mathbb{E} \left[\tanh(bW + \beta) \right]}{\partial b} = \mathbb{E} \left[\frac{W}{\cosh(bW + \beta)^2} \right]$$
$$= \mathbb{E} \left[\frac{W}{\cosh(bW + \beta)^2} - \frac{W}{\cosh(bW - \beta)^2} \mid W > 0 \right]$$
$$< 0.$$
(29)

We next analyze the minimal value $q(\beta) := \mathbb{E}[\tanh(C_f W + \beta)]$. It holds that $q(0) = \mathbb{E}[\tanh(C_f W)] = 0$ and that

$$q'(\beta) := \frac{\mathrm{d}q(\beta)}{\mathrm{d}\beta} = \mathbb{E}\left[\frac{1}{\cosh^2(C_f W + \beta)}\right]$$

and so $q'(0) = \mathbb{E}\left[\frac{1}{\cosh^2(C_f W)}\right] > 0$ and only depends on C_f . Also,

$$q''(\beta) := \frac{\mathrm{d}^2 q(\beta)}{\mathrm{d}\beta^2} = \mathbb{E}\left[\frac{-2\tanh(C_f W + \beta)}{\cosh^2(C_f W + \beta)}\right]$$
$$= \frac{1}{C_f} \mathbb{E}\left[\frac{W}{\cosh^2(C_f W + \beta)}\right]$$
$$< 0$$

by Stein's identity (see (55) in Appendix C.1), and where the inequality is as in (29). Hence, $\beta \mapsto q(\beta)$ is a concave function at $\beta \in \mathbb{R}_+$, and so for all $\beta \in [0, C_\beta]$, $q(\beta)$ is lower bounded by the straight line connecting q(0) and $q(C_\beta)$, to wit,

$$\mathbb{E}[\tanh(C_f W + \beta)] = q(\beta) \ge \frac{q(\mathsf{C}_\beta)}{\mathsf{C}_\beta}\beta = C_1\beta \ge C_1\underline{\mathsf{C}}_\beta\rho.$$

The claim then follows from (28) and $\mathbb{E}[V] = \rho \eta > 0$.

4. $|F(a,b)| \leq \mathbb{E}\left[|V \tanh(aV + bW + \beta)|\right] \leq \mathbb{E}|V| \leq \eta + \sqrt{2/\pi}$, and, similarly,

$$|G(a,b)| \le \mathbb{E}\left[|W \tanh(aV + bW + \beta)|\right] \le \mathbb{E}|W| \le \sqrt{2/\pi}.$$

5. We only show

$$\left|\frac{\partial F(a,b)}{\partial b}\right| \leq \mathbb{E}\left[\frac{|WV|}{\cosh^2(aV+bW+\beta)}\right] \leq \mathbb{E}\left[|WV|\right] \leq \sqrt{\mathbb{E}\left[W^2\right]\mathbb{E}\left[V^2\right]}$$

since $\cosh(t) \ge 1$. The other bounds are proved similarly.

6. Let $U \sim N(\eta, 1), U \perp W$. Then, for any $a, b \in [0, C_f]^2$

$$\begin{split} \frac{\partial F(a,b)}{\partial a} &= \mathbb{E} \left[\frac{V^2}{\cosh^2(aV + bW + \beta)} \right] \\ &= \mathbb{E} \left[\frac{2V^2}{1 + \cosh(2aV + 2bW + 2\beta)} \right] \\ &= \mathbb{E} \left[\frac{2(1 - \delta)U^2}{1 + \cosh(2aU + 2bW + 2\beta)} + \frac{2\delta U^2}{1 + \cosh(2aU - 2bW - 2\beta)} \right] \\ &\stackrel{(a)}{\geq} \mathbb{E} \left[\frac{(1 - \delta)U^2}{\cosh(2aU + 2bW + 2\beta)} + \frac{\delta U^2}{\cosh(2aU - 2bW - 2\beta)} \right] \\ &\stackrel{(b)}{\geq} \mathbb{E} \left[\frac{U^2}{\cosh(4aU + 2bW + 2\beta) \cdot \cosh(2aU - 2bW - 2\beta)} \right] \\ &= \mathbb{E} \left[\frac{2U^2}{\cosh(4aU) + \cosh(4bW + 4\beta)} \right] \\ &\stackrel{(c)}{\geq} \mathbb{E} \left[\frac{2U^2}{\cosh(4C_fU) + \cosh(4bW + 4\beta)} \right] \\ &\stackrel{(d)}{\geq} \mathbb{E} \left[\frac{4U^2}{2\cosh(4C_fU) + \exp(4b|W| + 4\beta)} \right] \\ &\stackrel{(d)}{\geq} \mathbb{E} \left[\frac{2U^2}{2\cosh(4C_fU) + \exp(4C_f|W| + 4\beta)} \right] \\ &\stackrel{(d)}{=} \mathbb{E} \left[\frac{2U^2}{2\cosh(4C_fU) + \exp(4C_f|W| + 4\beta)} \right] \\ &\stackrel{(d)}{=} \mathbb{E} \left[\frac{2U^2}{2\cosh(4C_fU) + \exp(4C_f|W| + 4\beta)} \right] \\ &\stackrel{(d)}{=} \mathbb{E} \left[\frac{2U^2}{2\cosh(4C_fU) + \exp(4C_f|W| + 4\beta)} \right] \end{aligned}$$

where (a) and (b) are since $\cosh(t) \ge 1$, (c) is since $\cosh(t)$ is an even function, and increasing for $t \ge 0$, (d) is since $\cosh(t) \ge \frac{1}{2}e^{|t|}$.

7. We have

$$\frac{\partial G(a,b)}{\partial b} = \mathbb{E}\left[\frac{W^2}{\cosh(aV + bW + \beta)^2}\right]$$

and

$$\begin{split} \frac{\partial G(a,b)}{\partial b} \bigg|_{b=0} &= \mathbb{E} \left[\frac{W^2}{\cosh(aV+\beta)^2} \right] \\ &= \mathbb{E} \left[\frac{1}{\cosh(aV+\beta)^2} \right] \\ &= 4\delta(1-\delta)\mathbb{E} \left[\frac{1}{\left((1-\delta)e^{aV}+\delta e^{-aV}\right)^2} \right] \,. \end{split}$$

At this point, for $a > \eta$, the proof follows the same steps of the proof of Lemma 15, item 2 and thus omitted. For $a \in [0, \eta]$ we let $Z \sim N(0, 1)$

$$\begin{aligned} \frac{\partial G(a,b)}{\partial b} \Big|_{b=0} &\stackrel{(a)}{=} 4\delta(1-\delta)e^{-\eta^2/2} \cdot \mathbb{E} \left[\frac{(1-\delta)e^{\eta Z} + \delta e^{-\eta Z}}{((1-\delta)e^{aV} + \delta e^{-aV})^2} \right] \\ &\stackrel{(b)}{=} 4\delta(1-\delta)e^{-\eta^2/2} \times \\ & \mathbb{E} \left[\frac{1}{2} \frac{(1-\delta)e^{\eta Z} + \delta e^{-\eta Z}}{((1-\delta)e^{aV} + \delta e^{-aV})^2} + \frac{1}{2} \frac{(1-\delta)e^{-\eta Z} + \delta e^{\eta Z}}{((1-\delta)e^{-aV} + \delta e^{aV})^2} \right] \\ &\stackrel{(c)}{\leq} 4\delta(1-\delta)e^{-\eta^2/2} \cdot \mathbb{E} \left[e^{\eta Z} \right] \\ &= 4\delta(1-\delta) \,, \end{aligned}$$

where (a) is by a change of measure (see Equation 52 in Appendix C.1) and (b) is by the symmetry of N(0,1). The inequality (c) can be proved pointwise as follows: We denote $\psi_{\eta} = e^{\eta Z}$ and $\psi_a = e^{aZ}$, and may assume that Z > 0 if we show it holds for all $\delta \in [0,1]$. Thus, it remains to show that

$$\max_{\psi_{\eta} \ge \psi_{a} > 1} \left[\frac{(1-\delta)\psi_{\eta} + \delta\psi_{\eta}^{-1}}{\left((1-\delta)\psi_{a} + \delta\psi_{a}^{-1}\right)^{2}} + \frac{(1-\delta)\psi_{\eta}^{-1} + \delta\psi_{\eta}}{\left((1-\delta)\psi_{a}^{-1} + \delta\psi_{a}\right)^{2}} - 2\psi_{\eta} \right] \le 0.$$
(30)

We prove this inequality by showing that it holds for $\psi_{\eta} = \psi_a$ and then show that the term in the l.h.s. of (30) is non-increasing in ψ_{η} for $\psi_{\eta} \in (\psi_a, \infty)$. We first verify the inequality (30) for $\psi_{\eta} = \psi_a$. In this case

$$\max_{\psi_a > 1} \left[\frac{1}{(1-\delta)\psi_a + \delta\psi_a^{-1}} + \frac{1}{(1-\delta)\psi_a^{-1} + \delta\psi_a} - 2\psi_a \right] \\ = \max_{\psi_a > 1} \psi_a \cdot \left[\frac{1}{(1-\delta)\psi_a^2 + \delta} + \frac{1}{(1-\delta) + \delta\psi_a^2} - 2 \right]$$

and the term in brackets is non-positive (its maximal value is 0 obtained by $\psi_a = 1$). To prove that the l.h.s. of (30) is monotonic w.r.t. ψ_{η} , we next differentiate w.r.t. to ψ_{η} :

$$\frac{\partial}{\partial\psi_{\eta}} \left[\frac{(1-\delta)\psi_{\eta} + \delta\psi_{\eta}^{-1}}{((1-\delta)\psi_{a} + \delta\psi_{a}^{-1})^{2}} + \frac{(1-\delta)\psi_{\eta}^{-1} + \delta\psi_{\eta}}{((1-\delta)\psi_{a}^{-1} + \delta\psi_{a})^{2}} - 2\psi_{\eta} \right] = \\
= \left(\frac{(1-\delta) - \frac{\delta}{\psi_{\eta}^{2}}}{\left[(1-\delta)\psi_{a} + \delta\psi_{a}^{-1}\right]^{2}} + \frac{\delta - \frac{1-\delta}{\psi_{\eta}^{2}}}{\left[(1-\delta)\psi_{a}^{-1} + \delta\psi_{a}\right]^{2}} \right) - 2 \\
\leq \left(\frac{1-\delta}{\left[(1-\delta)\psi_{a} + \delta\psi_{a}^{-1}\right]^{2}} + \frac{\delta}{\left[(1-\delta)\psi_{a}^{-1} + \delta\psi_{a}\right]^{2}} \right) - 2.$$
(31)

This last term in (31) is symmetric w.r.t. δ so we may return to assume $\delta \in [0, \frac{1}{2}]$, which along $\psi_a \geq 1$ satisfies $(1-\delta)\psi_a + \delta\psi_a^{-1} > 1$ and $(1-\delta)\psi_a^{-1} + \delta\psi_a \geq 2\sqrt{\delta(1-\delta)}$. With these properties, we may further upper bound (31) as

$$\left(1-\delta+\frac{1}{4(1-\delta)}\right)-2<0$$

8. We have

$$\left. \frac{\partial F(a,b)}{\partial b} \right|_{b=0} = \mathbb{E} \left[\frac{WV}{\cosh^2(aV+\beta)} \right] = 0.$$

9. We have

$$\frac{\partial^2 G(a,b)}{\partial a \partial b} = \frac{\partial^2 F(a,b)}{\partial b^2} = -2\mathbb{E}\left[\frac{W^2 V \tanh(aV + bW + \beta)}{\cosh^2(aV + bW + \beta)}\right]$$

and so using $|\tanh(t)| \le t$ and $\cosh(t) \ge 1$

$$\left| \frac{\partial^2 F(a,b)}{\partial b^2} \right|_{b=0} \right| \le \mathbb{E} \left[\frac{|V| \cdot |aV + \beta|}{\cosh^2(aV + \beta)} \right] \le a \mathbb{E} \left[|V|^2 \right] + \beta \mathbb{E} \left[|V| \right] \,.$$

10. We have

$$\begin{split} \left| \frac{\partial^3 F(a,b)}{\partial b^3} \right| &= \left| -2\mathbb{E} \left[W^3 V \frac{\left(1 - 2\sinh^2(aV + bW + \beta)\right)}{\cosh^4(aV + bW + \beta)} \right] \\ &\leq 2\mathbb{E} \left[\left| W^3 V \right| \right] \\ &\leq 2\sqrt{\mathbb{E} \left[W^6 \right] \mathbb{E} \left[V^2 \right]} \\ &\leq 2\sqrt{15(1 + \eta^2)} \end{split}$$

since $\left|\frac{1-2\sinh^2(t)}{\cosh^4(t)}\right|$ is maximized at t = 0 and its maximal value is 1.

We next turn to prove Proposition 9: **Proof** (of Proposition 9)

1. By Stein's identity (see Equation 55 in Appendix C.1), for $U \sim N(a\eta, a^2 + b^2)$

$$\frac{G(a,b \mid \eta, \delta)}{b} = \mathbb{E}\left[\frac{1-\delta}{\cosh^2(U+\beta)} + \frac{\delta}{\cosh^2(U+\beta)}\right] \,.$$

Then,

$$\frac{\partial \left[\frac{1}{b}G(a,b \mid \eta, \delta)\right]}{\partial \delta} = \mathbb{E}\left[\frac{1 - \frac{1}{1 - \delta} \tanh(U - \beta)}{\cosh^2(U - \beta)} - \frac{1 - \frac{1}{\delta} \tanh(U + \beta)}{\cosh^2(U + \beta)}\right]$$
$$= \mathbb{E}\left[s'(U)\right]$$
$$= \mathbb{E}\left[r\left(a\overline{U}\right)\right]$$
$$:= q(\eta),$$

where s(u) was defined in (20), and its derivative is denoted by $s'(u) \equiv \frac{ds}{du}$ (as in Equation 21), r(u) := s'(au) and $\overline{U} \sim N(\eta, 1 + \frac{b^2}{a^2})$. Recall that Lemma 16 implies that s'(u) has at most a single zero-crossing at some u < 0. As a > 0, r(u) also has a single zero-crossing at some u < 0. Hence, from Proposition 25, the total positivity of the Gaussian kernel implies that $\eta \mapsto q(\eta)$ has at most a single zero-crossing point

as a function of $\eta \in \mathbb{R}$ (note that for the sake of the proof we allow $\eta < 0$). We next show that the zero crossing must occur for $\eta < 0$. We do so by evaluating $q(\eta)$ for $\eta = 0$ and for large η . For $\eta = 0$, $\overline{U} \sim N(0, 1 + \frac{b^2}{a^2}) \stackrel{d}{=} -\overline{U}$ and so

$$q(0) = \left(\frac{1}{1-\delta} + \frac{1}{\delta}\right) \mathbb{E}\left[\frac{\tanh(a\overline{U}+\beta)}{\cosh^2(a\overline{U}+\beta)}\right] > 0$$
(32)

since $t \mapsto \frac{\tanh(t)}{\cosh^2(t)}$ is an odd function, positive (resp. negative) on \mathbb{R}_+ (resp. \mathbb{R}_-). Furthermore, noting that $r(0) = \frac{\frac{1}{\delta} \tanh(\beta) - \frac{1}{1-\delta} \tanh(\beta)}{\cosh^2(\beta)} > 0$, and using again the single zero-crossing of r(u) at some u < 0, we have that r(u) > 0 for all $u \in \mathbb{R}_+$. Since $q(\eta) = r(\eta) * \varphi(\eta \mid 1 + \frac{b^2}{a^2})$ where $\varphi(\eta \mid \sigma^2)$ is the Gaussian kernel with variance σ^2 , i.e., $\varphi(\eta \mid \sigma^2) := (2\pi\sigma^2)^{-1/2} \cdot e^{-\eta^2/(2\sigma^2)}$, there exists some $\eta_0 > 0$ such that $q(\eta) > 0$ for all $\eta > \eta_0$ (note that $q(\eta)$ is bounded because r(u) is). Since $q(\eta) > 0$ for $\eta = 0$ and all $\eta > \eta_0$, $q(\eta)$ must have an even number of zero-crossing in \mathbb{R}_+ . Since it cannot have more than one single crossing, it does not have any. Hence, $q(\eta) = \frac{1}{b} \frac{\partial[G(a,b|\eta,\delta)]}{\partial \delta} > 0$ for all $\eta > 0$, and thus $G(a, b \mid \eta, \delta) \leq G(a, b \mid \eta, \frac{1}{2})$.

2. Let $\tilde{V} \sim N(\eta, 1)$. We analyze the partial derivatives of

$$G(a,b \mid \eta, \delta) = \mathbb{E} \left[W \cdot \left((1-\delta) \tanh(a\tilde{V} + bW + \beta) + \delta \tanh(-a\tilde{V} + bW + \beta) \right) \right]$$
$$= \mathbb{E} \left[W \cdot \left((1-\delta) \tanh(a\tilde{V} + bW + \beta) + \delta \tanh(a\tilde{V} + bW - \beta) \right) \right]$$

w.r.t. δ around $\delta = \frac{1}{2}$ (i.e., $\beta = 0$) and then use Taylor expansion for $\frac{1}{b}G(a, b \mid \eta, \delta)$. For brevity, we denote $U = a\tilde{V} + bW \sim N(a\eta, a^2 + b^2)$.

(a) First derivative: Taking partial derivative w.r.t. δ^{11}

$$\frac{\partial \left[G(a,b \mid \eta, \delta)\right]}{\partial \delta} = \mathbb{E}\left[W \cdot \left(\tanh(U-\beta) - \tanh(U+\beta)\right)\right] \\ + \mathbb{E}\left[W \cdot \left(-\frac{1}{2\delta \cosh^2(U+\beta)} + \frac{1}{2(1-\delta)\cosh^2(U-\beta)}\right)\right]$$

we get $\frac{\partial [G(a,b|\eta,\delta)]}{\partial \delta}\Big|_{\delta=\frac{1}{2}} = 0.$

(b) Second derivative: Taking the next partial derivative w.r.t. δ

$$\frac{\partial^2 G(a,b \mid \eta, \delta)}{\partial \delta^2} = \frac{1}{2\delta^2 (1-\delta)^2} \times \\ \mathbb{E}\left[W \cdot \left(\frac{(1-\delta) \left[1-\tanh(U+\beta)\right]}{\cosh^2(U+\beta)} + \frac{\delta \left[1-\tanh(U-\beta)\right]}{\cosh^2(U-\beta)} \right) \right]$$
(33)

^{11.} Note that this form is different from the form used in the previous item, and is before applying Stein's identity.

and letting $\overline{U} = U - a\eta \sim N(0, a^2 + b^2),$

$$\begin{aligned} \frac{\partial^2 \left[\frac{1}{b}G(a,b \mid \eta, \delta)\right]}{\partial \delta^2} \bigg|_{\delta = \frac{1}{2}} &= \frac{4}{b} \cdot \mathbb{E} \left[W \cdot \frac{[1 - \tanh(U)]}{\cosh^2(U)} \right] \\ &= \frac{4}{b} \cdot \mathbb{E} \left[\frac{[1 - \tanh(U)]}{\cosh^2(U)} \cdot \mathbb{E} \left[W \mid U \right] \right] \\ &= \frac{4}{a^2 + b^2} \cdot \mathbb{E} \left[\overline{U} \cdot \frac{[1 - \tanh(\overline{U} + a\eta)]}{\cosh^2(\overline{U} + a\eta)} \right] \\ &:= \frac{4}{a^2 + b^2} \cdot A_0(a, b) \,, \end{aligned}$$

where the equality holds since $\mathbb{E}[W \mid U] = \frac{b}{a^2+b^2}(U-a\eta)$ and where $A_0(a,b)$ was implicitly defined. We next show that $A_0(a,b) < 0$. To this end, first assume that both a > 0 and b > 0, and let $h(t) := \frac{1-\tanh(t)}{\cosh^2(t)}$. It holds that $h(t) \ge 0$ for all $t \in \mathbb{R}$, $h(t) \le h(-t)$ for $t \ge 0$, and h(t) has unique maximum at $t = -\log\sqrt{2} < 0$. In addition, for any $\overline{u} > 0$, it holds that $h(-\overline{u} + a\eta) > h(\overline{u} + a\eta)$. Indeed, if $-\overline{u} + a\eta \ge 0$ then this is true since h(t) is strictly decreasing for $t \ge 0$, and if $-\overline{u} + a\eta < 0$ then $h(-\overline{u} + a\eta) > h(\overline{u} - a\eta) > h(\overline{u} + a\eta)$. Now, the conditional version of the expectation defining $A_0(a, b)$, when conditioned on $|\overline{U}| = \overline{u} > 0$ satisfies

$$\mathbb{E}\left[\overline{U}\cdot h(\overline{U}+a\eta)\mid |\overline{U}|=\overline{u}\right] = \frac{1}{2}\left[\overline{u}\cdot h(\overline{u}+a\eta)-\overline{u}\cdot h(-\overline{u}+a\eta)\right] < 0\,,$$

and so $A_0(a,b) < 0$. Therefore, any $(a,b,\eta) \in (0,C_f)^2 \times [0,\mathsf{C}_{\theta}]$ satisfies

$$\left. \frac{\partial^2 \left[\frac{1}{b} G(a, b \mid \eta, \delta) \right]}{\partial \delta^2} \right|_{\delta = \frac{1}{2}} := \Gamma(a, b, \eta) < 0.$$

We may now consider the cases a = 0 or b = 0. If a = 0 but $b \neq 0$ or vice-versa, similar analysis to before shows that $\Gamma(a, b, \eta) < 0$. For (a, b) = (0, 0) we use Stein's identity (see Equation 55 in Appendix C.1) to obtain

$$\frac{4}{a^2 + b^2} A_0(a, b) = 4 \cdot \mathbb{E}\left[\frac{e^{-2(\overline{U} + a\eta)} - 2}{\cosh^4(\overline{U} + a\eta)}\right]$$

and so $\frac{1}{b} \frac{\partial^2 [G(a,b|\eta,\delta)]}{\partial \delta^2} \Big|_{\delta = \frac{1}{2}} = -4$ for (a,b) = (0,0). So, there exists $C_2(C_f, \mathsf{C}_{\theta}, \mathsf{C}_{\beta}) > 0$ such that

$$\max_{(a,b,\eta)\in[0,C_f]^2\times[0,\mathsf{C}_\theta]}\Gamma(a,b,\eta)=-C_2<0\,.$$

(c) <u>Third derivative</u>: We show that its absolute value is upper bounded. As apparent from form (33), the second derivative $\frac{\partial^2 [G(a,b;\delta)]}{\partial \delta^2}$ can be written as the sum of two terms of the same form. We show how to bound the derivative of the first, and as

it is similar, omit the bounding of the second. Recalling that $\overline{U} \sim N(0, a^2 + b^2)$, the first term is,

$$\frac{1}{2\delta^2(1-\delta)} \mathbb{E}\left[W\frac{[1-\tanh(U+\beta)]}{\cosh^2(U+\beta)}\right] = \frac{1}{2\delta^2(1-\delta)} \frac{b}{a^2+b^2} \mathbb{E}\left[\overline{U} \cdot \frac{[1-\tanh(\overline{U}+a\eta+\beta)]}{\cosh^2(\overline{U}+a\eta+\beta)}\right]$$

using again $\mathbb{E}[W \mid U] = \frac{b}{a^2+b^2}(U - a\eta)$. Hence $\frac{1}{b} \cdot \frac{\partial^3[G(a,b;\delta)]}{\partial \delta^3}$ has two terms of a similar form, the first of them is

$$\begin{split} &\frac{1}{a^2+b^2} \cdot \frac{\partial}{\partial \delta} \left\{ \frac{1}{2\delta^2(1-\delta)} \mathbb{E} \left[\overline{U} \cdot \frac{\left[1-\tanh(\overline{U}+a\eta+\beta)\right]}{\cosh^2(\overline{U}+a\eta+\beta)} \right] \right\} \\ &= -\frac{1}{a^2+b^2} \cdot \frac{(1-\frac{3}{2}\delta)}{\delta^3(1-\delta)^2} \cdot \mathbb{E} \left[\overline{U} \cdot \frac{\left[1-\tanh(\overline{U}+a\eta+\beta)\right]}{\cosh^2(\overline{U}+a\eta+\beta)} \right] \\ &- \frac{1}{a^2+b^2} \cdot \frac{1}{\delta^3(1-\delta)^2} \mathbb{E} \left[\overline{U} \cdot \frac{e^{-2\overline{U}-2a\eta-2\beta}-2}{\left[1+\cosh(2\overline{U}+2a\eta+2\beta)\right]^2} \right] \\ &:= -\frac{(1-\frac{3}{2}\delta)}{\delta^3(1-\delta)^2} A_1(a,b) - \frac{1}{\delta^3(1-\delta)^2} A_2(a,b) \,, \end{split}$$

where $A_1(a, b), A_2(a, b)$ where implicitly defined. The multiplicative factors $\frac{(1-\frac{3}{2}\delta)}{\delta^3(1-\delta)^2}$ and $\frac{1}{\delta^3(1-\delta)^2}$ are upper bounded since δ is assume to be bounded away from zero $(\beta < C_{\beta})$, and so we focus on $A_1(a, b), A_2(a, b)$. Further,

$$A_1(a,b) = \frac{1}{a^2 + b^2} \cdot \mathbb{E}\left[\left| \overline{U} \cdot \frac{\left[1 - \tanh(\overline{U} + a\eta + \beta) \right]}{\cosh^2(\overline{U} + a\eta + \beta)} \right| \right] < 2\frac{1}{a^2 + b^2} \cdot \mathbb{E}\left| \overline{U} \right| < \frac{2}{\sqrt{a^2 + b^2}}$$

and

$$\begin{aligned} A_2(a,b) &= \frac{1}{a^2 + b^2} \cdot \mathbb{E}\left[\overline{U} \cdot \frac{e^{-2\overline{U} - 2a\eta - 2\beta} - 2}{\left[1 + \cosh(2\overline{U} + 2a\eta + 2\beta)\right]^2}\right] \\ &\leq \frac{4}{a^2 + b^2} \cdot \mathbb{E}\left[|\overline{U}| \cdot \frac{e^{-2\overline{U} - 2a\eta - 2\beta}}{\left[2 + e^{2\overline{U} + 2a\eta + 2\beta} + e^{-2\overline{U} - 2a\eta - 2\beta}\right]^2} \\ &+ \frac{1}{a^2 + b^2} \cdot \mathbb{E}\left[|\overline{U}| \cdot \frac{2}{\left[1 + \cosh(2\overline{U} + 2a\eta + 2\beta)\right]^2}\right] \\ &\leq \frac{6}{a^2 + b^2} \cdot \mathbb{E}\left|\overline{U}\right| < \frac{6}{\sqrt{a^2 + b^2}}.\end{aligned}$$

Thus, if either a > 0 or b > 0 then both $A_1(a, b) < \infty$ and $A_2(a, b) < \infty$. It remains to consider limits to (a, b) = (0, 0). The limits for $A_1(a, b)$ can be shown

to be finite by an analysis similar to the one made for the second derivative $\frac{\partial^2 G(a,b|\eta,\delta)}{\partial \delta^2}$. For $A_2(a,b)$, using Stein's identity (see Equation 55 in Appendix C.1)

$$A_{2}(a,b) = \frac{1}{a^{2} + b^{2}} \mathbb{E} \left[\overline{U} \frac{e^{-2\overline{U} - 2a\eta - 2\beta} - 2}{\left[1 + \cosh(2\overline{U} + 2a\eta + 2\beta) \right]^{2}} \right]$$
$$= -2 \cdot \mathbb{E} \left[\frac{e^{-2\overline{U} - 2a\eta - 2\beta}}{\left[1 + \cosh(2\overline{U} + 2a\eta + 2\beta) \right]^{2}} \right]$$
$$-4 \cdot \mathbb{E} \left[\frac{\left(e^{-2\overline{U} - 2a\eta - 2\beta} - 2 \right) \sinh(2\overline{U} + 2a\eta + 2\beta)}{\left[1 + \cosh(2\overline{U} + 2a\eta + 2\beta) \right]^{3}} \right]$$

and so $|A_2(0,0)| < 2e^{-2\beta} + 4 |e^{-2\beta} - 2|\sinh(2\beta) < \infty$. Hence, there exists $C_3(C_f, \mathsf{C}_\beta)$ such that

$$\sup_{\substack{(a,b,\eta)\in[0,C_f]^2\times[0,\mathsf{C}_{\theta}]}} \left| \frac{\partial^3 \left[\frac{1}{b} G(a,b \mid \eta, \delta) \right]}{\partial \delta^3} \right| \le C_3 \,.$$

From the analysis of the derivatives, and recalling that $\rho = 2(\frac{1}{2} - \delta)$, for any $(a, b, \eta) \in [0, C_f]^2 \times [0, \mathsf{C}_{\theta}]$ it holds that

$$\frac{G(a,b \mid \eta, \delta)}{b} \le \frac{G(a,b \mid \eta, \frac{1}{2})}{b} - \frac{C_2}{8} \cdot \rho^2 + \frac{C_3}{48}\rho^3$$

If C_{β} is such that $\rho \leq \frac{C_2}{3C_3} = \overline{\rho}$ then $\frac{1}{b}G(a, b \mid \eta, \delta) \leq \frac{1}{b}G(a, b \mid \eta, \frac{1}{2}) - \frac{C_2}{16} \cdot \rho^2$. Otherwise, by dominance of G w.r.t δ (item 1)

$$\begin{aligned} \frac{1}{b}G(a,b\mid\eta,\delta) &\leq \frac{1}{b}G\left(a,b\mid\eta,\frac{1-\overline{\rho}}{2}\right) \leq \frac{G(a,b\mid\eta,\frac{1}{2})}{b} - \frac{C_2}{8}\overline{\rho}^2\\ &\leq \frac{1}{b}G(a,b\mid\eta,\frac{1}{2}) - C_4\rho^2 \end{aligned}$$

for some constant C_4 (which depends on C_{β}). Taking $C_1^{(d)} = \min(\frac{1}{8}C_2, C_4)$

$$\begin{aligned} G(a,b \mid \eta, \delta) &\leq G(a,b \mid \eta, \frac{1}{2}) - \mathsf{C}_1^{(d)} \rho^2 b \\ &\leq b \left(1 - \frac{a^2 + b^2}{2 + 4(a^2 + b^2)} - \mathsf{C}_1^{(d)} \rho^2 \right) \end{aligned}$$

where the upper bound on $G(a, b \mid \eta, \frac{1}{2})$ was obtained in the analysis of the balanced iteration (Wu and Zhou, 2019, Lemma 5, item 8).

3. Let $Z \sim N(0,1)$. By Stein's identity for W (see Equation 55 in Appendix C.1), and a change of measure (see Equation 52 in Appendix C.1)

$$G(a, b \mid \eta, \delta) = \mathbb{E}\left[\frac{b}{\cosh^2(aV + bW + \beta)}\right]$$
$$= e^{-\eta^2/2} \mathbb{E}\left[\frac{b}{\cosh^2(aZ + bW + \beta)}\left((1 - \delta)e^{\eta Z} + \delta e^{-\eta Z}\right)\right]$$

Then,

$$\frac{\partial G(a,b \mid \eta, \delta)}{\partial \eta} = -\eta \cdot G(a,b \mid \eta, \delta) + e^{-\eta^2/2} \cdot \mathbb{E} \left[\frac{bZ}{\cosh(aZ + bW + \beta)^2} \left((1-\delta)e^{\eta Z} - \delta e^{-\eta Z} \right) \right] \\
= -2be^{-\eta^2/2} \cdot \mathbb{E} \left[\frac{\tanh(aZ + bW + \beta)}{\cosh^2(aZ + bW + \beta)} \left((1-\delta)e^{\eta Z} - \delta e^{-\eta Z} \right) \right],$$
(34)

by Stein's identity for Z. Letting $U = aZ + bW + \beta \sim N(\beta, a^2 + b^2)$, we have that $Z|U \sim N(\frac{a(U-\beta)}{a^2+b^2}, \frac{b^2}{a^2+b^2})$, and so

$$\frac{\partial G(a,b \mid \eta, \delta)}{\partial \eta} = -2 \exp\left(-\frac{\eta^2 a^2}{2(a^2 + b^2)}\right) \times \\ \mathbb{E}\left[\frac{b \tanh(U)}{\cosh^2(U)} \left((1 - \delta) \exp\left(\frac{\eta a}{a^2 + b^2}(U - \beta)\right) - \delta \exp\left(-\frac{\eta a}{a^2 + b^2}(U - \beta)\right)\right)\right].$$

Letting

$$p_{+} := (1-\delta) \exp\left(-\frac{\eta a}{a^{2}+b^{2}}\beta\right), \ p_{-} := \delta \exp\left(\frac{\eta a}{a^{2}+b^{2}}\beta\right),$$

then under the assumption $\frac{\eta a}{a^2+b^2} < 1$ and using $\exp(\beta) = \sqrt{(1-\delta)/\delta}$ it holds that $p_+ \ge p_-$. Now,

$$h(u) = \frac{\tanh(u)}{\cosh^2(u)} \left(p_+ \exp\left(\frac{\eta a u}{a^2 + b^2}\right) - p_- \exp\left(-\frac{\eta a u}{a^2 + b^2}\right) \right)$$

satisfies that for $u \ge 0$, $h(u) \ge 0$ and $|h(u)| \ge |h(-u)|$. Thus, we deduce that

$$\frac{\partial G(a,b\mid \eta,\delta)}{\partial \eta} = -2b \cdot e^{-\frac{\eta^2 a^2}{2(a^2+b^2)}} \mathbb{E}\left[h(U)\right] \le 0$$

(see the Gaussian average of odd function property in Appendix C.1).

- 4. We show that $\frac{1}{b} \frac{\partial G(a,b|\eta,\delta)}{\partial \eta} \Big|_{\eta=0} < 0$ and that $\frac{1}{b} \frac{\partial^2 G(a,b|\eta,\delta)}{\partial \eta^2}$ is uniformly bounded over all (a, b, η) , and the result then follows from Taylor expansion.
 - (a) <u>First derivative</u>: Let $\overline{U} \sim N(0, a^2 + b^2)$. If b = 0 then $\frac{\partial G(a, b|\eta, \delta)}{\partial \eta}\Big|_{\eta=0} = 0$ and so we next assume b > 0. From (34) and Stein's identity (see Equation 55 in Appendix C.1)

$$\frac{\partial G(a,b \mid \eta, \delta)}{\partial \eta} \Big|_{\eta=0} = -2(1-2\delta) \cdot b\mathbb{E}\left[\frac{\tanh(\overline{U}+\beta)}{\cosh^2(\overline{U}+\beta)}\right]$$
$$= (1-2\delta) \cdot b\frac{1}{a^2+b^2}\mathbb{E}\left[\frac{\overline{U}}{\cosh^2(\overline{U}+\beta)}\right]$$
$$< 0$$

since for $u > 0, \beta > 0$ it holds that $\cosh(u+\beta) > \cosh(-u+\beta) > 0$ and $\overline{U} \stackrel{d}{=} -\overline{U}$.

(b) <u>Second derivative</u>: Let $Z \sim N(0, 1)$. Taking the next partial derivative w.r.t. η in (34)

$$\begin{aligned} \frac{\partial^2 G(a,b \mid \eta, \delta)}{\partial \eta^2} &= -\eta \frac{\partial G(a,b \mid \eta, \delta)}{\partial \eta} \\ &- 2be^{-\eta^2/2} \cdot \mathbb{E} \left[Z \frac{\tanh(aZ + bW + \beta)}{\cosh^2(aZ + bW + \beta)} \left((1 - \delta)e^{\eta Z} + \delta e^{-\eta Z} \right) \right] \,. \end{aligned}$$

The absolute value of the first term is bounded by $2C_{\theta}b$ since

$$\left|\frac{\partial G(a,b\mid\eta,\delta)}{\partial\eta}\right| \le 2be^{-\eta^2/2}\mathbb{E}\left[(1-\delta)e^{\eta Z} + \delta e^{-\eta Z}\right] = 2$$

(using $\left|\frac{\tanh(t)}{\cosh^2(t)}\right| \leq 1$). The absolute value of the second term is bounded by $4C_{\theta}b$ since

$$\mathbb{E}\left[\left|Z\frac{\tanh(aZ+bW+\beta)}{\cosh^2(aZ+bW+\beta)}\left((1-\delta)e^{\eta Z}+\delta e^{-\eta Z}\right)\right|\right]$$

$$\leq \mathbb{E}\left[|Z|\left((1-\delta)e^{\eta Z}+\delta e^{-\eta Z}\right)\right]$$

$$=\mathbb{E}\left[|Z|e^{\eta Z}\right]$$

$$\leq 2 \cdot \mathbb{E}\left[Ze^{\eta Z}\right]$$

$$\stackrel{(a)}{=} 2 \cdot \eta \mathbb{E}\left[e^{\eta Z}\right]$$

$$= 2\eta e^{\eta^2/2}$$

where (a) follows from Stein's identity. Thus, $\left|\frac{\partial^2 G(a,b)}{\partial \eta^2}\right| \leq 6\mathsf{C}_{\theta}b.$

We may now prove that the population mean iteration converges.

Proof (of Theorem 4) If $a_0 \ge 0$ then $a_t \ge 0$ for all t > 1 (Lemma 17, item 2). Consider the upper envelope iteration $b_{t+1}^+ = G(a_t, b_t^+ \mid \eta, \frac{1}{2})$, where $b_0^+ = b_0$. Since $b \mapsto G(a, b \mid \eta, \delta)$ is increasing for a > 0 (Lemma 17, item 1), Proposition 9, item 1 and induction imply that $b_t^+ \ge b_t$ for all $t \ge 1$. It follows from the analysis of the balanced iteration (Wu and Zhou, 2019, Lemma 5, item 8) that (see Proposition 9, item 2 and its proof) that $b_t^+ \to 0$. Thus also $b_t \to 0$ as $t \to \infty$. As $\left|\frac{\partial F(a,b)}{\partial b}\right| \le \sqrt{1+\eta^2} \le \sqrt{1+C_{\theta}}$ is uniformly bounded (Lemma 17, item 5), for any given $\epsilon > 0$, there exists t > 0 such that

$$|F(a_t, b_t) - F(a_t, 0)| \le \epsilon,$$

where $F(a_t, 0) = f(\theta \mid \eta, \delta)$, i.e., the population mean iteration in d = 1. Theorem 6 shows that convergence is assured for any given sufficiently small absolute error, and that the error $|\theta_t - \eta|$ tends to zero as $\epsilon \to 0$.

4.2 Empirical Iteration

Proof (of Theorem 10) We analyze the empirical iteration $\theta_{t+1} = f_n(\theta_t) \equiv f_n(\theta_t, \delta \mid \theta_*, \delta)$. We will assume that $\rho \geq C_1 \sqrt{\omega}$ and specify conditions on C_1 along the proof. As for the population iteration (Lemma 8), we may write

$$\theta_t = a_t \cdot \hat{\theta}_* + b_t \cdot \xi_t$$

where $\eta = \|\theta_*\|$, $\hat{\theta}_* = \frac{\theta_*}{\eta}$, $\xi_t \perp \eta$ and $\|\xi_t\| = 1$ such that $\operatorname{span}\{\theta_*, \xi_t\} = \operatorname{span}\{\theta_*, \theta_t\}$ and $b_t \geq 0$. Assuming the high probability event (15) holds, we have that

$$||f_n(\theta) - f(\theta)|| \le \max\{\eta, \rho\} \cdot \omega$$

and so for the signal iteration

$$a_{t+1} = \langle \theta_{t+1}, \theta_* \rangle = \langle f_n(\theta_t), \theta_* \rangle$$

$$\leq F(a_t, b_t) + \max \{ |a_t| + b_t, \rho \} \cdot \omega$$

$$\leq F(a_t, b_t) + (|a_t| + b_t + \rho) \cdot \omega$$

$$:= F_+(a_t, b_t),$$

and, similarly,

$$a_{t+1} \ge F(a_t, b_t) - \max \{ |a_t| + b_t, \rho \} \cdot \omega$$
$$\ge F(a_t, b_t) - (|a_t| + b_t + \rho) \cdot \omega$$
$$:= F_-(a_t, b_t).$$

In the same spirit, for the orthogonal iteration, it holds that

$$b_{t+1} \leq G(a_t, b_t) + \max\left\{ |a_t| + b_t, \rho \right\} \cdot \omega.$$

We split the analysis into two regimes of $\eta \leq \frac{\omega}{\rho}$ and $\eta \geq \frac{\omega}{\rho}$. In the former regime, the iteration dwells around $\|\theta_t\| \leq \frac{\omega}{\rho}$, though the corresponding signal iteration a_t might be negative. In the later regime, it is assured that $a_t \geq 0$ for all t (given that $a_0 \geq 0$), and so properties such as dominance of the orthogonal iteration may be used. As a preliminary step, we show that the iteration is bounded:

<u>Step 0 (Boundedness)</u>: We prove that for all n sufficiently large, it holds that $|a_t|, b_t \leq C_f$ for all $t \geq 1$ if $C_f \geq \max\{2\mathsf{C}_{\theta}, \rho/2, 4(\mathsf{C}_{\theta}+1)\}$. By induction, when the iteration is initialized with $\theta_0 = 0$ then $|a_0| = b_0 = 0$. When $\theta_0 = \frac{1}{\rho}\mathbb{E}_n[X]$ then assuming the high probability event (15) it holds that $||\theta_0|| \leq \eta + \frac{\omega}{\rho} \leq 2\mathsf{C}_{\theta}$ for all $n > n_0(\mathsf{C}_{\theta}, \mathsf{C}_{\omega})$ (see the end of the proof of Theorem 6). Thus also $|a_0|, b_0 \leq 2\mathsf{C}_{\theta}$. Note that for all $n > n_1(\mathsf{C}_{\omega})$ it holds that $\omega \leq 1/4$. For the induction step, assume that $||a_t|, b_t \leq C_f$ for some t. Then, using Lemma 17, item 4

$$a_{t+1} \leq F(a_t, b_t) + \max \{ |a_t| + b_t, \rho \} \cdot \omega$$

$$\leq C_{\theta} + 1 + 2C_f \omega$$

$$\leq C_f ,$$

and a similar lower bound on a_{t+1} holds, as well as a similar upper bound b_{t+1} . We henceforth assume that $|a_t|, b_t \leq C_f$.

<u>Large signal case</u>: Assume that $\eta > C_0 \frac{\omega}{\rho}$ where $C_0 > 0$ is to be specified later on.

<u>Step 1 (Orthogonal iteration and Positivity)</u>: We prove by induction that there exists $c_1 > 0$ to be specified (large enough) such that if $a_0 \ge 0$ and $b_0 \le c_1 \frac{\omega}{\rho}$ then $a_t \ge 0$ and $b_t \le c_1 \frac{\omega}{\rho}$ for all t. For t = 0, this is satisfied when initializing with both $\theta_0 = 0$ since, trivially, $a_0 = b_0 = 0$, and also when initializing with $\theta_0 = \frac{1}{\rho} \mathbb{E}_n[X]$, since under the high probability event (15)

$$\|\frac{1}{\rho}\mathbb{E}_n[X] - \theta_*\| = \frac{1}{\rho^2} \|f_n(0) - f(0)\| \le \frac{\omega}{\rho}.$$

Taking $C_0 > 2$ (say) implies that $a_0 > 0$ and $b_0 \leq \frac{\omega}{\rho}$. We assume that $a_t \geq 0$ and that $b_t \leq c_1 \frac{\omega}{\rho}$ and show that these properties continue to hold after iteration t + 1. We first consider the orthogonal iteration which is analyzed through its upper bound. There are two differences compared to the balanced case (Wu and Zhou, 2019, Theorem 5): 1) The slope of the upper bound on b_t has additional $-C_{G,\rho}^{(d)}\rho^2$ term (which improves the bound on b_t and improves convergence to low values). 2) The empirical error has an additional $\omega\rho$ term which deteriorates the bound on b_t . Nonetheless, the first effect dominates the second. Specifically, from Proposition 9, item 2,¹² since $a_t > 0$ and $\eta > C_0 \frac{\omega}{\rho}$ was assumed,

$$b_{t+1} \leq b_t \left(1 - \frac{a_t^2 + b_t^2}{2 + 4(a_t^2 + b_t^2)} - \frac{\mathsf{C}_{G,\rho}^{(d)}}{2} \rho^2 \right) + \omega \left(a_t + b_t + \rho \right)$$
(35)
$$\stackrel{(a)}{\leq} b_t \left(1 + \omega - \frac{\mathsf{C}_{G,\rho}^{(d)}}{2} \rho^2 \right) - \frac{b_t^3}{C_2} + \sup_{0 \leq a_t \leq C_f} \left(\omega a_t - \frac{a_t^2}{C_2} \right) + \omega \rho$$

$$\stackrel{(b)}{\leq} b_t \left(1 - \frac{\mathsf{C}_{G,\rho}^{(d)}}{2} \rho^2 \right) - \frac{b_t^3}{C_2} + \frac{C_2 \omega^2}{4b_t} + \omega \rho$$

where in (a) we have used $C_2 = 2 + 8C_f^2$, and (b) holds by requiring that $C_1 \ge \sqrt{\frac{2}{\mathsf{C}_{G,\rho}^{(d)}}}$. We assume w.l.o.g. that $\mathsf{C}_{G,\rho}^{(d)} \le 1$ as otherwise, we may weaken the bound by setting $\mathsf{C}_{G,\rho}^{(d)} = 1$. Now, we may show that $b_{t+1} \le c_1 \frac{\omega}{\rho}$: Let $c_2 > 0$ be a constant to be specified.

• If $0 \leq b_t \leq c_2 \omega$ then the bound

$$b_{t+1} \le b_t \left(1 - \frac{\mathsf{C}_{G,\rho}^{(d)}}{2} \rho^2 \right) + \omega C_f + \omega \rho \le c_1 \frac{\omega}{\rho}$$

holds as long as $c_2 + \omega(C_f + \rho) \leq \frac{c_1}{\rho}$ (condition I).

• If $c_2 \omega \leq b_t \leq c_1 \frac{\omega}{\rho}$ we may use the bound

$$b_{t+1} \le b_t \left(1 - \frac{\mathsf{C}_{G,\rho}^{(d)}}{2} \rho^2 \right) - \frac{b_t^3}{C_2} + \frac{C_2 \omega^2}{4b_t} + \omega\rho := h(b_t)$$

12. For simplicity of later notation, the constant $C_{G,\rho}^{(d)}$ was reduced to $\frac{C_{G,\rho}^{(d)}}{2}$.

Under the assumption $\rho \geq C_1 \sqrt{\omega}$ it holds that $\frac{\omega^2}{\rho^2} \leq \frac{\omega}{C_1^2} \to 0$ as $n \to \infty$ Thus, we may assume that $c_1 < \frac{\rho^2}{\omega^2}$ and $c_2 \geq \sqrt{C_2}$ (condition II), so that for all $n > n_2(c_1, C_1, C_2, \mathsf{C}_\omega)$

$$\frac{\mathrm{d}h}{\mathrm{d}b} = \left(1 - \frac{\mathsf{C}_{G,\rho}^{(d)}}{2}\rho^2\right) - \frac{3b^2}{C_2} - \frac{C_2\omega^2}{4b^2} \ge \frac{1}{2} - \frac{3c_1^2\omega^2}{C_2\rho^2} - \frac{C_2}{4c_2^2} > 0.$$

In this event, $b \mapsto h(b)$ is increasing, and thus if $\frac{C_2}{4c_1} + 1 - c_1 \frac{\mathsf{C}_{G,\rho}^{(d)}}{2} < 0$ (condition III) then

$$b_{t+1} \leq \max_{c_2 \omega \leq b \leq c_1 \frac{\omega}{\rho}} h(b) = h(c_1 \frac{\omega}{\rho})$$
$$\leq c_1 \frac{\omega}{\rho} + \left(\frac{C_2}{4c_1} + 1 - c_1 \frac{\mathsf{C}_{G,\rho}^{(d)}}{2}\right) \omega\rho$$
$$\leq c_1 \frac{\omega}{\rho}$$

holds. We choose c_2 such that condition II holds, and then choose $c_1 \ge 1$ and large enough so that conditions I and III will hold (note that n_2 may be affected by these choices).

Thus, we have proved that $b_{t+1} \leq c_1 \frac{\omega}{\rho}$ in the next iteration. We next show that $a_{t+1} > 0$. Using the boundedness from step 0 and Lemma 17, items 1 and 3

$$a_{t+1} \ge F(a_t, b_t) - \max\left\{ |a_t| + b_t, \rho \right\} \cdot \omega$$

$$\stackrel{(a)}{\ge} F(a_t, b_t) - \omega a_t - c_1 \frac{\omega^2}{\rho} - \rho \omega$$

$$\stackrel{(b)}{\ge} F(0, b_t) + \mathsf{C}''_F a_t - \omega a_t - c_1 \frac{\omega^2}{\rho} - \rho \omega$$

$$\stackrel{(c)}{\ge} (\mathsf{C}''_F - \omega) a_t + \rho \left(\mathsf{C}_{F,0} \rho \eta - c_1 \frac{\omega^2}{\rho^2} - \omega \right)$$

$$> 0,$$

where (a) is by the induction assumption, (b) is by the uniform bound on $\frac{\partial F}{\partial a}$ in Lemma 17 item 6 and Taylor expansion, (c) is by the lower bound on F(0, b) in Lemma 17 item 3, and the final inequality holds as long as n is sufficiently large so that $\omega \leq C''_F$, and $\frac{\omega}{\rho} < 1$, when requiring that $C_0 \geq \frac{c_1+1}{C_{F,0}}$.

<u>Step 2 (Signal iteration)</u>: From the previous step, we may assume that $a_t \ge 0$ and $b_t \le c_1 \frac{\omega}{\rho}$ for all $t \ge 0$. Lemma 17 items 8, 9 and 10 characterize the derivative of F(a, b) w.r.t. b around b = 0. Using these claims and the global assumptions $\eta \le C_{\theta}$ and $\beta \le \overline{C}_{\beta}\rho$, Taylor expansion of F(a, b) around b = 0 results

$$F_{+}(a,b) \leq F(a,0) + \left[C_{3} \cdot (|a|+\rho)b^{2} + \mathsf{C}_{F}''b^{3} + \omega(|a|+b+\rho) \right] ,$$

and

$$F_{-}(a,b) \ge F(a,0) - \left[C_{3} \cdot (|a|+\rho)b^{2} + \mathsf{C}_{F}'''b^{3} + \omega(|a|+b+\rho)\right] \,.$$

Observe that for b = 0 it holds that $F(a, 0) = f(\theta, \delta \mid \eta, \delta)$ is simply the one-dimensional iteration with absolute mean η . Furthermore, the envelopes $F_{\pm}(a, b)$ are the same as one-dimensional envelopes $f_{\pm}(\theta)$ with $\theta \equiv a$ except for excess error $C_3 \cdot (|a|+\rho)b^2 + C_F''b^3 + \omega b$ which results from the orthogonal error when $b \neq 0$. From the previous step, we have that $b_t \leq c_1 \frac{\omega}{\rho} \leq \frac{c_1}{C_1} \sqrt{\omega} \leq \frac{c_1\rho}{C_1^2}$ for all t and thus we may evaluate the terms of this excess error under this assumption. Then, $C_3 \cdot |a|b^2 \leq C_3 \frac{c_1}{C_1} \omega |a|$, $C_3 \cdot \rho b^2 \leq C_3 \frac{c_1^2}{C_1^2} \omega \rho$, $C_F'' b^3 \leq C_F'' \frac{c_1^3}{C_1^2} \omega \rho$, and $\omega b \leq \frac{c_1}{C_1^2} \omega \rho$. Hence, the excess error is no more than $C_4(|a|+\rho)\omega$ for some $C_4 > 0$. Since the one-dimensional envelopes have error $\max\{|a|, \rho\}\omega \geq \frac{1}{2}(|a|+\rho)\omega$ and $\max\{|a|, \rho\}\omega \leq (|a|+\rho)\omega$ (see Equation 23 and Equation 24), the excess error due to $b \neq 0$ only contributes to increasing the factor multiplying $(|a|+\rho)\omega$. Thus, taking $F_{\pm}(a_t, b_t)$ as envelopes of one dimensional iteration for a_t (with b_t acting as bounded disturbance), we obtain that, orderwise, the statistical error and convergence time of a_t are the same as for θ_t in the one-dimensional empirical iteration given in Theorem 6. Thus, after the convergence time specified in Theorem 6, the error is $|a_t - \eta| \leq C_5 \min\{\frac{\omega}{\rho}, \frac{\omega}{\eta}\}$ where $C_5 \leq C_2^{(1)}(1 + C_4)$

(note, however, that $\omega = \sqrt{C_{\omega} \frac{d \log n}{n}}$ with d > 1). We denote this convergence time by T_a .

Step 3 (Refinement of the orthogonal iteration): At the end of the previous step, it was shown that the error in $|a_t - \eta| \lesssim \min\left\{\frac{\omega}{\rho}, \frac{\omega}{\eta}\right\}$, whereas in the proceeding step it was shown that $b_t \lesssim \frac{\omega}{\rho}$. We next refine the latter bound to $b_t \lesssim \frac{\omega}{\eta}$ in case $\eta > \rho$. Assume that $C_f \geq \frac{2}{3}C_5C_l$ so that after the previous step it holds that $a_t \in [\frac{\eta}{2}, 2\eta]$ for all $t \geq T_a$. Thus, it holds that

$$\frac{a^2 + b^2}{2 + 4(a^2 + b^2)} \ge \frac{\eta^2/4}{2 + 4(4\mathsf{C}_{\theta}^2 + c_1\frac{\omega^2}{\rho^2})} \ge C_7\eta^2$$

for some $C_7 > 0$. Utilizing the bound of Proposition 9 item 2, we get

$$b_{t+1} \le b_t \left(1 - C_7 \eta^2 - \mathsf{C}_1^{(d)} \rho^2 \right) + \max \left\{ |a_t| + b_t, \rho \right\} \cdot \omega \\ \le b_t \left(1 - C_8 (\eta^2 + \rho^2) \right) + C_9 \eta \cdot \omega$$

where $C_8 \leq C_7 + \mathsf{C}_1^{(d)}$ and $C_9 \leq \max\{2\mathsf{C}_{\theta}, 1 + \frac{c_1}{C_1^2}\}$. From convergence properties of onedimensional iterations, (Proposition 23, item 7) $b_t \leq \frac{8C_9}{C_8} \cdot \frac{\omega}{\eta}$ for all $t \geq T_a + T_b$ where

$$T_b \leq rac{2}{C_8 \eta^2} \cdot \log\left(rac{8C_9}{C_8}rac{\omega}{\eta}
ight) \,.$$

<u>Small signal case</u>: Assume that $\eta < C_0 \frac{\omega}{\rho}$. As the signal is small, we show that the EM iteration remains small for all iterations. There are only two steps—an analysis of the orthogonal iteration (without assuming that a_t is positive), and then the signal iteration.

<u>Step 1 (Orthogonal iteration)</u>: In this case $a_t < 0$ is possible, and so we cannot use the dominance relation to the balanced iteration (Proposition 9 item 1). However, since the signal is small, we may use Taylor expansion to relate $G(a, b \mid \eta, \delta)$ to $G(a, b \mid 0, \delta)$ (Proposition 9 item 4), and then use the fact that for $\eta = 0$, the weight δ does not affect the iteration at all. Specifically, Proposition 9, items 1 and 4, along with the assumption $\rho > C_1 \sqrt{\omega}$ while requiring that $C_1 \ge \left(\frac{2\mathsf{C}_{G,\eta}^{(d)}}{\mathsf{C}_1^{(d)}}\right)^{1/4} \sqrt{C_0}$ imply that

$$\begin{split} G(a,b \mid \eta, \delta) &\leq G(a,b \mid 0, \delta) + b\mathsf{C}_{G,\eta}^{(d)} C_0^2 \frac{\omega^2}{\rho^2} \\ &\leq b \left(1 - \frac{a^2 + b^2}{2 + 4(a^2 + b^2)} - \mathsf{C}_{G,\rho}^{(d)} \rho^2 + \mathsf{C}_{G,\eta}^{(d)} C_0^2 \frac{\omega^2}{\rho^2} \right) \\ &\leq b \left(1 - \frac{a^2 + b^2}{2 + 4(a^2 + b^2)} - \frac{\mathsf{C}_{G,\rho}^{(d)}}{2} \rho^2 \right) \end{split}$$

for all $(a, b, \eta) \in [-C_f, C_f]^2 \times [0, \mathsf{C}_{\theta}]$. Thus, the bound (35) holds for this case too (note that the error $\omega(a_t + b_t + \beta)$ with mixed signs for $a_t < 0$ and $b_t > 0$ is only lower than both being positive). Hence, for all $(a, b, \eta) \in [-C_f, C_f]^2 \times [0, \mathsf{C}_{\theta}]$ it holds that

$$b_{t+1} \le b_t \left(1 - \frac{\mathsf{C}_{G,\rho}^{(d)}}{2} \rho^2 \right) - \frac{b_t^3}{C_2} + \frac{C_2 \omega^2}{4b_t} + \omega \rho.$$

Similar analysis to the large signal case then yields $b_t \leq c_1 \frac{\omega}{\rho}$ for all t.

<u>Step 2 (Signal iteration)</u>: The analysis is similar to the large signal case, which shows that $|a_t - \eta| \le C_5 \frac{\omega}{\rho}$ for $t \ge T_a$. The conclusion then follows since for some $C_6 > 0$

$$|\theta_t - \theta_*| \le |a_t - \eta| + b_t \le C_6 \frac{\omega}{\rho}$$

We complete the proof of Theorem 2 with the case of $\rho \lesssim \sqrt{\omega}$: **Proof** (of Proposition 11) The balanced iteration $f_n(\theta, \delta = \frac{1}{2} \mid \theta_*, \delta = \frac{1}{2}) = \mathbb{E}_n[X \cdot \tanh(X\theta))]$ is insensitive to the actual signs generating the samples (X_1, \ldots, X_n) , and thus the convergence result of Theorem 1 holds, where we note that its error guarantee is w.r.t. ℓ_0 . It is thus remain to show that s_t correctly adjusts the sign of θ_t . Recall that $\rho = 1 - 2\delta$, and let $\varepsilon = \frac{1}{\rho} \mathbb{E}_n[X] - \theta_*$. Under the high probability event (15)

$$\|\varepsilon\| = \|\frac{1}{\rho^2} \mathbb{E}_n[X] - \frac{1}{\rho^2} \mathbb{E}[X]\| = \frac{1}{\rho^2} \|f_n(\theta, \delta \mid \theta_*, \delta) - f(\theta, \delta \mid \theta_*, \delta)\| \le \frac{\omega}{\rho}.$$

By the guarantees of the balanced iteration, there exists c_0 such that for t large enough (as specified in the theorem) $\|\theta_t - \theta_*\| \le c_0 \frac{\omega}{\eta}$. Thus, if $\eta > c_1 \sqrt{\omega}$ for properly large c_1 , then $|\langle \theta_t, \theta_* \rangle| \ge \frac{\omega}{\rho} \|\theta_t\| \ge |\langle \theta_t, \varepsilon_n \rangle|$. Hence,

$$s_t = \operatorname{sign}\langle \theta_t, \frac{1}{\rho} \mathbb{E}_n[X] \rangle = \operatorname{sign}\left(\langle \theta_t, \theta_* \rangle + \langle \theta_t, \varepsilon_n \rangle\right) = \operatorname{sign}\langle \theta_t, \theta_* \rangle$$

5. Proofs for Section 2.4

In this section we prove the results of Section 2.4.

5.1 Population Iteration

We begin with basic properties:

Lemma 18 Assume that $\rho_* \geq 0$ and that $\langle \theta, \theta_* \rangle > 0$. Then:

1. Iteration: The iteration is consistent $h(\rho_*, \theta_*) = \rho_*$, at the boundaries $\lim_{\rho \uparrow 1} h(\rho, \theta) = 1$ and $\lim_{\rho \downarrow -1} h(\rho, \theta) = -1$. At $\rho = 0$

$$h(0,\theta) \ge \rho_* \left[1 - e^{-\langle \theta, \theta_* \rangle/2} \right]$$
.

2. First order derivative: It holds that $\frac{d}{d\rho}h(\rho,\theta) > 0$ and so $\rho \mapsto h(\rho,\theta)$ is increasing on [-1,1]. At the left boundary $\lim_{\rho \downarrow -1} \frac{\partial}{\partial \rho}h(\rho,\theta) > 1$, and at the right boundary

$$\lim_{\rho \uparrow 1} \frac{\partial}{\partial \rho} h(\rho, \theta) = e^{2\|\theta\|^2} \left[\left(\frac{1+\rho_*}{2} \right) e^{-2\langle \theta, \theta_* \rangle} + \left(\frac{1-\rho_*}{2} \right) \cdot e^{2\langle \theta, \theta_* \rangle} \right]$$

for which $\lim_{\rho\uparrow 1} \frac{\partial}{\partial \rho} h(\rho, \theta) > 1$ if $\|\theta\| > |\langle \hat{\theta}, \theta_* \rangle|$.

- 3. Second order derivative: There exists $\overline{\rho} \leq \rho_*$ such that $h(\rho)$ is strictly concave on $[-1,\overline{\rho}]$ and strictly convex on $[\overline{\rho},1]$. Consequently, $\frac{\partial h(\rho,\theta)}{\partial \rho}$ is strictly decreasing on $[-1,\overline{\rho}]$ and strictly increasing on $[\overline{\rho},1]$.
- 4. Contractivity at $\rho \in [0, \rho_*]$: If $\|\theta\| > |\langle \hat{\theta}, \theta_* \rangle|$ then

$$\max_{\rho \in [0,\rho_*]} \frac{\partial h(\rho,\theta)}{\partial \rho} \le e^{-|\langle \hat{\theta}, \theta_* \rangle|^2/2} \cdot \max\left\{\frac{5}{6}, 1 - \frac{\|\theta\|^2}{6}\right\}$$

5. Bounded second derivative for $\theta = \theta_*$: $\max_{\rho \in (0, \mathsf{C}_{\rho})} \frac{\partial^2 h(\rho, \theta_*)}{\partial \rho^2} \leq \mathsf{C}''_h \cdot \eta^2$ for $\mathsf{C}''_h = \frac{32+36(4\mathsf{C}^2_{\theta}+1)}{(1-\mathsf{C}^2_{\rho})^2}.$

Proof Let $Z \sim N(0,1)$ and $U \sim N(\eta,1)$ where $\eta = \langle \hat{\theta}, \theta_* \rangle$.

1. Consistency for $\theta = \theta_*$ is well-known and can be proved as in the proof of Lemma 15, item 1. The limits at the boundaries are immediate. At $\rho = 0$

$$\begin{split} h(0,\theta) &= \mathbb{E}\left[\tanh\left(\|\theta\|V\right)\right] \\ &= \left(\frac{1+\rho_*}{2}\right) \cdot \mathbb{E}\left[\tanh\left(\|\theta\|U\right)\right] + \left(\frac{1-\rho_*}{2}\right) \cdot \mathbb{E}\left[\tanh\left(-\|\theta\|U\right)\right] \\ &= \rho_* \mathbb{E}\left[\tanh\left(\|\theta\|U\right)\right] \\ &\geq \rho_*\left[1-e^{-\langle\theta,\theta_*\rangle/2}\right], \end{split}$$

where the last inequality is from (53) in Appendix C.1.

2. By direct computation

$$\begin{aligned} h'(\rho) &:= \frac{\partial h(\rho, \theta)}{\partial \rho} = \frac{1}{1 - \rho^2} \cdot \mathbb{E}\left[\frac{1}{\cosh^2\left(\|\theta\|V + \beta_\rho\right)}\right] \\ &= \mathbb{E}\left[\frac{1}{\left[\left(\frac{1 + \rho}{2}\right)e^{\|\theta\|V} + \left(\frac{1 - \rho}{2}\right)e^{-\|\theta\|V}\right]^2}\right] > 0 \end{aligned}$$

and so the iteration is monotonically increasing. The limit at $\rho = -1$

$$\begin{split} \lim_{\rho \downarrow -1} h'(\rho) &= \mathbb{E}\left[e^{2\|\theta\|V}\right] = \left(\frac{1+\rho_*}{2}\right) \cdot \mathbb{E}\left[e^{2\|\theta\|U}\right] + \left(\frac{1-\rho_*}{2}\right) \cdot \mathbb{E}\left[e^{-2\|\theta\|U}\right] \\ &= e^{2\|\theta\|^2} \left[\left(\frac{1+\rho_*}{2}\right)e^{2\langle\theta,\theta_*\rangle} + \left(\frac{1-\rho_*}{2}\right) \cdot e^{-2\langle\theta,\theta_*\rangle}\right] \\ &> 1 \end{split}$$

where the last inequality is since $\left(\frac{1+\rho_*}{2}\right)s + \left(\frac{1-\rho_*}{2}\right)s^{-1}$ for $s \in [1,\infty)$ is minimized for s = 1 (assuming $\rho_* > 0$). Similarly, the limit at $\rho = 1$

$$\lim_{\rho \uparrow 1} h'(\rho) = \mathbb{E}\left[e^{-2\|\theta\|V}\right] = \left(\frac{1+\rho_*}{2}\right) \cdot \mathbb{E}\left[e^{-2\|\theta\|U}\right] + \left(\frac{1-\rho_*}{2}\right) \cdot \mathbb{E}\left[e^{2\|\theta\|U}\right]$$
$$= e^{2\|\theta\|^2}\left[\left(\frac{1+\rho_*}{2}\right)e^{-2\langle\theta,\theta_*\rangle} + \left(\frac{1-\rho_*}{2}\right) \cdot e^{2\langle\theta,\theta_*\rangle}\right].$$
(36)

3. By direct computation

$$h''(\rho) := \frac{\partial^2 h(\rho, \theta)}{\partial \rho^2} = \frac{2}{(1 - \rho^2)^2} \cdot \mathbb{E}\left[\frac{\rho - \tanh\left(\|\theta\|V + \beta_\rho\right)}{\cosh^2\left(\|\theta\|V + \beta_\rho\right)}\right],$$

and evidently, $\lim_{\rho \uparrow 1} h''(\rho) > 0$. At $\rho = 0$,

$$h''(0) = -2 \cdot \mathbb{E}\left[\frac{\tanh\left(\|\theta\|V\right)}{\cosh^2\left(\|\theta\|V\right)}\right] < 0,$$

since $\mathbb{P}[V = v] > \mathbb{P}[V = -v]$ for any v > 0 (see Equation 56 in Appendix C.1) and tanh is an odd function. To show that $h(\rho)$ changes its curvature from convex to concave as ρ increases from -1 to 1 only a single time at some $\overline{\rho}$, we note that

$$h'''(\rho) := \frac{\partial^3 h(\rho, \theta)}{\partial \rho^3} = \frac{3}{(1-\rho^2)^2} \cdot \mathbb{E}\left[\frac{\cosh\left(2\|\theta\|V\right) - 1}{\cosh^4\left(\|\theta\|V + \beta_\rho\right)}\right] > 0.$$

Thus, $h''(\rho)$ is monotonically increasing. The fact that $\overline{\rho} \leq \rho_*$ follows from $h''(\rho_*) > 0$ but we omit the full proof since this property is inconsequential for further analysis.

4. We prove the claimed bound at the edge points of the interval $[0, \rho_*]$, and then the same bound holds at the interior of the interval since the property of $h''(\rho)$ stated in item 3 implies that $\max_{\rho \in [0, \rho_*]} h'(\rho)$ is bounded by its values at the edge points. At

 $\rho = 0$, let $V_{\frac{1}{2}} \sim \frac{1}{2} \cdot N(\eta, 1) + \frac{1}{2} \cdot N(-\eta, 1)$ be a balanced version of V, where we recall that $\eta = \langle \hat{\theta}, \theta_* \rangle$ here. Then,

$$h'(0) = \mathbb{E}\left[\frac{1}{\cosh^{2}(||\theta||V)}\right]$$

$$\stackrel{(a)}{=} \mathbb{E}\left[\frac{1}{\cosh^{2}(||\theta||V_{\frac{1}{2}})}\right]$$

$$\stackrel{(b)}{=} e^{-\eta^{2}/2} \cdot \mathbb{E}\left[\frac{1}{\cosh(||\theta||Z)} \cdot \frac{e^{\eta Z} + e^{-\eta Z}}{e^{||\theta||Z} + e^{-||\theta||Z}} \mid Z > 0\right]$$

$$\stackrel{(c)}{\leq} e^{-\eta^{2}/2} \cdot \mathbb{E}\left[\frac{1}{\cosh(||\theta||Z)}\right]$$

$$\stackrel{(d)}{\leq} e^{-\eta^{2}/2} \cdot \left(1 - \frac{||\theta||^{2}}{2(1+2||\theta||^{2})}\right)$$

$$\leq e^{-\eta^{2}/2} \cdot \left\{\frac{5}{6}, \qquad ||\theta|| \le 1\\ 1 - \frac{||\theta||^{2}}{6}, \qquad ||\theta|| > 1, \end{cases}$$
(37)

where (a) is since $\cosh^2(t)$ is even, (b) is by a change of measure (see Equation 52 in Appendix C.1) and symmetry, (c) is since $\max_{a \ge b \ge 1} \frac{b+b^{-1}}{a+a^{-1}} = \max\left\{1, \max_{a \ge 1} \frac{2}{a+a^{-1}}\right\} \le 1$ (e.g., by the inequality of arithmetic and geometric means), and (d) is by the result of Wu and Zhou (2019, eq.(125) and Lemma 24). At $\rho = \rho_*$ it holds that

$$\begin{split} h'(\rho_*) &= \mathbb{E}\left[\frac{1}{\left[\left(\frac{1+\rho_*}{2}\right)e^{||\theta||V} + \left(\frac{1-\rho_*}{2}\right)e^{-||\theta||V}\right]^2}\right] \\ &\stackrel{(a)}{=} e^{-\eta^2/2} \cdot \mathbb{E}\left[\frac{1}{\left(\frac{1+\rho_*}{2}\right)e^{||\theta||Z} + \left(\frac{1-\rho_*}{2}\right)e^{-||\theta||Z}} \cdot \frac{\left(\frac{1+\rho_*}{2}\right)e^{\eta Z} + \left(\frac{1-\rho_*}{2}\right)e^{-\eta Z}}{\left(\frac{1+\rho_*}{2}\right)e^{||\theta||Z} + \left(\frac{1-\rho_*}{2}\right)e^{-||\theta||Z}}\right] \\ &\stackrel{(b)}{\leq} e^{-\eta^2/2} \cdot \mathbb{E}\left[\frac{1}{\left(\frac{1+\rho_*}{2}\right)e^{||\theta||Z} + \left(\frac{1-\rho_*}{2}\right)e^{-||\theta||Z}}\right] \\ &= e^{-\eta^2/2} \cdot \mathbb{E}\left[\frac{1}{\cosh(||\theta||Z+\beta)}\right] \\ &\stackrel{(c)}{\leq} e^{-\eta^2/2} \cdot \mathbb{E}\left[\frac{1}{\cosh(||\theta||Z)}\right] \\ &\stackrel{(d)}{\leq} e^{-\eta^2/2} \cdot \begin{cases} \frac{5}{6}, & ||\theta|| \le 1\\ 1 - \frac{||\theta||^2}{6}, & ||\theta|| > 1 \end{cases}, \end{split}$$

where (a) is again by a change of measure, (b) is as in (18) assuming $\|\theta\| \ge \eta = \langle \hat{\theta}, \theta_* \rangle$, (c) is since the argument inside the expectation is an even function of β , and using arguments similar to (32) to show that

$$\frac{\partial}{\partial\beta} \mathbb{E}\left[\frac{1}{\cosh(\|\theta\|Z+\beta)}\right] = -\mathbb{E}\left[\frac{\tanh(\|\theta\|Z+\beta)}{\cosh(\|\theta\|Z+\beta)}\right] < 0,$$

and (d) is as in (37).

5. To bound the second derivative let $\eta = \|\theta_*\|$ and $V \sim (1 - \delta_*) \cdot N(\eta, 1) + \delta_* \cdot N(-\eta, 1)$. Then, for any $\rho \in [0, \mathsf{C}_{\rho})$

$$h''(\rho) = \frac{2}{(1-\rho^2)^2} \cdot \mathbb{E}\left[\frac{\rho - \tanh(\eta V + \beta_{\rho})}{\cosh^2(\eta V + \beta_{\rho})}\right] := \frac{2}{(1-\rho^2)^2} \cdot a(\eta)$$

and using $\psi_{\pm} = \eta^2 + \eta Z \pm \beta_{\rho}$ with $Z \sim N(0, 1)$ we may write

$$a(\eta) = (1 - \delta_*) \cdot \mathbb{E}\left[\frac{\rho - \tanh(\psi_+)}{\cosh^2(\psi_+)}\right] + \delta_* \cdot \mathbb{E}\left[\frac{\rho + \tanh(\psi_-)}{\cosh^2(\psi_-)}\right].$$

We will bound $a(\eta)$ by its Taylor expansion around $\eta = 0$. Note that a(0) = 0 (since $\rho = \tanh(\beta_{\rho})$), and that the first derivative is

$$a'(\eta) = \frac{\partial a(\eta)}{\partial \eta} = -4(1 - \delta_*) \cdot \mathbb{E}\left[(2\eta + Z) \cdot \frac{2 + \rho \sinh(2\psi_+) - \cosh(2\psi_+)}{\left[1 + \cosh^2(2\psi_+)\right]^2} \right] + 4\delta_* \cdot \mathbb{E}\left[(2\eta + Z) \cdot \frac{2 + \rho \sinh(2\psi_-) - \cosh(2\psi_-)}{\left[1 + \cosh^2(2\psi_-)\right]^2} \right]$$

and so a'(0) = 0. Next we upper bound the second derivative $a''(\eta) = \frac{\partial a^2(\eta)}{\partial \eta^2}$. As $a'(\eta)$ in the last display is comprised from a mixture of two expectations, we only bound the first (and the second one can be bounded similarly by the same bound). So,

$$\begin{split} &\frac{\partial}{\partial \eta} \mathbb{E} \left[(2\eta + Z) \cdot \frac{2 + \rho \sinh(2\psi_+) - \cosh(2\psi_+)}{\left[1 + \cosh^2(2\psi_+)\right]^2} \right] \\ &= 2 \cdot \mathbb{E} \left[\frac{2 + \rho \sinh(2\psi_+) - \cosh(2\psi_+)}{\left[1 + \cosh^2(2\psi_+)\right]^2} \right] + \mathbb{E} \left[(2\eta + Z)^2 \times \frac{\rho + \rho \cosh(2\psi_+) - 5 \sinh(2\psi_+) + \cosh(2\psi_+) \sinh(2\psi_+) - \rho \sinh^2(2\psi_+)}{\left[1 + \cosh^2(2\psi_+)\right]^3} \right]. \end{split}$$

Using $|\sinh(t)| \le |\cosh(t)|$ and the triangle inequality, the absolute value of the above expression is bounded from above by

$$2(3+\rho) + (3\rho+6) \cdot \mathbb{E}\left[(2\eta+Z)^2\right] \le 8 + 9(4\eta^2+1)$$

Hence, $a''(\eta) \leq 32 + 36(4C_{\theta}^2 + 1)$ for all $\eta \in C_{\theta}$ and the result follows from Taylor expansion.

We may now prove the convergence of the population iteration.

Proof (of Theorem 12) For brevity, we denote the iteration by $h(\rho)$. Let $h'(\rho) = \frac{\partial}{\partial \rho}h(\rho,\theta)$ and recall that Lemma 18 states that: h'(-1) > 1; that there exists a $\overline{\rho}$ such that $h'(\rho)$ is strictly decreasing in $(-1,\overline{\rho})$ and strictly increasing in $(\overline{\rho},1)$; that $\rho = \pm 1$ are fixed points of $h(\rho) = h(\rho,\theta)$. Note also that an explicit expression for h'(1) is given in (36). We show that:

- 1. If $h'(1) \leq 1$ then $h(\rho)$ has no fixed points in (-1, 1).
- 2. If h'(1) > 1 then $h(\rho)$ has a unique fixed point $\rho_{\#} \in (-1, 1)$.

In the second case, we may deduce that $h(\rho) > \rho$ for $\rho \in (-1, \rho_{\#})$ and $h(\rho) < \rho$ for $\rho \in (\rho_{\#}, 1)$. By Lemma 18 item 2, $h(\rho)$ is increasing, and so Proposition 23, item 4 and analogous arguments imply that the iteration $\rho_{t+1} = h(\rho_t)$ will converge monotonically upwards (resp. downwards) to $\rho_{\#}$ if $\rho_0 \in (-1, \rho_{\#}]$ (resp. $\rho_0 \in [\rho_{\#}, 1)$). By consistency (Lemma 18) $\rho_{\#} = \rho_*$ for $\theta = \theta_*$.

<u>Case 1</u>: Assume h'(1) < 1. By the properties mentioned above, it must be that there exists $\tilde{\rho} \in (-1, 1]$ such that

$$h'(\rho) \begin{cases} > 1, & -1 \le \rho \le \tilde{\rho} \\ = 1, & \rho = \tilde{\rho} \\ < 1, & \tilde{\rho} < \rho \le 1 \end{cases}$$
(38)

Assume by contradiction that $\rho_1 \in (-1, 1)$ is a fixed point. Further assume that there are no other fixed points in $(-1, \rho_1)$.¹³ Since h(-1) > 1, Proposition 23, item 2 implies that $h'(\rho_1) \leq 1$. Hence, (38) implies that $\rho_1 \geq \tilde{\rho}$, and so $h'(\rho) < 1$ for all $\rho \in (\rho_1, 1)$. But this implies

$$h(1) = h(\rho_1) + \int_{\rho_1}^{1} h'(\rho) d\rho \le \rho_1 + (1 - \rho_1) \cdot \max_{\rho \in [\rho_1, 1]} h'(\rho) < 1$$
(39)

which contradicts the property h(1) = 1.

<u>Case 2</u>: Assume h'(1) > 1. In this case $h(\rho) < \rho$ for ρ close enough to $\rho = 1$ from below, and as h'(-1) > 1 then $h(\rho) > \rho$ for ρ close enough to $\rho = -1$ from above. By the intermediate value theorem for $h(\rho) - \rho$ for $\rho \in [-1, 1]$, there must exists at least a single fixed point $\rho_{\#}$ for $h(\rho)$ in (-1, 1). We show that $\rho_{\#}$ is unique. By the properties mentioned above, it must be that there exists $-1 < \tilde{\rho}_{-} < \tilde{\rho}_{+} < 1$ such that

$$h'(\rho) \begin{cases} > 1, & -1 \le \rho < \tilde{\rho}_{-} \\ = 1, & \rho = \tilde{\rho}_{-} \\ < 1 & \tilde{\rho}_{-} < \rho < \tilde{\rho}_{-} \\ = 1, & \rho = \tilde{\rho}_{+} \\ > 1, & \tilde{\rho}_{+} < \rho \le 1 \end{cases}$$
(40)

^{13.} The fixed points of $h(\rho)$ must be isolated; see Proposition 23, item 2.

(and also $h'(\rho)$ decreases in $(-1, \overline{\rho})$ and increases in $(\overline{\rho}, 1)$ where $\overline{\rho} \in (\tilde{\rho}_{-}, \tilde{\rho}_{+})$). If there are multiple fixed points in (-1, 1) then we denote by $\rho_{\#}$ the minimal one. Since h'(-1) > 1Proposition 23, item 2 implies that $h'(\rho_{\#}) \leq 1$, and, in fact, a similar argument to (39) together with (40) show that $h'(\rho_{\#}) < 1$. We next separately show that there are no fixed points in $(-1, \rho_{\#})$ and in $(\rho_{\#}, 1)$:

- Assume by contradiction that $\rho_1 \in (\rho_{\#}, 1)$ is a fixed point, and further assume that there are no other fixed points in $(\rho_{\#}, \rho_1)$. By Proposition 23, item 2, it holds that $h'(\rho_1) \geq 1$. Since $h'(\rho)$ has (strictly) increased from $h'(\rho_{\#}) < 1$ to $h'(\rho_1) \geq 1$, (40) implies that $h'(\rho)$ is strictly increasing on $(\rho_1, 1)$. Hence, $h(\rho) > \rho$ for all $\rho \in (\rho_1, 1)$. However, as $\rho = 1$ is a fixed point, and h'(1) > 1, continuity of $h(\rho)$ implies that there exists $\rho_1 < \tilde{\rho} < 1$ such that $h(\rho) < \rho$ for $\rho \in (\tilde{\rho}, 1)$; a contradiction.
- Assume by contradiction that ρ₁ ∈ (-1, ρ_{*}) is a fixed point, and further assume that ρ₁ is such that there are no other fixed points in (-1, ρ₁). Since h(-1) > 1, Proposition 23, item 2, implies that h'(ρ₁) ≤ 1. We consider separately the cases h'(ρ₁) < 1 and h'(ρ₁) = 1. First, if h'(ρ₁) < 1, then there exists p̄ such that h(ρ) < ρ for (ρ₁, p̄). Since h'(ρ_#) < 1 it holds that there exists ρ̀ such that h(ρ) > ρ for ρ ∈ (ρ̀, ρ_{*}). By the mean value theorem, there must exist at least one more fixed point ρ₂ ∈ (ρ₁, ρ_#) for which h'(ρ₂) > 1 (Proposition 23, item 2). Since h'(ρ) has increased from h'(ρ₁) < 1 to h(ρ₂) > 1, (40) implies that we must have that ρ̃₊ ≤ ρ₂. But since ρ_# > ρ₂ (40) implies that h'(ρ_#) > 1; a contradiction since it holds h'(ρ_#) < 1. Second, if h'(ρ₁) = 1, then if, in addition, ρ₁ = ρ̃₊ then h'(ρ) is strictly increasing on (ρ₁, 1) which will result h'(ρ_#) > 1; holds verbatim.

Proof (of Proposition 13) As discussed in the beginning of Section 2.4, we may assume d = 1, with $\eta = \langle \hat{\theta}, \theta_* \rangle$. Per the statement of the theorem, we assume that $\theta > 0$ and that there exists a fixed point $\rho_{\#} \in (-1, 1)$. According to Theorem 12, this fixed point must be unique and so $h(\rho, \theta\eta, \rho_*) > \rho$ for $\rho \in (-1, \rho_{\#})$ and $h(\rho, \theta \mid \eta, \rho_*) < \rho$ for $\rho \in (\rho_{\#}, 1)$. Consequently, the location of $\rho_{\#}$ with respect to ρ_* may be determined by comparing $h(\rho_*, \theta \mid \eta, \rho_*)$ to $= h(\rho_*, \eta \mid \eta, \rho_*) = \rho_*$. Specifically, it suffices to show that $h(\rho_*, \theta \mid \eta, \rho_*) > \rho_*$ for $\theta \in (0, \eta)$ and $h(\rho_*, \theta \mid \eta, \rho_*) < \rho_*$ for $\theta > \eta$. In the former case, this implies that $\rho_{\#} > \rho_*$ and in the latter case, this implies that $\rho_{\#} < \rho_*$ (and that such $\rho_{\#} \in (-1, 1)$ exists). To show that property, we take similar strategy as in the analysis of the mean iteration (Proposition 5), and prove this "global" property by exploring $h(\rho_*, \theta \mid \eta, \rho_*)$ as a function of η for a fixed θ . We thus denote it here explicitly as $k(\theta \mid \eta) := h(\rho_*, \theta \mid \eta, \rho_*)$. Thus, it boils down to show that for $\theta > 0$

$$\begin{cases} k(\theta \mid \eta) < k(\theta \mid \theta) = \rho_*, \quad \theta > \eta \\ k(\theta \mid \eta) > k(\theta \mid \theta) = \rho_*, \quad \theta < \eta \end{cases}$$
(41)

To this end, note that

$$k(\theta \mid \eta) - k(\theta \mid \theta)$$

= $\mathbb{E} \{ (1 - \delta_*) [\tanh(\theta U + \beta_{\delta_*}) - 1] - \delta_* [\tanh(\theta U - \beta_{\delta_*}) - 1] \}$
= $\mathbb{E} [s(\theta U)] = s(\theta \eta) * \varphi(\eta)$ (42)

where $\varphi(\eta) = \frac{1}{\sqrt{2\pi}} e^{-\eta^2/2}$ is the Gaussian kernel and

$$s(u) := (1 - \delta_*) \left[\tanh \left(u + \beta_{\delta_*} \right) - 1 \right] - \delta_* \left[\tanh \left(u - \beta_{\delta_*} \right) - 1 \right]$$

Note that $k(\theta \mid \eta) - k(\theta \mid \theta) = 0$ for $\eta = \theta$. We will show that this is a unique zero-crossing point of $\eta \mapsto k(\theta \mid \eta) - k(\theta \mid \theta)$ by analyzing s(u). The function s(u) has a single zerocrossing point at u = 0 since: (a) It can be shown by some simple algebra that the unique root of s(u) = 0 is u = 0, and (b) s(u) changes from negative to positive at u = 0 since $\lim_{u\to-\infty} s(u) = -2\rho_* < 0$ and

$$\left. \frac{\mathrm{d}s(u)}{\mathrm{d}u} \right|_{u=0} = (1 - 2\delta_*) \frac{1}{\cosh^2(\beta_{\delta_*})} > 0 \,.$$

Thus, s = 0 is a unique zero-crossing point of s(u). As in the proof of Proposition 5, the convolution relation (42) and the variation diminishing property of the Gaussian kernel (Proposition 25 in Appendix C.3) imply that $\eta \mapsto k(\theta \mid \eta) - k(\theta \mid \theta)$ has at most a single zero-crossing point as a function of $\eta \in \mathbb{R}$ (note that for the sake of the proof we allow $\eta < 0$). Clearly, this zero-crossing point can only be at $\eta = \theta$. To show that this is indeed a zero crossing point, we show that $k(\theta \mid \eta) - k(\theta \mid \theta)$ changes from negative to positive from $\eta = 0$ to $\eta \to \infty$. Indeed, for $\eta = 0$

$$k(\theta \mid \eta = 0) - k(\theta \mid \theta) = \mathbb{E} \left[\tanh \left(\theta Z + \beta_{\delta_*} \right) \right] - \rho_* < 0$$

because $k(\theta \mid \eta = 0) - k(\theta \mid \theta)|_{\theta=0} = \tanh(\beta_{\delta_*}) - \rho_* = 0$ and

$$\frac{\partial \left[k(\theta \mid \eta = 0) - k(\theta \mid \theta)\right]}{\partial \theta} = \mathbb{E}\left[\frac{Z}{\cosh^2\left(\theta Z + \beta_{\delta_*}\right)}\right] < 0$$

(by conditioning on |Z| and using $\delta_* \leq \frac{1}{2}$ and $\theta, \beta_{\delta_*} \geq 0$). For $\eta \to \infty$, since $s(u) \geq 0$ for all u > 0, (42) implies that $k(\theta \mid \eta) - k(\theta \mid \theta) > 0$ for all η large enough. Thus, $\eta = \theta$ is a unique zero-crossing point of $k(\theta \mid \eta) - k(\theta \mid \theta)$ and (41) holds.

5.2 Empirical Iteration

Proof (of Theorem 14) Let $h_n(\rho) \equiv h_n(\rho, \theta_*)$. Under the high probability event (15), it holds that $h_n(\rho)$ is sandwiched between the envelopes

$$h_n(\rho) \le h(\rho) + \eta \omega_1 := h_+(\rho)$$

and

$$h_n(\rho) \ge h(\rho) - \eta \omega_1 := h_-(\rho)$$

and where $\eta = \|\theta_*\|$. Thus, for the weight iteration, the empirical error is absolute, i.e., comprised of an additive term $\eta\omega_1$ which does not depend on ρ . Furthermore, the truncated empirical iteration $[h_n(\rho)]_{\mathsf{C}_{\rho}}$ is bounded by the truncated envelopes $[h_{\pm}(\rho)]_{\mathsf{C}_{\rho}}$. The truncation does not affect the analysis of the lower envelope, but will be used for the error analysis of the upper envelope.

By repeating the arguments in the proof of Theorem 12, it can be shown that $h_{-}(\rho)$ has only two fixed points in [-1, 1], denoted here by ρ_{-} and ρ_{-} such that $\rho_{-} \uparrow \rho_{*}$ and $\rho_{-} \downarrow -1$ as $\omega_{1} \to 0$ (or, $n \to \infty$).¹⁴ Hence, $h(\rho) > \rho$ for $\rho \in (\rho, \rho_{-})$, and if the iteration is initialized in $\rho_{0} \in (\rho, \rho_{-})$ it will converge to ρ_{-} . We next show that this holds for initialization at $\rho_{0} = 0$. It is readily verified that $\eta \mapsto \frac{1-e^{-\eta^{2}/2}}{\eta^{2}}$ is an even function of η which is strictly decreasing for $\eta > 0$. Since $\eta \leq C_{\theta}$ it holds that $1 - e^{-\eta^{2}/2} \geq C_{1}\eta^{2}$ for $C_{1} = \frac{1-e^{-C_{\theta}^{2}/2}}{C_{\theta}^{2}} > 0$. Then, Lemma 18, item 1 implies that if $\eta > \frac{2}{C_{1}} \cdot \frac{\omega_{1}}{\rho_{*}}$ then

$$h_{-}(0) \ge \rho_* \left[1 - e^{-\eta^2/2} \right] - \eta \omega_1 \ge C_1 \rho_* \eta^2 - \eta \omega_1 > 0.$$

Hence the iteration $\rho_{t+1} = h_{-}(\rho_t)$ with $\rho_0 = 0$ will converge to ρ_{-} . Analogous claims hold for the upper envelope for which clearly $h_{+}(0) > 0$. We next bound the errors $\rho_* - \rho_{-}$ and $\rho_+ - \rho_*$ and the convergence times of the envelops. For the lower envelope, the truncation is inconsequential. Lemma 18, item 4 implies that $h'_{-}(\rho) \leq \min\{e^{-1}, 1 - \frac{\eta^2}{12}\}$ for all $\rho \in [0, \rho_*]$, and so

$$\begin{split} \rho_{-} &= h_{-}(\rho_{-}) \\ &= h(\rho_{-}) - \eta \omega_{1} \\ &= h(\rho_{*}) - \int_{\rho_{-}}^{\rho_{*}} h'(\rho) d\rho - \eta \omega_{1} \\ &= \rho_{*} - \int_{\rho_{-}}^{\rho_{*}} h'(\rho) d\rho - \eta \omega_{1} \\ &\geq \rho_{*} - \min\{e^{-1}, 1 - \frac{\eta^{2}}{12}\} \cdot (\rho_{*} - \rho_{-}) - \eta \omega_{1} \end{split}$$

Thus, the error is at most

$$\rho_* - \rho_- \le \frac{\eta \omega_1}{1 - \max\{e^{-1}, 1 - \frac{\eta^2}{12}\}} \le \max\left\{12\frac{\omega_1}{\eta}, 2\mathsf{C}_{\theta}\omega_1\right\} \le 12\mathsf{C}_{\theta}^2 \cdot \frac{\omega_1}{\eta}$$

Further note that as $\rho_* > \frac{2}{C_1} \cdot \frac{\omega_1}{\eta}$ was assumed, this also implies that $\rho_- > \frac{\rho_*}{2}$. We now turn to the convergence time. Again, since $h'_-(\rho) \leq \min\{e^{-1}, 1 - \frac{\eta^2}{12}\} < 1$ for all $\rho \in (0, \rho_-)$, Proposition 23, item 6, implies that $|\rho_t - \rho_-| \leq \frac{\omega_1}{\eta}$ for all

$$t \geq \frac{1}{1 - \max\{e^{-1}, 1 - \frac{\eta^2}{12}\}} \log\left[\frac{\omega_1}{\eta \cdot \rho_-}\right]$$

^{14.} Indeed, the proof Theorem 12 mostly uses the first order derivative $h'(\rho)$ which is not changed by absolute errors.

The r.h.s. is at most $12C_{\theta}^2\eta^{-2}\log(C_1)$.

For the upper envelope, we use again Lemma 18, item 4 implies that $h'(\rho_*) \leq \max\{e^{-1}, 1-\frac{\eta^2}{12}\}$. Furthermore, by the truncation operation $\rho \leq C_{\rho}$ and Lemma 18, item 5 imply that $h''(\rho) \leq C''_h \eta^2$. Since $\rho_+ - \rho_* \to 0$ as $n \to \infty$ there exists n_0 such that $\frac{C''_h}{2}(\rho_+ - \rho_*) \leq \frac{1}{24}$ and so by Taylor expansion, for any $\rho \in [\rho_*, \rho_+]$

$$\begin{split} h'(\rho) &\leq h'(\rho_*) + \mathsf{C}''_h(\rho - \rho_*)\eta^2 \\ &\leq \max\{e^{-1}, 1 - \frac{\eta^2}{24}\}\,. \end{split}$$

With this bound on the first derivative, the analysis is similar to the one made for the lower envelope.

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Appendix A. A Proof for the Concentration Inequality of Section 2.1

The proof of Theorem 3 follows the analysis of Wu and Zhou (2019, Proof of Theorem 4), where here, uniform convergence of the relative error should be assured for all possible β_{ρ} , and uniform convergence of the error is also established for the weight iteration. For legibility of the proof, we summarize the required bounds on the moments and the tail bounds in the following lemma.

Lemma 19 Let $X \sim P_{\theta_*,\rho_*}$ for arbitrary $\rho_* \in (-1,1)$ and $\theta_* \in \mathbb{R}^d$. There exists an absolute constant c > 0 and $n_0 \in \mathbb{N}$ such that the following holds:

1. Population moments:

$$\mathbb{E}\|X\|^2 = d + \|\theta_*\|^2,$$

and

$$\mathbb{E} \|X\|^3 \le c(\|\theta_*\| + \sqrt{d})^3$$
.

2. Concentration of empirical moments:

$$\mathbb{P}\left[\mathbb{E}_n\left[\|X\|^2\right] > 2\|\theta_*\|^2 + 10d\right] \le e^{-dn}$$

and for all $n > n_0$

$$\mathbb{P}\left[\mathbb{E}_n\left[\|X\|^3\right] > 4\|\theta_*\|^3 + 16d^{3/2} + 16n^{3/2}\right] \le e^{-cn}.$$

3. Concentration of projections: For any $u, v \in \mathbb{S}^{d-1}$ and b > 0 and n > 0

$$\mathbb{P}\left[\mathbb{E}\left[\langle u, X \rangle\right] - \mathbb{E}_n\left[\langle u, X \rangle\right] > \sqrt{\left(1 + \|\theta_*\|^2\right)\frac{bd\log n}{n}}\right] \le 2\exp\left(-cbd\log n\right) \,,$$

and for any $n \ge bd \log n$

$$\mathbb{P}\left[|\mathbb{E}\left[\langle u, X \rangle \langle v, X \rangle\right] - \mathbb{E}_n\left[\langle u, X \rangle \langle v, X \rangle\right]| > (1 + \|\theta_*\|^2) \sqrt{\frac{bd \log n}{n}}\right] \le 2 \exp\left(-cbd \log n\right) \,.$$

4. Concentration of empirical EM iterations at a single point: For any $u, v \in \mathbb{S}^{d-1}$, b > 0and $n \ge bd \log n$

$$\mathbb{P}\left[|\langle u, f_n(\theta, \rho) \rangle - \langle u, f(\theta, \rho) \rangle| \ge (\|\theta\| + \beta_\rho) \cdot (1 + \|\theta_*\|^2) \sqrt{\frac{bd \log n}{n}} \right] \le 2 \exp\left(-cbd \log n\right) + \frac{bd \log n}{n} = \frac{1}{2} \exp\left(-cbd \log n\right) + \frac{bd \log n}{n} = \frac{1}{2} \exp\left(-cbd \log n\right) + \frac{bd \log n}{n} = \frac{1}{2} \exp\left(-cbd \log n\right) + \frac{bd \log n}{n} = \frac{1}{2} \exp\left(-cbd \log n\right) + \frac{bd \log n}{n} = \frac{1}{2} \exp\left(-cbd \log n\right) + \frac{bd \log n}{n} = \frac{1}{2} \exp\left(-cbd \log n\right) + \frac{bd \log n}{n} = \frac{1}{2} \exp\left(-cbd \log n\right) + \frac{bd \log n}{n} = \frac{1}{2} \exp\left(-cbd \log n\right) + \frac{bd \log n}{n} = \frac{1}{2} \exp\left(-cbd \log n\right) + \frac{bd \log n}{n} = \frac{1}{2} \exp\left(-cbd \log n\right) + \frac{bd \log n}{n} = \frac{1}{2} \exp\left(-cbd \log n\right) + \frac{bd \log n}{n} = \frac{1}{2} \exp\left(-cbd \log n\right) + \frac{bd \log n}{n} = \frac{1}{2} \exp\left(-cbd \log n\right) + \frac{bd \log n}{n} = \frac{1}{2} \exp\left(-cbd \log n\right) + \frac{bd \log n}{n} = \frac{1}{2} \exp\left(-cbd \log n\right) + \frac{bd \log n}{n} = \frac{1}{2} \exp\left(-cbd \log n\right) + \frac{bd \log n}{n} = \frac{1}{2} \exp\left(-cbd \log n\right) + \frac{bd \log n}{n} = \frac{1}{2} \exp\left(-cbd \log n\right) + \frac{bd \log n}{n} = \frac{1}{2} \exp\left(-cbd \log n\right) + \frac{bd \log n}{n} = \frac{1}{2} \exp\left(-cbd \log n\right) + \frac{bd \log n}{n} = \frac{1}{2} \exp\left(-cbd \log n\right) + \frac{bd \log n}{n} = \frac{1}{2} \exp\left(-cbd \log n\right) + \frac{bd \log n}{n} = \frac{1}{2} \exp\left(-cbd \log n\right) + \frac{bd \log n}{n} = \frac{1}{2} \exp\left(-cbd \log n\right) + \frac{bd \log n}{n} = \frac{1}{2} \exp\left(-cbd \log n\right) + \frac{bd \log n}{n} = \frac{bd \log n}{n}$$

Proof

- 1. The second moment follows from direct computation. For the third moment, we use $||X|| \leq ||\theta_*|| + ||Z||$ where $Z \sim N(0, I_d)$. By Vershynin (2018, Theorem 3.1.1) $|||Z|| \sqrt{d}||_{\psi_2} \leq 1$ and so also $|||Z|||_{\psi_2} \leq \sqrt{d}$. Hence, $|||X|||_{\psi_2} \leq ||\theta_*|| + \sqrt{d}$. The results then follows the moment property of the sub-gaussian ||X|| (Vershynin, 2018, Proposition 2.5.2).
- 2. Since $\mathbb{E}_n\left[\|X\|^2\right] \leq 2\|\theta_*\|^2 + 2\mathbb{E}_n\left[\|Z\|^2\right]$, where $n\mathbb{E}_n\left[\|Z\|^2\right] \sim \chi^2_{dn}$ using the χ^2 tail bound (54) in Appendix C.1 it holds that

$$\mathbb{P}\left[\mathbb{E}_n\left[\|Z\|^2\right] \ge 5d\right] \le e^{-dn}.$$

Hence,

$$\mathbb{P}\left[\mathbb{E}_n\left[\|X\|^2\right] > 2\|\theta_*\|^2 + 10d\right] \le e^{-dn}$$

For the third moment,

$$\mathbb{E}_{n}\left[\|X\|^{3}\right] \leq 4\|\theta_{*}\|^{3} + 4\mathbb{E}_{n}\left[\|Z\|^{3}\right] \leq 4\|\theta_{*}\|^{3} + 4\left(\max_{i\in[n]}\|Z_{i}\|\right)^{3}.$$

Since $||||Z_i|| - \sqrt{d}||_{\psi_2} \lesssim 1$ we have $\mathbb{P}[||Z_i|| - \sqrt{d} > \sqrt{n}] \leq e^{-c_0 n}$ for some $c_0 > 0$. By the union bound, there exists $n_0(c_0)$ and $c_1 > 0$ such that for all $n > n_0$

$$\mathbb{P}\left[\max_{i\in[n]} \|Z_i\| \ge \sqrt{d} + \sqrt{n}\right] \le ne^{-c_0n} \le e^{-c_1n}$$

Thus, $\mathbb{E}_n\left[\|Z\|^3\right] \leq (\sqrt{d} + \sqrt{n})^3 \leq 4d^{3/2} + 4n^{3/2}$ with probability larger than $1 - e^{-c_1 n}$.

3. We note that $\|\langle u, X \rangle\|_{\psi_2} \leq \sqrt{1 + \|\theta_*\|^2}$ for any $u \in \mathbb{S}^{n-1}$, and so the first claim follows from sub-gaussian concentration (Vershynin, 2018, Proposition 2.6.1). Next, by Vershynin (2018, Lemma 2.7.7)

$$\left\| \langle u, X \rangle \cdot \langle v, X \rangle \right\|_{\psi_1} \le \left\| \langle u, X \rangle \right\|_{\psi_2} \left\| \langle v, X \rangle \right\|_{\psi_2} = 1 + \|\theta_*\|^2$$

and Bernstein's inequality (Vershynin, 2018, Corollary 2.8.3) implies the required inequality for any b > 0 such that $n \ge bd \log n$.

4. For the mean iteration using the fact that product of sub-gaussian is sub-exponential (Vershynin, 2018, Lemma 2.7.7) (twice)

$$\begin{split} \left\| \langle u, X \rangle \cdot \tanh\left(\|\theta\| \langle \hat{\theta}, X \rangle + \beta_{\rho} \right) \right\|_{\psi_{1}} &\leq \|\theta\| \left\| \langle u, X \rangle \cdot \langle \hat{\theta}, X \rangle \right\|_{\psi_{1}} + \beta_{\rho} \| \langle u, X \rangle \|_{\psi_{1}} \\ &\leq \|\theta\| \cdot \| \langle u, X \rangle \|_{\psi_{2}} \left\| \langle \hat{\theta}, X \rangle \right\|_{\psi_{2}} + \beta_{\rho} \| \langle u, X \rangle \|_{\psi_{2}} \\ &\leq (\|\theta\| + \beta_{\rho}) \cdot (1 + \|\theta_{*}\|^{2}) \,. \end{split}$$

Bernstein's inequality (Vershynin, 2018, Corollary 2.8.3) implies the required inequality for any b > 0 such that $n \ge bd \log n$.

Define for some arbitrary nonnegative constants $\{C_j > 0\}_{j \in [3]}$ the events

$$\mathcal{E}_n^{(1)}(C_1) := \left\{ f_n(\theta, \rho) \in \mathbb{B}^d(C_1), \ \forall \theta \in \mathbb{R}^d, \ \forall \rho \in \mathbb{B}(\mathsf{C}_\rho) \right\} \,,$$

$$\begin{aligned} \mathcal{E}_n^{(2)}(C_2, C_1) &:= \\ & \left\{ \|f_n(\theta, \rho) - f(\theta, \rho)\| \le C_2 \left(\|\theta\| + \beta_\rho\right) \cdot \sqrt{\frac{d \log n}{n}}, \quad \forall \theta \in \mathbb{B}^d(C_1), \; \forall \rho \in \mathbb{B}(\mathsf{C}_\rho) \right\}, \\ & \mathcal{E}_n^{(3)}(C_3) := \left\{ |h_n(\rho, \theta) - h(\rho, \theta)| \le C_3 \|\theta\| \cdot \sqrt{\frac{\log n}{n}}, \; \; \forall \theta \in \mathbb{R}^d, \; \forall \rho \in (-1, 1) \right\}. \end{aligned}$$

To prove the theorem we will show that there exist constants $c, C, C_3 > 0$ which depend on (C_{θ}, C_{ρ}) such that for all $n \ge Cd \log n$

$$\mathbb{P}\left[\mathcal{E}_{n}^{(1)}(C_{1}) \cap \mathcal{E}_{n}^{(2)}(C_{2}, C_{1}) \cap \mathcal{E}_{n}^{(3)}(C_{3})\right] \ge 1 - \frac{1}{n^{cd}}$$

with $C_1 := 5(\sqrt{d} + \mathsf{C}_{\theta})$ and $C_2 = C(1 + \mathsf{C}_{\theta}^2)$. The proof is then completed using the relation $\underline{\mathsf{C}}_{\beta}\rho \leq |\beta_{\rho}| \leq \overline{\mathsf{C}}_{\beta}\rho$ (with $\underline{\mathsf{C}}_{\beta}$ and $\overline{\mathsf{C}}_{\beta}$ depending on C_{ρ}).

For $\mathcal{E}_n^{(1)}(C_1)$ we note that

$$\|f_n(\theta,\rho)\| \le \|\mathbb{E}_n[X \tanh(\langle \theta, X \rangle + \beta)]\| \le \mathbb{E}_n[\|X\|] \le \sqrt{\mathbb{E}_n[\|X\|^2]}$$

and then use Lemma 19.

For $\mathcal{E}_n^{(2)}(C_2, C_1)$, let $\epsilon \leq \frac{1}{2}$ be given, and let $\mathcal{C} \subset \mathbb{S}^{d-1}$ be an ϵ -net of \mathbb{S}^{d-1} in Euclidean distance, whose size satisfies $|\mathcal{C}| \leq (\frac{3}{\epsilon})^d$, whose existence is assured by Vershynin (2018, Corollary 4.2.13). By a standard argument (Vershynin, 2018, Exercise 4.4.2)

$$\|f_n(\theta,\rho) - f(\theta,\rho)\| \le 2 \cdot \max_{u \in \mathcal{C}} \langle u, f_n(\theta,\rho) - f(\theta,\rho) \rangle.$$

Furthermore, any $\hat{\theta} \in \mathbb{S}^{d-1}$ may be approximated by $v \in \mathcal{C}$ such that $\|\theta\| \cdot \|v - \hat{\theta}\| \le \epsilon \|\theta\|$. As tanh is 1-Lipschitz

$$\left| \mathbb{E}[\langle u, X \rangle \tanh(\|\theta\| \langle \hat{\theta}, X \rangle + \beta_{\rho})] - \mathbb{E}[\langle u, X \rangle \tanh(\|\theta\| \langle v, X \rangle + \beta_{\rho})] \right| \le \epsilon \|\theta\| \cdot \mathbb{E} \|X\|^2.$$

Repeating the same argument for the empirical iteration we get

$$\|f_n(\theta,\rho) - f(\theta,\rho)\| \le 2 \cdot \max_{(u,v) \in \mathcal{C}^2} \langle u, f_n(\|\theta\| \cdot v,\rho) - f(\|\theta\| \cdot v,\rho) \rangle + \epsilon \|\theta\| \cdot \left(\mathbb{E} \|X\|^2 + \mathbb{E}_n \|X\|^2\right)$$
$$:= \max_{(u,v) \in \mathcal{C}^2} \Phi(u,v,\|\theta\|,\rho).$$

Define the sets $\mathcal{A} = \mathbb{B}(\epsilon) \times \mathbb{B}(\epsilon)$ and $\overline{\mathcal{A}} = \mathbb{B}(C_1) \times \mathbb{B}(C_1) \setminus \mathcal{A}$. By the union bound, the required probability is bounded as:

$$\mathbb{P}\left[\mathcal{E}_{n}^{(2)}(C_{2},C_{1})\right] \leq \sum_{(u,v)\in\mathcal{C}^{2}} \mathbb{P}\left[\exists (\|\theta\|,\rho)\in\mathcal{A}: \Phi(u,v,\|\theta\|,\rho) > C_{2}\left(\|\theta\|+\beta_{\rho}\right)\cdot\sqrt{\frac{d}{n}\log n}\right]$$

$$(43)$$

$$+ \mathbb{P}\left[\exists (\|\theta\|, \rho) \in \overline{\mathcal{A}}: \Phi(u, v, \|\theta\|, \rho) > C_2 \left(\|\theta\| + \beta_{\rho}\right) \cdot \sqrt{\frac{d}{n} \log n}\right].$$
(44)

The probability pertaining to the set \mathcal{A} in (43) is analyzed as follows. Since $\tanh' \leq 1$ and $|\tanh''| \leq 1$ Taylor expansion of \tanh around 0 implies

$$\begin{split} & |\mathbb{E}\left[\langle u, X \rangle \tanh\left(\|\theta\|\langle v, X \rangle + \beta_{\rho}\right)\right] - \mathbb{E}\left[\langle u, X \rangle \left(\|\theta\|\langle v, X \rangle + \beta_{\rho}\right)\right] \\ & \leq \|\theta\|^{2} \cdot \mathbb{E}\left[|\langle u, X \rangle| \langle v, X \rangle^{2}\right] + \beta_{\rho}^{2} \cdot \mathbb{E}\left[|\langle u, X \rangle|\right] \,. \end{split}$$

Repeating the same argument for the empirical iteration, and then using the triangle and Cauchy-Schwartz inequalities, we obtain

$$\begin{split} \Phi(u,v,\|\theta\|,\rho) &\leq \|\theta\||\mathbb{E}\left[\langle u,X\rangle\langle v,X\rangle\right] - \mathbb{E}_n\left[\langle u,X\rangle\langle v,X\rangle\right]| + \beta_\rho\left|\mathbb{E}\left[\langle u,X\rangle\right] - \mathbb{E}_n\left[\langle u,X\rangle\right]| \\ &+ \|\theta\|^2 \mathbb{E}\left[\|X\|^3\right] + \beta_\rho^2 \sqrt{\mathbb{E}\left[\|X\|^2\right]} + \|\theta\|^2 \mathbb{E}_n\left[\|X\|^3\right] + \beta_\rho^2 \sqrt{\mathbb{E}_n\left[\|X\|^2\right]} \\ &+ \epsilon \|\theta\| \cdot \left(\mathbb{E}\|X\|^2 + \mathbb{E}_n\|X\|^2\right) \,. \end{split}$$

By Lemma 19, for any given $(u, v, ||\theta||, \beta_{\rho}) \in C^2 \times A$, as long as $n \geq bd \log n$, there exists absolute constants $\{c_i\}$ such that

$$\mathbb{P}\left[\frac{\Phi(u, v, \|\theta\|, \rho)}{\|\theta\| + \beta_{\rho}} > c_1 \left(1 + \|\theta_*\|^2\right) \sqrt{\frac{bd \log n}{n}} + \epsilon \cdot \left(\|\theta_*\|^3 + n^{3/2}\right)\right] \\ \leq 4 \exp\left(-c_2 bd \log n\right) + \exp(-c_2 n) + \exp(-dn) \leq \exp(-c_3 bd \log n) \,.$$

We will choose $\epsilon \leq \frac{c_4}{n^2}$ with sufficiently small c_4 and b to be sufficiently large so that the probability in (43) is bounded by $\exp(-c_4bd\log n)$ for $C_2 = (1 + C_{\theta}^2)\sqrt{\frac{bd}{n}\log n}$.

The probability of $\overline{\mathcal{A}}$ in (44) is analyzed as follows. Let \mathcal{R}_{β} be an ϵ^2 -net of $[-\mathsf{C}_{\beta},\mathsf{C}_{\beta}]$ of size $2\mathsf{C}_{\beta} \cdot \epsilon^{-2}$, and let \mathcal{R}_{θ} be an ϵ^2 -net of $[0, C_1]$ of size $C_1 \cdot \epsilon^{-2}$. As tanh is 1-Lipschitz, and by the triangle and Cauchy-Schwartz inequalities, for any $(u, v) \in \mathcal{C}^2$ and $(\|\theta\|, \beta_{\rho}) \in \overline{\mathcal{A}}$ there exists $(s, \gamma) \in \mathcal{R}_{\beta} \times \mathcal{R}_{\theta}$ such that

$$\begin{split} &|\mathbb{E}[\langle u, X \rangle \tanh(\|\theta\| \langle v, X \rangle + \beta_{\rho})] - \mathbb{E}[\langle u, X \rangle \tanh(s \langle v, X \rangle + \gamma)]| \\ &\leq \epsilon^{2} \left(\mathbb{E}\left[\|X\|^{2}\right] + \sqrt{\mathbb{E}\|X\|^{2}} \right) \\ &\leq \epsilon(\|\theta\| + \beta_{\rho}) \left(\mathbb{E}\left[\|X\|^{2}\right] + \sqrt{\mathbb{E}\|X\|^{2}} \right) \end{split}$$

where the first term in the r.h.s. (resp. second) corresponds to the approximation of $\|\theta\|$ with s (resp. β with γ), and the second inequality is since $(\|\theta\|, \rho) \in \overline{\mathcal{A}}$. Repeating the same argument for the empirical iteration, we deduce

$$\begin{split} \Phi(u,v,\|\theta\|,\rho) &\leq \max_{(s,\gamma)\in\mathcal{R}_{\theta}\times\mathcal{R}_{\beta}} \left|\mathbb{E}\left[\langle u,X\rangle\cdot\tanh\left(s\langle v,X\rangle+\gamma\right)\right] - \mathbb{E}_{n}\left[\langle u,X\rangle\cdot\tanh\left(s\langle v,X\rangle+\gamma\right)\right]\right| \\ &+ 2\epsilon(\|\theta\|+\beta_{\rho})\left(\mathbb{E}\left[\|X\|^{2}\right] + \mathbb{E}_{n}\left[\|X\|^{2}\right] + \sqrt{\mathbb{E}\|X\|^{2}} + \sqrt{\mathbb{E}_{n}\left[\|X\|^{2}\right]}\right) \\ &:= \Psi(u,v,s,\rho_{\gamma})\,. \end{split}$$

By Lemma 19, for any given $(u, v, s, \gamma) \in C^2 \times \mathcal{R}_\theta \times \mathcal{R}_\beta$, and any b > 0 such that $n \ge bd \log n$ there exists absolute constants $\{c_i\}$

$$\mathbb{P}\left[\Psi(u,v,s,\rho_{\gamma}) > (s+\gamma) \cdot (1+\|\theta_*\|^2) \sqrt{\frac{bd\log n}{n}} + c_1\epsilon(s+\gamma)(d+\|\theta_*\|^2)\right]$$

$$\leq 2\exp\left(-c_2bd\log n\right) + \exp(-dn) \leq \exp(-c_3bd\log n). \quad (45)$$

We will choose $\epsilon \leq c_4 \sqrt{\frac{d \log n}{n}}$ for sufficiently small c_4 so that the probability in (45) is bounded by $\exp(-c_3 b d \log n)$ for

$$C_2 = c_5 \cdot (\|\theta\| + \beta_{\rho}) \cdot (1 + \|\theta_*\|^2) \sqrt{\frac{bd \log n}{n}}.$$

By a union bound over $\mathcal{R}_{\theta} \times \mathcal{R}_{\beta}$ of size $2C_{\beta}C_{1}\epsilon^{-4}$, the probability in (44) is upper bounded by $\exp(-c_{6}bd\log n)$. The proof is then completed by another union bound over \mathcal{C}^{2} whose size is $(\frac{3}{\epsilon})^{2d}$, and taking b to be large enough.

We next turn to the analysis for $\mathcal{E}_n^{(3)}(C_3, C_1)$, which deals with the error of the weight iteration. Since this is, in essence, a one-dimensional iteration, the analysis is somewhat simpler. Since tanh is 1-Lipschitz, for all $\theta \in \mathbb{R}^d$

$$\left|\tanh(\|\theta\|u+\beta_{\rho})-\tanh(\|\theta\|v+\beta_{\rho})\right| \leq \|\theta\|\cdot|u-v|\,.$$

Let $X^{(n)}$ be a random variable distributed according to the empirical distribution of $\{X_i\}_{i=1}^n$. Hence, by coupling,

$$|h_{n}(\rho,\theta) - h(\rho,\theta)| \leq \left| \mathbb{E} \left[\tanh(\|\theta\| \langle \hat{\theta}, X \rangle + \beta_{\rho}) - \tanh(\|\theta\| \langle \hat{\theta}, X^{(n)} \rangle + \beta_{\rho}) \right] \right|$$

$$\leq \mathbb{E} \left[\left| \tanh(\|\theta\| \langle \hat{\theta}, X \rangle + \beta_{\rho}) - \tanh(\|\theta\| \langle \hat{\theta}, X^{(n)} \rangle + \beta_{\rho}) \right| \right]$$

$$\leq \|\theta\| \mathbb{E} \left[\left| \langle \hat{\theta}, X \rangle - \langle \hat{\theta}, X^{(n)} \rangle \right| \right]$$

$$\leq \|\theta\| \cdot W_{1}(\nu, \nu_{n})$$
(46)

where W_1 is the first order Wasserstein distance, $\nu = \mathcal{L}(\langle \hat{\theta}, X \rangle)$ and ν_n is the empirical law of $\{\langle \hat{\theta}, X_i \rangle\}_{i=1}^n$. Now, $\langle \hat{\theta}, X \rangle \sim (1 - \delta_*)N(\langle \hat{\theta}, \theta_* \rangle, 1) + \delta_*N(-\langle \hat{\theta}, \theta_* \rangle, 1)$ and so $\|\langle \hat{\theta}, X \rangle\|_{\psi_2} \leq \sqrt{1 + \|\theta_*\|^2}$ for any $\hat{\theta} \in \mathbb{S}^{n-1}$. The concentration inequality of Fournier and Guillin (2015, Theorem 2, Case 1) with the choices d = 1 (the dimension of $\langle \hat{\theta}, X \rangle$), p = 1 (Wasserstein distance order) and $\alpha = 2$ (for the ψ_α condition $\mathbb{E}[e^{\gamma|X|^\alpha}] < \infty$) implies that for $x_0 > 0$ there exists c, C > 0 such that

$$\mathbb{P}\left[W_1(\nu,\nu_n) > \sqrt{\frac{\log n}{n}}\right] \le C \cdot \exp\left(-c\log n\right) \,. \tag{47}$$

The bounds (46) and (47) imply that $\mathcal{E}_n^{(3)}(C_3)$ has high probability as stated in the theorem.

Appendix B. Minimax Rates

Theorem 20 (Minimax rates for mean estimation) For any $d \ge 2$, $n \in \mathbb{N}$ and $\eta \ge 0$, let $\tilde{\theta}$ be any estimator of θ_* based on $\underline{X} = (X_1, \ldots, X_n) \stackrel{\text{i.i.d.}}{\sim} P_{\theta_*, \rho_*}$. Then, for $d \le n$

$$\sup_{\tilde{\theta}(\rho_{*})} \inf_{\|\theta_{*}\|=\eta} \mathbb{E}_{\theta_{*},\rho_{*}} \left[\ell(\tilde{\theta},\theta_{*}) \right] \asymp \begin{cases} \eta, & \eta \leq \frac{1}{\rho_{*}} \sqrt{\frac{d}{n}} \\ \frac{1}{\rho_{*}} \sqrt{\frac{d}{n}}, & \frac{1}{\rho_{*}} \sqrt{\frac{d}{n}} < \eta < \rho_{*} \\ \frac{1}{\eta} \sqrt{\frac{d}{n}}, & \rho_{*} < \eta < 1 \\ \sqrt{\frac{d}{n}}, & \eta > 1 \end{cases}$$
(48)

if $\rho_* \geq (\frac{d}{n})^{1/4}$ and

$$\sup_{\tilde{\theta}(\rho_*)} \inf_{\|\theta_*\|=\eta} \mathbb{E}_{\theta_*,\rho_*} \left[\ell(\tilde{\theta},\theta_*) \right] \asymp \begin{cases} \eta, & \eta \leq \left(\frac{d}{n}\right)^{1/4} \\ \frac{1}{\eta}\sqrt{\frac{d}{n}}, & \left(\frac{d}{n}\right)^{1/4} < \eta < 1 \\ \sqrt{\frac{d}{n}}, & \eta > 1 \end{cases}$$

if $\rho_* \le (\frac{d}{n})^{1/4}$.

Proof

<u>Upper bounds</u>: The error rates in all cases except for the second case in (48) were shown to be achieved by a spectral method (Wu and Zhou, 2019, Appendix B). Specifically, in case $\rho_* \leq (\frac{d}{n})^{1/4}$ then the knowledge of the weight can be completely ignored by the estimator. Furthermore, the same method achieves $\frac{1}{\eta}\sqrt{\frac{d}{n}}$ in the third case of (48). We next show that an error rate of $\frac{1}{\rho_*}\sqrt{\frac{d}{n}}$ is also achievable by the estimator $\tilde{\theta}(\rho_*) = \frac{1}{\rho_*}\mathbb{E}_n[X]$. Indeed, let $X = S\theta_* + Z$ as in (2). Then,

$$\mathbb{E}_{\theta_*,\rho_*}\left[\ell(\tilde{\theta}(\rho_*),\theta_*)\right] \leq \mathbb{E}\|\tilde{\theta}(\rho_*) - \theta_*\|$$

$$\leq \frac{\|\theta_*\|}{\rho_*} \mathbb{E}\left[|\mathbb{E}_n[S] - \rho_*|\right] + \frac{1}{\rho_*} \mathbb{E}\left[\|\mathbb{E}_n[Z]\|\right]$$

$$\lesssim \frac{\|\theta_*\|}{\rho_*\sqrt{n}} + \frac{1}{\rho_*}\sqrt{\frac{d}{n}}$$

$$\leq \frac{1}{\rho_*}\sqrt{\frac{d}{n}}$$

where the penultimate asymptotic inequality follows from: (a) For the first term, as $\|\mathbb{E}_n[\mathbb{1}\{S = -1\}] - \delta_*\|_{\psi_2} \leq \frac{c_1}{\sqrt{n}}$ for some universal constant $c_1 > 0$ (Vershynin, 2018, Example 2.5.8. and Proposition 2.6.1), and so

$$\mathbb{E}[\|\mathbb{E}_{n}[S] - \rho_{*}\|] = 2\mathbb{E}[|\mathbb{E}_{n}[\mathbb{1}\{S = -1\}] - \delta_{*})|] \le \frac{c_{2}}{\sqrt{n}}$$

for some universal constant $c_2 > 0$ (Vershynin, 2018, Proposition 2.5.2). (b) For the second term, similarly, $\|\|\mathbb{E}_n[Z]\|\|_{\psi_2} \leq c_3 \sqrt{\frac{d}{n}}$ for some universal constant $c_3 > 0$ as in Lemma 19, and using the result of Vershynin (2018, Proposition 2.6.1).

<u>Lower bounds</u>: The proof follows that of Wu and Zhou (2019, Appendix B), which uses Fano's method (Yang and Barron, 1999) for all cases which are not lower bounded by the ℓ_2 error-rate of the standard Gaussian location model min $\{\eta, \sqrt{\frac{d}{n}}\}$. Thus, we mainly highlight the main difference and omit all other details. First note that if $|\rho_*| \ge \frac{1}{2}$ (say), then the lower bound (48) us again equivalent to the ℓ_2 error-rate of the standard Gaussian location model, and thus no proof is required. Thus, we may henceforth only consider the case $|\rho_*| \le \frac{1}{2}$. The lower bound of Wu and Zhou (2019) is based on Lemma 27 therein which is here generalized from $\rho = 0$ to any $\rho \in (-1, 1)$ as follows:

Lemma 21 Let $0 \le \eta \le 1$ and $|\rho| \le \frac{1}{2}$. Then there exists a universal constant C such that for any $d \ge 1$ and $u, v \in \mathbb{S}^{d-1}$

$$d_{\mathrm{KL}}(P_{\eta \cdot u,\rho}||P_{\eta \cdot v,\rho}) \le C \cdot \ell^2(u,v) \cdot \eta^2(\eta^2 + \rho^2).$$

Proof By symmetry, it suffice to prove

$$d_{\mathrm{KL}}(P_{\eta \cdot u,\rho} || P_{\eta \cdot v,\rho}) \le C \cdot ||\hat{\theta}_1 - \hat{\theta}_2 ||^2 \cdot \eta^2 (\eta^2 + \rho^2),$$

and by rotational invariance of the normal distribution it can be assumed that $v = e_1 = (1, 0, ..., 0)$. Let $\lambda = \max\{1 - u_1, ||u_\perp||\} < 1$ where $u_\perp = (u_2, ..., u_d)$ (and similar notation

will be used for any *d*-dimensional vector). Further, let Q be the distribution of $X = (X_1, \ldots, X_d) \in \mathbb{R}^d$ under $\theta_* = \eta v = \eta e_1$, to wit $Q = Q_{X_1,\ldots,X_d} = P_{\eta,\rho_*} \otimes N(0, I_{d-1})$ (which is a product distribution), and let P be the corresponding distribution under $\theta_* = \eta u$. From the chain rule of the KL divergence

$$d_{\mathrm{KL}}(P_{\eta \cdot u,\rho} || P_{\eta \cdot v,\rho}) = d_{\mathrm{KL}}(P_{X_1} || Q_{X_1}) + \mathbb{E}_{P_{X_1}} \left[d_{\mathrm{KL}}(P_{X_\perp | X_1} || N(0, I_{d-1})) \right] := (\mathrm{I}) + (\mathrm{II}).$$

We bound the two KL divergence terms using the corresponding chi-square divergence.

Bounding (I): In one dimension,

$$p_{\eta,\rho}(x) = e^{-\eta^2/2}\varphi(x) \left[\left(\frac{1+\rho}{2}\right) e^{\theta x} + \left(\frac{1-\rho}{2}\right) e^{-\theta x} \right]$$
$$= e^{-\eta^2/2}\varphi(x) \left[\cosh(\eta x) + \rho \sinh(\eta x) \right].$$

Hence, denoting for brevity

$$\alpha_{\epsilon,\eta,\rho}(x) := e^{-(\eta-\epsilon)^2/2} \left(\cosh\left((\eta-\epsilon)x\right) + \rho \sinh\left((\eta-\epsilon)x\right)\right) - e^{-\eta^2/2} \left(\cosh\left(\eta x\right) + \rho \sinh\left(\eta x\right)\right)$$

we get for $\epsilon = \eta \lambda$

$$\begin{aligned} \text{(I)} &= \mathrm{d}_{\mathrm{KL}}(P_{X_1}||Q_{X_1}) & (49) \\ &\leq \mathrm{d}_{\chi^2}(P_{\eta-\epsilon,\rho}||Q_{\eta,\rho}) \\ &= e^{\eta^2/2} \cdot \int \varphi(x) \cdot \frac{\alpha_{\epsilon,\eta,\rho}^2(x)}{\cosh(\eta x) + \rho \sinh(\eta x)} \mathrm{d}x \\ &\stackrel{(a)}{\leq} \sqrt{\frac{4e}{3}} \cdot \int \varphi(x) \cdot \alpha_{\epsilon,\eta,\rho}^2(x) \mathrm{d}x \\ &\stackrel{(b)}{=} \sqrt{\frac{4e}{3}} \cdot e^{-(\eta-\epsilon)^2} \int \varphi(x) \left[\cosh^2\left((\eta-\epsilon)x\right) + \rho^2 \sinh^2\left((\eta-\epsilon)x\right)\right] \mathrm{d}x \\ &- \sqrt{\frac{4e}{3}} \cdot 2e^{-(\eta-\epsilon)^2/2 - \eta^2/2} \int \varphi(x) \left[\cosh\left((\eta-\epsilon)x\right)\cosh\left(\eta x\right) + \rho^2 \sinh\left((\eta-\epsilon)x\right)\sinh\left(\eta x\right)\right] \mathrm{d}x \\ &+ \sqrt{\frac{4e}{3}} \cdot e^{-\eta^2/2} \int \varphi(x) \left[\cosh^2\left(\eta x\right) + \rho^2 \sinh^2\left(\eta x\right)\right]^2 \mathrm{d}x \\ &\quad \left(\stackrel{(e)}{=} \sqrt{\frac{4e}{3}} \cdot \left[\cosh\left((\eta-\epsilon)^2\right) + \cosh\left(\eta^2\right) - 2\cosh\left(\eta(\eta-\epsilon)\right)\right] \\ &+ \sqrt{\frac{4e}{3}} \left[\sinh\left((\eta-\epsilon)^2\right) + \sinh\left(\eta^2\right) - 2\sinh\left(\eta(\eta-\epsilon)\right)\right] \rho^2 \\ &\leq C_1 \epsilon^2 (\eta^2 + \rho^2) = C_1 \lambda^2 \eta^2 (\eta^2 + \rho^2) \,, \end{aligned}$$

where (a) is since by the inequality of arithmetic and geometric means $\cosh(t) + \rho \sinh(t) = \left(\frac{1+\rho}{2}\right)e^{\theta x} + \left(\frac{1-\rho}{2}\right)e^{-\theta x} \ge \sqrt{1-\rho^2}$ and using $0 < \eta < 1$ and $|\rho| < \frac{1}{2}$; (b) is obtained by expanding the square, and noting sinh is odd and that as $\varphi(x) \propto e^{-x^2/2}$ is an even function, $\int \varphi(x)f(x)dx = 0$ for any odd function f; (c) is obtained by the identities

$$\int \varphi(x) \cosh(\eta x)^2 dx = e^{\eta^2} \cosh(\eta^2), \ \int \varphi(x) \cosh(\eta x)^2 dx = e^{\eta^2} \sinh(\eta^2),$$

$$\int \varphi(x) \cosh(\eta_1 x) \cosh(\eta_2 x) dx = \frac{1}{2} e^{\frac{(\eta_1 + \eta_2)^2}{2}} + \frac{1}{2} e^{\frac{(\eta_1 - \eta_2)^2}{2}},$$
$$\int \varphi(x) \sinh(\eta_1 x) \sinh(\eta_2 x) dx = \frac{1}{2} e^{\frac{(\eta_1 + \eta_2)^2}{2}} - \frac{1}{2} e^{\frac{(\eta_1 - \eta_2)^2}{2}};$$

(d) is by Taylor expansion of cosh and sinh around η^2 , since $|\epsilon| \le \sqrt{2\eta} \le \sqrt{2}$ and where $C_1 > 0$ is a universal constant.

<u>Bounding (II)</u>: The proof follows that of Wu and Zhou (2019) up until almost the very last step. Recall that under P one can write $X = R_i + Z_i$ for $i \in [d]$ where $R_i = S \cdot \eta u_i$ where $S \in \{\pm 1\}$ and $\mathbb{P}[S = -1] = \delta_*$. Then,

$$\begin{aligned} \text{(II)} &= \mathbb{E}_{P_{X_{1}}} \left[\mathrm{d}_{\mathrm{KL}}(P_{X_{\perp}|X_{1}}||N(0, I_{d-1})) \right] \\ &\stackrel{(a)}{\leq} \mathbb{E} \left[\mathrm{d}_{\chi^{2}}(P_{X_{\perp}|X_{1}}||N(0, I_{d-1})) \right] \\ &\stackrel{(b)}{\leq} \eta^{2} \cdot \sum_{i=2}^{d} u_{i}^{2} \mathbb{E}_{P_{X_{1}}} \left[\mathbb{E}^{2}[R \mid X_{1}] \right] + C_{2}(\eta\lambda)^{4} \\ &\stackrel{(c)}{=} \eta^{2} \cdot \sum_{i=2}^{d} u_{i}^{2} \mathbb{E}_{P_{X_{1}}} \left[\tanh^{2}(u_{1}X_{1} + \beta_{\rho}) \right] + C_{2}(\eta\lambda)^{4} \\ &\stackrel{(d)}{\leq} \eta^{2} \cdot \sum_{i=2}^{d} u_{i}^{2} \mathbb{E}_{P_{X_{1}}} \left[2(u_{1}^{2}\eta^{2}X_{1}^{2} + \beta_{\rho}^{2}) \right] + C_{2}(\eta\lambda)^{4} \\ &\stackrel{(e)}{\leq} 4\eta^{4}\lambda^{2} + 2C_{3}\eta^{2}\rho^{2}\lambda^{2} + C_{2}(\eta\lambda)^{4} \\ &\stackrel{(f)}{\leq} C_{4}\eta^{2}(\eta^{2} + \rho^{2})\lambda^{2}, \end{aligned}$$

$$\tag{51}$$

where (a) is by bounding the KL divergence using the chi-square divergence; (b) stems from the Ingster-Suslina identity (Ingster and Suslina, 2012) along with Taylor expansion (see details in Wu and Zhou, 2019, Appendix B); (c) follows from $\mathbb{E}_{\eta,\rho}[S \mid X_1] = \tanh(\eta X_1 + \beta_{\rho})$ (see Equation 5); (d) follows from $\tanh^2(x) \leq x^2$; (e) follows from $|u_1| \leq 1$, $||u_{\perp}|| \leq \lambda$, $\mathbb{E}_{P_{X_1}}[X_1^2] = 1 + \eta^2 \leq 2$, and $\beta_{\rho} \leq C_3 \rho$ for all $|\rho| \leq \frac{1}{2}$ and $C_3 > 0$ is a universal constant; (f) holds for a universal constant $C_4 > 0$ since $\lambda < 1$.

Combining (50) and (51) we complete the proof of the lemma.

For completeness, we outline the proof of the lower bound using Fano's method. The method states that if there exists a set of M parameters $\Theta_M = \{\theta_1, \ldots, \theta_M\}$ such that $I(\theta; \underline{X}) \leq \log M$ and $\|\theta_m - \theta_{m'}\| \geq \epsilon \eta$ for all $m, m' \in [M], m' \neq m$ then the lower bound is of the order $\epsilon \eta$. This is shown by bounding the mutual information with the KL radius of Θ_M as $I(\theta; \underline{X}) \leq n \max_{m \in [m]} d_{\mathrm{KL}}(P_{\theta_m, \rho} || P_{\theta_0, \rho})$ for some θ_0 . Wu and Zhou (2019, Appendix B) constructed a set $\{\theta_0\} \cup \Theta_M$ with $M \geq e^{C_0 d}$ for some C_0 , and a small constant $c_0 > 0$ such that: (a) $\|\theta_m\| = \eta$ for all $m \in 0 \cup [m]$; (b) $\|\theta_m - \theta_{m'}\| \geq c_0 \epsilon \eta$ for all $m, m' \in [M], m' \neq m$; (c) $\|\theta_m - \theta_0\| \leq 2c_0 \epsilon \eta$ for all $m \in [m]$. By Lemma 21

$$\frac{I(\theta;\underline{X})}{\log M} \asymp \frac{I(\theta;\underline{X})}{d} \lesssim \frac{n}{d} \max_{m \in [m]} \mathrm{d}_{\mathrm{KL}}(P_{\theta_m,\rho} || P_{\theta_0,\rho}) \lesssim \frac{n}{d} \epsilon \cdot \eta^2 (\max\{\eta,\rho\})^2$$

and so choosing

$$\epsilon = \min\{1, \frac{1}{\eta \max\{\eta, \rho\}} \sqrt{\frac{d}{n}}\}$$

yields a minimax lower bound of rate $\min\{\eta, \frac{1}{\eta}\sqrt{\frac{d}{n}}, \frac{1}{\rho}\sqrt{\frac{d}{n}}\}.$

Theorem 22 (Minimax rates for weight estimation) For any $d, n \in \mathbb{N}$ let $\tilde{\rho}$ be any estimator of ρ_* based on $\underline{X} = (X_1, \ldots, X_n) \stackrel{\text{i.i.d.}}{\sim} P_{\theta_*, \rho_*}$. Then,

$$\sup_{\tilde{\rho}(\theta_*)} \inf_{\rho_* \in \mathbb{B}(\bar{\rho})} \mathbb{E}_{\theta_*,\rho_*} \left[\ell(\tilde{\rho},\rho_*) \right] \asymp \begin{cases} \overline{\rho}, & \|\theta_*\| \leq \frac{\bar{\rho}}{\sqrt{n}} \\ \frac{1}{\|\theta_*\|\sqrt{n}}, & \frac{\bar{\rho}}{\sqrt{n}} < \|\theta_*\| < 1 \\ \frac{1}{\sqrt{n}}, & \|\theta_*\| > 1 \end{cases}$$

Proof Given the measurements $\{X_i\}_{i=1}^n$ the projections $\{\langle \hat{\theta}_*, X_i \rangle\}_{i=1}^n$ are sufficient statistics for the estimation of ρ_* . Hence we may assume that d = 1, and we may write $X_i = S_i \theta_* + Z_i \in \mathbb{R}^d$ for $i \in [n]$ where $S_i \in \{\pm 1\}$ and $\mathbb{P}[S_i = -1] = \delta_*$

<u>Upper bound</u>: The first case can be achieved by the trivial estimator $\tilde{\rho} = 0$. For the other two cases, as in the proof of Theorem 20, the estimator $\tilde{\rho}(\theta_*) = \frac{1}{\|\theta_*\|} \langle \hat{\theta}_*, \mathbb{E}_n[X] \rangle$ can be shown to achieve an error rate of $\max\{\frac{1}{\sqrt{n}}, \frac{1}{\|\theta_*\|\sqrt{n}}\}$ where the first term stems from the empirical error of $\mathbb{E}_n[S]$, and the second term is due to the additive error Z.

<u>Lower bound</u>: If $\|\theta_*\| > 1$ we may bound the error rate of the given estimator by the error rate of an estimator which known the noise sequence $\{Z_i\}_{i=1}^n$, which, equivalently, has direct access to $\{S_i\}_{i=1}^n$. This is a simple Bernoulli model and the error rate is $\frac{1}{\sqrt{n}}$. We thus next assume that $\|\theta_*\| = \eta < 1$. As the calculation in the bound of term (I) in Lemma 21,

$$\begin{aligned} \mathrm{d}_{\mathrm{KL}}(P_{\eta,\rho}||P_{\eta,0}) &\leq \mathrm{d}_{\chi^2}(P_{\eta,\rho}||P_{\eta,0}) \\ &= e^{-\eta^2/2} \int \varphi(x) \frac{\rho^2 \cdot \sinh^2(\eta x)}{\cosh(\eta x)} \mathrm{d}x \\ &\leq e^{-\eta^2/2} \int \varphi(x) \rho^2 \cdot \sinh^2(\eta x) \mathrm{d}x \\ &= e^{\eta^2/2} \sinh(\eta^2) \rho^2 \\ &\leq C \eta^2 \rho^2 \,, \end{aligned}$$

for some C > 0 using $\sinh(t) \le C|t|$ for $t \le 1$. Le-Cam's two point argument with $\rho = c_0 \min\{\overline{\rho}, \frac{1}{\eta\sqrt{n}}\}$ and $c_0 > 0$ small enough then results a minimax error rate of $\frac{1}{\eta\sqrt{n}}$.

Appendix C. Miscellaneous

In this Appendix we summarize various results which are used in the proofs.
C.1 Useful Results

We collect here several useful results which are repeatedly used throughout the paper:

- Relations for inverse temperature parameter: For $\beta := \frac{1}{2} \log \frac{1-\delta}{\delta}$ it holds that $\tanh(\beta) = 1 2\delta$, $\cosh(\beta) = \frac{1}{\sqrt{4\delta(1-\delta)}}$, and $\frac{d\beta_{\delta}}{d\delta} = -\frac{1}{2\delta(1-\delta)}$ and $\frac{d\beta_{\rho}}{d\rho} = \frac{1}{1-\rho^2}$.
- Change of measure: Let $V \sim (1-\delta) \cdot N(\theta, 1) + (1-\delta) \cdot N(-\theta, 1)$ and let $Z \sim N(0, 1)$. Then, for any integrable function f

$$\mathbb{E}\left[f(V)\right] = e^{-\theta^2/2} \cdot \mathbb{E}\left[f(Z) \cdot \cosh(\theta Z + \beta_{\delta})\right]$$
$$= e^{-\theta^2/2} \cdot \mathbb{E}\left[f(Z) \cdot \left((1-\delta)e^{\theta Z} + \delta e^{-\theta Z}\right)\right].$$
(52)

• For $U \sim N(\eta, 1)$ (Daskalakis et al., 2017, Lemma 2)

$$\mathbb{E}\left[\tanh(U\theta)\right] \ge 1 - e^{-\eta\theta/2},\tag{53}$$

- $(a+b)^k \le 2^{k-1}(a^k+b^k)$ for $k \ge 1$.
- Chi-square tail bound: (Boucheron et al., 2013, Remark 2.11)

$$\mathbb{P}\left[\chi_k^2 \ge 2k + 3t\right] \le \mathbb{P}\left[\chi_k^2 - k \ge 2\sqrt{kt}k + 2t\right] \le e^{-t}.$$
(54)

• Stein's identity: (Vershynin, 2018, Lemma 7.2.3) Let $Z \sim N(0, \sigma^2)$. Let f be a differentiable function such that $\mathbb{E}|f'(Z)| < \infty$. Then,

$$\mathbb{E}\left[f(Z) \cdot Z\right] = \sigma^2 \mathbb{E}\left[f'(Z)\right].$$
(55)

• Let $V \sim (1 - \delta)N(\theta, 1) + \delta N(-\theta, 1)$ with $\theta > 0$ and $\delta < \frac{1}{2}$. Then $\mathbb{P}[V = v \mid |V| = v] > \mathbb{P}[V = -v \mid |V| = v]$ for any v > 0. This follows from Chebyshev's sum inequality

$$\frac{\mathbb{P}[V=v\mid |V|=v]}{\mathbb{P}[V=-v\mid |V|=v]} = \frac{(1-\delta)\varphi(\eta-v) + \delta\varphi(\eta+v)}{(1-\delta)\varphi(\eta+v) + \delta\varphi(\eta-v)} > 1$$
(56)

since $1 - \delta > \delta$ and $\varphi(\eta + v) < \varphi(\eta - v)$.

• Gaussian average of odd function. Let f(u) be an odd function which is positive on \mathbb{R}_+ and negative on \mathbb{R}_- . Let U be a continuous random variable such that $\mathbb{P}[U = u \mid |U| = u] \ge \mathbb{P}[U = -u \mid |U| = u]$. Then, $\mathbb{E}[f(U)] \ge 0$. This is satisfied for $U \sim N(\eta, \sigma^2)$ with $\eta > 0$.

C.2 Convergence Properties of One-Dimensional Iterations

Proposition 23 (Convergence properties of one-dimensional iterations) Let $\theta \mapsto h(\theta)$ be an analytic monotonically increasing function, and $h(\theta) - \theta$ is not identically 0. Let θ_0 be given, and suppose that either $\sup_{\theta > \theta_0} h(\theta) < \infty$ or $\lim_{\theta \to \infty} h'(\theta) < 1$. Let $h_+(\theta)$ be another function which satisfies the same properties as $h(\cdot)$.

- 1. If $h(\theta_0) > \theta_0$ for some θ_0 then $h(\theta)$ has at least a single fixed point in (θ_0, ∞) .
- 2. Let $\{\tilde{\theta}_k\}$ be an enumeration of the fixed points of $h(\theta)$. For all $k \ge 1$, if $h'(\tilde{\theta}_k) < 1$ then $h'(\tilde{\theta}_{k+1}) \ge 1$ and if $h'(\tilde{\theta}_k) > 1$ then $h'(\tilde{\theta}_{k+1}) \le 1$.
- 3. Assume that $h(\theta)$ is strictly concave on $[\theta_0, \infty)$. If $h(\theta_0) > \theta_0$ then $h(\theta)$ has a single fixed point in (θ_0, ∞) . If $h(\theta_0) \le \theta_0$ then $h(\theta)$ has at most two fixed points in (θ_0, ∞) .
- 4. Consider the iteration $\theta_{t+1} = h(\theta_t)$. If $\theta_1 = h(\theta_0) > \theta_0$ (resp. $\theta_1 < \theta_0$) then $\{\theta_{t+1}\}$ is monotonically increasing (resp. decreasing) and converges to a fixed point θ_{∞} . It holds that $h'(\theta_{\infty}) \leq 1$ (resp. $h'(\theta_{\infty}) \geq 1$).
- 5. Consider, in addition, the iteration $\theta_{t+1}^+ = h_+(\theta_t^+)$ such that $\theta_0 = \theta_0^+$, and suppose that $h_+(\theta) > h(\theta)$ on $[\theta_0, \infty)$. $\theta_t^+ \ge \theta_t$ for all $t \ge 1$, and this holds specifically in the limit $t \to \infty$. Hence, if, in addition, $\lim_{t\to\infty} \theta_t = \lim_{t\to\infty} \theta_t^+ = \theta_\infty$ then $\theta_\infty \theta_t^+ \le \theta_\infty \theta_t$, *i.e.*, the convergence of $\{\theta_t^+\}$ to the fixed point is faster than that of $\{\theta_t\}$.
- 6. Convergence rate of a contraction: If $\max_{\theta \in [\theta_0, \theta_\infty]} h'(\theta) = \zeta < 1$ then $\theta_\infty \theta_t \leq (\theta_\infty \theta_0) \cdot \zeta^t$, and $\theta_\infty \theta_t \leq c$ for all $t \geq \frac{1}{1-\zeta} \cdot \log \frac{c}{\theta_\infty \theta_0}$ (assuming $c \geq \theta_\infty \theta_0$, otherwise $t \geq 1$ suffice).
- 7. Suppose that $0 \le h(\theta) \le (1-a)\theta + b$ for $a \in (0,1)$. Then $h(\theta_t) \le \frac{2b}{a}$ for all $t \ge \frac{1}{a}\log \frac{a}{b}$

Proof

- 1. Under both conditions, there exists θ_1 such that $h(\theta_1) < \theta_1$. The claim follows from the intermediate value theorem for the function $h(\theta) \theta$.
- 2. First, we note that such an enumeration is possible since $h(\theta) \theta$ is analytic and not a constant, and so its zeros in \mathbb{R}_+ are isolated. Assume w.l.o.g. that $h'(\tilde{\theta}_1) > 1$. Thus, $h(\theta) > \theta$ for all $\theta \in (\tilde{\theta}_1, \tilde{\theta}_2)$ and so $h'(\tilde{\theta}_2) = \lim_{t \to 0} \frac{h(\tilde{\theta}_2) h(\tilde{\theta}_2 t)}{t} = \frac{\tilde{\theta}_2 h(\tilde{\theta}_2 t)}{t} \leq 1$. The analogous property is proved similarly.
- 3. Let θ_1 be the minimal fixed point which is larger than θ_0 . If $h(\theta_0) > \theta_0$ then we must have $h'(\theta_1) < 1$ and by concavity $h'(\theta) < 1$ for all $\theta \ge \theta_1$. Thus there are no fixed points in (θ_1, ∞) . If $h(\theta_0) \le \theta_0$ then assume by contradiction that there are more than or three fixed points $\{\tilde{\theta}_k\}$. By strict concavity, it is not possible that $h'(\tilde{\theta}_k) = 1$ for any of the fixed point since this fixed point would be unique. By the previous item, the signs $h'(\tilde{\theta}_k) - 1$ are alternating. Thus, there exists k such that $h'(\tilde{\theta}_k) > 1$ and $h'(\tilde{\theta}_{k+1}) < 1$. Strict concavity implies that no fixed points are possible in $(-\infty, \tilde{\theta}_k)$, $(\tilde{\theta}_k, \tilde{\theta}_{k+1})$ and $(\tilde{\theta}_k, \infty)$. So $h(\theta)$ cannot be more than two fixed points in (θ_0, ∞) .
- 4. Assume $\theta_1 > \theta_0$. Since *h* is increasing, then $\theta_2 = h(\theta_1) > h(\theta_0) = \theta_1$. By induction, $\{\theta_t\}$ is an increasing an bounded sequence, and thus has a limit $\tilde{\theta}$. Since *h* is continuous $\tilde{\theta} = \lim_{t \to \infty} \theta_{t+1} = \lim_{t \to \infty} h(\theta_t) = h(\lim_{t \to \infty} \theta_t) = h(\tilde{\theta})$, and so $\tilde{\theta}$ is a fixed point. The proof for $\theta_1 < \theta_0$ is similar.
- 5. By induction $\theta_{t+1}^+ = h^+(\theta_t^+) \ge h^+(\theta_t) \ge h(\theta_t) = \theta_{t+1}$.

- 6. By induction and $|\theta_{t+1} \theta_{\infty}| = |h(\theta_t) h(\theta_{\infty})| \le \zeta |\theta_t \theta_{\infty}|$. To achieve $\theta_{\infty} \theta_t \le c$ we may require $t \ge \frac{\log \frac{\theta_{\infty} - \theta_0}{c}}{\log(1/\zeta)}$, and the claim holds since $\frac{1}{\log(1/\zeta)} \le \frac{1}{1-\zeta}$.
- 7. By induction $\theta_{t+1} \leq (1-a)^t + \sum_{j=1}^t b(1-a)^j \leq (1-a)^t + \frac{b}{a}$. Using $-a \geq \log(1-a)$ we have $(1-a)^t \leq \frac{b}{a}$ if $t \geq \frac{1}{a} \log \frac{a}{b}$.

C.3 Totally Positive Kernels and Variation Diminishing Property

Let $A, B \subseteq \mathbb{R}$. A kernel $K : A \times B \mapsto \mathbb{R}$ is said to be *totally positive of order* k, TP_k if for all $m \in [k]$ and all $x_1 < \cdots < x_m$ and $y_1 < \cdots < y_m$ (with $x_i \in A$ and $y_i \in B$ for $i \in [k]$) it holds that

$$K\left(\begin{array}{c} x_1,\cdots,x_m\\ y_1,\cdots,y_m\end{array}\right) = \det \left[\begin{array}{ccc} K(x_1,y_1) & \cdots & K(x_1,y_m)\\ \vdots & & \vdots\\ K(x_m,y_1) & \cdots & K(x_m,y_m)\end{array}\right] \ge 0\,.$$

If K is TP_k for all $k \in \mathbb{N}$ then the kernel is said to be totally positive (resp. strictly totally positive), which is written $\operatorname{TP}_{\infty}$.

An important consequence of totally positive property is its variation diminishing property. The number of zero-crossings of a function $f: B \mapsto \mathbb{R}$ is the supremum of the numbers of sign changes in sequences of the form $f(x_1), \ldots f(x_m)$, for $m \in \mathbb{N}$, $x_i \in B$ for all $i \in [m]$ and $x_1 < \cdots < x_m$, where zero values in the sequence are discarded. The following is a result by Karlin (Marshall et al., 1979, Theorem A.5 p. 759):

Theorem 24 (Variation diminishing property of totally positive kernels) Let $A, B \subseteq \mathbb{R}$, and let $K: A \times B \mapsto \mathbb{R}$ be Borel-measurable and TP_k . Let σ be a regular σ -finite measure on B, and let $f: B \mapsto \mathbb{R}$ be a bounded measurable function such that

$$g(x) = \int_B K(x, y) f(y) \mathrm{d}\sigma(y)$$

converges absolutely. If f changes sign at most $j \leq k-1$ times on B, then g changes signs at most j times on A.

Proposition 25 Let $f: \mathbb{R} \to \mathbb{R}$ be a bounded and measurable function. If f has at most j sign-changes on \mathbb{R} , then $g: \mathbb{R} \to \mathbb{R}$ defined by $g(\eta) = \mathbb{E}_{U \sim N(\eta, 1)}[f(U)]$ has at most j signs-changes on \mathbb{R} .

Proof The Gaussian kernel $K(x, y) = e^{-(x-y)^2}$ for $A = B = \mathbb{R}$ is TP_{∞} (Marshall et al., 1979, Theorem A.6.B p. 759). We use Theorem 24 and

$$g(\eta) = \mathbb{E}\left[f(U)\right] = \int \varphi(u-\eta)f(u)du$$
$$= \frac{1}{\sqrt{2\pi}} \int e^{-(u-\eta)^2/2}f(u)du = \frac{1}{\sqrt{\pi}} \int e^{-(\tilde{u}-\tilde{\eta})^2}f(\tilde{u})d\tilde{u} = g(\sqrt{2}\tilde{\eta}) \quad (57)$$

with $\tilde{u} = \frac{u}{\sqrt{2}}$ and $\tilde{\eta} = \frac{\eta}{\sqrt{2}}$ as well as the observation that $f(\frac{u}{\sqrt{2}})$ (resp. $g(\sqrt{2}\eta)$) has the same zero-crossings as f(u) (resp. $g(\eta)$).

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