

A Distributed Method for Fitting Laplacian Regularized Stratified Models

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Editor: Massimiliano Pontil

Abstract

Stratified models are models that depend in an arbitrary way on a set of selected categorical features, and depend linearly on the other features. In a basic and traditional formulation a separate model is fit for each value of the categorical feature, using only the data that has the specific categorical value. To this formulation we add Laplacian regularization, which encourages the model parameters for neighboring categorical values to be similar. Laplacian regularization allows us to specify one or more weighted graphs on the stratification feature values. For example, stratifying over the days of the week, we can specify that the Sunday model parameter should be close to the Saturday and Monday model parameters. The regularization improves the performance of the model over the traditional stratified model, since the model for each value of the categorical ‘borrows strength’ from its neighbors. In particular, it produces a model even for categorical values that did not appear in the training data set.

We propose an efficient distributed method for fitting stratified models, based on the alternating direction method of multipliers (ADMM). When the fitting loss functions are convex, the stratified model fitting problem is convex, and our method computes the global minimizer of the loss plus regularization; in other cases it computes a local minimizer. The method is very efficient, and naturally scales to large data sets or numbers of stratified feature values. We illustrate our method with a variety of examples.

Keywords: convex optimization, stratified models, graphs, alternating direction method of multipliers, Laplacian regularization

1. Introduction

We consider the problem of fitting a model to some given data. One common and simple paradigm parametrizes the model by a parameter vector θ , and uses convex optimization to minimize an empirical loss on the (training) data set plus a regularization term that (hopefully) skews the model parameter toward one for which the model generalizes to new unseen data. This method usually includes one or more hyper-parameters that scale terms in the regularization. For each of a number of values of the hyper-parameters, a model parameter is found, and the resulting model is tested on previously unseen data. Among these models, we choose one that achieves a good fit on the test data. The requirement that

the loss function and regularization be convex limits how the features enter into the model; generally, they are linear (or affine) in the parameters. One advantage of such models is that they are generally interpretable.

Such models are widely used, and often work well in practice. Least squares regression (Legendre, 1805; Gauss, 1809), lasso (Tibshirani, 1996), logistic regression (Cox, 1958), support vector classifiers (Boser et al., 1992) are common methods that fall into this category (see (Hastie et al., 2009) for these and others). At the other extreme, we can use models that in principle fit arbitrary nonlinear dependence on the features. Popular examples include tree based models (Breiman et al., 1984) and neural networks (Goodfellow et al., 2016).

Stratification is a method to build a model of some data that depends in an arbitrary way on one or more of the categorical features. It identifies one or more categorical features and builds a separate model for the data that take on each of the possible values of these categorical features.

In this paper we propose augmenting basic stratification with an additional regularization term. We take into account the usual loss and regularization terms in the objective, plus an additional regularization term that encourages the parameters found for each value to be close to their neighbors on some specified weighted graph on the categorical values. We use the simplest possible term that encourages closeness of neighboring parameter values: a graph Laplacian on the stratification feature values. (As we will explain below, several recent papers use more sophisticated regularization on the parameters for different values of the categorical.) We refer to a stratified model with this objective function as a *Laplacian regularized stratified model*. Laplacian regularization can also be interpreted as a prior that our model parameters vary smoothly across the graph on the stratification feature values.

Stratification (without the Laplacian regularization) is an old and simple idea: Simply fit a different model for each value of the categorical used to stratify. As a simple example where the data are people, we can stratify on sex, *i.e.*, fit a separate model for females and males. (Whether or not this stratified model is better than a common model for both females and males is determined by out-of-sample or cross-validation.) To this old idea, we add an additional term that penalizes deviations between the model parameters for females and males. (This Laplacian regularization would be scaled by a hyper-parameter, whose value is chosen by validation on unseen or test data.) As a simple extension of the example mentioned above, we can stratify on sex and age, meaning we have a separate model for females and males, for each age from 1 to 100 (say). Thus we would create a total of 200 different models: one for each age/sex pair. The Laplacian regularization that we add encourages, for example, the model parameters for 37 year old females to be close to that for 37 year old males, as well as 36 and 38 year old females. We would have two hyper-parameters, one that scales the deviation of the model coefficients across sex, and another that scales the deviation of the model coefficients across adjacent ages. One would choose suitable values of these hyper-parameters by validation on a test set of data.

There are many other applications where a Laplacian regularized stratified model offers a simple and interpretable model. We can stratify over time, which gives time-varying models, with regularization that encourages our time-dependent model parameters to vary slowly over time. We can capture multiple periodicities in time-varying models, for example by asserting that the 11PM model parameter should be close to the midnight model parameter, the Tuesday and Wednesday parameters should be close to each other, and so on. We can

stratify over space, after discretizing location. The Laplacian regularization in this case encourages the model parameters to vary smoothly over space. This idea naturally falls in line with Waldo Tobler’s “first law of geography” (Tobler, 1970):

Everything is related to everything else, but near things are more related than distant things.

Compared to simple stratified models, our Laplacian regularized stratified models have several advantages. Without regularization, stratification is limited by the number of data points taking each value of the stratification feature, and of course fails (or does not perform well) when there are no data points with some value of the stratification feature. With regularization there is no such limit; we can even build a model when the training data has no points with some values of the stratification feature. In this case the model borrows strength from its neighbors. Continuing the example mentioned above, we can find a model for 37 year old females, even when our data set contains none. Unsurprisingly, the parameter for 37 year old females is a weighted average of the parameters for 36 and 38 year old females, and 37 year old males.

We can think of stratified models as a hybrid of complex and simple models. The stratified model has arbitrary dependence on the stratification feature, but simple (typically linear) dependence on the other features. It is essentially non-parametric in the stratified feature, and parametric with a simple form in the other features. The Laplacian regularization allows us to come up with a sensible model with respect to the stratified feature.

The simplest possible stratified model is a constant for each value of the stratification feature. In this case the stratified model is nothing more than a fully non-parametric model of the stratified feature. The Laplacian regularization in this case encourages smoothness of the predicted value relative to some graph on the possible stratification feature values. More sophisticated models predict a distribution of values of some features, given the stratified feature value, or build a stratified regression model, for example.

Contributions. Our contributions are two-fold. First, we provide a simple, cohesive discussion of stratified model fitting with Laplacian regularization, which previously was not unified. Furthermore, we describe stratified model fitting with Laplacian regularization as a convex optimization problem, with one model parameter vector for every value of the stratification feature. This problem is convex (when the loss and regularizers in the fitting method are), and so can be reliably solved (Boyd and Vandenberghe, 2004). Second, we propose an efficient distributed solution method based on the alternating direction method of multipliers (ADMM) (Boyd et al., 2011), which allows us to solve the optimization problem in a distributed fashion and at very large scale, in spite of coupling of the model parameters in the Laplacian regularization term. In each iteration of our method, we fit the models for each value of the stratified feature (independently in parallel), and then solve a number of Laplacian systems (one for each component of the model parameters, also in parallel). We illustrate the ideas and method with several examples.

2. Related work

Stratification, *i.e.*, the idea of separately fitting a different model for each value of some parameter, is routinely applied in various practical settings. For example, in clinical trials,

participants are often divided into subgroups, and one fits a separate model for the data from each subgroup (Kernan et al., 1999). Stratification by itself has immediate benefits; it can be helpful for dealing with confounding categorical variables, can help one gain insight into the nature of the data, and can also play a large role in experiment design in fields like clinical research (K. Rothman, 1986; Kestenbaum, 2009) and biology (Jacob and Vert, 2007).

The idea of adding regularization to fitting stratified models, however, is (unfortunately) not as well known in the data science, machine learning, and statistics communities. In this section, we outline some ideas related to stratified models, and also outline some prior work on Laplacian regularization.

Regularized lasso models. The data-shared lasso is a stratified model that encourages closeness of parameters by their difference as measured by the ℓ_1 -norm (Gross and Tibshirani, 2016). (Laplacian regularization penalizes their difference by the ℓ_2 -norm squared.) The pliable lasso is a generalization of the lasso that is also a stratified model, encouraging closeness of parameters as measured by a blend of the ℓ_1 - and ℓ_2 -norms (Tibshirani and Friedman, 2020; Du and Tibshirani, 2018). The network lasso is a stratified model that encourages closeness of parameters by their difference as measured by the ℓ_2 -norm (Hallac et al., 2015, 2017a). The network lasso problem results in groups of models with the same parameters, in effect clustering the stratification features. (In contrast, Laplacian regularization leads to smooth parameter values.) The ideas in the original papers on the network lasso were combined and made more general, resulting in the software package SnapVX (Hallac et al., 2017b), a general solver for convex optimization problems defined on graphs that is based on SNAP (Leskovec and Sosič, 2016) and CVXPY (Diamond and Boyd, 2016). One could, in principle, implement Laplacian regularized stratified models in SnapVX; instead we develop specialized methods for the specific case of Laplacian regularization, which leads to faster and more robust methods. We also have observed that, in most practical settings, Laplacian regularization is all you need.

Mixed effect models. In statistics, mixed effect models (also known as multilevel models) are used to model data that has some underlying dependent relationship (referred to as random effects in the literature) (Laird and Ware, 1982; Robinson, 1991; Jiang, 2007). In essence, a mixed effect model is similar to a stratified model. In fact, there are even cases where one fits mixed graphical models, generally using either ℓ_1 or group lasso regularization (Lee and Hastie, 2013; Chen et al., 2014; Lee and Hastie, 2015; Cheng et al., 2017). There are many efficient methods for fitting generalized linear mixed effect models, such as penalized least squares, expectation-maximization, proximal gradient, and proximal Newton algorithms (Lindstrom and Bates, 1988; Breslow and Clayton, 1993; Bates and DebRoy, 2004; Bates et al., 2015).

Varying-coefficient models. Varying-coefficient models are a class of regression and classification models in which the model parameters are smooth functions of some features (Hastie and Tibshirani, 1993). A stratified model can be thought of as a special case of varying-coefficient models, where the features used to choose the coefficients are categorical. Varying-coefficient models have been applied particularly to epidemiology, estimating parameters in Cox-type regression models (Murphy and Sen, 1991) and evaluating patient

risk of acquiring infections (Wiens et al., 2016). Estimating varying-coefficient models is generally nonconvex and computationally expensive (Fan and Zhang, 2008).

Geographically weighted regression. The method of geographically weighted regression (GWR) is widely used in the field of geographic information systems (GIS). It consists of a spatially-varying linear model with a location attribute (Brunsdon et al., 1996). GWR fits a model for each location using every data point, where each data point is weighted by a kernel function of the pairwise locations. (See, *e.g.*, McMillen, 2004, for a recent survey and applications.) GWR is an extremely special case of a stratified model, where the task is regression and the stratification feature is location.

Graph-based feature regularization. One can apply graph regularization to the features themselves. For example, the group lasso penalty enforces sparsity of model coefficients among groups of features (Yuan and Lin, 2006; Friedman et al., 2010), performing feature selection at the level of groups of features. The group lasso is often fit using a method based on ADMM, which is similar in vein to the one we describe. The group lasso penalty can be used as a regularization term to any linear model, *e.g.*, logistic regression (Meier et al., 2008). A related idea is to use a Laplacian regularization term on the features, leading to, *e.g.*, Laplacian regularized least-squares (LapRLS) and Laplacian regularized support vector machines (LapSVM) (Belkin et al., 2006; Melacci and Belkin, 2011). Laplacian regularized models have been applied to many disciplines and fields, *e.g.*, to semi-supervised learning (Zhu et al., 2003; Johnson and Zhang, 2007; Nadler et al., 2009; Alaoui et al., 2016), communication (Boyd, 2006; Chen et al., 2011; Zouzias and Freris, 2015), medical imaging (Zhang and Shen, 2011), computer vision (Wang et al., 2012), natural language processing (Wang et al., 2013), and microbiology (Wang et al., 2017).

Graph interpolation. In graph interpolation or regression on a graph, one is given vectors at some of the vertices of a graph, and is tasked with inferring the vectors at the other (unknown) vertices (Kovac and Smith, 2011). This can be viewed as a stratified model where the parameter at each vertex or node is a constant. This leads to, *e.g.*, the total variation denoising problem in signal processing (see Rudin et al., 1992).

Multi-task learning. In multi-task learning, the goal is to learn models for multiple related tasks by taking advantage of pair-wise relationships between the tasks (See, *e.g.*, Caruana, 1997; Zhang and Yang, 2017). Multi-task learning can be interpreted as a stratified model where the stratification feature is the task to be performed by that model. Laplacian regularization has also been investigated in the context of multi-task learning (Sheldon, 2008).

Laplacian systems. Laplacian matrices are very well studied in the field of spectral graph theory (Spielman, 2007; Teng, 2010). A set of linear equations with Laplacian coefficient matrix is called a *Laplacian system*. Many problems give rise to Laplacian systems, including in electrical engineering (resistor networks), physics (vibrations and heat), computer science, and spectral graph theory (see, *e.g.*, Spielman, 2010, for a survey) While solving a general linear system requires order K^3 flops, where K is the number of vertices in the graph, Laplacian system solvers have been developed that are (nearly) linear in the number of edges contained in the associated graph (Vishnoi, 2013; Cohen et al., 2014; Schaub et al., 2017).

In many cases, however, the graph can be large and dense enough that solving a Laplacian system is still a highly nontrivial computational issue; in these cases, graph sparsification can be used to yield results of moderate accuracy in much less time (Sadhanala et al., 2016). In practice, the conjugate gradient (CG) method (Hestenes and Stiefel, 1952b), with a suitable pre-conditioner, can be extremely efficient for solving the (positive definite) Tikhonov-regularized Laplacian systems that we encounter in this paper.

Laplacian regularized minimization problems. Stratified model fitting with Laplacian regularization is simply a convex optimization problem with Laplacian regularization. There are many general-purpose methods that solve this problem, indeed too many to name; in this paper we derive a problem-specific algorithm using ADMM. Another possibility would be majorization-minimization (MM), an algorithmic framework where one iteratively minimizes a majorizer of the original function at the current iterate (Sun et al., 2017). One possible majorizer for the Laplacian regularization term is a diagonal quadratic, allowing block separable problems to be solved in parallel; this was done in (Tuck et al., 2019). The MM and ADMM algorithms have been shown to be closely connected (Lu et al., 2018), since the proximal operator of a function minimizes a quadratic majorizer. However, convergence with MM depends heavily on the choice of majorizer and the problem structure (Hunter and Lange, 2004). In contrast, the ADMM-based algorithm we describe in this paper typically converges (at least to reasonable practical tolerance) within 100–200 iterations.

3. Stratified models

In this section we define stratified models and our fitting method; we describe our distributed method for carrying out the fitting in §4.

We consider data fitting problems with items or records of the form $(z, x, y) \in \mathcal{Z} \times \mathcal{X} \times \mathcal{Y}$. Here $z \in \mathcal{Z}$ is the feature over which we stratify, $x \in \mathcal{X}$ is the other features, and $y \in \mathcal{Y}$ is the outcome or dependent variable. For our purposes, it does not matter what \mathcal{X} or \mathcal{Y} are; they can consist of numerical, categorical, or other data types. The stratified feature values \mathcal{Z} , however, must consist of only K possible values, which we denote as $\mathcal{Z} = \{1, \dots, K\}$. What we call z can include several original features, for example, sex and age. If all combinations of these original features are possible, then K is the product of the numbers of values these features can take on. In some formulations, described below, we do not have x ; in this case, the records have the simplified form (z, y) .

Base model. We build a stratified model on top of a base model, which models pairs (x, y) (or, when x is absent, just y). The base model is parametrized by a parameter vector $\theta \in \Theta \subseteq \mathbf{R}^n$. In a stratified model, we use a different value of the parameter θ for each value of z . We denote these parameters as $\theta_1, \dots, \theta_K$, where θ_k is the parameter value used when $z = k$. We let $\theta = [\theta_1 \dots \theta_K] \in \mathbf{R}^{n \times K}$ denote the collection of parameter values, *i.e.*, the parameter value for the stratified model.

Local loss and regularization. Let (z_i, x_i, y_i) , $i = 1 \dots, N$, denote a set of N training data points or examples. We will use regularized empirical loss minimization to choose the parameters $\theta_1, \dots, \theta_K$. Let $l : \Theta \times \mathcal{X} \times \mathcal{Y} \rightarrow \mathbf{R}$ be a loss function. We define the k th (local)

empirical loss as

$$\ell_k(\theta) = \sum_{i:z_i=k} l(\theta, x_i, y_i) \quad (1)$$

(without x_i when x is absent).

We may additionally add a regularizer to the local loss function. The idea of regularization can be traced back to as early as the 1940s, where it was introduced as a method to stabilize ill-posed problems (Tikhonov, 1943, 1963). Let $r : \Theta \rightarrow \mathbf{R} \cup \{\infty\}$ be a regularization function or regularizer. Choosing θ_k to minimize $\ell_k(\theta_k) + r(\theta_k)$ gives the regularized empirical risk minimization model parameters, based only on the data records that take the particular value of the stratification feature $z = k$. This corresponds to the traditional stratified model, with no connection between the parameter values for different values of z . (Infinite values of the regularizer encode constraints on allowable model parameters.)

Laplacian regularization. Let $W \in \mathbf{R}^{K \times K}$ be a symmetric matrix with nonnegative entries. The associated *Laplacian regularization* is the function $\mathcal{L} : \mathbf{R}^{n \times K} \rightarrow \mathbf{R}$ given by

$$\mathcal{L}(\theta) = \mathcal{L}(\theta_1, \dots, \theta_K) = \frac{1}{2} \sum_{i=1}^K \sum_{j<i} W_{ij} \|\theta_i - \theta_j\|_2^2. \quad (2)$$

(To distinguish the Laplacian regularization \mathcal{L} from r in (1), we refer to r as the *local regularization*.) We can associate the Laplacian regularization with a graph with K vertices, which has an edge (i, j) for each positive W_{ij} , with weight W_{ij} . We refer to this graph as the regularization graph. We can express the Laplacian regularization as the positive semidefinite quadratic form

$$\mathcal{L}(\theta) = (1/2) \mathbf{Tr}(\theta L \theta^T),$$

where \otimes denotes the Kronecker product, and $L \in \mathbf{R}^{K \times K}$ is the (weighted) Laplacian matrix associated with the weighted graph, given by

$$L_{ij} = \begin{cases} -W_{ij} & i \neq j \\ \sum_{k=1}^K W_{ik} & i = j \end{cases}$$

for $i, j = 1, \dots, K$.

The Laplacian regularization $\mathcal{L}(\theta)$ evidently measures the aggregate deviation of the parameter vectors from their graph neighbors, weighted by the edge weights. Roughly speaking, it is a metric of how rough or non-smooth the mapping from z to θ_z is, measured by the edge weights.

Fitting the stratified model. To choose the parameters $\theta_1, \dots, \theta_K$, we minimize

$$F(\theta_1, \dots, \theta_k) = \sum_{k=1}^K (\ell_k(\theta_k) + r(\theta_k)) + \mathcal{L}(\theta_1, \dots, \theta_K). \quad (3)$$

The first term is the sum of the local objective functions, used in fitting a traditional stratified model; the second measures the non-smoothness of the model parameters as measured by the Laplacian. It encourages parameter values for neighboring values of z to be close to each other.

Convexity assumption. We will assume that the local loss function $l(\theta, x, y)$ and the local regularizer $r(\theta)$ are convex functions of θ , which implies that the local losses ℓ_k are convex functions of θ . The Laplacian is also convex, so the overall objective F is convex, and minimizing it (*i.e.*, fitting a stratified model) is a convex optimization problem. In §4 we will describe an effective distributed method for solving this problem. (Much of our development carries over to the case when l or r is not convex; in this case, of course, we can only expect to find a local minimizer of F ; see §6.)

The two extremes. Assuming the regularization graph is connected, taking the positive weights W_{ij} to ∞ forces all the parameters to be equal, *i.e.*, $\theta_1 = \dots = \theta_K$. We refer to this as the *common model* (*i.e.*, one which does not depend on z). At the other extreme we can take all W_{ij} to 0, which results in a traditional stratified model, with separate models independently fit for each value of z .

Hyper-parameters. The local regularizer and the weight matrix W typically contain some positive hyper-parameters, for example that scale the local regularization or one or more edges weights in the graph. As usual, these are varied over a range of values, and for each value a stratified model is found, and tested on a separate validation data set using an appropriate true objective. We choose values of the hyper-parameters that give good validation set performance; finally, we test this model on a new test data set.

Modeling with no data at nodes. Suppose that at a particular node on the graph (*i.e.*, value of stratification feature), there is no data to fit a model. Then, the model for that node will simply be a weighted average of the models of its neighboring nodes.

Feature engineering interpretation. We consider an interpretation of stratified model fitting versus typical model fitting in a linear model setting. Instead of being a scalar in $\{1, \dots, K\}$, let z be a one-hot vector in \mathbf{R}^K where the data record is in the k th category if $z = e_k$, the k th basis vector in \mathbf{R}^k . In a typical model fitting formulation with inputs x, z and outcomes y an estimate of y is given by $\hat{y} = (x, z)^T \theta$ with $\theta \in \mathbf{R}^{n+K}$; that is, the model is *linear* in x and z . With stratified model fitting, our estimate is instead $\hat{y} = x^T \theta z$ with $\theta \in \mathbf{R}^{n \times K}$; that is, the model is *bilinear* in x and z .

3.1 Data models

So far we have been vague about what exactly a data model is. In this section we list just a few of the many possibilities.

3.1.1 POINT ESTIMATES

The first type of data model that we consider is one where we wish to predict a single likely value, or point estimate, of y for a given x and z . In other words, we want to construct a function $f_z : \mathcal{X} \rightarrow \mathcal{Y}$ such that $f_z(x) \approx y$.

Regression. In a regression data model, $\mathcal{X} = \mathbf{R}^n$ and $\mathcal{Y} = \mathbf{R}$, with one component of x always having the value one. The loss has the form $l(\theta, x, y) = p(x^T \theta - y)$, where $p : \mathbf{R} \rightarrow \mathbf{R}$ is a penalty function. Some common (convex) choices include the square penalty (Legendre, 1805; Gauss, 1809), absolute value penalty (Boscovich, 1757), Huber penalty (Huber, 1964), and tilted absolute value (for quantile regression). Common generic regularizers include

zero, sum of squares, and the ℓ_1 norm (Tibshirani, 1996); these typically do not include the coefficient in θ associated with the constant feature value one, and are scaled by a positive hyper-parameter. Various combinations of these choices lead to ordinary least squares regression, ridge regression, the lasso, Huber regression, and quantile regression. Multiple regularizers can also be employed, each with a different hyper-parameter, as in the elastic net. Constraints on model parameters (for example, nonnegativity) can be imposed by infinite values of the regularizer.

The stratified regression model gives the predictor of y , given z and x , given by

$$f_z(x) = x^T \theta_z.$$

The stratified model uses a different set of regression coefficients for each value of z . For example, we can have a stratified lasso model, or a stratified nonnegative least squares model.

An interesting extension of the regression model, sometimes called multivariate or multi-task regression, takes $\mathcal{Y} = \mathbf{R}^m$ with $m > 1$. In this case we take $\Theta = \mathbf{R}^{n \times m}$, so θ_z is a matrix, with $f_z(x) = x^T \theta_z$ as our predictor for y . An interesting regularizer for multi-task regression is the nuclear norm, which is the sum of singular values, scaled by a hyper-parameter (Vandenberghe and Boyd, 1996). This encourages the matrices θ_z to have low rank.

Boolean classification. In a boolean classification data model, $\mathcal{X} = \mathbf{R}^n$ and $\mathcal{Y} = \{-1, 1\}$. The loss has the form $l(\theta, x, y) = p(yx^T \theta)$, where $p: \mathbf{R} \rightarrow \mathbf{R}$ is a penalty function. Common (convex) choices of p are $p(u) = (u - 1)^2$ (square loss); $p(u) = (u - 1)_+$ (hinge loss), and $p(u) = \log(1 + \exp -u)$ (logistic loss). The predictor is

$$f_z(x) = \mathbf{sign}(x^T \theta_z).$$

The same regularizers mentioned in regression can be used. Various choices of these loss functions and regularizers lead to least squares classification, support vector machines (SVM) (Cortes and Vapnik, 1995), logistic regression (Cox, 1958; Hosmer and Lemeshow, 2005), and so on (Hastie et al., 2009). For example, a stratified SVM model develops an SVM model for each value of z ; the Laplacian regularization encourages the parameters associated with neighboring values of z to be close.

Multi-class classification. Here $\mathcal{X} = \mathbf{R}^n$, and \mathcal{Y} is finite, say, $\{1, \dots, M\}$. We usually take $\Theta = \mathbf{R}^{n \times M}$, with associated predictor $f_z(x) = \operatorname{argmax}_i (x^T \theta_z)_i$. Common (convex) loss functions are the multi-class logistic (multinomial) loss (Engel, 1988),

$$l(\theta, x, y) = \log \left(\sum_{j=1}^M \exp(x^T \theta)_j \right) - (x^T \theta)_y, \quad y = 1, \dots, M,$$

and the multi-class SVM loss (Yang et al., 2007; Manning et al., 2008),

$$l(\theta, x, y) = \sum_{i:i \neq y} ((x^T \theta)_i - (x^T \theta)_y + 1)_+, \quad y = 1, \dots, M.$$

The same regularizers mentioned in multivariate regression can be used.

Point estimates without x . As mentioned above, x can be absent. In this case, we predict y given only z . We can also interpret this as a point estimate with an x that is always constant, *e.g.*, $x = 1$. In a regression problem without x , the parameter θ_z is a scalar, and corresponds simply to a prediction of the value y . The loss has the form $l(\theta, y) = p(\theta - y)$, where p is any of the penalty functions mentioned in the regression section. If, for example, p were the square (absolute value) penalty, then θ_k would correspond to the average (median) of the y_i that take on the particular stratification feature k , or $z_i = k$. In a boolean classification problem, $\theta_z \in \mathbf{R}$, and the predictor is $\mathbf{sign}(\theta_z)$, the most likely class. The loss has the form $l(\theta, y) = p(y\theta)$, where p is any of the penalty functions mentioned in the boolean classification section. A similar predictor can be derived for the case of multi-class classification.

3.1.2 CONDITIONAL DISTRIBUTION ESTIMATES

A more sophisticated data model predicts the conditional probability distribution of y given x (rather than a specific value of y given x , in a point estimate). We parametrize this conditional probability distribution by a vector θ , which we denote as $\mathbf{Prob}(y \mid x, \theta)$. The data model could be any generalized linear model (Nelder and Wedderburn, 1972); here we describe a few common ones.

Logistic regression. Here $\mathcal{X} = \mathbf{R}^n$ and $\mathcal{Y} = \{-1, 1\}$, with one component of x always having the value one. The conditional probability has the form

$$\mathbf{Prob}(y = 1 \mid x, \theta) = \frac{1}{1 + e^{-x^T \theta}}.$$

(So $\mathbf{Prob}(y = -1 \mid x, \theta) = 1 - \mathbf{Prob}(y = 1 \mid x, \theta)$.) The loss, often called the logistic loss, has the form $l(\theta, x, y) = \log(1 + \exp(-y\theta^T x))$, and corresponds to the negative log-likelihood of the data record (x, y) , when the parameter vector is θ . The same regularizers mentioned in regression can be used. Validating a logistic regression data model using the average logistic loss on a test set is the same (up to a constant factor) as the average log probability of the observed values in the test data, under the predicted conditional distributions.

Multinomial logistic regression. Here $\mathcal{X} = \mathbf{R}^n$ and \mathcal{Y} is finite, say $\{1, \dots, M\}$ with one component of x equal to one. The parameter vector is a matrix $\theta \in \mathbf{R}^{n \times M}$. The conditional probability has the form

$$\mathbf{Prob}(y = i \mid x, \theta) = \frac{\exp(x^T \theta)_i}{\sum_{j=1}^M \exp(x^T \theta)_j}, \quad i = 1, \dots, M.$$

The loss has the form

$$l(\theta, x, y = i) = \log \left(\sum_{j=1}^M \exp(x^T \theta)_j \right) - (x^T \theta)_i, \quad i = 1, \dots, M,$$

and corresponds to the negative log-likelihood of the data record (x, y) .

Exponential regression. Here $\mathcal{X} = \mathbf{R}^n$ and $\mathcal{Y} = \mathbf{R}_+$ (*i.e.*, the nonnegative reals). The conditional probability distribution in exponential regression has the form

$$\mathbf{Prob}(y \mid x, \theta) = \exp(x^T \theta) e^{-\exp(x^T \theta) y},$$

where $\theta \in \mathbf{R}^n$ is the parameter vector. This is an exponential distribution over y , with rate parameter given by $\omega = \exp(x^T \theta)$. The loss has the form

$$l(\theta, x, y) = -x^T \theta + \exp(x^T \theta) y,$$

which corresponds to the negative log-likelihood of the data record (x, y) under the exponential distribution with parameter $\omega = \exp(x^T \theta)$. Exponential regression is useful when the outcome y is positive. A similar conditional probability distribution can be derived for the other distributions, *e.g.*, the Poisson distribution.

3.1.3 DISTRIBUTION ESTIMATES

A distribution estimate is an estimate of the probability distribution of y when x is absent, denoted $p(y \mid \theta)$. This data model can also be interpreted as a conditional distribution estimate when $x = 1$. The stratified distribution model consists of a separate distribution for y , for each value of the stratification parameter z . The Laplacian regularization in this case encourages closeness between distributions that have similar stratification parameters, measured by the distance between their model parameters.

Gaussian distribution. Here $\mathcal{Y} = \mathbf{R}^m$, and we fit a density to the observed values of y , given z . For example θ can parametrize a Gaussian on \mathbf{R}^m , $\mathcal{N}(\mu, \Sigma)$. The standard parametrization uses the parameters $\theta = (\Sigma^{-1}, \Sigma^{-1} \mu)$, with $\Theta = \mathbf{S}_{++}^m \times \mathbf{R}^m$ (\mathbf{S}_{++}^n denotes the set of $n \times n$ positive definite matrices.) The probability density function of y is

$$p(y \mid \theta) = (2\pi)^{-m/2} \det(\Sigma)^{-1/2} \exp\left(-\frac{1}{2}(y - \mu)^T \Sigma^{-1}(y - \mu)\right)$$

The loss function (in the standard parametrization) is

$$l(\theta, y) = -\log \det S + y^T S y - 2y^T \nu + \nu^T S^{-1} \nu$$

where $\theta = (S, \nu) = (\Sigma^{-1}, \Sigma^{-1} \mu)$. This loss function is jointly convex in S and ν ; the first three terms are evidently convex and the fourth is the matrix fractional function (see (Boyd and Vandenberghe, 2004, p76)). Some common (convex) choices for the local regularization function include the trace of Σ^{-1} (encourages the harmonic mean of the eigenvalues of Σ , and hence volume, to be large), sum of squares of Σ^{-1} (shrinks the overall conditional dependence between the variables), ℓ_1 -norm of Σ^{-1} (encourages conditional independence between the variables) (Friedman et al., 2008), or a prior on Σ^{-1} or $\Sigma^{-1} \mu$.

When $m = 1$, this model corresponds to the standard normal distribution, with mean μ and variance σ^2 . A stratified Gaussian distribution model has a separate mean and covariance of y for each value of the stratification parameter z . This model can be validated by evaluating the average log density of the observed values y_i , under the predicted distributions, over a test set of data.

Bernoulli distribution. Here $\mathcal{Y} = \mathbf{R}_+^n$. The probability density function of a Bernoulli distribution has the form

$$p(y | \theta) = \theta^{\mathbf{1}^T y} (1 - \theta)^{n - \mathbf{1}^T y},$$

where $\theta \in \Theta = [0, 1]$. The loss function has the form

$$l(\theta, y) = -(\mathbf{1}^T y) \log(\theta) - (n - \mathbf{1}^T y) \log(1 - \theta),$$

which corresponds to the negative log-likelihood of the Bernoulli distribution.

Poisson distribution. Here $\mathcal{Y} = \mathbb{Z}_+$ (*i.e.*, the nonnegative integers). The probability density function of a Poisson distribution has the form

$$p(y = k | \theta) = \frac{\theta^k e^{-\theta}}{k!}, \quad k = 0, 1, \dots,$$

where $\theta \in \Theta = \mathbf{R}_+$. If $\theta = 0$, then $p(y = 0 | \theta) = 1$. The loss function has the form

$$l(\theta, y = k) = -k \log \theta + \theta, \quad k = 0, 1, \dots,$$

which corresponds to the negative log-likelihood of the Poisson distribution. A similar data model can be derived for the exponential distribution.

Non-parametric discrete distribution. Here \mathcal{Y} is finite, say $\{1, \dots, M\}$ where $M > 1$. We fit a non-parametric discrete distribution to y , which has the form

$$p(y = k | \theta) = \theta_k, \quad k = 1, \dots, M,$$

where $\theta \in \Theta = \{p \in \mathbf{R}^M \mid \mathbf{1}^T p = 1, p \succeq 0\}$, *i.e.*, the probability simplex. The loss function has the form

$$l(\theta, y = k) = -\log(\theta_k), \quad k = 1, \dots, M.$$

A common (convex) regularization function is the negative entropy, given by $\sum_{i=1}^M \theta_i \log(\theta_i)$.

Exponential families. A probability distribution that can be expressed as

$$p(y | \theta) = e^{M(\theta, y)}$$

where $M : \mathbf{R}^n \times \mathcal{Y} \rightarrow \mathbf{R}$ is a concave function of θ , is an exponential family (Koopman, 1936; Pitman, 1936). Some important special cases include the Bernoulli, multinomial, Gaussian, and Poisson distributions. A probability distribution that has this form naturally leads to the following (convex) loss function

$$l(\theta, y) = -\log p(y | \theta) = -M(\theta, y).$$

3.2 Regularization graphs

In this section we outline some common regularization graphs, which are undirected weighted graphs where each vertex corresponds to a possible value of z . We also detail some possible uses of each type of regularization graph in stratified model fitting.

Complete graph. A complete graph is a (fully connected) graph that contains every possible edge. In this case, all of the models for each stratification feature are encouraged to be close to each other.

Star graph. A star graph has one vertex with edges to every other vertex. The vertex that is connected to every other vertex is sometimes called the *internal* vertex. In a stratified model with a star regularization graph, the parameters of all of the non-internal vertices are encouraged to be similar to the parameter of the internal vertex. We refer to the internal vertex as the *common model*. A common use of a star graph is when the stratification feature relates many vertices only to the internal vertex.

It is possible to have no data associated with the common model or internal vertex. In this case the common model parameter is a weighted average of other model parameters; it serves to pull the other parameter values together.

It is a simple exercise to show that a stratified model with the complete graph can also be found using a star graph, with a central or internal vertex that is connected to all others, but has no data. (That is, it corresponds to a new fictitious value of the stratification feature, that does not occur in the real data.)

Path graph. A path graph, or linear/chain graph, is a graph whose vertices can be listed in order, with edges between adjacent vertices in that order. The first and last vertices only have one edge, whereas the other vertices have two edges. Path graphs are a natural choice for when the stratification feature corresponds to time, or location in one dimension. When the stratification feature corresponds to time, a stratified model with a path regularization graph correspond to a time-varying model, where the model varies smoothly with time.

Cycle graph. A cycle graph or circular graph is a graph where the vertices are connected in a closed chain. Every vertex in a cycle graph has two edges. A common use of a cycle graph is when the stratification feature corresponds to a periodic variables, *e.g.*, the day of the week; in this case, we fit a separate model for each day of the week, and the model parameter for Sunday is close to both the model parameter for Monday and the model parameter for Saturday. Other examples include days of the year, the season, and non-time variables such as angle.

Tree graph. A tree graph is a graph where any two vertices are connected by exactly one path (which may consist of multiple edges). Tree graphs can be useful for stratification features that naturally have hierarchical structure, *e.g.*, the location in a corporate hierarchy, or in finance, hierarchical classification of individual stocks into sectors, industries, and sub-industries. As in the star graph, which is a special case of a tree graph, internal vertices need not have any data associated with them, *i.e.*, the data is only at the leaves of the tree.

Grid graph. A grid graph is a graph where the vertices correspond to points with integer coordinates, and two vertices are connected if their maximum distance in each coordinate is less than or equal to one. For example, a path graph is a one-dimensional grid graph.

Grid graphs are useful for when the stratification feature corresponds to locations. We discretize the locations into bins, and connect adjacent bins in each dimension to create a grid graph. A space-stratified model with grid graph regularization is encouraged to have model parameters that vary smoothly through physical space.

Entity graph. There can be a vertex for every value of some entity, *e.g.*, a person. The entity graph has an edge between two entities if they are perceived to be similar. For example, two people could be connected in a (friendship) entity graph if they were friends on a social networking site. In this case, we would fit a separate model for each person, and encourage friends to have similar models. We can have multiple relations among the entities, each one associated with its own graph; these would typically be weighted by separate hyper-parameters.

Products of graphs. As mentioned earlier, z can include several original features, and K , the number of possible values of z , is the product of the number of values that these features take on. Each original stratification feature can have its own regularization graph, with the resulting regularization graph for z given by the (weighted) Cartesian product of the graphs of each of the features. For example, the product of two path graphs is a grid graph, with the horizontal and vertical edges having different weights, associated with the two original stratification features.

4. Distributed method for stratified model fitting

In this section we describe a distributed algorithm for solving the fitting problem (3). This algorithm is based off of ADMM, a well-known algorithm that is well suited for solving convex optimization problems in parallel (and works well in practice when the problem is nonconvex) (Boyd et al., 2011; Wang et al., 2019). The method alternates between computing (in parallel) the proximal operator of the local loss and local regularizer for each model, and computing the proximal operator of the Laplacian regularization term, which requires the solution of a number of regularized Laplacian linear systems (which can also be done in parallel). The use of an ADMM-based algorithm allows for parallelizability over the objective, which is not separable due to the Laplacian regularization.

To derive the algorithm, we first express (3) in the equivalent form

$$\begin{aligned} & \text{minimize} && \sum_{k=1}^K (\ell_k(\theta_k) + r(\tilde{\theta}_k)) + \mathcal{L}(\hat{\theta}_1, \dots, \hat{\theta}_K) \\ & \text{subject to} && \theta = \hat{\theta}, \quad \tilde{\theta} = \hat{\theta}, \end{aligned} \tag{4}$$

where we have introduced two additional optimization variables $\tilde{\theta} \in \mathbf{R}^{n \times K}$ and $\hat{\theta} \in \mathbf{R}^{n \times K}$. The augmented Lagrangian L_λ of (4) has the form

$$\begin{aligned} L_\lambda(\theta, \tilde{\theta}, \hat{\theta}, u, \tilde{u}) &= \sum_{k=1}^K (\ell_k(\theta_k) + r(\tilde{\theta}_k)) + \mathcal{L}(\hat{\theta}_1, \dots, \hat{\theta}_K) \\ &\quad + (1/2\lambda) \|\theta - \hat{\theta} + u\|_2^2 + (1/2\lambda) \|\tilde{\theta} - \hat{\theta} + \tilde{u}\|_2^2, \end{aligned}$$

where $u \in \mathbf{R}^{n \times K}$ and $\tilde{u} \in \mathbf{R}^{n \times K}$ are the (scaled) dual variables associated with the two constraints in (4), respectively, and $\lambda > 0$ is the penalty parameter. The ADMM algorithm

(in scaled dual form) for the splitting $(\theta, \tilde{\theta})$ and $\hat{\theta}$ consists of the iterations

$$\begin{aligned}\theta^{i+1}, \tilde{\theta}^{i+1} &:= \underset{\theta, \tilde{\theta}}{\operatorname{argmin}} L_\lambda(\theta, \tilde{\theta}, \hat{\theta}^i, u^i, \tilde{u}^i) \\ \hat{\theta}^{i+1} &:= \underset{\hat{\theta}}{\operatorname{argmin}} L_\lambda(\theta^i, \tilde{\theta}^i, \hat{\theta}, u^i, \tilde{u}^i) \\ u^{i+1} &:= u^i + \theta^{i+1} - \hat{\theta}^{i+1} \\ \tilde{u}^{i+1} &:= \tilde{u}^i + \tilde{\theta}^{i+1} - \hat{\theta}^{i+1}.\end{aligned}$$

Since the problem is convex, the iterates θ^i , $\tilde{\theta}^i$, and $\hat{\theta}^i$ are guaranteed to converge to each other and to a primal optimal point of (3) (Boyd et al., 2011).

This algorithm can be greatly simplified (and parallelized) with a few simple observations. Our first observation is that the first step in ADMM can be expressed as

$$\theta_k^{i+1} = \mathbf{prox}_{\lambda l_k}(\hat{\theta}_k^i - u_k^i), \quad \tilde{\theta}_k^{i+1} = \mathbf{prox}_{\lambda r}(\hat{\theta}_k^i - \tilde{u}_k^i), \quad k = 1, \dots, K,$$

where $\mathbf{prox}_g : \mathbf{R}^n \rightarrow \mathbf{R}^n$ is the proximal operator of the function g (Parikh and Boyd, 2014) (see the Appendix for the definition and some examples of proximal operators). This means that we can compute θ^{i+1} and $\tilde{\theta}^{i+1}$ at the same time, since they do not depend on each other. Also, we can compute $\theta_1^{i+1}, \dots, \theta_K^{i+1}$ (and $\tilde{\theta}_1^{i+1}, \dots, \tilde{\theta}_K^{i+1}$) in parallel.

Our second observation is that the second step in ADMM can be expressed as the solution to the n regularized Laplacian systems

$$\left(L + (2/\lambda)I \right) \begin{bmatrix} (\hat{\theta}_1^{i+1})_j \\ (\hat{\theta}_2^{i+1})_j \\ \vdots \\ (\hat{\theta}_K^{i+1})_j \end{bmatrix} = (1/\lambda) \begin{bmatrix} (\theta_1^{i+1} + u_1^i + \tilde{\theta}_1^{i+1} + \tilde{u}_1^i)_j \\ (\theta_2^{i+1} + u_2^i + \tilde{\theta}_2^{i+1} + \tilde{u}_2^i)_j \\ \vdots \\ (\theta_K^{i+1} + u_K^i + \tilde{\theta}_K^{i+1} + \tilde{u}_K^i)_j \end{bmatrix}, \quad j = 1, \dots, n. \quad (5)$$

These systems can be solved in parallel. Many efficient methods for solving these systems have been developed; we find that the conjugate gradient (CG) method (Hestenes and Stiefel, 1952a), with a diagonal pre-conditioner, can efficiently and reliably solve these systems. (We can also warm-start CG with $\hat{\theta}^i$.) Combining these observations leads to Algorithm 4.1.

Algorithm 4.1 *Distributed method for fitting stratified models with Laplacian regularization.*

given Loss functions ℓ_1, \dots, ℓ_K , local regularization function r , graph Laplacian matrix L , and penalty parameter $\lambda > 0$.

Initialize. $\theta^0 = \tilde{\theta}^0 = \hat{\theta}^0 = u^0 = \tilde{u}^0 = 0$.

repeat

in parallel

1. Evaluate proximal operator of l_k . $\theta_k^{i+1} = \mathbf{prox}_{\lambda \ell_k}(\hat{\theta}_k^i - u_k^i)$, $k = 1, \dots, K$
2. Evaluate proximal operator of r . $\tilde{\theta}_k^{i+1} = \mathbf{prox}_{\lambda r}(\hat{\theta}_k^i - \tilde{u}_k^i)$, $k = 1, \dots, K$
3. Evaluate proximal operator of \mathcal{L} in parallel. $\hat{\theta}^{i+1} = \mathbf{prox}_{\lambda \mathcal{L}/2}(\theta^{i+1} + u^i + \tilde{\theta}^{i+1} + \tilde{u}^i)$
4. Update the dual variables. $u^{i+1} := u^i + \theta^{i+1} - \hat{\theta}^{i+1}$; $\tilde{u}^{i+1} := \tilde{u}^i + \tilde{\theta}^{i+1} - \hat{\theta}^{i+1}$

until convergence

Evaluating the proximal operator of l_k . Evaluating the proximal operator of l_k corresponds to solving a fitting problem with sum-of-squares regularization. In some cases, this has a closed-form expression, and in others, it requires solving a small convex optimization problem (Parikh and Boyd, 2014; Polson et al., 2015). When the loss is differentiable, we can use, for example, the L-BFGS algorithm to solve it (Liu and Nocedal, 1989). (We can also warm start with θ^i .) We can also re-use factorizations of matrices (*e.g.*, Hessians) used in previous evaluations of the proximal operator.

Evaluating the proximal operator of r . The proximal operator of r often has a closed-form expression. For example, if $r(\theta) = 0$, then the proximal operator of r corresponds to the projection onto Θ . If r is the sum of squares function and $\Theta = \mathbf{R}^n$, then the proximal operator of r corresponds to the (linear) shrinkage operator. If r is the ℓ_1 norm and $\Theta = \mathbf{R}^n$, then the proximal operator of r corresponds to soft-thresholding, which can be performed in parallel.

Complexity. Generally, as the proximal operators of the l_k , r , and \mathcal{L} can all be computed in parallel, the complexity of this algorithm is the dominant cost of computing a single proximal operator of l_k , r , or \mathcal{L} , assuming access to at least $\max(n, K)$ parallelizations.

Stopping criterion. The primal and dual residuals

$$r^{i+1} = (\theta^{i+1} - \hat{\theta}^{i+1}, \tilde{\theta}^{i+1} - \hat{\theta}^{i+1}), \quad s^{i+1} = -(1/\lambda)(\hat{\theta}^{i+1} - \hat{\theta}^i, \hat{\theta}^{i+1} - \hat{\theta}^i),$$

converge to zero (Boyd et al., 2011). This suggests the stopping criterion

$$\|r^{i+1}\|_2 \leq \epsilon_{\text{pri}}, \quad \|s^{i+1}\|_2 \leq \epsilon_{\text{dual}},$$

where ϵ_{pri} and ϵ_{dual} are given by

$$\epsilon_{\text{pri}} = \sqrt{2Kn}\epsilon_{\text{abs}} + \epsilon_{\text{rel}} \max\{\|r^{i+1}\|_2, \|s^{i+1}\|_2\}, \quad \epsilon_{\text{dual}} = \sqrt{2Kn}\epsilon_{\text{abs}} + (\epsilon_{\text{rel}}/\lambda)\|(u^i, \tilde{u}^i)\|_2,$$

for some absolute tolerance $\epsilon_{\text{abs}} > 0$ and relative tolerance $\epsilon_{\text{rel}} > 0$.

Selecting the penalty parameter. Algorithm 4.1 will converge regardless of the choice of the penalty parameter λ . However, the choice of the penalty parameter can affect the speed of convergence. We adopt the simple adaptive scheme (He et al., 2000; Wang and Liao, 2001)

$$\lambda^{i+1} := \begin{cases} \lambda^i/\tau^{\text{incr}} & \text{if } \|r^i\|_2 > \mu\|s^i\|_2 \\ \tau^{\text{decr}}\lambda^i & \text{if } \|s^i\|_2 > \mu\|r^i\|_2 \\ \lambda^i & \text{otherwise,} \end{cases}$$

where $\mu > 1$, $\tau^{\text{incr}} > 1$, and $\tau^{\text{decr}} > 1$ are parameters. (We recommend $\mu = 5$, $\tau^{\text{incr}} = 2$, and $\tau^{\text{decr}} = 2$.) We found that this simple scheme with $\lambda^0 = 1$ worked very well across all of our experiments. When $\lambda^{i+1} \neq \lambda^i$, we must re-scale the dual variables, since we are using with scaled dual variables. The re-scaling is given by

$$u^{i+1} = cu^{i+1}, \quad \tilde{u}^{i+1} = c\tilde{u}^{i+1},$$

where $c = \lambda^{i+1}/\lambda^i$.

Regularization path via warm-start. Our algorithm supports *warm starting* by choosing the initial point θ^0 as an estimate of the solution, for example, the solution of a closely related problem (*e.g.*, a problem with slightly varying hyper-parameters.)

Software implementation. We provide an (easily extensible) implementation of the ideas described in the paper, available at www.github.com/cvxgrp/strat_models. We use `numpy` for dense matrix representation and operations (Van Der Walt et al., 2011), `scipy` for sparse matrix operations and statistics functions (Jones et al., 2001), `networkx` for graph factory functions and Laplacian matrix computation (Hagberg et al., 2008), `torch` for L-BFGS and GPU computation (Paszke et al., 2017), and `multiprocessing` for parallel processing. We provide implementations for local loss and local regularizers for creating a custom stratified model. A stratified model can be instantiated with the following code:

```
base_model = strat_models.BaseModel(loss,reg)
model = strat_models.StratifiedModel(base_model, G).
```

Here, `loss` and `reg` are implementations for the local loss and local regularizer, respectively, and `G` is a `networkx` graph with nodes corresponding to \mathcal{Z} describing the Laplacian. The stratified model class supports the method

```
model.fit(data),
```

where `data` is a Python dictionary with with the data records (x, y, z) (or just (y, z) for distribution estimates). We also provide methods that automatically compute cross validation scores.

We note that our implementation is for the most part expository and for experimentation with stratified models; its speed could evidently be improved by using a compiled language (*e.g.*, C or C++). Practitioners looking to use these methods at a large scale should develop specialized codes for their particular application using the ideas that we have described.

5. Examples

In this section we illustrate the effectiveness of stratified models by combining base fitting methods and regularization graphs to create stratified models. In each example, we fit three models: a stratified model without Laplacian regularization (which we refer to as a *separate model*), a *common model* without stratification, and a *stratified model* with non-trivial edge weights. For each model, we performed a validation technique and selected the hyper-parameters that performed best over this technique. We note that these examples are all highly simplified in order to illustrate their usage; better models can be devised using the very same techniques illustrated. For example, in all examples we utilize one hyper-parameter per regularization graph, where we could in fact utilize one hyper-parameter per edge weight (though this would greatly increase the amount of hyper-parameters to be tuned). Even with these highly simplified Laplacian regularized stratified models, we find that the stratified model significantly outperforms the other two methods in each example.

The code is available online at https://github.com/cvxgrp/strat_models. All numerical experiments were performed on an unloaded Intel i7-8700K CPU.

Table 1: Mesothelioma results.

Model	Cross-validated ANLL	Cross-validated error
Separate	0.70 ± 0.016	0.51 ± 0.039
Stratified	0.59 ± 0.019	0.27 ± 0.021
Common	1.82 ± 0.34	0.47 ± 0.064

5.1 Mesothelioma classification

We consider the problem of predicting whether a patient has mesothelioma, a form of cancer, given their sex, age, and other medical features that were gathered during a series of patient encounters and laboratory studies.

Dataset. We obtained data describing 324 patients from the Dicle University Faculty of Medicine (Er et al., 2012; Dua and Graff, 2019). The dataset is comprised of males and females between (and including) the ages of 19 and 85, with 96 (29.6%) of the patients diagnosed with mesothelioma. The 32 medical features in this dataset include: city, asbestos exposure, type of MM, duration of asbestos exposure, diagnosis method, keep side, cytology, duration of symptoms, dyspnoea, ache on chest, weakness, habit of cigarette, performance status, white blood cell count (WBC), hemoglobin (HGB), platelet count (PLT), sedimentation, blood lactic dehydrogenase (LDH), alkaline phosphatase (ALP), total protein, albumin, glucose, pleural lactic dehydrogenase, pleural protein, pleural albumin, pleural glucose, dead or not, pleural effusion, pleural thickness on tomography, pleural level of acidity (pH), C-reactive protein (CRP), class of diagnosis (whether or not the patient has mesothelioma). We randomly split the data into five folds.

Data records. The ‘diagnosis method’ feature is perfectly correlated with the output, so we removed it (this was not done in many other studies on this dataset which led to near-perfect classifiers). We performed rudimentary feature engineering on the raw medical features to derive a feature vector $x \in \mathbf{R}^{46}$. The outcomes $y \in \{0, 1\}$ denote whether or not the patient has mesothelioma, with $y = 1$ meaning the patient has mesothelioma. The stratification feature z is a tuple consisting of the patient’s sex and age; for example, $z = (\text{Male}, 62)$ corresponds to a 62 year old male. Here the number of stratification features $K = 2 \cdot 67 = 134$.

Data model. We model the conditional probability of contracting mesothelioma given the features using logistic regression, as described in §3.1.2. We employ sum of squares regularization on the model parameters, with weight γ_{local} .

Regularization graph. We take the Cartesian product of two regularization graphs:

- *Sex.* The regularization graph has one edge between male and female, with edge weight γ_{sex} .
- *Age.* The regularization graph is a path graph between ages, with edge weight γ_{age} .

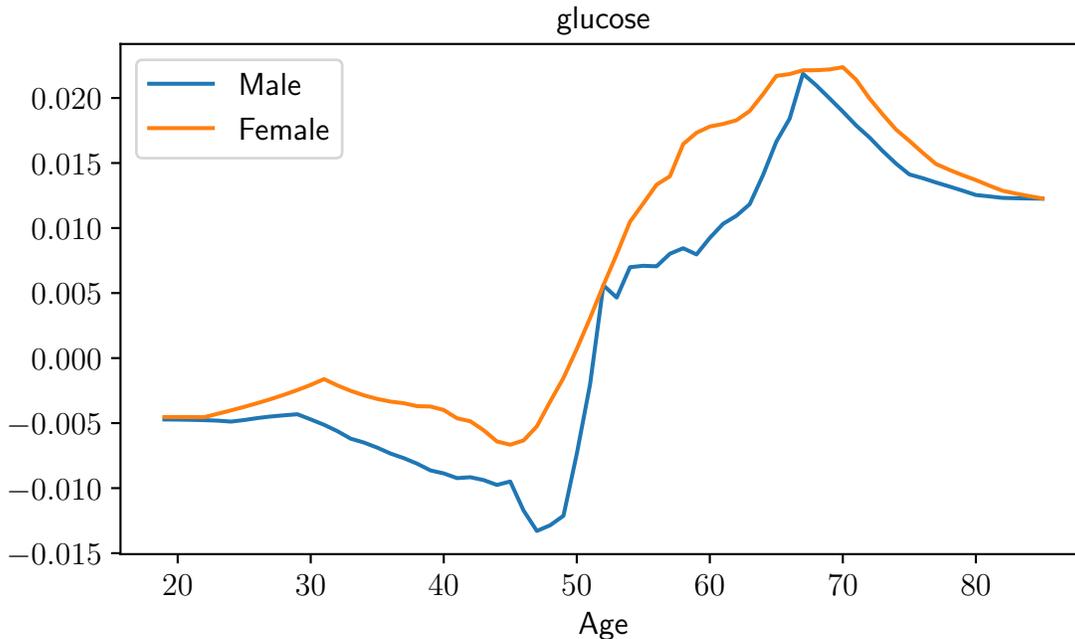


Figure 1: Glucose parameter versus age, for males and females.

Results. We used $\gamma_{\text{local}} = 12.9$ for the separate model and $\gamma_{\text{local}} = 0.004$ for the common model; we used $\gamma_{\text{local}} = .52$, $\gamma_{\text{sex}} = 10$, and $\gamma_{\text{age}} = 500$ for the stratified model, which were obtained by selecting the hyper-parameter combination that minimized the 5-fold cross-validated average negative log likelihood (ANLL). We compare the cross-validated ANLL and prediction error on the test set between all three models in table 1. The stratified model performs much better at predicting the presence of mesothelioma than the common model and the separate model. Figure 1 displays the stratified model glucose parameter over age and sex.

5.2 House price prediction

We consider the problem of predicting the logarithm of a house’s sale price based on its geographical location (given as latitude and longitude), and various features describing the house.

Data records. We gathered a dataset of sales data for homes in King County, WA from May 2014 to May 2015. Each record includes the latitude/longitude of the sale and $n = 10$ features: the number of bedrooms, number of bathrooms, number of floors, waterfront (binary), condition (1-5), grade (1-13), year the house was built (1900-2015), square footage of living space, square footage of the lot, and a constant feature (1). We randomly split the dataset into five folds, and we standardized the features so that they have zero mean and unit variance.

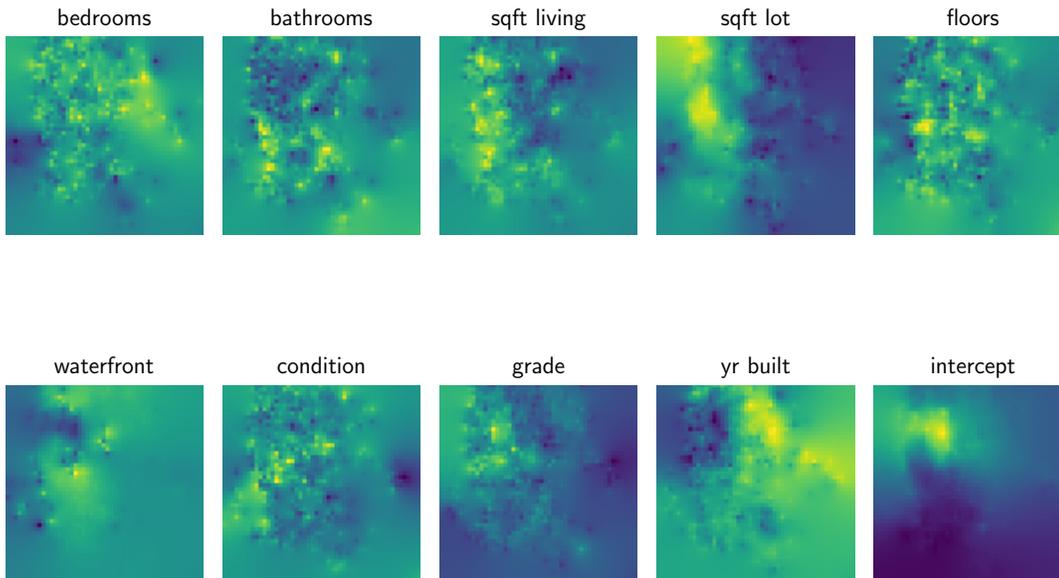


Figure 2: House price prediction coefficients.

Table 2: House price prediction results.

Model	No. parameters	Cross-validated RMS error
Separate	22500	2.503 ± 0.159
Stratified	22500	0.177 ± 0.001
Common	10	0.316 ± 0.002
Random forest	1070412	0.299 ± 0.003

Data model. The data model here is ordinary regression with square loss. We use the sum of squares local regularization function (excluding the intercept) with regularization weight γ_{local} .

Regularization graph. We binned latitude/longitude into 50×50 equally sized bins. The regularization graph here is a grid graph with edge weight γ_{geo} .

Results. We compared a stratified model to a separate model, a common model, and a random forest regressor with 100 trees (widely considered to be the best “out of the box” model). We used $\gamma_{\text{local}} = 0.001$ for the separate model, $\gamma_{\text{local}} = 0.001$ for the common model, and $\gamma_{\text{local}} = 0.001$ and $\gamma_{\text{geo}} = 18.5$ for the stratified model. All of these hyper-parameters were selected by performing 5-fold cross-validation and selecting the hyper-parameters that minimized the 5-fold RMS error.

We gave the latitude and longitude as raw features to the random forest model. In table 2, we show the size of these models (for the random forest this is the total number of nodes) and their cross-validated RMS error. The Laplacian regularized stratified model performs better than the other models, and in particular, outperforms the random forest, which has almost two orders of magnitude more parameters and is much less interpretable.

In figure 2, we show the model parameters for each feature across location. In this visualization, the brightness of a particular location can be interpreted as the influence that increasing that feature would have on log sales price. (A dark spot means that an increase in that feature in fact decreases log sales price.) For example, the waterfront feature seems to have a positive effect on sales price only in particular coastal areas.

5.3 Senate elections

We model the probability that a United States Senate election in a particular state and election year is won by the Democratic party.

Dataset. We obtained data describing the outcome of every United States Senate election from 1976 to 2016 (every two years, 21 time periods) for all 50 states (Data and Lab, 2017). At most one Senator is elected per state per election, and approximately 2/3 of the states elect a new Senator each election. We created a training dataset consisting of the outcomes of every Senate election from 1976 to 2012, and a test dataset using 2014 and 2016.

Data records. In this problem, there is no x . The outcome is $y \in \{0, 1\}$, with $y = 1$ meaning the candidate from the Democratic party won. The stratification feature z is a tuple consisting of the state (there are 50) and election year (there are 21); for example, $z = (\text{GA}, 1994)$ corresponds to the 1994 election in Georgia. Here the number of stratification features $K = 50 \cdot 21 = 1050$. There are 639 training records and 68 test records.

Data model. Our model is a Bernoulli model of the probability that the election goes to a Democrat (see §3.1.3). For each state and election year, we have a single Bernoulli parameter that can be interpreted as the probability that state will elect a candidate from the Democratic party. To be sure that our model never assigns zero likelihood, we let $r(\theta) = 0$ and $\Theta = [\epsilon, 1 - \epsilon]$, where ϵ is some small positive constant; we used $\epsilon = 1 \times 10^{-5}$. Only approximately 2/3 of states hold Senate elections each election year, so our model makes a prediction of how a Senate race might unfold in years when a particular states' seats are not up for re-election.

Regularization graph. We take the Cartesian product of two regularization graphs:

- *State location.* The regularization graph is defined by a graph that has an edge with edge weight γ_{state} between two states if they share a border. (To keep the graph connected, we assume that Alaska borders Washington and that Hawaii borders California. There are 109 edges in this graph.)
- *Year.* The regularization graph is a path graph, with edge weight γ_{year} . (There are 20 edges in this graph.)

Table 3: Congressional elections results.

Model	Train ANLL	Test ANLL
Separate	0.69	1.00
Stratified	0.48	0.61
Common	0.69	0.70

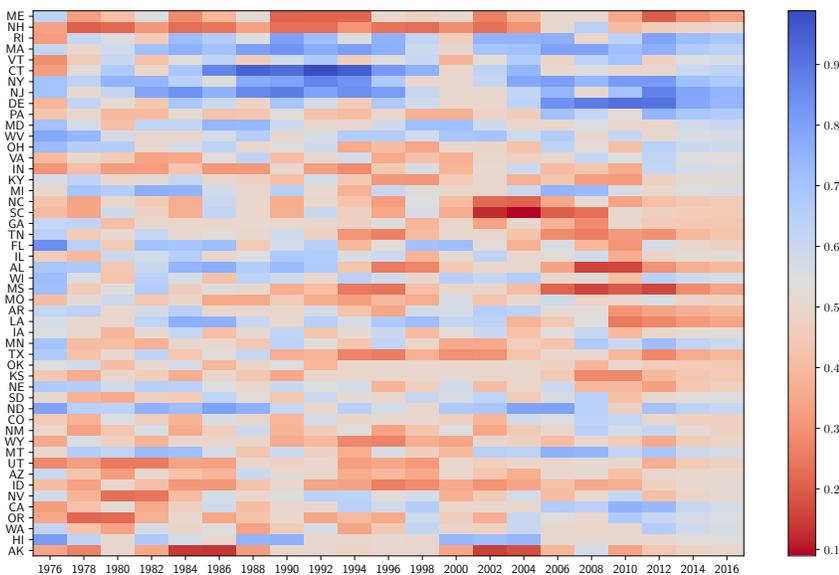


Figure 3: A heatmap representing the Bernoulli parameters across election year and state.

Results. We ran the fitting method with $\gamma_{\text{state}} = 1$ and $\gamma_{\text{year}} = 4$. Table 3 shows the train and test ANLL of the three models on the training and test sets. We see that the stratified model outperforms the other two models. Figure 3 shows a heatmap of the estimated Bernoulli parameter in the stratified model for each state and election year. The states are sorted according to the Fiedler eigenvector (the eigenvector corresponding to the smallest nonzero eigenvalue) of the Laplacian matrix of the state location regularization graph, which groups states with similar parameters near each other. High model parameters correspond to blue (Democrat) and low model parameters correspond to red (Republican and other parties). We additionally note that the model parameters for the entire test years 2014 and 2016 were estimated using no data.

5.4 Chicago crime prediction

We consider the problem of predicting the number of crimes that will occur at a given location and time in the greater Chicago area in the United States.

Dataset. We downloaded a dataset of crime records from the greater Chicago area, collected by the Chicago police department, which include the time, location, and type of crime (Department, 2019). There are 35 types of recorded crimes, ranging from theft and battery to arson. (For our purposes, we ignore the type of the crime.) From the dataset, we created a training set, composed of the recorded crimes in 2017, and a test set, composed of the recorded crimes in 2018. The training set has 263 752 records and the test set has 262 365 records.

Data records. We binned latitude/longitude into 20×20 equally sized bins. Here there are no features x , the outcome y is the number of crimes, and the stratification feature z is a tuple consisting of location bin, week of the year, day of the week, and hour of day. For example, $z = ((10, 10), 1, 2, 2)$ could correspond to a latitude between 41.796 and 41.811, a longitude between -87.68 and -87.667, on the first week of January on a Tuesday between 1AM and 2AM. Here the number of stratification features $K = 20^2 \cdot 52 \cdot 7 \cdot 24 = 3\,494\,400$.

Creating the dataset. Recall that there are 263 752 recorded crimes in our training data set. However, the fact that there were no recorded crimes in a time period is itself a data point. We count the number of recorded crimes for each location bin, day, and hour in 2017 (which could be zero), and assign that number as the single data point for that stratification feature. Therefore, we have 3 494 400 training data points, one for each value of the stratification feature. We do the same for the test set.

Data model. We model the distribution of the number of crimes y using a Poisson distribution, as described in §3.1.3. To be sure that our model never assigns zero log likelihood, we let $r(\theta) = 0$ and $\Theta = [\epsilon, \infty)$, where ϵ is some small constant; we used $\epsilon = 1 \times 10^{-5}$.

Regularization graph. We take the Cartesian product of three regularization graphs:

- *Latitude/longitude bin.* The regularization graph is a two-dimensional grid graph, with edge weight γ_{loc} .
- *Week of the year.* The regularization graph is a cycle graph, with edge weight γ_{week} .
- *Day of the week.* The regularization graph is a cycle graph, with edge weight γ_{day} .
- *Hour of day.* The regularization graph is a cycle graph, with edge weight γ_{hour} .

The Laplacian matrix has over 37 million nonzero entries and the hyper-parameters are γ_{loc} , γ_{week} , γ_{day} , and γ_{hour} .

Results. We ran the fitting method with

$$\gamma_{\text{loc}} = \gamma_{\text{week}} = \gamma_{\text{day}} = \gamma_{\text{hour}} = 100.$$

The method converged to tolerances of $\epsilon_{\text{rel}} = 1 \times 10^{-6}$ and $\epsilon_{\text{abs}} = 1 \times 10^{-6}$ in 464 iterations, which took about 434 seconds. For each of the three models, we calculated the average

Table 4: Chicago crime results.

Model	Train ANLL	Test ANLL
Separate	0.068	0.740
Stratified	0.221	0.234
Common	0.279	0.278

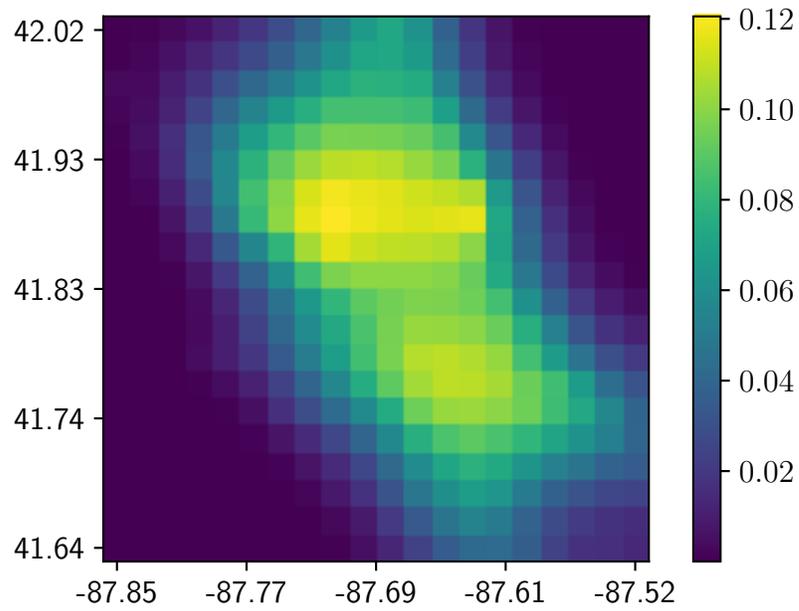


Figure 4: Rate of crime in Chicago for each latitude/longitude bin averaged over time, according to the stratified model.

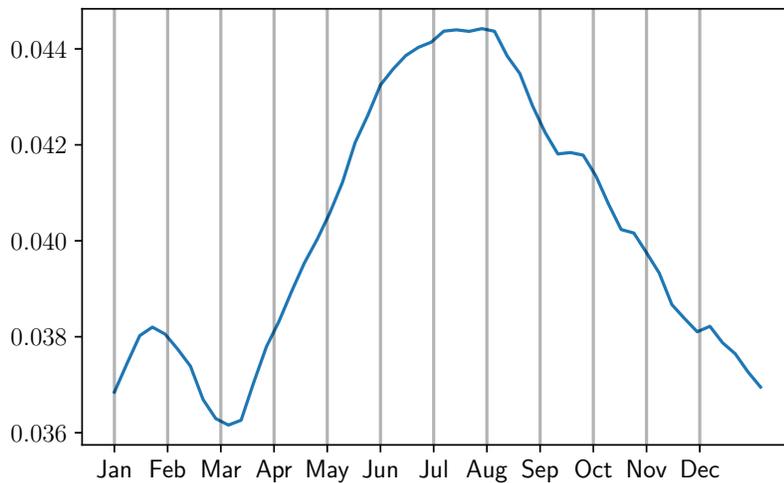


Figure 5: Rate of crime in Chicago versus week of the year averaged over latitude/longitude bins, according to the stratified model.

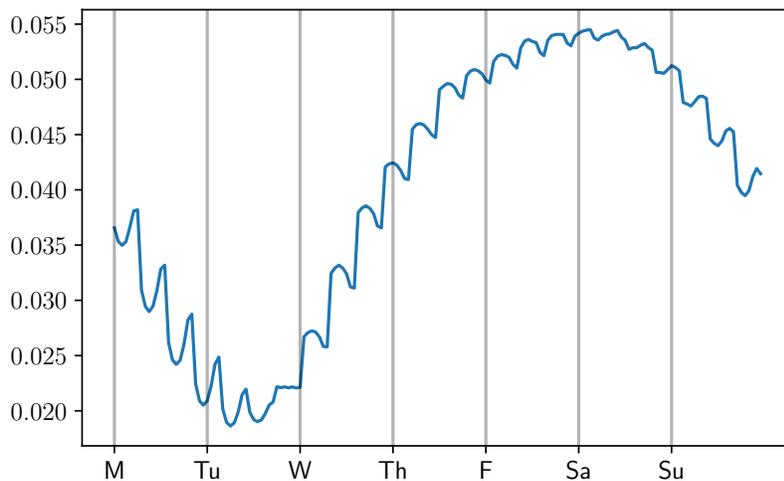


Figure 6: Rate of crime in Chicago versus hour of the week averaged over latitude/longitude bins, according to the stratified model.

negative log-likelihood (ANLL) of the training and test set (see table 4). We also provide visualizations of the parameters of the fitted stratified model. Figure 4 shows the rate of crime, according to each model, in each location (averaged over time), figure 5 shows the rate of crime, according to each model, for each week of the year (averaged over location and day), and figure 6 shows the rate of crime, according to each model, for each hour of the day (averaged over location and week). (This figure shows oscillations in crime rate with a period around 8 hours. We are not sure what this is, but suspect it may have to do with work shifts.)

6. Extensions and variations

In §3 and §4 we introduced the general idea of stratified model fitting and a distributed fitting method. In this section, we discuss possible extensions and variations to the fitting and the solution method.

Varied loss and regularizers. In our formulation of stratified model fitting, the local loss and regularizer in the objective is a sum of the K local losses and regularizers, which are all the same (save for problem data). With slight alterations, the ideas described in this paper can extend to the case where the model parameter for each stratification feature has different local loss and regularization functions.

Nonconvex base fitting methods. We now explore the idea of fitting stratified models with *nonconvex* local loss and regularization functions. The algorithm is exactly the same, except that we replace the θ and $\tilde{\theta}$ update with approximate minimization. ADMM no longer has the guarantees of converging to an optimal point (or even converging at all), so this method must be viewed as a *local* optimization method for stratified model fitting, and its performance will depend heavily on the parameter initialization. Despite the lack of convergence guarantees, it can be very effective in practice, given a good approximate minimization method.

Different sized parameter vectors. It is possible to handle θ_k that have different sizes with minor modifications to the ideas that we have described. This can happen, *e.g.*, when a feature is not applicable to one category of the stratification. A simple example is when one is stratifying on sex and one of the features corresponds to number of pregnancies. (It would not make sense to assign a number of pregnancies to men.) In this case, the Laplacian regularization can be modified so that only a subset of the entries of the model parameters are compared.

Laplacian eigenvector expansions. If the Laplacian regularization term is small, meaning that if θ_k varies smoothly over the graph, then it can be well approximated by a linear combination of a modest number, say M , of the Laplacian eigenvectors (Tuck and Boyd, 2020). The smallest eigenvalue is always zero, with associated eigenvector $\mathbf{1}$; this corresponds to the common model, *i.e.*, all θ_k are the same. The other $M - 1$ eigenvectors can be computed from the graph, and we can change variables so that the coefficients of the expansion are the variables. This technique can potentially drastically reduce the number of variables in the problem.

Coordinate descent Laplacian solver. It is possible to solve a regularized Laplacian system $Ax = b$ where $A = L + (1/\lambda)I$ by applying randomized coordinate descent (Nesterov, 2012) to the optimization problem

$$\text{minimize } \frac{1}{2}x^T Ax - b^T x,$$

which has solution $x = A^{-1}b$. The algorithm picks a random row $i \in \{1, \dots, K\}$, then minimizes the objective over x_i , to give

$$x_i = \frac{b_i - \sum_{j \neq i} a_{ij}x_j}{a_{ii}}, \quad (6)$$

and repeats this process until convergence. We observe that to compute the update for x_i , a vertex only needs the values of x at its neighbors (since a_{ij} is only nonzero for connected vertices). This algorithm is guaranteed to converge under very general conditions (Richtárik and Takáč, 2014).

Decentralized implementation. Algorithm 4.1 can be implemented in a decentralized manner, *i.e.*, where each vertex only has access to its own parameters, dual variables, and edge weights, and can only communicate these quantities to adjacent vertices in the graph. Line 1, line 2, and line 4 can be obviously be performed in parallel at each vertex of the graph, using only local information. Line 3 requires coordination across the graph, and can be implemented using a decentralized version of the coordinate descent Laplacian solver described above.

The full decentralized implementation of the coordinate descent method goes as follows. Each vertex broadcasts its value to adjacent vertices, and starts a random length timer. Once a vertex's timer ends, it stops broadcasting and collects the values of the adjacent vertices (if one of them is not broadcasting, then it restarts the timer), then computes the update (6). It then starts another random length timer and begins broadcasting again. The vertices agree beforehand on a periodic interval (*e.g.*, every 15 minutes) to complete line 3 and continue with the algorithm.

Acknowledgments

Jonathan Tuck is supported by the Stanford Graduate Fellowship in Science and Engineering. Shane Barratt is supported by the National Science Foundation Graduate Research Fellowship under Grant No. DGE-1656518. The authors thank Trevor Hastie and Robert Tibshirani for helpful comments on an early draft of this paper.

Appendix A. Proximal operators

Recall that for $\theta \in \mathbf{R}^n$, the proximal operator $\mathbf{prox}_{tf} : \mathbf{R}^n \rightarrow \mathbf{R}^n$ of a function $f : \mathbf{R}^n \rightarrow \mathbf{R} \cup \{+\infty\}$ and parameter $t > 0$ is defined as

$$\mathbf{prox}_{tf}(\nu) = \operatorname{argmin}_{\theta \in \operatorname{dom} f} (tf(\theta) + (1/2)\|\theta - \nu\|_2^2).$$

In this section, we list some functions encountered in this paper and their associated proximal operators.

Indicator function of a convex set. If \mathcal{C} is a closed nonempty convex set, and we define $f(\theta)$ as 0 if $\theta \in \mathcal{C}$ and $+\infty$ otherwise, then

$$\mathbf{prox}_{tf}(\nu) = \Pi_{\mathcal{C}}(\nu),$$

i.e., the projection of ν onto \mathcal{C} . (Note: If we allow \mathcal{C} to be nonconvex, then $\mathbf{prox}_{tf}(\nu)$ is still of this form, but the projection is not guaranteed to be unique.) For example, if $\mathcal{C} = \mathbf{R}_+^n$, then $(\mathbf{prox}_{tf}(\nu))_i = \max\{\nu_i, 0\}$.

Sum of squares. When $f(\theta) = (1/2)\|\theta\|_2^2$, the proximal operator is given by

$$\mathbf{prox}_{tf}(\nu) = \frac{\nu}{t+1}.$$

ℓ_1 norm. When $f(\theta) = \|\theta\|_1$, the proximal operator is given by soft-thresholding, or

$$\mathbf{prox}_{tf}(\nu) = (\nu - t)_+ - (-\nu - t)_+.$$

ℓ_2 norm. The proximal operator of $f(\theta) = \|\theta\|_2$ is

$$\mathbf{prox}_{tf}(\nu) = \left(1 - \frac{t}{\|\nu\|_2}\right)_+ \nu.$$

Negative logarithm. The proximal operator of $f(\theta) = -\log \theta$ is

$$\mathbf{prox}_{tf}(\nu) = \frac{\nu + \sqrt{\nu^2 + 4t}}{2}.$$

Sum of ℓ_1 and ℓ_2 -squared. The proximal operator of $f(\theta) = \|\theta\|_1 + (\gamma/2)\|\theta\|_2^2$ for $\gamma \geq 0$, is

$$\mathbf{prox}_{tf}(\nu) = \frac{1}{1 + \gamma t} \mathbf{prox}_{t\|\cdot\|_1}(\nu).$$

Quadratic. If $f(\theta) = (1/2)\theta^T A \theta + b^T \theta + c$, with $A \in \mathbf{S}_+^n$, $b \in \mathbf{R}^n$, and $c \in \mathbf{R}$, then

$$\mathbf{prox}_{tf}(\nu) = (I + tA)^{-1}(\nu - tb).$$

If, *e.g.*, $f(\theta) = \frac{1}{2}\|A\theta - b\|_2^2$, then $\mathbf{prox}_{tf}(\nu) = (I + tA^T A)^{-1}(\nu - tA^T b)$.

Poisson negative log likelihood. Here $f(\theta) = \sum_{i=1}^N \theta - y_i \log \theta$, where $y_i \in \mathbb{Z}_+$ and $\theta > 0$. If we let $S = \sum_{i=1}^N y_i$, then

$$\mathbf{prox}_{tf}(\nu) = \frac{\nu - tN + \sqrt{(tN - \nu)^2 + 4tS}}{2}.$$

Covariance maximum likelihood. Here

$$f(\theta) = \mathbf{Tr}(S\theta) - \log \det(\theta).$$

We want to find $\mathbf{prox}_{tf}(V) := \underset{\theta}{\operatorname{argmin}} (\mathbf{Tr}(S\theta) - \log \det(\theta) + (1/2t)\|\theta - V\|_F^2)$. The first-order optimality condition (along with the implicit constraint that $\theta \succ 0$) is that the gradient should vanish, *i.e.*,

$$S - \theta^{-1} + (1/t)(\theta - V) = 0.$$

Rewriting, this is

$$(1/t)\theta - \theta^{-1} = (1/t)V - S,$$

implying that θ and $S - (1/t)V$ share the same eigenvectors (Witten and Tibshirani, 2009), stored in Q . Let w_i denote the i th eigenvalue of θ , and s_i the i th eigenvalue of $S - (1/t)V$. Then we have

$$1/w_i + (1/t)w_i = s_i, \quad i = 1, \dots, n.$$

To solve for $w = (w_1, \dots, w_n)$, we solve these n 1-dimensional quadratic equations, with the i th equation solved by

$$w_i = \frac{ts_i + \sqrt{t^2s_i^2 + 4t}}{2}.$$

The proximal operator is then

$$\mathbf{prox}_{tf}(V) = Q \mathbf{diag}(w) Q^T.$$

Bernoulli negative log-likelihood. Here

$$f(\theta) = -(\mathbf{1}^T y) \log(\theta) - (n - \mathbf{1}^T y) \log(1 - \theta),$$

with $y \in \mathbf{R}^n$ is problem data and $\theta \in [0, 1]$. We want to find

$$\mathbf{prox}_{tf}(\nu) := \underset{\theta}{\operatorname{argmin}} (-\mathbf{1}^T y \log(\theta) - (n - \mathbf{1}^T y) \log(1 - \theta) + (1/2t)(\theta - \nu)^2).$$

By setting the derivative of the above argument with respect to θ to zero, we find that

$$\theta^3 - \theta^2(1 - \nu) - \theta(nt - \nu) + t\mathbf{1}^T y = 0.$$

Solving this cubic equation (with respect to θ) for the solution that lies in $[0, 1]$ yields the result of the proximal operator.

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