Submodularity in Batch Active Learning and Survey Problems on Gaussian Random Fields

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Abstract

Many real-world datasets can be represented in the form of a graph whose edge weights designate similarities between instances. A discrete Gaussian random field (GRF) model is a finite-dimensional Gaussian process (GP) whose prior covariance is the inverse of a graph Laplacian. Minimizing the trace of the prediction covariance \( \Sigma \) (V-optimality) on GRFs has proven successful in batch active learning classification problems with budget constraints. However, its worst-case bound has been missing. We show that the V-optimality on GRFs as a function of the batch query set is submodular and hence its greedy selection algorithm guarantees an \( (1 - 1/e) \) approximation ratio. Moreover, GRF models have the absence-of-suppressor (AoS) condition. For active survey problems, we propose a similar survey criterion which minimizes \( 1^T \Sigma 1 \). In practice, V-optimality criterion performs better than GPs with mutual information gain criteria and allows nonuniform costs for different nodes.

1 Introduction

In many real-world applications, such as author classification based on coauthorship graphs, one or more output variables need to be predicted from a subset of queryable inputs, constrained by a budget. In batch active learning applications, an algorithm refines its prediction by generating a list of queries for domain experts to answer [2, 5, 8]. In both cases, we consider the situation where the similarities between all instances, both labeled and unlabeled, are known a-priori. We formulate these similarities by a graph \( G = (V, E) \) with edge weights \( W \). The goal is to optimize the subset of nodes to query within the budget so that the risk in prediction can be minimized. One common risk is the predictive variance, measured by the trace of the covariance matrix of multivariate outputs. Minimizing this risk is known as the V-optimality criterion.

Commonly used models for these subset selection or batch active learning problems are discrete Gaussian random fields (GRF) [2, 5], finite-dimensional Gaussian processes (GP) [1], and linear regression with prior knowledge of covariances [3, 4]. GRFs formulate the input-output correspondence by the conditional distribution of a (maybe improper) gaussian prior whose inverse covariance is set to be the graph Laplacian, sometimes with diagonal regularization. Finite-dimensional GPs define the prior as \( \mathcal{N}(0, W) \), where \( W \) is an arbitrary covariance matrix. Finally, linear regression with prior knowledge of covariance is essentially a finite-dimensional GP with linear covariance.

GPs have been used as a base model for both subset selection and active learning [1]. One minor issue is that they require \( W \) to be positive-semidefinite. However a major issue is that they do not have a provable lower bound for optimality [4]. Instead, [1] used an alternative mutual information gain (MIG) criterion for selecting nodes for query. The MIG-criterion is naturally a normalized, monotone, and submodular function. As a result, a greedy algorithm garantuees an \( (1 - 1/e) \) approximation ratio. However, there is not classification-related risk function associated and the log determinates of covariance submatrices are sensitive to small eigenvalues, which can be a problem.
Another direction with GP models is to constrain the prior kernel matrix. [4] constrained the prior covariance matrix such that its diagonal entries are 1s and off-diagonal entries some very small values. However, these models can be approximated by regularized GRF models in that 
\[(I + \varepsilon W)^{-1} = I - \varepsilon W + \varepsilon^2 W^2 - \cdots \approx I - \varepsilon W, \text{ when } \lim_{\varepsilon \to 0} \varepsilon^2 W^2 = 0, \text{ with small } \varepsilon > 0.\]
[4] also proposed an absence-of-suppressors (AoS) condition that is sufficient for submodularity. However, it is generally hard to verify if a discrete GP meets the AoS condition, whereas we will show that every GRF is AoS.

Finally, [5] demonstrates semi-supervised and active learning using GRFs. Their motivation is that unlabeled nodes can reasonably influence the prediction by their edge weights with other nodes, because these weights can encode information such as sample density (e.g. using a radial basis function kernel to calculate the weight matrix). Later research [1] used spectral methods to boost the computation speed for subset selection in batch active learning. However, they only solved the subset selection case where every node query has a unit cost. Moreover, in both works, the optimization lacks worst-case guarantees.

In this paper, we properly define a (regularized) discrete GRF model and prove an \((1 - 1/\varepsilon)\) approximation ratio lower bound with the V-optimality criterion under a limited budget for a greedy subset selection algorithm. We also extend this bound for the scenario where different nodes have different costs. GRF models are a special type of AoS GP models. Conversely, any GP model whose conditional covariance matrices are always nonnegative is a GRF model and is AoS. From real-world experiments we show that GRF models using the V-optimality criterion present advantages over GP models with the MIG criterion and random selection.

## 2 Gaussian Random Fields and Subset Selection Problems

### 2.1 The Gaussian Random Field (GRF) model

Suppose the dataset can be represented in the form of a connected undirected graph \(G = (V, E)\) where each node has an (either known or unknown) label and each edge \(e_{ij}\) has a fixed nonnegative weight \(w_{ij}(= w_{ji})\) that reflects the proximity, similarity, etc between nodes \(v_i\) and \(v_j\). Define the graph Laplacian of \(G\) to be \(L_0 = \text{diag}(W) - W\) and the regularized graph Laplacian to be \(L_\sigma = L_0 + \text{diag}(\sigma_1^{-2}, ..., \sigma_N^{-2})\) with \(\sigma_i > 0, \forall i = 1, ..., N\). We use \(L\) to generalize both.

The discrete Gaussian Random Field (GRF) is a joint continuous distribution on both labeled and unlabeled nodes, containing one tunable “heat” parameter \(\beta > 0\), as

\[
P(y) \propto \exp \left( -\frac{\beta}{2} y^T L y \right) = \begin{cases} \exp \left( -\frac{\beta}{2} \sum_{i,j} w_{ij} (y_i - y_j)^2 \right) & \text{(unregularized)} \\ \exp \left( -\frac{\beta}{2} \sum_{i,j} w_{ij} (y_i - y_j)^2 + \sum_i \frac{1}{\sigma_i^2} y_i^2 \right) & \text{(regularized).} \end{cases} \tag{1}
\]

Assuming labels \(y_L = \{y_{i,1}, ..., y_{i,|L|}\}\) are tagged as \(t_L \in [0, 1]^{|L|}\), a Gaussian Harmonic predictor predicts all unlabeled continuous nodes \(y_U = \{y_{u,1}, ..., y_{u,|U|}\}\) by factoring out known variables [5],

\[
P(y_U | y_L = t_L) \sim \mathcal{N}(f_U, \beta L_U^{-1}) = \mathcal{N}(f_U, \beta L_U^{-1}_{(V-L)}), \tag{2}
\]

where \(L_U\) is the submatrix consisting of the unlabeled row and column indices in \(L\), for example the lower right block of \(L = \begin{pmatrix} L_{ll} & L_{lu} \\ L_{ul} & L_{uu} \end{pmatrix}\) and \(f_U = (-L_U^{-1} L_{ul} t_L)\). By convention, \(L_{(V-L)}\) means the inverse of the submatrix. We use \(L_{(V-L)}\) and \(L_U\) interchangeably because \(L\) and \(U\) partition the set of all nodes \(V\).

In some problems, a test set \(T \subset U\) is specified. Define \(T\) to be a \(|T| \times |U|\) matrix such that \(t_{ij} = \delta(v_i, v_T)\), i.e. \(T y_U = y_T\). Otherwise, a default value of \(T\) is the identity matrix of size \(|U|\). By marginalizing out node variables in \(U \setminus T\) from (2), we have \(P(y_T | t_L) \sim \mathcal{N}(T f_U, \beta T L_{(V-L)}^{-1} T^T)\).

Notice that GRFs differ from general GPs in that the predictive mean \(f_U \in [0, 1]^{N-|L|}\) (Corollary 1). Unlike GPs, GRFs do not “squeeze” regression responses to \([0, 1]\) to get probability predictions.
2.2 Risk Minimization for Classification

Since in GRFs regression responses are taken directly as probability predictions, it is computationally and analytically more convenient to apply the regression loss and risk directly in the GRF as in [2]. Assume the L2 loss to be our classification loss, \( L_c(y, f) = \sum_{v_i \in \mathcal{E}} (y_i - f_i)^2 \), and a risk function whose input variable is the subset \( \mathcal{L} \) as

\[
R_c(\mathcal{L}) = \mathbb{E}[L_c(y, f) \mid y \in \mathcal{L}] = \mathbb{E} \left[ \sum_i (y_i + (TL^{-1}_u L_u y_\mathcal{L}))_i^2 \right] = \text{tr}(TL_u^{-1} T^T) \tag{3}
\]

2.3 The Subset Selection Problem (the Active Learning for Classification Problem)

Assume every vertex on the graph has a cost, (a unit cost if not specified), the major objective in this paper is to choose a subset of nodes \( \mathcal{L} = \{v_1, ..., v_{|L|}\} \) to query for labels, constrained by a given budget \( C \), such that the risk is minimized. Formally,

\[
\arg \min \mathcal{L} \quad R(\mathcal{L}) = R_c(\mathcal{L}) = \text{tr}(TL_{(\mathcal{Y} - \mathcal{L})}^{-1} T^T) \tag{4}
\]

Though not explicitly denoted, the specific matrix \( T = (\delta(v_i, v_u))_{i=1,j=1}^{T,|U|} \) depends on \( U = \mathcal{Y} - \mathcal{L} \).

3 Submodularity, Suppressor-free, and Bounds for Greedy Method

In § 3, we assume that \( L \) is nonsingular. This could be achieved by either deleting a node (a row and a column) from the original undirected connected graph Laplacian, i.e. assuming that the dataset always contains a fixed label, or by using the regularized \( L_g \). In these cases, \( L \) satisfies the following.

- \( L \) has proper signs, i.e. \( l_{ij} \geq 0 \) if \( i = j \) and \( l_{ij} \leq 0 \) if \( i \neq j \); \( \tag{5} \)
- \( L \) is undirected and connected, i.e. \( l_{ij} = l_{ji} \forall i, j \) and \( \sum_{j \neq i} (-l_{ij}) > 0 \ \forall i \); \( \tag{6} \)
- Node degree no less than number of edges, i.e. \( \sum_j l_{ij} = \sum_j l_{ji} \geq 0 \ \forall i = 1, ..., N \); \( \tag{7} \)
- \( L \) is nonsingular and therefore positive definite, i.e. \( \exists \text{s.t. } \sum_j l_{ij} = \sum_j l_{ji} > 0 \). \( \tag{8} \)

Conversely, our results hold if a finite-dimensional GP has covariance \( = (L^{-1}) \) and \( L \) satisfies (5-8).

3.1 Major results

- **Submodularity.** Under conditions (5-8), the risk reduction function \( R_\Delta(\mathcal{L}) := R(\emptyset) - R(\mathcal{L}) \) is normalized, monotone, and submodular, i.e.,

\[
R_\Delta(\emptyset) = 0 \tag{9}
\]

\[
R_\Delta(\mathcal{L}_1 \cup \mathcal{L}_2) \geq R_\Delta(\mathcal{L}_1) \tag{10}
\]

\[
R_\Delta(\mathcal{L}_1 \cup \{v\}) - R_\Delta(\mathcal{L}_1) \geq R_\Delta(\mathcal{L}_1 \cup \mathcal{L}_2 \cup \{v\}) - R_\Delta(\mathcal{L}_1 \cup \mathcal{L}_2) \tag{11}
\]

\( \forall \mathcal{L}_1, \mathcal{L}_2, v \)

- **Greedy Algorithm and near-optimal bounds.** If (9-11) is satisfied, the optimization problem (4) is NP-hard and the greedy selection algorithm (Alg 1) produces a query set \( \mathcal{L}_g \) that guarantee an \( (1 - 1/e) \) optimality bound [6],

\[
R_\Delta(\mathcal{L}_g) \geq (1 - \frac{1}{e}) \cdot R_\Delta(\mathcal{L}_*) \tag{12}
\]

where \( \mathcal{L}_* \) is the global (NP) optimizer under the constraint \( \sum_{v \in \mathcal{L}_*} c_v \leq \sum_{v \in \mathcal{L}_g} c_v \).

- **Relationship with suppressor-free models.** An absence-of suppressor (AoS) condition in regression models guarantees submodularity. With our notation, this condition is \( |\text{Corr}(y_i, y_j | \mathcal{L}_1 \cup \mathcal{L}_2)| \leq |\text{Corr}(y_i, y_j | \mathcal{L}_1)| \\forall v_i, v_j, \mathcal{L}_1, \mathcal{L}_2 \). An example of suppressor variable is some node \( v_k \in \mathcal{L}_2 - \mathcal{L}_1 \) such that \( y_i + y_j = y_k \). Such variable is counter-tuitive in prediction models because knowing \( y_k \) suppresses an unmodeled correlation between the predictors. We show that the GRF model is a perfect example for AoS condition.

\[^1|\text{Corr}(Z, \text{Res}(X_i, S))/\text{Res}(X_j, S))| \leq |\rho(Z, \text{Res}(X_i, S))| \] in the original paper.
Now that every term on the right side of (16) is nonnegative, the left side also has to be.

Thus, by assumption (8), the invertibility of $L$ implies that $(I - D^{-1} W)$ is invertible, i.e. having no 0 eigenvalue. Hence, $|\lambda_k| < 1, \forall k = 1, ..., N$ and $\lim_{n \to \infty} (D^{-1} W)^n = 0$. The latter yields the following,

$$ L^{-1} = (I - D^{-1} W)^{-1} = [I + D^{-1} W + (D^{-1} W)^2 + \cdots ] D^{-1}. \tag{15} $$

Since every term in the right hand side of (15) is nonnegative, $L^{-1}$ should also be nonnegative.

Corollary 1. GRF prediction functor $L_{ul}^{-1}$ maps $y_L \in [0,1]^{|L|}$ to $f_{ul} = -L_{ul}^{-1} L_{ul} y_L \in [0,1]^{[ul]}$.

Proof. Since $L_{ul} \geq 0$ and $-L_{ul} \geq 0$, we have $y_L \geq 0 \Rightarrow L_{ul}^{-1} (-L_{ul}) y_L \geq 0$ and $y_L \geq y_L' \Rightarrow L_{ul}^{-1} (-L_{ul}) y_L \geq L_{ul}^{-1} (-L_{ul}) y_L'$. On the other hand, $(L_{ul}, L_{ul}) \cdot 1 \geq 0$ and $L_{ul}^{-1} \geq 0$ imply $(I, L_{ul}^{-1} L_{ul}) \cdot 1 \geq 0$, i.e. $1 + L_{ul} L_{ul} \geq 0$. Hence, $1 \geq L_{ul}^{-1} L_{ul} \geq -L_{ul}^{-1} L_{ul} y_L$.

Lemma 2. Suppose $L = \begin{pmatrix} L_{11} & L_{12} \\ L_{21} & L_{22} \end{pmatrix}$ satisfies (5-8), then $L^{-1} - \begin{pmatrix} L_{11}^{-1} & 0 \\ 0 & 0 \end{pmatrix}$ is positive-semidefinite and nonnegative.

Proof. By block matrix inversion theorem,

$$ L^{-1} - \begin{pmatrix} L_{11} & 0 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} -L_{11}^{-1} & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} L_{22} - L_{12} L_{11}^{-1} L_{21} & -L_{21} L_{11}^{-1} \\ L_{11}^{-1} & I \end{pmatrix} \begin{pmatrix} -L_{11}^{-1} & 0 \\ 0 & 0 \end{pmatrix} \tag{16} $$

By assumption (8), $L^{-1}$ is positive-definite, so is its lower right corner $(L_{22} - L_{21} L_{11}^{-1} L_{12})^{-1}$. Thus, $L^{-1} - \begin{pmatrix} L_{11} & 0 \\ 0 & 0 \end{pmatrix}$ is positive-semidefinite.

By Lemma 1, $L^{-1} \geq 0$ and this implies that its lower right $(L_{22} - L_{21} L_{11}^{-1} L_{12})^{-1} \geq 0$. The submatrix $L_{11}$ also satisfies (5-8) and by Lemma 1, $L_{11} \geq 0$. By sign rule (5), $(-L_{12}) = (-L_{21})^T \geq 0$. Now that every term on the right side of (16) is nonnegative, the left side also has to be.

Lemma 3 (Monotonicity). For function $R_\Delta (L)$ defined in § 2.3, $R_\Delta (L_1 \cup L_2) \geq R_\Delta (L_1), \forall L_1, L_2.$

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Algorithm 1: Greedy subset selection. Fast realization of $*$ in [2], [5], and § 4.

Input: Node costs $c_v$, budget $C$, queryable pool $P$, objective function $R(L)$.

Output: A subset $L \subset \mathcal{P}$ by greedy selection.

Define $L \leftarrow \emptyset$, $R_{old} \leftarrow R(\emptyset)$.

while available pool $P' = \{ v' \in \mathcal{P} - L : c_{v'} + \sum_{v \in L} c_v \leq C \}$ is not empty do

- Find $v'_* \leftarrow \arg \min_{v' \in P'} R(L \cup \{v'_*\}) - R_{old}$.
- Update $L \leftarrow L \cup \{v'_*\}$, $R_{old} \leftarrow R(L)$.

3.2 Proofs

Lemma 1. For any $L$ satisfying (5-8), the inverse of $L$ is nonnegative, i.e. $L^{-1} \geq 0$ (entry-wise).

Proof. Define $D = \text{diag}(L)$ and $W = D - L$, we have $L = D - W = D(I - D^{-1} W)$.

According to (5), entry-wise $D \geq 0, W \geq 0$ and $D^{-1} W \geq 0$. Furthermore, by (7),

$$ 0 \leq D^{-1} W = \left( \frac{w_{ij}}{d_{ii}} \right)^N_{i,j=1} \leq \left( \frac{w_{ij}}{\sum_k w_{ik}} \right)^N_{i,j=1}, \tag{13} $$

$$ \|D^{-1} W\|_\infty := \sup_{\mathbf{x} \neq \mathbf{0}} \max_i \left| \frac{\|D^{-1} W \mathbf{x}\|_i}{\max_i |x_i|} \right| = \max_i \sum_j |\|D^{-1} W\|_{ij}| \leq \max_i \sum_j \frac{w_{ij}}{\sum_k w_{ik}} \leq 1. \tag{14} $$

Thus, any eigenvalue $\lambda_k$ and its corresponding eigenvector $v_k$ of $D^{-1} W$ needs to satisfy $|\lambda_k| \|v_k\|_\infty = \|\lambda_k v_k\|_\infty = \|D^{-1} W v_k\|_\infty \leq \|v_k\|_\infty$, i.e. $|\lambda_k| \leq 1 \ \forall k = 1, ..., N$.

Moreover, (8) the invertibility of $L$ implies that $(I - D^{-1} W)$ is invertible, i.e. having no 0 eigenvalue. Hence, $|\lambda_k| < 1, \forall k = 1, ..., N$ and $\lim_{n \to \infty} (D^{-1} W)^n = 0$. The latter yields the following,

$$ L^{-1} = (I - D^{-1} W)^{-1} = [I + D^{-1} W + (D^{-1} W)^2 + \cdots ] D^{-1}. \tag{15} $$

In the following, for any vector or matrix $A, A \geq 0$ always stands for $A$ being (entry-wise) nonnegative.
Lemma 4 (Submodularity). For function $R_\Delta(\mathcal{L})$ defined in § 2.3, $R_\Delta(\mathcal{L}_1 \cup \{v\}) - R_\Delta(\mathcal{L}_1) \geq R_\Delta(\mathcal{L}_1 \cup \mathcal{L}_2 \setminus \{v\}) - R_\Delta(\mathcal{L}_1 \cup \mathcal{L}_2)$, $\forall \mathcal{L}_1, \mathcal{L}_2, v$.

Proof. We may assume that $\mathcal{L}_1, \mathcal{L}_2$, and $\{v\}$ are disjoint. Without loss of generality, suppose

\[
L_{(V-\mathcal{L}_1)} = \begin{pmatrix}
L_{(V-\mathcal{L}_1),\mathcal{L}_2} & L_{(V-\mathcal{L}_1),\mathcal{L}_2,\{v\}} \\
L_{(V-\mathcal{L}_1),\mathcal{L}_2} & L_{\mathcal{L}_2}
\end{pmatrix}
\]

and $L_{(V-\mathcal{L}_1 \cup \mathcal{L}_2)} = \begin{pmatrix}
L_{(V-\mathcal{L}_1 \cup \mathcal{L}_2),\{v\}} \\
L_{(V-\mathcal{L}_1 \cup \mathcal{L}_2,\{v\})}
\end{pmatrix}$. Apply block matrix inversion theorem, when a test set is not specified, i.e. $T = I$ of size $|\mathcal{L}|$,

\[
R_\Delta(\mathcal{L}_1 \cup \{v\}) - R_\Delta(\mathcal{L}_1) = R_\Delta(\mathcal{L}_1 \cup \mathcal{L}_2) - R_\Delta(\mathcal{L}_1 \cup \mathcal{L}_2) = tr\left(\begin{pmatrix}
A & b \\
0 & c
\end{pmatrix}^{-1} - \begin{pmatrix}
A & 0 \\
0 & 0
\end{pmatrix}\right) = \begin{pmatrix}
A & b \\
0 & c
\end{pmatrix}^{-1} \left(\begin{pmatrix}
-1 \\
0
\end{pmatrix}\right)
\]

Notice that by sign rule (5), $-b \geq -\hat{b} \geq 0$ and by Lemma 2, $A^{-1} \geq \begin{pmatrix}
A^{-1} & 0 \\
0 & 0
\end{pmatrix} \geq 0$. Thus, $(-b^T)A^{-1}(-b) \geq (\hat{b}^T)A^{-1}(\hat{b}) \geq 0$ and $A^{-1}(-b) \geq \begin{pmatrix}
A^{-1} & 0 \\
0 & 0
\end{pmatrix} \hat{b} = A^{-1}(\hat{b}) \geq 0$. The proof when a test set $\mathcal{T}$ is specified is fundamentally similar because the indicator matrix $T$ is always applied to nonnegative vectors or matrices.
4 Extension to Active Survey and Tricks to Improve Efficiency

In an active survey problem[7], our goal is to actively query points to ultimately predict the proportion of a given class. Embedded in GRF models, it changes the loss function to the Mean Squared Error (MSE) \( L_s(y^*, f_T) = (\sum_{v_i \in T} (y_{v_i} - f_{v_i}))^2 \) and the risk to \( R_s(L) = T^T L^{-1} L T^T 1 \).

For the subset selection problem with this new objective function, all results in § 3 hold and the proofs are similar. Besides, we developed an algorithm with \( O(N^2.36 + kN^2) \) runtime complexity for \( k \) queries (\( O(kN^{3.36}) \) if implemented natively) similar to [2].

4.1 The Active Surveying Problem and The Proofs

Similar to (4), define the subset selection (active surveying) problem as

\[
\begin{align*}
\arg \min_{\mathcal{L}} \quad & R(\mathcal{L}) = R_s(\mathcal{L}) = 1^T T L^{-1}_{(\mathcal{V} \setminus \mathcal{L})} T 1 \\
\text{s.t.} \quad & \sum_{v \in \mathcal{L}} c_v \leq C.
\end{align*}
\]

(25)

We also assume (5-8) and \( R_\Delta(\mathcal{L}) := R(\emptyset) - R(\mathcal{L}) \). To prove Theorem 1 via Lemma 2 and 3, the only adjustment is with (20),

\[
R_\Delta(\mathcal{L}_1 \cup \{v\}) - R_\Delta(\mathcal{L}_1) = R_s(\mathcal{L}_1) - R_s(\mathcal{L}_1 \cup \{v\}) = 1^T T \left( \left( \begin{array}{c|c}
A & b \\
\hline
b^T & c
\end{array} \right)^{-1} - \left( \begin{array}{c}
A^{-1} \\
0
\end{array} \right) \right) T 1
\]

\[= 1^T T \left( \left( \begin{array}{c}
-A^{-1} b \\
1
\end{array} \right) \frac{1}{c - b^T A^{-1} b} \left( -b^T A^{-1}, 1 \right) \right) T 1 = \frac{1}{c - b^T A^{-1} b} \left( 1^T T \left( \begin{array}{c}
-A^{-1} b \\
1
\end{array} \right) \right)^2. \]  

(26)

Still, because \( -b \geq -\tilde{b} \geq 0, A^{-1} \geq \left( \begin{array}{c}
\tilde{A}^{-1} \\
0
\end{array} \right) \geq 0 \), and \( T \geq (T, 0) \geq 0 \), the above is larger than its counterpart in \( R_\Delta(\mathcal{L}_1 \cup \mathcal{L}_2 \cup \{v\}) - R_\Delta(\mathcal{L}_1 \cup \mathcal{L}_2) \). \( \Box \)

4.2 Tricks to Improve Efficiency: With Precomputed Covariance

In Algo 1, the most time-consuming step is to compute \( R(\mathcal{L} \cup \{v'\}) \) for every possible \( v' \in \mathcal{P} \), which in general involves taking the inverse of \( L_{(\mathcal{V} \setminus \mathcal{L}) \cup \{v'\}} \). Zhu et al. [5] presented a fast way to do this. Actually it can get even faster in the following way, assuming \( L_{(\mathcal{V} \setminus \mathcal{L}) \cup \{v'\}}^{-1} = \Sigma' = A^{-1}, \)

\[
L_{(\mathcal{V} \setminus \mathcal{L})}^{-1} = \Sigma = \left( \begin{array}{c|c}
A & b \\
\hline
b^T & c
\end{array} \right)^{-1} = \left( \begin{array}{c|c}
C & d \\
\hline
d^T & e
\end{array} \right), \text{ and } \Sigma_{v'v'} \text{ to be the last column of } \Sigma,
\]

\[
\left( \begin{array}{c|c}
C & d \\
\hline
d^T & e
\end{array} \right) = \left( \begin{array}{c|c}
A^{-1} & 0 \\
\hline
0 & 0
\end{array} \right) + \left( \begin{array}{c|c}
\Sigma_{v'v'} & \Sigma_{v'v} \\
\hline
\Sigma_{v'v} & \Sigma_{v'v'}
\end{array} \right) \left( \begin{array}{c|c}
\Sigma_{v'v'} & \Sigma_{v'v} \\
\hline
\Sigma_{v'v} & \Sigma_{v'v'}
\end{array} \right)^{-1} \left( \begin{array}{c}
\Sigma_{v'v'} \\
\hline
\Sigma_{v'v}
\end{array} \right)
\]

(27)

\[
\Rightarrow \left( \begin{array}{c|c}
A^{-1} & 0 \\
\hline
0 & 0
\end{array} \right) = \left( \begin{array}{c|c}
C & d \\
\hline
d^T & e
\end{array} \right) - \frac{1}{e} \cdot \left( \begin{array}{c}
d^T \\
e
\end{array} \right) \left( \begin{array}{c}
d^T \\
e
\end{array} \right)^T. \]

(28)

\[
\Rightarrow \left( \begin{array}{c}
\Sigma' \\
0
\end{array} \right) = \Sigma - \frac{1}{\Sigma_{v'v'}} \cdot \Sigma_{v'v'} \Sigma_{v'v} \Sigma_{v'v}'. \]

(29)

In Algo 2, only linear time is needed to evaluate the marginal gain of a candidate because

\[
R_v(\mathcal{L} \cup \{v'\}) = tr(\Sigma') = tr(\Sigma) - tr(\left( \frac{1}{\Sigma_{v'v'}} \cdot \Sigma_{v'v'} \Sigma_{v'v} \right)) = const - \frac{\Sigma_{v'v} \Sigma_{v'v}'}{\Sigma_{v'v'}}
\]

\[
R_s(\mathcal{L} \cup \{v'\}) = 1^T \Sigma' 1 = 1^T \Sigma 1 - 1^T \frac{1}{\Sigma_{v'v'}} \cdot \Sigma_{v'v'} 1 = const - \frac{(1^T \Sigma_{v'v})^2}{\Sigma_{v'v'}}
\]
Algorithm 2: Fast progressive $R(\mathcal{L} \cup \{v^t\})$ evaluation with precomputed covariance.

**Input:** Labeled set $\mathcal{L}$, current $R(\mathcal{L})$, $\Sigma$ (covariance of $y|\mathcal{L}$ conditioned on $y|\mathcal{L}$), queryable pool $\mathcal{P}$, and test set $T \subset \mathcal{U}$ if applicable (otherwise $T \leftarrow I$ of size $|\mathcal{U}|$).

**Output:** $R(\mathcal{L} \cup \{v_{p_1}\})$, ..., $R(\mathcal{L} \cup \{v_{p_k}\})$.

$T \leftarrow (\delta(v_{i_1}, \delta_{u_1}))_{1 \leq i_1, j_1 \leq 1}$, or $T \leftarrow I$ of size $|\mathcal{U}|$ if $T$ not specified.

for $v_{p_i} \in \mathcal{P} - \mathcal{L}$ do

\[ v^t \leftarrow j \text{ if } \delta_{v_{u_j}} = v_{p_i}. \]

$R(\mathcal{L} \cup \{v_{p_i}\}) \leftarrow R(\mathcal{L}) - \frac{(\Sigma_{v_{u'}}T^T)(T\Sigma_{v_{u'}})}{\Sigma_{v_{u'}}}$ if classification or $R(\mathcal{L}) - \frac{(1^T \Sigma_{v_{u'}})^2}{\Sigma_{v_{u'}}}$ if survey.

4.3 Tricks to Improve Efficiency: Singular Laplacian

However, we still have one question unsolved—how to compute the first $L^{-1}$ when $L$ for a connected graph is singular?

The algorithm for classification problem $\arg\min_{v_{b_0}} \text{tr}(L^{-1}(\mathcal{V} - (v_{b_0})))$ has been optimized in [2]. We can follow a similar method to compute $\arg\min_{v_{b_0}} 1^T L^{-1}(\mathcal{V} - (v_{b_0})) 1$ and also the criterion with specified test sets. Essentially, we want to avoid numerical inverse of large matrices as much as possible. In fact, both the algorithm in [2] and the following require only one eigen-decomposition of $L$, which has the same order of complexity as matrix inversion.

**Definition 2 (First Query in Survey Problem).** Suppose $L$ satisfies (5-7), i.e. every property including connectivity but singularity. Also suppose $L$ has eigen-decomposition $L = QAQ^T$, where $A = \text{diag}(\lambda_1, \lambda_2, ..., \lambda_N)$ with $\lambda_1 = 0$, $\lambda_k > 0$, $\forall k \neq 1$ and $Q$ is the orthogonal matrix whose every column is the regularized eigenvector corresponding to the eigenvalue in $A$. Denote the row vector representation\(^3\) of $Q$ as $Q = \begin{pmatrix} r_1 \\ r_2 \\ \vdots \\ r_N \end{pmatrix}$ and its miss-i-th-row form $Q_{-i,*} = \begin{pmatrix} r_1 \\ \vdots \\ r_{i-1} \\ r_{i+1} \\ \vdots \\ r_N \end{pmatrix}$. The first query in survey problem asks to optimize

\[ \arg\min_i R_s(\{v_i\}) = 1^T L_{\mathcal{V} - \{v_i\}}^{-1} 1 = 1^T \cdot (Q_{-i,*} \Lambda Q_{-i,*}^{-1}) \cdot 1 \] \hspace{1cm} (30)

**Solution (First Query in Survey Problem).**

For any fixed $i$, denote $(n-1)$-by-$n$ $\hat{Q} = Q_{-i,*}$. Thus $\hat{Q}^T \hat{Q} = I_{N-1}$, $\hat{Q}^T \hat{Q} = I_{N} - r_i^T r_i$, and $R_s(\{v_i\}) = 1^T (\hat{Q} \Lambda \hat{Q}^T)^{-1}$. Also denote $\hat{A} = \begin{pmatrix} \lambda_1 & 0 \\ 0 & \hat{A} \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & \hat{A} \end{pmatrix}$, where $\hat{A}$ is $(n-1)$-by-$(n-1)$ nonsingular diagonal matrix and $\hat{L} = L_{\mathcal{V} - \{v_i\}} = \hat{Q} \Lambda \hat{Q}^T$. By matrix inversion theorem,

\[ \hat{L}^{-1} = (-\hat{Q}^T \hat{Q} + \hat{Q}(I_N + \hat{A}) \hat{Q}^T)^{-1} \] \hspace{1cm} (31)

\[ = (-\hat{Q}^T \hat{Q})^{-1} - \hat{Q}^T \hat{Q}^{-1} \hat{Q} \left[ (I_N + \hat{A})^{-1} + \hat{Q}^T (-\hat{Q} \hat{Q}^T)^{-1} \hat{Q} \right]^{-1} \hat{Q}^T (\hat{Q} \hat{Q}^T)^{-1} \] \hspace{1cm} (32)

\[ = -I_{N-1} - \hat{Q} \left[ (I_N + \hat{A})^{-1} - \hat{Q}^T \hat{Q} \right]^{-1} \hat{Q}^T \] \hspace{1cm} (33)

\[ = -I_{N-1} - \hat{Q} \left[ (I_N + \hat{A})^{-1} - I_N + r_i^T r_i \right]^{-1} \hat{Q}^T \] \hspace{1cm} (34)

Since $L$ is a connected graph Laplacian, the normalized eigenvector for $\lambda_1 = 0$ is $\begin{pmatrix} \frac{1}{\sqrt{N}} \\ \vdots \\ \frac{1}{\sqrt{N}} \end{pmatrix}^T$. Therefore, we can denote $r_i = \begin{pmatrix} \frac{1}{\sqrt{N}} \\ \vdots \\ \frac{1}{\sqrt{N}} \end{pmatrix}$, where $\alpha_i$ is $(N-1)$-dimensional. Apply matrix inver-

\(^3\)Notice this $r_i$ representation is the only row vector representation in this paper.
Theorem again,

\[ \left[ (I_N + \Lambda)^{-1} - I_N \right] + r_i^T r_i \right]^{-1} = \left( \frac{1}{N} \mathbf{a}_N \mathbf{a}_N^T \right) - \frac{1}{m \sqrt{N}} \tilde{M}^{-1} \mathbf{a}_i \mathbf{a}_i^T \right)^{-1} \]

where \( \tilde{B}^{-1} = \tilde{M}^{-1} - \tilde{M}^{-1} \mathbf{a}_i \cdot \frac{1}{1 + \mathbf{a}_i^T \tilde{M}^{-1} \mathbf{a}_i} \cdot \mathbf{a}_i^T \tilde{M}^{-1} \) and \( m = \frac{1}{N} - \frac{1}{N} \mathbf{a}_i^T \tilde{B}^{-1} \mathbf{a}_i \).

Assign \( \mathbf{a}_i = \mathbf{a}_i^T \tilde{M}^{-1} \mathbf{a}_i \) and we have

\[ \alpha_i^T \tilde{B}^{-1} \mathbf{a}_i = \alpha_i^T \tilde{M}^{-1} \mathbf{a}_i - \frac{(\alpha_i^T \tilde{M}^{-1} \mathbf{a}_i)^2}{1 + \alpha_i^T \tilde{M}^{-1} \mathbf{a}_i} = a_i - \frac{a_i^2}{1 + a_i} = \frac{a_i}{1 + a_i} \]

\[ \frac{1}{m} = \left( \frac{1}{N} - \frac{1}{N} \frac{a_i}{1 + a_i} \right) \]

Finally, because the first column of the orthogonal \( \mathbf{Q} \) is \( \frac{1}{\sqrt{N}} \mathbf{1} \), we have \( \mathbf{1}^T \mathbf{Q} = \left( \sqrt{N}, 0^T \right) \) and

\[ R_s(\{v_i\}) = \mathbf{1}^T \cdot \tilde{L}^{-1} \cdot \mathbf{1} \]

\[ = - (N - 1) - \left( \mathbf{1}^T \mathbf{Q} - r_i \right) \left( -\frac{1}{m \sqrt{N}} \tilde{B}^{-1} \mathbf{a}_i - \frac{1}{m \sqrt{N}} \mathbf{a}_i^T \tilde{B}^{-1} \right) \left( \mathbf{1}^T \mathbf{Q} - r_i \right)^T \]

\[ = - (N - 1) - \left( \frac{N - 1}{\sqrt{N}}, -\mathbf{a}_i \right) \left( -\frac{1}{m \sqrt{N}} \tilde{B}^{-1} \mathbf{a}_i - \frac{1}{m \sqrt{N}} \mathbf{a}_i^T \tilde{B}^{-1} \right) \left( \frac{N - 1}{\sqrt{N}}, -\mathbf{a}_i \right)^T \]

\[ = - (N - 1) - \left[ (N - 1)^2 (1 + a_i) + 2(N - 1) a_i + \frac{a_i^2}{1 + a_i} \right] \]

\[ = - N(N - 1) - N^2 a_i, \]

where \( a_i = (q_{i,2}, ..., q_{i,N}) \mathbf{diag} \left( \frac{1 + \lambda_2}{-\lambda_2}, ..., \frac{1 + \lambda_N}{-\lambda_N} \right) (q_{i,2}, ..., q_{i,N})^T. \]

When a test set \( \mathcal{T} \) is specified, since \( v_i \notin \mathcal{T} \),

\[ R_s(\{v_i\}) = \mathbf{1}^T \tilde{T} \tilde{L}^{-1} \mathbf{1} \]

\[ = - (|\mathcal{T}| - 1) - \mathbf{1}^T \tilde{Q} \left[ (I_N + \Lambda)^{-1} + r_i^T r_i \right]^{-1} \tilde{Q}^T \mathbf{1}. \]

A similar algorithm can be derived, though the runtime complexity may have a factor \(|\mathcal{T}|\).

**Algorithm 3:** Fast first-step \( R_s(\{v\}) \) evaluation with singular Laplacian.

**Input:** Singular connected graph Laplacian \( L \).

**Output:** \( R_s(\{v_i\}) = \mathbf{1}^T \tilde{L}^{-1} \mathbf{1} \), \( i = 1, ..., N \).

Perform eigen-decomposition \( L = \mathbf{Q} \mathbf{\Lambda} \mathbf{Q}^T \), where \( \mathbf{\Lambda} = \mathbf{diag} (\lambda_1, ..., \lambda_N) \) in ascending order.

Denote \( \mathbf{M}^{-1} \leftarrow \mathbf{diag} \left( 0, \frac{1 + \lambda_2}{-\lambda_2}, ..., \frac{1 + \lambda_N}{-\lambda_N} \right) \) and \( \mathbf{Q} = \left( \begin{array}{c} \mathbf{r}_1 \\ \vdots \\ \mathbf{r}_N \end{array} \right) \).

for \( i = 1, ..., N \) do

\[
\left\{
\begin{array}{l}
\mathbf{a}_i \leftarrow \mathbf{r}_i \mathbf{M}^{-1} \mathbf{r}_i^T.
R_s(\{v_i\}) = -N(N - 1) - N^2 a_i.
\end{array}
\right.
\]
5 Experiment

We performed various active learning methods on the DBLP coauthorship graph dataset on four areas: machine learning, data mining, information retrieval and database. Edge weights are the number of papers coauthored. We took its largest connected component, which contains 1711 nodes and 0.3% of all possible edges. We used the V-optimality criterion (§2), mutual information gain \(\max_{\mathcal{L}} \mathcal{M}(\mathcal{L}; \mathcal{Y} - \mathcal{L})\) [1], and random selection. For fair comparison, every method was assigned the same random seed to start and the curves are the mean and the standard error of the mean after 120 repetitions (Figure 1). The V-optimality criterion performs better than others.

![Figure 1: Batch active learning to classify the unlabeled authors on DBLP coauthorship graph.](image)

6 Conclusion

In this paper, we introduced the GRF model (1) and the Gaussian harmonic prediction (2). The batch active learning with V-optimality criterion, whose risk function is (3) can be formulated as the subset selection problem (4). Our major contribution is to prove the submodularity conditions (9-11) and an \((1 - 1/e)\) optimality bound (12) for a greedy selection algorithm (Algo 1) when the graph Laplacian is nonsingular (5-8), via either extracting a subgraph from the original connected graph or regularizing the GRF model. Furthermore, the fact that all GRFs meet the AofS condition (Theorem 2) may shed light on this otherwise obscure condition.

In §4, we also proposed an active survey problem and its related risk \(R_s(\mathcal{L})\). We can show that this batch active survey problem also meet the submodularity conditions and its greedy subset selection algorithm achieves a similar \((1 - 1/e)\) optimality bound.

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