Fiedler Regularization: Learning Neural Networks with Graph Sparsity

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Abstract
We introduce a novel regularization approach for deep learning that incorporates and respects the underlying graphical structure of the neural network. Existing regularization methods often focus on dropping/penalizing weights in a global manner that ignores the connectivity structure of the neural network. We propose to use the Fiedler value of the neural network’s underlying graph as a tool for regularization. We provide theoretical support for this approach via spectral graph theory. We demonstrate the convexity of this penalty and provide an approximate, variational approach for fast computation in practical training of neural networks. We provide bounds on such approximations. We provide an alternative but equivalent formulation of this framework in the form of a structurally weighted L1 penalty, thus linking our approach to sparsity induction. We performed experiments on datasets that compare Fiedler regularization with traditional regularization methods such as dropout and weight decay. Results demonstrate the efficacy of Fiedler regularization.

1. Introduction
Neural networks (NN) are important tools with many applications in various machine learning domains such as Computer Vision, Natural Language Processing and Reinforcement Learning. NNs have been very effective in settings where large labeled datasets are available. Empirical and theoretical evidence has point to the ever-increasing capacity of recent NN models, both in depth and width, as an important contributor to their modeling flexibility and empirical success. However, even the largest datasets can still be potentially overfitted by large NNs with millions of parameters. A wide range of techniques for regularizing NNs have thus been developed. These techniques often regularize the networks from a global penalization perspective, e.g. weight decay (Krogh & Hertz, 1992) (L2 penalization of weights in the stochastic gradient descent context), dropping nodes or weights in a Bernoulli manner with uniform probability (Hinton et al., 2012; Srivastava et al., 2014; Wan et al., 2013), or stopping training early. These commonly used approaches ignore the neural networks’ underlying graphical structure, which can provide valuable connectivity information for regularization.

One natural generalization of these existing approaches is to take the graph structure of the NN into consideration during regularization. Existing feedforward neural network architectures, e.g. multi-layer perceptrons, frequently employ fully connected layers that lead to many redundant paths between nodes of the network. These redundant connections can contribute to over-fitting through the phenomenon of co-adaptation, where weights become dependent on one another, leading to highly correlated behavior amongst different hidden units (Hinton et al., 2012). Empirical work has shown that dropping weights and nodes randomly during training can significantly improve test performance by reducing co-adaptation (Hinton et al., 2012; Srivastava et al., 2014; Wan et al., 2013).

In this work, we would like to regularize the neural network through reducing co-adaptation and extraneous connections in such a way that, informally, "less important" weights will be penalized more in a manner that depends on the graph structure. We formalize the above intuition via the notion of Fiedler regularization, borrowing from advances in spectral graph theory (Godsil & Royle, 2013; Chung & Graham, 1997; Spielman, 2019). The Fiedler value of a connected graph, denoted \( \lambda_2 \), also known as the algebraic connectivity, is the second smallest eigenvalue of the graph’s Laplacian matrix. Its magnitude characterizes how well connected a graph is. By adding the Fiedler value as a penalty term to the loss function during training, we can reduce the connectedness of the neural network and reduce co-adaptation in a way that takes into account the graph structure. The dependency of the Fiedler value on the sizes of the network’s weights is convex, and we provide a closed form expression of its gradient, thus allowing for direct employment of existing gradient-based stochastic optimization techniques.

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We would like to use structural information from where we would like to emphasize the dependency of this L1 formulation allows us to link Fiedler regularization, along with strong theoretical guarantees and experimental performances.

2. Spectral Graph Theory

2.1. Setup and Background

Let \( W \) denote the set of weights of a feedforward neural network \( f \). We denote \( f \)'s underlying graph structure as \( G \). We would like to use structural information from \( G \) to regularize \( f \) during training. Feedforward neural networks do not allow for self-loops or recurrent connections, hence it suffices that \( G \) be a finite, connected, simple, weighted and undirected graph in this setting. Such a graph \( G \) can be fully specified by a triplet \( (V, E, |W|) \), where \(| \cdot |\) denotes the absolute value mapping. The vertex set \( V \) of \( G \) corresponds to all the units (including input and output layers) in the neural network \( f \), while the edge set \( E \) of \( G \) corresponds to all the edges in \( f \). For our purposes of regularization, \( G \) is restricted to have non-negative weights \(|W|\), which is taken to be the absolute value of the corresponding weights \( W \) in the neural network \( f \). Throughout the paper we will use \( n \) to denote the number of vertices in \( G \). \(|W|\) and \( E \) can be jointly represented by an \( n \times n \) weighted adjacency matrix \(|W|\), where \(|W|_{ij}\) is the weight on the edge \((i, j)\) if vertices \( i \) and \( j \) are connected, and 0 otherwise. The degree matrix \( D \) of the graph is a \( n \times n \) diagonal matrix, where \( D_{ii} = \sum_{j=1}^{n} |W|_{ij} \). The Laplacian matrix \( L \), which is a central object of study in spectral graph theory, is defined as the difference between the degree and the adjacency matrix, i.e. \( L = D - |W| \). In certain contexts where we would like to emphasize the dependence of \( L \) on the particular graph \( G \), we will adopt the notation \( L_G \). We use \(|M|\) to denote the set \( \{1, 2, \cdots, M\} \) for positive integer \( M \). Throughout the paper, eigenvalues are real-valued since the matrices under consideration are symmetric. We adopt the convention where all eigenvectors are taken to be unit vectors. We order the eigenvalues in ascending order, so \( \lambda_i \leq \lambda_j \) for \( i < j \). When we want to emphasize the dependence of \( \lambda_i \) on the weights, we use \( \lambda_i(|W|) \). We use \( v_i \) to denote the corresponding eigenvector for \( \lambda_i \).

2.2. Graph Laplacian

The Laplacian matrix encodes much information about the structure of a graph. One particularly useful characterization of the graph Laplacian is through the so called Laplacian quadratic form (Batson et al., 2012; Spielman, 2019; Chung & Graham, 1997), defined below.

**Definition 2.2.1 (Laplacian quadratic form)** Given a graph \( G = (V, E, |W|) \), for every vector \( z \in \mathbb{R}^{|V|} \) we can associate a Laplacian quadratic form \( Q_G : \mathbb{R}^{|V|} \rightarrow \mathbb{R}^+ \), defined as

\[
Q_G(z) := z^T L_G z = \sum_{(i, j) \in E} |W|_{ij} (z(i) - z(j))^2
\]

where \( z(k) \) denotes the \( k \)th entry of the vector \( z \).

The Laplacian quadratic form demonstrates how a graph’s boundary information can be recovered from its Laplacian matrix. One can think of \( z \) as a mapping that assigns to each vertex a value. If we denote the characteristic vector of a subset of vertices \( S \subset V \) as \( 1_S \), i.e. \( 1_S(i) = 1 \) if \( i \in S \) and \( 1_S(i) = 0 \) otherwise, and apply it to the Laplacian quadratic form, we obtain

\[
\sum_{(i, j) \in E, i \in S, j \notin S} |W|_{ij}.
\]

This expression characterizes the size of the graph cut \((S, V - S)\), which is the sum of the weights of edges crossing the boundary between \( S \) and \( V - S \). The size of any graph cut can therefore be obtained by application of the corresponding characteristic vector on the Laplacian quadratic form.

2.3. Graph Conductance and Cheeger’s Inequality

The above discussion on the sizes of graph cuts is highly related to our study of regularizing a neural network. Reducing the sizes of graph cuts in a NN would imply reducing the NN’s connectivity and potentially co-adaptation. A related but more convenient construct that captures this notion of boundary sizes in a graph is the conductance, which can be informally thought of as normalized version of the graph cut.

**Definition 2.3.1 (Conductance of a cut)** The conductance \( \phi(S) \) of a cut \((S, V - S)\) in a graph \( G = (V, E, |W|) \) is defined as

\[
\phi(S) = \frac{\sum_{i \in S, j \notin S} |W|_{ij}}{\min(\text{Vol}(S), \text{Vol}(V - S))},
\]

where \( \text{Vol}(S) = \sum_{u \in S} \deg(u) \) is the sum of the weighted degrees of all vertices in \( S \).

The conductance of a graph \( \phi_G \) is then defined as the mini-
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minimum conductance out of all possible cuts in the graph $G$

\[ \phi_G = \min_S \phi(S) \]

One can think of the conductance of a graph as characterizing the connectivity bottleneck of a graph. It is highly related to how sparse the graph is and whether there exist nice planar embeddings of the graph (Hall, 1970).

We would like to control the conductance of the neural network’s underlying graph for regularization. Direct optimization of conductance is a difficult problem due to the combinatorial structure. Instead, we control the conductance indirectly through the Fiedler value $\lambda_2$, the second smallest eigenvalue of the graph’s Laplacian $L$. It is related to the conductance of the graph through Cheeger’s inequality (Spielman, 2019; Chung & Graham, 1997; Godsil & Royle, 2013).

**Proposition 2.3.2 (Cheeger’s inequality)** Given a graph $G = (V, E, |W|)$, the conductance constant $\phi_G$ is upper and lower bounded as follows:

\[ \sqrt{2\lambda_2 d_{\text{max}}(G)} \geq \phi_G \geq \frac{\lambda_2}{2}, \]

where $d_{\text{max}}(G)$ is the maximum (weighted) degree of $G$ and $\lambda_2$, the Fiedler value, is the second smallest eigenvalue of $G$’s Laplacian matrix.

Cheeger’s inequality originally arose from the study of Riemannian manifolds and was later extended to graphs. There are several versions of this classic inequality depending on the types of graphs and Laplacians considered. The proofs can be found in many references, including (Spielman, 2019; Chung & Graham, 1997; Godsil & Royle, 2013). We remark that both sides of Cheeger’s inequality are tight asymptotically up to constant factors.

The Fiedler value is also known as the algebraic connectivity because it encodes considerable information about the connectedness of a graph. Cheeger’s inequality allows sharp control over the conductance of $G$ via the Fiedler value. It demonstrates that by making the Fiedler value small, we can force the conductance of the graph to be small, thus reducing the connectedness of the graph and potentially alleviating co-adaptation in the neural network setting. On the other hand, a large Fiedler value necessarily implies a large conductance. This shows that penalization of the Fiedler value during neural network training is a promising regularization strategy to reduce connectivity and thus co-adaptation.

3. Fiedler Regularization

3.1. Supervised Classification Setup

We now consider the classical setup for using neural networks for classification. Given training data $\{x_i, y_i\}_{i=1}^N$, where $i$ indexes the $N$ data points, $x_i \in \mathbb{R}^d$ are independent $d$-dimensional feature vectors, $y_i \in [M]$ are the labels and $M$ is the number of categories, we aim to find a mapping $f$ that predicts $y$ through $f(x)$ so that some pre-specified loss $L(f(x), y)$ is minimized in the test data. Typical choices of $L(\cdot, \cdot)$ include the cross-entropy loss, hinge loss etc. It is assumed that new observations in the testing set follow the same distribution as the training data $\{x_i, y_i\}$. We will denote the estimator of $f$ as $\hat{f}$. When we want to emphasize the estimator’s dependence on the weights, we will use $\hat{f}_W$.

For feedforward neural networks, $f$ is characterized as a composition of non-linear functions $\{g^{(l)}\}_{l=1}^L$, i.e. $\hat{f} = g^{(L)} \circ g^{(L-1)} \circ \cdots \circ g^{(1)}(x)$, where $L$ is the number of layers in the network. The outputs of the $l$th layer have the form $h'(i) := g^{(l)}(h^{(l-1)}) := \sigma^{(l)}(W^{(l)}h^{(l-1)} + b^{(l)})$, where $\sigma^{(l)}, W^{(l)}$ and $b^{(l)}$ are the activation function, weight matrix and bias of the $l$th layer of the neural network, respectively. In essence, each unit in a hidden layer of the feedforward neural network performs a linear regression on the previous layer’s outputs, followed by a non-linear transformation. For an excellent review of related approaches, refer to (Fan et al., 2019).

3.2. Penalizing with Fiedler Value

In our proposed Fiedler regularization approach, we add a penalty term that depends on the graphical connectivity structure of the NN. In particular, we penalize the Fiedler value, under the motivation from the previous subsection.

**Definition 3.2.1 (Fiedler regularization)** In training the neural network to find $\hat{f}_W$, we optimize the following objective:

\[ \min_{W} L(Y, \hat{f}_W(X)) + \delta \lambda_2(\|W\|), \]

where $\lambda_2(\|W\|)$ is the Fiedler value of the neural network’s underlying graph, $W$ is the weight matrix of the NN and $\delta$ is a tuning parameter. $Y$ and $X$ denote the sets of training labels and training features respectively.

We remark that the actual neural network $\hat{f}_W$ will have weights that can be negative, but for the regularization term $\lambda_2(\|W\|)$ will only depend on the underlying graph $G$ of the neural network, which has non-negative edge weights $\|W\|$ (the absolute value of $W$).

Note that one can modify the penalty by applying a differentiable, non-negative, convex function $Q$ to $\lambda_2$. For our discussion below, we will focus on the case where no $Q$ is applied (or that $Q$ is the identity mapping $Q(\lambda_2) = \lambda_2$) in order to focus the analysis on the Fiedler value. However, incorporating $Q$ is straightforward and desirable properties such as convexity and having a closed-form gradient can be retained. We also note that, without loss of generality, one can consider the biases of the units in the neural network as...
additional weights with constant inputs, so it is straightforward to include consideration of both biases and weights in Fiedler regularization.

We remark that for our purposes of regularization, we consider the parameters of interest in the neural network to be the edge weights and the biases of the units. The choice of activation function, the architecture of the neural network, as well as the choice of hyperparameters such as the learning rate or the tuning factor etc are all considered to be pre-specified in our study. There is a separate and rich literature devoted to methods for selecting activation functions/architectures/hyperparameters that we won’t consider here.

### 3.3. Convexity of Fiedler Regularization

We show in the following proposition that that Fiedler penalty is convex; this implies that adding the penalty does not add to the difficulty of the optimization problem and standard algorithms routinely used for neural network optimization can be used directly.

**Proposition 3.3.1 (Convexity of Fiedler Penalty)** The problem of optimizing

\[
\min_{\mathbf{W}} \delta \lambda_2(|\mathbf{W}|)
\]

is convex.

**Proof**: To show that this minimization problem is convex, we need to show that the objective function is convex and that the constraints are convex.

For the objective function, since multiplication by the constant $\delta$ does not change convexity, we only need to concern ourselves with the eigenvalue $\lambda_2(|\mathbf{W}|)$. If we consider the Rayleigh-Ritz variational characterization of this eigenvalue, we have:

\[
\lambda_2(|\mathbf{W}|) = \inf_{||\mathbf{u}||=1} \mathbf{u}^T \mathbf{L} \mathbf{u} = \inf_{||\mathbf{u}||=1} \sum_{(i,j) \in E} |\mathbf{W}|_{ij} (\mathbf{u}(i) - \mathbf{u}(j))^2
\]

Note that this is a pointwise infimum of a linear function of $|\mathbf{W}|_{ij}$. Since linear functions are convex, and pointwise infimums preserves convexity, we have that $\lambda_2$ is a convex function of the weights.

For the constraints, in our setup we already mentioned that the underlying graphs of neural networks can only have non-negative weights $|\mathbf{W}|$. This implies each entry $|\mathbf{W}|_{ij} \geq 0$, which is a convex constraint. $\square$

This is a Laplacian eigenvalue optimization problem and we refer to [Boyd, 2006] and [Sun et al., 2006] for a more general treatment. The essence of their approach is that the problem can be reformulated as optimizing linear objective functions on the cone of positive semi-definite matrices under affine constraints and thus is a semi-definite program, which is convex.

From the above convexity result on optimizing the Fiedler penalty, we immediately obtain the corollary that commonly used algorithms such as stochastic gradient descent, which are guaranteed to converge on convex problems, will work on this penalty term as well.

### 3.4. Closed-form Expression of Gradient

In all except the most simple of cases, optimizing the loss function $\min_{\mathbf{W}} \mathcal{L}(\mathbf{Y} - \mathbf{f}_{\mathbf{W}}(\mathbf{X}))$ is a nonconvex problem. There are a variety of scalable, stochastic algorithms for practical optimization on such objectives. Virtually all of the widely used methods, such as stochastic gradient descent ([Ruder, 2016], [Adam (Kingma & Ba, 2014), Adagrad ([Duchi et al., 2011]), RMSProp ([Graves, 2013]) etc, require computation of the gradient of the objective with respect to the parameters. We provide a closed form analytical expression of the gradients of a general Laplacian eigenvalue with respect to the entries of the Laplacian matrix. From that, as a straightforward corollary, a closed form analytical expression of the Fiedler value’s gradient is obtained.

**Proposition 3.4.1 (Gradient of Laplacian Eigenvalue)**

Assuming that the $k^{th}$ smallest eigenvalue $\lambda_k$ of the Graph Laplacian $\mathbf{L}$ is not repeated, the gradient of $\lambda_k$ with respect to $\mathbf{L}$’s $(ij)^{th}$ entry $\mathbf{L}_{ij}$ can be analytically expressed as

\[
\frac{d\lambda_k}{d\mathbf{L}_{ij}} = \mathbf{v}_k(i) \times \mathbf{v}_k(j),
\]

where $\mathbf{v}_k(i)$ denotes the $i^{th}$ entry of the $k^{th}$ eigenvector of the Laplacian. We adopt the convention in which all eigenvectors under consideration are unit vectors.

**Proof**: To compute $\frac{d\lambda_k}{d\mathbf{L}_{ij}}$, note that since the Laplacian matrix is symmetric, all eigenvalues are real. By assumption, the second smallest eigenvalue is not repeated. By the existing closed form formulae under this situation (see [Petersen et al., 2008]),

\[
\mathbf{v}_k^T (\frac{\partial}{\partial \mathbf{L}}) \mathbf{v}_k = d\lambda_k.
\]

Specializing to individual entries, we get

\[
\frac{d\lambda_k}{d\mathbf{L}_{ij}} = \mathbf{v}_k(i) \times \mathbf{v}_k(j).
\]

We note that any non-diagonal element $\mathbf{L}_{ij}$ is equal to $-\mathbf{W}_{ij}$. As an immediate special case of Proposition 3.4.1, the gradient of the Fiedler value $\lambda_2$ can be expressed as:

\[
\frac{d\lambda_2}{d\mathbf{L}_{ij}} = \mathbf{v}_2(i) \times \mathbf{v}_2(j).
\]

Using this expression of the gradient for the Fiedler penalty, we can perform weight updates in existing deep learning libraries using a wide variety of stochastic optimization methods.

We remark that our assumption that $\lambda_2$ is not repeated generally holds in the context of neural networks. The weights
in a NN are usually initialized as independent draws from certain continuous distributions, such as the uniform or the Gaussian. Repeated Laplacian eigenvalues often occur when there are strong symmetries in the graph, and such symmetries are usually broken since the probability of any subset of the weights taking the same non-zero value at initialization or during training is negligible.

4. Variational, Approximate Approach for Computational Speedup

We have given theoretical motivation and outlined the use of the Fiedler value of the neural network as a penalization term for regularization. However, we note that typical matrix computations for eigenvalues and eigenvectors are of order \( O(n^3) \), where \( n = |V| \). This can be computationally prohibitive for moderate to large networks. Even though there exist theoretically more efficient algorithms to compute eigenvalues/eigenvectors of graph-related matrices (e.g. the power method), in practice computing the Fiedler value in every iteration of training can prove costly. To circumvent this issue, we propose an approximate, variational approach to speed up the computation to \( O(|E|) \), where \( |E| \) is the number of edges in the graph. This proposed approach can be readily implemented in popular deep learning packages such as Tensorflow and PyTorch.

We make the following observations. First, for the purposes of regularizing a neural network, we do not need the exact Fiedler value of the Laplacian matrix. Approximate solutions suffice. Second, there is no need to update our approximate \( \lambda_2 \) at every iteration during training. One can set an update schedule to update \( \lambda_2 \) periodically, say every 100 iterations or every training epoch. Both of these observations allow for substantial speedup in practice. An outline of the pseudo-code for this approximate, variational approach is provided in Algorithm 1 below.

To obtain an approximate Fiedler value for regularization, we provide a variational upper bound that can be used for penalization. We additionally provide a perturbation bound, giving justification for algorithms that periodically update the Fiedler value, in terms of closeness guarantees for the resulting eigenvalues/eigenvectors after weight updates.

4.1. Rayleigh Quotient Characterization of Eigenvalues

We can closely upper-bound the Fiedler value via the notion of test vectors (Spielman, 2019), which depends crucially upon the Rayleigh quotient characterization of eigenvalues.

**Proposition 4.1.1 (Test Vector Bound)** For any unit vector \( u \) that is perpendicular to the constant vector \( I \), we have:

\[
\lambda_2 \leq u^T L u
\]

Any such unit vectors are called test vectors. Equality is achieved when \( u = v_2 \).

**Proof:** The Laplacian matrix of a non-negatively weighted graph is symmetric and positive semidefinite. Thus all eigenvalues are real and non-negative. In particular, the smallest eigenvalue of the Laplacian is 0, with the constant vector being the first eigenvector. For a connected graph, the second smallest eigenvalue, which is the Fiedler value, can thus be characterized by the Raleigh quotient

\[
\lambda_2 = \min_{||u|| = 1, u^T I = 0} u^T L u.
\]

This gives us a tight upper bound.

The above description implies that by appropriately choosing test vectors, we can effectively upper bound the Fiedler value. This in turn implies that during training, instead of penalizing by the exact Fiedler value, we can penalize by the quadratic form upper bound instead, speeding up computation considerably to \( O(|E|) \) since

\[
\sum_{(i,j) \in E} |W|_{ij} (u(i) - u(j))^2.
\]

The core question now becomes how to choose appropriate test vectors that are close to \( v_2 \).

We propose to initialize training with the exact \( v_2 \) (or an accurate numerical approximation) and update \( v_2 \) only periodically during training. By the Rayleigh quotient characterization above, the quadratic form of such a test vector will always upper-bound the true \( \lambda_2 \). In other words, during each \( v_2 \) update step, the Fiedler vector used will be exact, and in between updates, the previous \( v_2 \) will be used as a test vector.

During training, weights of the neural network are updated at each iteration. This is equivalent to adding a symmetric matrix \( H \) to the Laplacian matrix \( L \), which is also symmetric, at every iteration. This perturbation \( H \) to the matrix \( L \), if small, will have a small effect on the eigenvalues/eigenvectors of \( L \). We can bound the effect of such a perturbation on the eigenvalues via Weyl’s inequality (Horn & Johnson, 2012; Horn et al., 1998).

**Proposition 4.1.2 (Weyl’s Inequality)** Given a symmetric matrix \( L \) and a symmetric perturbation matrix \( H \), both with dimension \( n \times n \), for any \( 1 \leq i \leq n \), we have:

\[
|\lambda_i(L + H) - \lambda_i(L)| \leq ||H||_{op}
\]

where \( || \cdot ||_{op} \) denote the operator norm.

Weyl’s inequality is a classic result in matrix analysis, and its proof can be found in the excellent reference (Horn & Johnson, 2012) as a straightforward result of linearity and the Courant-Fischer theorem. As an immediate special case, \( |\lambda_2(L + H) - \lambda_2(L)| \leq ||H||_{op} \). Proposition 4.1.2 tells us that as long as the perturbation \( H \) is small, the change in Fiedler value caused by the perturbation will also be small. In fact, this shows that the map \( L \rightarrow \lambda_2(L) \) is Lipschitz continuous on the space of symmetric matrices.
Algorithm 1 Variational Fiedler Regularization with SGD

**Input:** Training data \( \{x_i, y_i\}_{i=1}^{N} \)

**Hyperparameters:** Learning rate \( \eta \), batch size \( m \), penalty parameter \( \delta \), updating period \( T \)

Initialize parameters \( W \) of the neural network

Compute the Laplacian \( L_W \) of the neural network

Compute the Fiedler vector \( v_2 \) of the Laplacian \( L_W \)

Initialize counter \( c = 0 \)

**while** Stopping criterion not met **do**

Sample minibatch \( \{x^{(i)}, y^{(i)}\}_{i=1}^{m} \) from training set

Set gradient \( \gamma = 0 \)

**for** \( i = 1 \) to \( m \) **do**

Compute gradient \( \gamma \leftarrow \gamma + \nabla W L_W (f_W (x^{(i)}), y^{(i)}) + \delta \nabla W v^2_W L_W v_2 \)

Apply gradient update \( W \leftarrow W - \eta \gamma \)

Update Laplacian matrix \( L_W \)

Update counter \( c \leftarrow c + 1 \)

**if** \( c \mod T = 0 \) **then**

Update second Laplacian eigenvector \( v_2 \)

**end if**

**end while**

In the context of training neural networks, \( H \) represents the updates to the weights of the network during training. This justifies updating \( \lambda_2 \) only periodically for the purposes of regularization. It suggests that with a smaller learning rate, \( H \) would be smaller, and therefore the change to \( \lambda_2 \) would also be smaller, and updates of the test vectors can be more spaced apart. On the other hand, for larger learning rates we recommend using updating test vectors more frequently. Alternatively, a similar bound on eigenvector perturbation could be established via the Davis-Kahan Sin-\( \Theta \) inequality, but is omitted here since the eigenvalue bound suffices for Fiedler regularization.

5. Weighted-L1 formulation and Sparsity

We now expand on an equivalent formulation of Fiedler regularization via a weighted L1 penalty. We note that the Laplacian quadratic form can be written as \( u^T L u = \sum_{(i,j) \in E} |W|_{ij} (u(i) - u(j))^2 \). This, combined with the Rayleigh quotient characterization of eigenvalues, yields the equivalent objective:

\[
\min_W L(Y - f_W(X)) + \delta \sum_{(i,j) \in E} |W|_{ij} (u(i) - u(j))^2
\]

We note that both \( |W|_{ij} \) and \( (u(i) - u(j))^2 \) are non-negative. This is equivalent to performing \( L_1 \) penalization on \( W_{ij} \) with weights \( u(i) - u(j) \).

There is an immense literature on modified \( L_1 \) penalties in shallow models (Zou, 2006; Candès et al., 2008). It is well known that optimizing an objective under (weighted) \( L_1 \) constraints often yields sparse solutions. This thus connects our Fiedler regularization approach with sparsity induction on the weights of the neural network.

In Fiedler regularization, the weights \( |W|_{ij} \) are scaled by a factor of \( (u(i) - u(j))^2 \), where \( u \) is a test vector that approximates \( v_2 \). From the spectral clustering literature (Hagen & Kahng, 1992; Donath & Hoffman, 1972), we understand that \( v_2 \) is very useful for approximating the minimum conductance cut of a graph. The usual heuristic is that one sorts entries of \( v_2 \) in ascending order, sets a threshold \( t \), and groups all vertices \( i \) having \( v_2 > t \) into one cluster and the rest into another cluster. If the threshold \( t \) is chosen optimally, this clustering will be a good approximation to the minimum conductance cut of a graph. As such, the farther apart \( v_2(i) \) and \( v_2(j) \) are, (1) the less connected the nodes \( i \) and \( j \) should be and (2) the more likely that nodes \( i \) and \( j \) belong to different clusters.

This is also connected to spectral drawing of graphs (Spielman, 2019; Hall, 1970), where it can be shown that "nice" planar embeddings/drawings of the graph do not exist if \( \lambda_2 \) is large. In this sense, Fiedler regularization is forcing the neural network to be "more planar" while respecting its connectivity structure.

Hence, with Fiedler regularization, the penalization on \( |W|_{ij} \) is the strongest when nodes \( i \) and \( j \) are more disconnected. This would in theory lead to greater sparsity in edges that have low weights and connect distant vertices belonging to different clusters. Thus, Fiedler regularization sparsifies the neural network in a way that respects its connectivity structure.

To this end, an alternative guarantee is the ordering property of Laplacian eigenvalues with respect to a sequence of graphs (Godsil & Royle, 2013).

**Proposition 5.1 (Laplacian Eigenvalue Ordering)** Given the graph \( G \) with non-negative weights, if we remove an edge \( (a, b) \) to obtain \( G \setminus (a, b) \), we have that

\[
\lambda_2(G \setminus (a, b)) \leq \lambda_2(G)
\]

**Proof:** The proof is a simple generalization of (Godsil & Royle, 2013). Pick \( q_2 \) and \( r_2 \) to be second eigenvectors of \( G \) and \( G \setminus (a, b) \) respectively. By the Laplacian quadratic form characterization of eigenvalues, we have

\[
\lambda_2(G) = q_2^T L_G q_2 = \sum_{(c,d) \in E} |W|_{cd} (q_2(c) - q_2(d))^2
\]

\[
\geq \left[ \sum_{(c,d) \in E} |W|_{cd} (q_2(c) - q_2(d))^2 \right] - |W|_{ab} (q_2(a) - q_2(b))^2
\]

\[
= q_2^T L_G \setminus (a,b) q_2 \geq \sum_{(c,d) \in E} |W|_{cd} (q_2(c) - q_2(d))^2
\]

\[
= \lambda_2(G \setminus (a, b))
\]
where the first inequality follows from the non-negativity of the weights under consideration and the second inequality follows from the Rayleigh-Ritz variational characterization of eigenvalues. □

Hence, by sparsifying edges and reducing edge weights, we are in effect reducing the Fiedler value of the NN. The above ordering property is a special case of the more general Laplacian eigenvalue interlacing property, where \( \lambda_2(G \setminus (a, b)) \) also admits a corresponding lower bound. For a general treatment, see (Godsil & Royle, 2013).

6. Experiments and Results

Deep/multilayer feedforward neural networks are useful in many classification problems, with image recognition being a particularly notable example. We examine a variety of standard image recognition datasets used as benchmarks in prior studies. We compare the performances of several standard regularization approaches for neural networks on these datasets, including dropout, L1 regularization and weight decay. Extension of such experiments to non-image classification tasks is straightforward.

The purpose of the experiments below is not to use the deepest neural networks or the latest architectures. Nor is the purpose to show the supremacy of neural networks versus other traditional classification algorithms like SVM or logistic regression. Rather, we attempt to compare the efficacy of Fiedler regularization against other neural network regularization techniques as a proof of concept. Extensions to more complicated and general network architectures are explored in the discussion section.

For the experiments below, we used standard 5-layer neural networks with ReLU activations, batch size of 100 and a learning rate of 0.001. Each hidden layer is 500 units wide, and all layers are fully connected. The networks were trained with 20 epochs. We used PyTorch 1.4 and Python 3.6 for all experiments, and Adam for optimization. For dropout, we used a standard dropout probability of 0.5. For L1, Fiedler regularization and weight decay, we used a penalty parameter value of 0.05. Each experiment was run 5 times, with the median and the standard deviation of the performances reported. All experiments were run on a Unix machine with an Intel Core i7 processor. All code used for the experiments are included in the supplementary material.

6.1. MNIST

Dataset MNIST is a standard handwriting recognition dataset that consist of 60,000 \( 28 \times 28 \) training images of individual hand-written digits and 10,000 testing images.

Results The results for MNIST are displayed in Table 1.

| Regularization | Training | Testing |
|----------------|----------|---------|
| L1             | 9.915 ± 0.79 | 10.01 ± 0.87 |
| WEIGHT DECAY   | 11.24 ± 35.84 | 11.35 ± 35.76 |
| DROPOUT        | 99.81 ± 0.08 | 98.25 ± 0.2  |
| FIEDLER        | 99.72 ± 0.04 | 98.16 ± 0.06 |

1. For the MNIST dataset, we obtained superb accuracies that are near perfect for dropout and Fiedler regularization, followed by weight decay. L1 regularization performed poorly, classifying only marginally better than chance. The high accuracies obtained for the MNIST dataset with dropout is consistent with results from previous studies (Srivastava et al., 2014). Fiedler regularization showed comparable performance to dropout and substantial gains over L1 and weight decay.

6.2. CIFAR10

Dataset CIFAR10 is a benchmark object recognition dataset that consists of \( 32 \times 32 \times 3 \) down-sampled RGB color images of 10 different object classes. There are 50,000 training images and 10,000 test images.

Results The results for CIFAR10 are displayed in Table 2. The ordering among the regularization methods is similar for CIFAR10 to what we obtained for MNIST. While this is known as a more difficult dataset than MNIST, the same pattern persists: Dropout and Fiedler regularization performed the best, followed by weight decay, followed by L1 regularization, which performed no better than chance.

We remark that Fiedler regularization enjoys practical running speeds that are very fast, comparable to that of dropout, weight decay and L1. After running for a long enough period of time (20 epochs), we observe that the training accuracy of the 5 layer neural network generally stabilizes, a sign of convergence.

L1 regularization has long been an unpopular choice for deep learning, perhaps partly due to its poor empirical performance in training multi-layer neural networks that we observed in our experiments. We experimented with a
range of penalty values ranging from 0.001 to 0.05 for L1, but performance changed only negligibly. Another potential factor for its poor performance is the choice of optimization technique. When we switched to using Stochastic Gradient Descent without momentum rather than Adam, we observe an increase in L1 performance to around 30 percent classification accuracy, still substantially lower than the performance of Dropout and Fiedler regularization.

7. Discussion

The above experiments demonstrated several points of interest. The poor performance of L1 regularization stands in sharp contrast to the performance of Fiedler regularization, a weighted L1 penalty. The precise reason why this happens is unknown. Previous studies have adopted a group-lasso formulation for regularization of deep neural networks and have obtained good performance. It appears that modifications of L1 through weighting or other similar schemes can drastically improve empirical performance.

We note that while we only considered relatively simple feedforward neural architectures, extensions to more sophisticated structures are straightforward. Many convolutional neural networks contain fully connected layers after the initial convolutional layers. Dropout regularization of such networks usually only concerns dropping nodes in the fully connected layers. One could easily extend Fiedler regularization to this case. In the context of ResNets, where there are skip connections, the spectral graph properties we have utilized still hold, and hence Fiedler regularization could be directly applied. An open direction is to establish appropriate spectral graph theory for directed, weighted graphs so that Fiedler regularization could be applied to recurrent neural networks.

We also note that while in theory Fiedler regularization could lead to sparsely connected neural networks, in practice it can take a higher penalty to achieve sparsity. This might be in part due to the penalty weights \(|(u(i) - u(j))^2|\): \(u\) is a unit vector and squaring the difference between its entries could lead to small penalties for \(|W|_{ij}\). This could be offset by setting a larger value of \(\delta\).

We also note that while Fiedler regularization emphasizes regularization based on graph connectivity structure, global penalization approaches such as Dropout, L2 etc could still prove useful. One could combine the two regularization methodologies to achieve simultaneous regularization based on both graph structure and global scale.

Last, we have adopted a version of spectral graph theory that considers the unnormalized Laplacian \(L = D - |W|\). A similar theory could be developed for the normalized Laplacian \(L' = I - D^\frac{1}{2}|W||D|^\frac{1}{2}\) after appropriately accounting for the total scale of the neural network. While the unnormalized Laplacian that we considered is related to the notion of RatioCut, the normalized Laplacian is associated with the notion of NCuts. Both notions could in theory be used for reducing connectivity/co-adaptation of the neural network.

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