Scalable Semi-Supervised Learning over Networks using Nonsmooth Convex Optimization

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Abstract

We propose a scalable method for semi-supervised (transductive) learning from massive network-structured datasets. Our approach to semi-supervised learning is based on representing the underlying hypothesis as a graph signal with small total variation. Requiring a small total variation of the graph signal representing the underlying hypothesis corresponds to the central smoothness assumption that forms the basis for semi-supervised learning, i.e., input points forming clusters have similar output values or labels. We formulate the learning problem as a nonsmooth convex optimization problem which we solve by appealing to Nesterov’s optimal first-order method for nonsmooth optimization. We also provide a message passing formulation of the learning method which allows for a highly scalable implementation in big data frameworks.

I. INTRODUCTION

Modern technological systems generate (heterogeneous) data at unprecedented scale, i.e., “Big Data” [9], [11], [16], [23]. While lacking a precise formal definition, Big Data problems typically share four main characteristics: (i) large data volume, (ii) high speed of data generation, (iii) data is heterogeneous, i.e., partially labeled or unlabeled, mixture of audio, video and text data and (iv) data is noisy, i.e., there are statistical variations due to missing labels, labeling errors, or poor data curation [23]. Moreover, in a wide range of big data applications, e.g., social networks, sensor networks, communication networks, and biological networks an intrinsic graph (or network) structure is present. This graph structure reflects either the physical properties of a system (e.g., public transportation networks) or statistical dependencies (e.g., probabilistic graphical models for bioinformatics). Quite often, these two notions of graph structure coincide: in a wireless sensor network, the graph modeling the communication links between nodes and the graph formed by statistical dependencies between sensor measurements resemble each other since both graphs are induced by the nodes mutual proximity [17], [21], [24].

On the algorithmic side, having a graph model for the observed datapoints facilitates scalable distributed data processing, in the form of message passing on the graph. On a higher-level, graph models are suitable to deal with data of diverse nature, since they only require a weak notion of similarity between datapoints. Moreover, graph models allow to capitalize on massive amounts of unlabeled data via semi-supervised learning. In particular, semi-supervised learning exploits the information contained in large amounts of unlabeled datapoints by considering their similarities to a small number of labeled datapoints.

In this paper, we consider the problem of semi-supervised learning using a graph model for the raw data. The observed data consists of a small number of labeled datapoints and a huge amount of unlabeled datapoints. We tackle this learning problem by casting the dataset as a graph signal. In this graph signal model, the different dimensions of the data are identified as variables and the observed values of these variables are called signals. These signals are represented by nodes of a (empirical) graph whose edges represent pairwise dependencies between signals. Imposition of such graph signal structure on the data is

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analogous to making the smoothness assumption of semi-supervised learning \[7\]: signals that are connected by an edge in the graph have similar labels. In other words, the graph signal is expected to reflect the underlying graph structure in the sense that the labels of signals on closely connected nodes have high mutual correlation and thus these signals form close-knit clusters or communities \[12\]. In order to quantify the smoothness assumption underlying semi-supervised learning, one can use different measures to incorporate the topological dependency structure of graphs signals. For example, one can project the signals onto the column space of the graph Laplacian matrix, using the squared norm of the projected signals, i.e., the graph Laplacian form, as a measure of smoothness. This is the basis for many well-known label propagation methods \[7\].

In contrast, the approach proposed in this paper is based on using (graph) total variation \[22\], which provides a more natural match between smoothness and the community structure of the data, i.e., input or feature signal nodes forming a community or cluster should yield similar output values or labels.

Conclusions and Outline

In Section II, we formulate semi-supervised learning using a graph model for the observed data as a convex optimization problem. By adapting Nesterov’s method for nonsmooth convex optimization, which is reviewed in Section III, we propose an efficient learning algorithm in Section IV. We then present a message passing formulation of our learning algorithm in Section V, which only requires local information updating. We also discuss how to implement the message passing formulation for graphs of massive size.

Notation

Matrices are denoted by boldcase uppercase letters (e.g. \(A\)) and column vectors are denoted by boldface lowercase letters (e.g. \(x\)). The \(i\)th entry of the vector \(x\) is denoted by \(x_i\), and the entry in the \(i\)th row and \(j\)th column of matrix \(A\) is \(A_{ij}\). For vectors \(x, y \in \mathbb{R}^N\) and matrices \(X, Y \in \mathbb{R}^{N \times N}\), we define the inner products \(\langle x, y \rangle_2 := \sum_i x_i y_i\) and \(\langle X, Y \rangle_F := \sum_{i,j} X_{ij} Y_{ij}\) with induced norms \(\|x\|_2 := \sqrt{\langle x, x \rangle_2}\) and \(\|X\|_F := \sqrt{\langle X, X \rangle_F}\). For a generic Hilbert space \(\mathcal{H}\), we denote its inner product by \(\langle \cdot, \cdot \rangle_{\mathcal{H}}\). Given a linear operator \(B\) mapping the Hilbert space \(\mathcal{H}_1\) into the Hilbert space \(\mathcal{H}_2\), we denote its adjoint by \(B^*\) and by \(\|B\|_{op} := \sup_{\|x\|_{\mathcal{H}_1} \leq 1} \|Bx\|_{\mathcal{H}_2}\) its operator norm. The operator norm of a matrix \(A \in \mathbb{R}^{M \times N}\), interpreted as a mapping from Hilbert space \(\mathbb{R}^M\) to \(\mathbb{R}^N\), reduces to the spectral norm \(\|A\|_2 := \sup_{x \in \mathbb{R}^N \setminus \{0\}} \|Ax\|_2 / \|x\|_2\). The \(i\)th column of the identity matrix \(I\) is denoted by \(e_i\). Given a closed convex subset \(C \subseteq \mathcal{H}\) of a Hilbert space, we denote by \(\pi_C(x) = \arg \min_{z \in C} \|z - x\|_{\mathcal{H}}\) the orthogonal projection on \(C\). For a diagonal matrix \(D \in \mathbb{R}^{N \times N}\) with non-negative main diagonal entries \(d_{i,i}\), we denote by \(D^{1/2}\) the diagonal matrix with main diagonal entries \(\sqrt{d_{i,i}}\).

II. Problem Formulation

We consider a heterogenous dataset \(D = \{z_i\}_{i=1}^N \subseteq \mathcal{Z}\) consisting of \(N\) datapoints \(z_i \in \mathcal{Z}\), which might be of significantly different nature, e.g., \(z_1 \in \mathbb{R}^d\), \(z_2\) is a continuous-time signal (i.e., \(z_2 : \mathbb{R} \rightarrow \mathbb{R}\)) and \(z_3\) might represent the bag-of-words histogram of a text document. Thus, we assume the input space \(\mathcal{Z}\) rich enough to accomodate for strongly heterogeneous data. Associated with the dataset \(D\) is an undirected empirical graph \(\mathcal{G} = (\mathcal{V}, \mathcal{E}, \mathcal{W})\) with node set \(\mathcal{V} = \{1, \ldots, N\}\), edge set \(\mathcal{E} \subseteq \mathcal{V} \times \mathcal{V}\) and symmetric weight matrix \(\mathcal{W} \in \mathbb{R}^{N \times N}\). The nodes represent the datapoints, i.e., node \(i\) corresponds to the datapoint \(z_i\). An undirected edge \((i, j) \in \mathcal{E}\) encodes some notion of (physical or statistical) similarity from datapoint \(z_i\) to datapoint \(z_j\). Moreover, the presence of an edge \((i, j) \in \mathcal{E}\) between nodes \(i, j \in \mathcal{V}\) is indicated by a nonzero entry \(W_{i,j} = W_{j,i}\) of the weight matrix \(\mathcal{W}\). Given an edge \((i, j) \in \mathcal{E}\), the nonzero value \(W_{i,j} > 0\) represents the strength of the connection from node \(i\) to node \(j\). We assume the empirical graph to be simple, i.e., it contains no self-loops (\(W_{i,i} = 0\) for all \(i \in \mathcal{V}\)). The neighborhood \(\mathcal{N}(i)\) and degree \(d_i\) of node \(i \in \mathcal{V}\) is defined, respectively, as

\[
\mathcal{N}(i) := \{j \in \mathcal{V} : (i, j) \in \mathcal{E}\}
\]
We emphasize that the label which represents the deviation of the learned labels if we fix a maximum level values (i.e., \(x_i \in \{0, 1\}\), multi-level discrete values (i.e., \(x_i \in \{1, \ldots, K\}\), with \(K\) being the number of classes or clusters), or continuous values in \(\mathbb{R}\). We can represent the entire labeling of the empirical graph conveniently by a vector \(x \in \mathbb{R}^N\) whose \(i\)th entry is the label \(x_i\) of node \(i \in \mathcal{V}\). For a small subset \(S\) of datapoints \(z_i\) we are provided with initial labels \(y_i\). With slight abuse of notation, we refer by \(S\) also to the subset of nodes \(i \in \mathcal{V}\) representing the datapoints \(z_i\) for which initial labels \(y_i\) are available. We refer to the set \(S \subseteq \mathcal{V}\) as the sampling set, where typically \(M := |S| \ll N\).

In order to learn the entire labeling \(x\) from the initial labels \(\{y_i\}_{i \in S}\), we invoke the basic smoothness assumption for semi-supervised learning \([7]\): If two points \(z_1, z_2\) are close, with respect to a given topology on the input space \(Z\), then so should be the corresponding labels \(x_1, x_2\), with respect to some distance measure on the label space \(\mathbb{R}\). For quantifying the smoothness of a labeling, we appeal to the discrete calculus for graph signals, which rests on the concept of a gradient for graph signals \([7, \text{Sec. 13.2}]\). In order to draw on discrete calculus for quantifying smoothness of a labeling, we interpret the labels \(x_i\), for \(i \in \mathcal{V}\), as the values of a graph signal, i.e., a mapping \(x[\cdot] : \mathcal{V} \to \mathbb{R}\) which maps node \(i \in \mathcal{V}\) to graph signal value \(x[i] = x_i\). Using this interpretation, we measure the smoothness of the labels via the (local) gradient \(\nabla x\) at node \(i \in \mathcal{V}\), given as \([22]\)

\[
(\nabla x)_j := \sqrt{W_{i,j}}(x_j - x_i).
\]  

The norm \(\|\nabla x\|_2 = \sqrt{\sum_{j \in \mathcal{V}} W_{i,j}(x_j - x_i)^2}\) provides a measure for the local variation of the graph signal \(x\) at node \(i \in \mathcal{V}\). The (global) smoothness of the labels \(x_i\) is then quantified by the total variation \([22]\):

\[
\|x\|_{TV} := \sum_{i \in \mathcal{V}} \|\nabla x\|_2 = \sum_{i \in \mathcal{V}} \sqrt{\sum_{j \in \mathcal{V}} W_{i,j}(x_j - x_i)^2}.
\]  

Note that the total variation \((5)\) is a seminorm, being equal to 0 for labelings that are constant over connected graph components.

The basic idea of semi-supervised learning is to find a labeling \(x\) of the datapoints \(z_i\) by balancing the empirical error

\[
\text{Err}[x] := \sqrt{\frac{1}{2|S|} \sum_{i \in S} (x_i - y_i)^2},
\]  

which represents the deviation of the learned labels \(x_i\) from the initial labels \(y_i\), with the smoothness \(\|x\|_{TV}\). If we fix a maximum level \(\varepsilon > 0\) tolerated for the empirical error \(\text{Err}[x]\), we can formulate semi-supervised learning as the optimization problem

\[
\hat{x} \in \arg \min_{x \in Q} \|x\|_{TV}
\]

with \(Q := \{x \in \mathbb{R}^N : \text{Err}[x] \leq \varepsilon\}\). \(\text{Err}[x] \leq \varepsilon\)
Since the objective function in (7) is the seminorm $\|z\|_{TV}$, which is a convex function and also the constraint set $Q$ is a convex set, problem (7) is a convex optimization problem. As the notation in (7) suggests, and which can be verified by simple examples, there typically exist several solutions for this optimization problem. However, the methods we consider for solving (7) in the following do not require uniqueness of the solution, i.e., they work even if there are multiple optimal labelings $\hat{x}$.

For completeness, we also mention an alternative convex formulation of the recovery problem (7), based on using a penalty term for the total variation instead of constraining the empirical error:

$$\hat{x} \in \arg \min_{x \in \mathbb{R}^N} \text{Err}[x] + \lambda \|x\|_{TV}. \quad (8)$$

The regularization parameter $\lambda > 0$ trades off small empirical risk $\text{Err}[\hat{x}]$ against small total variation $\|\hat{x}\|_{TV}$ of the learned labeling $\hat{x}$.

The convex optimization problems (7) and (8) are related by convex duality [2], [5]: For each choice for $\varepsilon$ there is a choice for $\lambda$ (and vice-versa) such that the solutions of (7) and (8) coincide. However, the relation between $\varepsilon$ and $\lambda$ for this equivalence to hold is non-trivial and determining the corresponding $\lambda$ for a given $\varepsilon$ is as challenging as solving the problem (7) itself [11].

From a practical viewpoint, an advantage of the formulations (7) is that the parameter $\varepsilon$ may be interpreted as a noise level, which can be estimated or adjusted more easily than the parameter $\lambda$ of the learning problem (8). For the rest of the paper, we will focus on the learning problem (7).

Finally, for a dataset $D$ whose empirical graph $G$ is composed of several (weakly connected) components [20], the learning problem (7) decompose into independent subproblems, i.e., one learning problem of the form (7) for each of the components. Therefore, we will henceforth, without loss of generality, consider datasets whose empirical graph $G$ is (weakly) connected.

### III. Optimal Nonsmooth Convex Optimization

We will now briefly review a recently proposed method [19] for solving nonsmooth convex optimization problems, i.e., optimization problems with a non-differentiable objective function, such as (7). This method exploits a particular structure, which is present in the problems (7). In particular, this optimization method is based on (i) approximating a nonsmooth objective function by a smooth proxy and (ii) then applying an optimal first order (gradient based) method for minimizing this proxy.

Consider a structured convex optimization problem of the generic form

$$\hat{x} \in \arg \min_{x \in \mathcal{Q}_1} f(x) := \hat{f}(x) + \max_{u \in \mathcal{Q}_2} \langle u, Bx \rangle_{\mathcal{H}_2} - \hat{g}(u). \quad (9)$$

Here, $B : \mathcal{H}_1 \to \mathcal{H}_2$ is a linear operator from a finite dimensional Hilbert space $\mathcal{H}_1$ to another finite dimensional Hilbert space $\mathcal{H}_2$, both defined over the real numbers. The set $\mathcal{Q}_1 \subseteq \mathcal{H}_1$ is required to be a closed convex set and the set $\mathcal{Q}_2 \subseteq \mathcal{H}_2$ is a bounded, closed convex set. The functions $\hat{f}$ and $\hat{g}$ in (9) are required to be continuous and convex on $\mathcal{Q}_1$ and $\mathcal{Q}_2$, respectively. Moreover, the function $\hat{f}$ is assumed differentiable with gradient $\nabla \hat{f}$ being Lipschitz-continuous with constant $L \geq 0$, i.e.,

$$\|\nabla \hat{f}(y) - \nabla \hat{f}(x)\|_{\mathcal{H}_1} \leq L \|y - x\|_{\mathcal{H}_1}. \quad (10)$$

**Smooth Approximation of Nonsmooth Objective**

In order to solve the nonsmooth problem (9), we approximate the non-differentiable component $\hat{h}_0(x)$ by the smooth function

$$h_\mu(x) := \max_{u \in \mathcal{Q}_2} \langle u, Bx \rangle_{\mathcal{H}_2} - \hat{g}(u) - (\mu/2) \|u\|_{\mathcal{H}_2}^2 \quad (11)$$

The seminorm $\|x\|_{TV}$ is convex since it is homogeneous ($\|\alpha x\|_{TV} = |\alpha| \|x\|_{TV}$ for $\alpha \in \mathbb{R}$) and satisfies the triangle inequality ($\|x+y\|_{TV} \leq \|x\|_{TV} + \|y\|_{TV}$). These two properties imply convexity [3] Section 3.1.5].
with the smoothing parameter \( \mu > 0 \), yielding
\[
f_\mu(x) := \hat{f}(x) + \max_{u \in Q_2} \langle u, Bx \rangle_{\mathcal{H}_2} - \hat{g}(u) - (\mu/2)\|u\|_{\mathcal{H}_2}^2. \tag{12}
\]
The objective function \( f(x) \) of the original problem (9) is obtained formally from (12) for the choice \( \mu = 0 \), i.e., \( f(x) = f_0(x) \). Since the function \( g(u) = \|u\|_{\mathcal{H}_2}^2 \) is strongly convex, the optimization problem (11) has a unique optimal point
\[
u_\mu(x) = \arg\max_{u \in Q_2} \langle u, Bx \rangle_{\mathcal{H}_2} - \hat{g}(u) - (\mu/2)\|u\|_{\mathcal{H}_2}^2. \tag{13}
\]
According to [19, Theorem 1], the function \( h_\mu(x) \) (cf. (11)) is differentiable with gradient
\[
\nabla h_\mu(x) = B^*u_\mu(x),
\]
which can be shown to be Lipschitz continuous with constant \((1/\mu)\|B\|_{\text{op}}^2\). Since the gradient \( \nabla \hat{f}(x) \) of \( \hat{f}(x) \) is assumed Lipschitz continuous with constant \( L \) (cf. (10)), the function \( f_\mu(x) \) (cf. (12)) has gradient
\[
\nabla f_\mu(x) = \nabla \hat{f}(x) + B^*u_\mu(x) \tag{14}
\]
which is Lipschitz continuous with constant
\[
L_\mu := L + (1/\mu)\|B\|_{\text{op}}^2. \tag{15}
\]
Furthermore, by evaluating [19, Eq. (2.7)], we have
\[
f_\mu(x) \leq f_0(x) = f(x) \leq f_\mu(x) + (\mu/2)\max_{u \in Q_2} \|u\|_{\mathcal{H}_2}^2, \tag{16}
\]
which verifies that \( f_\mu(x) \) is a uniform smooth approximation of the objective function \( f(x) \) in (9).

By replacing the objective \( f(x) \) in (9) with its smooth approximation \( f_\mu(x) \), we obtain the smooth optimization problem
\[
\hat{x}_\mu \in \arg\min_{x \in Q_1 \subseteq \mathcal{H}_1} f_\mu(x). \tag{17}
\]
The original nonsmooth problem (9) is obtained formally from the smooth approximation (17) for the particular choice \( \mu = 0 \). For nonzero \( \mu > 0 \), the solutions \( \hat{x} \) of (9) will be different from the solutions \( \hat{x}_\mu \) of (17) in general. However, for sufficiently small \( \mu \) any solution \( \hat{x}_\mu \) of (17) will be also an approximate solution to (9). We can relate the optimal values \( f(\hat{x}) \) and \( f_\mu(\hat{x}_\mu) \) of the original problem (9) and its smooth approximation (17), respectively, with the help of (16). Indeed, by inserting the optimal points \( \hat{x}_\mu \) and \( \hat{x} \) into the corresponding objective functions in (16), we obtain
\[
f_\mu(\hat{x}_\mu) \leq f(\hat{x}) \leq f_\mu(\hat{x}_\mu) + (\mu/2)\max_{u \in Q_2} \|u\|_{\mathcal{H}_2}^2. \tag{18}
\]
Thus, the optimal value \( f_\mu(\hat{x}_\mu) \) of the smoothed problem (12) provides an estimate for the optimal value \( f(\hat{x}) \) of the original problem (9).

**Optimal Gradient Method for Smooth Minimization**

For solving the smooth optimization problem (17), being a proxy for the original nonsmooth problem (9), we apply an optimal first-order method [11, 19]. This method achieves the optimal worst-case rate of convergence among all gradient based methods [18, 19]. We summarize this method for solving (17) in Alg. 1 which requires as input the smoothing parameter \( \mu > 0 \), an initial guess \( x_0 \) and a valid Lipschitz constant \( L \) for the gradient (14), i.e., satisfying \( L \geq L_\mu = L + (1/\mu)\|B\|_{\text{op}}^2 \). For a particular stopping criterion of Alg. 1 one can monitor the relative decrease in the objective function \( f_\mu(x_k) \) (cf. Section V.6), is to run Alg. 1 for a fixed number of iterations.
Theorem 2.1.7. methods for the class of continuously differentiable functions with Lipschitz continuous gradient \[18, \text{decaying proportional to} \]

The approximation to the objective function.

Let \( \text{proxy} \)

obtained in step

Lemma III.1.

For the choice

Input:

smoothing parameter \( \mu \), initial guess \( x_0 \), Lipschitz constant \( \hat{L} \geq L_{\mu} = L + (1/\mu) \| B \|_{opt}^2 \) (cf. (15))

Initialize: iteration counter \( k := 0 \)

1: repeat
2: \( g_k := \nabla f_{\mu}(x_k) = \nabla \hat{f}(x) + B^* u_{\mu}(x) \) with \( u_{\mu}(x) \) given by (13)
3: \( x_k := \arg \min_{x \in Q_1} (\hat{L}/2)\| x - x_k \|_{\mathcal{H}_1}^2 + \langle g_k, x - x_k \rangle_{\mathcal{H}_1} \)
4: \( z_k := \arg \min_{x \in Q_1} (\hat{L}/2)\| x - x_0 \|_{\mathcal{H}_1}^2 + \sum_{i=0}^{k} \frac{1}{\mu+1} \langle g_i, x - x_i \rangle_{\mathcal{H}_1} \)
5: \( x_{k+1} := \frac{2}{\mu+1} z_k + \left(1 - \frac{2}{\mu+1}\right) x_k \)
6: \( k := k + 1 \)
7: until stopping criterion is satisfied

Output: \( \hat{x}_k \)

Theorem 2.1.7. methods for the class of continuously differentiable functions with Lipschitz continuous gradient \[18, \text{decaying proportional to} \]

The approximation to the objective function.

The output \( \hat{x}_k \) of Alg. 1 satisfies [19, Theorem 2]

\[
f_{\mu}(\hat{x}_k) - f_{\mu}(\hat{x}_\mu) \leq \frac{2\hat{L}\| \hat{x}_\mu - x_k \|_2^2}{(k+1)(k+2)}
\]  

for any optimal point \( \hat{x}_\mu \) of [17]. The convergence rate predicted by [19], i.e., the error \( f_{\mu}(\hat{x}_k) - f_{\mu}(\hat{x}_\mu) \) decaying proportional to \( 1/k^2 \) with the iteration counter \( k \), is optimal among all gradient-based minimization methods for the class of continuously differentiable functions with Lipschitz continuous gradient [18, Theorem 2.1.7].

The characterization [19] can be used to bound the number of iterations needed to run Alg. 1 such that it delivers an approximate solution \( \hat{x}_k \in Q_1 \) for the nonsmooth problem [9] with prescribed accuracy \( \delta \), i.e., the output \( \hat{x}_k \) satisfies \( f(\hat{x}_k) - f(\hat{x}) \leq \delta \).

Lemma III.1. Let \( \hat{x} \in \mathbb{R}^N \) and \( \hat{x}_\mu \in \mathbb{R}^N \) be optimal points of the original problem [9] and its smoothed proxy [17], respectively. Denote \( D := \max_{u \in Q_2} \| u \|_{\mathcal{H}_2}^2 \) and assume Alg. 1 is used with Lipschitz constant \( \hat{L} = L + (1/\mu) \| B \|_{opt}^2 \). Then, the output \( \hat{x}_k \) after \( k \) iterations of Alg. 1 satisfies

\[
f(\hat{x}_k) - f(\hat{x}) \leq f_{\mu}(\hat{x}_k) - f_{\mu}(\hat{x}_\mu) + (\mu/2)D.
\]  

For the choice \( \mu = \delta/D \), Alg. 1 delivers a solution \( \hat{x}_k \) for the non-smooth problem [9] with accuracy \( \delta \), i.e.,

\[
f(\hat{x}_k) - f(\hat{x}) \leq \delta \text{ for all } k \geq k_\delta
\]

\[
k_\delta := (2/\delta)\| \hat{x}_\mu - x_0 \|_2 \sqrt{\hat{L}\delta + D\| B \|_{opt}^2}.
\]

Proof: By combining (16) (for the choice \( x = \hat{x}_k \)) with (18), we have

\[
f(\hat{x}_k) - f(\hat{x}) \leq f_{\mu}(\hat{x}_k) - f_{\mu}(\hat{x}_\mu) + (\mu/2)D.
\]  

Algorithm 1 Nesterov’s algorithm for solving (17)

Input: smoothing parameter \( \mu \), initial guess \( x_0 \), Lipschitz constant \( \hat{L} = L + (1/\mu) \| B \|_{opt}^2 \) (cf. (15))

Initialize: iteration counter \( k := 0 \)

1: repeat
2: \( g_k := \nabla f_{\mu}(x_k) = \nabla \hat{f}(x) + B^* u_{\mu}(x) \) with \( u_{\mu}(x) \) given by (13)
3: \( x_k := \arg \min_{x \in Q_1} (\hat{L}/2)\| x - x_k \|_{\mathcal{H}_1}^2 + \langle g_k, x - x_k \rangle_{\mathcal{H}_1} \)
4: \( z_k := \arg \min_{x \in Q_1} (\hat{L}/2)\| x - x_0 \|_{\mathcal{H}_1}^2 + \sum_{i=0}^{k} \frac{1}{\mu+1} \langle g_i, x - x_i \rangle_{\mathcal{H}_1} \)
5: \( x_{k+1} := \frac{2}{\mu+1} z_k + \left(1 - \frac{2}{\mu+1}\right) x_k \)
6: \( k := k + 1 \)
7: until stopping criterion is satisfied

Output: \( \hat{x}_k \)
Choosing $\mu = \delta/D$ and using (19) for the particular choice $\hat{L} = L + (1/\mu)\|B\|^2_{op}$, we obtain

$$f(\hat{x}_k) - f(\bar{x}) \leq (2/\delta)\|\hat{x}_\mu - x_0\|^2(2L\delta + D\|B\|^2_{op})(1/k^2) + \delta/2,$$

which implies (21).

According to Lemma III.1 we need $k \propto 1/\delta$ iterations of Alg. 1 for solving the nonsmooth optimization problem (9) with accuracy $\delta$ (cf. [19, Theorem 3]). This iteration complexity is essentially optimal for any first-order (sub-)gradient method solving problems of the form (9) [14].

The lower bound (21) on the iteration complexity of Alg. 1 depends on both the desired accuracy $\delta$ (which is enforced by choosing the smoothing parameter as $\mu = \delta/D$) and the choice for the initial guess $\|\hat{x}_\mu - x_0\|_2$. As discussed in [1], an effective approach to speed up the convergence of Alg. 1 is to run it repeatedly with increasing accuracy (corresponding to decreasing values of the smoothing parameter $\mu$) and using the output of Alg. 1 in a particular run as initial guess for the next run. Since the initial guesses used for Alg. 1 in a new run becomes more accurate, it is possible to use a smaller value for the smoothing parameter $\mu$, which effects an increased accuracy of the output of Alg. 1 according to (21). However, a simpler option is to adapt the smoothing parameter directly “on-the-fly” within the iterations of Alg. 1. This results in Alg. 2 being an accelerated version of Alg. 1.

### Algorithm 2 Accelerated Nesterov for solving (17)

**Input:** initial smoothing parameter $\mu_0$, decreasing factor $\kappa$, initial guess $x_0$

**Initialize:** iteration counter $k = 0$

1. repeat
   2. $\mu := \mu_0 \kappa^k$
   3. $\hat{L} := L + (1/\mu)\|B\|^2_{op}$
   4. $g_k := \nabla f_\mu(x_k) = \nabla \hat{f}(x) + B^* u_\mu(x)$ with $u_\mu(x)$ given by (13)
   5. $\hat{x}_k := \arg\min_{x \in Q_1} \langle \hat{L}/2, x - x_k \rangle_{H_1} + \langle g_k, x - x_k \rangle_{H_1}$
   6. $z_k := \arg\min_{x \in Q_1} \langle \hat{L}/2, x - x_0 \rangle_{H_1} + \sum_{l=0}^{k-1} \frac{\mu_1}{2} \langle g_l, x - x_l \rangle_{H_1}$
   7. $x_{k+1} := \frac{2}{\mu_0 \kappa^k} z_k + \left(1 - \frac{2}{\kappa^k}\right) \hat{x}_k$
   8. $k := k + 1$
   9. until stopping criterion is satisfied

**Output:** $x_k$

### IV. EFFICIENT LEARNING OF GRAPH SIGNALS

We will now show that the semi-supervised learning problem (7) can be rephrased in the generic form (9). This will then allow us to apply Alg. 1 for semi-supervised learning from big data, i.e., from high-dimensional heterogeneous data, over networks. To this end, we need to introduce the graph gradient operator $\nabla_G$ as a mapping from the Hilbert space $\mathbb{R}^N$ endowed with inner product $\langle a, b \rangle_2 = a^T b$ into the Hilbert space $\mathbb{R}^{N \times N}$ endowed with inner product $\langle A, B \rangle_F = \text{Tr}\{A B^T\}$ [13], [15]. In particular, the gradient operator $\nabla_G$ maps a graph signal $x \in \mathbb{R}^N$ to the matrix

$$\nabla_G x := (\nabla_1 x, \ldots, \nabla_N x)^T \in \mathbb{R}^{N \times N}.$$

(24)

The $i$th row of the matrix $\nabla_G x$ is given by the local gradient $\nabla_i x$ of the graph signal $x$ at node $i \in V$ (cf. (4)). Let us also highlight the close relation between the gradient operator $\nabla_G : \mathbb{R}^N \rightarrow \mathbb{R}^{N \times N}$ and the
normalized graph Laplacian matrix \( L \) [8], defined element-wise as
\[
(L)_{i,j} := \begin{cases} 
1 & \text{if } i = j \text{ and } d_i \neq 0, \\
-1/\sqrt{d_id_j} & \text{if } (i,j) \in \mathcal{E}, \\
0 & \text{otherwise}, 
\end{cases} \tag{25}
\]
with \( d_i \) being the degree of node \( i \in V \) (cf. [2]). If we define the diagonal matrix \( D \) with diagonal elements \( d_{i,i} = d_i \), we have for any graph signal \( x \) (cf. [22] Eq. (6)) the identity
\[
\|\nabla_G x\|_F^2 = x^T D^{1/2} L D^{1/2} x. \tag{26}
\]
We then define the divergence operator \( \text{div}_G : \mathbb{R}^{N \times N} \to \mathbb{R}^N \) as the negative adjoint of the gradient operator \( \nabla_G : \mathbb{R}^N \to \mathbb{R}^{N \times N} \) (cf. [7] Chapter 13), i.e.,
\[
\text{div}_G := -\nabla_G. \tag{27}
\]
A straightforward calculation (cf. [7] Proposition 13.4) reveals that the operator \( \text{div}_G \) maps a matrix \( P \in \mathbb{R}^{N \times N} \) to the vector \( \text{div}_G P \in \mathbb{R}^N \) with entries
\[
(\text{div}_G P)_i = \sum_{j \in V} \sqrt{W_{i,j}} P_{i,j} - \sqrt{W_{j,i}} P_{j,i} \tag{28}
\]
We highlight the fact that both, the gradient \( \nabla_G : \mathbb{R}^N \to \mathbb{R}^{N \times N} \) as well as the divergence operator \( \text{div}_G \) depend on the graph structure due to the presence of the weights \( W_{i,j} \) in (4) and (28). Moreover, the above definitions for the gradient and divergence operator over complex networks are straightforward generalizations of the well-known gradient and divergence operator for grid graphs representing 2D-images [6].

Using the identity \( \|\nabla x\|_2 = \max \langle p_i, \nabla x \rangle_2 \), we can represent the total variation (5) as
\[
\|x\|_{TV} = \sum_{i \in V} \max_{\|p_i\|_2 \leq 1} \langle p_i, \nabla x \rangle_2 = \max_{P \in \mathcal{P}} \langle P, \nabla_G x \rangle_F. \tag{29}
\]
with the closed convex set
\[
\mathcal{P} := \{ P = (p_1, \ldots, p_N)^T \in \mathbb{R}^{N \times N} : \|p_i\|_2 \leq 1 \text{ for every } i = 1, \ldots, N \}. \tag{30}
\]
Using (29), the learning problem (7) can be written as
\[
\min_{x \in \mathcal{Q}} f_0(x) \quad \text{with} \quad f_0(x) := \max_{P \in \mathcal{P}} \langle P, \nabla_G x \rangle_F \tag{31}
\]
with constraint set \( \mathcal{Q} = \{ x \in \mathbb{R}^N : \text{Err}[x] \leq \varepsilon \} \) (cf. (6) and (7)). The optimization problem (31) is exactly of the form (2) with the linear operator \( B = \nabla_G \), the functions \( f(x) \equiv 0 \) and \( g(u) \equiv 0 \), and the sets \( \mathcal{Q}_1 = \mathcal{Q} \) and \( \mathcal{Q}_2 = \mathcal{P} \). The smoothed version (cf. (12)) of the problem (7) is then obtained as
\[
\min_{x \in \mathcal{Q}} f_\mu(x) \quad \text{with} \quad f_\mu(x) := \max_{P \in \mathcal{P}} \left( \langle P, \nabla_G x \rangle_F - (\mu/2)\|P\|_2^2 \right). \tag{32}
\]
In order to apply Alg. 1 to the smoothed version (32) of the learning problem (7), we have to determine the gradient \( \nabla f_\mu(x) \) and a corresponding valid Lipschitz constant \( L \geq L_\mu \) (cf. (15)). The gradient \( \nabla f_\mu(x) \)
is obtained by specializing (14) for the objective in (32), yielding
\[ \nabla f_\mu(x) = -\text{div}_G P_\mu(x) \] (33)
with
\[ P_\mu(x) = \arg \max_{P \in P} \left( \langle P, \nabla G x \rangle_F - (\mu/2)\|P\|_2^2 \right). \] (34)

By the KKT conditions for constrained convex optimization problems [5], [15],
\[ P_\mu(x) = (q_1, \ldots, q_N)^T \] (35)
with \[ q_i = \max\{\mu, \|\nabla_i x\|_2\} \nabla_i x \]
A particular Lipschitz constant for the gradient \( \nabla f_\mu(x) \) is obtained, by specializing (15) to \( B = \nabla G \), as
\[ L_\mu = (1/\mu)\|\nabla G\|_{\text{op}}^2 \] (36)
However, since evaluating the exact operator norm of the gradient (or divergence) operator is difficult for an arbitrary large-scale graph, we will rely on a simple upper bound.

Lemma IV.1. Let \( \mathcal{G} = (V, E, W) \) be a weighted undirected graph and let \( \nabla G \) denote the corresponding gradient operator (24). The norm of the gradient operator satisfies
\[ \|\nabla G\|_{\text{op}} \leq \sqrt{2d_{\text{max}}} \] (37)
with the maximum node degree \( d_{\text{max}} \) (cf. (3)).

Proof: Due to (26), we have
\[ \|\nabla G\|_{\text{op}}^2 = \|D^{1/2}LD^{1/2}\|_2, \] (38)
which, since obviously \( \|D\|_2 \leq d_{\text{max}} \), implies
\[ \|\nabla G\|_{\text{op}}^2 \leq d_{\text{max}}\|L\|_2. \] (39)
The bound (37) follows from the well-known upper bound \( \|L\|_2 \leq 2 \) for the maximum eigenvalue (which is equal to the spectral norm) of the normalized Laplacian matrix \( L \) (cf. [8, Lemma 1.7])

According to Lemma IV.1, the gradient \( \nabla f_\mu(x) \) (cf. (33)) of \( f_\mu(x) \) is Lipschitz with constant
\[ \tilde{L} = 2d_{\text{max}}/\mu, \] (40)
which we can use as input to Alg. 1.

In order to apply Alg. 1 to the smoothed learning problem (32), we now present closed-form expressions for the updates in step 3 and 4 of Alg. 1 for \( Q_1 = Q \) (cf. (7)).

Lemma IV.2. Consider the convex set \( Q = \{x : \text{Err}[x] \leq \varepsilon\} \) and let \( y \) denote any labeling which is consistent with the initial labels \( y_i \), i.e., \( (y)_i = y_i \) for all \( i \in S \). Then, using the shorthand \( D(S) := \sum_{i \in S} e_i e_i^T \), the solution \( \hat{x}_k \) of the optimization problem
\[ \hat{x}_k = \arg \min_{x \in Q} (\tilde{L}/2)\|x - x_k\|_2^2 + g_k^T(x - x_k) \] (41)

3In many big data applications it is not possible to have a complete description of the graph, e.g. in form of an edge list, available. Instead, one typically has only knowledge about some basic parameters, e.g., the maximum node degree \( d_{\text{max}} \) (cf. (3)).
is given by
\[
\hat{x}_k = (I + \lambda \varepsilon D(S))^{-1}(q + \lambda \varepsilon D(S)y)
\]

\[
= (I - D(S))q + \begin{cases} 
D(S)[y + (\varepsilon/r)(q - y)] & \text{if } r > \varepsilon \\
D(S)q & \text{otherwise}
\end{cases}
\]

with
\[
q := x_k - (1/\hat{L})g_k, \quad r := \text{Err}[q - y]
\]

In a similar manner, the solution \(z_k\) of the optimization problem
\[
z_k = \arg \min_{x \in \mathcal{Q}} \| x - x_0 \|_2 + (1/2) \sum_{l=0}^{k} (l+1)g_l^T(x - x_l)
\]
is given by
\[
z_k = (I - \tilde{\lambda} \varepsilon D(S))\tilde{q} + \begin{cases} 
D(S)[y + (\varepsilon/r)(\tilde{q} - y)] & \text{if } r > \varepsilon \\
D(S)\tilde{q} & \text{otherwise}
\end{cases}
\]

with
\[
\tilde{q} := x_0 - (1/2\hat{L}) \sum_{l=0}^{k} (l+1)g_l, \quad \tilde{r} := \text{Err}[\tilde{q} - y]
\]

\[\text{Proof: see Appendix A}\]

The closed-form expressions (42) and (45) are suitable modifications of those presented in [1, Sec. 3] to our setting of semi-supervised learning over complex networks. We are now in the position to specialize Alg. I to the smoothed learning problem (32) by using the closed-form expressions (42) and (45) for step 3 and 4 of Alg. I. This results in Alg. 3 for semi-supervised learning from big data over networks.

The steps 2 and 3 of Alg. 3 amount to computing the gradient \(g_k = \nabla f_\mu(x_k)\) of the objective function \(f_\mu(x)\) in the learning problem (32). The steps 4-6 of Alg. 3 implement a projected gradient descent step, while steps 7-9 amount to computing the minimizer \(z_k\) of the approximation in step 4 of Alg. 1.

Combining (19) with (40), yields the following characterization of the convergence rate of Alg. 3:
\[
f_\mu(\hat{x}_k) - f_\mu(\hat{x}_\mu) \leq \frac{4d_{\max}||\hat{x}_\mu - x_0||^2_2}{\mu(k+1)(k+2)}
\]
for any solution \(\hat{x}_\mu\) of (32). The bound (47) suggests that the convergence is faster for graphs which are more sparse, i.e., have a smaller maximum node degree \(d_{\max}\). As for Alg. I, the convergence speed of Alg. 3 depends on the accuracy of the initial guess as well as on the smoothing parameter \(\mu\). The accelerated version of Alg. 3 is then obtained from Alg. 2, yielding Alg. 4.

V. MESSAGE PASSING FORMULATIONS

In order to make semi-supervised learning via the optimization problem (32) feasible for massive (internet-scale) datasets, we will now discuss a message passing formulation of Alg. 3 which is summarized as Alg. 5 (being an adaptation of [13, Alg. 2] to undirected graphs): The steps 2-6 of Alg. 5 amount to computing the (scaled) gradient \(\nabla f_\mu(x)\) (cf. (33)) of the objective function \(f_\mu(x)\) for the problem (32) in a distributed manner. The quantities \(P_{i,j}\) are the entries of the matrix \(P_\mu(x)\) (cf. (34)). The steps 11-15 and 17-21 of
Algorithm 3  Semi-Supervised Learning via Nesterov’s Method

**Input:** dataset \( \mathcal{D} \) with empirical graph \( \mathcal{G} \), subset \( S = \{i_1, \ldots, i_M\} \) of datapoints with initial labels \( \{y_j\}_{j \in S} \), error level \( \varepsilon \), smoothing parameter \( \mu \), initial guess for the labeling \( x_0 \in \mathbb{R}^N \)

**Initialize:** \( k := 0 \), Lipschitz constant \( \tilde{L} := (2/\mu) d_{\text{max}} \), \( q_0 := x_0 \), \( \alpha := 1/2 \)

1. repeat
   2. \( \forall i \in \mathcal{V} : p_i := \max\{\mu, ||x_k||_2\} \nabla_i x_k \)
   3. \( g_k := -\text{div}_\mathcal{G}(P) \) with \( P = (p_1, \ldots, p_N)^T \)
   4. \( q_k := x_k - (1/\tilde{L}) g_k \)
   5. \( r := \text{Err}[q_k] \) (cf. (6))
   6. \( \forall i \in \mathcal{V} : \tilde{x}_{k,i} := \begin{cases} y_i + (\varepsilon/r)(q_{k,i} - y_i) & \text{if } i \in S \text{ and } r > \varepsilon \\ q_{k,i} & \text{otherwise} \end{cases} \)
   7. \( \tilde{q}_k := \tilde{q}_k - (\alpha/\tilde{L}) g_k \)
   8. \( \tilde{r} := \text{Err}[\tilde{q}_k] \)
   9. \( \forall i \in \mathcal{V} : z_{k,i} := \begin{cases} y_i + (\varepsilon/\tilde{r})(\tilde{q}_{k,i} - y_i) & \text{if } i \in S \text{ and } \tilde{r} > \varepsilon \\ \tilde{q}_{k,i} & \text{otherwise} \end{cases} \)
   10. \( x_{k+1} := \frac{2}{k+3} z_k + (1 - \frac{2}{k+3}) x_k \)
   11. \( k := k + 1 \)
   12. \( \alpha := \alpha + 1/2 \)
13. until stopping criterion is satisfied

**Output:** learned labeling \( x_k \) for all datapoints

Algorithm 4  Semi-Supervised Learning via Accelerated Nesterov

**Input:** dataset \( \mathcal{D} \) with empirical graph \( \mathcal{G} \), subset \( S = \{i_1, \ldots, i_M\} \) of datapoints with initial labels \( \{y_j\}_{j \in S} \), error level \( \varepsilon \), initial smoothing parameter \( \mu_0 \), decreasing factor \( \kappa \), initial guess for the labeling \( x_0 \in \mathbb{R}^N \)

**Initialize:** \( k := 0 \), \( q_0 := x_0 \), \( \alpha := 1/2 \)

1. repeat
   2. \( \mu := \mu_0 \kappa^k \)
   3. \( \tilde{L} := (2/\mu) d_{\text{max}} \)
   4. \( \forall i \in \mathcal{V} : p_i := \max\{\mu, ||x_k||_2\} \nabla_i x_k \)
   5. \( g_k := -\text{div}_\mathcal{G}(P) \) with \( P = (p_1, \ldots, p_N)^T \)
   6. \( q_k := x_k - (1/\tilde{L}) g_k \)
   7. \( r := \text{Err}[q_k] \) (cf. (6))
   8. \( \forall i \in \mathcal{V} : \tilde{x}_{k,i} := \begin{cases} y_i + (\varepsilon/r)(q_{k,i} - y_i) & \text{if } i \in S \text{ and } r > \varepsilon \\ q_{k,i} & \text{otherwise} \end{cases} \)
   9. \( \tilde{q}_k := \tilde{q}_k - (\alpha/\tilde{L}) g_k \)
   10. \( \tilde{r} := \text{Err}[\tilde{q}_k] \)
   11. \( \forall i \in \mathcal{V} : z_{k,i} := \begin{cases} y_i + (\varepsilon/\tilde{r})(\tilde{q}_{k,i} - y_i) & \text{if } i \in S \text{ and } \tilde{r} > \varepsilon \\ \tilde{q}_{k,i} & \text{otherwise} \end{cases} \)
   12. \( x_{k+1} := \frac{2}{k+3} z_k + (1 - \frac{2}{k+3}) x_k \)
   13. \( k := k + 1 \)
   14. \( \alpha := \alpha + 1/2 \)
15. until stopping criterion is satisfied

**Output:** learned labeling \( x_k \) for all datapoints
Alg. 5 implement a finite number $K$ of iterations of the average consensus algorithm, using Metropolis-Hastings weights [26], for (approximately) computing the sums \( \frac{1}{N} \sum_{j \in V} b_j = \frac{1}{N} \sum_{j \in S} (y_j - q_j)^2 \) and \( \frac{1}{N} \sum_{j \in V} \tilde{b}_j = \frac{1}{N} \sum_{j \in S} (y_j - \tilde{q}_j)^2 \), respectively. In particular, for sufficiently large $K$, the results $r_i$ and $\tilde{r}_i$ in step 16 and 22 of Alg. 5 satisfy $r_i \approx r$ and $\tilde{r}_i \approx \tilde{r}$ for every node $i \in V$ (cf. step 6,7 of Alg. 3). The choice for the number $K$ of average consensus iterations can be guided by a wide range of results characterizing the convergence rate of average consensus [4], [10], [26]. As a rule of thumb, $K$ should be significantly larger than the diameter $d(G)$ of the underlying graph $G$ [10, Thm. 4.3.]. We highlight that Alg. 5 requires each node $i \in V$ to have access to local information only. In particular, to implement Alg. 5 on a given node $i \in V$, the measurement $y_j$, the value $x_j$, the matrix entries $P_{i,j}$ and the edge weights $W_{i,j}$ are required only for node $i$ itself and its neighborhood $N(i)$.

We implemented Alg. 5 using the big data framework AKKA [25], which is a toolkit for building distributed and resilient message-driven applications. The AKKA implementation was run on a computing cluster composed of nine virtual machines (one master and eight slave workers) obtained via the cloud computing service Amazon EC2. Each virtual machine has been configured with a 64-bit CPU, 3.75 GB of main memory, and 8 GB of local disk storage. In Figure 1 we sketch the basic architecture of the AKKA implementation of our graph learning methods. First, we partition the graph in a simple uniform manner, i.e., node $i \in \{1, \ldots, N\}$ is assigned to partition $(i \mod 8) + 1$. After partitioning $G$, the master machine assigns the obtained partitions to the eight workers and manages the execution of the message passing algorithm between the workers. There are two alternating phases in the execution of the AKKA implementation: the master phase, where the states of the worker machines are synchronized and the worker phase. Two types of operations are executed in the worker phase:

- intra-block operations: each worker performs local computations within its associated partition, and
- inter-block operations: workers exchange messages across their partitions.

We then compared the runtime of the AKKA implementation to the centralized implementation in MATLAB used in [13]. The results indicate a runtime reduction by almost a factor 10 which is reasonable since we are using a cluster of nine machines.

**VI. Numerical Experiments**

We assess the performance of (the accelerated version of) the proposed learning algorithm Alg. 4 empirically by applying it to an synthetic dataset with empirical graph $G = (V, E, W)$, depicted in Fig. 2 whose nodes are made up of 2 disjoint clusters $C_c$ of same size $|C_c| = 100$ giving a total graph size of
Algorithm 5: Distributed Semi-Supervised Learning via Nesterov’s Method

Input: sampling set $S = \{i_1, \ldots, i_M\}$, samples $\{y_j\}_{j\in S}$, error level $\varepsilon$, edge weights $\{W_{i,j}\}_{i,j\in V}$, smoothing parameter $\mu$, initial guess $\{x_{0,i}\}_{i\in V}$, number $K$ of average consensus iterations

Initialize: $L := (2/\mu)d_{\text{max}}$, $\forall i \in V : x_i = x_{0,i}$, $\alpha := 1/2$, $\tau := 2/3$, $\{u_{i,j} := 1/(\max\{d_i, d_j\} + 1)\}_{j\in N(i)}$

1: repeat
2: $\forall i \in V :$ broadcast $x_i$ to neighbors $N(i)$/ collect $\{x_j\}_{j\in N(i)}$ from neighbors $N(i)$
3: $\forall i \in V :$ update $\gamma_i = \sqrt{\sum_{j\in N(i)}(x_j - x_i)^2W_{i,j}}$
4: $\forall i \in V :$ for neighbor $j \in N(i)$ update $P_{i,j} = \frac{1}{\max\{\mu, \gamma_j\}}(x_j - x_i)\sqrt{W_{i,j}}$
5: $\forall i \in V :$ broadcast $P_{i,j}$ to neighbors $N(i)$/ collect $\{P_{j,i}\}_{j\in N(i)}$ from neighbors $N(i)$
6: $\forall i \in V :$ update $\tilde{x}_i = (1/\tilde{L})(\sum_{j\in N(i)}\sqrt{W_{i,j}}P_{j,i} - \sum_{j\in N(i)}\sqrt{W_{i,j}}P_{i,j})$
7: $\forall i \in V :$ update $\tilde{q}_i = x_{0,i} - \tilde{x}_i$
8: $\forall i \in V :$ update $\tilde{g}_i = \tilde{q}_i - \alpha g_i$
9: $\forall i \in V :$ update $\alpha = \alpha + 1/2$
10: $\forall i \in V :$ update $\tilde{q}_i = x_{0,i} - \tilde{g}_i$
11: $\forall i \in V :$ update $b_i = \begin{cases} (y_i - q_i)^2 & \text{for } i \in \mathcal{S} \\ 0 & \text{else} \end{cases}$
12: for $l = 1 : K$ do
13: $\forall i \in V :$ broadcast $b_i$ to neighbors $N(i)$/ collect $\{b_j\}_{j\in N(i)}$ from $N(i)$
14: $\forall i \in V :$ update $b_i = (1 - \sum_{j\in N(i)}u_{i,j})b_i + \sum_{j\in N(i)}u_{i,j}b_j$
15: end for
16: $\forall i \in V :$ update $r_i = \sqrt{N_{bi}}$
17: $\forall i \in V :$ update $\hat{b}_i = \begin{cases} (y_i - q_i)^2 & \text{for } i \in \mathcal{S} \\ 0 & \text{else} \end{cases}$
18: for $l = 1 : K$ do
19: $\forall i \in V :$ broadcast $\hat{b}_i$ to neighbors $N(i)$/collect $\{\hat{b}_j\}_{j\in N(i)}$ from $N(i)$
20: $\forall i \in V :$ update $\hat{b}_i = (1 - \sum_{j\in N(i)}u_{i,j})\hat{b}_i + \sum_{j\in N(i)}u_{i,j}\hat{b}_j$
21: end for
22: $\forall i \in V :$ update $\tilde{r}_i = \sqrt{N_{bi}}$
23: $\forall i \in V :$ update $\tilde{x}_i = \begin{cases} y_i + (\varepsilon / r)(\hat{r}_i - y_i) & \text{if } i \in \mathcal{S} \text{ and } r > \varepsilon \\ q_i & \text{otherwise} \end{cases}$
24: $\forall i \in V :$ update $z_i = \begin{cases} y_i + (\varepsilon / \tilde{r})(\tilde{r}_i - y_i) & \text{if } i \in \mathcal{S} \text{ and } \tilde{r} > \varepsilon \\ \tilde{q}_i & \text{otherwise} \end{cases}$
25: $\forall i \in V :$ update $x_i = \tau z_i + (1 - \tau)\tilde{x}_i$
26: $\forall i \in V :$ update $\tau = \left(\frac{1}{\tau} + (1/2)\right)^{-1}$
27: until stopping criterion is satisfied

Output: $\hat{x}_i$

$N = 2 \cdot 100$ nodes. The clusters are connected through few “gate” nodes. The maximum node degree of $G$ is $d_{\text{max}} = 8$. Given the empirical graph $G$, we generated a labeling $x^{(g)}$ by labeling the nodes for each cluster $C_c$ by a random number $t_c \sim \mathcal{N}(0, 1)$, i.e., $x^{(g)}_i = t_c$ for all nodes $i \in C_c$ in the cluster $C_c$. For each cluster $C_c$ we assume that we are provided initial labels $y_i = x_i$ for 100 randomly chosen nodes $i \in C_c$, giving rise to an overall sampling set $S$ with $M = 2 \cdot 100$ nodes. We run Alg. 4 with initial smoothing parameter $\mu = 1$, decreasing factor $\kappa = (2 \cdot 10^{-5})^{1/2000}$, error bound $\varepsilon := \|x^{(g)}\|_2/10^2$ and a fixed number of 2000 iterations, to obtain the learned labels $\hat{x}_i$ for every node $i \in V$. In Fig. 3 we show the learned labeling $\hat{x}_i$ output by Alg. 4. We also show the learned labeling $\hat{x}^{LP}_i$ obtained using the well-known label propagation (LP)
algorithm \[7\] Alg. 11.1] which is run for the same number of iterations. From Fig. 3 it is evident that Alg. 4 yields better learning accuracy compared to plain LP, which is also reflected in the empirical normalized MSEs \(\text{NMSE}_{\text{test}} \approx 2.1 \times 10^{-4}\) and \(\text{NMSE}_{\text{LP}} \approx 2.4 \times 10^{-3}\) obtained by averaging \(\|\hat{x} - x^{(g)}\|_2^2 / \|x^{(g)}\|_2^2\) and \(\|\hat{x}_{\text{LP}} - x^{(g)}\|_2^2 / \|x^{(g)}\|_2^2\) over 100 independent Monte Carlo runs. We have also depicted the dependence of the NMSE of Alg. 4 and LP on the iteration number \(k\) in Fig. 4, which shows that after some initial phase, which comprises \(\approx 100\) iterations, the NMSE obtained by Alg. 4 converges quickly to its stationary value.

![Empirical graph \(G\) made up of 2 clusters \(C_1\) and \(C_2\), each consisting of 100 nodes.](image)

![True labels \(x_i^{(g)}\) and labelings \(\hat{x}_i\) and \(\hat{x}_{\text{LP}}^i\), obtained by our method (Alg. 4) and from LP.](image)
Remarkably, according to Fig. 4, the simple LP method provides smaller NMSE for the first few iterations. However, the comparison of the convergence speed of Alg. 4 and LP should be interpreted carefully, since the optimization problem underlying LP is based on the smooth Laplacian quadratic form [7, Sec. 11.3.], whereas Alg. 4 amounts to solving the non-smooth problem (7).

![Graph showing log_{10} NMSE after k iterations](image)

**Fig. 4:** Overall NMSE of Alg. 4 (NMSE_{nest}) and label propagation (NMSE_{LP}) vs. iteration number $k$.

**VII. CONCLUSIONS**

The problem of semi-supervised learning from massive datasets over networks has been formulated as a nonsmooth convex optimization problem based on penalizing the total variation of the labeling. We applied the smoothing technique of Nesterov to this optimization problem for obtaining an efficient learning algorithm which can capitalize on huge amounts of unlabeled data using only few labeled datapoints. Moreover, we proposed an implementation of the learning method as message passing over the underlying data graph. This message passing algorithm can be easily implemented in a big data platform such as AKKA to allow for scalable learning algorithms. Future work includes the extension of the optimization framework to accommodate loss functions, different from the mean squared error, that better characterize the training error for discrete valued or categorical labels.

**APPENDIX A**

**PROOF OF LEMMA IV.2**

We only detail the derivation of (42), since the derivation of (45) is very similar. Our argument closely follows the derivations used in [1, Sec. 3]. Consider the constrained convex optimization problem (41), which we repeat here for convenience:

$$
\hat{x}_k = \arg \min_{x \in Q} \frac{\hat{L}}{2} \| x - x_k \|^2 + g_k^T (x - x_k)
$$

with constraint set $Q := \{ x : \operatorname{Err}[x] \leq \varepsilon \} = \{ x : (\operatorname{Err}[x])^2 \leq \varepsilon^2 \}$. The Lagrangian associated with (48) is

$$
\mathcal{L}(x, \lambda) = \left( \frac{\hat{L}}{2} \| x - x_k \|^2 + g_k^T (x - x_k) \right) + \lambda ((\operatorname{Err}[x])^2 - \varepsilon^2),
$$

where $\lambda$ is a Lagrange multiplier.

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and the corresponding KKT conditions for \( \hat{x}_k \) and \( \lambda_e \) to be primal and dual optimal read [5, Section 5.5.3]

\[
\hat{L}(\hat{x}_k - x_k) + g_k + (\lambda_e/|S|)D(S)(\hat{x}_k - y) = 0, \tag{50}
\]

\[
\lambda_e (\text{Err}[\hat{x}_k] - \varepsilon) = 0, \tag{51}
\]

\[
\text{Err}[\hat{x}_k] \leq \varepsilon, \tag{52}
\]

\[
\lambda_e \geq 0, \tag{53}
\]

with the diagonal matrix \( D(S) = \sum_{i \in S} e_i e_i^T \). From condition (50), we obtain

\[
\hat{x}_k = (I + \tilde{\lambda}_e D(S))^{-1}(x_k - (1/\hat{L})g_k + \tilde{\lambda}_e D(S)y). \tag{54}
\]

with

\[
\tilde{\lambda}_e := \frac{\lambda_e}{\hat{L}|S|} \tag{55}
\]

Using the elementary identity

\[
(I + aD(S))^{-1} = I - \frac{a}{1 + a}D(S) \tag{56}
\]

which is valid for any \( a \geq 0 \), we can develop (54) further to

\[
\hat{x}_k = \left(I - \frac{\tilde{\lambda}_e}{1 + \tilde{\lambda}_e}D(S)\right)(x_k - (1/\hat{L})g_k + \tilde{\lambda}_e D(S)y). \tag{57}
\]

Inserting (57) into (52) yields

\[
\text{Err}[\hat{x}_k] \leq \varepsilon. \tag{58}
\]

From (58), we have

\[
\tilde{\lambda}_e \geq (1/\varepsilon)\text{Err}[x_k - (1/\hat{L})g_k - y] - 1. \tag{59}
\]

Thus if \( (1/\varepsilon)\text{Err}[x_k - (1/\hat{L})g_k - y] > 1 \), then (59) implies \( \lambda_e > 0 \), which, via (51), requires the inequality (58) to become an equality, i.e.,

\[
\tilde{\lambda}_e = (1/\varepsilon)\text{Err}[x_k - (1/\hat{L})g_k - y] - 1 \tag{60}
\]

This equality holds also if \( \text{Err}[x_k - (1/\hat{L})g_k - y]/\varepsilon = 1 \). For \( \text{Err}[x_k - (1/\hat{L})g_k - y]/\varepsilon < 1 \), complementary slackness (51) requires \( \tilde{\lambda}_e = 0 \). Thus the optimal dual variable \( \lambda_e \) is fully determined by the quantity \( \text{Err}[x_k - (1/\hat{L})g_k - y] \) via

\[
\lambda_e = \max\{0, (1/\varepsilon)\text{Err}[x_k - (1/\hat{L})g_k - y] - 1\}. \tag{61}
\]
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