ABSTRACT
Predicting the occurrence of links is a fundamental problem in networks. In the link prediction problem we are given a snapshot of a network and would like to infer which interactions among existing members are likely to occur in the near future or which existing interactions are we missing. Although this problem has been extensively studied, the challenge of how to effectively combine the information from the network structure with rich node and edge attribute data remains largely open.

We develop an algorithm based on Supervised Random Walks that naturally combines the information from the network structure with node and edge level attributes. We achieve this by using these attributes to guide a random walk on the graph. We formulate a supervised learning task where the goal is to learn a function that assigns strengths to edges in the network such that a random walker is more likely to visit the nodes to which new links will be created in the future. We develop an efficient training algorithm to directly learn the edge strength estimation function.

Our experiments on the Facebook social graph and large collaboration networks show that our approach outperforms state-of-the-art unsupervised approaches as well as approaches that are based on feature extraction.

Categories and Subject Descriptors: H.2.8 [Database Management]: Database applications—Data mining

General Terms: Algorithms; Experimentation.

Keywords: Link prediction, Social networks

1. INTRODUCTION
Large real-world networks exhibit a range of interesting properties and patterns [20]. One of the recurring themes in this line of research is to design models that predict and reproduce the emergence of such network structures. Research then seeks to develop models that will accurately predict the global structure of the network [7][20][19][5].

Many types of networks and especially social networks are highly dynamic; they grow and change quickly through the additions of new edges which signify the appearance of new interactions between the nodes of the network. Thus, studying the networks at a level of individual edge creations is also interesting and in some respects more difficult than global network modeling. Identifying the mechanisms by which such social networks evolve at the level of individual edges is a fundamental question that is still not well understood, and it forms the motivation for our work here.

We consider the classical problem of link prediction [21] where we are given a snapshot of a social network at time $t$, and we seek to accurately predict the edges that will be added to the network during the interval from time $t$ to a given future time $t'$. More concretely, we are given a large network, say Facebook, at time $t$ and for each user we would like to predict what new edges (friendships) that user will create between $t$ and some future time $t'$. The problem can be also viewed as a link recommendation problem, where we aim to suggest to each user a list of people that the user is likely to create new connections to.

The processes guiding link creation are of interest from more than a purely scientific point of view. The current Facebook system for suggesting friends is responsible for a significant fraction of link creations, and adds value for Facebook users. By making better predictions, we will be able to increase the usage of this feature, and make it more useful to Facebook members.

Challenges. The link prediction and link recommendation problems are challenging from at least two points of view. First, real networks are extremely sparse, i.e., nodes have connections to only a very small fraction of all nodes in the network. For example, in the case of Facebook a typical user is connected to about 100 out of more than 500 million nodes of the network. Thus, a very good (but unfortunately useless) way to predict edges is to predict no new edges since this achieves near perfect predictive accuracy (i.e., out of 500 million possible predictions it makes only 100 mistakes).

The second challenge is more subtle; to what extent can the links of the social network be modeled using the features intrinsic to the network itself? Similarly, how do characteristics of users (e.g., age, gender, home town) interact with the creation of new edges? Consider the Facebook social network, for example. There can be many reasons exogenous to the network for two users to become connected: it could be that they met at a party, and then connected on Facebook. However, since they met at a party they are likely to be about the same age, and they also probably live in the same town. Moreover, this link might also be hinted at by the structure of the network: two people are more likely to meet at the same party if they are “close” in the network. Such a pair of people likely has friends in common, and travel in similar social circles. Thus, despite the fact that they became friends due to the exogenous event (i.e., a party) there are clues in their social networks which suggest a high probability of a future friendship.

Thus the question is how do network and node features interact
in the creation of new links. From the link creation point of view: how important is it to have common interests and characteristics? Furthermore, how important is it to be in the same social circle and be “close” in the network in order to eventually connect. From the technical point of view it is not clear how to develop a method that, in a principled way, combines the features of nodes (i.e., user profile information) and edges (i.e., interaction information) with the network structure. A common, but somewhat unsatisfactory, approach is to simply extract a set of features describing the network structure (like node degree, number of common friends, shortest path length) around the two nodes of interest and combine it with the user profile information.

Present work: Supervised Random Walks. To address these challenges we develop a method for both link prediction and link recommendation. We develop a concept of Supervised Random Walks that naturally and in a principled way combines the network structure with the characteristics (attributes, features) of nodes and edges of the network into a unified link prediction algorithm.

We develop a method based on Supervised Random Walks that in a supervised way learns how to bias a PageRank-like random walk on the network so that it visits given nodes (i.e., positive training examples) more often than the others.

We achieve this by using node and edge features to learn edge strengths (i.e., random walk transition probabilities) such that the random walk on a such weighted network is more likely to visit “positive” than “negative” nodes. In the context of link prediction, positive nodes are nodes to which new edges will be created in the future, and negative are all other nodes. We formulate a supervised learning task where we are given a source node \( s \) and training examples about which nodes \( s \) will create links to in the future. The goal is to then learn a function that assigns a strength (i.e., random walk transition probability) to each edge so that when computing the random walk scores in such a weighted network nodes to which \( s \) creates new links have higher scores to \( s \) than nodes to which \( s \) does not create links.

From a technical perspective, we show that such edge strength function can be learned directly and efficiently. This means, that we do not postulate what it means for edge to be “strong” in an ad-hoc way and then use this heuristic estimate. Rather, we show how to directly find the parameters of the edge strength function which give optimal performance. This means we are able to compute the gradient of the parameters of the edge strength function with respect to the PageRank-like random walk scores. The formulation results in an optimization problem for which we derive an efficient estimation procedure.

From the practical point of view, we experiment with large collaboration networks and data from the Facebook network, showing that our approach outperforms state-of-the-art unsupervised approaches as well as supervised approaches based on complex network feature extraction. An additional benefit of our approach is that no complex network feature extraction or domain expertise are required as our algorithm nicely combines the node attribute and network structure information.

Applications and consequences. As networks evolve and grow by addition of new edges, the link prediction problem offers insights into the factors behind creation of individual edges as well as into network formation in general.

Moreover, the link-prediction and the link-recommendation problems are relevant to a number of interesting current applications of social networks. First, for online social networking websites, like Facebook and Myspace, being able to predict future interactions has direct business consequences. More broadly, large organizations can directly benefit from the interactions within the informal social network among its members and link-prediction methods can be used to suggest possible new collaborations and interactions within the organization. Research in security has recently recognized the role of social network analysis for this domain (e.g., terrorist networks). In this context link prediction can be used to suggest the most likely links that may form in the future. Similarly, link prediction can also be used for prediction of missing or unobserved links in networks or to suggest which individuals may be working together even though their interaction has yet been directly observed. Applications go well beyond social networks, as our techniques can be used to predict unobserved links in protein-protein interaction networks in systems biology or give suggestions to bloggers about which relevant pages on the Web to link to.

Furthermore, the framework we develop is more general than link prediction, and could be used for any sort of interaction. For instance, in a collaboration network, it could easily be used not to predict who \( s \) will link to next (write a paper with a previously un-collaborated-with person) but to predict who \( s \) will coauthor a paper with next, including all those with whom \( s \) has previously coauthored.

Further related work. The link prediction problem in networks comes in many flavors and variants. For example, the network inference problem can be cast as a link prediction problem where no knowledge of the network is given. Moreover, even models of complex networks, like Preferential Attachment, have been extensively evaluated by Liben-Nowell and Kleinberg who found that the Adamic-Adar measure of node similarity performed best. More recently approaches based on network community detection have been tested on small networks. Link prediction in supervised machine learning setting was mainly studied by the relational learning community. However, the challenge with these approaches is primarily scalability.

Random walks on graphs have been considered for computing node proximities in large graphs. They have also been used for learning to rank nodes in graphs. Next we describe our algorithm for link prediction and recommendation. The general setting is that we are given a graph and a node \( s \) for which we would like to predict/recommend new links. The idea is that \( s \) has already created some links and we would like to predict which links it will create next (or will be created to it, since the direction of the links is often not clear). For simplicity the following discussion will focus on a single node \( s \) and how to predict the links it will create in the future.

Note that our setting is much more general than it appears. We require that for a node \( s \) we are given a set of “positive” and “negative” training nodes and our algorithm then learns how to distinguish them. This can be used for link prediction (positive nodes are those to which links are created in the future), link recommendation (positive nodes are those which user clicks on), link anomaly detection (positive nodes are those to which \( s \) has anomalous links) or missing link prediction (positive nodes are those to which \( s \) has missing links), to name a few. Moreover, our approach can also be generalized to a setting where prediction/recommendation is not being made for only a single node \( s \) but also for a group of nodes.

General considerations. A first general approach to link prediction would be to view it as a classification task. We take pairs
of nodes to which \( s \) has created edges as positive training examples, and all other nodes as negative training examples. We then learn a classifier that predicts where node \( s \) is going to create links. There are several problems with such an approach. The first is the class imbalance; \( s \) will create edges to a very small fraction of the total nodes in the network and learning is particularly hard in domains with high class imbalance. Second, extracting the features that the learning algorithm would use is a challenging and cumbersome task. Deciding which node features (e.g., node demographics like, age, gender, hometown) and edge features (e.g., interaction activity) to use is already hard. However, it is even less clear how to extract good features that describe the network structure and patterns of connectivity between the pair of nodes under consideration.

Even in a simple undirected graph with no node/edge attributes, there are countless ways to describe the proximity of two nodes. For example, we might start by counting the number of common neighbors between the two nodes. We might then adjust the proximity score based on the degrees of the two nodes (with the intuition being that high-degree nodes are likely to have common neighbors by mere happenstance). We might go further giving different length two paths different weights based on things like the centrality or degree of the intermediate nodes. The possibilities are endless, and extracting useful features is typically done by trial and error rather than any principled approach. The problem becomes even harder when annotations are added to edges. For instance, in many networks we know the creation times of edges, and this is likely to be useful. But how do we combine the creation times of all the edges to get a feature relevant to a pair of nodes?

A second general approach to the link prediction problem is to think about it as a task to rank the nodes of the network. The idea is to design an algorithm that will assign higher scores to nodes \( s \) did not link to. PageRank \([28]\), and variants like Personalized PageRank \([17, 53]\) and Random Walks with Restarts \([51]\) are popular methods for ranking nodes on graphs. Thus, one simple idea would be to start a random walk at node \( s \) and compute the proximity of each other node to node \( s \) \([40]\). This can be done by setting the random jump vector so that the walk only jumps back to \( s \) and thus restarts the walk. The stationary distribution of such random walk assigns each node a score (i.e., a PageRank score) which gives us a ranking of how “close” to the node \( s \) are other nodes in the network. This method takes advantage of the structure of the network but does not consider the impact of other properties, like age, gender, and creation time.

Overview of our approach. We combine the two above approaches into a single framework that will at the same time consider rich node and edge features as well as the structure of the network. As Random Walks with Restarts have proven to be a powerful tool for computing node proximities on graphs we use them as a way to consider the network structure. However, we then use the node and edge attribute data to bias the random walk so that it will more often visit nodes to which \( s \) creates edges in the future.

More precisely, we are given a source node \( s \). Then we are also given a set of destination nodes \( d_1, \ldots, d_k \in D \) to which \( s \) will create edges in the near future. Now, we aim to bias the random walk originating from \( s \) so that it will visit nodes \( d_i \) more often than other nodes in the network. One way to bias the random walk is to assign each edge a random walk transition probability (i.e., strength). Whereas the traditional PageRank assumes that transition probabilities of all edges to be the same, we learn how to assign each edge a transition probability so that the random walk is more likely to visit target nodes \( d_i \) than other nodes of the network. However, directly setting an arbitrary transition probability to each edge would make the task trivial, and would result in drastic overfitting. Thus, we aim to learn a model (a function) that will assign the transition probability for each edge \((u, v)\) based on features of nodes \( u \) and \( v \), as well as the features of the edge \((u, v)\). The question we address next is, how to directly and in a principled way estimate the parameters of such random walk biasing function?

Problem formulation. We are given a directed graph \( G(V, E) \), a node \( s \) and a set of candidates to which \( s \) could create an edge. We label nodes to which \( s \) creates edges in the future as destination nodes \( D = \{d_1, \ldots, d_k\} \), while we call other nodes to which \( s \) does not create edges no-link nodes \( L = \{l_1, \ldots, l_n\} \). We label candidate nodes with a set \( C = \{c_i\} = D \cup L \). We think of nodes in \( D \) as positive and nodes in \( L \) as negative training examples. Later we generalize to multiple instances of \( s \), \( L \) and \( D \). Each node and each edge in \( G \) is further described with a set of features. We assume that each edge \((u, v)\) has a corresponding feature vector \( \psi_{uv} \) that describes the nodes \( u \) and \( v \) (e.g., age, gender, hometown) and the interaction attributes (e.g., when the edge was created, how many messages \( u \) and \( v \) exchanged, or how many photos they appeared together in).

For edge \((u, v)\) in \( G \) we compute the strength \( a_{uv} = f_w(\psi_{uv}) \). Function \( f_w \) parameterized by \( w \) takes the edge feature vector \( \psi_{uv} \) as input and computes the corresponding edge strength \( a_{uv} \) that models the random walk transition probability. It is exactly the function \( f_w(\psi) \) that we learn in the training phase of the algorithm.

To predict new edges of node \( s \), first edge strengths of all edges are calculated using \( f_w \). Then a random walk with restarts is run from \( s \). The stationary distribution \( p \) of the random walk assigns each node \( u \) a probability \( p_u \). Nodes are ordered by \( p_u \) and top ranked nodes are then predicted as destinations of future links of \( s \).

Now our task is to learn the parameters \( w \) of function \( f_w(\psi_{uv}) \) that assigns each edge a transition probability \( a_{uv} \). One can think of the weights \( a_{uv} \) as edge strengths and the random walk is more likely to traverse edges of high strength and thus nodes connected to node \( s \) via paths of strong edges will likely be visited by the random walk and will thus rank higher.

The optimization problem. The training data contains information that source node \( s \) will create edges to nodes \( d \in D \) and not to nodes \( l \in L \). So, we aim to set the parameters \( w \) of function \( f_w(\psi_{uv}) \) so that it will assign edge weights \( a_{uv} \) in such a way that the random walk will be more likely to visit nodes in \( D \) than \( L \); i.e., \( p_l < p_d \) for each \( d \in D \) and \( l \in L \).

Thus, we define the optimization problem to find the optimal set of parameters \( w \) of edge strength function \( f_w(\psi_{uv}) \) as follows:

\[
\min_w \mathcal{F}(w) = ||w||^2 \\
\text{such that} \\
\forall d \in D, l \in L : p_l < p_d
\]

(1)

where \( p \) is the vector of PageRank scores. Note that PageRank scores \( p_l \) depend on edge strengths \( a_{uv} \) and thus actually depend on \( f_w(\psi_{uv}) \) that is parameterized by \( w \). The idea here is that we want to find the parameter vector \( w \) such that the PageRank scores of nodes in \( D \) will be greater than the scores of nodes in \( L \). We prefer the shortest \( w \) parameter vector simply for regularization.

However, Eq. [1] is a “hard” version of the optimization problem as it allows no constraints to be violated. In practice it is unlikely that a solution satisfying all the constraints exists. Thus similarly to formulations of Support Vector Machines we make the constraints “soft” by introducing a loss function \( h \) that penalizes violated con-
connection between the parameters \( p \) of the edge strength function \( f_w(\psi_{uv}) \) and the random walk scores \( p \). Then we show how to obtain the derivative of the loss function and the random walk scores \( p \) with respect to \( w \) and then perform gradient based optimization method to minimize the loss and find the optimal parameters \( p \).

Function \( f_w(\psi_{uv}) \) combines the attributes \( \psi_{uv} \) and the parameter vector \( w \) to output a non-negative weight \( a_{uv} \) for each edge. We then build the random walk stochastic transition matrix \( Q' \):

\[
Q'_{uv} = \begin{cases} 
\sum a_{uv} & \text{if } (u, v) \in E, \\
0 & \text{otherwise}.
\end{cases}
\]

To obtain the final random walk transition probability matrix \( Q \), we also incorporate the restart probability \( \alpha \), i.e., with probability \( \alpha \) the random walk jumps back to seed node \( s \) and thus “restarts”:

\[
Q_{uv} = (1 - \alpha) Q'_{uv} + \alpha \mathbf{1}(v = s).
\]

Note that each row of \( Q \) sums to 1 and thus each entry \( Q_{uv} \) defines the conditional probability that a path will traverse edge \( (u, v) \) given that it is currently at node \( u \).

The vector \( p \) is the stationary distribution of the Random walk with restarts (also known as Personalized PageRank), and is the solution to the following eigenvector equation:

\[
p^T = p^T Q
\]

Equation 4 establishes the connection between the node PageRank scores \( p_s \in p \), and parameters \( w \) of function \( f_w(\psi_{uv}) \) via the random walk transition matrix \( Q \). Our goal now is to minimize Eq. 2 with respect to the parameter vector \( w \). We approach this by first deriving the gradient of \( F(w) \) with respect to \( w \), and then use a gradient based optimization method to find \( w \) that minimize \( F(w) \).

Note that non-trivial due to the recursive relation in Eq. 4.

First, we introduce a new variable \( \delta_d = p_l - p_d \) and then we can write the derivative:

\[
\frac{\partial F(w)}{\partial w} = 2w + \sum_{l,d} \frac{\partial h(p_l - p_d)}{\delta_d} \frac{\partial h}{\partial h(p_l - p_d)}
\]

For commonly used loss functions \( h(\cdot) \) (like, hinge-loss or squared loss), it is simple to compute the derivative \( \frac{\partial h(\cdot)}{\partial h(\cdot)} \). However, it is not clear how to compute \( \frac{\partial h}{\partial h(p_l - p_d)} \), the derivative of the score \( p_w \) with respect to the vector \( w \). Next we show how to do this.

Note that \( p \) is the principal eigenvector of matrix \( Q \). Eq. 2 can be rewritten as \( p_s = \sum_j p_j Q_{ju} \) and taking the derivative now gives:

\[
\frac{\partial p_s}{\partial w} = \sum_j Q_{ju} \frac{\partial p_j}{\partial w} + p_j \frac{\partial Q_{ju}}{\partial w}
\]

Notice that \( p_s \) and \( \frac{\partial p_s}{\partial w} \) are recursively entangled in the equation. However, we can still compute the gradient iteratively. By recursively applying the chain rule to Eq. 2 we can use a power-method like algorithm to compute the derivative. We repeatedly compute the derivative \( \frac{\partial h}{\partial h(p_l - p_d)} \) based on the estimate obtained in the previous iteration. Thus, we first compute \( p \) and then update the estimate of the gradient \( \frac{\partial h}{\partial h(p_l - p_d)} \). We stop the algorithm when both \( p \) and \( \frac{\partial h}{\partial h(p_l - p_d)} \) do not change (i.e., \( \epsilon = 10^{-12} \) in our experiments) between iterations. We arrive at Algorithm 1 that iteratively computes the eigenvector \( p \) as well as the partial derivatives of \( p \). Convergence of Algorithm 1 is similar to those of power-iteration.

To solve Eq. 4 we further need to compute \( \frac{\partial \psi_{uv}}{\partial w} \) which is the partial derivative of entry \( Q_{ju} \) (Eq. 2). This calculation is straightforward. When \( j, u \) in \( E \) we find \( \frac{\partial \psi_{uv}}{\partial w} = (1 - \alpha) \frac{\partial f_w(\psi_{uv})}{\partial w} (\sum_k f_w(\psi_{vk}) - f_w(\psi_{ju})) (\sum_k \frac{\partial f_w(\psi_{vk})}{\partial w}) - \frac{\partial f_w(\psi_{ju})}{\partial w} \frac{\partial f_w(\psi_{ju})}{\partial w} \)

and otherwise \( \frac{\partial \psi_{uv}}{\partial w} = 0 \). The edge strength function \( f_w(\psi_{uv}) \) must be differentiable and so \( \frac{\partial \psi_{uv}}{\partial w} \) can be easily computed.

This completes the derivation and shows how to evaluate the derivative of \( F(w) \) (Eq. 2). Now we apply a gradient descent based method, like a quasi-Newton method, and directly minimize \( F(w) \).

Final remarks. First we note that our problem is not convex in general, and thus gradient descent methods will not necessarily find the global minimum. In practice we resolve this by using several different starting points to find a good solution.

Second, since we are only interested in the values of \( p \) for nodes in \( C \), it makes sense to evaluate the loss function at a slightly different point: \( h(p_l^* - p_d^*) \) where \( p_l^* \) is a normalized version of \( p \) such that \( p_d^* = \frac{p_d}{\sum_{v \in V} p_v} \). This adds one more chain rule application to the derivative calculation, but does not change the algorithm. The effect of this is mostly to allow larger values of \( \alpha \) to be used without having to change \( h(\cdot) \) (We omit the tick marks in our notation for the rest of this paper, using \( p \) to refer to the normalized score).

So far we only considered training and estimating the parameter vector \( w \) for predicting the edges of a particular node \( s \). However, our aim to estimate \( w \) that make good predictions across many different nodes \( s \) in \( S \). We easily extend the algorithm to multiple source nodes \( s \) in \( S \), that may even reside in different graphs. We do this by taking the sum of losses over all source nodes \( s \) and the Initialization: PageRank scores \( p \) and partial derivatives \( \frac{\partial p_s}{\partial w_k} \):

\[
\text{foreach } u \in V \text{ do } \frac{\partial p_s}{\partial w_k}(0) = \frac{1}{w}
\]

\[
\text{foreach } u \in V, k = 1, \ldots, |w| \text{ do } \frac{\partial p_s}{\partial w_k}(t) = 0
\]

\[
\text{while not converged do}
\]

\[
\text{foreach } u \in V \text{ do }
\]

\[
\left\lfloor \frac{\partial p_s}{\partial w_k}(t) = \sum_j Q_{ju} \frac{\partial p_s}{\partial w_k}(t-1) + p_j \frac{\partial Q_{ju}}{\partial w}
\right\rfloor
\]

\[
t = t + 1
\]

\[
\text{foreach } k = 1, \ldots, |w| \text{ do }
\]

\[
\left\lfloor \frac{\partial p_s}{\partial w_k}(t) = \sum_j Q_{ju} \frac{\partial p_s}{\partial w_k}(t-1) + p_j \frac{\partial Q_{ju}}{\partial w}
\right\rfloor
\]

\[
t = t + 1
\]

\[
\text{return } \frac{\partial p_s}{\partial w_k}(t)
\]

Algorithm 1: Iterative power-method like computation of PageRank vector \( p \) and its derivative \( \frac{\partial p_s}{\partial w} \).
corresponding pairs of positive $D_s$ and negative $L_s$ training examples. We slightly modify the Eq. [2] to obtain:

$$\min_w F(w) = ||w||^2 + \lambda \sum_{s \in S} \sum_{d \in D_s} h(p_l - p_d)$$

The gradients of each instance $s \in S$ remain independent, and can thus be computed independently for all instances of $s$ (Alg. 1). By optimizing parameters $w$ over many individuals $s$, the algorithm is less likely to overfit, which improves the generalization.

As a final implementation note, we point out that gradient descent often makes many small steps which have small impact on the eigenvector and its derivative. A 20% speedup can be achieved by using the solutions from the previous position (in the gradient descent) as initialization for the eigenvector and derivative calculations in Alg. 1. Our implementation of Supervised Random Walks uses the L-BFGS algorithm [22]. Given a function and its partial derivatives, the solver iteratively improves the estimate of $w$, converging to a local optima. The exact runtime of the method depends on how many iterations are required for convergence of both the PageRank and derivative computations, as well as of the overall process (quasi-Newton iterations).

3. EXPERIMENTS ON SYNTHETIC DATA

Before experimenting with real data, we examine the soundness and robustness of the proposed algorithm using synthetic data. Our goal here is to generate synthetic graphs, edge features and training data (triples $(s, D, L)$) and then try to recover the original model.

Synthetic data. We generate scale-free graphs $G$ on 10,000 nodes by using the Copying model [18]: Graph starts with three nodes connected in a triad. Remaining nodes arrive one by one, each creating exactly three edges. When a node $u$ arrives, it adds three edges $(u, v_i)$. Existing node $v_i$ is selected uniformly at random with probability 0.8, and otherwise $v_i$ is selected with probability proportional to its current degree. For each edge $(u, v)$ we create two independent Gaussian features with mean 0 and variance 1. We set the edge strength $\theta_{uv} = \exp(\psi_{uv1} - \psi_{uv2})$, i.e., $w^* = [1, -1]$.

For each $G$, we randomly select one of the oldest 3 nodes of $G$ as the start node, $s$. To generate a set of destination $D$ and no-link nodes $L$ for a given $s$ we use the following approach.

On the graph with edge strengths $\theta_{uv}$ we run the random walk ($\alpha = 0.2$) starting from $s$ and obtain node PageRank scores $p^*$. We use these scores to generate the destinations $D$ in one of two ways. First is deterministic and selects the top $K$ nodes according to $p^*$ to which $s$ is not already connected. Second is probabilistic and selects $K$ nodes, selecting each node $u$ with probability $p_u^*$. Now given the graph $G$, attributes $\psi_{uv}$ and targets $D$ our goal is to recover the true edge strength parameter vector $w^* = [1, -1]$. To make the task more interesting we also add random noise to all of the attributes, so that $\psi'_{uv} = \psi_{uv} + N(0, \sigma^2)$, where $N(0, \sigma^2)$ is a Gaussian random variable with mean 0 and variance $\sigma^2$.

Results. After applying our algorithm, we are interested in two things. First, how well does the model perform in terms of the classification accuracy and second, whether it recovers the edge strength function parameters $w^* = [1, -1]$. In the deterministic case of creating $D$ and with 0 noise added, we hope that the algorithm is able achieve near perfect classification. As the noise increases, we expect the performance to drop, but even then, we hope that the recovered values of $\hat{w}$ will be close to true $w^*$.

In running the experiment we generated 100 synthetic graphs. We used 50 of them for training the weights $w$, and report results on the other 50. We compute Area under the ROC curve (AUC) of each of 50 test graphs, and report the mean (AUC of 1.0 means perfect classification, while random guessing scores 0.5).

Figures 1 and 2 show the results. We plot the performance of the model that ignores edge weights (red), the model with true weights $w^*$ (green) and a model with learned weights $\hat{w}$ (blue).

For the deterministically generated $D$ (Fig. 1), the performance is perfect in the absence of any noise. This is good news as it demonstrates that our training procedure is able to recover the correct parameters. As the noise increases, the performance slowly drops. When the noise reaches $\sigma^2 \approx 1.5$, using the true parameters $w^*$ (green) actually becomes worse than simply ignoring them (red). Moreover, our algorithm learns the true parameters $[+1, -1]$ almost perfectly in the noise-free case, and decreases their magnitude as the noise level increases. This matches the intuition that, as more and more noise is added, the signal in the edge attributes becomes weaker and weaker relatively to the signal in the graph structure. Thus, with more noise, the parameter values $w$ decrease as they are given less and less credence.

In the probabilistic case (Fig. 2), we see that our algorithm does better (statistically significant at $p = 0.01$) than the model with true parameters $w^*$, regardless of the presence or absence of noise. Even though the data was generated using parameters $w^* = [+1, -1]$, these values are not optimal and our model gets better AUC by finding different (smaller) values. Again, as we add noise, the overall performance slowly drops, but still does much better than the baseline method of ignoring edge strengths (red), and continues to do better than the model that uses true parameter values $w^*$ (green).

We also note that regardless of where we initialize the parameter
work degree) $k_u$ and let $t_0$ be the time when $u$ created it’s $k_u/2$-th edge. Then we define $m_u$ to be the number of co-authorship links that $u$ created after time $t_0$ and that at the time of creation spanned 2-hops (i.e., closed a triangle). We attempt to make predictions only for “active” authors, where we define a node $u$ to be active if $k_u \geq K$ and $m_u \geq \Delta$. In this work, we set $K = 10$ and $\Delta = 5$. For every source node $s$ that is above this threshold, we extract the network at time $t_s$ and try to predict the $d_s$ new edges that $s$ creates in the time after $t_s$. Table 1 gives dataset statistics.

For every edge $(i, j)$ of the network around the source node $u$ at time $t_u$ we generate the following six features:

- Number of papers $i$ written before $t_u$
- Number of papers $j$ written before $t_u$
- Number of papers $i$ and $j$ co-authored
- Cosine similarity between the titles of papers written by $i$ and titles of $j$’s papers
- Time since $i$ and $j$ last co-authored a paper
- The number of common friends between $j$ and $s$

The Facebook network. Our second set of data comes from the Facebook online social network. We first selected Iceland since it has high Facebook penetration, but relatively few edges pointing to users in other countries. We generated our data based on the state of the Facebook graph on November 1, 2009. The destination nodes $D$ from a node $s$ are those that $s$ became friends with between November 1 2009 and January 13 2010. The Iceland graph contains more than 174 thousand people, or 55% of the country’s population. The average user had 168 friends, and during the period Nov 1 – Jan 23, an average person added 26 new friends.

From these users, we randomly selected 200 as the nodes $s$. Again, we only selected “active” nodes, this time with the criteria $|D| > 20$. As Figure 5 shows, individuals without many mutual friends are exceedingly unlikely to become friends. As the Facebook graph contains users whose 2-hop neighborhood has several million nodes we can prune such graphs and speed-up the computations without losing much on prediction performance. Since we know that individuals with only a few mutual friends are unlikely to form friendships, and our goal is to predict the most likely friendships, we remove all individuals with less than 4 mutual friends with practically no loss in performance. As demonstrated in Figure 5 if a user creates an edge, then the probability that she links to a node with whom she has less than 4 friends is about $0.1\%$.

We annotated each edge of the Facebook network with seven features. For each edge $(i, j)$, we created:

- Edge age: $(T - t)^{-\beta}$, where $T$ is the time cutoff Nov. 1, and $t$ is the edge creation time. We create three features like this with $\beta = \{0.1, 0.3, 0.5\}$.
- Edge initiator: Individual making the friend request is encoded as $+1$ or $-1$.
- Communication and observation features. They represent the probability of communication and profile observation in a one week period.

| Network  | $N$ | $E$ | $S$ | $\bar{D}$ | $C$ | $\bar{D}/C$ |
|----------|----|----|----|--------|----|-----------|
| Astro-Ph | 19,144 | 197,110 | 1,123 | 18.0 | 775.6 | 0.023 |
| Cond-Mat | 23,608 | 94,492 | 140 | 9.1 | 335.3 | 0.027 |
| Hep-Ph   | 12,527 | 118,515 | 340 | 29.2 | 345.3 | 0.084 |
| Hep-Th   | 10,700 | 25,997 | 55 | 6.3 | 110.5 | 0.057 |
| Facebook | 174,000 | 29M | 200 | 43.6 | 1987 | 0.022 |

Table 1: Dataset statistics. $N, E$: number of nodes and edges in the full network, $S$: number of sources, $C$: avg. number of candidates per source, $\bar{D}$: avg. number of destination nodes.
The number of common friends between $j$ and $s$.

All features in all datasets are re-scaled to have mean 0 and standard deviation 1. We also add a constant feature with value 1.

**Evaluation methodology.** For each dataset, we assign half of the nodes $s$ into training and half into test set. We use the training set to train the algorithm (i.e., estimate $w$). We evaluate the method on the test set, considering two performance metrics: the Area under the ROC curve (AUC) and the Precision at Top 20 (Prec@20), i.e., how many of top 20 nodes suggested by our algorithm actually receive links from $s$. This measure is particularly appropriate in the context of link-recommendation where we present a user with a set of friendship suggestions and aim that most of them are correct.

## 5. EXPERIMENTS ON REAL DATA

Next we describe the results of on five real datasets: four co-authorship networks and the Facebook network of Iceland.

### 5.1 General considerations

First we evaluate several aspects of our algorithm: (A) the choice of the loss function, (B) the choice of the edge strength function $f_w(*)$, (C) the choice of random walk restart (jump) parameter $\alpha$, and (D) choice of regularization parameter $\lambda$. We also consider the extension where we learn a separate edge weight vector depending on the type of the edge, i.e., whether an edge touches $s$ or any of the candidate nodes $c \in C$.

(A) **Choice of the loss function.** As is the case with most machine learning algorithms, the choice of loss function plays an important role. Ideally we would like to optimize the loss function $h(*)$ which directly corresponds to our evaluation metric (i.e., AUC or Precision at top $k$). However, as such loss functions are not continuous and not differentiable and so it is not clear how to optimize over them. Instead, we experiment with three common loss functions:

- **Squared loss with margin $b$:**
  
  $$h(x) = \max(x + b, 0)^2$$

- **Huber loss with margin $b$ and window $z > b$:**
  
  $$h(x) = \begin{cases} 0 & \text{if } x \leq -b, \\ (x + b)^2/(2z)^2 & \text{if } -b < x \leq -z + b, \\ (x + b) - z/2 & \text{if } x > z - b \end{cases}$$

- **Wilcoxon-Mann-Whitney (WMW) loss with width $b$ (Proposed to be used when one aims to maximize AUC):**
  
  $$h(x) = \frac{1}{1 + \exp(-x/b)}$$

Each of these loss functions is differentiable and needs to be evaluated for all pairs of nodes $d \in D$ and $l \in L$ (see Eq. 1). Performing this naively takes approximately $O(c^2)$ where $c = |D \cup L|$. However, we next show that the first two loss functions have the advantage that they can be computed in $O(c \log c)$. For example, we rewrite the squared loss as:

$$\sum_{d,l} h(p_l - p_d) = \sum_{d,l,p_l > p_d} (p_l - p_d + b)^2$$

$$= \sum_l \sum_{d:p_l + b > p_d} (p_l + b)^2 - 2(p_l + b)p_d + p_d^2$$

$$= \sum_l |\{d : p_l + b > p_d\}|(p_l + b)^2 - 2(p_l + b) \sum_{d:p_l + b > p_d} p_d + \sum_{d:p_l + b > p_d} p_d^2$$

Once we have the lists $\{p_l\}$ and $\{p_d\}$ sorted, we can iterate over the list $\{p_l\}$ in reverse order. As we do this, we can incrementally update the two terms which sum over $d$ above. The Huber loss can as well be quickly evaluated using a similar calculation.

Computation of the WMW loss is more expensive, as there is no way to go around the summation over all pairs. Evaluating WMW loss thus takes time $O(|D| \cdot |L|)$. In our case, $|D|$ is typically relatively small, and so the computation is not a significant part of total runtime. However, the primary advantage of it is that it performs slightly better. Indeed, in the limit as $b$ goes to 0, it reflects AUC, as it measures the number of inversions in the ordering.

In our experiments we notice that while the gradient descent achieves significant reduction in the value of the loss for all three loss functions, this only translates to improved AUC and Prec@20 for the WMW loss. In fact, the model trained with the squared or the Huber loss does not perform much better than the baseline we obtain through unweighted PageRank. Consequently, we use the WMW loss function for the remainder of this work.

(B) **Choice of edge strength function $f_w(*)$.** The edge strength function $f_w(*)$ must be non-negative and differentiable. While more complex functions are certainly possible, we experiment with two functions. In both cases, we start by taking the inner product of the weight vector $w$ and the feature vector $\psi_{uv}$ of an edge $(u, v)$. This yields a single scalar value, which may be negative. To transform this into the desired domain, we apply either an exponential or logistic function:

- **Exponential edge strength:** $a_{uv} = \exp(\psi_{uv} \cdot w)$
- **Logistic edge strength:** $a_{uv} = \left(1 + \exp(-\psi_{uv} \cdot w)\right)^{-1}$

Our experiments show that the choice of the edge strength function does not seem to make a significant impact on performance. There is slight evidence from our experiments that the logistic function performs better. One problem that can occur with the exponential version is underflow and overflow of double precision floating point numbers. As the performance seems quite comparable, we recommend the use of the logistic to avoid this potential pitfall.

(C) **Choice of $\alpha$.** To get a handle on the impact of random walk restart parameter $\alpha$, it is useful to think of the extreme cases, for unweighted graphs. When $\alpha = 0$, the PageRank of a node in an undirected graph is simply its degree. On the other hand, when $\alpha$ approaches 1, the score will be exactly proportional to the “Random-Random” model which simply makes two random hops from $s$, as random walks of length greater than 2 become increasingly unlikely, and hence the normalized eigenvector scores become the same as the Random-Random scores. When we add the notion of edge strengths, these properties remain. Intuitively, $\alpha$ controls...
for how “far” the walk wanders from seed node $s$ before it restarts and jumps back to $s$. High values of $\alpha$ give very short and local random walks, while low values allow the walk to go farther away.

When evaluating on real data we observe that $\alpha$ plays an important role in the simple unweighted case when we ignore the edge strengths, but as we give the algorithm more power to assign different strengths to edges, the role of $\alpha$ diminishes, and we see no significant difference in performance for a broad range of choices $\alpha$. Figure 5 illustrates this; in the unweighted case (i.e., ignoring edge strengths) $\alpha = 0.3$ performs best, while in the weighted case a broad range from 0.3 to 0.7 seem to do about equally well.

(D) Regularization parameter $\lambda$. Empirically we find that overfitting is not an issue in our model as the number of parameters $w$ is relatively small. Setting $\lambda = 1$ gives best performance.

Extension: Edge types. The Supervised Random Walks framework we have presented so far captures the idea that some edges are stronger than others. However, it doesn’t allow for different types of edges. For instance, it might be that an edge $(u, v)$ between $s$’s friends $u$ and $v$ should be treated differently than the edge $(s, u)$ between $s$ and $u$. Our model can easily capture this idea by declaring different edges to be of different types, and learning a different set of feature weights $w$ for each edge type. We can take the same approach to learning each of these weights, computing partial derivatives with respect to each one weight. The price for this is potential overfitting and slower runtime.

In our experiments, we find that dividing the edges up into multiple types provides significant benefit. Given a seed node $s$ we label the edges according to the hop-distance from $s$ of their endpoints, e.g., edges $(s, u)$ are of type (0,1), edges $(u, v)$ are either of type (1,1) (if both $u$ and $v$ link to $s$) or (1,2) (if $v$ does not link to $s$). Since the nodes are at distance 0, 1, or 2 from $s$, there are 6 possible edge types: (0,1), (1,0), (1,1), (1,2), (2,1) and (2,2). While learning six sets of more parameters $w$ increases the runtime, using multiple edge types gives a significant increase in performance.

Extension: Social capital. Before moving on to the experimental results, we also briefly examine somewhat counterintuitive behavior of the Random Walk with Restarts. Consider a graph in Figure 6 with the seed node $s$. There are two nodes which $s$ could form a new connection to $v_1$ and $v_2$. These two are symmetric except for the fact that the two paths connecting $s$ to $v_1$ are connected themselves. Now we ask, is $s$ more likely to link to $v_1$ or to $v_2$?

Building on the theory of embeddedness and social capital [10] one would postulate that $s$ is more likely to link to $v_1$ than to $v_2$. However, the result of an edge $(u_1, u_2)$ is that when $\alpha > 0$, $v_2$ ends up with a higher PageRank score than $v_1$. This is somewhat counterintuitive, as $s$ somehow seems “more connected” to $s$ than to $v_2$. Can we remedy this in a natural way?

One solution could be that carefully setting $\alpha$ resolves the issue. However, there is no value of $\alpha > 0$ which will make the score of $v_1$ higher than $v_2$ and changing to other simple teleporting schemes (such as a random jump to a random node) does not help either. However, a simple correction that works is to add the number of friends a node $w$ has in common with $s$, and use this as an additional feature $\gamma$ on each edge $(u, w)$. If we apply this to the graph shown in Figure 6 and set the weight along each edge to $1 + \gamma$, then the PageRank score $p_{v_1}$ of node $v_1$ is 1.9 greater than of $v_2$ (as opposed to 0.1 smaller as in Fig 6). In practice, we find that introducing this additional feature $\gamma$ helps on the Facebook graph. In Facebook, connection $(u_1, u_2)$ increases the probability of a link forming to $v_1$ by about 50%. In the co-authorship networks, the presence of $(u_1, u_2)$ actually decreases the link formation probability by 37%. Such behavior of co-authorship networks can be explained by the argument that long range weak ties help in access to new information [14] (i.e., $s$ is more likely to link to $v_2$ than $v_1$ of Fig 6). Having two independent paths is a stronger connection in the co-authorship graph, as this indicates that $s$ has written papers with two people, on two different occasions, and both of these people have written with the target $v$, also on two different occasions. Thus, there must be at least four papers between these four people when the edge $(u_1, u_2)$ is absent, and there may be as few as two when it is present. Note this is exactly the opposite to the social capital argument [10]. Which postulates that individuals who are well embedded in a network or a community have higher trust and get more support and information. This is interesting as it shows that Facebook is about social contacts, norms, trying to fit in and be well embedded in a circle of friends, while co-authorship networks are about access to information and establishing long-range weak ties.

5.2 Experiments on real data

Next we evaluate the predictive performance of Supervised Random Walks (SRW) on real datasets. We examine the performance of the parameter estimation and then compare Supervised Random Walks to other link-prediction methods.

Parameter estimation. Figure 7 shows the results of gradient descent on the Facebook dataset. At iteration 0, we start with unweighted random walks, by setting $w = 0$. Using L-BFGS we perform gradient descent on the WMW loss. Notice the strong correlation between AUC and WMW loss, i.e., as the value of the loss decreases, AUC increases. We also note that the method basically converges in only about 25 iterations.

Comparison to other methods. Next we compare the predictive performance of Supervised Random Walks (SRW) to a number of simple unsupervised baselines, along with two supervised machine learning methods. All results are evaluated by creating two inde-
Table 2: Hep-Ph co-authorship network. DT: decision tree, LR: logistic regression, and SRW: Supervised Random Walks.

| Learning Method       | AUC  | Prec@20 |
|-----------------------|------|---------|
| Random Walk with Restart | 0.81725 | 6.80    |
| Adamic-Adar           | 0.81856 | 7.35    |
| Common Friends        | 0.80054 | 7.35    |
| Degree                | 0.58535 | 3.25    |
| DT: Node features     | 0.59248 | 2.38    |
| DT: Network features  | 0.76979 | 5.38    |
| DT: Node+Network      | 0.76217 | 5.86    |
| DT: Path features     | 0.62836 | 2.46    |
| DT: All features      | 0.72986 | 5.34    |
| LR: Node features     | 0.54134 | 1.38    |
| LR: Network features  | 0.80560 | 7.56    |
| LR: Node+Network      | 0.80280 | 7.56    |
| LR: Path features     | 0.51418 | 0.74    |
| LR: All features      | 0.81681 | 7.52    |
| SRW: one edge type    | 0.82502 | 6.87    |
| SRW: multiple edge types | 0.82799 | 7.57    |

Table 3: Results for the Facebook dataset.

| Learning Method       | AUC  | Prec@20 |
|-----------------------|------|---------|
| Random Walk with Restart | 0.63831 | 3.41    |
| Adamic-Adar           | 0.60570 | 3.13    |
| Common Friends        | 0.59370 | 3.11    |
| Degree                | 0.56522 | 3.05    |
| DT: Node features     | 0.60961 | 3.54    |
| DT: Network features  | 0.59302 | 3.69    |
| DT: Node+Network      | 0.63711 | 3.95    |
| DT: Path features     | 0.56213 | 1.72    |
| DT: All features      | 0.61820 | 3.77    |
| LR: Node features     | 0.64754 | 3.19    |
| LR: Network features  | 0.58732 | 3.27    |
| LR: Node+Network      | 0.64644 | 3.81    |
| LR: Path features     | 0.67237 | 2.78    |
| LR: All features      | 0.67426 | 3.82    |
| SRW: one edge type    | 0.69996 | 4.24    |
| SRW: multiple edge types | 0.71238 | 4.25    |

Table 4: Results for all datasets. We compare favorably to logistic features as run on all features. Our Supervised Random Walks (SRW) perform significantly better than the baseline in all cases on ROC area. The variance is too high on the Top20 metric, and the two methods are statistically tied on this metric.

| Dataset                  | AUC   | Prec@20 |
|--------------------------|-------|---------|
| Co-authorship Astro-Ph   | 0.70548 | 2.55  |
| Co-authorship Cond-Mat   | 0.74173 | 2.54  |
| Co-authorship Hep-Ph     | 0.71238 | 4.18  |
| Co-authorship Hep-Th     | 0.72505 | 2.59  |
| Facebook (Iceland)       | 0.82799 | 7.57  |

Figure 8: ROC curve of Astro-Ph test data.
makes sense as if a user has just made a new friend u, she is likely to have also recently met some of u’s friends. In the co-authorship networks, we find that the number of co-authored papers and the cosine similarity amongst titles were the features with highest weights.

Runtime. While the exact runtime of Supervised Random Walks is highly dependent on the graph structure and features used, we give some rough guidelines. The results here are for single runs on a single 2.3Ghz processor on the Facebook dataset.

When putting all edges in the same category, we have 8 weights to learn. It took 98 iterations of the quasi-Newton method to converge and minimize the loss. This required computing the PageRanks of all the nodes in all the graphs (100 of them) 123 times, along with the partial derivatives of each of the 8 parameters 123 times. On average, each PageRank computation took 13.2 steps of power-iteration before convergence, while each partial derivative computation took 6.3 iterations. Each iteration for PageRank or its derivative takes $O(|E|)$. Overall, the parameter estimation on Facebook network took 96 minutes. By contrast, increasing the number of edge types to 6 (which gives best performance) required learning 48 weights, and increased the training time to 13 hours on the Facebook dataset.

6. CONCLUSION

We have proposed Supervised Random Walks, a new learning algorithm for link prediction and link recommendation. By utilizing node and edge attribute data our method guides the random walks towards the desired target nodes. Experiments on Facebook and co-authorship networks demonstrate good generalization and overall performance of Supervised Random Walks. The resulting predictions show large improvements over Random Walks with Restarts and compare favorably to supervised machine learning techniques that require tedious feature extraction and generation. In contrast, our approach requires no network feature generation and in a principled way combines rich node and edge features with the structure of the network to make reliable predictions.

Supervised Random Walks are not limited to link prediction, and can be applied to many other problems that require learning to rank nodes in a graph, like recommendations, anomaly detection, missing link, and expertise search and ranking.

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