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Classification in Networked Data: A Toolkit and a Univariate Case Study

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Abstract

This paper[1] is about classifying entities that are interlinked with entities for which the class is known. After surveying prior work, we present NetKit, a modular toolkit for classification in networked data, and a case-study of its application to networked data used in prior machine learning research. NetKit is based on a node-centric framework in which classifiers comprise a local classifier, a relational classifier, and a collective inference procedure. Various existing node-centric relational learning algorithms can be instantiated with appropriate choices for these components, and new combinations of components realize new algorithms. The case study focuses on univariate network classification, for which the only information used is the structure of class linkage in the network (i.e., only links and some class labels). To our knowledge, no work previously has evaluated systematically the power of class-linkage alone for classification in machine learning benchmark data sets. The results demonstrate that very simple network-classification models perform quite well—well enough that they should be used regularly as baseline classifiers for studies of learning with networked data. The simplest method (which performs remarkably well) highlights the close correspondence between several existing methods introduced for different purposes—that is, Gaussian-field classifiers, Hopfield networks, and relational-neighbor classifiers. The case study also shows that there are two sets of techniques that are preferable in different situations, namely when few versus many labels are known initially. We also demonstrate that link selection plays an important role similar to traditional feature selection.

Keywords: relational learning, network learning, collective inference, collective classification, networked data, probabilistic relational models, network analysis, network data

1. Introduction

Networked data contain interconnected entities for which inferences are to be made. For example, web pages are interconnected by hyperlinks, research papers are connected by citations, telephone accounts are linked by calls, possible terrorists are linked by communications. This paper is about

1. Versions of this paper have been available as S.A. Macskassy and Provost, F.J., “Classification in Networked Data: A toolkit and a univariate case study” CeDER Working Paper CeDER-04-08, Stern School of Business, New York University, NY, NY 10012. December 2004. Updated December 2006.

within-network classification: entities for which the class is known are linked to entities for which the class must be estimated. For example, telephone accounts previously determined to be fraudulent may be linked, perhaps indirectly, to those for which no assessment yet has been made.

Such networked data present both complications and opportunities for classification and machine learning. The data are patently not independent and identically distributed, which introduces bias to learning and inference procedures (Jensen and Neville, 2002b). The usual careful separation of data into training and test sets is difficult, and more importantly, thinking in terms of separating training and test sets obscures an important facet of the data: entities with known classifications can serve two roles. They act first as training data and subsequently as background knowledge during inference. Relatedly, within-network inference allows models to use specific node identifiers to aid inference (see Section 3.5.3).

Networked data allow *collective inference*, meaning that various interrelated values can be inferred simultaneously. For example, inference in Markov random fields (MRFs, Dobrushin, 1968; Besag, 1974; Geman and Geman, 1984) uses estimates of a node's neighbors' labels to influence the estimation of the node's label—and vice versa. Within-network inference complicates such procedures by pinning certain values, but also offers opportunities such as the application of network-flow algorithms to inference (see Section 3.5.1). More generally, networked data allow the use of the features of a node's neighbors, although that must be done with care to avoid greatly increasing estimation variance and thereby error (Jensen et al., 2004).

To our knowledge there previously has been no large-scale, systematic experimental study of machine learning methods for within-network classification. A serious obstacle to undertaking such a study is the scarcity of available tools and source code, making it hard to compare various methodologies and algorithms. A systematic study is further hindered by the fact that many relational learning algorithms can be separated into various sub-components; ideally the relative contributions of the sub-components and alternatives should be assessed.

As a main contribution of this paper, we introduce a network learning toolkit (NetKit-SRL) that enables in-depth, component-wise studies of techniques for statistical relational learning and classification with networked data. We abstract prior, published methods into a modular framework on which the toolkit is based.[2]

NetKit is interesting for several reasons. First, various systems from prior work can be realized by choosing particular instantiations for the different components. A common platform allows one to compare and contrast the different systems on equal footing. Perhaps more importantly, the modularity of the toolkit broadens the design space of possible systems beyond those that have appeared in prior work, either by mixing and matching the components of the prior systems, or by introducing new alternatives for components.

In the second half of the paper, we use NetKit to conduct a case study of within-network classification in homogeneous, univariate networks, which are important both practically and scientifically (as we discuss in Section 5). We compare various learning and inference techniques on twelve benchmark data sets from four domains used in prior machine learning research. Beyond illustrating the value of the toolkit, the case study provides systematic evidence that with networked data even univariate classification can be remarkably effective. One implication is that such methods should be used as baselines against which to compare more sophisticated relational learning algorithms (Macskassy and Provost, 2003). One particular very simple and very effective technique

2. NetKit-SRL, or NetKit for short, is written in Java 1.5 and is available as open source from `http://www.research.rutgers.edu/~sofmac/NetKit.html`.

highlights the close correspondence between several types of methods introduced for different purposes: "node-centric" methods, which focus on each node individually; random-field methods; and classic connectionist methods. The case study also illustrates a bias/variance trade-off in networked classification, based on the principle of homophily (the principle that a contact between similar people occurs at a higher rate than among dissimilar people, Blau, 1977; McPherson et al., 2001, page 416; cf., assortativity, Newman, 2003, and relational autocorrelation, Jensen and Neville, 2002b) and suggests network-classification analogues to feature selection and active learning.

To further motivate and to put the rest of the paper into context, we start by reviewing some (published) applications of classification in networked data. Section 3 describes the problem of network learning and classification more formally, introduces the modular framework, and surveys existing work on network classification. Section 4 describes NetKit. Then Section 5 covers the case study, including motivation for studying univariate network inference, the experimental methodology, data used, toolkit components used, and the results and analysis.

2. Applications

The earliest work on classification in networked data arose in scientific applications, with the networks based on regular grids of physical locations. Statistical physics introduced, for example, the Ising model (Ising, 1925) and the Potts model (Potts, 1952), which were used to find minimum energy configurations in physical systems with components exhibiting discrete states, such as magnetic moments in ferromagnetic materials. Network-based techniques then saw application in spatial statistics (Besag, 1974) and in image processing (e.g., Geman and Geman, 1984; Besag, 1986), where the networks were based on grids of pixels.

More recent work has concentrated on networks of arbitrary topology, for example, for the classification of linked documents such as patents (Chakrabarti et al., 1998), scientific research papers (e.g., Taskar et al., 2001; Lu and Getoor, 2003), and web pages (e.g., Neville et al., 2003; Lu and Getoor, 2003). Segal et al. (2003a,b) apply network classification (specifically, relational Markov networks, Taskar et al., 2002) to protein interaction and gene expression data, where protein interactions form a network over which inferences are drawn about pathways, that is, sets of genes that coordinate to achieve a particular task. In computational linguistics network classification is applied to tasks such as the segmentation and labeling of text (e.g., part-of-speech tagging, Lafferty et al., 2001).

Explicit social-network data play an important role in counterterrorism, law enforcement, and fraud detection, because suspicious people may interact with known malicious people. The U.S. Government recently has received attention for its gathering of telephone call-detail records to build a network for counterterrorism analysis (Tumulty, 2006). The simple relational-neighbor technique that performs so well in the case study below (wvRN), combined with a protocol for acquiring network link data, can be applied to communication or surveillance networks for suspicion scoring—ranking candidates by their estimated likelihood of being malicious (Macskassy and Provost, 2005) (cf., Galstyan and Cohen, 2005). In fraud detection, entities to be classified as being fraudulent or legitimate are linked by chains of transactions to those for which classifications are known. For more than a decade "state-of-the-art" fraud detection techniques have included network-based methods such as the "dialed-digit monitor" (Fawcett and Provost, 1997) that examines indirect (two-hop) connections to prior fraudulent accounts in the call network. Cortes et al. (2001) and Hill et al. (2006b) explicitly represent and reason with accounts' local network neighborhoods, for identifying telecommunications fraud. Similarly, networks of relationships between brokers can help in identifying securities fraud (Neville et al., 2005).

For marketing, consumers can be connected into a network based on the products that they buy (or that they rate in a collaborative filtering system), and then network-based techniques can be applied for making product recommendations (Domingos and Richardson, 2001; Huang et al., 2004). If a firm can know actual social-network links between consumers, for example through communications records, statistical, network-based marketing techniques can perform significantly better than traditional targeted marketing based on demographics and prior purchase data (Hill et al., 2006a).

Finally, network classification approaches have seen elegant application to problems that initially do not present themselves as *network* classification. Section 3.5.1 discusses how for "transductive" inference (Vapnik, 1998a), data points can be linked into a network based on any similarity measure. Thus, any transductive classification problem can be treated as a (within-)network classification problem.

3. Network Classification and Learning

Traditionally, machine learning methods have treated entities as being independent, which makes it possible to infer class membership on an entity-by-entity basis. With networked data, the class membership of one entity may have an influence on the class membership of a related entity. Furthermore, entities not directly linked may be related by chains of links, which suggests that it may be beneficial to infer the class memberships of all entities simultaneously. Collective inferencing in relational data (Jensen et al., 2004) makes simultaneous statistical judgments regarding the values of an attribute or attributes for multiple linked entities for which some attribute values are not known.

3.1 Univariate Collective Inferencing

For the univariate case study presented below, the (single) attribute X_i of a vertex v_i, representing the class, can take on some categorical value $c \in \mathcal{X}$—for m classes, $\mathcal{X} = \{c_1, \ldots, c_m\}$. We will use c to refer to a non-specified class value.

> Given graph $\mathbf{G} = (\mathbf{V}, \mathbf{E}, \mathbf{X})$ where X_i is the (single) attribute of vertex $v_i \in \mathbf{V}$, and given known values x_i of X_i for some subset of vertices $\mathbf{V}^K$, *univariate collective inferencing* is the process of simultaneously inferring the values x_i of X_i for the remaining vertices, $\mathbf{V}^U = \mathbf{V} - \mathbf{V}^K$, or a probability distribution over those values.

As a shorthand, we will use $\mathbf{x}^K$ to denote the (vector of) class values for $\mathbf{V}^K$, and similarly for $\mathbf{x}^U$. Then, $\mathbf{G}^K = (\mathbf{V}, \mathbf{E}, \mathbf{x}^K)$ denotes everything that is known about the graph (we do not consider the possibility of unknown edges). Edge $e_{ij} \in \mathbf{E}$ represents the edge between vertices v_i and v_j, and w_{ij} represents the edge weight. For this paper we consider only undirected edges (i.e., $w_{ij} = w_{ji}$), if necessary simply ignoring directionality for a particular application.

Rather than estimating the full joint probability distribution $P(\mathbf{x}^U | \mathbf{G}^K)$ explicitly, relational learning often enhances tractability by making a Markov assumption:

$$P(x_i | \mathbf{G}) = P(x_i | \mathcal{N}_i),$$

where $\mathcal{N}_i$ is a set of "neighbors" of vertex v_i such that $P(x_i | \mathcal{N}_i)$ is independent of $\mathbf{G} - \mathcal{N}_i$ (i.e., $P(x_i | \mathcal{N}_i) = P(x_i | \mathbf{G})$). For this paper, we make the ("first-order") assumption that $\mathcal{N}_i$ comprises only the immediate neighbors of v_i in the graph. As one would expect, and as we will see in Section 5.3.5, this assumption can be violated to a greater or lesser degree based on how edges are defined.

Given $\mathcal{N}_i$, a relational model can be used to estimate x_i. Note that $\mathcal{N}_i^U$ $(= \mathcal{N}_i \cap \mathbf{V}^U)$—the set of neighbors of v_i whose values of attribute X are not known—could be non-empty. Therefore, even if the Markov assumption holds, a simple application of the relational model may be insufficient. However, the relational model also may be used to estimate the labels of $\mathcal{N}_i^U$. Further, just as estimates for the labels of $\mathcal{N}_i^U$ influence the estimate for x_i, x_i also influences the estimate of the labels of $v_j \in \mathcal{N}_i^U$ (because edges are undirected, so $v_j \in \mathcal{N}_i \implies v_i \in \mathcal{N}_j$). In order to simultaneously estimate these interdependent values $\mathbf{x}^U$, various collective inference methods can be applied, which we discuss below.

Many of the algorithms developed for within-network classification are heuristic methods without a formal probabilistic semantics (and others are heuristic methods with a formal probabilistic semantics). Nevertheless, let us suppose that at inference time we are presented with a probability distribution structured as a graphical model.[3] In general, there are various inference tasks we might be interested in undertaking (Pearl, 1988). We focus primarily on within-network, univariate classification: the computation of the marginal probability of class membership of a particular node (i.e., the variable represented by the node taking on a particular value), conditioned on knowledge of the class membership of certain other nodes in the network. We also discuss methods for the related problem of computing the maximum a posteriori (MAP) joint labeling for $\mathbf{V}$ or $\mathbf{V}^U$.

For the sort of graphs we expect to encounter in the aforementioned applications, such probabilistic inference is quite difficult. As discussed by Wainwright and Jordan (2003), the naive method of marginalizing by summing over all configurations of the remaining variables is intractable even for graphs of modest size; for binary classification with around 400 unknown nodes, the summation involves more terms than atoms in the visible universe. Inference via belief propagation (Pearl, 1988) is applicable only as a heuristic approximation, because directed versions of many network classification graphs will contain cycles.

An important alternative to heuristic ("loopy") belief propagation is the junction-tree algorithm (Cowell et al., 1999), which provides exact solutions for arbitrary graphs. Unfortunately, the computational complexity of the junction-tree algorithm is exponential in the "treewidth" of the junction tree formed by the graph (Wainwright and Jordan, 2003). Since the treewidth is one less than the size of the largest clique, and the junction tree is formed by triangulating the original graph, the complexity is likely to be prohibitive for graphs such as social networks, which can have dense local connectivity and long cycles.

3.2 A Node-centric Network Learning Framework and Historical Background: Local, Relational, and Collective Inference

A large set of approaches to the problem of network classification can be viewed as "node centric," in the sense that they focus on a single node at a time. For a couple reasons, which we elaborate presently, it is useful to divide such systems into three components. One component, the *relational classifier*, addresses the question: given a node and the node's neighborhood, how should a classification or a class-probability estimate be produced? For example, the relational classifier might

3. For this paper, we assume that the structure of the network resulting from the chosen links corresponds at least partially to the structure of the network of probabilistic dependencies. This of course will be more or less true based on the choice of links, as we will see in Section 5.3.5.

1. **Non-relational (“local”) model.** This component consists of a (learned) model, which uses only local information—namely information about (attributes of) the entities whose target variable is to be estimated. The local models can be used to generate priors that comprise the initial state for the relational learning and collective inference components. They also can be used as one source of evidence during collective inference. These models typically are produced by traditional machine learning methods.
2. **Relational model.** In contrast to the non-relational component, the relational model makes use of the relations in the network as well as the values of attributes of related entities, possibly through long chains of relations. Relational models also may use local attributes of the entities.
3. **Collective inferencing.** The collective inferencing component determines how the unknown values are estimated together, possibly influencing each other, as described above.

Table 1: The three main components making up a (node-centric) network learning system.

combine local features and the labels of neighbors using a naive Bayes model (Chakrabarti et al., 1998) or a logistic regression (Lu and Getoor, 2003). A second component addresses the problem of *collective inference*: what should we do when a classification depends on a neighbor's classification, and vice versa? Finally, most such methods require initial (“prior”) estimates of the values for $P(\mathbf{x}^U|\mathbf{G}^K)$. The priors could be Bayesian subjective priors (Savage, 1954), or they could be estimated from data. A common estimation method is to employ a non-relational learner, using available “local” attributes of v_i to estimate x_i (e.g., as done by Besag, 1986). We propose a general “node-centric” network classification framework consisting of these three main components, listed in Table 1.

Viewing network classification approaches through this decomposition is useful for two main reasons. First, it provides a way of describing certain approaches that highlights the similarities and differences among them. Secondly, it expands the small set of existing methods to a design space of methods, since components can be mixed and matched in new ways. In fact, some novel combination may well perform better than those previously proposed; there has been little systematic experimentation along these lines. Local and relational classifiers can be drawn from the vast space of classifiers introduced over the decades in machine learning, statistics, pattern recognition, etc., and treated in great detail elsewhere. Collective inference has received much less attention in all these fields, and therefore warrants additional introduction.

Collective inference has its roots mainly in pattern recognition and statistical physics. Markov random fields have been used extensively for univariate network classification for vision and image restoration. Introductions to MRFs fill textbooks (Winkler, 2003); for our purposes, it is important to point out that they are the basis both directly and indirectly for many network classification approaches. MRFs are used to estimate a joint probability distribution over the free variables of a set of nodes under the first-order Markov assumption that $P(x_i|\mathbf{G}/v_i) = P(x_i|\mathcal{N}_i)$, where x_i is the (estimated) label of vertex v_i, $\mathbf{G}/v_i$ means all nodes in $\mathbf{G}$ except v_i, and $\mathcal{N}_i$ is a neighborhood function returning the neighbors of v_i. In a typical image application, nodes in the network are pixels and the labels are image properties such as whether a pixel is part of a vertical or horizontal border.

Because of the obvious interdependencies among the nodes in an MRF, computing the joint probability of assignments of labels to the nodes ("configurations") requires collective inference. Gibbs sampling (Geman and Geman, 1984) was developed for this purpose for restoring degraded images. Geman and Geman enforce that the Gibbs sampler settles to a final state by using simulated annealing where the temperature is dropped slowly until nodes no longer change state. Gibbs sampling is discussed in more detail below.

Two problems with Gibbs sampling (Besag, 1986) are particularly relevant for machine learning applications of network classification. First, prior to Besag's paper Gibbs sampling typically was used in vision not to compute the final marginal posteriors, as required by many "scoring" applications where the goal is to rank individuals, but rather to get final MAP classifications. Second, Gibbs sampling can be very time consuming, especially for large networks (not to mention the problems detecting convergence in the first place). With his Iterated Conditional Modes (ICM) algorithm, Besag introduced the notion of *iterative classification* for scene reconstruction. In brief, iterative classification repeatedly classifies labels for $v_i \in \mathbf{V}^U$, based on the "current" state of the graph, until no vertices change their label. ICM is presented as being efficient and particularly well suited to maximum marginal classification by node (pixel), as opposed to maximum joint classification over all the nodes (the scene).

Two other, closely related, collective inference techniques are (loopy) belief propagation (Pearl, 1988) and relaxation labeling (Rosenfeld et al., 1976; Hummel and Zucker, 1983). Loopy belief propagation was introduced above. Relaxation labeling originally was proposed as a class of parallel iterative numerical procedures that use contextual constraints to reduce ambiguities in image analysis; an instance of relaxation labeling is described in detail below. Both methods use the estimated class distributions directly, rather than the hard labelings used by iterative classification. Therefore, one requirement for applying these methods is that the relational classifier, when estimating x_i, must be able to use the estimated class distributions of $v_j \in N_i^U$.

Graph-cut techniques recently have been used in vision research as an alternative to using Gibbs sampling (Boykov et al., 2001). In essence, these are collective inference procedures, and are the basis of a collection of modern machine learning techniques. However, they do not quite fit in the node-centric framework, so we treat them separately below.

3.3 Node-centric Network Classification Approaches

The node-centric framework allows us to describe several prior systems by how they solve the problems of local classification, relational classification, and collective inference. The components of these systems are the basis for composing methods in NetKit.

For classifying web-pages based on the text and (possibly inferred) class labels of neighboring pages, Chakrabarti et al. (1998) combined naive Bayes local and relational classifiers with relaxation labeling for collective inference. In their experiments, performing network classification using the web-pages' link structure substantially improved classification as compared to using only the local (text) information. Specifically, considering the text of neighboring pages generally hurt performance, whereas using only the (inferred) class labels improved performance.

The iterated conditional modes procedure (ICM, Besag, 1986) is a node-centric approach where the local and relational classifiers are domain-dependent probabilistic models (based on local attributes and a MRF), and iterative classification is used for collective inference. Iterative classification has been used for collective inference elsewhere as well, for example Neville and Jensen (2000) use it in combination with naive Bayes for local and relational classification (with a simulated annealing procedure to settle on the final labeling).

We will look in more detail at the procedure known as "link-based classification" (Lu and Getoor, 2003), also introduced for the classification of linked documents (web pages and published manuscripts with an accompanying citation graph). Similarly to the work of Chakrabarti et al. (1998), linked-based classification uses the (local) text of the document as well as neighbor labels. More specifically, the relational classifier is a logistic regression model applied to a vector of aggregations of properties of the sets of neighbor labels linked with different types of links (in-, out-, co-links). Various aggregates could be used and are examined by Lu and Getoor (2003), such as the mode (the value of the most often occurring neighbor class), a binary vector with a value of 1 at cell i if there was a neighbor whose class label was c_i, and a count vector where cell i contained the number of neighbors belonging to class c_i. In their experiments, the count model performed best. They used logistic regression on the local (text) attributes of the instances to initialize the priors for each vertex in their graph and then applied the link-based classifiers as their relational model.

The simplest network classification technique we will consider was introduced to highlight the remarkable amount of "power" for classification present just in the structure of the network, a notion that we will investigate in depth in the case study below. The weighted-vote relational neighbor (wvRN) procedure (Macskassy and Provost, 2003) performs relational classification via a weighted average of the (potentially estimated) class membership scores ("probabilities") of the node's neighbors. Collective inference is performed via a relaxation labeling method similar to that used by Chakrabarti et al. (1998). If local attributes such as text are ignored, the node priors can be instantiated with the unconditional marginal class distribution estimated from the training data.

Since wvRN performs so well in the case study below, it is noteworthy to point out its close relationship to Hopfield networks (Hopfield, 1982) and Boltzmann machines (Hinton and Sejnowski, 1986). A Hopfield network is a graph of homogeneous nodes and undirected edges, where each node is a binary threshold unit. Hopfield networks were designed to recover previously seen graph configurations from a partially observed configuration, by repeatedly estimating the states of nodes one at a time. The state of a node is determined by whether or not its input exceeds its threshold, where the input is the weighted sum of the states of its immediate neighbors. wvRN differs in that it retains uncertainty at the nodes rather than assigning each a binary state (also allowing multi-class networks). *Learning* in Hopfield networks consists of learning the weights of edges and the thresholds of nodes, given one or more input graphs. Given a partially observed graph state and repeatedly applying, node-by-node, the node-activation equation will provably converge to a stable graph state—the low-energy state of the graph. If the partial input state is "close" to one of the training states, the Hopfield network will converge to that state.

A Boltzmann machine, like a Hopfield network, is a network of units with an "energy" defined for the network (Hinton and Sejnowski, 1986). Unlike Hopfield networks, Boltzmann machine nodes are stochastic and the machines use simulated annealing to find a stable state. Boltzmann machines also often have both visible and hidden nodes. The visible nodes' states can be observed, whereas the states of the hidden nodes cannot—as with hidden Markov models.

3.4 Modeling Homophily for Classification

The case study below demonstrates the remarkable power of a simple assumption: linked entities have a propensity to belong to the same class. This autocorrelation in the class variable of related entities is one form of homophily (the principle that a contact between similar people occurs at a higher rate than among dissimilar people), which is ubiquitous in observations and theories of social networks (Blau, 1977; McPherson et al., 2001). The relational neighbor classifier, which performs well in the case study below, was introduced as a very simple classifier based solely on homophily, that might provide a baseline to other relational classification techniques (Macskassy and Provost, 2003). As we discuss in Section 3.5.4 some more complex relational classification techniques can deal well with (arbitrary) homophily, and others cannot.

Homophily was one of the first characteristics noted by early social network researchers (Almack, 1922; Bott, 1928; Richardson, 1940; Loomis, 1946; Lazarsfeld and Merton, 1954), and holds for a wide variety of different relationships (McPherson et al., 2001). It seems reasonable to conjecture that homophily may also be present in other sorts of networks, especially networks of artifacts created by people. (Recently *assortativity*, a link-centric notion of homophily, has become the focus of mathematical studies of network structure, Newman, 2003).

Shared membership in groups such as communities with shared interests is an important reason for similarity among interconnected nodes (Neville and Jensen, 2005). Inference can be more effective if these groups are modeled explicitly, such as by using latent group models (LGMs, Neville and Jensen, 2005) to specify joint models of attributes, links, and *groups*. LGMs are especially promising for within-network classification, since the existence of known classes will facilitate the identification of (hidden) group membership, which in turn may aid in the estimation of $\mathbf{x}^U$.

3.5 Other Methods for Network Classification

Before describing the node-centric network classification toolkit, for completeness we first will discuss three other types of methods that are suited to univariate, within-network classification. Graph-based methods (Sections 3.5.1 and 3.5.2) that are used for semi-supervised learning, could apply as well to within-network classification. Within-network classification also offers the opportunity to take advantage of node identifiers, discussed in Section 3.5.3. Finally, although there are important reasons to study univariate network classification (see below), recently the field has seen a flurry of development of multivariate methods applicable to classification in networked data (Section 3.5.4).

3.5.1 GRAPH-CUT METHODS AND THEIR RELATIONSHIP TO TRANSDUCTIVE INFERENCE

As mentioned above, one complication to within-network classification is that the to-be-classified nodes and the nodes for which the labels are known are intermixed in the same network. Most prior work on network learning and classification assumes that the classes of all the nodes in the network need to be estimated (perhaps having learned something from a separate, related network). Pinning the values of certain nodes intuitively should be advantageous, since it gives to the classification procedure clear points of reference.

This complication is addressed directly by several lines of recent work (Blum and Chawla, 2001; Joachims, 2003; Zhu et al., 2003; Blum et al., 2004). The setting is not initially one of network classification, but rather, semi-supervised learning in a transductive setting (Vapnik, 1998b). Nevertheless, the methods introduced may have direct application to certain instances of univariate network classification. Specifically, they consider data sets where labels are given for a subset of cases, and classifications are desired for a subset of the rest. To form an "induced" weighted network, edges are added between data points based on similarity between cases.

Finding the minimum energy configuration of a MRF, the partition of the nodes that maximizes self-consistency under the constraint that the configuration be consistent with the known labels, is equivalent to finding a minimum cut of the graph (Greig et al., 1989). Following this idea and subsequent work connecting classification to the problem of computing minimum cuts (Kleinberg and Tardos, 1999), Blum and Chawla (2001) investigate how to define weighted edges for a transductive classification problem such that polynomial-time mincut algorithms give optimal solutions to objective functions of interest. For example, they show elegantly how forms of leave-one-out-cross-validation error (on the predicted labels) can be minimized for various nearest-neighbor algorithms, including a weighted-voting algorithm. This procedure corresponds to optimizing the consistency of the predictions in particular ways—as Blum and Chawla put it, optimizing the "happiness" of the classification algorithm.

Of course, optimizing the consistency of the labeling may not be ideal. For example in the case of a highly unbalanced class frequency it is necessary to preprocess the graph to avoid degenerate cuts, for example those cutting off the one positive example (Joachims, 2003). This seeming pathology stems from the basic objective: the minimum of the sum of cut-through edge weights depends directly on the sizes of the cut sets; normalizing for the cut size leads to ratiocut optimization (Dhillon, 2001) constrained by the known labels (Joachims, 2003).

The mincut partition corresponds to the most probable joint labeling of the graph (taking an MRF perspective), whereas as discussed earlier we often would like a per-node (marginal) class-probability estimation (Blum et al., 2004). Unfortunately, in the case we are considering—when some node labels are known in a general graph—there is no known efficient algorithm for determining these estimates. There are several other drawbacks (Blum et al., 2004), including that there may be many minimum cuts for a graph (from which mincut algorithms choose rather arbitrarily), and that the mincut approach does not yield a measure of confidence on the classifications. Blum et al. address these drawbacks by repeatedly adding artificial noise to the edge weights in the induced graph. They then can compute fractional labels for each node corresponding to the frequency of labeling by the various mincut instances. As mentioned above, this method (and the one discussed next) was intended to be applied to an induced graph, which can be designed specifically for the application. Mincut approaches are appropriate for graphs that have at least some small, balanced cuts (whether or not these correspond to the labeled data) (Blum et al., 2004). It is not clear whether methods like this that discard highly unbalanced cuts will be effective for network classification problems such as fraud detection in transaction networks, with extremely unbalanced class distributions.

3.5.2 THE GAUSSIAN-FIELD CLASSIFIER

In the experiments of Blum et al. (2004), their randomized mincut method empirically does not perform as well as a method introduced by Zhu et al. (2003). Therefore, we will revisit this latter method in an experimental comparison following the main case study. Zhu et al. treat the induced network as a Gaussian field (Besag, 1975) (a random field with soft node labels) constrained such that the labeled nodes maintain their values. The value of the energy function is the weighted average of the function's values at the neighboring points. Zhu et al. show that this function is a harmonic function and that the solution over the complete graph can be computed using a few matrix operations. The result is a classifier essentially identical to the wvRN classifier (Macskassy and Provost, 2003) discussed above (paired with relaxation labeling), except with a principled semantics and exact inference.[4] The energy function then can be normalized based on desired class posteriors ("class mass normalization"). Zhu et al. also discuss various physical interpretations of this procedure, including random walks, electric networks, and spectral graph theory, that can be intriguing in the context of particular applications. For example, applying the random walk interpretation to a telecommunications network including legitimate and fraudulent accounts: consider starting at an account of interest and walking randomly through the call graph based on the link weights; the node score is the probability that the walk hits a known fraudulent account before hitting a known legitimate account.

3.5.3 USING NODE IDENTIFIERS

As mentioned in the introduction, another unique aspect of within-network classification is that *node identifiers*, unique symbols for individual nodes, can be used in learning and inference. For example, for suspicion scoring in social networks, the fact that someone met with a particular individual may be informative (e.g., having had repeated meetings with a known terrorist leader). Very little work has incorporated identifiers, because of the obvious difficulty of modeling with very high cardinality categorical attributes. Identifiers (telephone numbers) have been used for fraud detection (Fawcett and Provost, 1997; Cortes et al., 2001; Hill et al., 2006b), but to our knowledge, Perlich and Provost (2006) provide the only comprehensive treatment of the use of identifiers for relational learning.

3.5.4 BEYOND UNIVARIATE CLASSIFICATION

Besides the methods already discussed (e.g., Besag, 1986; Lu and Getoor, 2003; Chakrabarti et al., 1998), several other methods go beyond the homogeneous, univariate case on which this paper focuses. Conditional random fields (CRFs, Lafferty et al., 2001) are random fields where the probability of a node's label is conditioned not only on the labels of neighbors (as in MRFs), but also on all the observed attribute data.

Relational Bayesian networks (RBNs, a.k.a. probabilistic relational models, Koller and Pfeffer, 1998; Friedman et al., 1999; Taskar et al., 2001) extend Bayesian networks (BNs, Pearl, 1988) by taking advantage of the fact that a variable used in one instantiation of a BN may refer to the exact same variable in another BN. For example, consider that the grade of a student depends to some extent upon his professor; this professor is the same for all students in the class. Therefore, rather than building one BN and using it in isolation for each entity, RBNs directly link shared variables, thereby generating one big network of connected entities for which collective inferencing can be performed.

Unfortunately, because the BN representation must be acyclic, RBNs cannot model arbitrary relational autocorrelation, such as the homophily that plays a large role in the case study below. However, undirected relational graphical models can model relational autocorrelation. Relational dependency networks (RDNs, Neville and Jensen, 2003, 2004, 2007), extend dependency networks (Heckerman et al., 2000) in much the same way that RBNs extend Bayesian networks. RDNs learn the dependency structure by learning a conditional model individually for each variable of interest, conditioning on the other variables, including variables of other nodes in the network. Cyclic de-

4. Experiments show these two procedures to yield almost identical generalization performance, albeit the matrix-based procedure of Zhu et al. is much slower than the iterative wvRN.

```
Input: $\mathbf{G}^K, \mathbf{V}^U, \mathrm{RC}_{\mathrm{type}}, \mathrm{LC}_{\mathrm{type}}, \mathrm{CI}_{\mathrm{type}}$
Induce a local classification model, LC, of type $\mathrm{LC}_{\mathrm{type}}$, using $\mathbf{G}^K$
Induce a relational classification model, RC, of type $\mathrm{RC}_{\mathrm{type}}$, using $\mathbf{G}^K$
Estimate $x_i \in \mathbf{V}^U$ using LC.
Apply collective inferencing of type $\mathrm{CI}_{\mathrm{type}}$, using RC as the model.
Output: Final estimates for $x_i \in \mathbf{V}^U$
```

Table 2: High-level pseudo-code for the core routine of the Network Learning Toolkit.

pendencies such as homophily are modeled when the conditional modeling for a particular variable includes instantiations of the same variable from linked nodes. Relational extensions to Markov networks (Pearl, 1988) also can model arbitrary autocorrelation dependencies. In relational Markov networks (RMNs, Taskar et al., 2002) the clique potential functions are based on functional templates, each of which is a (learned, class-conditional) probability function based on a user-specified set of relations. In associative Markov networks (AMNs, Taskar et al., 2004) autocorrelation of labels is explicitly modeled by extending the *generalized Potts model* (Potts, 1952) (specifically, to allow different labels to have different penalties). Of particular interest, exact inference can be performed in AMNs (formulated as a quadratic programming problem for binary classification, which can be relaxed for multi-class problems).

These methods for network classification use only a few of the many relational learning techniques. There are many more, for example from the rich literature of inductive logic programming (ILP, such as, De Raedt et al., 2001; Dzeroski and Lavrac, 2001; Kramer et al., 2001; Flach and Lachiche, 2004; Richardson and Domingos, 2006), or based on using relational database joins to generate relational features (e.g., Perlich and Provost, 2003; Popescul and Ungar, 2003; Perlich and Provost, 2006).

4. Network Learning Toolkit (NetKit-SRL)

NetKit is designed to accommodate the interchange of components and the introduction of new components. As outlined in Section 3.2, the node-centric learning framework comprises three main components: the relational classifier, the local classifier and collective inference. Any local classifier can be paired with any relational classifier, which can then be combined with any collective inference method. NetKit's core routine is simple and is outlined in Table 2; it consists of these five general modules:

1. **Input:** This module reads data into a memory-resident graph $\mathbf{G}$.

2. **Local classifier inducer:** Given as training data $\mathbf{V}^K$, this module returns a model $\mathcal{M}_L$ that will estimate x_i using only attributes of a node $v_i \in \mathbf{V}^U$. Ideally, $\mathcal{M}_L$ will estimate a probability distribution over the possible values for x_i.

3. **Relational classifier inducer:** Given $\mathbf{G}^K$, this module returns a model $\mathcal{M}_R$ that will estimate x_i using v_i and $\mathcal{N}_i$. Ideally, $\mathcal{M}_R$ will estimate a probability distribution over the possible values for x_i.

4. **Collective Inferencing:** Given a graph $\mathbf{G}$ possibly with some x_i known, a set of prior estimates for $\mathbf{x}^U$, and a relational model $\mathcal{M}_R$, this module applies collective inferencing to estimate $\mathbf{x}^U$.

5. **Weka Wrapper:** This module is a wrapper for Weka[5] (Witten and Frank, 2000) and can convert the graph representation of v_i into an entity that can either be learned from or be used to estimate x_i. NetKit can use a Weka classifier either as a local classifier or as a relational classifier (by using various aggregation methods to summarize the values of attributes in $\mathcal{N}_i$).

The current version of NetKit-SRL, while able to read in heterogeneous graphs, only supports classification in graphs consisting of a single type of node. Algorithms based on expectation maximization are possible to implement through the NetKit collective inference module, by having the collective inference module repeatedly apply a relational classifier to learn a new relational model and then apply the new relational model to $\mathbf{G}$ (rather than repeatedly apply the same learned model at every iteration).

The rest of this section describes the particular relational classifiers and collective inference methods implemented in NetKit for the case study. First, we describe the four (univariate[6]) relational classifiers. Then, we describe the three collective inference methods.

4.1 Relational Classifiers

All four relational classifiers take advantage of the first-order Markov assumption on the network: only a node's local neighborhood is necessary for classification. The univariate case renders this assumption particularly restrictive: only the class labels of the local neighbors are necessary. The local network is defined by the user, analogous to the user's definition of the feature set for propositional learning. Entities whose class labels are not known are either ignored or are assigned a prior probability, depending upon the choice of local classifier.

4.1.1 WEIGHTED-VOTE RELATIONAL NEIGHBOR CLASSIFIER (WVRN)

The case study's simplest classifier (Macskassy and Provost, 2003)[7] estimates class-membership probabilities by assuming the existence of homophily (see Section 3.4).

Definition. Given $v_i \in \mathbf{V}^U$, the weighted-vote relational-neighbor classifier (wvRN) estimates $P(x_i|\mathcal{N}_i)$ as the (weighted) mean of the class-membership probabilities of the entities in $\mathcal{N}_i$:

$$P(x_i = c|\mathcal{N}_i) = \frac{1}{Z} \sum_{v_j \in \mathcal{N}_i} w_{i,j} \cdot P(x_j = c|\mathcal{N}_j),$$

where Z is the usual normalizer. This can be viewed simply as an inference procedure, or as a probability model. In the latter case, it corresponds exactly to the Gaussian-field model discussed below in Section 3.5.2. How to conduct the inference/estimate the model falls on the collective inference procedure.

5. We use version 3.4.2. Weka is available at `http://www.cs.waikato.ac.nz/~ml/weka/`.
6. The open-source NetKit release contains multivariate versions of these classifiers.
7. Previously called the probabilistic Relational Neighbor classifier (pRN).

4.1.2 CLASS-DISTRIBUTION RELATIONAL NEIGHBOR CLASSIFIER (CDRN)

The simple wvRN assumes that neighboring class labels were likely to be the same. *Learning* a model of the distribution of neighbor class labels is more flexible, and may lead to better discrimination. Following Perlich and Provost (2003, 2006), and in the spirit of Rocchio's method (Rocchio, 1971), we define node v_i's *class vector* $\mathrm{CV}(v_i)$ to be the vector of summed linkage weights to the various (known) classes, and class c's *reference vector* $\mathrm{RV}(c)$ to be the average of the class vectors for nodes known to be of class c. Specifically:

$$\mathrm{CV}(v_i)_k = \sum_{v_j \in \mathcal{N}_i, x_j = c_k} w_{i,j}, \tag{1}$$

where $\mathrm{CV}(v_i)_k$ represents the kth position in the class vector and $c_k \in \mathcal{X}$ is the kth class. Based on these class vectors, the reference vectors can then be defined as the normalized vector sum:

$$\mathrm{RV}(c) = \frac{1}{|\mathbf{V}_c^K|} \sum_{v_i \in \mathbf{V}_c^K} \mathrm{CV}(v_i), \tag{2}$$

where $\mathbf{V}_c^K = \{v_i | v_i \in \mathbf{V}^K, x_i = c\}$.

For the case study, during training, neighbors in $\mathbf{V}^U$ are ignored. For prediction, estimated class membership probabilities are used for neighbors in $\mathbf{V}^U$, and Equation 1 becomes:

$$\mathrm{CV}(v_i)_k = \sum_{v_j \in \mathcal{N}_i} w_{i,j} \cdot P(x_j = c_k | \mathcal{N}_j). \tag{3}$$

Definition. Given $v_i \in \mathbf{V}^U$, the *class-distribution relational-neighbor classifier (cdRN)* estimates the probability of class membership, $P(x_i = c|\mathcal{N}_i)$, by the normalized vector similarity between v_i's class vector and class c's reference vector:

$$P(x_i = c|\mathcal{N}_i) = \mathrm{sim}(\mathrm{CV}(v_i), \mathrm{RV}(c)),$$

where $\mathrm{sim}(a,b)$ is any vector similarity function (L_1, L_2, cosine, etc.), normalized to lie in the range $[0,1]$. For the results presented below, we use cosine similarity.

As with wvRN, Equation 3 is a recursive definition, and therefore the value of $P(x_j = c|\mathcal{N}_j)$ is approximated by the "current" estimate as defined by the selected collective inference technique.

4.1.3 NETWORK-ONLY BAYES CLASSIFIER (NBC)

NetKit's network-only Bayes classifier (nBC) is based on the algorithm described by Chakrabarti et al. (1998). To start, assume there is a single node v_i in $\mathbf{V}^U$. The nBC uses multinomial naive Bayesian classification based on the classes of v_i's neighbors.

$$P(x_i = c|\mathcal{N}_i) = \frac{P(\mathcal{N}_i|c) \cdot P(c)}{P(\mathcal{N}_i)},$$

where

$$P(\mathcal{N}_i|c) = \frac{1}{Z} \prod_{v_j \in \mathcal{N}_i} P(x_j = \tilde{x}_j | x_i = c)^{w_{i,j}}$$

where Z is a normalizing constant and $\tilde{x}_j$ is the class observed at node v_j. As usual, because $P(\mathcal{N}_i)$ is the same for all classes, normalization across the classes allows us to avoid explicitly computing it.

We call nBC "network-only" to emphasize that in the application to the univariate case study below, we do not use local attributes of a node. As discussed above, Chakrabarti et al. initialize nodes' priors based on a naive Bayes model over the local document text and add a text-based term to the node probability formula.[8] In the univariate setting, local text is not available. We therefore use the same scheme as for the other relational classifiers: initialize unknown labels as decided by the local classifier being used (in our study: either the class prior or 'null', depending on the collective inference component, as described below). If a neighbor's label is 'null', then it is ignored for classification. Also, Chakrabarti et al. differentiated between incoming and outgoing links, whereas we do not. Finally, Chakrabarti et al. do not mention how or whether they account for possible zeros in the estimations of the marginal conditional probabilities; we apply traditional Laplace smoothing where $m = |\mathcal{X}|$, the number of classes.

The foregoing assumes all neighbor labels are known. When the values of some neighbors are unknown, but estimations are available, we follow Chakrabarti et al. (1998) and perform a Bayesian combination based on (estimated) configuration priors and the entity's known neighbors. Chakrabarti et al. (1998) describe this procedure in detail. For our case study, such an estimation is necessary only when using relaxation labeling (described below).

4.1.4 NETWORK-ONLY LINK-BASED CLASSIFICATION (nLB)

The final relational classifier used in the case study is a network-only derivative of the link-based classifier (Lu and Getoor, 2003). The network-only Link-Based classifier (nLB) creates a feature vector for a node by aggregating the labels of neighboring nodes, and then uses logistic regression to build a discriminative model based on these feature vectors. This learned model is then applied to estimate $P(x_i = c|\mathcal{N}_i)$. As with the nBC, the difference between the "network-only" link-based classifier and Lu and Getoor's version is that for the univariate case study we do not consider local attributes (e.g., text).

As described above, Lu and Getoor (2003) considered various aggregation methods: existence (binary), the mode, and value counts. The last aggregation method, the count model, is equivalent to the class vector $\mathrm{CV}(v_i)$ defined in Equation 3. This was the best performing method in the study by Lu and Getoor, and is the method on which we base nLB. The logistic regression classifier used by nLB is the multiclass implementation from Weka version 3.4.2.

We made one minor modification to the original link-based classifier. Perlich (2003) argues that in different situations it may be preferable to use either vectors based on raw counts (as given above) or vectors based on normalized counts. We did preliminary runs using both. The normalized vectors generally performed better, and so we use them for the case study.

4.2 Collective Inference Methods

This section describes three collective inferencing methods implemented in NetKit and used in the case study. As described above, given (i) a network initialized by the local model, and (ii) a relational model, a collective inference method infers a set of class labels for $\mathbf{x}^U$. Depending

8. The original classifier was defined as: $P(x_i = c|\mathcal{N}_i) = P(\mathcal{N}_i|c) \cdot P(\tau_i|v_i) \cdot P(c)$, with τ_i being the text of the document-entity represented by vertex v_i.

```
1. Initialize $v_i \in \mathbf{V}^U$ using the local classifier model, $\mathcal{M}_L$. Specifically, for $v_i \in \mathbf{V}^U$:
    (a) $\widehat{\mathbf{c}}_i \leftarrow \mathcal{M}_L(v_i)$, where $\widehat{\mathbf{c}}_i$ is a vector of probabilities representing $\mathcal{M}_L$'s estimates
        of $P(x_i|\mathcal{N}_i)$. We use $\widehat{\mathbf{c}}_i(k)$ to mean the $k^{\text{th}}$ value in $\widehat{\mathbf{c}}_i$, which represents
        $P(x_i = c_k|\mathcal{N}_i)$.

        For the case study, the local classifier model returns the unconditional
        marginal class distribution estimated from $\mathbf{x}^K$.
    (b) Sample a value $c_s$ from $\widehat{\mathbf{c}}_i$, such that $P(c_s = c_k|\widehat{\mathbf{c}}_i) = \widehat{\mathbf{c}}_i(k)$.
    (c) Set $x_i \leftarrow c_s$.
2. Generate a random ordering, $O$, of vertices in $\mathbf{V}^U$.
3. For elements $v_i \in O$ in order:
    (a) Apply the relational classifier model: $\widehat{\mathbf{c}}_i \leftarrow \mathcal{M}_R(v_i)$.
    (b) Sample a value $c_s$ from $\widehat{\mathbf{c}}_i$, such that $P(c_s = c_k|\widehat{\mathbf{c}}_i) = \widehat{\mathbf{c}}_i(k)$.
    (c) Set $x_i \leftarrow c_s$.
        Note that when $\mathcal{M}_R$ is applied to estimate $\widehat{\mathbf{c}}_\mathbf{i}$ it uses the "new" labelings
        from elements $1, \ldots, (i-1)$, while using the "current" labelings for elements
        $(i+1), \ldots, n$.
4. Repeat prior step 200 times without keeping any statistics. This is known as the
   burnin period.
5. Repeat again for 2000 iterations, counting the number of times each $X_i$ is assigned
   a particular value $c \in \mathcal{X}$. Normalizing these counts forms the final class probability
   estimates.
```

Table 3: Pseudo-code for Gibbs sampling.

on the application, the goal ideally would be to infer the class labels with either the maximum joint probability or the maximum marginal probability for each node. Alternatively, if estimates of entities' class-membership probabilities are needed, the collective inference method estimates the marginal probability distribution $P(X_i = c|\mathbf{G}^K, \Lambda)$ for each $X_i \in \mathbf{x}^U$ and $c \in \mathcal{X}$, where Λ stands for the priors returned by the local classifier.

4.2.1 GIBBS SAMPLING (GS)

Gibbs sampling (Geman and Geman, 1984) is commonly used for collective inferencing with relational learning systems. The algorithm is straightforward and is shown in Table 3.[9] The use of 200 and 2000 for the burnin period and number of iterations are commonly used values.[10] Ideally, we would iterate until the estimations converge. Although there are convergence tests for the Gibbs sampler, they are neither robust nor well understood (cf., Gilks et al., 1995), so we simply use a fixed number of iterations.

9. This instance of Gibbs sampling uses a single random ordering ("chain"), as this is what we used in the case study. In the case study, averaging over 10 chains (the default in NetKit) had no effect on the final accuracies.
10. As it turns out, in our case study Gibbs sampling invariably reached a seemingly final plateau in fewer than 1000 iterations, and often in fewer than 500.

```
1. For $v_i \in \mathbf{V}^U$, initialize the prior: $\widehat{\mathbf{c}}_i^{(0)} \leftarrow \mathcal{M}_L(v_i)$, where $\widehat{\mathbf{c}}_i$ is defined as in Table 3.

   For the case study, the local classifier model returns the unconditional marginal class
   distribution estimated from $\mathbf{x}^K$.
2. For elements $v_i \in \mathbf{V}^U$:
   (a) Estimate $x_i$ by applying the relational model:

       $\widehat{\mathbf{c}}_i^{(t+1)} \leftarrow \mathcal{M}_R(v_i^{(t)})$,   (4)

       where $\mathcal{M}_R(v_i^{(t)})$ denotes using the estimates $\widehat{\mathbf{c}}_j^{(t)}$ for $v_j \in \mathcal{N}_i$, and $t$ is the
       iteration count. This has the effect that all predictions are done pseudo-
       simultaneously based on the state of the graph after iteration $t$.
3. Repeat for $T$ iterations, where $T = 99$ for the case study. $\widehat{\mathbf{c}}^{(T)}$ will comprise the final
   class probability estimations.
```

Table 4: Pseudo-code for relaxation labeling.

Notably, because all nodes are assigned a class at every iteration, when Gibbs sampling is used the relational models will always see a fully labeled/classified neighborhood, making prediction straightforward. For example, nBC does not need to compute its Bayesian combination (see Section 4.1.3).

4.2.2 RELAXATION LABELING (RL)

The second collective inferencing method used in the study is relaxation labeling, based on the method of Chakrabarti et al. (1998). Rather than treat $\mathbf{G}$ as being in a specific labeling "state" at every point (as Gibbs sampling does), relaxation labeling retains the uncertainty, keeping track of the current probability estimations for $\mathbf{x}^U$. The relational model must be able to use these estimations. Further, rather than estimating one node at a time and updating the graph right away, relaxation labeling "freezes" the current estimations so that at step $t+1$ all vertices will be updated based on the estimations from step t. The algorithm is shown in Table 4.

Preliminary runs showed that relaxation labeling sometimes does not converge, but rather ends up oscillating between two or more graph states.[11] NetKit performs simulated annealing—on each subsequent iteration giving more weight to a node's own current estimate and less to the influence of its neighbors.

The new updating step, replacing Equation 4 is:

$$\widehat{\mathbf{c}}_i^{(t+1)} = \beta^{(t+1)} \cdot \mathcal{M}_R(v_i^{(t)}) + (1-\beta^{(t+1)}) \cdot \widehat{\mathbf{c}}_i^{(t)},$$

where

$$\begin{aligned} \beta^0 &= k, \\ \beta^{(t+1)} &= \beta^{(t)} \cdot \alpha, \end{aligned}$$

11. Such oscillation has been noted elsewhere for closely related methods (Murphy et al., 1999).

```
1. For $v_i \in \mathbf{V}^U$, initialize the prior: $\widehat{\mathbf{c}}_i \leftarrow \mathcal{M}_L(v_i)$, where $\widehat{\mathbf{c}}_i$ is defined as in Table 3. The
   link-based classification work of Lu and Getoor (2003) uses a local classifier to set
   initial classifications. This will clearly not work in our case (all unknowns would be
   classified as the majority class), and we therefore use a local classifier model which
   returns null (i.e., it does not return an estimation.)
2. Generate a random ordering, $O$, of elements in $\mathbf{V}^U$.
3. For elements $v_i \in O$:
   (a) Apply the relational classifier model, $\widehat{\mathbf{c}}_i \leftarrow \mathcal{M}_R$, using all non-null labels (en-
       tities which have not yet been classified will be ignored.) If all neighbor enti-
       ties are null, then return null.
   (b) Classify $v_i$:
           $x_i = c_k, k = \text{argmax}_j \widehat{\mathbf{c}}_i(j)$,
       where $\widehat{\mathbf{c}}_i(j)$ is the $j^{\text{th}}$ value in vector $\widehat{\mathbf{c}}_i$. (Remember, $\widehat{\mathbf{c}}_i$ is a vector of $|\mathcal{X}|$
       elements. We classify $v_i$ by predicting the class with the highest likelihood).
4. Repeat for $T = 1000$ iterations, or until no entities receive a new class label.[a] The
   estimates from the final iteration will be used as the final class probability estimates.
```

[a]. A post-mortem of the results showed that iterative classification often stopped within $10-20$ iterations when paired with cdRN, nBC or nLB. For wvRN, it generally ran the full 1000 iterations, although the accuracy quickly plateaued and wvRN ended up moving within a small range of similar accuracies.

Table 5: Pseudo-code for Iterative classification.

where k is a constant between 0 and 1, which for the case study we set to 1.0, and α is a decay constant, which we set to 0.99. Preliminary testing showed that final performance is very robust as long as $0.9 < \alpha < 1$. Smaller values of α can lead to neighbors losing their influence too quickly, which can hurt performance when only very few labels are known. A post-mortem of the results showed that the accuracies often converged within the first 20 iterations.

4.2.3 ITERATIVE CLASSIFICATION (IC)

The third and final collective inferencing method implemented in NetKit and used in the case study is the variant of iterative classification described in the work on link-based classification (Lu and Getoor, 2003) and shown in Table 5. As with Gibbs sampling, the relational model never sees uncertainty in the labels of (neighbor) entities. Either the label of a neighbor is `null` and ignored (which only happens in the first iteration or if all its neighbors are also `null`), or it is assigned a definite label.

5. Case Study

The study presented in this section has two goals. First, it showcases NetKit, demonstrating that the modular framework indeed facilitates the comparison of systems for learning and inference in networked data. Second, it examines the simple-but-important special case of univariate learning and inference in homogeneous networks, comparing alternative techniques that have not before been compared systematically, if at all. The setting for the case study is simple: For some entities in the network, the value of x_i is known; for others it must be estimated.

Univariate classification, albeit a simplification for many domains, is important for several reasons. First, it is a representation that is used in some applications. Above we mentioned fraud detection; as a specific example, a telephone account that calls the same numbers as a known fraudulent account (and hence the accounts are connected through these intermediary numbers) is suspicious (Fawcett and Provost, 1997; Cortes et al., 2001). For phone fraud, univariate network classification often provides alarms with reasonable coverage and remarkably low false-positive rates. Generally speaking, a homogeneous, univariate network is an inexpensive (in terms of data gathering, processing, storage) approximation of many complex networked data problems. Fraud detection applications certainly do have a variety of additional attributes of importance; nevertheless, univariate simplifications are very useful and are used in practice.

The univariate case also is important scientifically. It isolates a primary difference between networked data and non-networked data, facilitating the analysis and comparison of relevant classification and learning methods. One thesis of this study is that there is considerable information inherent in the structure of the networked data and that this information can be readily taken advantage of, using simple models, to estimate the labels of unknown entities. This thesis is tested by isolating this characteristic—namely ignoring any auxiliary attributes and only allowing the use of known class labels—and empirically evaluating how well univariate models perform in this setting on benchmark data sets.

Considering homogeneous networks plays a similar role. Although the domains we consider have obvious representations consisting of multiple entity types and edges (e.g., people and papers for node types and same-author-as and cited-by as edge types in a citation-graph domain), a homogeneous representation is much simpler. In order to assess whether a more complex representation is worthwhile, it is necessary to assess standard techniques on the simpler representation (as we do in this case study). Of course, the way a network is "homogenized" may have a considerable effect on classification performance. We will revisit this below in Section 5.3.6.

5.1 Data

The case study reported in this paper makes use of 12 benchmark data sets from four domains that have been the subject of prior study in machine learning. As this study focuses on networked data, any singleton (disconnected) entities in the data were removed. Therefore, the statistics we present may differ from those reported previously.

5.1.1 IMDB

Networked data from the Internet Movie Database (IMDb)[12] have been used to build models predicting movie success as determined by box-office receipts (Jensen and Neville, 2002a). Following the work of Neville et al. (2003), we focus on movies released in the United States between 1996 and 2001 with the goal of estimating whether the opening weekend box-office receipts "will" exceed \$2 million (Neville et al., 2003). Obtaining data from the IMDb web-site, we identified 1169 movies released between 1996 and 2001 that we were able to link up with a revenue classification

12. See `http://www.imdb.com`.

Category	Size
High-revenue	572
Low-revenue	597
Total	1169
Base accuracy	51.07%

Table 6: Class distribution for the IMDb data set.

Category	Size
Case-based	402
Genetic Algorithms	551
Neural Networks	1064
Probabilistic Methods	529
Reinforcement Learning	335
Rule Learning	230
Theory	472
Total	3583
Base accuracy	29.70%

Table 7: Class distribution for the cora data set.

in the database given to us by the authors of the original study. The class distribution of the data set is shown in Table 6.

We link movies if they share a production company, based on observations from previous work (Macskassy and Provost, 2003).[13] The weight of an edge in the resulting graph is the number of production companies two movies have in common. Notably, we ignore the temporal aspect of the movies in this study, simply labeling movies at random for the training set. This can result in a movie in the test set being released earlier than a movie in the training set.

5.1.2 CORA

The cora data set (McCallum et al., 2000) comprises computer science research papers. It includes the full citation graph as well as labels for the topic of each paper (and potentially sub- and sub-sub-topics).[14] Following a prior study (Taskar et al., 2001), we focused on papers within the machine learning topic with the classification task of predicting a paper's sub-topic (of which there are seven). The class distribution of the data set is shown in Table 7.

Papers can be linked if they share a common author, or if one cites the other. Following prior work (Lu and Getoor, 2003), we link two papers if one cites the other. The weight of an edge would normally be one unless the two papers cite each other (in which case it is two—there can be no other weight for existing edges).

13. And on a suggestion from David Jensen.
14. These labels were assigned by a naive Bayes classifier (McCallum et al., 2000).

	Number of web-pages			
Class	**Cornell**	**Texas**	**Washington**	**Wisconsin**
student	145	163	151	155
not-student	201	171	283	193
Total	346	334	434	348
Base accuracy	58.1%	51.2%	60.8%	55.5%

Table 8: Class distribution for the WebKB data set using binary class labels.

5.1.3 WEBKB

The third domain we draw from is based on the WebKB Project (Craven et al., 1998).[15] It consists of sets of web pages from four computer science departments, with each page manually labeled into 7 categories: course, department, faculty, project, staff, student, or other. As with other work (Neville et al., 2003; Lu and Getoor, 2003), we ignore pages in the "other" category except as described below.

From the WebKB data we produce eight networked data sets for within-network classification. For each of the four universities, we consider two different classification problems: the six-class problem, and following a prior study, the binary classification task of predicting whether a page belongs to a student (Neville et al., 2003).[16] The binary task results in an approximately balanced class distribution.

Following prior work on web-page classification, we link two pages by co-citations (if x links to z and y links to z, then x and y are co-citing z) (Chakrabarti et al., 1998; Lu and Getoor, 2003). To weight the link between x and y, we sum the number of hyperlinks from x to z and separately the number from y to z, and multiply these two quantities. For example, if student x has 2 edges to a group page, and a fellow student y has 3 edges to the same group page, then the weight along that path between those 2 students would be 6. This weight represents the number of possible co-citation paths between the pages. Co-citation relations are not uniquely useful to domains involving documents; for example, as mentioned above, for phone-fraud detection bandits often call the same numbers as previously identified bandits. We chose co-citations for this case study based on the prior observation that a student is more likely to have a hyperlink to her advisor or a group/project page rather than to one of her peers (Craven et al., 1998).[17]

To produce the final data sets, we extracted the pages that have at least one incoming and one outgoing link. We removed pages in the "other" category from the classification task, although they were used as "background" knowledge—allowing 2 pages to be linked by a path through an "other" page. For the binary tasks, the remaining pages were categorized into either student or not-student. The composition of the data sets is shown in Tables 8 and 9.

5.1.4 INDUSTRY CLASSIFICATION

The final domain we draw from involves classifying companies by industry sector. Companies are linked via cooccurrence in text documents. We use two different data sets, representing different

15. We use the WebKB-ILP-98 data.
16. It turns out that the relative performance of the methods is quite different on these two variants.
17. We return to these data in Section 5.3.5, where we show and discuss how using the hyperlinks directly is not sufficient for any of the univariate methods to do well.

	Number of web-pages			
Category	**cornell**	**texas**	**washington**	**wisconsin**
course	54	51	170	83
department	25	36	20	37
faculty	62	50	44	37
project	54	28	39	25
staff	6	6	10	11
student	145	163	151	155
Total	346	334	434	348
Base accuracy	41.9%	48.8%	39.2%	44.5%

Table 9: Class distribution for the WebKB data set using six-class labels.

	Number of companies	
Sector	industry-yh	industry-pr
Basic Materials	104	83
Capital Goods	83	78
Conglomerates	14	13
Consumer Cyclical	99	94
Consumer NonCyclical	60	59
Energy	71	112
Financial	170	268
Healthcare	180	279
Services	444	478
Technology	505	609
Transportation	38	47
Utilities	30	69
Total	1798	2189
Base accuracy	28.1%	27.8%

Table 10: Class distribution for the industry-yh and industry-pr data sets.

sources and distributions of documents and different time periods (which correspond to different topic distributions).

INDUSTRY CLASSIFICATION (YH)

As part of a study of activity monitoring, Fawcett and Provost (1999) collected 22,170 business news stories from the web between 4/1/1999 and 8/4/1999. Following the study by Bernstein et al. (2003), we placed an edge between two companies if they appeared together in a story. The weight of an edge is the number of such cooccurrences found in the complete corpus. The resulting network comprises 1798 companies that cooccurred with at least one other company. To classify a company, we used Yahoo!'s 12 industry sectors. Table 10 shows the details of the class memberships.

INDUSTRY CLASSIFICATION (PR)

The second industry classification data set is based on 35,318 PR Newswire press releases gathered from April 1, 2003 through September 30, 2003. As above, the companies mentioned in each press release were extracted and an edge was placed between two companies if they appeared together in a press release. The weight of an edge is the number of such cooccurrences found in the complete corpus. The resulting network comprises 2189 companies that cooccurred with at least one other company. To classify a company, we use the same classification scheme from Yahoo! as before. Table 10 shows the details of the class memberships.

5.2 Experimental Methodology

NetKit allows for any combination of a local classifier (LC), a relational classifier (RC) and a collective inferencing method (CI). If we consider an LC-RC-CI configuration to be a complete *network-classification method*, we have 12 to compare on each data set. Since, for this paper, the local classifier component is directly tied to the collective inference component (our local classifier components determine priors based on which collective inference component is being used), we henceforth consider a network-classification method to be an RC-CI configuration.

We first verify that the network structure alone (linkages plus known class labels) often contains a considerable amount of useful information for entity classification. We vary from 10% to 90% the percentage of nodes in the network for which class membership is known initially.[18] The study assesses: (1) whether the network structure enables accurate classification; (2) how much prior information is needed in order to perform well, and (3) whether there are regular patterns of improvement across methods as the percentage of initially known labels increases.

Accuracy is averaged over 10 runs. Specifically, given a data set, $\mathbf{G} = (\mathbf{V}, \mathbf{E})$, the subset of entities with known labels $\mathbf{V}^K$ (the "training" data set[19]) is created by selecting a class-stratified random sample of $(100 \times r)\%$ of the entities in $\mathbf{V}$. The test set, $\mathbf{V}^U$, is then defined as $\mathbf{V} - \mathbf{V}^K$. We prune $\mathbf{V}^U$ by removing all nodes in *zero-knowledge* components—nodes for which there is no path to any node in $\mathbf{V}^K$. We use the same 10 training/test partitions for each network-classification method. Although it would be desirable to keep the test data disjoint (and therefore independent) as done in traditional machine learning via methods such as cross-validation, this is not applicable for within-network learning. We keep the test node sets disjoint as much as possible between the different runs. For example, at $r = 0.90$ (90% labeled data), our sets of training and testing nodes follow standard class-stratified 10-fold cross-validation.

5.3 Results

This section describes the results for our case study as well as follow-up experiments that clarify some of our findings. We start by verifying that there is information in the network structure alone (Section 5.3.1), then study the collective inference (Section 5.3.2) and relational classifier (Section 5.3.3) components separately, and then compare the network-classification methods (Section 5.3.4). We then revisit how edges were selected—we study the effects of badly chosen edges (Section 5.3.5) and then provide one method for automatic selection of edges (Section 5.3.6). We end in Section 5.3.7 with a discussion of the use of network-only methods as a baseline method that is as important as the standard non-relational-classifier baseline comparison.

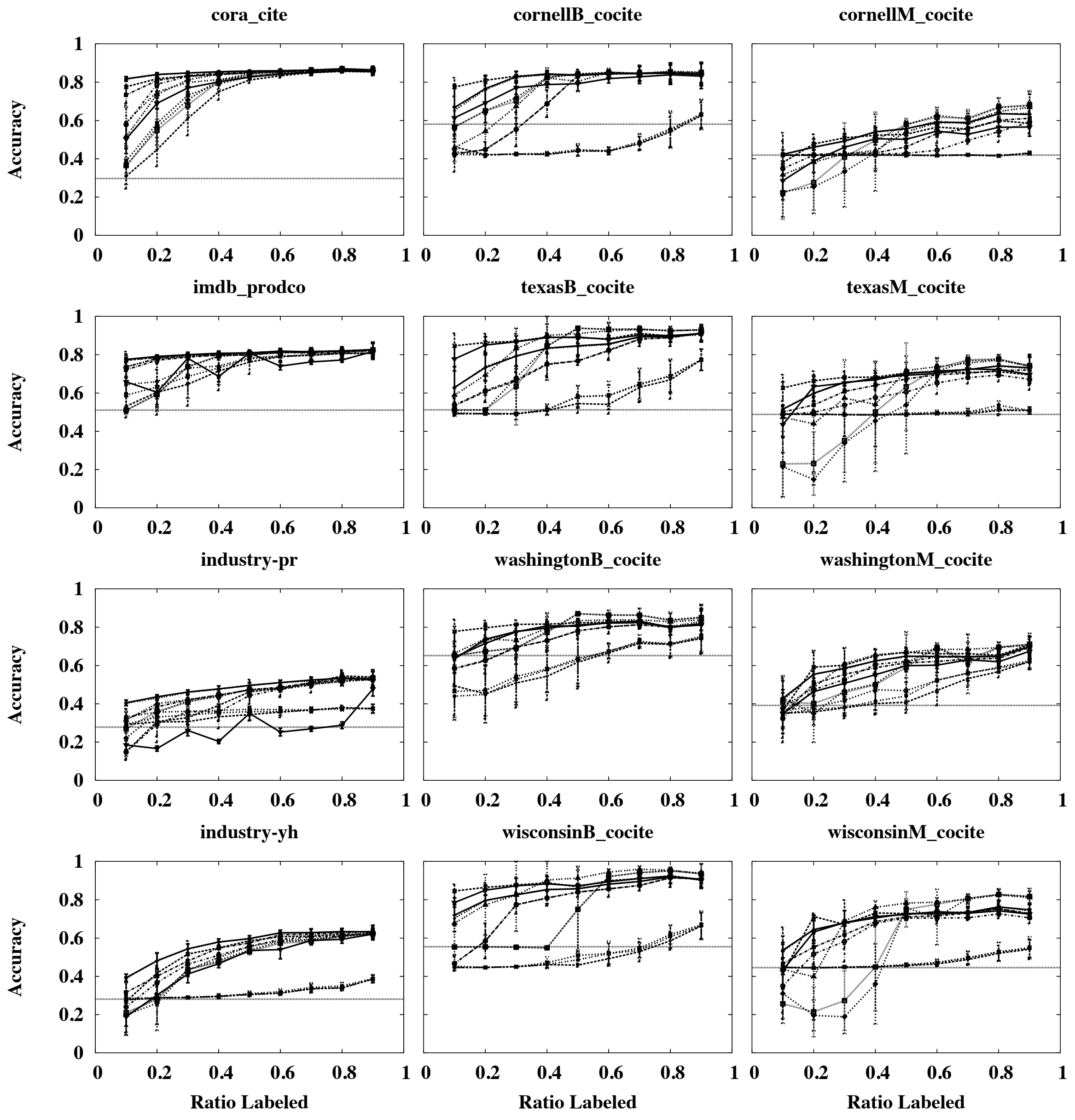


Figure 1: Overall classification accuracies on the twelve data sets. Horizontal lines represent predicting the most prevalent class. These graphs are shown to display trends and not to distinguish the twelve methods; individual methods will be clarified in subsequent discussion. The horizontal axis plots the fraction (r) of a network's nodes for which the class label is known. In each case, when many labels are known (right end) there is a set of methods that performs well. When few labels are known (left end) there is much more variation in performance. Data sets are tagged based on the edge-type used, where 'prodco' on the IMDb data is short for 'production company', and 'B' and 'M' in the WebKB data sets represent 'binary' and 'multi-class' respectively.

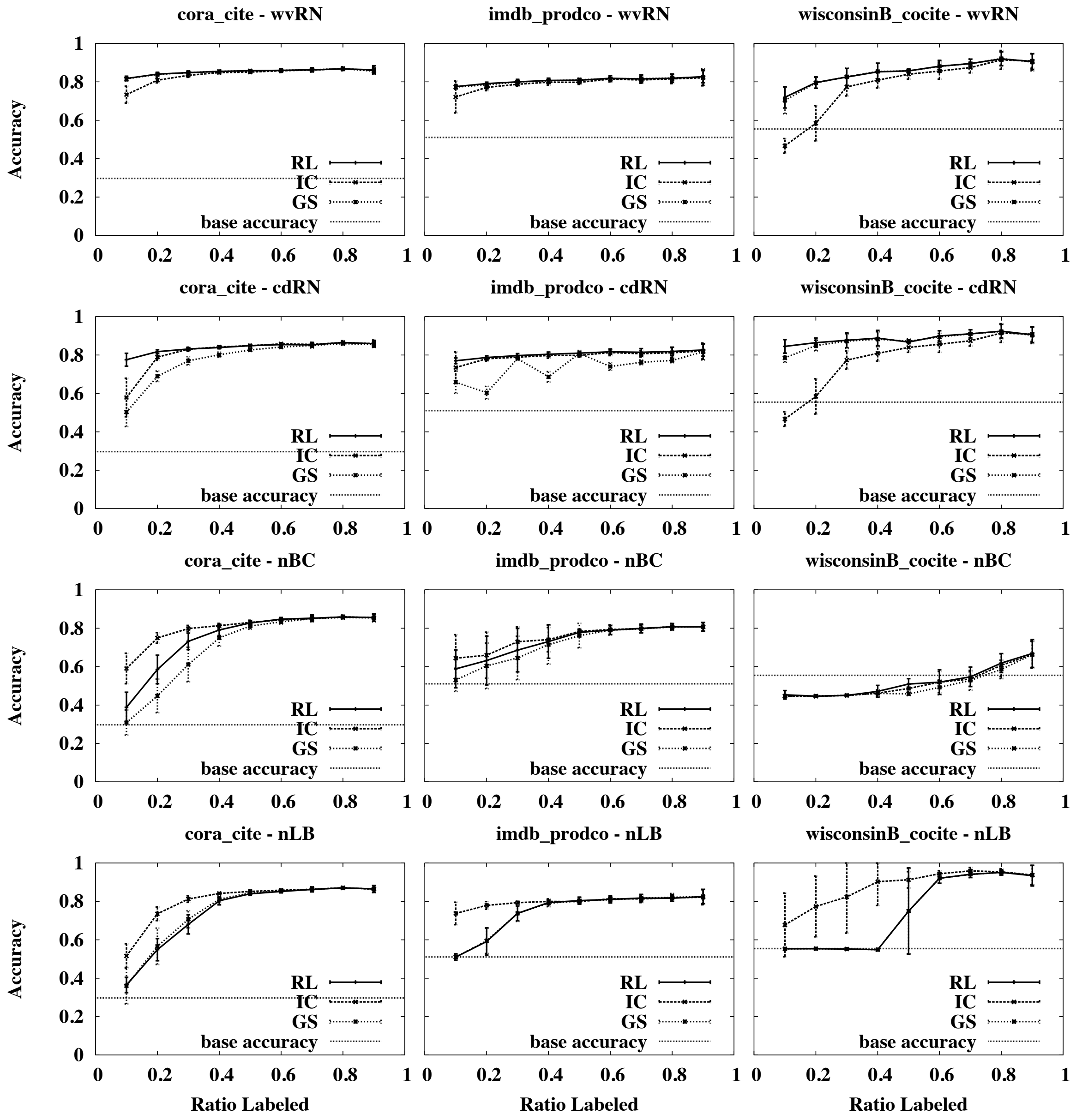


Figure 2: Comparison of collective inference methods on a few data sets. The three collective inference methods are relaxation labeling (RL), iterative classification (IC), and Gibbs sampling (GS). The data set and the relational classifier component are listed above each graph. The horizontal line represents predicting the most prevalent class.

5.3.1 INFORMATION IN THE NETWORK STRUCTURE

Figure 1 shows the accuracies of the 12 network-classification methods across the 12 data sets as the fraction (r) of entities for which class memberships are known increases from $r = 0.1$ to $r = 0.9$. The purpose of these graphs is not to differentiate the curves, but to compare the general trends and the levels of the accuracies to the baseline accuracies. In the univariate case, if the linkage structure is not known, the only non-subjective alternative is to estimate using the class base rate (prior), which is shown by the horizontal line in the graphs. As is clear from Figure 1, all of the data sets contain considerable information in the class-linkage structure. The worst relative performance is on industry-pr, where at the right end of the curves the error rate nonetheless is reduced by 30–40%. The best performance is on the binary-class WebKB-texas, where the best methods reduce the error rate by close to 90%. And in most cases, the better methods reduce the error rate by over 50% toward the right end of the curves.

Machine learning studies on networked data sets seldom have compared to simple network-classification methods like these, opting instead for comparing to non-relational classification. These results argue strongly that comparisons also should be made to univariate network classification, if the purpose is to demonstrate the power of a more sophisticated relational learning method. We return to this argument in Section 5.3.7.

5.3.2 COLLECTIVE INFERENCE COMPONENT

Figure 2 shows, for three of the data sets, the comparative performances of the three collective inference components. Each graph is for a particular relational classifier. The graphs show that while the three components often perform similarly, their performances are clearly separated for low values of r.

Table 11 shows the p-values for a Wilcoxon signed-rank test assessing whether the first method listed in column 1 is significantly better than the second. Specifically, for a given data set and label ratio (r), each network-classification experiment consists of 10 random train/test splits—the same for all configurations. For each pair of collective inference components, averaging the accuracies of the 10 splits across the 4 relational classifier components gives one average accuracy score for each of the 12 data sets yielding 12 paired data points for each collective inference method. The results show clearly that relaxation labeling, across the board, outperforms Gibbs sampling at $p \leq 0.01$ and that relaxation labeling is also better than iterative classification across the board. Further, we see that iterative classification and Gibbs sampling are roughly comparable.

The foregoing gives some evidence that relaxation labeling is consistently better than iterative classification and Gibbs sampling when the results are pooled, especially at low values of r. Table 12 quantifies the differences. In order to be comparable across data sets with different base rates, the table shows the amount of error reduction over the base rate. As a simple example, assume the base error rate is 0.4, method A yields an error rate of 0.1, and method B yields an error rate of 0.2. Method A reduces the error by 75%. Method B reduces the error by 50%.

18. We also performed boundary experiments using the weighted-vote relational neighbor classifier with relaxation labeling, where we decreased the number of initially known labels down to 0.1% of the graph. The classification accuracy generally degrades gracefully to doing no better than random guessing at this extreme.
19. These data will be used not only for training models, but also as existing background knowledge during classification.

	sample ratio (r)								
	0.10	0.20	0.30	0.40	0.50	0.60	0.70	0.80	0.90
RL v *GS*	**0.002**	**0.001**	**0.001**	**0.001**	**0.002**	**0.001**	**0.001**	**0.010**	**0.010**
RL v *IC*	**0.025**	**0.100**	**0.100**	**0.025**	**0.002**	**0.002**	**0.001**	**0.005**	**0.002**
IC v *GS*	*0.400*	**0.450**	—	**0.450**	*0.400*	—	*0.250*	—	**0.400**

Table 11: p-values for the Wilcoxon signed-rank test, comparing the accuracies of pairs of three collective inference methods across all data sets and relational classifier methods. (The three collective inference methods are relaxation labeling (RL), iterative classification (IC), and Gibbs sampling (GS)). For each cell, bold text means that the first method was better than the second method and italics means it was worse. The cells with '—' means there was no significant difference.

	sample ratio (r)									
	0.10	0.20	0.30	0.40	0.50	0.60	0.70	0.80	0.90	**overall**
RL	**0.081**	**0.184**	**0.262**	**0.339**	**0.409**	**0.446**	**0.468**	**0.491**	**0.509**	**0.354**
IC	0.000	0.116	0.235	0.314	0.382	0.423	0.452	0.482	0.503	0.323
GS	0.029	0.126	0.231	0.301	0.385	0.421	0.450	0.474	0.502	0.324

Table 12: Relative error reductions (ER_{REL}) for each collective inference method across all data sets and relational classifier methods. (The three collective inference methods are relaxation labeling (RL), iterative classification (IC), and Gibbs sampling (GS)). The last column, **overall**, is the average error reduction for each method across all sample ratios. Bold entries indicate the largest relative error reduction for each sample ratio.

	sample ratio (r)									
	0.10	0.20	0.30	0.40	0.50	0.60	0.70	0.80	0.90	**total**
RL	11	11	10	7	4	5	6	4	6	64
GS	1	1	0	1	5	3	4	4	4	23
IC	0	0	2	4	3	4	2	4	2	21

Table 13: Number of times each collective inference method was the best across the 12 data sets. The three methods are relaxation labeling (RL), iterative classification (IC), and Gibbs sampling (GS).

The relative error reduction of the collective inference (CI) components is defined as follows:

$$\begin{aligned}
\mathrm{ER}_{\mathrm{ABS}}(\mathrm{RC},\mathrm{CI},D,r) &= (\mathrm{base\_err}(D) - \mathrm{err}(\mathrm{RC\text{-}CI},D,r)),\\
\mathrm{ER}_{\mathrm{REL}}(\mathrm{RC},\mathrm{CI},D,r) &= \frac{\mathrm{ER}_{\mathrm{ABS}}(\mathrm{RC},\mathrm{CI},D,r)}{\mathrm{base\_err}(D)},\\
\mathrm{ER}_{\mathrm{REL}}(\mathrm{RC},\mathrm{CI},r) &= \frac{1}{|\mathbf{D}|}\sum_{D\in\mathbf{D}} \mathrm{ER}_{\mathrm{REL}}(\mathrm{RC},\mathrm{CI},D,r),\\
\mathrm{ER}_{\mathrm{REL}}(\mathrm{CI},r) &= \frac{1}{|\mathbf{RC}|}\sum_{\mathrm{RC}\in\mathbf{RC}} \mathrm{ER}_{\mathrm{REL}}(\mathrm{RC},\mathrm{CI},r),
\end{aligned}$$

where err(RC-CI,D,r) is the error for the RC-CI configuration (a relational classifier paired with a collective inference method) on data set D with r% of the graph being labeled.

Table 12 shows the relative error reductions for each collective inference component. Relaxation labeling outperformed iterative classification across the board, from as low as a 1.3% improvement ($r = 0.90$) to as high as 59% or better improvement ($r \leq 0.2$) when averaged over all the data sets and relational classifier methods. Overall relaxation labeling improved performance over iterative classification by about 10% as seen in the last column. Notably, relaxation labeling's advantage over iterative classification improves monotonically as less is known in the network. Similar numbers and a similar pattern are seen for relaxation labeling versus Gibbs sampling. Iterative classification and Gibbs sampling are comparable.

For another perspective, Table 13 shows, for each ratio as well as a total across all ratios, the number of times each collective inference implementation took part in the best-performing network-classification combination for each of the 12 data sets. Specifically, for each sampling ratio, each win for an RC-CI configuration (relational classifier paired with a collective inference method) counted as a win for the collective inference module of the pair (as well as a win for the relational classifier module in the next section). For example, in Figure 2, the first column of four graphs shows the performances of the 12 network-classification combinations on the cora data; at the left end of the curves, wvRN-RL is the best performing combination. Table 13 adds further support to the conclusion that relaxation labeling was the overall best component, primarily due to its advantage at low values of r. We also see again that Gibbs sampling and iterative classification were comparable.

5.3.3 RELATIONAL CLASSIFIER COMPONENT

Comparing relational models, we would expect to see a certain pattern: if even moderate homophily is present in the data, we would expect wvRN to perform well. Its nonexistent training variance[20] should allow it to perform relatively well, even with small numbers of known labels in the network. The higher-variance nLB may perform relatively poorly with small numbers of known labels (primarily because of the lack of training data). On the other hand, wvRN is potentially a very-high-bias classifier—it does not learn a relational model at all. The learning-based classifiers may well perform better with large numbers of known labels if there are patterns beyond homophily to be learned. As a worst case for wvRN, consider a bipartite graph between two classes. In a leave-one-out cross-validation, wvRN would be wrong on every prediction. The relational learners should notice the true pattern immediately. More generally, one should expect a pattern of curves crossing with increasing numbers of known labels, similar to learning curves crossing (Perlich et al., 2003): lower variance methods (such as wvRN) should be preferable with fewer known labels; more flexible learning methods should be preferable with more known labels (thus, more training data).

Figure 3 shows for four of the data sets the performances of the four relational classifier implementations. The rows of graphs correspond to data sets and the columns to the three different collective inference methods. The graphs show several things. As would be expected, accuracy improves as more of the network is labeled, although in certain cases classification is remarkably accurate with very few known labels (e.g., see cora). One method is substantially worse than the others. Among the remaining methods, performance often differs greatly with few known labels, and tends to converge with many known labels. More subtly, as expected there often is a crossing of curves when about half the nodes are labeled (e.g., see Washington).

20. There still will be variance due to the set of known labels.

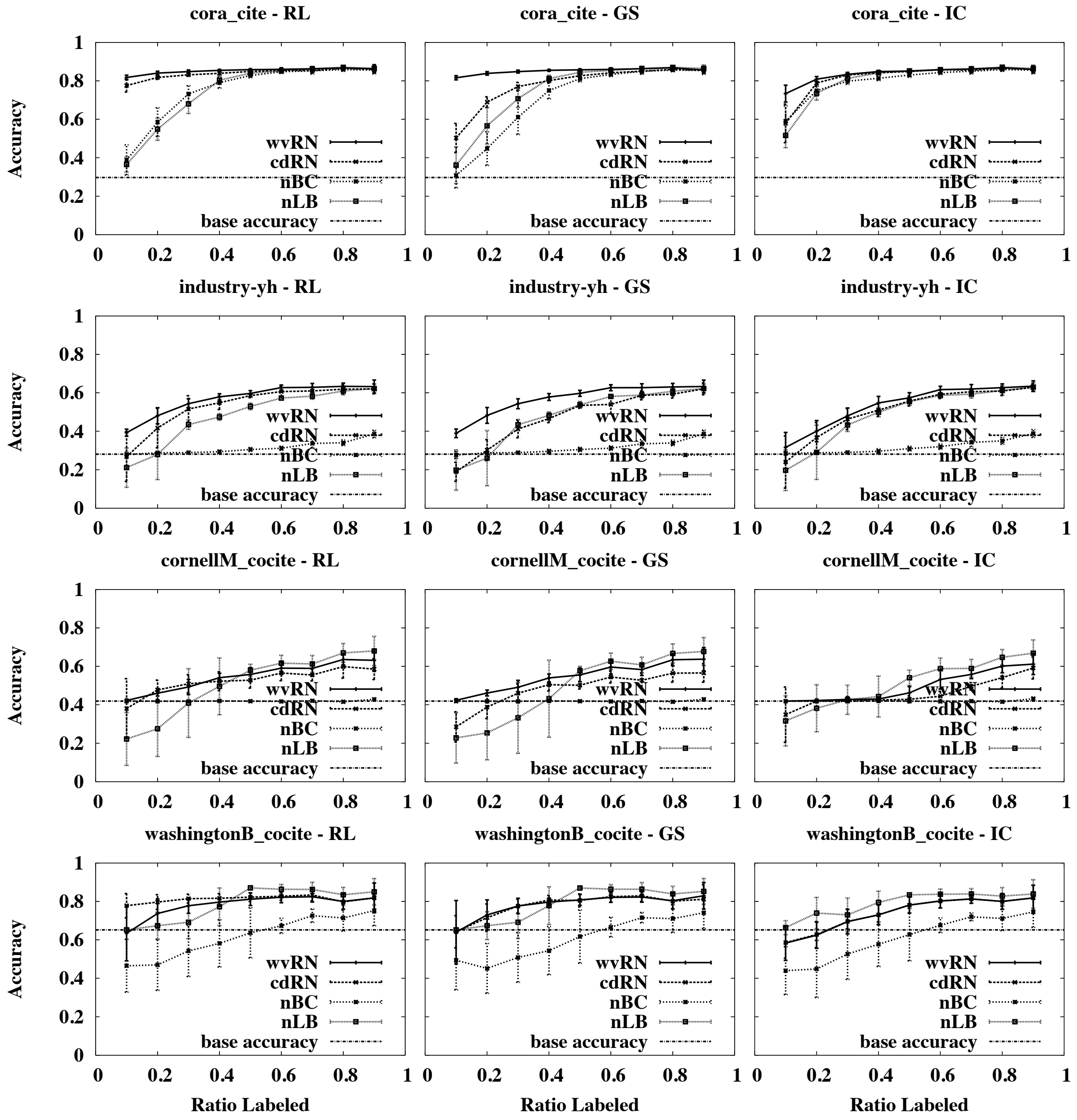


Figure 3: Comparison of the relational classifiers on a few data sets. The data set (and link-type) and the paired collective inference component are listed above each graph. (The three collective inference methods are relaxation labeling (RL), iterative classification (IC), and Gibbs sampling (GS)). The horizontal line represents predicting the most prevalent class.

	sample ratio (r)								
	0.10	0.20	0.30	0.40	0.50	0.60	0.70	0.80	0.90
wvRN v *cdRN*	**0.025**	**0.200**	**0.050**	**0.100**	**0.025**	**0.025**	**0.010**	**0.002**	**0.001**
wvRN v *nBC*	**0.001**	**0.001**	**0.001**	**0.001**	**0.001**	**0.001**	**0.001**	**0.001**	**0.001**
wvRN v *nLB*	**0.001**	**0.001**	**0.001**	**0.005**	*0.400*	*0.005*	*0.002*	*0.001*	*0.001*
cdRN v *nBC*	**0.050**	**0.001**	**0.001**	**0.001**	**0.001**	**0.001**	**0.001**	**0.001**	**0.001**
cdRN v *nLB*	**0.010**	**0.001**	**0.010**	**0.200**	*0.050*	*0.001*	*0.001*	*0.001*	*0.001*
nLB v *nBC*	—	**0.200**	**0.001**	**0.001**	**0.001**	**0.001**	**0.001**	**0.001**	**0.001**

Table 14: p-values for the Wilcoxon signed-rank test, comparing the accuracies between pairs of relational classifiers across all data sets and collective inference methods. For each cell, bold text means that the first method was better than the second method and italic text means it was worse. The cells with '—' showed no significant difference.

	sample ratio (r)									
	0.10	0.20	0.30	0.40	0.50	0.60	0.70	0.80	0.90	**overall**
cdRN	0.106	0.273	0.370	0.423	0.474	0.496	0.519	0.533	0.549	0.416
nLB	−0.049	0.039	0.206	0.354	**0.508**	**0.573**	**0.587**	**0.609**	**0.609**	0.382
wvRN	**0.157**	**0.299**	**0.392**	**0.453**	0.494	0.525	0.543	0.563	0.571	**0.444**

Table 15: Relative error reductions (ER_{REL}) for each relational classifier component across all data sets. Each cell shows the error reduction of the given method. The last column, **overall**, is the average error reduction for the methods across all sample ratios. Bold entries indicate the largest relative error reduction for each sample ratio.

	sample ratio (r)									
	0.10	0.20	0.30	0.40	0.50	0.60	0.70	0.80	0.90	**total**
wvRN	7	4	4	6	4	4	2	1	2	34
cdRN	5	8	6	2	1	0	0	1	1	24
nLB	0	0	2	4	7	8	10	10	9	50

Table 16: Number of times each relational classifier implementation was the best across the 12 data sets.

Table 14 shows statistical significance results, computed as described in the previous section (except here varying the relational classifier component). nBC was almost always significantly and often substantially worse than the other three relational classifiers and therefore for clarity is eliminated from the remainder of this analysis. Although cdRN and wvRN were close, wvRN was generally better than cdRN. Examining the wvRN and cdRN methods versus nLB we see the same pattern: at $r = 0.5$, the advantage shifts from the wvRN/cdRN methods to nLB, consistent with our expectations discussed above.

Table 15 shows the error reductions for each relational classifier comparison, computed as in the previous section with the obvious changes between relational classifier and collective inference.

The same patterns are evident as observed from Table 14. Further, we see that the differences can be large: when the wvRN/cdRN methods are better, they often are much better. The link-based (nLB) classifier also can be considerably better than wvRN/cdRN.

Table 16 shows how often each relational classifier method participated in the best combination, as described in the previous section. nLB is the overall winner, but we see the same clear pattern that the wvRN/cdRN methods dominate for fewer labels, and nLB dominates for more labels, with the advantage changing hands at $r = 0.5$.

5.3.4 INTERACTION BETWEEN COMPONENTS

Table 17 shows how many times each of the 9 individual relational classifier/collective inference (RC-CI) configurations was the best, across the 12 data sets and 9 labeling ratios.[21] Strikingly, two sets of closely related configurations stand out: wvRN-RL and cdRN-RL; and nLB with any of the collective inference methods. The wvRN-RL/cdRN-RL methods dominate for $r < 0.5$; the nLB methods (nLB paired with any collective inference method) dominate for $r \geq 0.5$. Table 18 and Table 19 compare these five methods analogously to the previous sections. (As before, each cell comprises 12 data points, each being an average accuracy of one data set over 10 repetitions.) The clear pattern is in line with that shown in the prior sections, showing that of this set of best methods, the wvRN/cdRN methods excel for fewer labeled data, and the nLB-based method excels for more labeled data.

In addition, these results show that the wvRN-/cdRN-methods clearly should be paired with relaxation labeling, possibly because RL allows them to average estimates between zero and one, resulting in lower variance, especially with few known labels. nLB, on the other hand, does not favor one collective inference method over the others.

Following up on these results, a 2-way ANOVA shows a strong interaction between the relational classifier and collective inference components for most data sets for small numbers of labeled nodes, as would be expected given the strong performance of the specific pairings wvRN-RL and cdRN-RL. As more nodes are labeled, the interaction becomes insignificant for almost all data sets, as might be expected given that nLB dominates but no collective inference method does. The ANOVA adds weight to the conclusion that for very many known labels, it matters little which collective inference method is used for accuracy maximization, so perhaps the most efficient method can be chosen.

5.3.5 THE IMPORTANCE OF EDGE SELECTION

To create homogeneous graphs, we had to select the edges to use. As mentioned briefly above, the type of edge selected can have a substantial impact on classification accuracy. For these data sets, the worst case (we have found) occurs for WebKB. As described in Section 5.1.3, for the results presented so far we have used co-citation links, based on observations in prior published work. An obvious alternative is to use the hyperlinks themselves.

Figures 4 and 5 compare the results using hyperlinks with those using co-citation links. Using hyperlinks, the network-classification methods perform much worse than with co-citations. Although there is some lift at large values of r, especially for the Washington data, the performance is not comparable to that with the co-citation formulation. The transformation from the hyperlink-

21. As mentioned before, we are no longer including nBC in the comparisons. As it turns out, nBC did not have any wins, regardless of the collective inference method it was paired with.

	sample ratio (r)									
	0.10	0.20	0.30	0.40	0.50	0.60	0.70	0.80	0.90	**total**
wvRN-IC	0	0	0	0	0	0	0	0	1	1
wvRN-GS	1	1	0	1	3	0	0	0	0	6
wvRN-RL	6	3	4	5	1	4	2	1	1	27
cdRN-IC	0	0	0	0	0	0	0	0	0	0
cdRN-GS	0	0	0	0	0	0	0	0	0	0
cdRN-RL	5	8	6	2	1	0	0	1	1	24
nLB-IC	0	0	2	4	3	4	2	4	1	20
nLB-GS	0	0	0	0	2	3	4	4	4	17
nLB-RL	0	0	0	0	2	1	4	2	4	13

Table 17: Number of times each relational classifier and collective inference configuration was the best across the 12 data sets. The three collective inference methods are relaxation labeling (RL), iterative classification (IC), and Gibbs sampling (GS).

	sample ratio (r)								
	0.10	0.20	0.30	0.40	0.50	0.60	0.70	0.80	0.90
wvRN-RL v *cdRN-RL*	*0.450*	*0.200*	*0.250*	*0.400*	—	**0.450**	**0.400**	**0.200**	**0.100**
wvRN-RL v *nLB-GS*	**0.010**	**0.010**	**0.010**	**0.010**	**0.300**	*0.250*	*0.100*	*0.025*	*0.025*
wvRN-RL v *nLB-IC*	**0.010**	**0.010**	**0.050**	**0.300**	*0.300*	*0.200*	*0.200*	*0.050*	*0.025*
wvRN-RL v *nLB-RL*	**0.010**	**0.010**	**0.010**	**0.010**	**0.250**	*0.200*	*0.100*	*0.025*	*0.020*
cdRN-RL v *nLB-GS*	**0.010**	**0.010**	**0.010**	**0.020**	**0.400**	*0.200*	*0.100*	*0.050*	*0.025*
cdRN-RL v *nLB-IC*	**0.050**	**0.020**	**0.050**	**0.300**	*0.200*	*0.025*	*0.050*	*0.025*	*0.025*
cdRN-RL v *nLB-RL*	**0.010**	**0.010**	**0.010**	**0.025**	**0.400**	*0.050*	*0.100*	*0.025*	*0.020*
nLB-IC v *nLB-GS*	**0.050**	**0.010**	**0.020**	**0.010**	**0.400**	**0.400**	*0.300*	*0.300*	*0.400*
nLB-IC v *nLB-RL*	**0.050**	**0.025**	**0.020**	**0.025**	**0.400**	**0.400**	*0.250*	*0.200*	*0.100*
nLB-RL v *nLB-GS*	**0.450**	**0.100**	—	**0.300**	*0.200*	**0.400**	**0.200**	**0.300**	**0.100**

Table 18: p-values for the Wilcoxon signed-rank test, comparing the accuracies among the five best relational classifier/collective inference configurations across all data sets. (The three collective inference methods are relaxation labeling (RL), iterative classification (IC), and Gibbs sampling (GS)). For each cell, bold text means that the first method was better than the second method and italic text means it was worse. The cells with '—' showed no significant difference.

	sample ratio (r)									
	0.10	0.20	0.30	0.40	0.50	0.60	0.70	0.80	0.90	**overall**
wvRN-RL	0.222	0.369	0.444	0.489	0.514	0.537	0.551	0.568	0.573	0.474
cdRN-RL	**0.274**	**0.430**	**0.462**	**0.501**	0.519	0.538	0.549	0.556	0.558	**0.488**
nLB-RL	−0.101	−0.024	0.131	0.311	0.499	**0.577**	**0.590**	**0.611**	**0.612**	0.356
nLB-IC	0.054	0.191	0.367	0.468	**0.535**	0.575	0.587	0.606	0.606	0.443
nLB-GS	−0.100	−0.051	0.121	0.284	0.489	0.567	0.585	**0.611**	0.610	0.346

Table 19: Relative error reduction (ER_{REL}) improvements for the 5 best relational classifier/collective inference configurations across all data sets. (The three collective inference methods are relaxation labeling (RL), iterative classification (IC), and Gibbs sampling (GS)). Each cell shows the error reduction of the given method. The last column, **overall**, is the average error reduction for the methods across all sample ratios. Bold entries indicate the largest relative error reduction for each sample ratio.

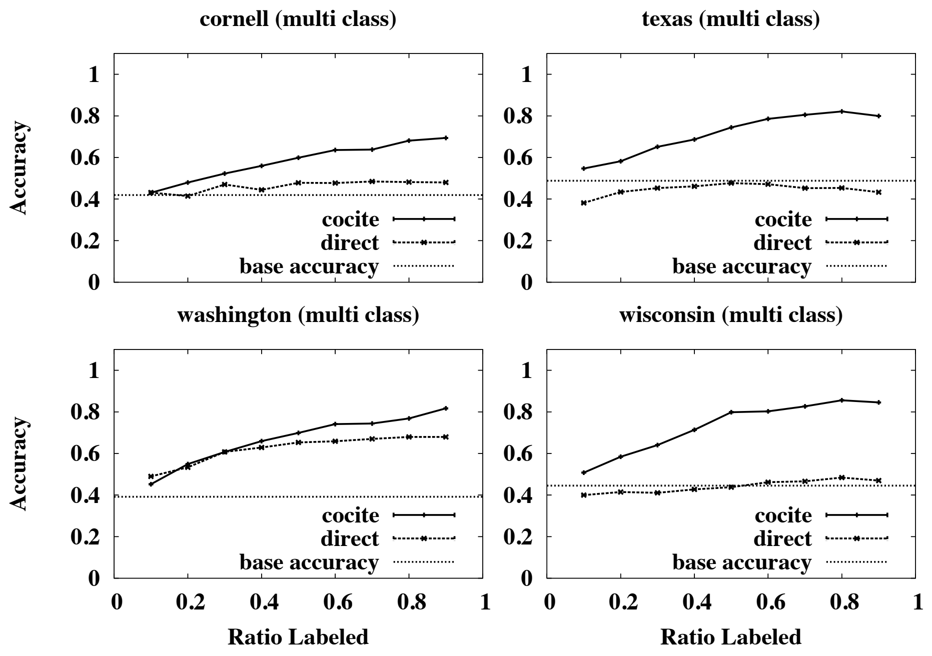


Figure 4: Comparative performances on WebKB multi-class problems using co-citation links versus using direct hyperlinks as edges. We show here the average performance of the 12 network learners.

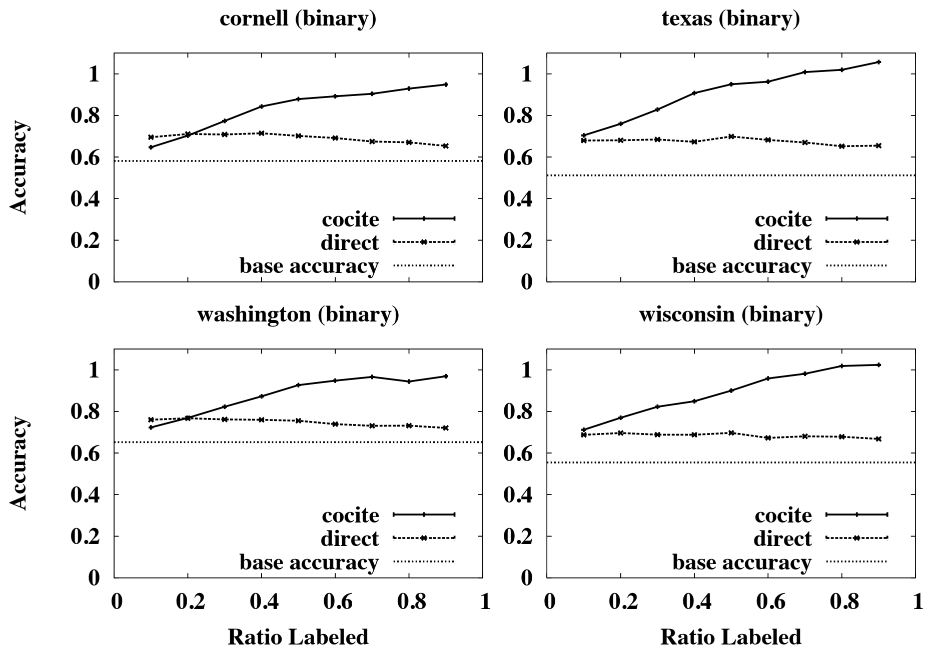


Figure 5: Comparative performances on WebKB binary-class problems using co-citation links versus using direct hyperlinks as edges. We show here the average performance of the 12 network learners.

based network to the co-citation-based network adds no new information to the graph. However, in the hyperlink formulation the network classification methods cannot take full advantage of the information present—mainly because of the stark violation of the first-order Markov assumption made by the relational classifiers. These results demonstrate that the choice of edges can be crucial for good performance.

5.3.6 AUTOMATIC EDGE SELECTION

Creating a graph with a single type of edge from a problem where various possible links exist is a representation engineering problem reminiscent of the selection of a small set of useful features for traditional classification.[22] For feature selection, practitioners use a combination of domain knowledge, analysis, and trial and error to select a good representation. To create the networked data for our study, we chose edges based on suggestions from prior work—which indirectly combines domain knowledge, prior analysis and prior trial and error, although we explicitly avoided choosing the representations based on their performance using NetKit.

Pursuing the analogy with choosing features, it may be possible to select edges automatically. It is beyond the scope of this paper to address the general (open and important) problem of edge selection; however, the excellence (on these data sets) and simplicity of wvRN suggests straightforward techniques.

If we consider the data sets used in the study, all but the industry classification data sets have more than one reasonable choice for defining the edges:

1. **cora**: We linked entities through citations (*cite*). Alternatively, we could have linked by the sharing of an author (*author*), or by either relationship (combined as a single generic link).

2. **imdb**: There are many types of ways to connect two movies, but we focus here on four that were suggested to us by David Jensen: *actor*, *director*, *producer* and production company (*prodco*). Again, we could use any or all of them (we do not consider all possible combinations here).

3. **WebKB**: Based on prior work, we chose co-citations (*cocite*) for the case study and later showed that the original hyperlinks (*hyper*) were a poor choice.

Kohavi and John (1997) differentiate between wrapper approaches and filter approaches to feature selection, and this notion extends directly to edge selection. For any network classification method we can take a wrapper approach, computing the error reduction over $\mathbf{G}^K$ using cross-validation. wvRN is an attractive candidate for such an approach, because it is very fast and requires no training; we can use a simple leave-one-out (loo) estimation.

The homophily-based wvRN also lends itself to a filter approach, selecting the edge type simply by measuring the homophily in $\mathbf{G}^K$. Heckathorn and Jeffri (2003) define a homophily index, but it computes homophily for a specific group, or class, rather than a general value across all classes. The *assortativity coefficient* (Newman, 2003) is based on the correlation between the classes linked by edges in a graph. Specifically, it is based on the graph's assortativity matrix—a CxC matrix, where

22. We required a single edge type for our homogeneous case study; it is reasonable to conjecture that even if heterogeneous links are allowed, a small set of good links would be preferable. For example, a link-based classifier produces a feature-vector representation with multiple positions per link type.

cell e_{ij} represents the fraction of (all) edges that link nodes of class c_i to nodes of class c_j, such that $\sum_{ij} e_{ij} = 1$. The assortativity coefficient, A_E, is calculated as follows:

$$\begin{aligned} a_i &= \sum_j e_{ij}, \\ b_j &= \sum_i e_{ij}, \\ A_E &= \frac{\sum_i e_{ii} - \sum_i a_i \cdot b_i}{1 - \sum_i a_i \cdot b_i}. \end{aligned}$$

However, A_E measures homophily across edges, while wvRN is based on homophily across nodes. It is possible to create (sometimes weird) graphs with high A_E but for which wvRN performs poorly, and vice versa. However, we can modify A_E to be a *node-based assortativity* coefficient, A_N, by defining e^*_{ij}, a node-based cell-value in the assortativity matrix as follows:

$$e^*_{ij} = \frac{1}{Z}\mathrm{RV}(X_i)_j,$$

where $\mathrm{RV}(X_i)_j$ is the j^{th} element in $\mathrm{RV}(X_i)$ as defined in Equation 2, and Z is a normalizing constant such that all e_{ij} sum to 1.

To assess their value for edge selection for wvRN, we compute the actual error reduction for each different edge type (and all edges) for the benchmark data sets, and compare with the edge selected by each of these three methods (loo, A_E, A_N). In Table 20 the first six columns show the data set, the number of nodes, the base accuracy, the number of edges, the average edge weight, and the average node degree. The next columns show A_E and A_N. The following column shows the estimated $\widehat{\mathrm{ER}}_{\mathrm{REL}}$ based on the leave-one-out estimation, and the last column shows the $\mathrm{ER}_{\mathrm{REL}}$ values on the test set. Each data set group is sorted by the $\mathrm{ER}_{\mathrm{REL}}$ performance on its various edge types, so the top row of each group is the "best" edge selection. Note that as the edge types differ, we get different connectivities and different coverages, and hence different the values are not completely comparable.

The results show that the links used in our study generally resulted in the highest node-based assortativity.[23] In 8 out of 10 cases, A_N chose the best edge. Neither the leave-one-out (loo) method nor A_E performed as well, but they nevertheless yield networks on which wvRN performs relatively well. Notice that for IMDb, although director has the highest A_E, it also has very low coverage (only 554 nodes were connected), and with such a slight difference in assortativity between that and prodco there should be no question which should be used for classification. A_N and the leave-one-out estimates are much more volatile than A_E as the amount of labeled data decreases, because typically there are many more edges than nodes. If we believe that assortativity is relatively stable across the network, it may be beneficial to use A_E when little is known. However, for our data sets, A_N performs just as well as A_E even when $r = 0.1$.

In summary, these results show that the differences in the results by domain, and even within domains, depend on the level of homophily. This is almost tautological for wvRN. We also computed many other graph statistics besides the homophily measures (e.g., average degree, number of connected clusters, graph diameter, shortest paths, etc.) none of which were as strongly correlated with performance.

23. We had picked the edge types for the study before performing this analysis. However, common sense and domain knowledge would lead one to conclude that the edge types we used in the case study would have high assortativity.

				mean	mean	Assortativity		$\widehat{\text{ER}}_{\text{REL}}$	ER_{REL}
		base	num	edge	node	(edge)	(node)	loo (wvRN)	wvRN at
Data set	size	acc.	edges	weight	degree	A_E	A_N	$r = 0.90$	$r = 0.90$
$\text{cora}_{\text{cite}}$	3583	0.297	22516	2.061	6.284	**0.737**	0.642	0.5373	0.805
cora_{all}	4025	0.315	71824	2.418	17.844	0.656	**0.656**	**0.6122**	0.767
$\text{cora}_{\text{author}}$	3604	0.317	56268	2.262	15.613	0.623	0.558	0.4662	0.711
$\text{imdb}_{\text{prodco}}$	1169	0.511	40634	1.077	34.760	0.501	**0.392**	**0.3711**	0.647
$\text{imdb}_{\text{producers}}$	1195	0.520	13148	1.598	11.003	0.283	0.389	0.3618	0.547
imdb_{all}	1377	0.564	92248	1.307	66.992	0.279	0.308	0.3415	0.531
$\text{imdb}_{\text{directors}}$	554	0.549	826	1.031	1.491	**0.503**	0.210	0.0369	0.498
$\text{imdb}_{\text{actors}}$	1285	0.541	48354	1.135	37.630	0.131	0.174	0.1372	0.246
$\text{cornellB}_{\text{all}}$	349	0.585	27539	3.000	78.908	0.325	**0.399**	**0.5655**	0.629
$\text{cornellB}_{\text{cocite}}$	346	0.581	26832	2.974	77.549	**0.360**	0.394	0.5345	0.618
$\text{cornellB}_{\text{hyper}}$	349	0.585	1393	2.349	3.991	−0.169	−0.068	−0.1621	−0.114
$\text{cornellM}_{\text{all}}$	349	0.415	27539	3.000	78.908	0.219	**0.286**	**0.3209**	0.382
$\text{cornellM}_{\text{cocite}}$	346	0.419	26832	2.974	77.549	**0.227**	0.273	0.2481	0.366
$\text{cornellM}_{\text{hyper}}$	349	0.415	1393	2.349	3.991	0.054	0.102	−0.2883	−0.212
$\text{texasB}_{\text{cocite}}$	334	0.512	32988	2.961	98.766	**0.577**	**0.617**	**0.7166**	0.819
$\text{texasB}_{\text{all}}$	338	0.518	33364	2.995	98.710	0.523	0.585	0.6939	0.768
$\text{texasB}_{\text{hyper}}$	285	0.547	1001	2.605	3.512	−0.179	−0.114	−0.1368	−0.232
$\text{texasM}_{\text{cocite}}$	334	0.488	32988	2.961	98.766	**0.461**	**0.477**	0.3737	0.475
$\text{texasM}_{\text{all}}$	338	0.482	33364	2.995	98.710	0.420	0.458	**0.3874**	0.466
$\text{texasM}_{\text{hyper}}$	285	0.453	1001	2.605	3.512	−0.033	−0.044	−0.6583	−0.490
$\text{washingtonB}_{\text{all}}$	434	0.652	31253	3.800	72.012	**0.388**	**0.455**	**0.4225**	0.530
$\text{washingtonB}_{\text{cocite}}$	434	0.652	30462	3.773	70.189	0.375	0.446	0.3940	0.477
$\text{washingtonB}_{\text{hyper}}$	433	0.651	1941	2.374	4.483	−0.095	0.076	−0.1126	−0.069
$\text{washingtonM}_{\text{cocite}}$	434	0.392	30462	3.773	70.189	0.301	0.359	0.3481	0.503
$\text{washingtonM}_{\text{all}}$	434	0.392	31253	3.800	72.012	**0.331**	**0.377**	**0.4023**	0.453
$\text{washingtonM}_{\text{hyper}}$	433	0.390	1941	2.374	4.483	0.084	0.233	−0.0167	0.004
$\text{wisconsinB}_{\text{all}}$	352	0.560	33587	3.543	95.418	0.524	**0.587**	**0.7219**	0.855
$\text{wisconsinB}_{\text{cocite}}$	348	0.555	33250	3.499	95.546	**0.673**	0.585	0.7168	0.788
$\text{wisconsinB}_{\text{hyper}}$	297	0.616	1152	2.500	3.879	−0.147	−0.103	−0.2123	−0.331
$\text{wisconsinM}_{\text{cocite}}$	348	0.445	33250	3.499	95.546	**0.577**	**0.489**	0.4286	0.544
$\text{wisconsinM}_{\text{all}}$	352	0.440	33587	3.543	95.418	0.416	0.474	**0.4518**	0.503
$\text{wisconsinM}_{\text{hyper}}$	297	0.384	1152	2.500	3.879	0.160	0.021	−0.4729	−0.275
# mistakes						5	2	4	

Table 20: Graph metrics for networks formed by various edge types. Each data set grouping is sorted on ER_{REL}. A_E, A_N, $\widehat{\text{ER}}_{\text{REL}}$ and ER_{REL} values were all averaged over the 10 data splits used throughout the case study. The leave-one-out (loo) measure used only $\mathbf{G}^K$ to calculate the $\widehat{\text{ER}}_{\text{REL}}$ value.

5.3.7 NETWORK-ONLY CLASSIFICATION AS A BASELINE FOR RELATIONAL LEARNING STUDIES

The foregoing results support the claim that network-only classification should be used as a baseline against which more sophisticated network-classification methods should be compared. Therefore, for example, when evaluating a system for the classification of interconnected web pages, their connectivity alone should be considered in addition to their text alone. This of course is sound scientific methodology, requiring one to look for simpler explanations for a phenomenon once a complex explanation has been found. When considering a sophisticated relational learning method on networked data, using the network alone is one sort of lesion or ablation study (Langley, 2000). Our point here is that the absolute classification performance based only on the network of class labels is remarkable in several of the cases examined above. For example, who would have thought that on the University of Texas student/not-student classification task, accuracy could be increased from 62.9% to 91.2% using just the network structure—with no text and no learning?

Nevertheless, it is enlightening to compare these simple methods to alternatives. In this section we provide several such comparisons. We compare to text-only methods and to a relational learning technique that uses both local and relational information, and we see that one might be led to be overly optimistic by comparing solely to local-only baselines. We also compare to a graph-based method that does not fall into the "node-centric" framework. Finally, we replicate a prior, published study, showing that conclusions would have changed if a network-only baseline had been used.

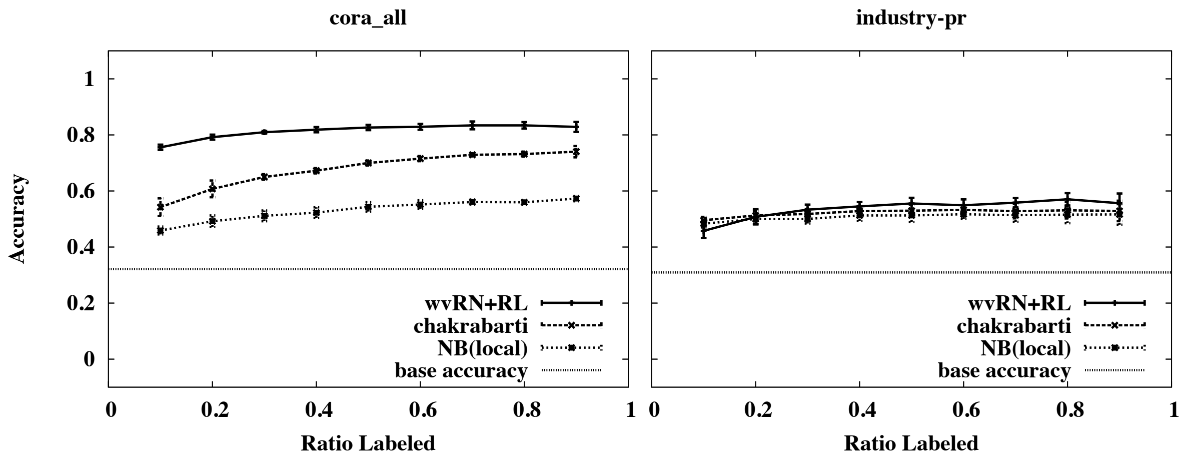
COMPARISON TO A MULTIVARIATE TECHNIQUE

In real networks, the amount of local information and its relevance to the classification task vary widely. In certain social network classification applications, for example in support of counterterrorism, no information at all may be available about certain individuals other than their connections to others (Tumulty, 2006). In applications such as fraud detection in telecommunications little reliable information may be available about potential fraudsters, beyond the calls they make (or as discussed above, local information may be ignored for many individuals because network-only classification works so well). On the other hand, the text of certain web pages contains a wealth of information relevant for classifying the topic of the web page.

For determining how much better can be done by using both the text and the interconnectivity information, even for existing techniques and benchmark data sets, a definitive answer would involve a comparison of a large number of alternative relational learning systems on equal experimental footing. Such a comparison is beyond the scope of this paper; to our knowledge, no such comparison has yet been attempted, but one would be facilitated by a platform such as NetKit. To demonstrate, we compare to a reimplementation in NetKit of the highly cited approach by Chakrabarti et al. (1998), which we will call NetKit-CDI.

Thus, for those of our data sets that contained local information, we compared the accuracies using only the local information with the accuracies using only the network as well as both relational and local information.[24] It must be noted that even within these data sets, there are nodes that have no local information, just as there are nodes with no connectivity information.[25] We compare classification accuracies only for those nodes that have both local information and connectivity information. Specifically, the local information is text, and for local classification we use naive

24. We have no local information on the IMDb data or the industry-yh data.
25. The industry-pr and WebKB data sets only have local information for roughly half the instances.



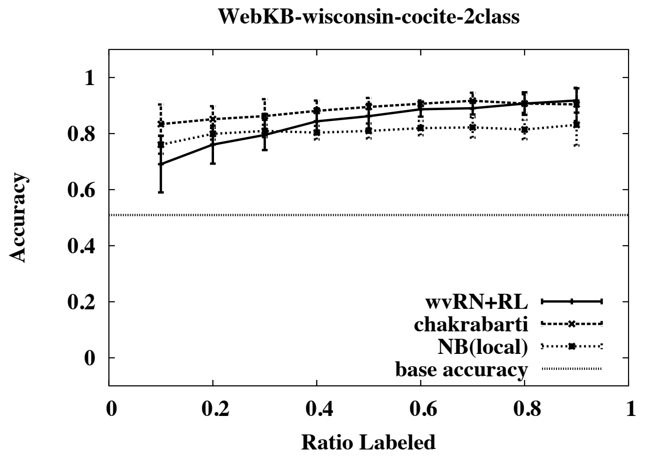


Figure 6: Comparisons of wvRN-RL (relaxation labeling), a reimplementation of the method of Chakrabarti et al. (NetKit-CDI), and a local-only naive Bayes classifier (NB(local)).

Bayes classification (which in preliminary studies, when averaged over the data sets, performed better than Rocchio's algorithm and multinomial Naive Bayes).

Figure 6 shows the accuracies on three of the ten data sets. We show these three to highlight the variance in relative performances, making it clear that neither network-only nor local-only should be the sole baseline of choice. We performed the same statistical analyses of these results as we did in the main study. Table 21 shows the p-values of the Wilcoxon signed-rank test across the ten data sets. The table shows that no method is significantly better than any other at $r = 0.1$, but the network-only is significantly better than both the full relational classifier and the local-only for $r \geq 0.3$ ($p \leq 0.100$) and $r \geq 0.4$ ($p \leq 0.025$ except against NetKit-CDI at $r = 0.9$). We also found that the relational classifier generally performed better than the local-only method at $r \geq 0.4$,

	sample ratio (r)								
	0.10	0.20	0.30	0.40	0.50	0.60	0.70	0.80	0.90
wvRN-RL v *NB-local*	*0.200*	—	**0.100**	**0.025**	**0.025**	**0.025**	**0.025**	**0.025**	**0.025**
wvRN-RL v *NetKit-CDI*	**0.400**	**0.100**	**0.050**	**0.025**	**0.025**	**0.025**	**0.025**	**0.025**	**0.050**
NetKit-CDI v *NB-local*	*0.400*	*0.400*	—	**0.450**	**0.450**	**0.250**	**0.400**	**0.200**	**0.200**

Table 21: p-values for the Wilcoxon signed-rank test comparing the performances of wvRN-RL (relaxation labeling), the method of Chakrabarti et al. (NetKit-CDI), and a local-only naive Bayes classifier. For each cell, bold text means that the first method was better than the second method and italics means it was worse. The cell with '—' means there was no significant difference.

although not significantly so in this comparison.[26] Most importantly, there are clear cases where using local-only methods as the sole baseline would lead to overly optimistic conclusions about the value of the full-blown relational learning technique.

This has an interesting implication: for classification purposes, as more labels are available in these networks, the network structure carries more information than what can be gotten from the local text, at least as measured using naive Bayes. It is important to reiterate that for different applications, the amount of local information and its relevance to the classification task can differ greatly, so these results are suggestive at best. Furthermore, aggregate classification accuracies tell only part of the story. Different subpopulations may be more or less amenable to local- or network-only classification (cf., fraud detection, Fawcett and Provost, 1997).

COMPARISON TO A GRAPH-BASED METHOD

Since there is a close relationship between wvRN and the "graph-based" methods that use only labels (as discussed in Sections 3.5.1 and 3.5.2), a question that follows from wvRN's excellent performance is whether such a graph-based method might provide an even better baseline than wvRN-RL. Blum et al. (2004) found that their randomized mincut method empirically did not perform as well as the method introduced by Zhu et al. (2003), so we compare the method of Zhu et al. to wvRN-RL on all the data from the case study. Their performances are nearly identical. This should come as no surprise as the two methods are nearly identical. Which method then should one use? By our experiments, the method of Zhu et al. gives slightly better scores for ranking entities by likelihood of class membership. Therefore, when their class mass normalization technique was employed to match the class posteriors to the class priors, Zhu's method generally improved more than when using class mass normalization with wvRN, making Zhu's method slightly but statistically significantly better than wvRN at $0.3 \leq r \leq 0.8$. However, one important reason to favor wvRN over the method of Zhu et al. is that the latter does not scale well: it requires inverting an NxN matrix and then doing a matrix multiplication, an O(N^3) operation. wvRN-RL is linear in the number of edges. In the worst case this is O(N^2), although most networks we have examined have a small average degree per node. For example, whereas for a modest-sized network (e.g., cora, N=4000) on a state-of-the-art compute server, wvRN finishes in just a few seconds, the method of Zhu et al.

26. The multi-data-set comparison has only 10 data points for the computation of statistical significance. The graphs also show standard-deviation error bars based on the 10 runs for each method, which suggest data-set specific conclusions of superiority. For example, in cora there is a clear ranking of the three methods.

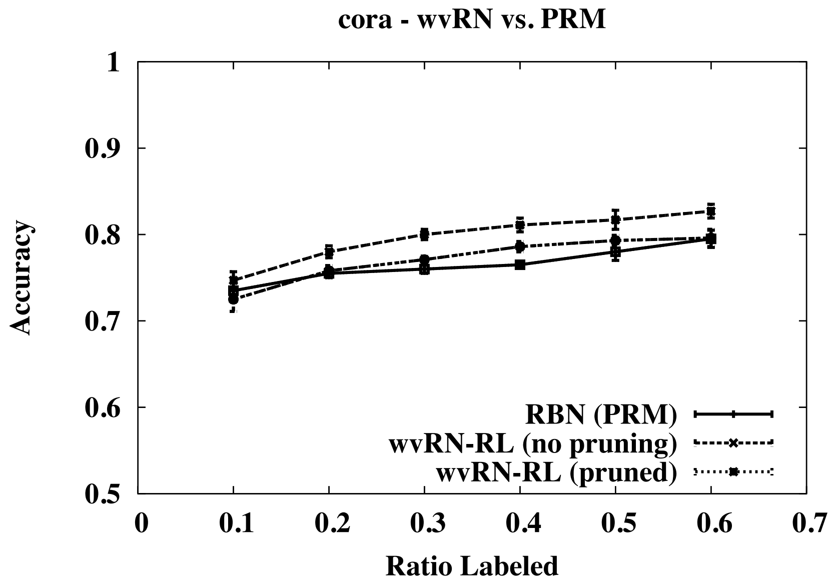


Figure 7: Comparison on cora of wvRN-RL (relaxation labeling) to RBN (PRM, Taskar et al., 2001). The graph shows wvRN using both citation and author links as in the original study. The "pruned" results follow the methodology of the case study in this paper by removing zero-knowledge components (see page 957) and singletons from the test set.

takes about 20 minutes. While this may not be a considerable burden for modest-sized data, some social network data sets are significantly larger (e.g., consider the many millions of communications records mined for fraud detection Fawcett and Provost, 1997; Cortes et al., 2001; Hill et al., 2006b or for network-based marketing Hill et al., 2006a, or by the NSA for counterterrorism, Tumulty, 2006). On a state-of-the-art machine, wvRN-RL can generate predictions on graphs consisting of a million nodes and millions of edges in minutes, whereas the method of Zhu et al. would not be tractable.

COMPARISON TO PRIOR PUBLISHED RESULTS

Yet another way to support the claim that network-only classification should be considered as a baseline is to a find published study for which using network-only classification would have changed the resulting conclusions. Consider cora. In a prior study, Taskar et al. (2001) show that a relational Bayesian network (RBN), there called a Probabilistic Relational Model (PRM), using author and citation links in conjunction with the text of the paper, was able to achieve a higher accuracy than a non-relational naive Bayesian classifier for $r = \{0.1, \ldots, 0.6\}$ (which did not use the links). However, as we saw above, wvRN performed quite well on this data set.

Figure 7 compares the accuracies of the RBN (transcribed from the graphs in the paper) with wvRN-RL. Note that in the prior work, they used fewer values of r and only had 5 cross-validation runs. Other than that, our setup is identical to the original study. Also note that to make a direct comparison, we here use both author edges and citation edges as was done in the original study (as opposed to only citation edges in our main study). We see clearly that wvRN was able to perform

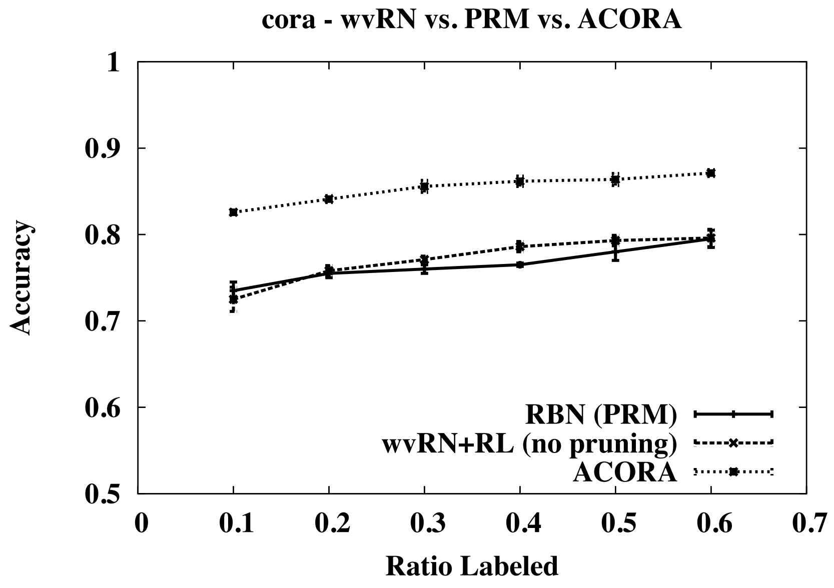


Figure 8: Comparison on cora of wvRN-RL (relaxation labeling) (no pruning, see Figure 7) to RBN (PRM, Taskar et al., 2001) and the use of identifier attributes via ACORA (Perlich and Provost, 2006).

comparably.[27] This demonstrates that cora is not a good data set to showcase the advantages of RBNs for classification. Had a method such as wvRN been readily available as a baseline, then Taskar et al. would most likely have used a more appropriate data set.

5.4 Limitations

We would like to characterize how much classification ability comes from the structure of the network alone. We have examined a limited notion: these methods all assume that "the structure of the network" can be reduced to "the structure of the neighborhood," bolstered by collective inference, rather than using relational models that look deeper.

Furthermore, we only considered links and class labels as comprising the structure of the network. We did not consider aspects of network structure such as the positions of individual nodes (as discussed in Section 3.5.3 on using node identifiers). For example, Figure 8 shows that accuracy can be improved substantially by reasoning with node identifiers via the ACORA system (Perlich and Provost, 2006). To our knowledge, no existing network classification system combines local attributes, node identifiers, and collective inference.

In the homogeneous, univariate case study we ignored much of the complexity of real networked data, such as heterogeneous edges, heterogeneous nodes, directed edges, and attributes of nodes and edges. Each of these introduces complications and opportunities for modeling. There are no

27. The "pruned" results show the accuracy after eliminating the zero-knowledge components, for which wvRN-RL can only predict the most prevalent class. Recall that zero-knowledge components (as defined on page 957) are nodes for which there is no path to any node in $\mathbf{V}^K$.

comprehensive, empirical machine learning studies that consider these dimensions systematically. For example, when using attributes of nodes, how much is gained by using them in the relational classifier, as opposed to using them simply to initialize priors? (For example, Chakrabarti et al. 1998 found that using the text of hyperlinked documents reduced performance.) Similarly, how much value is added by considering multiple edge types explicitly?

An important limitation of this work, with respect to its relevance to practical problems, is that we chose training data randomly to be labeled. It is likely that the data for which labels are available are interdependent. For example, all the members from one terrorist cell may be known and none from another. If other attributes are available more uniformly, then studies such as this may artificially favor network-only methods over attribute-based methods.

5.5 Conclusions and Future Work

We introduced a modular toolkit, NetKit-SRL, for classification in networked data. The importance of NetKit is three-fold: (1) it generalizes several existing methods for classification in networked data, thereby making comparison to existing methods possible; (2) it enables the creation and use of many new algorithms by its modularity and extensibility, and (3) it enables the analysis/comparison of individual components and configurations.

We then used NetKit to perform a case study of within-network, univariate classification for homogeneous networked data. The case study makes several contributions. It provides demonstrative support for points 2 and 3 above. Of the five network classifiers that stood clearly above the rest, three were novel combinations of components (and thus, novel relational classifiers). Certain collective inference and relational classification components stood out with consistently better performance. For collective inference, relaxation labeling was best when there are few known labels; it mattered little which collective inference method is used when there were many known labels. For relational classification, the link-based classifier clearly was preferable when many labels were known. The lower-variance methods (wvRN and cdRN) dominated when fewer labels were known. In combination, two pairs of relational classifier/collective inference combinations stand out strikingly: nLB with any of the collective inference methods dominates when many labels are known; the relational neighbor methods with relaxation labeling (wvRN-RL and cdRN-RL) dominate when fewer labels are known. Of particular relevance given this latter result, we also show the close correspondence of several simple, network classification methods: the node-centric wvRN-RL (Macskassy and Provost, 2003), the random-field method of Zhu et al. (2003), and classic connectionist techniques such as Hopfield networks (Hopfield, 1982).

The case study demonstrates the power of simple network classification models, and argues that they must be included when evaluating relational learning methods on networked data. On the benchmark data sets, error rates were reduced substantially by taking into account only the class-linkage structure of the network. Although learning helped in many cases, the no-learning wvRN was a very strong competitor—performing very well especially when few labels were known. This result was supported further by followup analyses showing cases where one would draw overly optimistic conclusions about the value of more-sophisticated methods if these network-only techniques were not used as baselines. It also raises the question of whether we need "better" benchmark data sets—to showcase the value of more-powerful techniques.

More generally, the results showcase two different modes of within-network classification that call for different types of methods: when many labels are known versus when few labels are known.

These modes correspond to different application scenarios. The former may correspond (for example) to networks that evolve over time with new nodes needing classification before their labels become known naturally, as would be the case for predicting movie box-office receipts. Examples of the little-known scenario can be found in counter-terrorism and law enforcement, where analysts form complex interaction networks containing a few, known bad guys. The little-known scenario has an economic component, similar to active learning: it may be worthwhile to incur costs to label additional nodes in the network, because this will lead to much improved classification. This suggests another direction for future work—identifying the most beneficial nodes for labeling (cf., Domingos and Richardson, 2001).

The case study also showcases a problem of representation for network classification: the selection of which edges to use. We show that edge selection can make a considerable difference, and suggest techniques analogous to those used in traditional feature selection. It is straightforward to extend NetKit's relational classification methods to handle heterogeneous links. However, that would not solve the fundamental problem that edge selection (like feature selection) may improve generalization performance, as well as provide simpler models.

Classification in networked data is important for real-world applications and presents many opportunities for machine-learning research. The field is beginning to amass benchmark domains containing networked data. We hope that NetKit can facilitate systematic study.

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