

Automating the Construction of Internet Portals with Machine Learning

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Abstract. Internet portals are growing in popularity because they gather content from the Web and organize it for easy access, retrieval and search. For example, *www.campsearch.com* allows complex queries by age-group, size, location and cost over summer camps. This functionality is not possible with general, Web-wide search engines. Unfortunately these portals are difficult and time-consuming to maintain. This paper proposes the use of machine learning techniques to greatly automate the creation and maintenance of Internet portals. We describe new research in reinforcement learning, information extraction and text classification that enables efficient spidering, the identification of informative text segments, and the population of topic hierarchies. Using these techniques, we have built a demonstration system: a portal for computer science research papers. It already contains over 50,000 papers and is publicly available at *www.cora.justresearch.com*. These techniques are widely applicable to portal creation in other domains.

Keywords: spidering, reinforcement learning, information extraction, hidden Markov models, text classification, naive Bayes, Expectation-Maximization, unlabeled data

1. Introduction

As the amount of information on the World Wide Web grows, it becomes increasingly difficult to find just what we want. While general-purpose search engines, such as AltaVista and NorthernLight offer relatively high coverage, they often provide only low precision, even for detailed queries. When we know that we want information of a certain type, or on a certain topic, an Internet portal can be a powerful tool. A *portal* is an information gateway that often includes a search engine, and additional organization and content. Portals are often, though not always, concentrated on a particular topic. They usually offer powerful methods for finding domain-specific information. For example:



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- Camp Search (*www.campsearch.com*) allows the user to search for summer camps for children and adults. The user can query and browse the system based on geographic location, cost, duration and other requirements.
- LinuxStart (*www.linuxstart.com*) provides a clearinghouse for Linux resources. It has a hierarchy of topics and a search engine over Linux pages.
- Movie Review Query Engine (*www.mrqe.com*) allows the user to search for reviews of movies. Type a movie title, and it provides links to relevant reviews from newspapers, magazines, and individuals from all over the world.
- Crafts Search (*www.bella-decor.com*) lets the user search web pages about crafts. It also provides search capabilities over classified ads and auctions of crafts, as well as a browseable topic hierarchy.
- Travel-Finder (*www.travel-finder.com*) allows the user to search web pages about travel, with special facilities for searching by activity, category and location.

Performing any of these searches with a traditional, general-purpose search engine would be extremely tedious or impossible. For this reason, portals are becoming increasingly popular. Unfortunately, however, building these portals is a labor-intensive process, typically requiring significant and ongoing human effort.

This paper describes the automation of many aspects of creating and maintaining portals by using machine learning techniques. These techniques allow portals to be created quickly with minimal effort and are suited for re-use across many domains. We present machine learning methods for spidering in an efficient topic-directed manner, extracting topic-relevant information, and building a browseable topic hierarchy. These approaches are briefly described in the following three paragraphs.

Every search engine or portal must begin with a collection of documents to index. A spider (or crawler) is an agent that traverses the Web, looking for documents to add to the collection. When aiming to populate a domain-specific collection, the spider need not explore the Web indiscriminantly, but should explore in a directed fashion in order to find domain-relevant documents efficiently. We set up the spidering task in a reinforcement learning framework (Kaelbling, Littman, & Moore, 1996), which allows us to precisely and mathematically define optimal behavior. This approach provides guidance for designing an intelligent

spider that aims to select hyperlinks optimally. It also indicates how the agent should learn from delayed reward. Our experimental results show that a reinforcement learning spider is three times more efficient in finding domain-relevant documents than a spider with a breadth-first search strategy.

Extracting characteristic pieces of information from the documents of a domain-specific collection allows the user to search over these features in a way that general search engines cannot. Information extraction, the process of automatically finding certain categories of textual substrings in a document, is well suited to this task. We approach information extraction with a technique from statistical language modeling and speech recognition, namely *hidden Markov models* (Rabiner, 1989). We learn model structure and parameters from a combination of labeled and distantly labeled data. Our model extracts fifteen different fields from spidered documents with 93% accuracy.

Search engines often provide a hierarchical organization of materials into relevant topics; Yahoo is the prototypical example. Automatically adding documents into a topic hierarchy can be framed as a text classification task. We present extensions to a probabilistic text classifier known as *naive Bayes* (Lewis, 1998; McCallum & Nigam, 1998) that succeed in this task without requiring large sets of labeled training data. The extensions reduce the need for human effort in training the classifier by using a few keywords per class, a class hierarchy and unlabeled documents in a bootstrapping process to build a classifier. Use of the resulting classifier places documents into a 70-leaf topic hierarchy with 66% accuracy—performance approaching human agreement levels.

The remainder of the paper is organized as follows. We describe the design of an Internet portal built using these techniques in the next section. The following three sections describe machine learning research introduced above and present their experimental results. We then discuss related work and present conclusions.

2. The Cora Search Engine

We have brought all the above-described machine learning techniques together in a demonstration system: an Internet portal for computer science research papers named Cora. The system is publicly available at www.cora.justresearch.com. Not only does it provide keyword search facilities over 50,000 collected papers, it also places these papers into a computer science topic hierarchy, maps the citation links between papers, and provides bibliographic information about each paper. Our hope is that in addition to providing a platform for testing machine



Figure 1. A screen shot of the Cora homepage. It has a search interface and a hierarchy interface.

learning research, this search engine will become a valuable tool for other computer scientists, and will complement similar efforts, such as the Computing Research Repository (xxx.lanl.gov/archive/cs), by providing functionality and coverage not available online elsewhere.

We provide three ways for a user to access papers in the repository. The first is through a topic hierarchy, similar to that provided by Yahoo, but customized specifically for computer science research. It is available on the homepage of Cora, as shown in Figure 1. This hierarchy was hand-constructed, and contains 70 leaves, varying in depth from one to three. Using text classification techniques, each research paper is automatically placed into a topic node. The topic hierarchy may be traversed by following hyperlinks from the homepage. Each node in the tree contains a list of the most-cited papers in that research topic.

All papers are indexed into a search engine available through a standard search interface. It supports commonly-used searching syn-

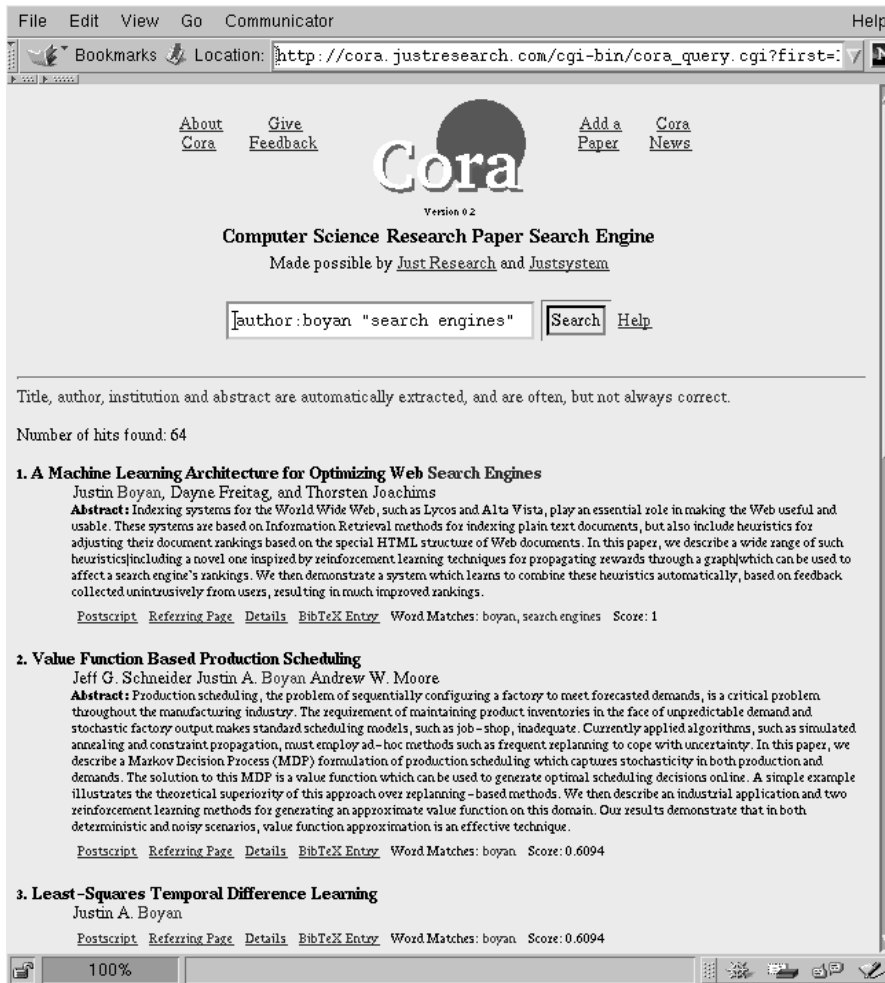


Figure 2. A screen shot of the query results page of the Cora search engine (www.cora.justresearch.com). Extracted paper titles, authors and abstracts are provided at this level.

tax for queries, including +, -, and phrase searching with ". It also allows searches restricted to extracted fields, such as authors and titles. Search result matches are ranked by the weighted log of term frequency, summed over all query terms. Query response time is usually less than a second. The results of search queries are presented as in Figure 2.

From both the topic hierarchy and the results of searching, links are provided to individual paper "details" pages. Each of these pages shows all the relevant information for a single paper, such as title and authors, links to the actual postscript paper, and a citation map that can be traversed either forwards or backwards. One example of this is

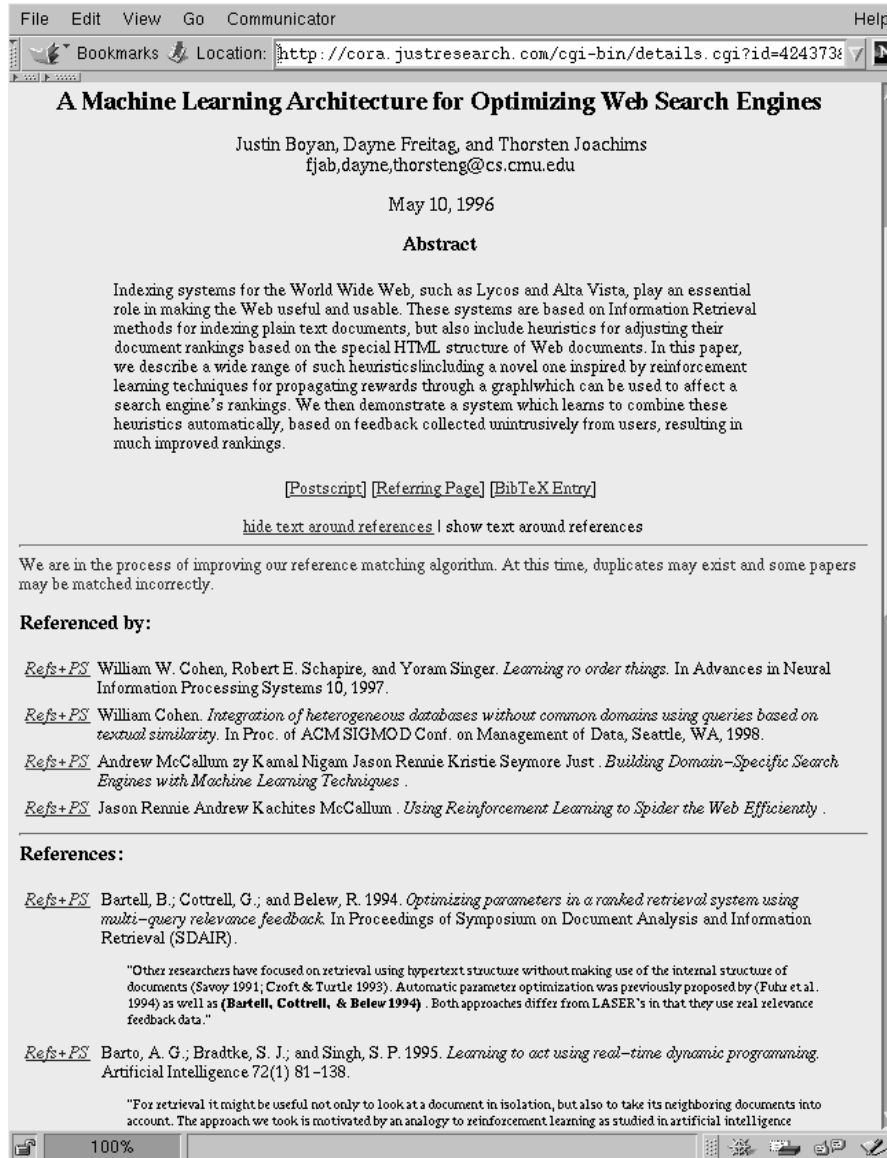


Figure 3. A screen shot of a details page of the Cora search engine. At this level, all extracted information about a paper is displayed, including the citation linking, which are hyperlinks to other details pages.

shown in Figure 3. The citation map allows a user to find details on cited papers, as well as papers that cite the detailed paper. The context of each reference is also provided, giving a brief summary of how the reference is used by the detailed paper. We also provide automatically

constructed BibTeX entries, a mechanism for submitting new papers and web sites for spidering, and general Cora information links.

The collection and organization of the research papers for Cora is automated by drawing upon the machine learning techniques described in this paper. The first step of building any portal is the collection of relevant information from the Web. A spider crawls the Web, starting from the home pages of computer science departments and laboratories and looks for research papers. Using reinforcement learning, our spider efficiently explores the Web, following links that are more likely to lead to research papers, and collects all postscript documents it finds.¹ The details of this spidering are described in Section 3. The postscript documents are then converted into plain text. If the document can be reliably determined to have the format of a research paper (*e.g.* by having Abstract and Reference sections), it is added to Cora. Using this system, we have found 50,000 computer science research papers, and are continuing to spider for even more.

The beginning of each paper is passed through a learned information extraction system that automatically finds the title, authors, affiliations and other important header information. Additionally, the bibliography section of each paper is located, individual references identified, and each reference automatically broken down into the appropriate fields, such as author, title, journal, and date. This information extraction process is described in Section 4.

Using the extracted information, reference and paper matches are made—grouping citations to the same paper together, and matching citations to papers in Cora. Of course, many papers that are cited do not appear in the repository. This matching procedure is similar to one described by Bollacker, Lawrence, and Giles (Bollacker et al., 1998), except that we use additional field-level constraints provided by knowing, for example, the title and authors of each paper. Finally, each paper is placed into the computer science hierarchy using a text classification algorithm. This process is described in Section 5.

These steps complete the processing of the data necessary to build Cora. The creation of other Internet portals also involves directed spidering, information extraction, and classification. The machine learning techniques described in the following sections are widely applicable to the construction and maintenance of any Internet portal.

¹ Nearly all computer science papers are in postscript format, though we are adding more formats, such as PDF.

3. Efficient Spidering

Spiders are agents that explore the hyperlink graph of the Web, often for the purpose of finding documents with which to populate a portal. Extensive spidering is the key to obtaining high coverage by the major Web search engines, such as AltaVista, Excite and NorthernLight. Since the goal of these general-purpose search engines is to provide search capabilities over the Web as a whole, for the most part they simply aim to find as many distinct web pages as possible. Such a goal lends itself to strategies like breadth-first search. If, on the other hand, the task is to populate a domain-specific portal, then an intelligent spider should try to avoid hyperlinks that lead to off-topic areas, and concentrate on links that lead to documents of interest.

In Cora, efficient spidering is a major concern. The majority of the pages in computer science department web sites do not contain links to research papers, but instead are about courses, homework, schedules and admissions information. Avoiding whole branches and neighborhoods of departmental web graphs can significantly improve efficiency and increase the number of research papers found given a finite amount of crawling time. We use reinforcement learning as the setting for efficient spidering in order to provide a formal framework.

Several other systems have also studied spidering, but without a framework defining optimal behavior. ARACHNID (Menczer, 1997) maintains a collection of competitive, reproducing and mutating agents for finding information on the Web. Cho, Garcia-Molina, and Page (Cho et al., 1998) suggest a number of heuristic ordering metrics for choosing which link to crawl next when searching for certain categories of web pages. Chakrabarti, van der Berg, and Dom (Chakrabarti et al., 1999) produced a crawler to locate documents that are textually similar to a set of training documents. This spider only requires a handful of relevant example pages, whereas we also require example Web graphs where such relevant pages are likely to be found. However, with this additional training data, our framework is able to explicitly capture knowledge of future reward—the fact that many pages leading to "goal" pages may contain text that is drastically different from goal pages. Additionally, there are other systems that use reinforcement learning for non-spidering Web tasks. WebWatcher (Joachims, Freitag, & Mitchell, 1997) is a browsing assistant that uses a combination of supervised and reinforcement learning to help a user find information by recommending which hyperlinks to follow. Laser uses reinforcement learning to tune the search parameters of a search engine (Boyan, Freitag, & Joachims, 1996).

The spidering algorithm we present here is unique in that it represents and takes advantage of future reward—learning features that predict an on-topic document several hyperlink hops away from the current hyperlink. This is particularly important when reward is sparse, in other words, on-topic documents are few and far between. Our experimental results bear this out. In a domain *without* sparse rewards, our reinforcement learning spider that represents future reward performs about the same as another reinforcement learning spider that does not (both out-perform a breadth-first search spider by three-fold). However, on another domain in which reward is more sparse, explicitly representing future reward increases efficiency by a factor of two.

3.1. REINFORCEMENT LEARNING

The term “reinforcement learning” refers to a framework for learning optimal decision making from rewards or punishment (Kaelbling et al., 1996). It differs from supervised learning in that the learner is never told the correct action for a particular state, but is simply told how good or bad the selected action was, expressed in the form of a scalar “reward.” We now describe the framework, and define optimal behavior in this context.

A task is defined by a set of states, $s \in \mathcal{S}$, a set of actions, $a \in \mathcal{A}$, a state-action transition function (mapping state/action pairs to the resulting state), $T : \mathcal{S} \times \mathcal{A} \rightarrow \mathcal{S}$, and a reward function (mapping state/action pairs to a scalar reward), $R : \mathcal{S} \times \mathcal{A} \rightarrow \mathfrak{R}$. At each time step, the learner (also called the *agent*) selects an action, and then as a result is given a reward and transitions to a new state. The goal of reinforcement learning is to learn a *policy*, a mapping from states to actions, $\pi : \mathcal{S} \rightarrow \mathcal{A}$, that maximizes the sum of its reward over time. The most common formulation of “reward over time” is a discounted sum of rewards into an infinite future. We use the infinite-horizon discounted model where reward over time is a geometrically discounted sum in which the discount, $0 \leq \gamma < 1$, devalues rewards received in the future. Accordingly, when following policy π , we can define the *value* of each state to be:

$$V^\pi(s) = \sum_{t=0}^{\infty} \gamma^t r_t, \quad (1)$$

where r_t is the reward received t time steps after starting in state s . The optimal policy, written π^* , is the one that maximizes the value, $V^\pi(s)$, for all states s .

In order to learn the optimal policy, we learn its value function, V^* , and its more specific correlate, called Q . Let $Q^*(s, a)$ be the value of

selecting action a from state s , and thereafter following the optimal policy. This is expressed as:

$$Q^*(s, a) = R(s, a) + \gamma V^*(T(s, a)). \quad (2)$$

We can now define the optimal policy in terms of Q by selecting from each state the action with the highest expected future reward: $\pi^*(s) = \arg \max_a Q^*(s, a)$. The seminal work by Bellman (Bellman, 1957) shows that the optimal policy can be found straightforwardly by dynamic programming.

3.2. SPIDERING AS REINFORCEMENT LEARNING

As an aid to understanding how reinforcement learning relates to spidering, consider the common reinforcement learning task of a mouse exploring a maze to find several pieces of cheese. The mouse can perform actions for moving among the grid squares of the maze. The mouse receives a reward for finding each piece of cheese. The state is both the position of the mouse and the locations of the cheese pieces remaining to be consumed (since the cheese can only be consumed and provide reward once). Note that the mouse only receives immediate reward for finding a maze square containing cheese, but that in order to act optimally it must choose actions based on future rewards as well.

In the spidering task, the on-topic documents are immediate rewards, like the pieces of cheese. The actions are following a particular hyperlink. The state does not include the current “position” of the agent since a crawler can go next to any URL it has previously encountered. The state is the set of on-topic documents that remain to be consumed, and the set of URLs that have been encountered.² The number of actions is large and dynamic, in that it depends on which pages the spider has visited so far.

The most important features of topic-specific spidering that make reinforcement learning an especially good framework for defining the optimal solution are: (1) performance is measured in terms of reward over time (because it is better to locate on-topic documents sooner, given time limitations), and (2) the environment presents situations with delayed reward, (in that on-topic documents may be several hyperlink traversals away from the current choice point, but the text on the current page may offer indications of which hyperlinks will lead to reward soonest).

² It is as if the mouse can jump to any square, as long as it has already visited a bordering square. Thus the state is not a single position, but the position and shape of the boundary.

3.3. PRACTICAL APPROXIMATIONS

The problem now is how to apply reinforcement learning to spidering in such a way that it can be practically solved. Unfortunately, the state space is huge: exponential in the number of on-topic documents on the Web. The action space is also large: the number of unique hyperlinks that the spider could possibly visit. Thus we need to make some simplifying assumptions in order to make the problem tractable and to allow the spider to generalize to hyperlinks it has not already followed.³

We begin by assuming that the states are not distinguished by which on-topic documents have already been consumed—this means that the state is represented only by the set of URLs encountered so far. We refer to the set of URLs encountered so far as the “fringe.” Although this assumption reduces the size of the state space drastically, the number of possible fringes is still exponential in the number of pages the spider could visit, so straightforward dynamic programming or Q -learning is impractical.

We turn instead to a *roll-out* solution with a model, and a form of reinforcement learning policy evaluation called TD-1 (Sutton, 1988). We gather training data and build a model consisting of all the pages and hyperlinks found by exhaustively spidering a few web sites.⁴ By knowing the complete web graph of the training data, we can easily define a near-optimal policy. We then execute that policy for a finite number of steps from state/action pairs for some subset of the states; these executions result in a sequence of immediate rewards. We then assign to these state/action pairs the Q -value calculated as the discounted sum of the reward sequence. Finally, a value function approximator is trained using the chosen subset of state/action/ Q -value triples as training data. The spider that emerges from this training procedure efficiently explores new web graphs by estimating the expected future reward associated with new hyperlinks using this function approximator. In the next two sub-sections we describe the near-optimal policy on known web graphs, and the value function approximation.

3.4. NEAR-OPTIMAL POLICY ON KNOWN HYPERLINK GRAPHS

Given full knowledge of a hyperlink graph built by exhaustively spidering a web site, it is straightforward to specify the near-optimal policy

³ Note, that by defining the exact solution in terms of the optimal policy, and making our assumptions explicit, we better understand the approximations we introduce, and how to select areas of future work that will improve performance further.

⁴ This is the off-line version of our algorithm; the on-line version would be a form of policy improvement using roll-outs, as in (Tesauro & Galperin, 1997).

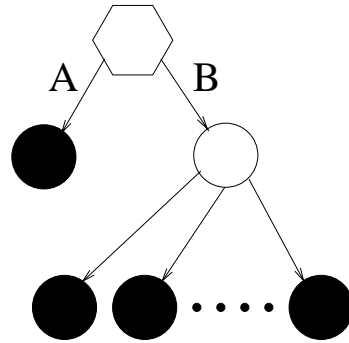


Figure 4. A representation of spidering space where arrows are hyperlinks and nodes are web documents. The hexagonal node represents an already-explored node; the circular nodes are unexplored. Filled-in circles denote the presence of immediate reward (target pages). When a spider is given the choice between an action that provides immediate reward and one that provides future reward, the spider always achieves the maximum discounted reward by choosing the immediate reward first.

for restricted values of the discount factor, γ . The policy must choose from among all the hyperlinks it knows about so far, the “fringe.” At each time step, the near-optimal policy selects from the fringe the action that follows the hyperlink on the path to the closest immediate reward. For example, in Figure 4, the policy would choose action A at time 0 because it provides a reward at time 1, where choosing action B would delay the first immediate reward until time 2.

This policy closely approximates the optimal policy in cases where $\gamma \leq 0.5$ and all non-zero immediate rewards have the same value—both conditions that hold in our spidering scenario. Under these conditions, the optimal action is the one that brings immediate reward as soon as possible. Even an infinite stream of constant reward discounted by 0.5 at each step is only equal in value to a single immediate reward starting one time step sooner. Thus, finding a single immediate reward at time step 1 and none thereafter provides more discounted reward than any continuous finite stream of immediate reward starting at time step 2. Our policy, which follows the path leading to the closest immediate reward, correctly distinguishes between these two scenarios and any others where the first rewards are different number of steps away. The policy may not make the optimal choice in cases where two or more actions provide the first immediate reward equidistantly from the fringe. The heuristic policy arbitrarily selects one of these; in contrast, the optimal policy would select the hyperlink leading to the most additional reward, beyond just the first one.

3.5. VALUE FUNCTION APPROXIMATION

Using the above policy, the training procedure can generate state/action/ Q -value triples. As in most reinforcement learning solutions to problems with large state spaces, these triples then act as training data for supervised training of an approximation to the value function, $V(s)$, or a Q function.

First we must choose the subset of the states from which we will execute roll-outs and estimate Q -values. For the experiments in this paper, we choose all fringes that contain exactly one hyperlink. Thus, for each known hyperlink a , we estimate $Q(\{a\}, a)$ by roll-out to generate training data.

Next we must specify the features of the training data used by the value function approximator. We assume that the Q -value of a state-action pair is a function of an unordered list of the words in the neighborhood of the hyperlink; that is $Q(s, a) = F(\text{text}(a))$. Note this assumption states that the Q -value is independent of the state, and thus the fringe as well.

The $\text{text}()$ function selects which textual features will be the inputs to the regression function F . In the experiments presented in this paper, we select two sets of words, 1) the anchor text and tokens from the URL of the hyperlink and 2) the full text of the web page where the hyperlink is located. This associates a significant portion of text with each hyperlink and allows each hyperlink to be identified uniquely. Experiments not presented in this paper show that using a more restricted set of neighborhood text does not enhance spidering performance.

Now using these features we must define a regression function, F , that maps text to real-valued Q -values. We perform the mapping by casting this regression problem as classification (Torgo & Gama, 1997). We discretize the discounted sum of future reward values of our training data into bins and treat each bin as a class. For each hyperlink, we calculate the probabilistic class membership of each bin using naive Bayes (which is described in section 5.2.1). Then the Q -value of a new, unseen hyperlink is estimated by taking a weighted average of each bins' Q -value, using the probabilistic class memberships as weights.

3.6. EXPERIMENTAL RESULTS

In August 1998 we completely mapped the documents and hyperlinks of the web sites of computer science departments at Brown University, Cornell University, University of Pittsburgh and University of Texas. They include 53,012 documents and 592,216 hyperlinks. We perform a series of four test/train splits, in which the data from three universities is used to train a spider that is then tested on the fourth. The

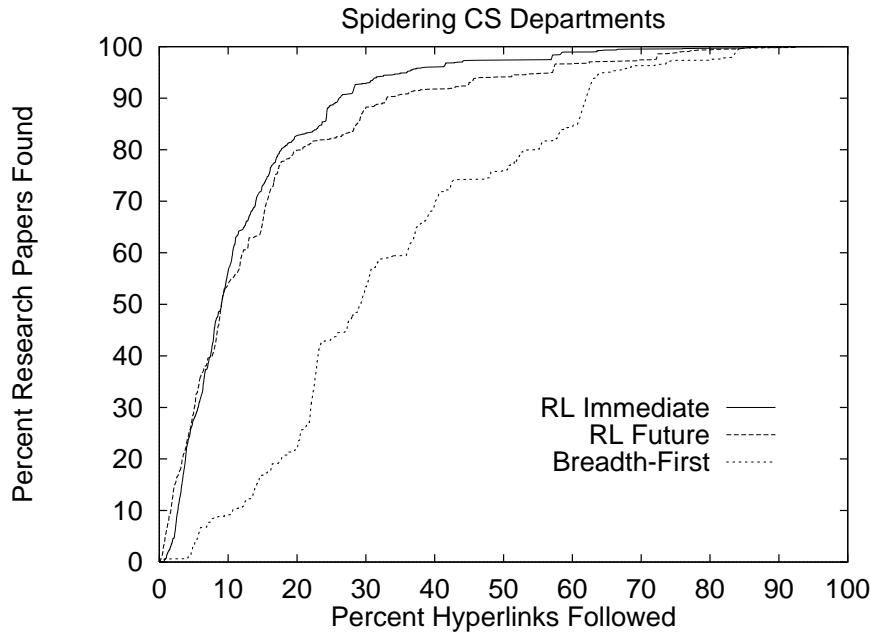


Figure 5. The performance of different spidering strategies, averaged over four test/train splits. The reinforcement learning spiders find target documents significantly faster than traditional breadth-first search.

target pages (for which a reward of 1 is given) are computer science research papers. They are identified with very high precision by a simple hand-coded algorithm that locates abstracts and reference sections with regular expressions. Each spidering run begins at the homepage of the test department.

We present results of two different reinforcement learning spiders and compare them to a breadth-first-search spider. *Immediate* uses $\gamma = 0$, utilizing only immediate reward in its assignment of hyperlink values. This spider employs a binary classifier that distinguishes between links that do and do not point directly to a research paper. *Future* uses $\gamma = 0.5$ and represents the Q -function that makes use of future reward with a more finely-discriminating 3-bin classifier, where the data are partitioned into bins equally based on the Q -value of the training documents.

The three spiders are evaluated on each test/train split by spidering the test university. Figure 5 plots the number of research papers found over the course of all the pages visited, averaged over all four universities.

At all times during its progress, both reinforcement learning spiders have found more research papers than breadth-first search. One

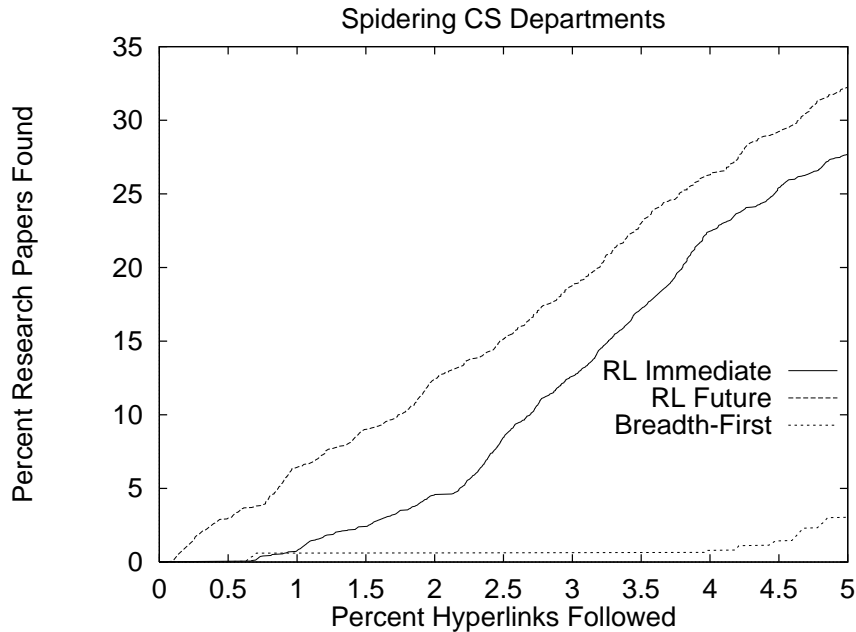


Figure 6. The performance of different spidering strategies during the initial stages of each spidering run. Here, the Future spider performs best, because identifying future rewards are crucial.

measure of performance is the number of hyperlinks followed before 75% of the research papers are found. Both reinforcement learners are significantly more efficient, requiring exploration of less than 16% of the hyperlinks; in comparison, Breadth-first requires 48%. This represents a factor of three increase in spidering efficiency.

In the early stages of each spidering run, the task of identifying future rewards is more crucial, because no immediate reward actions are available. In these cases, we would expect the Future spider to outperform the Immediate one. Figure 6 shows the average performance of the spiders during the initial stages of each spidering run. Here, we indeed see that a spider using future rewards does better than one using only immediate rewards. On average the Immediate spider takes nearly three times as long as Future to find the first 28 (5%) of the papers.

In Figure 5, after the first 50% of the papers are found, however, the Immediate spider performs slightly better than the Future spider. This is because the system has uncovered many links that will give immediate reward if followed, and the Immediate spider recognizes them more accurately. In future work we are investigating techniques for improving classification to recognize these immediate rewards when

the spider uses the larger number of bins required for regression with future reward.

These results indicate that when modeling future reward is particularly important, the `Future` spider gathers information more efficiently than the `Immediate` spider. This case is particularly evident in spidering tasks where immediate reward is very sparse. In other work (Rennie & McCallum, 1999), we have run experiments on the task of finding web pages listing corporate officers in a company web site. Usually there is only a single page with this information in a company web site, and thus this is a task with a single reward, a “goal of achievement.” In this case, the `Future` spider retrieves target pages twice as efficiently as the `Immediate` spider.

As the Internet continues to prosper, it will continually become more and more difficult to gather a sizable portion of the Web. Our research suggests that this is no longer important. The Web is so vast that even if we could amass all of the available documents, current techniques are such that we could not find the information that we are looking for. Thus, the future is in building specialized Internet portals that are domain specific. The spidering research presented here is the first step in building such portals. Instead of requiring a search over the entire Internet to find a large collection of relevant documents, our reinforcement learning framework can find such documents in a very efficient fashion, up to three times faster than breadth-first search.

4. Information Extraction

Information extraction is concerned with identifying phrases of interest in textual data. For many applications, extracting items such as names, places, events, dates, and prices is a powerful way to summarize the information relevant to a user’s needs. In the case of a domain-specific portal, the automatic identification of important information can increase the accuracy and efficiency of a directed search.

In `Cora` we use hidden Markov models (HMMs) to extract the fields relevant to computer science research papers, such as titles, authors, affiliations and dates. One HMM extracts information from each paper’s header (the words preceding the main body of the paper.) A second HMM processes the individual references in each paper’s reference section. The extracted text segments are used (1) to allow searches over specific fields, (2) to provide useful effective presentation of search results (*e.g.* showing title in bold), and (3) to match references to papers during citation grouping.

Our research interest in HMMs for information extraction is particularly focused on learning the appropriate state and transition structure of the models from training data, and estimating model parameters with labeled and unlabeled data. We show that models with structures learned from data outperform models built with one state per extraction class. We also demonstrate that using distantly-labeled data, for parameter estimation improves extraction accuracy, but that Baum-Welch estimation of model parameters with unlabeled data degrades performance.

4.1. HIDDEN MARKOV MODELS

Hidden Markov modeling is a powerful statistical machine learning technique that is just beginning to gain use in information extraction tasks (*e.g.* Leek, 1997; Bikel, Miller, Schwartz, & Weischedel, 1997; Freitag & McCallum, 1999). HMMs offer the advantages of having strong statistical foundations that are well-suited to natural language domains and handling new data robustly. They are also computationally efficient to develop and evaluate due to the existence of established training algorithms. The disadvantages of using HMMs are the need for an *a priori* notion of the model topology and, as with any statistical technique, large amounts of training data.

Discrete output, first-order HMMs are composed of a set of states Q , with specified initial and final states q_I and q_F , a set of transitions between states ($q \rightarrow q'$), and a discrete vocabulary of output symbols $\Sigma = \{\sigma_1, \sigma_2, \dots, \sigma_M\}$. The model generates a string $\mathbf{w} = w_1 w_2 \dots w_l$ by beginning in the initial state, transitioning to a new state, emitting an output symbol, transitioning to another state, emitting another symbol, and so on, until a transition is made into the final state. The parameters of the model are the transition probabilities $P(q \rightarrow q')$ that one state follows another and the emission probabilities $P(q \uparrow \sigma)$ that a state emits a particular output symbol. The probability of a string \mathbf{w} being emitted by an HMM M is computed as a sum over all possible paths by:

$$P(\mathbf{w}|M) = \sum_{q_1, \dots, q_l \in Q^l} \prod_{k=1}^{l+1} P(q_{k-1} \rightarrow q_k) P(q_k \uparrow w_k), \quad (3)$$

where q_0 and q_{l+1} are restricted to be q_I and q_F respectively, and w_{l+1} is an end-of-string token. The Forward algorithm can be used to calculate this probability efficiently (Rabiner, 1989).

The observable output of the system is the sequence of symbols that the states emit, but the underlying state sequence itself is hidden. One common goal of learning problems that use HMMs is to recover

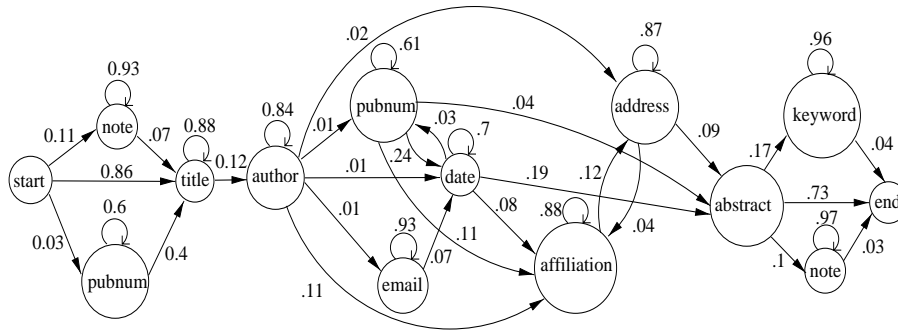


Figure 7. Example header HMM. Each state emits words from a class-specific multinomial distribution.

the state sequence $V(\mathbf{w}|M)$ that has the highest probability of having produced an observation sequence:

$$V(\mathbf{w}|M) = \arg \max_{q_1 \dots q_l \in Q^l} \prod_{k=1}^{l+1} P(q_{k-1} \rightarrow q_k) P(q_k \uparrow w_k). \quad (4)$$

Fortunately, the Viterbi algorithm (Viterbi, 1967) efficiently recovers this state sequence.

4.2. HMMs FOR INFORMATION EXTRACTION

Hidden Markov models provide a natural framework for modeling the production of the headers and references of research papers. We want to label each word of a header or reference as belonging to a class such as title, author, journal, or keyword. We do this by modeling the entire header or reference (and all of the classes to extract) with one HMM. This task varies from the more classic extraction task of identifying a small set of target words from a large document containing mostly uninformative text.

HMMs may be used for information extraction by formulating a model in the following way: each state is associated with a class that we want to extract, such as title, author or affiliation. Each state emits words from a class-specific multinomial (unigram) distribution. We can learn the class-specific multinomial distributions and the state transition probabilities from training data. In order to label a new header or reference with classes, we treat the words from the header or reference as observations and recover the most-likely state sequence with the Viterbi algorithm. The state that produces each word is the class tag for that word. An example HMM for headers, annotated with class labels and transition probabilities, is shown in Figure 7.

Hidden Markov models, while relatively new to information extraction, have enjoyed success in related natural language tasks. They have been widely used for part-of-speech tagging (Kupiec, 1992), and have more recently been applied to topic detection and tracking (Yamron, Carp, Gillick, Lowe, & van Mulbregt, 1998) and dialog act modeling (Stolcke, Shriberg, Bates, Coccaro, Jurafsky, Martin, Meteer, Ries, Taylor, & Ess-Dykema, 1998). Other systems using HMMs for information extraction include those by Leek (1997), who extracts gene names and locations from scientific abstracts, and the Nymble system (Bikel et al., 1997) for named-entity extraction. Unlike our work, these systems do not consider automatically determining model structure from data; they either use one state per class, or use hand-built models assembled by inspecting training examples. Freitag and McCallum (1999) hand-build multiple HMMs, one for each field to be extracted, and focus on modeling the immediate prefix, suffix, and internal structure of each field; in contrast, we focus on learning the structure of one HMM to extract all the relevant fields, taking into account field sequence.

4.2.1. *Learning model structure from data*

In order to build an HMM for information extraction, we must first decide how many states the model should contain, and what transitions between states should be allowed. A reasonable initial model is to use one state per class, and to allow transitions from any state to any other state (a fully-connected model). However, this model may not be optimal in all cases. When a specific hidden sequence structure is expected in the extraction domain, we may do better by building a model with multiple states per class, with only a few transitions out of each state. Such a model can make finer distinctions about the likelihood of encountering a class at a particular location in the document, and can model specific local emission distribution differences between states of the same class.

An alternative to simply assigning one state per class is to learn the model structure from training data. Training data labeled with class information can be used to build a maximally-specific model. An example of this model built from just four labeled examples is shown in Figure 8. Each word in the training data is assigned its own state, which transitions to the state of the word that follows it. Each state is associated with the class label of its word token. A transition is placed from the start state to the first state of each training instance, as well as between the last state of each training instance and the end state.

This model can be used as the starting point for a variety of state merging techniques. We propose two simple types of merges that can be used to generalize the maximally-specific model. First, “neighbor-

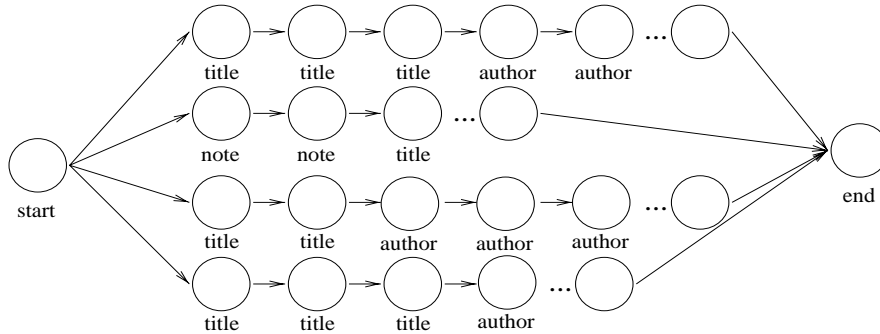


Figure 8. Example of a maximally specific HMM built from four training instances, which is used as the starting point for state merging.

merging” combines all states that share a transition and have the same class label. For example, in Figure 8, the three adjacent title states from the first header would be merged into a single title state. As multiple neighbor states with the same class label are merged into one, a self-transition loop is introduced, whose probability represents the expected state duration for that class.

Second, “V-merging” merges any two states that have the same label and share transitions from or to a common state. V-merging reduces the branching factor of the maximally-specific model. We apply V-merging to models that have already undergone neighbor-merging. For example, again in Figure 8, instead of selecting from among three transitions from the start state into title states, the V-merged model would merge the children title states into one, so that only one transition from the start state to the title state would remain. The V-merged model can be used for extraction directly, or more state merges can be made automatically or by hand to generalize the model further.

4.2.2. Labeled, unlabeled, and distantly-labeled data

Once a model structure has been selected, the transition and emission parameters need to be estimated from training data. While obtaining unlabeled training data is generally not too difficult, acquiring labeled training data is more problematic. Labeled data is expensive and tedious to produce, since manual effort is involved. It is also valuable, since the counts of class transitions $N(q \rightarrow q')$ and the counts of a word occurring in a class $N(q \uparrow \sigma)$ can be used to derive maximum likelihood estimates for the parameters of the HMM:

$$\hat{P}(q \rightarrow q') = \frac{N(q \rightarrow q')}{\sum_{s \in Q} N(q \rightarrow s)}, \quad (5)$$

$$\hat{P}(q \uparrow \sigma) = \frac{N(q \uparrow \sigma)}{\sum_{\rho \in \Sigma} N(q \uparrow \rho)}. \quad (6)$$

Smoothing of the distributions is often necessary to avoid probabilities of zero for the transitions or emissions that do not occur in the training data.

Unlabeled data, on the other hand, can be used with the Baum-Welch training algorithm (Baum, 1972) to train model parameters. The Baum-Welch algorithm is an iterative Expectation-Maximization (EM) algorithm that, given an initial parameter configuration, adjusts model parameters to locally maximize the likelihood of unlabeled data. Baum-Welch training suffers from the fact that it finds local maxima, and is thus sensitive to initial parameter settings.

A third source of valuable training data is what we refer to as *distantly-labeled* data. Sometimes it is possible to find data that is labeled for another purpose, but which can be partially applied to the domain at hand. In these cases, it may be that only a portion of the labels are relevant, but the corresponding data can still be added into the model estimation process in a helpful way. For example, BibTeX files are bibliography databases that contain labeled citation information. Several of the labels that occur in citations, such as title and author, also occur in the headers of papers, and this labeled data can be used in training emission distributions for header extraction. However, other BibTeX fields are not relevant to the header extraction task, and not all of the header fields occur in the BibTeX data. In addition, the data does not include any information about sequences of classes in headers and therefore cannot be used for transition distribution estimation.

Class emission distributions can be trained directly using either the labeled training data (L), a combination of the labeled and distantly-labeled data (L+D), or a linear interpolation of the labeled and distantly-labeled data (L*D). In the L+D case, the word counts of the labeled and distantly-labeled data are added together before deriving the emission distributions. In the L*D case, separate emission distributions are trained for the labeled and distantly-labeled data, and then the two distributions are interpolated together using a mixture weight derived from leave-one-out Expectation-Maximization of the labeled data. These three cases are shown below:

$$\hat{P}_L(w_i) = \frac{f(N_L(w_i))}{\sum_{i=1}^V N_L(w_i)} \quad (7)$$

$$\hat{P}_{L+D}(w_i) = \frac{f(N_L(w_i) + N_D(w_i))}{\sum_{i=1}^V N_L(w_i) + N_D(w_i)} \quad (8)$$

$$\hat{P}_{L^*D}(w_i) = \lambda \hat{P}_L(w_i) + (1 - \lambda) \hat{P}_D(w_i), \quad (9)$$

where $N(w_i)$ is the count of word w_i in the class, λ is the mixture weight, and $f()$ represents a smoothing function, used to avoid probabilities of zero for the vocabulary words that are not observed for a particular class.

4.3. EXPERIMENTAL RESULTS

We focus our information extraction experiments on extracting relevant information from the headers of computer science research papers, though the techniques described here apply equally well to reference extraction. We define the header of a research paper to be all of the words from the beginning of the paper up to either the first section of the paper, usually the introduction, or to the end of the first page, whichever occurs first. The abstract is automatically located using regular expression matching and changed to a single ‘abstract’ token. Likewise, an ‘intro’ or ‘page’ token is added to the end of each header to indicate whether a section or page break terminated the header. A few special classes of words are identified using simple regular expressions and converted to special identifying tokens: email addresses, web addresses, year numbers, zip codes, technical report numbers, and all other numbers. All punctuation, case and newline information is removed from the text.

The target classes we wish to identify include the following fifteen categories: title, author, affiliation, address, note, email, date, abstract, introduction (intro), phone, keywords, URL, degree, publication number (pubnum), and page. The abstract, intro and page classes are each represented by a state that outputs only the token of that class. The degree class captures the language associated with Ph.D. or Master’s theses, such as “submitted in partial fulfillment of...” and “a thesis by...”. The note field commonly accounts for phrases from acknowledgements, copyright notices, and citations.

One thousand headers were manually tagged with class labels. Sixty-five of the headers were discarded due to poor formatting, and the rest were split into a 500-header, 23,557 word token labeled training set and a 435-header, 20,308 word token test set. Distantly-labeled training data was acquired from 176 BibTeX files that were collected from the Web. These files consist of 2.4 million words, which contribute to the following nine header classes: address, affiliation, author, date, email, keyword, note, title, and URL.

For each emission distribution training case (L, L+D, L*D), a fixed vocabulary is derived from all of the words in the training data used.

Table I. Extraction accuracy (%) for models with one state per class when the transition parameters are estimated from labeled (L) data, a combination of labeled and distantly-labeled (L+D) and an interpolation of labeled and distantly-labeled (L*D) data. Using the interpolation of the two data sources provides the best extraction performance.

Model	# States	# Transitions	L	L+D	L*D
Full	17	255	62.8	57.4	64.5
Self	17	252	85.9	83.1	89.4
ML	17	149	90.5	89.4	92.4
Smooth	17	255	89.9	88.8	92.0

The labeled data results in a 4,914-word vocabulary, and the labeled and distantly-labeled data together contain 92,426 distinct words. Absolute discounting (Ney, Essen, & Kneser, 1994) is used as the smoothing function. An unknown word token is added to the vocabularies to model out-of-vocabulary words. Any words in the testing data that are not in the vocabulary are mapped to this token. The probability of the unknown word is estimated separately for each class, and is assigned a portion of the discount mass proportional to the fraction of singleton words observed only in the current class.

We build several HMM models, varying model structures and training conditions, and test the models by finding the Viterbi paths for the test set headers. Performance is measured by word classification accuracy, which is the percentage of header words that are emitted by a state with the label of the words' true label.

4.3.1. Model selection – One state per class

The first set of models each use one state per class. Emission distributions are trained for each class on either the labeled data (L), the combination of the labeled and distantly-labeled data (L+D), or the interpolation of the labeled and distantly-labeled data (L*D). Extraction accuracy results for these models are reported in Table I.

The Full model is a fully-connected model where all transitions are assigned uniform probabilities. It relies only on the emission distributions to choose the best path through the model, and achieves a maximum accuracy of 64.5%. The Self model is similar, except that the self-transition probability is set according to the maximum likelihood estimate from the labeled data, with all other transitions set uniformly. This model benefits from the additional information of the expected number of words to be emitted by each state, and its accuracy jumps to

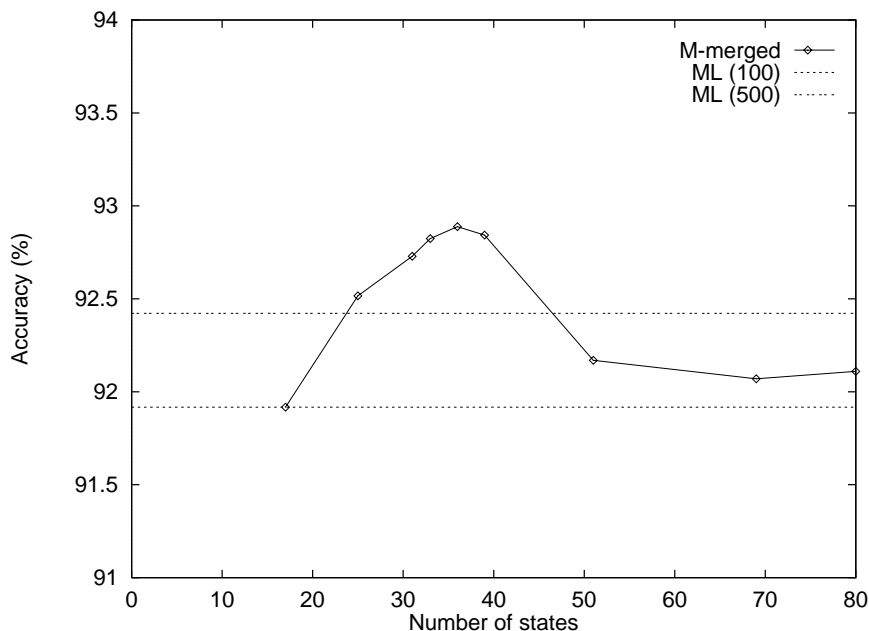


Figure 9. Extraction accuracy for multi-state models as states are merged. The dashed lines represent the baseline performances of the ML model, trained on all 500 headers and on the same 100 headers as the multi-state models.

89.4%. The ML model sets all transition parameters to their maximum likelihood estimates, and achieves the best result of 92.4% among this set of models. The Smooth model adds an additional smoothing count of one to each transition, so that all transitions have non-zero probabilities, but smoothing the transition probabilities does not improve tagging accuracy. For all models, the combination of the labeled and distantly-labeled data (L+D) negatively affects performance relative to the labeled data results. However, the interpolation of the distantly-labeled data with the labeled data (L*D) consistently provides several percentage points improvement in accuracy over training on the labeled data alone. We will refer back to the ML model results in the next comparisons, as the best representative of the models with one state per class.

4.3.2. Model selection – Deriving structure from data

The next set of models are learned from data; both the number of states and the transitions between the states are derived by state merging techniques. We first consider models built from a combination of automated and manual techniques. Starting from a neighbor-merged model of 805 states built from 100 randomly selected labeled training headers, states with the same class label are manually merged in an iterative

Table II. Extraction accuracy (%) for models learned from data compared to the best model that uses one state per class. Transition probabilities are estimated in three different ways.

Model	# States	# Transitions	L	L+D	L*D
ML	17	149	90.5	89.4	92.4
M-merged	36	164	91.3	90.5	92.9
V-merged	155	402	90.6	89.7	92.7

manner. The manual merges are performed by a domain expert, and only 100 of the 500 headers are used in order to keep the manual state selection process manageable. Transition counts are preserved throughout the merges to estimate maximum likelihood transition probabilities. Each state uses its smoothed class emission distribution estimated from the interpolation of the labeled and distantly-labeled data (L*D). Extraction performance, measured as the number of states decreases during the merging, is plotted in Figure 9. The dashed lines on the figure represent the baseline performances of the ML model, trained on all 500 headers and on the same 100 headers as the multi-state models. The models with multiple states per class outperform the ML model for both training conditions, particularly when 30 to 40 states are present. Note that when trained on the same amount of data, the multi-state models outperform the ML model for any number of states greater than one per class. The best performance of 92.9% is obtained by the model containing 36 states. We refer to this model as the **M-merged** model. This result shows that more complex model structure benefits extraction performance of HMMs on the header task.

We compare this result to the performance of a 155-state V-merged model created entirely automatically from all of the labeled training data. A summary of the results of the ML model, the M-merged model, and the V-merged model is presented in Table II. Once again, the L*D results are superior to the L and L+D results. In addition, both the M-merged and V-merged models outperform the ML model by a statistically significant margin in the L*D case, as determined with McNemar’s test ($p < 0.005$ each).

For comparison, a V-merged model trained only on the 100 headers used to train the M-merged model achieves an accuracy of 91.8% in the L*D case. The performance of the ML model trained on 100 headers, as shown in Figure 9, is 91.9%. It is interesting to note that for a very small amount of training data, the two models perform equivalently, but that with more training data, the V-merged model performs significantly

Table III. Individual class extraction accuracy (%) for the ML, M-merged and V-merged models. Classes noted in bold occur in distantly-labeled data.

Tag	ML		M-merged		V-merged	
	L	L*D	L	L*D	L	L*D
Abstract	100.0	100.0	98.4	98.7	99.7	99.7
Address	95.8	95.5	95.2	95.1	95.8	95.6
Affiliation	87.9	91.4	88.4	90.7	88.3	91.4
Author	95.8	97.7	95.1	97.2	95.5	97.8
Date	97.6	96.9	96.9	97.2	97.6	96.5
Degree	75.8	70.8	80.3	73.2	77.1	72.5
Email	89.2	89.0	87.5	86.9	89.2	89.2
Keyword	92.2	98.1	97.3	98.9	94.5	99.0
Note	84.9	85.1	88.1	89.0	85.1	86.2
Phone	93.7	93.1	89.7	87.4	93.1	92.0
Pubnum	65.0	65.0	61.3	60.6	65.0	65.0
Title	93.4	98.4	93.2	97.8	92.8	98.2
URL	80.6	83.3	41.7	41.7	63.9	66.7
Overall	90.5	92.4	91.3	92.9	90.6	92.7

better. This indicates that, while learning model structure can give better performance, it requires more training data. This requirement is expected because there are many more parameters to estimate in the V-merged model, because it has multiple states per class.

Yet, the M-merged model, trained on this same amount of data, attains a far superior accuracy of 92.9%.

Table III provides a closer look at the errors in each class for the ML, M-merged and V-merged models when using emission distributions trained on labeled (L) and interpolated (L*D) data. Classes for which there is distantly-labeled training data are indicated in bold. For several of the classes, such as title and author, there is a noticeable increase in accuracy when the distantly-labeled data is included. The poorest performing individual classes are the degree, publication number, and URL classes. The URL class has a particularly low accuracy for the M-merged model, when limited URL class examples in the 100 training headers probably kept the URL state from having transitions to and from as many states as necessary.

Table IV. Extraction accuracy (%) and test set perplexity (PP) for the ML and M-merged models after Baum-Welch training.

	ML		M-merged	
	Accuracy	Perplexity	Accuracy	Perplexity
Initial (L*D)	92.4	471	92.9	482
$\lambda = 0.5$	90.1	374	89.4	361
λ varies	89.7	364	88.8	349

4.3.3. Incorporating Unlabeled Data

Next, we demonstrate that using unlabeled data for parameter estimation does not help classification accuracy for this extraction task. Baum-Welch training, the standard technique for estimating HMM parameters from unlabeled data, produces new transition and emission parameter values that locally maximize the likelihood of the unlabeled data. Careful selection of the initial parameter values is thus essential for finding a good local maximum.

Five thousand unlabeled headers, composed of 287,770 word tokens are used as training data. Baum-Welch training is run on the ML and M-merged models. Model parameters are initialized to the maximum likelihood transition probabilities from the labeled data and the interpolated (L*D) emission distributions. The models are tested under three different conditions; the extraction results, as well as the model perplexities on the test set, are shown in Table IV. Perplexity is a measure of how well the HMMs model the data; a lower value indicates a model that assigns a higher likelihood to the observations from the test set.

The “initial” result is the performance of the models using the initial parameter estimates. These results are the same as the L*D case in Table II. After Baum-Welch training, the vocabulary words that do not occur in the unlabeled data are given a probability of zero in the newly-estimated emission distributions. Thus, the new distributions need to be smoothed; we choose to do this by interpolating them with the initial parameter estimates. Each state’s newly-estimated emission distribution is linearly interpolated with its initial distribution using a mixture weight of λ . For the “ $\lambda = 0.5$ ” setting, both distributions for each state use a weight of 0.5. Alternatively, the Viterbi paths of the labeled training data can be computed for each model using the “ $\lambda = 0.5$ ” emission distributions. The words emitted by each state are then used to estimate optimal mixture weights for the local and initial

distributions using the EM algorithm. These mixture weights are used in the “ λ varies” case.

Baum-Welch training degrades classification performance for both the ML and M-merged models. The lack of improvement in classification accuracy can be partly explained by the fact that Baum-Welch training maximizes the likelihood of the unlabeled data, not the classification accuracy. However, Baum-Welch training does result in improved predictive modeling of the header domain. This improvement is pointed out through the decrease in test set perplexity. The perplexity of the test set improves over the initial settings with Baum-Welch reestimation, and improves even further with careful selection of the emission distribution mixture weights. Merialdo (1994) finds a similar effect on tagging accuracy when training part-of-speech taggers using Baum-Welch training when starting from well-estimated initial parameter estimates.

4.4. DISCUSSION

Our experiments show that hidden Markov models do well at extracting important information from the headers of research papers. We achieve an accuracy of 92.9% over all classes of the headers, and class-specific accuracies of 97.8% for titles and 97.2% for authors. We have demonstrated that models that contain multiple states per class do provide increased extraction accuracy over models that use only one state per class. This improvement is due to more specific transition context modeling that is possible with more states. We expect that it is also beneficial to have localized emission distributions, which can capture distribution variations that are dependent on the position of the class in the header.

Distantly-labeled data has proven to be valuable in providing robust parameter estimates. The interpolation of distantly-labeled data provides a consistent increase in extraction accuracy for headers. In cases where little labeled training data is available, distantly-labeled data is a helpful resource.

The high accuracy of our header extraction results allows Cora to process and present search results effectively. The success of these extraction techniques is not limited to this single application, however. For example, applying these techniques to reference extraction achieves an accuracy of 93.4%. These techniques are also applicable beyond the domain of research papers. We have shown how distantly-labeled data can improve extraction accuracy; this data is available in electronic form for many other domains. For example, lists of names (with relative frequencies) are provided by the U.S Census Bureau, street names and

addresses can be found in online phone books, and discussion groups and news sites provide focused, topic-specific collections of text. These sources of data can be used to derive class-specific words and relative frequencies, which can then be applied to HMM development for a vast array of domain-specific portals.

5. Classification into a Topic Hierarchy

Topic hierarchies are an efficient way to organize, view and explore large quantities of information that would otherwise be cumbersome. The U.S. Patent database, Yahoo, MEDLINE and the Dewey Decimal system are all examples of topic hierarchies that exist to make information more manageable.

As Yahoo has shown, a topic hierarchy can be a useful, integral part of a portal. Many search engines (*e.g.* Lycos, Excite, and HotBot) now display hierarchies on their front page. This feature is equally or more valuable for domain-specific Internet portals. We have created a 70-leaf hierarchy of computer science topics for Cora, part of which is shown in Figures 1 and 10.

A difficult and time-consuming part of creating a hierarchy is populating it with documents by placing them into the correct topic nodes. Yahoo has hired large numbers of people to categorize web pages into their hierarchy. The U.S. patent office also employs people to perform the job of categorizing patents. In contrast, we automate the process of placing documents into leaf nodes of the hierarchy with learned text classifiers.

Traditional text classification algorithms learn representations from a set of labeled data. Unfortunately, these algorithms typically require on the order of hundreds of examples per class. Since labeled data is tedious and expensive to obtain, and our class hierarchy is large, using the traditional supervised approach is not feasible. In this section we describe how to create a text classifier by bootstrapping without any labeled documents, using only a few keywords per class and a class hierarchy. Both of these information sources are easily obtained. Keywords are quicker to generate than even a small number of labeled documents. Many classification problems naturally come with hierarchically-organized classes.

Bootstrapping is a general framework for iteratively improving a learner using unlabeled data. Bootstrapping is initialized with a small amount of seed information that can take many forms. Each iteration has two steps: (1) labels are estimated for unlabeled data from the currently learned model, and (2) the unlabeled data and these

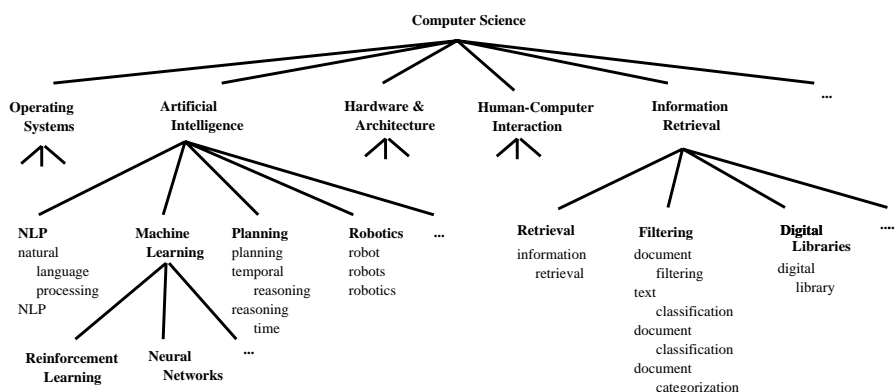


Figure 10. A subset of Cora’s computer science hierarchy with the complete keywords for each of several categories. These keywords are used to initialize bootstrapping.

estimated labels are incorporated as training data into the learner. Bootstrapping approaches have been used for information extraction (Riloff & Jones, 1999), word sense disambiguation (Yarowsky, 1995), and hypertext classification (Blum & Mitchell, 1998).

Our algorithm for text classification is initialized by using the keywords to generate preliminary labels for some documents by term-matching. The bootstrapping iterations are EM steps that use unlabeled data and hierarchical shrinkage to estimate parameters of a naive Bayes classifier. An outline of the entire algorithm is presented in Table V. In experimental results, we show that the learned classifier has accuracy that approaches human agreement levels for this domain.

5.1. INITIALIZING BOOTSTRAPPING WITH KEYWORDS

The initialization step in the bootstrapping process uses the keywords to generate preliminary labels for as many of the unlabeled documents as possible. For each class a few keywords are generated by a human trainer. Figure 10 shows examples of the number and type of keywords given in our experimental domain—the human-provided keywords are shown in the nodes in non-italic font.

We generate preliminary labels from the keywords by term-matching in a rule-list fashion: for each document, we step through the keywords and place the document in the category of the first keyword that matches. Since we provide only a few keywords for each class, classification by keyword matching is both inaccurate and incomplete. Keywords tend to provide high-precision and low-recall; this brittleness will leave many documents unlabeled. Some documents will match

Table V. An outline of the bootstrapping algorithm described in Sections 5.1 and 5.2.

-
- **Inputs:** A collection of unlabeled training documents, a class hierarchy, and a few keywords for each class.
 - Generate preliminary labels for as many of the unlabeled documents as possible by term-matching with the keywords in a rule-list fashion.
 - Initialize all the λ_j 's to be uniform along each path from a leaf class to the root of the class hierarchy.
 - Iterate the EM algorithm:
 - **(M-step)** Build the maximum likelihood multinomial at each node in the hierarchy given the class probability estimates for each document (Equations 10 and 11). Normalize all the λ_j 's along each path from a leaf class to the root of the class hierarchy so that they sum to 1.
 - **(E-step)** Calculate the expectation of the class labels of each document using the classifier created in the M-step (Equation 12). Increment the new λ_j 's by attributing each word of held-out data probabilistically to the ancestors of each class.
 - **Output:** A naive Bayes classifier that takes an unlabeled test document and predicts a class label.
-

keywords from the wrong class. In general we expect the low recall of the keywords to be the dominating factor in overall error. In our experimental domain, for example, 59% of the unlabeled documents do not contain any keywords.

5.2. THE BOOTSTRAPPING ITERATIONS

The goal of the bootstrapping iterations is to generate a naive Bayes classifier from seed information and the inputs: the (inaccurate and incomplete) preliminary labels, the unlabeled data and the class hierarchy. Many bootstrapping algorithms assign labels to the unlabeled data, and then choose just a few of these to incorporate into training at each step. In our algorithm, we take a different approach. At each bootstrapping step we assign *probabilistic* labels to *all* the unlabeled data, and incorporate the entire set into training. Expectation-Maximization is the bootstrapping process we use to iteratively estimate these probabilistic labels and the parameters of the naive Bayes classifier. We begin a detailed description of the bootstrapping iteration with a short overview of supervised naive Bayes text classification, then proceed to explain EM as a bootstrapping process, and conclude by presenting

hierarchical shrinkage, an augmentation to basic EM estimation that uses the class hierarchy.

5.2.1. *The naive Bayes framework*

We build on the framework of multinomial naive Bayes text classification (Lewis, 1998; McCallum & Nigam, 1998). It is useful to think of naive Bayes as estimating the parameters of a probabilistic generative model for text documents. In this model, first the class of the document is selected. The words of the document are then generated based on the parameters of a class-specific multinomial (*i.e.* unigram model). Thus, the classifier parameters consist of the class prior probabilities and the class-conditioned word probabilities. Each class, c_j , has a document frequency relative to all other classes, written $P(c_j)$. For every word w_t in the vocabulary V , $P(w_t|c_j)$ indicates the frequency that the classifier expects word w_t to occur in documents in class c_j .

In the standard supervised setting, learning of the parameters is accomplished using a set of labeled training documents, \mathcal{D} . To estimate the word probability parameters, $P(w_t|c_j)$, we count the frequency with which word w_t occurs among all word occurrences for documents in class c_j . We supplement this with Laplace smoothing that primes each estimate with a count of one to avoid probabilities of zero. Let $N(w_t, d_i)$ be the count of the number of times word w_t occurs in document d_i , and define $P(c_j|d_i) \in \{0, 1\}$, as given by the document's class label. Then, the estimate of the probability of word w_t in class c_j is:

$$P(w_t|c_j) = \frac{1 + \sum_{d_i \in \mathcal{D}} N(w_t, d_i) P(c_j|d_i)}{|V| + \sum_{s=1}^{|V|} \sum_{d_i \in \mathcal{D}} N(w_s, d_i) P(c_j|d_i)}. \quad (10)$$

The class prior probability parameters are set in the same way, where $|\mathcal{C}|$ indicates the number of classes:

$$P(c_j) = \frac{1 + \sum_{d_i \in \mathcal{D}} P(c_j|d_i)}{|\mathcal{C}| + |\mathcal{D}|}. \quad (11)$$

Given an unlabeled document and a classifier, we determine the probability that the document belongs in class c_j using Bayes' rule and the naive Bayes assumption—that the words in a document occur independently of each other given the class. If we denote $w_{d_i,k}$ to be the k th word in document d_i , then classification becomes:

$$\begin{aligned} P(c_j|d_i) &\propto P(c_j)P(d_i|c_j) \\ &\propto P(c_j) \prod_{k=1}^{|d_i|} P(w_{d_i,k}|c_j). \end{aligned} \quad (12)$$

Empirically, when given a large number of training documents, naive Bayes does a good job of classifying text documents (Lewis, 1998). More complete presentations of naive Bayes for text classification are provided by Mitchell (1997) and McCallum and Nigam (1998).

5.2.2. *Parameter estimation from unlabeled data with EM*

In a standard supervised setting, each document comes with a label. In our bootstrapping scenario, the documents are unlabeled, except for the preliminary labels from keyword matching that are incomplete and not completely correct. In order to estimate the parameters of a naive Bayes classifier using all the documents, we use EM to generate probabilistically-weighted class labels. This results in classifier parameters that are more likely given all the data.

EM is a class of iterative algorithms for maximum likelihood or maximum a posteriori parameter estimation in problems with incomplete data (Dempster, Laird, & Rubin, 1977). Given a model of data generation, and data with some missing values, EM iteratively uses the current model to estimate the missing values, and then uses the missing value estimates to improve the model. Using all the available data, EM will locally maximize the likelihood of the parameters and give estimates for the missing values. In our scenario, the class labels of the documents are the missing values.

In implementation, using EM for bootstrapping is an iterative two-step process. Initially, the parameter estimates are set in the standard naive Bayes way from just the preliminarily labeled documents. Then we iterate the E- and M-steps. The E-step calculates probabilistically-weighted class labels, $P(c_j|d_i)$, for every document using the classifier and Equation 12. The M-step estimates new classifier parameters using all the documents, by Equations 10 and 11, where $P(c_j|d_i)$ is now continuous, as given by the E-step. We iterate the E- and M-steps until the classifier converges. The initialization step from the preliminary labels identifies a starting point for EM to find a good local maxima for the classification task.

In previous work (Nigam, McCallum, Thrun, & Mitchell, 1999), we have shown this technique significantly increases text classification accuracy when given limited amounts of labeled data and large amounts of unlabeled data. Here, we use the preliminary labels to provide the starting point for EM. The EM iterations both correct the preliminary labels and complete the labeling for the remaining documents.

5.2.3. *Improving sparse data estimates with shrinkage*

Even when provided with a large pool of documents, naive Bayes parameter estimation during bootstrapping will suffer from sparse data problems because there are so many parameters to estimate ($|V||C| + |C|$). Fortunately we can further alleviate the sparse data problem by leveraging the class hierarchy with a statistical technique called *shrinkage*.

Consider trying to estimate the probability of the word “intelligence” in the class NLP. This word should clearly have non-negligible probability there; however, with limited training data we may be unlucky, and the observed frequency of “intelligence” in NLP may be very far from its true expected value. One level up the hierarchy, however, the Artificial Intelligence class contains many more documents (the union of all the children). There, the probability of the word “intelligence” can be more reliably estimated.

Shrinkage calculates new word probability estimates for each leaf class by a *weighted average* of the estimates on the path from the leaf to the root. The technique balances a trade-off between specificity and reliability. Estimates in the leaf are most specific but unreliable; further up the hierarchy estimates are more reliable but unspecific. We can calculate mixture weights for the averaging that are guaranteed to maximize the likelihood of held-out data with the EM algorithm during bootstrapping.

One can think of hierarchical shrinkage as a generative model that is slightly augmented from the one described in Section 5.2.1. As before, a class (leaf) is selected first. Then, for each word position in the document, an ancestor of the class (including itself) is selected according to the shrinkage weights. Then, the word itself is chosen based on the multinomial word distribution of that ancestor. If each word in the training data were labeled with which ancestor was responsible for generating it, then estimating the mixture weights would be a simple matter of maximum likelihood estimation from the ancestor emission counts. But these ancestor labels are not provided in the training data, and hence we use EM to fill in these missing values. During EM, we estimate these vertical mixture weights concurrently with the class word probabilities.

More formally, let $\{P^1(w_t|c_j), \dots, P^k(w_t|c_j)\}$ be word probability estimates, where $P^1(w_t|c_j)$ is the maximum likelihood estimate using training data just in the leaf, $P^2(w_t|c_j)$ is the maximum likelihood estimate in the parent using the training data from the union of the parent’s children, $P^{k-1}(w_t|c_j)$ is the estimate at the root using all the training data, and $P^k(w_t|c_j)$ is the uniform estimate ($P^k(w_t|c_j) = 1/|V|$). The interpolation weights among c_j ’s “ancestors” (which we de-

fine to include c_j itself) are written $\{\lambda_j^1, \lambda_j^2, \dots, \lambda_j^k\}$, where $\sum_{a=1}^k \lambda_j^a = 1$. The new word probability estimate based on shrinkage, denoted $\check{P}(w_t|c_j)$, is then

$$\check{P}(w_t|c_j) = \lambda_j^1 P^1(w_t|c_j) + \dots + \lambda_j^k P^k(w_t|c_j). \quad (13)$$

The λ_j vectors are calculated by the iterations of EM. In the E-step we calculate for each class c_j and each word of unlabeled held-out data \mathcal{H} , the probability that the word was generated by the i th ancestor. In the M-step, we normalize the sum of these expectations to obtain new mixture weights λ_j . Without the use of held-out data, all the mixture weights would concentrate in the leaves.

Specifically, we begin by initializing the λ mixture weights along each path from a leaf to a uniform distribution. Let $\beta_j^a(w_{d_{i,k}})$ denote the probability that the a th ancestor of c_j was used to generate word occurrence $w_{d_{i,k}}$. The E-step consists of estimating the β 's:

$$\beta_j^a(w_{d_{i,k}}) = \frac{\lambda_j^a P^a(w_{d_{i,k}}|c_j)}{\sum_m \lambda_j^m P^m(w_{d_{i,k}}|c_j)}. \quad (14)$$

In the M-step, we derive new and guaranteed improved weights, λ , by summing and normalizing the β 's:

$$\lambda_j^a = \frac{\sum_{w_{d_{i,k}} \in \mathcal{H}} \beta_j^a(w_{d_{i,k}}) P(c_j|d_i)}{\sum_b \sum_{w_{d_{i,k}} \in \mathcal{H}} \beta_j^b(w_{d_{i,k}}) P(c_j|d_i)}. \quad (15)$$

The E- and M-steps iterate until the λ 's converge. These weights are then used to calculate new shrinkage-based word probability estimates, as in Equation 13. Classification of new test documents is performed just as before (Equation 12), where the Laplace estimates of the word probability estimates are replaced by shrinkage-based estimates.

A more complete description of hierarchical shrinkage for text classification is presented by McCallum, Rosenfeld, Mitchell, and Ng (1998).

5.3. EXPERIMENTAL RESULTS

In this section, we provide empirical evidence that bootstrapping a text classifier from unlabeled data can produce a high-accuracy text classifier. As a test domain, we use computer science research papers. We have created a 70-leaf hierarchy of computer science topics, part of which is shown in Figure 10. Creating the hierarchy took about 60 minutes, during which we examined conference proceedings, and explored computer science sites on the Web. Selecting a few keywords associated with each node took about 90 minutes. A test set was created

Table VI. Classification results with different techniques: keyword matching, naive Bayes, Bootstrapping and Human agreement. The classification accuracy, and the number of labeled, keyword-matched preliminarily-labeled (P-Labeled), and unlabeled documents used by each variant are shown.

Method	# Labeled	# P-Labeled	# Unlabeled	Accuracy
Keyword Matching	—	—	—	45%
Naive Bayes	100	—	—	30%
Naive Bayes	399	—	—	47%
Naive Bayes	—	12,657	—	47%
Bootstrapping	—	12,657	—	63%
Bootstrapping	—	12,657	18,025	66%
Human Agreement	—	—	—	72%

by expert hand-labeling of a random sample of 625 research papers from the 30,682 papers in the Cora archive at the time we began these experiments. Of these, 225 (about one-third) did not fit into any category, and were discarded—resulting in a 400 document test set. Labeling these documents took about six hours. Some of the discarded papers were outside the area of computer science (*e.g.* astrophysics papers), but most of these were papers that with a more complete hierarchy would be considered computer science papers. The class frequencies of the data are not drastically skewed; on the test set, the most populous class accounted for only 7% of the documents.

Each research paper is represented as the words of the title, author, institution, references, and abstract. A detailed description of how these segments are automatically extracted is provided in Section 4. Words occurring in fewer than five documents and words on a standard stoplist were discarded. No stemming was used. Bootstrapping was performed using the algorithm outlined in Table V.

Table VI shows results with different classification techniques used. The rule-list classifier based on the keywords alone provides 45% accuracy.⁵ As an interesting time comparison, about 100 documents could have been labeled in the time it took to generate the keyword lists. Naive Bayes accuracy with 100 labeled documents is only 30%. It takes about four times as much labeled training data to provide comparable accuracy to simple keyword matching; with 399 labeled documents (using our test set in a leave-one-out-fashion), naive Bayes reaches 47%.

⁵ The 43% of documents in the test set containing no keywords are not assigned a class by the rule-list classifier, and are counted as incorrect.

This result alone shows that hand-labeling sets of data for supervised learning can be expensive in comparison to alternate techniques.

When running the bootstrapping algorithm, 12,657 documents are given preliminary labels by keyword matching. EM and shrinkage incorporate the remaining 18,025 documents, “fix” the preliminary labels and leverage the hierarchy; the resulting accuracy is 66%. As an interesting comparison, agreement on the test set between two human experts was 72%. These results show that our bootstrapping algorithm can generate competitive classifications without the use of large hand-labeled sets of data.

A few further experiments reveal some of the inner-workings of bootstrapping. If we build a naive Bayes classifier in the standard supervised way from the 12,657 preliminarily labeled documents the classifier gets 47% accuracy. This corresponds to the performance for the first iteration of bootstrapping. Note that this matches the accuracy of traditional naive Bayes with 399 labeled training documents, but that it requires less than a quarter the human labeling effort. If we run bootstrapping without the 18,025 documents left unlabeled by keyword matching, accuracy reaches 63%. This indicates that shrinkage and EM on the preliminarily labeled documents is providing substantially more benefit than the remaining unlabeled documents.

5.4. DISCUSSION

One explanation for the small impact of the 18,025 documents left unlabeled by keyword matching is that many of these do not fall naturally into the hierarchy. Remember that about one-third of the 30,000 documents fall outside the hierarchy. Most of these will not be given preliminary labels by keyword matching. The presence of these outlier documents skews EM parameter estimation. A more inclusive computer science hierarchy would allow the unlabeled documents to benefit classification more.

However, even without a complete hierarchy, we could use these documents if we could identify these outliers. Some techniques for robust estimation with EM are discussed by McLachlan and Basford (McLachlan & Basford, 1988). One specific technique for these text hierarchies is to add extra leaf nodes containing uniform word distributions to each interior node of the hierarchy in order to capture documents not belonging in any of the predefined topic leaves. This should allow EM to perform well even when a large percentage of the documents do not fall into the given classification hierarchy. A similar approach is also planned for research in topic detection and tracking

(TDT) (Baker, Hofmann, McCallum, & Yang, 1999). Experimentation with these techniques is an area of ongoing research.

In other future work we will investigate different ways of initializing bootstrapping, with keywords and otherwise. We plan to refine our probabilistic model to allow for documents to be placed in interior hierarchy nodes, documents to have multiple class assignments, and classes to be modeled with multiple mixture components. We are also investigating principled methods of re-weighting the word features for “semi-supervised” clustering that will provide better discriminative training with unlabeled data.

Here, we have shown the application of our bootstrapping process to populating a hierarchy for Cora, a portal for computer science research papers. Topic hierarchies are often an integral part of most portals, although they are typically hand-built and maintained. The techniques demonstrated here are generally applicable to any topic hierarchy, and should become a powerful tool for populating topic hierarchies with a minimum of human effort.

6. Related Work

Several related research projects investigate the gathering and organization of specialized information on the Internet. The WebKB project (Craven, DiPasquo, Freitag, McCallum, Mitchell, Nigam, & Slattery, 1998) focuses on the collection and organization of information from the Web into knowledge bases. This project also has a strong emphasis on using machine learning techniques, including text classification and information extraction, to promote easy re-use across domains. Two example domains, computer science departments and companies, have been developed.

The CiteSeer project (Bollacker et al., 1998) has also developed a search engine for computer science research papers. It provides similar functionality for searching and linking of research papers, but does not currently provide a topic hierarchy of the field. CiteSeer focuses on the domain of research papers, and has particularly strong features for autonomous citation indexing and the viewing of the textual context in which a citation was made. The project does not aim to automate with machine learning the construction of Internet portals on arbitrary domains.

The New Zealand Digital Library project (Witten, Nevill-Manning, McNab, & Cunningham, 1998) has created publicly-available search engines for domains from computer science technical reports to song melodies. The emphasis of this project is on the creation of full-text

searchable digital libraries, and not on machine learning techniques that can be used to autonomously generate such repositories. The web sources for their libraries are manually identified. No high-level organization of the information is given. No information extraction is performed and, for the paper repositories, no citation linking is provided.

The WHIRL project (Cohen, 1998) is an effort to integrate a variety of topic-specific sources into a single domain-specific search engine. Two demonstration domains of computer games and North American birds integrate information from many sources. The emphasis is on providing soft matching for information retrieval searching. Information is extracted from web pages by hand-written extraction patterns that are customized for each web source. Recent WHIRL research (Cohen & Fan, 1999) learns general wrapper extractors from examples.

7. Conclusions and Future Work

The amount of information available on the Internet continues to grow exponentially. As this trend continues, we argue that not only will the public need powerful tools to help them sort through this information, but the *creators* of these tools will need intelligent techniques to help them build and maintain these services. This paper has shown that machine learning techniques can significantly aid the creation and maintenance of portals and domain-specific search engines. We have presented new research in reinforcement learning, text classification and information extraction towards this end.

In addition to the future work discussed earlier, we also see many other areas where machine learning can further automate the construction and maintenance of domain-specific search engines. For example, text classification can decide which documents on the Web are relevant to the domain. Unsupervised clustering can automatically create a topic hierarchy and generate keywords. Citation graph analysis can identify seminal papers. We anticipate developing a suite of many machine learning techniques so that the creation of portals can be accomplished quickly and easily.

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