Web-Prospector – An Automatic, Site-Wide Wrapper Induction Approach for Scientific Deep-Web Databases

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Abstract: Wrapper induction techniques traditionally focus on learning wrappers based on examples from one *class* of Web pages, i.e. from Web pages that are all similar in structure and content. Thereby, traditional wrapper induction targets the understanding of Web pages generated from a database using the same generation template as observed in the example set. Applying such techniques to Web sites generated from biological databases, however, we found that there is a need for wrapping of structurally diverse web pages from *multiple classes* making the problem more challenging. Furthermore, we observed that such scientific web sites do not just provide mere data, but they also tend to provide schema information in terms of data labels – giving further cues for solving the web site wrapping task. In this paper we present a novel approach to automatic information extraction from whole Web sites that considers the novel challenge and takes advantage of the additional clues commonly available in scientific deep Web databases. The solution consists of a sequence of steps: 1. classification of similar Web pages into classes, 2. discovery of these classes and 3. wrapper induction for each class. Our approach thus allows us to perform unsupervised information retrieval from across an entire Web site. We test our algorithm against three real-world biochemical deep Web sources and report our preliminary results, which are very promising.

1. Introduction

Hundreds of freely-accessible databases are available on the Web in the Life Sciences domain, covering areas such as Genomics, Proteomics, Systems Biology and Micro Array Gene Expression, to name a few. These databases often provide complementary data, pertaining to narrow specialized sub-domains. Life Science researchers thus need to search, collect and aggregate data from multiple online resources. This Web site *hopping* is time consuming and error-prone, whereby a user must learn search interfaces of various Web sites, perform multiple copy-paste actions, create temporary text-files and manually link extracted records of interest.

"Deep Web" research aims to *virtually* integrate such Web-accessible databases, provide a unified query interface and, typically, aggregate query results. Deep Web data integration consists of a number of distinct sub-tasks (See [CC06] for a survey):

1. *Source Searching and Clustering* – Searching domain-specific databases on the Web. ([BF05], [HTC04], [Lu06])

2. *Interface Extraction* – Learning query capabilities of forms ([Ku03], [ZHC04])
3. *Interface Matching* – Determining semantic correspondences between query-form attributes across sources. ([Wa04], [Ma05], [WDT06], [HC03])
4. *Interface Merging & Query Translation* – Deriving a unified query interface, translating queries from this interface to source interfaces. ([He03], [KLC05])
5. *Wrapper Generation/Data Extraction* – Learning templates to extract data from result pages. (See section 5 for related work)

We focus on unsupervised wrapper induction and data extraction in this paper. Automatic wrapper induction has received considerable attention in recent years. However, most techniques learn wrappers for one class of Web pages. They assume structurally and content-wise similar pages are manually provided as an input for their wrapper induction methods.

As we shall explain in section 2, in our target domain, data are spread across multiple pages of a Web site, which often differ considerably in their structure and layout (template) as well as content. We therefore need an approach to automatically group similar pages in a Web site for our wrapper induction process. Additionally, we need to automatically discover the Web-site structure, so that we may predict which wrapper to use for a Web page encountered in that Web site. These requirements go beyond traditional wrapper induction methods. We term this compound problem of Web-page classification, site-structure discovery and wrapper induction as *Site-Wide Wrapper Induction*. Though this task is extremely hard in general, in our target domain, i.e. Web-accessible Life Science databases, we may benefit from additional cues in terms of labeling of data. Consequently, we restrict our attention to Web pages from Web sites with labeled data.

In order to solve the challenge of Site-Wide Wrapper Induction in our target domain, we provide the following original contributions in this paper:

I. A novel approach for unsupervised wrapper induction to extract labeled data (Section 3.1). The approach is unsupervised as sample pages (required for induction) belonging to the same *class* or *template* are collected automatically, and no labeling is required.
II. An original integrated approach for Web-page classification and site structure discovery (Section 3.2)
III. An automatic mechanism for detecting and correcting errors in our wrapper learning process (Section 3.3)

The rest of this paper is organized as follows. Section 2 makes some observations about deep Web scientific sources. Based on these observations, we formulate our problem and present our approach for site-wide wrapper induction in section 3. Section 4 presents our results, followed by a review of the related work and comparison to our contributions in section 5. We conclude the paper in section 6 with a brief discussion about future work.

2. Life Science Databases on the Web: Observations and Implications

We observe the following about result pages of Life Science Web sources:

I) Structured Data – The results are highly structured. This owes to the fact that the backend relational schemas are very complex, and entities in scientific domains generally have complex relations and associations.

II) Highly Dynamic Page Structures – Data fields that are NULL are often omitted from the results displayed, resulting in pages with widely varying structure. A wrapper induction method which ties its learning process to the page structure only would require numerous training pages, covering all possibilities of data arrangement. One drawback of such an approach would be the need for a large number of input seed queries to probe the deep Web source. Additionally, this would make the learning process slow and put strain on the Web database. A related observation is that Web pages undergo frequent updates [KK02]. An approach which circumvents the need to learn the page structure would hence be desirable.

III) Labeled Data – Scientific data require precision and clear annotation. A natural consequence of this observation is that scientific data are labeled and, often, annotated to controlled vocabularies. This differs from other domains such as E-commerce, where many data fields are often unlabeled because they have become self-explaining in the public domain (e.g. price, title). This labeling can be exploited to not only help determine data regions, but can also serve as anchors for these data regions, allowing us to disregard the portion of the page which does not contain data. We further observe that labels for the same real-world entity can be different across Web pages of the same source. Finally, labels of real-world entities, such as names of biological concepts, rarely change, which can be beneficial with respect to wrapper maintenance.

IV) Rich Site Structure – Data is scattered across multiple Web pages. This gives such Web sites a comprehensive structure. Therefore, the wrapper must be able to navigate through the result pages to extract data. We also observe that some data fields, together with their labels, reappear on multiple pages. This reoccurrence can be used for mutual reinforcement, to detect and correct errors in the wrapper induction process.

One final observation is that of Web service API access. While some Life Science databases do provide such APIs, our survey[1] of 100 online databases showed that only 11 sources provide programmatic access, and even among these the coverage of the database in some cases is not complete. Therefore, Web pages still remain the primary form of data dissemination.

These observations serve to clarify the two broad characteristics of our work: Firstly, at the Web site level, the challenge is to extract data from a number of pages, generated from many templates. This requires determining homogenous clusters of pages having similar templates so that we can induce wrappers for these clusters. Another implicit requirement is that of learning the structure of a Web site through navigational steps. This is essential because our system needs to know which wrapper to apply during data extraction while traversing through the Web site. Secondly, at the Web page level, the

[1] Databases indexed by the Nucleic Acids Research Journal (http://www3.oup.co.uk/nar/database/c/). Complete survey available at http://sabiork.villa-bosch.de/index.html/survey.html

presence of labeled data gives us the opportunity to segment data records and fields based on these labels, and to accommodate the dynamic structure of pages by using these labels to extract data, rather than analyzing and learning the entire Web page structure in a regular expression-like syntax. However, these labels must themselves be identified. Although the vocabulary for labels converges across different sources in a domain [CHZ04], it is not trivial to manually provide a set of possible labels (which can number in their hundreds) to aid in identification of data regions. Therefore, a desirable approach would be to automatically identify these labels.

3. The Web-Prospector Wrapper Induction Approach

We follow the divide-and-conquer approach and present our algorithm for page-level wrapper induction in section 3.1. Subsequently, in section 3.2, we describe how this algorithm is used in our site-wide wrapper-induction method. In section 3.3, we discuss a technique to automatically detect and correct certain erroneous results of our induction algorithm presented in section 3.1.

3.1 Page-Level Wrapper Induction

Our wrapper induction algorithm relies on multiple sample *instance pages* from a *class of pages*. We borrow this terminology from [CMM01], which describes *a class of pages* in a site as a collection of pages which are generated by the same server-side script or program. Different inputs to this script result in different *instance pages*. We clarify this further using Figure 1, our running example, which shows two instance pages of a class of pages[2]. The wrapper induction algorithm is shown in Figure 2.

Entry	C00221 Compound
Name	beta-D-Glucose
Formula	C6H12O6
Mass	180.0634
Reaction	R00026 R01520 R01521 R01522 R01600 R01601 R01602 R02187 R02887 R03256 R04783 R06077 R06092 R06110 R06144
Enzyme	1.1.1.47 1.1.3.4 1.1.3.5 2.7.1.1 2.7.1.2 2.7.1.63 3.1.6.3 3.2.1.21 3.2.1.23 3.2.1.85 5.1.3.3

Entry	C00185 Compound
Name	Cellobiose; 1-beta-D-Glucopyranosyl-4-D-glucopyranose
Formula	C12H22O11
Mass	342.1162
Reaction	R00026 R00306 R00952 R01441 R01442 R01443 R01444 R01445 R02365 R02886
Enzyme	1.1.99.18 2.4.1.20 2.7.1.85 3.2.1.4 3.2.1.21 3.2.1.74 3.2.1.91 5.1.3.11

Figure 1: Our running example – The results obtained by probing KEGG Compound with C00221 and C00185 respectively.

[2] From KEGG [Ka02]. Portions of these pages have been removed to simplify the discussion and to save space, while remaining true to the challenges encountered

We note that, upon querying, the initial response pages generated by a deep Web source belong to the same class[3]. Therefore, we can probe a source with different inputs, and use the resulting initial pages to learn a wrapper, without having to cluster similarly structured pages. In fact, for a given Web site, the site-wide wrapper induction process is bootstrapped by using these initial result pages and learning a wrapper for this class.
Briefly, the algorithm compares text entries on the sample pages and identifies some (possibly not all) data entries among them. These data entries are subsequently used to identify bigger data regions, so that more data entries can be discovered. A label is then selected for each data entry from text entries outside the data regions, based on vicinity. Our approach is based on the DOM[4] representation of Web pages, and uses XPath[5] for performing the above operations on the DOM tree. The output of the wrapper is a collection of XPath expressions, each pointing to a label and associated data region.

```
   Input: n Web pages P
   Output: R: L => X_gr        //L is a set of labels. X_gr is a set of XPaths to data entries. R is a map from
                               each label l in L to each data XPath dx in X_gr.
   Start
   For each sample page p_i in P{
1        For each text entry t in p_i
2                If t is unique to p_i
                                Add t to D_i;
                        Else
                                Add t to O_i; }
3  For each p_i in P{
           X^d_i = get_XPath(D_i);
           X^o_i = get_XPath(O_i);}
4  D_i', O_i', X^o_i', X^d_i' = reclassify(X^o_i, X^d_i);      // grow the data regions, and reclassify data
   For each XPath dx in X^d_i'{
5          Find closest XPath lx in X^o_i';          // search for XPath of most suitable label in O
           If the corresponding text (label) in O_i' is not in R
                   X = {dx};                         // X is a set containing all data XPaths associated
                                                        with one label
           Else
                   X = X ∪ {dx};
             R = lx => X;}              // XPath of label is mapped to set of corresponding data XPaths
   For each lx in R{
6          Generalize corresponding X to X_g ;    // Create a single XPath from all paths in set X
7          Find relative path X_gr from lx to X_g ;   // relative path from label to data
           Replace X with  X_gr ;
           Replace lx with l';                       // replace Xpath with the corresponding label
   }
   End
```

Figure 2: Wrapper Induction Algorithm

[3] In certain cases, probing a source with an imprecise keyword leads to a disambiguation step. This is a separate research issue and we don't address it in this paper. We assume exact keywords are used to perform the search, as explained in Figure 2.

[4] W3C. Document Object Model. http://www.w3.org/DOM/

[5] W3C. XML Path Language (XPath 2.0) Recommendation. http://www.w3.org/TR/xpath20/

We now explain each step of the algorithm in detail using our running example. Each step is annotated to its corresponding location in the algorithm in Figure 2.
1. The two HTML pages are converted to well-formed XHTML using an HTML-parsing library, i.e. TagSoup[6], so that standard XML tools can be applied to them. Additionally, these pages are subjected to pre-processing, where certain visual formatting features are removed. This is done so that a logically single text entry is located under the same text node in the DOM tree. For example, if there is an underline or bold HTML tag on one word in a sentence, it splits the text of the sentence into more than one text node. While visually this formatting might be important, logically it segments single entries into multiple ones, which is undesirable. Finally, each page is *screen-scraped* to obtain a set T of values contained in all text nodes. Both sets (T_1 and T_2 in our example) thus contain a union of presentation text, labels and data entries.

2. We compare both sets to initially classify some data entries. Mutually exclusive entries in T_1 and T_2 are classified as data entries (D_1, D_2), and the remaining as non-data entries, or "*Other"* (O_1, O_2). For example:

```
D1 = {C00221, beta-D-Glucose, …, R01520, 1.1.1.47,…}
D2 = {C00185, Cellobiose,…, R00306, 1.1.99.18,… }
O1 = {Entry, Name,…, Reaction, R00026, Enzyme,…, 3.2.1.21}
O2 = {Entry, Name,…, Reaction, R00026, Enzyme,…, 3.2.1.21}
```

Notice that since the data entry R00026 occurs in both instance pages, it is erroneously classified as *Other* at this point.

3. We compute XPath expressions for each entry in the above sets. The expression determines the unique path along the DOM tree for the XHTML file, from the root node to the node containing the entry. For example, the XPath for C00221 is:

```
html/body/…/code[1]/table[1]/tr[1]/td[1]/code[1]/text()
```

4. We use the XPath expressions to reclassify some data entries which might have been wrongly classified in the previous step (such as R00026, 3.2.1.21). This can be considered as *growing* of a data region, whereby data entries are used to reclassify other entries in their vicinity as data, based on their relative positions in the DOM tree. This reclassification step compares an XPath of a data entry with that of an entry not classified as data by applying the following two rules:

Rule 1 (Last Element Node Rule): If two XPaths are identical and differ only at the ordering of the last element node, and this last element node in the data XPath precedes the last element node in the non-data XPath, the non-data entry is re-classified as data.

This rule can be explained from an example in Figure 3(a). As shown in the figure, this rule uses data elements to automatically grow data regions towards the right in a table-row. While Figure 3 only shows the example of a table, it is important to emphasize that since this rule is independent of tag names, it works on tags other than those associated to HTML tables, for example, downwards in a list or in a succession of anchor tags. For instance, for the latter case, the XPaths for successive anchor tags (even if they are separated by line breaks) could be: `html/body/a[1]`, `html/body/a[2]`

[6] A SAX-compliant HTML Parser. http://home.ccil.org/~cowan/XML/tagsoup/

It is easy to see from the above example that this rule grows data regions in many types of HTML structures.

Rule 2 (Penultimate Element Node Rule) If the two XPaths are identical and differ only at the ordering of the penultimate element node, and this penultimate element node in the data XPath precedes the penultimate element node in the non-data XPath, the non-data entry is re-classified as a data entry

This rule is similar to Rule 1, except it grows data regions down a table-column as shown in Figure 3(b)

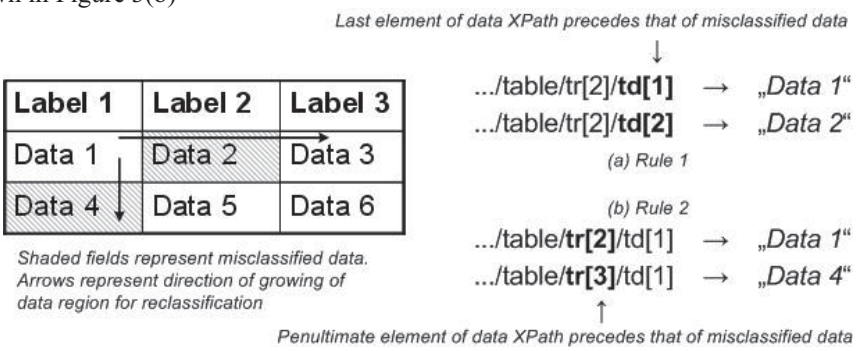

Figure 3: Growing of data region using (a) Rule 1 - Last Element Node Rule (b) Rule 2 - Penultimate Element Node Rule

We note that our rules for growing data-regions operate in only two directions. This is based on the observation that labels generally occur above or towards the left of data [WL03]. Therefore, we restrict our re-classification in these two directions, to avoid incorrectly re-classifying labels as data. There might also be occasions where the above observation does not hold true, though as noted in [WL03], they are rare. In such a case, our rules will erroneously classify labels as data.

After this re-classification step, we have the modified sets:

D_1' = {C00221, beta-D-Glucose, …, R01520, 1.1.1.47,…, 3.2.1.21}
D_2' = {C00185, Cellobiose,…, R00306, 1.1.99.18,…, 3.2.1.21}
O_1' = {Entry, Name,…, Reaction, R00026, Enzyme,…}
O_2' = {Entry, Name,…, Reaction, R00026, Enzyme,…,}

Note that R00026 is not re-classified (incorrectly) because there are no data entries which can grow the data region in its direction. The sets of non-data entries, O_1' and O_2', now contain both presentation text, as well as labels for our data entries.

5. For each data entry in a data set, we now select the closest non-data entry as its label. This can be achieved by comparing XPath of the data entry against the XPaths of the non-data entries. The closer a non-data entry is to a data entry, the more element nodes in their corresponding XPath expressions will be matched before a mismatch. The closest element will have the longest common leading path, which is classified as the label. For example, the XPath for data entry 1.1.1.47 in our example is given by:

```
html/…./table[1]/tr[8]/td[1]/…/code[1]/a[1]
```

Some XPath expressions for the set of non-data entries include, for example;

```
html/…./table[1]/tr[6]/th[1]/…/code[1]/   ("Reaction")
```

`html/…./table[1]/tr[8]/th[1]/…/code[1]/ ("Enzyme")`

The latter XPath has the longest sequence of matching nodes with the XPath of our data element (indicated by the bold-face font above). Therefore, the label ("Enzyme") and corresponding XPath are associated with data entry 1.1.1.47 and its XPath (This association is represented by the "=>" symbol in Figure 5).

Note that multiple data elements can be associated with a single label in such a manner, as shown in Table 1. The last row of the table shows that the data entry R00026, which has been misclassified previously, has been selected as a label for data entries R01520, R01521 etc, as it found to be the closest non-data entry.

Label – With XPath	**Data Entry**	**XPath of Data Entry**
Enzyme - html/…./th[1]/…/code[1]/	1.1.1.47	html/…/td[1]/…/code[1]/a[1]
	1.1.3.4	html/…/td[1]/…/code[1]/a[2]
	…..	…..
R00026 - html/…/th[1]/…/code[1]/a[1]	R01520	html/…/td[1]/…/code[1]/a[2]
	R01521	html/…/td[1]/…/code[1]/a[3]
	….	….

Table 1: Two labels inferred, with corresponding data entries and their XPath expressions.

6. The XPaths of data entries classified to the same label are then generalized to form a single XPath expression. The XPaths for data entries in Table 1, for example, can be generalized as given below:

```
html/…./table[1]/tr[8]/td[1]/…/code[1]/a[position()≥1]/text()
html/…./table[1]/tr[6]/td[1]/…/code[1]/a[position()≥2]/text()
```

The last XPath expression above, for example, selects all text entries pointed to by a collection of anchor tags, starting from the second anchor tag. This is required as sample pages may only contain a small number of multiple data entries associated to a label. What is required is that we recognize and generalize that multiple number of data entries are associated for that label, rather than the number of data entries *seen* by the wrapper induction algorithm.

7. A relative path from the label to its corresponding generalized data path is computed. For the "Enzyme" label in Table 1, the relative path to its data is:

```
../…./../ td[1]/…/code[1]/a[position()≥2]/text()          (1)
```

Finally, the XPath for the label is replaced with an *anchored* XPath expression, i.e., an XPath which directly access the text node, and does not utilize ancestor nodes. For the "Enzyme" label:

```
//*[text()='Enzyme']                                      (2)
```

Concatenating (1) with (2) gives us, for label "Enzyme":

```
//*[text()='Enzyme']../…./td[1]/…/code[1]/a[position()≥2]/text()
```

The wrapper, thus, comprises of a collection of labels associated with a generalized anchored XPath expression to extract corresponding data.

Discussion It is worth noting here that the wrapper learnt by our algorithm is not tied to the structure of a class of pages. The wrapper anchors, or pivots, to a particular label, and finds a relative path from the label to associated data entries. As noted in section 2, data pages returned by Web databases can be very dynamic, where some labels can be

omitted completely. Our approach is beneficial in this case, as well as in the case that a Web site undergoes a template redesign, for instance. As long as the relative path from a label to its corresponding data remains the same, there would be no need to re-learn the wrapper. The only other limitation is that of labels remaining constant, and as we mentioned in section 2, changes in names of real-world entities, such as biological concepts, is extremely rare. Finally, recall that the wrapper-induction process for our running example results in the misclassification of "R00026" as a label. We discuss a technique to automatically detect and possibly correct such errors in section 3.3.

3.2 Site-Wide Wrapper Induction

As we noted in section 1, data-intensive sites, such as those in the Life Sciences domain, have their data scattered across multiple pages. Therefore, we need a wrapper-induction strategy that extracts data from multiple pages, which might belong to different page classes. This implies that we need to not only discover which pages returned by the server belong to the same class, but also to distinguish between classes and the navigational steps between them. Here, we make the following observations:

1. Not all pages of a Web site contain data, for example, pages pointed to by navigational menus, help pages, contact information etc. Therefore, we do not wish to discover all page classes. Rather, we wish to perform *targeted crawling* to only seek out *data-pages* and discover their classes.
2. We observe the concept of *link-collection* [CMM03], which refers to anchor links in a page (class) that share the same path in the DOM tree, from the root element to their parent or grandparent element. As a result, these hyperlinks appear grouped together in the rendered page. In our running example of Figure 1, the links on the reaction names form a link-collection, as well as those on the enzyme names. A link collection may be a singleton as well, comprising only a single hyperlink. We also note that hyperlinks in such a collection might not point to the same class of pages. For example, links in a navigation bar or those in categorization menus. However, link-collections that have been *classified* as being over data regions point to the same class of pages. For example, all hyperlinks on enzyme names point to "enzyme details" pages.
3. Pages belonging to the same class contain similar set of labels. However, due to the highly dynamic nature of pages, some labels may be omitted (e.g. NULL values in databases), but their ordering typically remains the same, as they are generated by scripts. If the order of labels on two pages is different, then their page-structures will most likely be different as well. Furthermore, it is highly unlikely that a site will have two different templates to display the same set of labels in the same order.

We, therefore, base our approach for site-wide wrapper induction on these assumptions:
1. Given the initial result output of a deep Web source, all data-intensive pages can be reached by iteratively following link-collections that occur on data regions. This assumption allows us to do targeted crawling for data-intensive pages, and eliminate navigation bars and menus etc.
2. A pre-classified link-collection points to the same class of pages.
3. Classes of pages can be distinguished from each other based on the labels they contain, and their order.

We now model our site-wide wrapper-induction problem as follows:
A page class C_i is defined by $C_i = SEQ_i$, where $SEQ_i = (\ell_{i1}, \ell_{i2},\ldots)$, a sequence of labels ℓ_{i1}, ℓ_{i2}, … described in page class C_i in this order of arrangement. These labels may have link-collections associated with them. Two classes C_i and C_j are considered not equal if $SEQ_i \neq SEQ_j$

Our site model is given by a collection of navigation steps:
$R_{ijn} = C_i \rightarrow \ell_{im} \rightarrow C_j$ $(i \neq j, i, j, n, m \geq 0)$
Where ℓ_{im} is the m-th label in page class C_i, the associated link-collection of which points to pages of class C_j. The site model is schematically depicted in Figure 4.

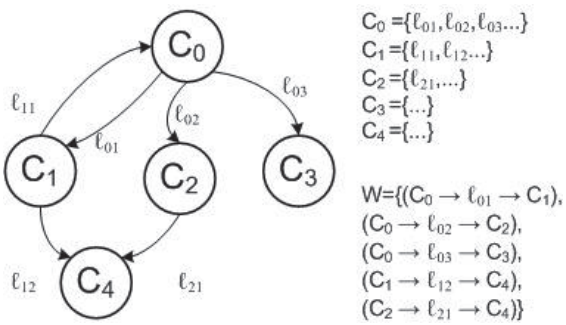

Figure 4: Schematic representation of a Web site Model as a labeled directed graph, with page-classe C composed of labels ℓ, the navigation steps between classes represented with → symbol.

The goal of the site-wide wrapper induction algorithm is to find the following:
1. $C_i \neq C_j$ $(i \neq j, i, j \geq 0)$
2. $R_{ijn} = C_i \rightarrow \ell_{im} \rightarrow C_j$ $(i \neq j, i, j, n, m \geq 0)$
That is, all possible data-intensive page classes, and the navigation steps between them.

The algorithm for site-wide wrapper induction is presented in Figure 5. We explain the algorithm using our running example of Figure 1. As in section 3.1, each step explained below is annotated to its corresponding location in the algorithm in Figure 5.

1. The algorithm starts with an input of the initial page class C_0, which corresponds to the initial response pages of the Web source. In our case, this is the page class that is generated by the sample pages of our running example, shown in Figure 1.
2. For each label in this class, the corresponding link-collections are followed. Let's assume we follow the link-collection of "Enzyme". Portions of sample results are shown in Figure 6.
3. According to our assumption 2, these pages belong to the same class. We learn a wrapper for this page class using our algorithm in Figure 2, with these sample pages as input. We note that not all links in a link-collection need to be followed. Our initial experiments have shown that ~9 sample pages yield a very good result (See section 4).
4. If this wrapper learning process results in a new class, according to our assumption 3, we add this new class to our sets, and define its corresponding navigational steps. In our example, a new class is created, C_1 = (Entry, Name, Class,…), as well as a navigation step $R = (C_0 \rightarrow$ "Enzyme" $\rightarrow C_1)$.
5. The above steps are repeated for each new page class that is learnt in step 3.

```
1  Input: S={C0}, C0=(ℓ01, ℓ02,…); // Set of all page classes discovered. C0 corresponds to the
                                    initial results page of a deep Web source.
   W = {};                          //Set of navigation steps between page classes.
   Output: S={Ci} (i≥0)
   W={Rij} (i,j≥0, i≠j)
   Start
   S´ = S;
   Do{
2      For each C in S´{            // for each class in our set
          For each ℓ in C{          // for each link-collection associated with a label
                    Follow ℓ;       // follow the link-collection
3                   induceWrapper Cnew;   // induce wrapper
4                   if (Cnew ∉ S) {          // if this is a new class
                                 Add Cnew in S and S´;}   // add it to our set
                    R = (C →ℓ→Cnew);      // form the navigation step
                    Add R in W;}          // add the step
                        }
           Remove C from S´;
5  }While(S´ ≠ NULL)             // all classes' link-collections have been explored
   End
```

Figure 5: Site-Wide Wrapper Generation Algorithm

Entry	EC 2.7.1.2 Enzyme
Name	glucokinase; glucokinase (phosphorylating)
Class	Transferases; Transferring phosphorus-containing groups; Phosphotransferases with an alcohol group as acceptor

Entry	EC 1.1.1.47 Enzyme
Name	glucose 1-dehydrogenase; D-glucose dehydrogenase (NAD(P)+); hexose phosphate dehydrogenase
Class	Oxidoreductases; Acting on the CH-OH group of donors; With NAD+ or NADP+ as acceptor

Figure 6: Small excerpts of pages obtained from following "Enzyme" link-collection

3.3 Error-Detection by Mutual Reinforcement

The natural residual output of our site-wide wrapper-induction approach is labeled data. These labels and data can be used to automatically detect and possibly correct errors in our wrapper-induction method for a page-class. We observe that some data entries reappear on different page classes. For example, the enzyme classification numbers in Figures 1 and 6. If the reappearing entries have been correctly classified as data across different page-class wrapper induction runs, then this enforces our confidence that the classification is correct. On the other hand, if, for example, some entries are classified as labels or presentation text by some wrappers and data by others, then this clearly points to a misclassification. This indicates that not enough sample pages were available to distinguish between data, labels and presentation text. We can address this by providing more samples for these page classes. We call such a mismatch as *label-data mismatch*.

For example, recall from Section 3.1 that the data entry R00026 was misclassified as a label in our running example (for page class C_0). When we follow the "Reaction" link-collection, we come across the page shown in Figure 7. While learning the wrapper for this class of pages (C_1), R00026 will be (correctly) classified as data. Based on this mismatch, we introduce more learning pages for both C_0 and C_1. In our example, any page for class C_0 which does not contain "R00026" as an entry will force our algorithm to classify this entry as data, thereby correcting the label to "Reaction" as well. The other type of mismatch is *label-label mismatch*, where the same data entry is assigned different labels across page classes. Recall our observation from section 2 that the same data entries can be labeled differently across different page classes. This can be observed from Figures 1 and 7, where R00026 is labeled as "Reaction" and "Entry", respectively. Based on this observation, it is not possible to detect whether a label-label mismatch was an error or a correct classification.

Entry	R00026 Reaction
Name	beta-D-Glucoside glucohydrolase
Definition	Cellobiose + H2O <=> 2 beta-D-Glucose
Equation	C00185 + C00001 <=> 2 C00221

Figure 7: Top-most portion of "Reaction" page of R00026 From KEGG

We slightly modify our site-wide wrapper induction algorithm to incorporate automatic error detection and correction for label-data mismatches. We introduce this mutual reinforcement step each time a new page class is created. The entries classified as data in this new class are compared with labels of previously formed page classes. If a mismatch is found, more sample pages for this new class, and conflicting page class, are introduced for wrapper generation until the mismatch is resolved.

4. Results and Evaluation

We have developed a prototype in Java which implements our algorithms. We use it to perform some preliminary experiments on three real-world biochemical sources, namely KEGG[Ka02], ChEBI[De08] and MSDChem[Go04]. All these sources provide basic qualitative data, and are often used for reference or annotation in more specialized domains, such as Genetics, Proteomics and Systems Biology. We use a simple random sample of input values for search forms of these sites in order to probe and induce their initial results page[7]. A Web-crawler based on httpUnit[8] was manually configured to fill the search forms with these values and submit them. We first report the results of our page-level wrapper-induction algorithm in section 4.1, and in section 4.2, describe our findings on site-wide wrapper-induction.

4.1 Page-Level Wrapper Induction Results

We perform two evaluations of the wrapper induction algorithm: The first evaluation (section 4.1.1) is that of the XPaths retrieved, which is beneficial for analyzing the

[7] The values can be collected from downloadable flat files or Web services provided by each source.

[8] A Java library for automated testing of Web sites. http://httpunit.sourceforge.net/

specific cases under which our algorithm misclassifies labels and data, and can help in improving the algorithm. It is also useful for determining how many samples are required in general by our algorithm for learning a wrapper for a class of pages. The second evaluation (section 4.1.2) is of the accuracy of the learnt wrapper in a traditional information retrieval evaluation.

4.1.1 XPath Analysis

We determine the precision and recall of our algorithm in retrieving the labels and corresponding data present in a page class. The total number of labels in each class was determined a priori by a domain expert.[9] In addition, the expert also determined the cardinality of the data associated with each label – specifically whether the label had one or possibly multiple data entries as its values. (Recall from section 3.1 that the algorithm *generalizes* multiple XPaths into a single expression for multiple data entries associated with the same label).

The correctness of each XPath returned by the algorithm is determined by the following three factors: (1) The correctness of the label, (2) that of the relative path from the label to the data, and (3) that of the generalization in case of a cardinality relation of greater than one between the label and data. We manually check these a posteriori. Verifications of labels and of generalization of the XPath are done manually. Note that since the relative path between a label and its data is always constant, we can verify the retrieved relative path by executing the XPath on a single test page by observing if it returns the correct data. The results are shown in Table 2. For each page-class, Table 2 shows the total number of label-data pairs contained in that class (#LD), the number of sample pages used for wrapper induction (#s), the number of label-data pairs successfully learnt, i.e. our *true-positives* (TP), the number of pairs not learnt, i.e. our *false-negatives* (FN) and the ones incorrectly learnt, i.e. *false-positives* (FP). We report our precision P and recall R in the last two columns respectively.

Before discussing the results, we briefly explain some conditions under which false-negatives and false-positives occur. False-positives generally occur when there is unlabeled data present in the pages. These data usually occur at the top of a page, such as a heading or a large caption, and are often *redundant* data entries, as they reappear as labeled data later in the same page (e.g, compound and reaction identification numbers etc). The other occurrence of false-positives is when data entries are misclassified as labels (as "R00026" in our example, section 3.1). This *may* also result in a corresponding false-negative for the *missed* label (as "Enzyme" due to the misclassification of "R00026"). Lastly, false-negatives also occur when sample pages used for the induction process simply do not contain the labels. This is a limitation for all wrapper induction approaches – you can only learn what you see.

As Table 2 indicates, our best results are obtained for KEGG Reaction, with a precision and recall of 100%, with 6 sample pages. This owes to the fact that there are frequent pages in KEGG Reaction which contain all labels. The results for KEGG Compound and ChEBI are quite similar. In both cases, our wrapper was unable to learn one label

[9] The total number of labels can be manually obtained from help pages and FAQs of the sources.

("Sequence" and "IN Number" respectively) for each source. Manual inspection revealed that none of our 15 sample pages contained those labels, which leads us to believe that they occur rarely. As noted above, this is a general problem for learning systems, and can only be removed with more sample pages.

Source	#LD	#S	TP	FN	FP	P	R
KEGG Compound http://www.genome.jp/kegg/compound/	10	3	5	5	2	71.4%	50%
		6	8	2	2	80%	80%
		9	9	1	1	90%	90%
		12	9	1	0	100%	90%
		15	9	1	0	100%	90%
KEGG Reaction http://www.genome.jp/kegg/reaction/	10	3	8	2	0	100%	80%
		6	10	0	0	100%	100%
ChEBI http://www.ebi.ac.uk/chebi/	22	3	18	4	3	85.7%	81%
		6	20	2	0	100%	90.9%
		9	21	1	0	100%	95.4%
		12	21	1	0	100%	95.4%
		15	21	1	0	100%	95.4%
MSDChem http://www.ebi.ac.uk/msd-srv/msdchem/cgi-bin/cgi.pl	30	3	30	0	1	96.7%	100%
		6	30	0	1	96.7%	100%
		9	30	0	1	96.7%	100%
Average (based on final wrappers for each source)						99.1%	96.3%

Table 2: Results for page-wide wrapper induction algorithm. (LD is label-data pairs, s is samples)

Formula	C10 H16 N5 O13 P3
Defined at	1999-07-08
Last modified at	2007-08-16
EBI name	ADENOSINE-5'-TRIPHOSPHATE
EBI Id	not assigned
Additional name	ADENOSINE-5'-TRIPHOSPHATE
Classification	NUCLEOTIDES
Cas reg number	not assigned
Therapeutic category	not assigned
Merck Id	not assigned
Polymer topology	not assigned
Polymer code	not assigned
Polymer sub type	not assigned
Hetgroup type	NON-POLYMER
Obsoleted	not assigned
Parent	not assigned
Topological variant	not assigned

Figure 8: Portion of MSDChem page for "ATP", showing unassigned values

The results for MSDChem are quite interesting, as they demonstrate the usefulness of our *data-region growing* approach. Unlike other sources, pages in MSDChem have a very static structure – no labels are omitted from the pages when corresponding data entry is NULL, as shown in Figure 8. This means that the frequency of data fields being NULL (or "Not Assigned" in this example) is very high. Such fields are not classified as data in our algorithm, as they are constant across many pages. However, we note that the label-data pairs are arranged in a (invisible) table, as shown in Figure 8. Therefore, through rule 2 in Section 3.1, an entry classified as data at the top of the data column in Figure 8 reclassifies all entries below it in the column as data as well. This accounts for a perfect recall, with only 3 sample pages. Overall, we observe that we can get very high

precision and recall (~97%, ~96% respectively) from ~9 samples. The precision can be improved with more samples, especially if they contain rarely occurring labels.

4.1.2 Wrapper Evaluation

We verify the accuracy of our wrappers by applying them to sets of five test pages. We manually count the total number of data entries and note corresponding labels across these five test pages a priori, and determine the precision and recall of our algorithm in retrieving these data entries and classifying them with the right label. These results are summarized in Table 3. The wrapper for the page class belonging to KEGG Reaction has a perfect precision and recall. This reinforces our observation in the previous section that there are frequent pages in this class which contain all labels. Our algorithm is thus able to correctly induce a wrapper for this class with only a few samples. The wrappers for KEGG Compound and ChEBI are unable to retrieve data entries corresponding to the labels which were not learnt (see Table 2). The wrapper for MSDChem has FPs as a result of false classification of redundant data entries to some presentation text in the learning phase.

SOURCE	#T	(TP) #RC	(FN) #NR	FP		PRECISION	RECALL
				#R	#IR		
KEGG Compound	186	184	2	0	0	100%	98.9%
KEGG Reaction	45	45	0	0	0	100%	100%
ChEBI	204	203	1	0	0	100%	99.5%
MSDChem	150	150	0	0	5	96.7%	100%
Average						99.1%	99.6%

Table 3: Results from applying wrappers to five sample pages each. (T = Total number of data entries across 5 test pages, RC = Retrieved and Classified correctly, NR = Not Retrieved, R = Retrieved but not classified correctly, IR = Incorrect Retrieval)

4.2 Site-Wide Wrapper Induction

In this section, we present our results for site-structure discovery, which together with the wrapper induction algorithm constitutes our site-wide wrapper induction approach. As in section 4.1, we perform two evaluations: The first determines to what extent we were able to determine the Web site structures (section 4.2.1), which gives us cues to modify and improve our algorithm. The second determines the accuracy of our Web site wrapper induction algorithm, by applying the algorithm to small portions of the site to retrieve data (section 4.2.2).

4.2.1 Analysis of Retrieved Site Models

We manually model all three sources, which involves manually determining classes for data pages for a source, and the navigation steps for generating these classes[10]. We then compare our algorithm's results and measure its accuracy by comparing the navigation steps generated (section 3.2) with the manually determined steps.

[10] We ignore classes of pages which describe content using Flash or Java applets etc., as our system can only process HTML pages. This restriction limits the amount of information our algorithm can extract. However, such content is still quite limited in our target domain, and the vast amount of data is typically available in textual form on HTML pages.

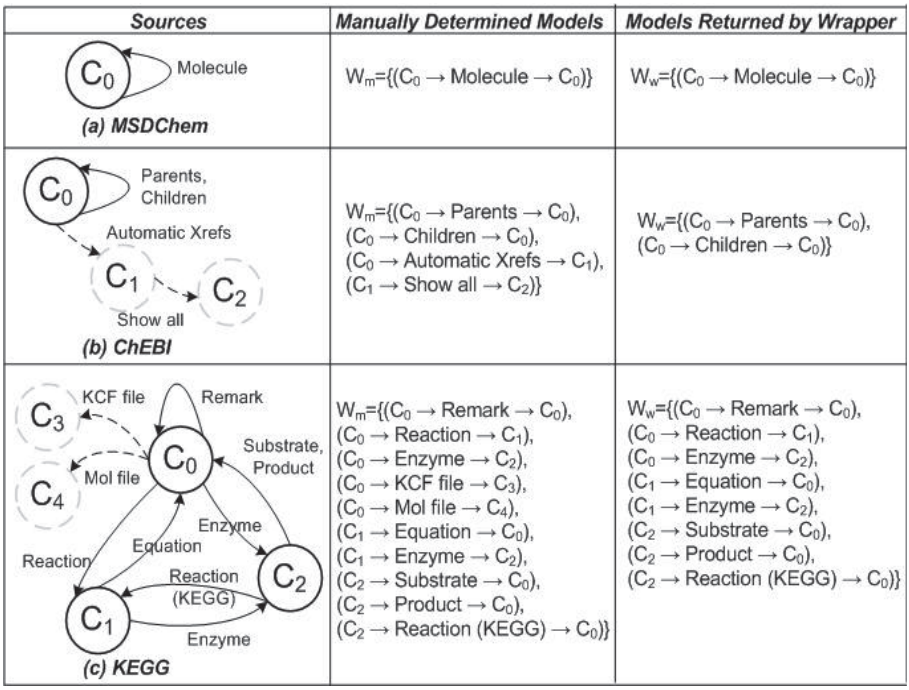

Figure 9: Manual and retrieved site models for (a) MSDChem, (b) ChEBI (c) KEGG (partial). Solid lines: Portions of the model discovered correctly. Dashed lines: portions not retrieved.

These results are partially shown in Figure 9, along with schematic representations of the Web site models, with the complete results in Table 4. MSDchem and ChEBI have relatively simple models. KEGG on the other hand has a very complex model. It actually consist of a number of back-end database schemas, each having its unique Web interface, with extensive links between all interfaces to form a large Web portal, with more than 30 page classes. For this paper, we restrict our manual model to a specific sub-site (KEGG Compound, Drug, Reaction, RPair, Enyzme and Orthology). We restrict our algorithm from exploring the portal outside this boundary, allowing it to discover navigation steps within this sub-site. It is immediately apparent from Table 4, based on perfect precision, that our assumption that all link-collections associated with data regions point to classes of pages containing data, is indeed correct. However, the relatively low recall seems to suggest that we need to relax the restriction that only link-collections associated with data regions should be followed. Indeed, in the site models that our algorithm retrieves, we notice that certain page-classes have not been discovered. Therefore, we probably need to adjust our algorithm to follow link-collections that are also close to data regions, but not necessarily directly on them.

SOURCE	#NS	TP	FN	FP	P	R
MSDChem	1	1	0	0	100%	100%
ChEBI	4	2	2	0	100%	50%
KEGG	21	16	5	0	100%	76.19%

Table 4: Results for site-structure discovery. (#NS is total number of navigation steps)

4.2.2 Site-Wide Wrapper Evaluation

We apply our site-wide wrappers to the three sources to extract data. We limit the execution so that our system extracts data from only five test instances of each class of the Web site. We manually count the total number of data entries and note corresponding labels across all test pages a priori, and determine the accuracy of the algorithm similarly to section 4.1.2, with results displayed in Table 5.

SOURCE	#C	#C'	#T	(TP) #RC	(FN) #NR	FP		P	R
						#R	#IR		
MSDChem	1	1	N/A	N/A	N/A	N/A	N/A	N/A	N/A
ChEBI	3	1	412	247	165	0	0	100%	59.9%
KEGG	10	7	1618	1422	109	87	0	94.2%	87.8%
Average								97.1%	73.9%

Table 5: Site-wide wrapper evaluation. (#C = Total number of classes, #C' = Number of classes discovered, T = Total number of data entries across 5 test pages, RC = Retrieved and Classified correctly, NR = Not Retrieved, R = Retrieved but not classified correctly, IR = Incorrect Retrieval)

We observe that for MSDChem, even though the navigation steps constituting the site model are correct, the site-wide wrapper induction fails. Upon closer inspection, we notice that the navigation step from a page instance actually results in the same page instance. For example, following the "Molecule" link-collection (Figure 9) from a page of ADP results in the same page. This implies that the MSDChem Web site consists of a large number of leaf nodes only, having no hyperlinks connecting them to each other. For ChEBI, we have a perfect precision, but a low recall. This indicates that the two classes our algorithm failed to retrieve (Figure 9) had rich data regions. Our algorithm also fails to retrieve 3 classes in the KEGG sub-site, though a relatively higher recall suggests these missing classes did not contain as big a data region as in the case of ChEBI. Furthermore, we have some misclassifications in some page wrappers for KEGG which slightly lower the precision for the corresponding site-wide wrapper for KEGG.

5. Related Work

5.1 Wrapper Induction

Wrapper generation has received considerable attention for a long time now. The earliest approaches, including [Ku98] and [MMK00] required training examples. Due to the large size of the Web and its dynamic nature, supervised techniques do not scale well. Recent attempts have focused on fully automatic wrapper induction techniques. The reader is instructed to read [La02] for a survey on wrapper induction techniques. RoadRunner [CMM01 ,CMM04] is an automatic wrapper induction algorithm that is closest to our approach, as it uses multiple sample pages of a page-class. However, unlike our approach, it compares the structures of the sample pages to learn a regular expression, which takes into consideration the mismatches between text and HTML tags across the samples. This regular expression based wrapper is thus tied directly to the page structure. As we noted in section 2, pages from deep Web sources are often very dynamic, where concepts that are NULL are often omitted. RoadRunner would thus

require a large number of sample pages, covering all possible types of such omissions, so that its regular expression can accommodate for this dynamic behavior.

Lixto [BFG01] and W4F [SA01] use XPath-like languages "Elog" and "HEL" respectively, and both offer visual tools for creating wrappers in an unsupervised manner. The user selects data of interest in a Web page, and a path from the root of the page to the target node is generated in the respective languages. Therefore, manual identification of data elements is required for each page, which can be labourious for pages containing numerous data entries. ANDES [MJ02] is based on XPath and requires the user to manually provide XPath expressions to extract data. [An06] builds on ANDES to induce the XPath expressions using tree traversal patterns but requires annotated examples. IEPAD [CCL03], DeLA [WL03], ViNTs [MRY05], DEPTA [ZL06] and ViPER [SL05] are unsupervised wrapper induction techniques that are all based on one common assumption: Data regions in Web pages are constituted by at least two spatially consecutive records that are structurally and visibly similar. This assumption partially holds for result pages of search engines, online listings and E-commerce Web sites, but not for scientific repositories on the Web, as is apparent from our example in Figure 1. Even in the case of E-commerce sites and listings, the initial response pages of a search do exhibit a repetitive structure comprising of records, but the *details* pages describing each result do not exhibit this repetitiveness. All approaches cited above perform wrapper induction on a single class of pages, whereas our approach attempts to automatically classify pages in a Web site into appropriate classes, learn wrappers for each class and discover rules for applying these wrappers on Web pages encountered on the Web site. IDE [ZL07] extracts structured data from different classes of Web pages. It starts with one labeled training page, indicating the information to be extracted. It proceeds to extract corresponding data from test pages based on the similarity between a consecutive sequence of tags before and after the labeled data and the data in the test pages. Whenever extraction fails for a page, it is manually labeled. However, this requires foreknowledge about which information must be extracted, and assumes that the same information is present and to be extracted from all classes. This is very useful in E-Commerce, but not always true in scientific sources, as shown by examples in Section 3.

5.2 Site-Structure Discovery

We are only aware of one approach to automatic site-structure discovery [CMM03], which also constitutes the main motivation for our approach. The focus of their work is slightly different from ours – It tries to efficiently discover the entire site-structure, whereas we focus on discovering only portions of the site which contain data extracted from the backend database. Their approach to clustering of Web pages into classes is based on the assumption that pages belonging to the same class contain link-collections that are in a structurally similar arrangement and position. Based on structural similarity of these link collections, they group Web pages into classes. This is a good assumption for sites that do not have *leaf* pages which do not have any links, such as help pages, FAQs, contacts, legal disclaimers etc. In the absence of hyperlinks, all these pages would be classified into a single class (because their link-collections have the same structure), even though these pages may exhibit considerable structural variations. Our approach is also based on an assumption over link-collections, but contrary to their assumption, we

assume that link-collections that have been classified as belonging to the same concept point to pages which belong to the same class.

6. Conclusions and Future Work

We have described a novel wrapper induction technique to extract labeled data from data-intensive Web pages of deep Web sources. The approach takes advantage of the peculiarities typically associated with scientific Web sites, most notably that they contain labeled data. Our approach is unique in that it automatically classifies structurally similar pages into classes which can then be used for learning wrappers. Navigation steps that are retrieved during the site-wide wrapper induction phase are used to associate wrappers to classes of pages, allowing us to automatically select and apply a wrapper for a page in the Web site. The approach is fully automatic, the samples required for page-level wrapper induction are collected automatically and do not require any manual labeling. The approach does not need fine-tuning of any heuristics or parameters, but does require the presence of labels. Our approach is less prone to structural changes or updates of the Web pages, as it does not marry the induced wrapper to the pages structures, and only requires the relative path in the HTML tree between the label and data. Our ultimate goal is to be able to integrate and query data from multiple deep Web sources. We briefly mention our future work in this direction: As mentioned in section 2, data extracted from a single source may have multiple labels. Furthermore, different sources may also have different labels for the same entity. A first step is to homogenize this labeling. This is a *matching* problem in traditional data integration systems. Secondly, data extracted from applying the wrapper lack a schema associated with it, whereas querying and using these data requires a rich schema, similar to that of the hidden database, or an ontology. The arrangement of different labels, repetitive patterns and cardinalities of the data might give us some clues to discovering the hidden schema.

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