OpBerg: Discovering causal sentences using optimal alignments

Justin Wood\textsuperscript{a}, Nicholas J. Matiasz\textsuperscript{b}, Alcino J. Silva\textsuperscript{c}, William Hsu\textsuperscript{b}, Alexej Abyzov\textsuperscript{d}, Wei Wang\textsuperscript{a},\textsuperscript{*}

\textsuperscript{a}Department of Computer Science, UCLA, 3551 Boelter Hall, 580 Portola Plaza, Los Angeles, CA 90095
\textsuperscript{b}Department of Bioengineering, UCLA, 924 Westwood Blvd., Ste. 420, Los Angeles, CA 90024
\textsuperscript{c}Department of Neuroscience, UCLA, 695 Charles Young Dr. S., Rm. 2357, Los Angeles, CA 90095
\textsuperscript{d}Center for Individualized Medicine, Department of Health Sciences Research, Mayo Clinic, 200 First St. SW Rochester, MN 55905

Abstract

Background: The biological literature is rich with sentences that describe causal relations. Methods that automatically extract such sentences can help biologists to synthesize the literature and even discover latent relations that had not been articulated explicitly. Current methods for extracting causal sentences are based on either machine learning or a predefined database of causal terms. Machine learning approaches require a large set of labeled training data and can be susceptible to noise. Methods based on predefined databases are limited by the quality of their curation and are unable to capture new concepts or mistakes in the input.

Objectives: This paper presents a novel and outperforming method for extracting causal relations from text by aligning the part-of-speech (POS) representations of an input set with that of known causal sentences.

Methods: This method extracts causal relations by adapting and improving a method designed for a seemingly unrelated problem: finding alignments between genomic sequences. Each sentence for training and testing is converted to a representation where each word is replaced by its corresponding POS token. Given a set of POS tokens labeled as causal and non-causal, we take an unlabeled token sequence to be of the same class as its best aligning labeled match. Paramount to this approach is finding the best number of alignments (breakpoints) along with the best alignment for each breakpoint.

Results: The execution time of OpBerg is compared against the state-of-the-art machine learning algorithms for the task of causality extraction using a training set size of 100 sentences and a test size ranging from 1,000 to 10,000 sentences. OpBerg is shown to run faster by a factor of 10 over the compared methods. Next OpBerg is compared against the same methods in a causality retrieval task. The task is to correctly retrieve the causal statements from a set of research articles. Again, OpBerg significantly outperforms the competing methods.

Conclusion: Our experiments show that when applied to the task of finding causal sentences in biological literature, our method improves on the accuracy of other methods in a computationally efficient manner.

Keywords: Causality extraction, Natural language processing, AGE

1. Introduction

Researchers who perform biological experiments convey their discovery in published research articles, which contain descriptions of causal relations. This growing literature provides an enormous amount of information and represents the current state of biological understanding. This documentation of scientific discovery can verify previous experiments, provide insights to researchers \cite{1}, and motivate future research \cite{2}.

These corpora of biological text are growing at an exponential rate. Algorithms and approaches are thus needed to extract the relevant information, allowing biologists to understand and connect biological processes. Since researchers describe causal connections among biological entities in free-text research papers, it is logical to extract
these connections using natural language processing (NLP).

A causal assertion can be thought of as a relation between an agent and a target. Often in biological studies, an agent is either passively observed or actively manipulated, and a change or lack thereof is noted in a target. Although this type of result can be described across many different and sometimes nonadjacent sentences, this paper focuses only on causal assertions appearing in a single sentence. This approach has the advantage of limiting the search range for descriptions of causality and takes advantage of existing methods that can reliably fragment documents into collections of sentences [3].

Existing methods for causality extraction use either predefined knowledge bases, word lists, other types of databases [4, 5, 6, 7, 8], or are based on statistical techniques—often some form of machine learning [9, 10, 11, 12, 13]. Predefined knowledge bases are of course limited by the quality of the knowledge base itself. Often, these sources are manually curated and do not always contain all possible words or phrases of interest. Additionally, they require exact matches to be useful. For instance, if a knowledge base contains causal verbs and a potential causal sentence contains the misspelled verb “cuases” (instead of “causes”), the sentence will be dismissed due to the misspelling. These predefined knowledge bases are also not able to capture new words or concepts, and they are not extensible to other tasks such as extracting causality from text in other languages.

One solution to these problems is to use existing machine learning techniques. But these approaches often require large amounts of labeled training data, something that can be expensive and tedious to obtain. These barriers of time and cost are expanded when the task is to discover more fine-grained details pertaining to causality, such as that of finding the specific types of studies and outcomes that lend evidence for a causal assertion. Additionally, the vocabulary for biomedical free text can be quite large, as it contains not only common words but also domain-specific terms. This large vocabulary set requires an even larger training data for the machine-learning model to predict the necessary components for representing causal phenomena.

Thus, to automatically extract causal sentences, an approach is required that does not suffer from limitations in the size of the training data, and that can be performed efficiently. The approach presented in this paper is inspired by the analogy of the aforementioned problem to that of comparing a set of genomic sequences in bioinformatics.

Though it may not be obvious, there is indeed a connection between aligning sequences in genomic data and finding causal sentences in free text. While each sentence may contain a unique set of words, the part-of-speech (POS) sequence of each sentence is likely to be much more common. Breaking each sentence into its grammatical structures can thus help to identify patterns in the way that causal relations are described. Thus, applying an alignment method to the grammatical structures of sentences has the potential to discover similarities that may be missed by approaches that focus only on words. We further illustrate this with the following example of three sentences and their corresponding POS mappings (for brevity we replace the POS label with a single character: A = pronoun, B = verb, C = determiner, E = adjective, F = noun, G = preposition):

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We noticed a rather large increase in insulin after eating.
We observed that we are running out of melatonin today.
Today we observed an increase in melatonin after running.
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Here the first two sentences are talking about two different things; yet both are causal sentences. Their POS structures are similar. In comparison, the second and third sentence share a lot of words, more so than the first and second sentences, yet their POS representations have fewer matching elements, with long gaps in between matches. Therefore, knowing that the second sentence is causal, we cannot determine whether the third sentence is causal. It is our hypothesis that given a labeled set of causal sentences $C^+$ and non-causal sentences $C^-$, a new sentence $s$ is classified as a causal sentence if its POS structure is most similar to a causal sentence (than any non-causal sentences) and the
similarity ($S$) is above a threshold $\delta$,
\[
\max_{c \in C^+} S(c, s) > \max_{c \in C^-} S(c, s) \wedge \max_{c \in C^+} S(c, s) > \delta
\]
The approach presented here finds causal relations by comparing the POS mappings of unlabeled sentences to that of labeled sentences. A new causal sentence is discovered by identifying the optimal number of alignments between the grammatical representations of the sentences. This alignment approach can thus classify causal sentences accurately and efficiently, and it has the potential to be used for other problems as well.

However, existing methods of sequence alignment are insufficient for aligning POS representations of free text: either (1) they require the user to specify the number of local alignments [15] or (2) they introduce a gap penalty for each new local alignment [16], possibly leading to erroneous alignments [15]. Given the nature of free text, it is unreasonable to ask the users to pre-specify the number of alignments or to efficiently apply the algorithm to NLP. The techniques presented in this paper need not be limited to extracting causality. We recommend using our approach for information retrieval tasks dealing with sequential similarity when the input data set is too small to be sufficient for machine learning.

2. Methods

The proposed approach, named OpBerg, builds upon the AGE algorithm: it uses a similar strategy to find the optimal number of local alignments. AGE can be thought of as splitting the input sequences into segments and then running a local alignment algorithm on those segments. The original form of AGE that involves going forward and reverse in two matrices makes any additional alignment gaps difficult to compute and store. It is thus the linear-space algorithm that holds the key to solving the problem of optimal local alignments. Because the directionality moves from left to right (or right to left), this approach can be used to split the strings into an arbitrary number of segments. Further information is needed to implement the proposed approaches that retain necessary information about the locations of the gaps in the alignments. The change required to the original AGE equation is the addition of a matrix that stores the location of a newly created gap.

This optimal solution also uses our proposed concept of score length, whose definition is as follows:

**Definition: score length.** The score length for the alignment of POS tokens $a_i a_{i+1} \ldots a_{i+d_1}$ and $b_j b_{j+1} \ldots b_{j+d_2}$ is defined as the difference between the max score in the alignment matrix at cell locations $(i + d_1, j + d_2)$ and $(i, j)$.

A naive algorithm for solving the optimal alignment problem is to run the existing AGE method on every possible number of local alignments that could reasonably occur:

\[
L(i, j, 0) = \max \begin{cases} 
L(i-1, j, 0) + Q \\
L(i-1, j-1, 0) + S(a_i, b_j) \\
L(i, j-1, 0) + Q \\
0
\end{cases}
\]

\[
L(i, j, k) = \max \begin{cases} 
L(i-1, j, k) + Q \\
L(i-1, j-1, k) + S(a_i, b_j) \\
L(i, j-1, k) + Q \\
M(i-1, j-1, k) + S(a_i, b_j) \\
0
\end{cases}
\]

\[
M(i, j, 0) = \max \begin{cases} 
M(i-1, j, 0) \\
L(i, j, 0) \\
M(i, j-1, 0)
\end{cases}
\]

\[
M(i, j, k) = \max \begin{cases} 
M(i-1, j, k) \\
L(i, j, k-1) \\
M(i, j-1, k)
\end{cases}
\]

\[
X_i(i, j) = X(i-1, j, k) \\
X_M(i, j) = X(i-1, j-1, k)
\]
The linear penalty can be thought of as an additional larger gap penalty, thus taking the form of a generalized global alignment \[16\]. It has already been shown \[15\] that this can lead to improper alignments.

The question then becomes: What is the optimal number of alignments? For example, a user may prefer to find an alignment that has only 1 large segment aligned and a score of 28 over 10 alignments and a score of 29. To determine the correct number of alignments, this work focuses on three major trade-offs:

1. Number of alignments.
2. Score length to break apart an alignment (\(\alpha\)).
3. Minimum score length to start an alignment (\(\beta\)).

The naive algorithm solves the problem of finding the optimal number of local alignments, but it does so at a considerable cost. For causal sentences, this increase is not infeasible due to the relatively low input size of sentences. But running this algorithm over a very large corpus like the entirety of PubMed Central would carry a considerable execution cost. Thus, it is advantageous to seek solutions that are more efficient in both time and space. Opberg, the approach we present here, seeks to reduce memory by a factor of \(n^2\) and execution time by a factor of \(n^2\).

### 2.1. OpBerg

Note that during execution of the naive algorithm described above, once it is decided that a new local alignment is a better choice, the optimal solution can then only be of the same or more alignments. This allows us to reuse the existing \(M\) matrix and shave off the \(k\) dimension, allowing for much simpler bookkeeping. We introduce a new matrix \(L\) that represents the values of a local alignment. The \(M\) matrix then takes on the interpretation of a matrix whose values are the max of the previous max \(M\) cell value and the corresponding \(L\) cell value. The optimal solution then can be in the \(L\) matrix (that is, performing a local alignment) or in the \(M\) matrix (that is, moving through the cells of the matrix and not decreasing in value). We use the notation that if the optimal solution is in the \(L\) matrix, then it is in the “\(L\)” or “alignment” state; and if the optimal solution is in the \(M\) matrix, then it is in the

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\[
X_D(i,j) = X(i,j-1,k)
\]

\[
X_X(i,j) = X(i,j,k-1) \cup (i-1,j-1)
\]

\[
X_0 = (0,0)
\]

\[
L_I(i,j,k) = L(i-1,j,k) + Q
\]

\[
L_M(i,j,k) = L(i-1,j-1,k) + S(a_i,b_j)
\]

\[
L_D(i,j,k) = L(i,j-1,k) + Q
\]

\[
L_X(i,j,k) = M(i-1,j-1,k) + S(a_i,b_j)
\]

\[
X(i,j,k) = \begin{cases} 
X_I(i,j), & \text{if } L(i,j,k) = L_I(i,j,k) \\
X_M(i,j), & \text{if } L(i,j,k) = L_M(i,j,k) \\
X_X(i,j), & \text{if } L(i,j,k) = L_X(i,j,k) \\
X_0, & \text{if } L(i,j,k) = 0
\end{cases}
\]

Although this may seem to be an unreasonable solution, the running time and memory usage remain polynomial and thus feasible for small input sizes.

As shown by Equation 2, the change required is to compute and store the possible different alignments using a separate matrix for each split. A new variable is introduced, \(k\), which represents the current number of local alignments to run on the given input sequences. The results of these additions require an \(n\) factor increase in both running time and memory retention, where \(n\) is defined as the size of the largest input POS token sequence. The running time becomes \(O(n^3)\) with memory required as \(O(n^3)\).

Like the segmented least squares problem \[17\], it is intuitive to add a penalty (\(P\)) for each additional increase in local alignments. This penalty is needed since otherwise, the optimal alignment would always just match individual POS tokens. Because this penalty is proportional to the number of local alignments, we make the penalty a simple linear constant. The maximum alignment score can then be defined as:

\[
\max_{1 \leq k \leq n} \left[ P \times k + M(|A|, |B|, k) \right],
\]

where \(A\) and \(B\) are the input POS token sequences mapped from two sentences. \(M\) is the three-dimensional maximum matrix which holds the maximum alignment score for each \(a_i\), \(b_j\), and \(k\); where \(a_i \in A\) and \(b_j \in B\).

A simple linear penalty constant reveals that returning one such alignment is not a trivial and deterministic task.

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\[\text{https://www.ncbi.nlm.nih.gov/pmc/}\]
“M” or “max” state. Given that there is only one L state, it is entirely possible for the optimal solution to transition multiple times from the M state to the L state before beginning an alignment. We store the values of a transition in a new matrix N which holds the point of a transition in and out of the M state. Another matrix X holds the points of all transitions through the optimal solution.

The three trade-offs discussed above can be dealt with in various ways. To account for the number of alignments, we can leave in the original penalty $P$, but instead of considering this as a larger gap penalty, one can think of it as a value less than 1 and possibly even 0 (with the original gap penalty greater than 1). By doing so, one can easily gauge at what point a new alignment gap starts to weigh negatively on the score and thus becomes less desirable.

To consider the minimum score length that is considered to break apart an alignment, we need only consider the point at which the algorithm exits the max state. If the current alignment has not dropped below the input score length $\alpha$, then we will restrict the transition until the appropriate threshold has been reached.

Likewise for the start of an alignment, with the change only to the entering of the max state. This requires storing the score at the start of entering the alignment state so that we can compare the difference to see if we are above threshold. This value is stored in the matrix $H$. This allows us to restrict the length as we do for breaking apart an alignment, but a key difference happens when an alternative alignment is nonexistent. For example, a user may prefer not to start a segment of only 3 matched characters unless this is the max score out of any alternative alignments by a score of 3 matches. We must introduce into this restriction of a transition into the max state a way to keep track of how a score length smaller than $\beta$ influences the score. That is, we do not necessarily want to discard these alignments unless there is a better alignment available. A new parameter is introduced, $\gamma(x)$, which allows the user to specify a function to weigh how important a certain score length is when it is below threshold, but no higher scoring alternatives exist.

With these parameters, the algorithm is bound to a running time of $O(n^2)$ and memory requirements of $O(n^3)$. The intuition for this algorithm follows the intuition of segmented least squares. In the segmented least squares problem, we are searching for a balance between accuracy and number of lines, whereas in OpBerg we seek this parsimony between alignment score and number of jumps through the matrix to start a new local alignment. The trade-off is then enforced by the penalty constants $P$, $\alpha$, $\beta$, and function $\gamma(x)$.

### 2.1.1. Affine Gap

It should not always be the case that insertions and deletions (indels) between the inputs are weighted equally, regardless of where they occur. For instance, in certain causal sentences, a large cluster of indels may represent a tangential segment of words. To capture these occurrences, an affine gap model that takes into account segments of tangential words must be adapted to OpBerg.

The changes required of OpBerg for an affine gap are similar to those in the original local alignment algorithm [18]. Three matrices—representing a match/mismatch ($L_G$), insertion ($L_I$), and deletion ($L_D$) transitions, respectively—must be used in place of the original L matrix. The max matrix $M$ cannot enter into any of these three states because it represents a jump through the inputs, so it remains the same. Also, since a local alignment must start and end with a match (diagonal move), the transition between the L states to the M states can occur only through the new $L_G$ matrix. This also applies to the X and N matrices, as they only must monitor jumps between the $L_G$ and the M matrices.

The recurrent relations needed for the affine gap OpBerg model are given in their entirety as:

$$L_I(i, j) = \max \begin{cases} L_I(i - 1, j) + E \\ L_G(i - 1, j) + O + E \\ L_D(i - 1, j) + O + E \end{cases}$$

$$H_I(i, j) = \begin{cases} H_I(i - 1, j) & \text{if } L_I(i, j) = L_I(i - 1, j) + E \\ H_G(i - 1, j) & \text{if } L_I(i, j) = L_G(i - 1, j) + O + E \\ H_D(i - 1, j) & \text{if } L_I(i, j) = L_D(i - 1, j) + O + E \end{cases}$$

$$\theta(i, j) = \max \begin{cases} M(i - 1, j) \\ M(i, j - 1) \end{cases}$$
H(i,j) = Max \[ \begin{cases} 0, & \text{if } \delta(i,j) = 0 \\ L_I(i-1,j-1) + S(a_i,b_j), & \text{if } \delta(i,j) = \psi(i,j) \end{cases} \]
L_{G,H}(i,j) = L_G(i-1,j-1) + S(a_i,b_j)
L_{D,H}(i,j) = L_D(i-1,j-1) + S(a_i,b_j)
L_{G,M,H}(i,j) = M(i-1,j-1) + S(a_i,b_j) + P
\psi(i,j) = \begin{cases} \theta(i,j), & \text{if } \delta(i,j) = \psi(i,j) \\ H_I(i-1,j-1), & \text{if } \delta(i,j) = L_{G,I,H}(i,j) \\ H_G(i-1,j-1), & \text{if } \delta(i,j) = L_{G,G,H}(i,j) \\ H_D(i-1,j-1), & \text{if } \delta(i,j) = L_{G,D,H}(i,j) \\ \theta(i,j), & \text{if } \delta(i,j) = L_{G,M}(i,j) \end{cases}
\pi(i,j) = M(i-1,j-1) + S(a_i,b_j) + P
\epsilon(i,j) = \begin{cases} \pi(i,j), & \text{if } \delta(i,j) = \psi(i,j) \leq \alpha \\ -\infty, & \text{otherwise} \end{cases}
L_G(i,j) = Max \{ \delta(i,j), \epsilon(i,j) \}
H_G(i,j) = \begin{cases} \theta(i,j), & \text{if } L_G(i,j) = 0 \\ H_I(i-1,j-1), & \text{if } L_G(i,j) = L_{G,I,H}(i,j) \\ H_G(i-1,j-1), & \text{if } L_G(i,j) = L_{G,G,H}(i,j) \\ H_D(i-1,j-1), & \text{if } L_G(i,j) = L_{G,D,H}(i,j) \\ \theta(i,j), & \text{if } L_G(i,j) = L_{G,M}(i,j) \end{cases}
L_D(i,j) = Max \{ L_I(i,j-1) + O + E, L_G(i,j-1) + O + E, L_D(i,j-1) + E \}
L_{D,I,H}(i,j) = L_I(i,j-1) + O + E
L_{D,G,H}(i,j) = L_G(i,j-1) + O + E
L_{D,D,H}(i,j) = L_D(i,j-1) + E
H_D(i,j) = \begin{cases} H_I(i,j-1), & \text{if } L_D(i,j) = L_{D,I,H}(i,j) \\ H_G(i,j-1), & \text{if } L_D(i,j) = L_{D,G,H}(i,j) \\ H_D(i,j-1), & \text{if } L_D(i,j) = L_{D,D,H}(i,j) \end{cases}
\zeta(i,j) = \begin{cases} L_G(i,j), & \text{if } L_G(i,j) \geq \beta \\ \gamma(L_G(i,j)), & \text{otherwise} \end{cases}
M(i,j) = Max \{ \zeta(i,j), M(i-1,j), M(i,j-1) \}
L_{G,I,X}(i,j) = L_I(i-1,j-1) + Q
L_{G,G,X}(i,j) = L_G(i-1,j-1) + S(a_i,b_j)
L_{G,D,X}(i,j) = L_D(i-1,j-1) + Q
N_X(i,j) = N(i-1,j-1) \cup (i,j)
X_D(i,j) = X(i-1,j-1)
X(i,j) = \begin{cases} X(i-1,j), & \text{if } L_G(i,j) = L_{G,I,X}(i,j) \\ X_D(i,j), & \text{if } L_G(i,j) = L_{G,G,X}(i,j) \\ X(i,j-1), & \text{if } L_G(i,j) = L_{G,D,X}(i,j) \\ N_X(i,j), & \text{if } L_G(i,j) = \epsilon(i,j) \\ \emptyset, & \text{if } L_G(i,j) = 0 \end{cases}
\text{where } (i,j) \text{ represents the cell location of both matrices and the } k \text{th POS token in } A \text{ and the } j \text{th POS token in } B.
S \text{ is a function that takes in two POS tokens and returns a score value. The opening gap penalty is represented by } O \text{ and the extension penalty by } E.
\text{Even with the newly created matrices and additional processing that must take place to populate the matrices, the running time will be } O(n^2), \text{ with memory as } O(n^2).

3. Conclusion

This paper introduces a novel approach to causality discovery by considering alignments among POS mappings of sentences. This approach considers restrictions on the score size to break apart an alignment and enforces a minimum length requirement while also considering the number of alignments. OpBerg discovers meaningful alignments that return from alignment query results that are more useful in finding semantic similarity of two causal sentences. The improved model and efficient implementation make OpBerg the best model to use when performing tasks that involve the alignment of two or more sets of input, particularly in that of POS mappings for causal extraction.
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