Structural Isomprphism in Mathematical Expressions: A Simple Coding Scheme

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Abstract

While there exist many methods in machine learning for comparison of letter string data, most are better equipped to handle strings that represent natural language, and their performance will not hold up when presented with strings that correspond to mathematical expressions. Based on the graphical representation of the expression tree, here I propose a simple method for encoding such expressions that is only sensitive to their structural properties, and invariant to the specifics which can vary between two seemingly different, but semantically similar mathematical expressions.

1 Introduction

The toolbag of Natural Language Processing contains several methods for measuring similarity between textual data. From superficial metrics like Levenshtein (edit) distance (Levenshtein, 1965), to somewhat superficial ones like TF-IDF (Sparck Jones, 1972), and to heavily semantic metrics that emerge from the depths of encoding neural networks (Vaswani et al., 2017; Kiros et al., 2015). In general these methods are particularly suited to analyzing text that represent natural language. However, there are occasions where the string data consist of more than normal text, and contain, for instance, mathematical formulæ. The existing metrics are less than optimal in such scenarios, and one has to employ other means of representing the similarity between such data strings.

An example of this comes up in correlation of school standards to textbook headings. School districts are required to follow certain curricular standards that are usually designated at the state or federal level. These standards state the specific topics that should be covered for each subject in each grade. For instance under biology for grade 11, one of California standards about DNA reads “Construct an explanation based on evidence for how the structure of DNA determines the structure of proteins which carry out the essential functions of life through systems of specialized cells (NGSS, 2018).” Therefore, teachers need to know the correspondence between the material in the textbook they adopt and the standards their district follows. Seeing as this correspondence relies on the semantics of the standard and the text in the book, a semantic matching can be used (e.g. document embedding) to measure the similarity between the two, and pick the most similar candidates.

This strategy works well for most scientific subjects (e.g. Biology, Earth Sciences, etc.) but falls short when the subject at hand involves mathematical expressions, because often the matching
algorithms do not have a default method of encoding mathematical expressions. A simple approach for such occasions would be to opt for a standard format (e.g., LaTeX) and store the formulae as they are. During matching, one only needs to look for an exact match between the formula in the query and the ones stored in the database. However, this approach falls apart quickly as we notice that the same expression may be stated using $x$ and $y$ in the database, but using $\alpha$ and $\beta$ in the query. For instance $(x + y)^2$ vs. $(\alpha + \beta)^2$.

2 Motivation

Looking at the following two expressions, we can tell that they are expressing the same symbolic mathematical relationship\(^1\), even though they look quite different.

\[ a^2 + b^2 + 2ab \]
\[ (x + y)^2 \]  

(1)

How do we capture this similarity? Part of the problem lies in recognizing the identity $(s + t)^2 = s^2 + t^2 + 2st$. Thankfully, there exist libraries and platforms that can easily handle such identities (e.g., Maple and SymPy). The more cumbersome issue is that one expression is stated in terms of $a$ and $b$ while the other is expressed via $x$ and $y$. Since we already have the means of resolving the identity, let us reformulate the problem and focus on the issue that requires our attention:

\[ a^2 + b \]
\[ x + y^2 \]  

(2)

Note that the isomorphy of the two expressions is in the structure of the algebraic operation they suggest, which in words would be something along “one variable plus the square of another variable”. Therefore, what we need is to encode the expression in such a way that exposes this structure.

I propose to use the expression tree for this purpose, namely, a convenient way to represent the structure of a mathematical expression. The useful property of such a graph is that it makes explicit the property of interest, which is otherwise only implied in the nominal representation of the above expressions. Once we have the desired graph, then the problem of matching two expressions changes to that of graph isomorphism. Graph isomorphism is the well established problem of deciding whether two different graphs employ the same toplogical structure, regardless of their apparently different representation. For instance, in figure 1, bottom, a and b are isomorphic to each other, but neither is isomorphic to c.

It should be noted that the question of whether two mathematical expressions are equal is akin to the halting problem\(^2\), and in general undecidable\(^1\). Therefore, the algorithm I propose here would be better considered a heuristic which can handle most ordinary cases likely to appear in school textbooks, but will nevertheless fail in the face self referential statements. To make matters worse, in the proposed approach, once the expressions are converted

\(^{1}\)Of course if we were to specify them further, they may become different expressions. For instance, if one were defined only on complex numbers and the other on positive integers, then obviously they wouldn’t be the same.
Figure 1: Top: The expression tree for $x^2 + y$. Bottom: $a$ and $b$ are isomorphic, even though they appear different. Neither is isomorphic with $c$. 
into their graphical representation, their equality amounts to isomorphism of their corresponding trees, which is conjectured to be NP-complete (Lewis 1983). But the algorithm will not actually test for isomorphism of trees (more on that later).

3 Algorithm

We start by parsing the expression and building an expression tree. Expression trees are undirected acyclic graphs built from a prefix notation of the expression. Specifically, we are interested in the algebraic expression trees. Figure 1, top, illustrates an example of an expression tree for \( x^2 + y \).

While it is common for these trees to be binary, here we are relaxing this constraint and allowing each sub-tree to have more than two children. However, note that since \( T(c_0, c_1, ... c_n) \), an N-ary branch, can be rewritten as \( T_0(T_1(...T_{n-1}(c_{n-1}, c_n), c_1), c_0) \), a binary sub-tree, our discussion here extends to binary trees too.

With the expression tree built, the adjacency matrix\(^2\) together with the set of vertices will uniquely identify a symbolic expression. From there, the proper way to test whether two expressions thus coded are equal, will be to test whether they have the same vertices, and more importantly, if their graphs are isomorphic, a rather expensive task (Lewis 1983). However, if we are willing to accept less than perfect results, we can systematically organize the vertices to be consistent across all expressions and obviate the need to test for isomorphism. The test of graph isomorphism is only necessary because the adjacency matrix for the same graph can be rewritten multiple ways for each possible ordering of the vertices. For instance, for the example in figure 1, top, we can have \( x, 2, y, \text{Pow}, \text{Add}, \) or \( 2, x, y, \text{Pow}, \text{Add}, \) or ... each resulting in a different matrix. But if the vertices always appear in the same order (e.g. from largest power to smallest, trig functions last, etc.), the adjacency matrix will usually look the same for different expressions that share the same structure. The consistency of the ordering can break, however, where there is ambiguity in the order, and the algorithm has to resort to a secondary tie breaking policy. For instance, when there are multiple terms of the same order, sorting them alphabetically seems like a natural solution. But, this can lead to imperfect results because the letter representing the symbol is the very entity that we want to be invariant to. Consequently, this is a decision on the trade-off between computational expense and error tolerance, which the designer will need to consider for the particular application of interest.

Since the expression tree is undirected, the adjacency matrix will be symmetric. Therefore, instead of the entire matrix, the upper triangular (or the lower triangular) matrix alone will suffice. Putting together the two main ingredients (adjacency matrix and vertex set), one possible coding scheme will then be to concatenate the upper triangular adjacency matrix and the the set of vertices into one long string representation. For instance, for the expression \( x^2 + y \) (figure 1), we have:

\[
\begin{align*}
\text{Vertices} & : x, 2, y, \text{Pow}, \text{Add} \\
\text{Adjacency Matrix} = & [[0, 0, 0, 1, 0], [0, 0, 0, 1, 0], [0, 0, 0, 0, 1], [1, 1, 0, 0, 1], [0, 0, 1, 1, 0]] \\
\text{Upper Triangular} = & [[0, 0, 1, 0], [0, 1, 0], [0, 1, 0], [0, 1, 0], [0, 1, 0], [0, 1, 0], [0, 1, 0]] \\
\text{Coded} & :0010010011SymNumSymPowAdd
\end{align*}
\]

\(^2\)A common representation for graphs is a square matrix with as many rows and columns as the number of vertices in the graph. If there is an edge connecting vertex \( i \) to vertex \( j \) then the \( ij^{th} \) entry in the matrix will be 1, otherwise 0. This is called the adjacency matrix.
Table 1: Examples of expressions and their corresponding expression trees, as well as the final coded strings.

\[
\begin{align*}
(x + y)^2 & : 0010010011SymSymNumAddPow \\
\sin(x)\cos(x) & : 110011SymSinCosAdd \\
\frac{2xy+5}{y} & : 00010000101010010101SymSymNumNumMulAddDiv
\end{align*}
\]

Figure 2: Examples of expression trees. a: \((x + y)^2\); b: \(\sin(x)\cos(x)\); c: \(\frac{2xy+5}{y}\)

Where the final coded representation is the concatenation of the rows from the upper triangular matrix and the vertices, with Sym and Num denoting symbolic and numerical vertices. Note that had the expression been \(a^2 + b\) or \(t + s^2\), the final representation would still be the same. Table 1 lists a few more examples of coded expressions.

4 Discussion

The basic implementation of this coding scheme is truly invariant to both variables and constants. As long as the structure of the expression is the same, it cares not what the specifics of the variables or constants are and treats them all the same. For instance, \((a+b)^7\) and \((u+v)^5\) are both coded the same way. While this may be desired for the purpose of measuring similarity, it can pose a problem when the specific variable or constant used bears a significance not shared by other choices for that
variable or constant. Examples are variables of particular meaning in Physics (e.g. $R, C, V, G, \rho, \epsilon$ etc.), exponents of 2 and 3 which are generally treated separately and given special attention (e.g. many books cover $(a + b)^2$ and $(a + b)^3$ in isolation before generalizing to $(a + b)^n$), and constants such as 3.14 and 9.8. Therefore, it is important for the designer to consider carefully how much invariance is desired and include in the algorithm a list of special cases that require a different treatment.

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