Exploring Einsum as a Universal Inference Language

Master's Thesis

zur Erlangung des akademischen Grades

Master of Science (M.Sc.)

im Studiengang Informatik

Friedrich-Schiller-Universität Jena

Fakultät für Mathematik und Informatik

von Maurice Wenig **geboren am** 11.08.1999 **in** Jena

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Abstract

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1 Introduction

1.1 Einsum

Definition 1. Let S be a collection of symbols that correspond to non-empty sets of tensor axes. For $i \in [n]$, let $T^{(i)}$ be a $d^{(i)}$-th order tensor with axis symbols $s^{(i)} \in S^{d^{(i)}}$ for their unique axes $a_j^{(i)} \in \mathcal{N}$. The actual value of $a_j^{(i)}$ does not matter. These variables are just used as a unique identifier for the axes so that the definition is more rigorous.

The size of the tensor $T^{(i)}$ on the axis $a_j^{(i)}$ is denoted as $d_j^{(i)}$ for $j \in [d_i]$. For this definition it must hold that $s_j^{(i)} = s_{j'}^{(i')} \implies d_j^{(i)} = d_{j'}^{(i')}$ for all $i, i' \in [n], j \in [d^{(i)}], j' \in [d^{(i')}]$. This means that the set of axes that a symbol $s \in S$ corresponds to, must all have the same size.

Therefore we can also denote the size of the axes that a symbol $s \in S$ corresponds to as $d_s := d_j^{(i)}$ for all $i \in [n], j \in [d^{(i)}]$ with $s = s_j^{(i)}$. Note that not all same size axes have to assigned the same symbol. E.g. with $S = \{i, j\}$, a square matrix $T^{(1)}$ could have axes $s^{(1)} = (i, i)$ or $s^{(1)} = (i, j)$.

Let $T^{(0)}$ be a $d^{(0)}$-th order tensor with axis symbols $s^{(0)} \in S^{d^{(0)}}$. This tensor will be the result of the computation. Its axis symbols decide which axes are kept and which axes will be summed over. The symbols S are partitioned into bound symbols $B = \{s_j^{(0)} \mid j \in [d^{(0)}]\}$ and free symbols $F = S \setminus B$. We will keep all axes corresponding to symbols in B and sum over all axes corresponding to symbols in F.

Let $\mathcal{I} := \prod_{s \in B} [d_s]$ and $\mathcal{J} := \prod_{s \in F} [d_s]$. These will be the space of multi-indices which we iterate over. For $I \in \mathcal{I}, J \in \mathcal{J}$, the concatenation of the indices is denoted as IJ. The projection of the multi-index over all tensors IJ on the multi-index for tensor $T^{(i)}$ is denoted as $IJ : s^{(i)}$. $I : s^{(0)}$ is defined analogously.

Given a semiring $R = (M, \oplus, \odot)$. Then the einsum-notation denotes the following:

$$
\begin{aligned}
& T^{(0)} = (s^{(1)}, \ldots, s^{(n)} \to s^{(0)}, T^{(1)}, \ldots, T^{(n)})_R \\
:\Longleftrightarrow\ & \forall I \in \mathcal{I} : T^{(0)}_{I:s^{(0)}} = \bigoplus_{J \in \mathcal{J}} \bigodot_{i=1}^{n} T^{(i)}_{IJ:s^{(i)}}
\end{aligned}
$$

if B, F are non-empty. However, if there are no free symbols, the summation is removed:

$$
\begin{aligned}
T^{(0)} &= (s^{(1)}, \ldots, s^{(n)} \to s^{(0)}, T^{(1)}, \ldots, T^{(n)})_R \\
:\Longleftrightarrow\ \forall I \in \mathcal{I} : T^{(0)}_{I:s^{(0)}} &= \bigodot_{i=1}^{n} T^{(i)}_{IJ:s^{(i)}}
\end{aligned}
$$

If there are no bound symbols, then $s^{(0)}$ is empty and $T^{(0)}$ is a scalar:

$$
\begin{aligned}
T^{(0)} &= (s^{(1)}, \ldots, s^{(n)} \to s^{(0)}, T^{(1)}, \ldots, T^{(n)})_R \\
:\Longleftrightarrow\ T^{(0)} &= \bigoplus_{J \in \mathcal{J}} \bigodot_{i=1}^{n} T^{(i)}_{J:s^{(i)}}
\end{aligned}
$$

Note that duplicate entries in $s^{(i)}, i \in [n]$ will result in the expression iterating over the input tensors in a sort of *diagonal* way. Duplicate entries in $s^{(0)}$ will result in some entries of $T^{(0)}$ not being defined. These can be set to an arbitrary value like 0.

In case the semiring can be derived from the context, or if it is irrelevant, it can be left out from the expression.

1.1.1 Examples

All following examples use the standard semiring $R = (\mathbb{R}, +, \cdot)$.

- matrix-vector multiplication: Let $A \in \mathbb{R}^{m \times n}, v \in \mathbb{R}^n$. Then

$$A \cdot v = (ij, j \to i, A, v)$$

- matrix-matrix multiplication: Let $A \in \mathbb{R}^{m \times r}, B \in \mathbb{R}^{r \times n}$. Then

$$A \cdot B = (ik, kj \to ij, A, B)$$

- trace: Let $A \in \mathbb{R}^{n \times n}$. Then

$$\text{trace}(A) = (ii \to, A)$$

- squared frobenius norm: Let $A \in \mathbb{R}^{n \times n}$. Then

$$|A|_2^2 = (ij, ij \to, A, A)$$

- diagonal matrix: Let $v \in \mathbb{R}^n$. Then

$$\text{diag}(v) = (i \to ii, v)$$

1.1.2 Nested Einsum Expressions

Theorem 1: For $i \in [m+n+1]$, let $T^{(i)}$ be a $d^{(i)}$-th order tensor with axis symbols $s^{(i)} \in S^{d^{(i)}}$, $o := m+n+1$. Let

$$T^{(0)} := (s^{(1)}, \dots, s^{(m)}, s^{(x)} \to s^{(0)}, T^{(1)}, \dots, T^{(m)}, T^{(o)})$$

and

$$T^{(o)} = (s^{(m+1)}, \dots, s^{(m+n)} \to s^{(o)}, T^{(m+1)}, \dots, T^{(m+n)})$$

where the free symbols of the second einsum expression share no symbols with the first einsum expression.

Then

$$T^{(0)} = (s^{(1)}, \dots, s^{(m+n)} \to s^{(0)}, T^{(1)}, \dots, T^{(m+n)})$$

Proof. Let B, B', F, F' be the bound and free symbols of the first and second einsum expression respectively. W.l.o.g. they are all non-empty. From them we can derive $\mathcal{I}, \mathcal{I}', \mathcal{J}, \mathcal{J}'$ as above. Then

$$\begin{aligned}
& T^{(0)} = (s^{(1)}, \dots, s^{(m)}, s^{(o)} \to s^{(0)}, T^{(1)}, \dots, T^{(m)}, T^{(o)}) \\
\iff \forall I \in \mathcal{I} : T^{(0)}_{I:s^{(0)}} &= \bigoplus_{J \in \mathcal{J}} \bigodot_{i=1}^{m} T^{(i)}_{IJ:s^{(i)}} \odot T^{(o)}_{IJ:s^{(o)}} \\
&= \bigoplus_{J \in \mathcal{J}} \bigodot_{i=1}^{m} T^{(i)}_{IJ:s^{(i)}} \odot \bigoplus_{J' \in \mathcal{J}'} \bigodot_{i'=m+1}^{m+n} T^{(i')}_{IJJ':s^{(i')}} \\
&= \bigoplus_{J \in \mathcal{J}} \bigoplus_{J' \in \mathcal{J}'} \bigodot_{i=1}^{m} T^{(i)}_{IJ:s^{(i)}} \odot \bigodot_{i=m+1}^{m+n} T^{(i)}_{IJJ':s^{(i)}} \\
&= \bigoplus_{J \in \mathcal{J} \times \mathcal{J}'} \bigodot_{i=1}^{m+n} T^{(i)}_{IJ:s^{(i)}} \\
\iff & T^{(0)} = (s^{(1)}, \dots, s^{(m+n)} \to s^{(0)}, T^{(1)}, \dots, T^{(m+n)})
\end{aligned}$$

where the third equality follows from

$$\forall I' \in \mathcal{I}' : T^{(o)}_{I':s^{(o)}} = \bigoplus_{J' \in \mathcal{J}'} \bigodot_{i'=m+1}^{m+n} T^{(i')}_{I'J':s^{(i')}},$$

$B' \subseteq B \cup F$, and $(B \cup F) \cap F' = \emptyset$. The last two facts are required so that $IJJ' : s^{(i')}$ is well-defined and projects on the same indices as $I'J' : s^{(i')}$. The fourth equality follows from the distributivity in a semiring. □

1.1.3 A More General Result

Theorem 2: For $i \in [m+n+1]$, let $T^{(i)}$ be a $d^{(i)}$-th order tensor with axis symbols $s^{(i)} \in S^{d^{(i)}}$, $o := m+n+1$. Also let $\hat{s}^{(o)}$ be alternative axis symbols for $T^{(o)}$ with $s^{(o)}_j = s^{(o)}_{j'} \implies \hat{s}^{(o)}_j = \hat{s}^{(o)}_{j'}$ for all $j, j' \in [d^{(o)}]$. Let

$$T^{(0)} := (s^{(1)}, \ldots, s^{(m)}, \hat{s}^{(o)} \rightarrow s^{(0)}, T^{(1)}, \ldots, T^{(m)}, T^{(o)})$$

and

$$T^{(o)} = (s^{(m+1)}, \ldots, s^{(m+n)} \rightarrow s^{(o)}, T^{(m+1)}, \ldots, T^{(m+n)})$$

where the free symbols of the second einsum expression share no symbols with the first einsum expression. Let $\nu : S \rightarrow S$ such that

$$\nu(s) = \begin{cases} \hat{s}^{(o)}_j & \text{if } \exists j \in [d^{(o)}] : s^{(o)}_j = s \\ s & \text{else} \end{cases}$$

which maps symbols in $s^{(o)}$ to the symbol at the same index in $\hat{s}^{(o)}$ and all other symbols to themselves. ν can be extended to map from axis symbol tuples by setting $\nu(s^{(i)}) \in S^{d^{(i)}}, \nu(s^{(i)})_j := \nu(s^{(i)}_j)$.

Let $\hat{s}^{(i)} := \nu(s^{(i)})$ Then

$$T^{(0)} = (s^{(1)}, \ldots, s^{(m)}, \hat{s}^{(m+1)}, \ldots, \hat{s}^{(m+n)} \rightarrow s^{(0)}, T^{(1)}, \ldots, T^{(m+n)})$$

Proof. Let ...

$$\begin{aligned}
& T^{(0)} = (s^{(1)}, \ldots, s^{(m)}, s^{(o)} \rightarrow \hat{s}^{(0)}, T^{(1)}, \ldots, T^{(m)}, T^{(o)}) \\
\iff \forall I \in \mathcal{I} : T^{(0)}_{I:s^{(0)}} &= \bigoplus_{J \in \mathcal{J}} \bigodot_{i=1}^{m} T^{(i)}_{IJ:s^{(i)}} \odot T^{(o)}_{IJ:\hat{s}^{(o)}} \\
&= \bigoplus_{J \in \mathcal{J}} \bigodot_{i=1}^{m} T^{(i)}_{IJ:s^{(i)}} \odot \mu \left(\bigoplus_{J' \in \mathcal{J}'} \bigodot_{i'=m+1}^{m+n} T^{(i')}_{IJJ':s^{(i')}} \right) \\
&= \bigoplus_{J \in \mathcal{J}} \bigodot_{i=1}^{m} T^{(i)}_{IJ:s^{(i)}} \odot \bigoplus_{J' \in \mathcal{J}'} \bigodot_{i'=m+1}^{m+n} \mu \left(T^{(i')}_{IJJ':s^{(i')}} \right) \\
&= \bigoplus_{J \in \mathcal{J}} \bigodot_{i=1}^{m} T^{(i)}_{IJ:s^{(i)}} \odot \bigoplus_{J' \in \mathcal{J}'} \bigodot_{i'=m+1}^{m+n} T^{(i')}_{IJJ':\hat{s}^{(i')}} \\
&= \bigoplus_{J \in \mathcal{J} \times \mathcal{J}'} \bigodot_{i=1}^{m} T^{(i)}_{IJ:s^{(i)}} \odot \bigodot_{i=m+1}^{m+n} T^{(i)}_{IJ:\hat{s}^{(i)}} \\
\iff T^{(0)} &= (s^{(1)}, \ldots, s^{(m)}, \hat{s}^{(m+1)}, \ldots, \hat{s}^{(m+n)} \rightarrow s^{(0)}, T^{(1)}, \ldots, T^{(m+n)})
\end{aligned}$$

□

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2 Methods

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3 Results

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4 Discussion

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5 Conclusion

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Proofs

Proof that expanding the matrix multiplication in a neural network results in an exponentially big term in terms of the width of the skipped layer of the neural network:

Given: fully connected neural network with 2 layers ($n \to m \to l$ neurons), ReLU Activations, maps inputs $x \in \mathbb{R}^n$ to outputs $y \in R^l$, with parameters $A^{(0)} \in \mathbb{R}^{m \times n}, A^{(1)} \in \mathbb{R}^{l \times m}, b^{(0)} \in \mathbb{R}^m, b^{(1)} \in \mathbb{R}^l$. Then the computation of the neural network is:

$$y = \max(A^{(1)} \max(A^{(0)} x + b^{(0)}, 0) + b^{(1)}, 0)$$

To reasonably work with matrix multiplication in the tropcial semiring, we can only view matrices with positive integer entries. Making the entries integers does not impact the strength of the neural network, because [...] (quote the paper).

Now to only use positive valued matrices, we can rewrite the expression of computing the next layer from a previous layer:

$$\max(Ax + b, 0) = \max(A_+ x + b, A_- x) - A_- x$$

where $A_+ = \max(A, 0), A_- = \max(-A, 0)$ and therefore $A = A_+ - A_-$.

This turns the network output into a tropical rational function (quote):

$$\begin{aligned} y = \max(&\overbrace{A_+^{(1)} \max(A_+^{(0)} x + b^{(0)}, A_-^{(0)} x)}^{z} + A_-^{(1)} A_+^{(0)} x + b^{(1)}, \\ &A_-^{(1)} \max(A_+^{(0)} x + b^{(0)}, A_-^{(0)} x) + A_+^{(1)} A_+^{(0)} x) \\ &- \left[A_-^{(1)} \max(A_+^{(0)} x + b^{(0)}, A_-^{(0)} x) + A_+^{(1)} A_+^{(0)} x\right] \end{aligned}$$

We focus on the subexpression z, which makes the calculation a bit simpler, but keeps the point.

Now if we want to avoid the switch of semirings, we need to apply the distributive law a bunch of times.

$$
\begin{aligned}
z &= A_+^{(1)} \max(A_+^{(0)} x + b^{(0)}, A_-^{(0)} x) \\
z_i &= \bigodot_{j=1}^{m} \left(b_j^{(0)} \odot \bigodot_{k=1}^{n} x_k^{\odot A_{jk+}^{(0)}} \oplus \bigodot_{k=1}^{n} x_k^{\odot A_{jk-}^{(0)}} \right)^{\odot A_{ij+}^{(1)}} \\
&= \bigodot_{j=1}^{m} \left(\left(b_j^{(0)} \right)^{\odot A_{ij+}^{(1)}} \odot \bigodot_{k=1}^{n} x_k^{\odot\left(A_{ij+}^{(1)} + A_{jk+}^{(0)} \right)} \oplus \bigodot_{k=1}^{n} x_k^{\odot\left(A_{ij+}^{(1)} + A_{jk-}^{(0)} \right)} \right) \\
&= \bigoplus_{J \in 2^{[m]}} \bigodot_{j \in J} \left[\left(b_j^{(0)} \right)^{\odot A_{ij+}^{(1)}} \odot \bigodot_{k=1}^{n} x_k^{\odot\left(A_{ij+}^{(1)} + A_{jk+}^{(0)} \right)} \right] \odot \bigodot_{j \in [n] \setminus J} \left[\bigodot_{k=1}^{n} x_k^{\odot\left(A_{ij+}^{(1)} + A_{jk-}^{(0)} \right)} \right]
\end{aligned}
$$

Where the second equality is just the first equality written with the operations of the tropical semiring, the third equality follows from the distributive law with standard operations, and the last equality follows from the distributive law in the tropical semiring.

This expression maximizes over a number of subexpressions that grows exponentially in the width of the inner layer. Which subexpressions can be removed before the evaluation remains an open question. Note that it depends on the non-linearities of the neural network, which might make it hard to find a general answer to this question.

1 General Einsum Stuff

Nested einsum expressions in the same semiring can be combined into one smaller einsum expression.

(proof: basically distributive law.) Let $R = (M, \oplus, \odot)$ be a semiring, and $f : M \to M, g : M \to M$

2 Expressing Stuff as Einsum

Fully connected Feed-Forward Neural Net with ReLU activations (1 layer) $\nu : \mathbb{R}^n \to \mathbb{R}^m$ with weights $A \in \mathbb{R}^{m \times n}$ and biases $b \in \mathbb{R}^m$, input $x \in \mathbb{R}^n$

- $(\text{einsum\_expression})_R$ indicates that the einsum expression uses the semiring R
- $R_{(+,\cdot)}$ indicates the standard semiring
- $R_{(\max,+)}$ indicates the tropical semiring
- $R_{(\min,\max)}$ indicates the minimax semiring

$$\begin{aligned}\nu(x) &= \max(Ax+b,0)\\ &= (i,i\to i,0,(i,i\to i,b,(ij,j\to i,A,x)_{R_{(+,\cdot)}})_{R_{(\max,+)}})_{R_{(\min,\max)}}\end{aligned}$$

Attention with einsum:

$$\begin{aligned}
(QK^\top)_{ij} &= \sum_k Q_{ik}K_{jk}\\
QK^\top &= (ik,jk\to ij,Q,K)\\
\mathrm{softmax}(X)_{ij} &= \frac{\exp(X_{ij})}{\sum_{j'}\exp(X_{ij'})}\\
&= \exp(X_{ij})\cdot\sum_{j'}\exp(-X_{ij'})\\
\mathrm{softmax}(X) &= (ij,i\to ij,\exp(X),(ij\to i,\exp(-X)))\\
(XV)_{ij} &= \sum_k X_{ik}V_{kj}\\
XV &= (ik,kj\to ij,X,V)\\
\mathrm{Attention}(Q,K,V) &= \mathrm{softmax}\left(\frac{QK^\top}{\sqrt{d_K}}\right)V\\
&= (ik,kj\to ij,(ij,i\to ij,\exp(\frac{1}{\sqrt{d_k}}\cdot(ik,jk\to ij,Q,K)),\\
&\qquad (ij\to i,\exp(-\frac{1}{\sqrt{d_k}}\cdot(ik,jk\to ij,Q,K)))),V)\\
&= (ik,i,kj\to ij,\exp(\frac{1}{\sqrt{d_k}}\cdot(ik,jk\to ij,Q,K)),\\
&\qquad (ij\to i,\exp(-\frac{1}{\sqrt{d_k}}\cdot(ik,jk\to ij,Q,K))),\\
&\qquad V)
\end{aligned}$$

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Selbständigkeitserklärung

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Jena, 16.05.2023