Exploring Einsum as a Universal Inference Language

Masterarbeit

zur Erlangung des akademischen Grades

Master of Science (M.Sc.)

im Studiengang Informatik

Friedrich-Schiller-Universität Jena

Fakultät für Mathematik und Informatik

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Abstract

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1.1 Some Section

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1.2 Some Other Section

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2 Einsum

Given two third-order tensors $A \in \mathbb{R}^{3 \times 4 \times 5}$ and $B \in \mathbb{R}^{3 \times 3 \times 5}$, and a vector $v \in \mathbb{R}^4$. Consider the following computation resulting in a matrix $C \in \mathbb{R}^{3 \times 3}$:

$$\forall i \in [3] : \forall j \in [4] : C_{ij} = \sum_{k=1}^{5} A_{ijk} B_{iik} v_j$$

The original Einstein-notation for summation removes redundant formalism ("boilerplate") from this expression:

$$C_{ij} = A_{ijk} B_{iik} v_j$$

where it is assumed that C is defined for all possible i, j. We sum over all indices that are not used to index the output. In this example, we therefore have to sum over all possible values of k, because it is not used to index C_{ij}. Note how it is clear what the shape of C is, because i and j were used to index the tensors A, B, and v, for which we defined the dimensions on every axis.

This notation is essentially the inspiration for Einsum, which might be apparent given the name Einsum. Einsum is just an adaptation of this style, which makes it easier to use in programming. With it, we can write the above expression like this:

$$C := (ijk, iik, j \to ij, A, B, v)$$

Through the following definition, we hope to clear up why this Einsum expression results in the computation above, and what computation a general Einsum expression results in.

Definition 1. Einsum expressions specify how several input tensors are combined into a single output tensor. Let $T^{(1)}, \ldots, T^{(n)}$ be our input tensors, where $T^{(i)}$ is an n_i-th order tensor for $i \in [n]$. The core of the Einsum expression are index strings. For this, we first need a collection of symbols S. The respective index string for a tensor $T^{(i)}$ is then just a tuple $\boldsymbol{s_i} \in S^{n_i}$, composed of symbols $s_{ij} \in S$ for $j \in [n_i]$. The index string that is right of the arrow ($\to$) belongs to the output tensor T and is referred to as output string $\boldsymbol{s_t}$.

In our example this could be $S = \{i, j, k\}$ with respective index strings $\boldsymbol{s_1} = ijk$ for $T^{(1)} = A$, $\boldsymbol{s_2} = iik$ for $T^{(2)} = B$, $\boldsymbol{s_3} = j$ for $T^{(3)} = v$, and $\boldsymbol{s_t} = ij$. The individual symbols are $s_{11} = i$, $s_{12} = j$, $s_{13} = k$, $s_{12} = i$, $s_{22} = i$, $s_{23} = k$, $s_{31} = j$, $s_{t1} = i$, $s_{t2} = j$.

In order to refer to individual tensor axes, let us numerate them with $a_{ij} \in \mathbb{N}$, where a_{ij} denotes the j-th axis of the tensor i-th tensor $T^{(i)}$. The actual value of a_{ij} does not matter. These variables are just used as unique identifiers for the axes. Note that we can combine the axes to describe the set of axes of a tensor $T^{(i)}$ with $\boldsymbol{a_i} = \{a_{ij} \mid j \in [n_i]\}$. In contrast to $\boldsymbol{s_i}$, this is a set and not a tuple. This is because tensors can reuse symbols as indices, but cannot reuse axes.

The next step in the definition is to speak about the axis sizes. If we want to iterate over shared indices, it is necessary that the axes, that these indices are used for, share the same size. In our example, A_{ijk} and v_j share the symbol $s_{12} = s_{31} = j$. This means that the respective axes a_{12} and a_{31} have to have the same size, which happens to be 4 (four?). Let us express this formally.

Let $d_{ij} \in \mathbb{N}$ denote the size of the axis a_{ij} for $i \in [n], j \in [n_i]$. Then it must hold that $s_{ij} = s_{i'j'} \implies d_{ij} = d_{i'j'}$ for all $i, i' \in [n], j \in [n_i], j' \in [n_{i'}]$.

Therefore we can also denote the size of all axes that a symbol $s \in S$ corresponds to as $d_s := d_{ij}$ for all $i \in [n], j \in [n_i]$ with $s = s_{ij}$. Note that not all same size axes have to assigned the same symbol. For instance a square matrix could have index strings $\boldsymbol{s} = (i, i)$ or $\boldsymbol{s} = (i, j)$.

The next step of the definition is figuring out which symbols are used for summation and which symbols are used for saving the result of the computation. In order to do this, it is useful to know which symbols are in an index string, because symbols can occur more than once in just one index string (as seen in B_{iik} in our example). Therefore, let $\sigma(\boldsymbol{s})$ denote the set with all symbols used in an index string $\boldsymbol{s}$. That is, in out example $\sigma(\boldsymbol{s_2}) = \sigma(iik) = \{i, k\}$.

All symbols to the right of the arrow ($\rightarrow$) are used as an index for the result of the computation. These symbols are called *free* symbols $F = \sigma(\boldsymbol{s_t})$. All other symbols used in the expression are called *bound* symbols $B = \bigcup_{i \in [n]} \sigma(\boldsymbol{s_i}) \setminus \sigma(\boldsymbol{s_t})$. The reasoning behind this name is, that these symbols are bound by the summation symbol in the original computation. In Einsum, we sum over all axes that belong to bound symbols. It follows that the multi-index space that we iterate over is $\mathcal{I} = \prod_{s \in F}[d_s]$ and the multi-index space we sum over is $\mathcal{J} = \prod_{s \in B}[d_s]$. In our example, the free symbols are $F = \{ij\}$ and the bound symbols are $B = \{k\}$. The multi-index space we iterate over is $d_i \times d_j = [3] \times [4]$. The multi-index space we sum over is $d_k = [5]$.

From the definition of $\mathcal{I}$, it follows that d_s has to be defined for all symbols $s \in F$. This means we have to add the constraint $\sigma(\boldsymbol{s_t}) \subseteq \bigcup_{i \in [n]} \sigma(\boldsymbol{s_i})$.

However, we do not use every symbol in the multi-index spaces to index every input tensor. Instead, we use the index strings $\boldsymbol{s}$ to index the tensor. To formally express this, we need a projection from a multi-index $(\boldsymbol{i}, \boldsymbol{j}) \in \mathcal{I} \times \mathcal{J}$ to another multi-index, which includes only the symbols used in $\boldsymbol{s}$, in the same order as present in $\boldsymbol{s}$. We denote this as $(\boldsymbol{i}, \boldsymbol{j}) : \boldsymbol{s}$. Notice how this still allows duplication of indices given in $(\boldsymbol{i}, \boldsymbol{j})$. This is needed, as can be seen in our example for B_{iik}, where a multi-index, e.g. $(1, 4, 2) \in \mathcal{I} \times \mathcal{J}$, is projected on the index string iik, which results in the multi-index $(1, 4, 2) : iik = (1, 1, 2)$.

In our example, we used the standard sum and multiplication as operators for computing our result. But with Einsum, we allow the more general use of any semiring $R = (M, \oplus, \odot)$. With this, we can finally define a general Einsum expression

$$T := (\boldsymbol{s_1}, \dots, \boldsymbol{s_n} \to \boldsymbol{s_t}, T^{(1)}, \dots, T^{(n)})_R$$

in terms of semiring operations. Namely, T is the $|\boldsymbol{s_t}|$-th order tensor

$$\forall \boldsymbol{i} \in \mathcal{I} : T_{\boldsymbol{i}:\boldsymbol{s_t}} = \bigoplus_{\boldsymbol{j} \in \mathcal{J}} \bigodot_{k=1}^{n} T^{(k)}_{(\boldsymbol{i},\boldsymbol{j}):\boldsymbol{s_t}}$$

Because we also project the indices $\boldsymbol{i}$ on the output string $\boldsymbol{s_t}$, we allow to iterate over duplicate indices, e.g. $\mathrm{diag}(v) = (j \to jj, v)$. This leaves some entries of the result undefined. We define these entries to be the additive neutral element in the given semiring R. This may sound arbitrary at first, but will be useful for later.

There are still some special case which need to be considered. If there are no bound symbols in the expression, then the sum will be empty. But we still want the result of the computation of the product. Therefore, if $F = \emptyset$, then

$$T := (\boldsymbol{s_1}, \dots, \boldsymbol{s_n} \to \boldsymbol{s_t}, T^{(1)}, \dots, T^{(n)})_R$$

results in the computation of a $|\boldsymbol{s_t}|$-th order tensor T with

$$\forall \boldsymbol{i} \in \mathcal{I} : T_{\boldsymbol{I}:\boldsymbol{s_t}} = \bigodot_{k=1}^{n} T^{(k)}_{\boldsymbol{i}:\boldsymbol{s_t}}$$

If there are no free symbols, we will sum over all axes given by the symbols in the expression. Therefore, if $B = \emptyset$, then

$$T := (\boldsymbol{s_1}, \dots, \boldsymbol{s_n} \to, T^{(1)}, \dots, T^{(n)})_R$$

results in the computation of a scalar T with

$$T = \bigoplus_{\boldsymbol{j} \in \mathcal{J}} \bigodot_{k=1}^{n} T^{(k)}_{\boldsymbol{j}:\boldsymbol{s_t}}$$

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

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

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

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

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

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

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

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

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

3 Nested Expressions

In practice, concatenations of operations come naturally, e.g. computing the squared norm of a matrix-vector product $|A \cdot v|_2^2$ for $A \in \mathbb{R}^{m \times n}, v \in \mathbb{R}^n$. This would lead to a nested Einsum expression $|A \cdot v|_2^2 = (i, i \to, (ij, j \to i, A, v), (ij, j \to i, A, v))$. This expression dictates the order of evaluating the expression. In the example of the norm, the expression $(ij, j \to i, A, v)$ has to be evaluated before squaring and summing over the results of this computation.

This is limiting, because the order of evaluation might not yield optimal runtime. This can be seen with a simple matrix-matrix-vector multiplication, which can be written as follows:

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

which is clearly worse than the optimal contraction order

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

for $A \in \mathbb{R}^{m \times r}, B \in \mathbb{R}^{r \times n}, v \in \mathbb{R}^r$.

But fortunately, all nested Einsum expressions can be compressed into a single Einsum expression, if they are computed over the same semiring. This leaves the path of contraction up to the implementation. In the following theorems, we assume that the computations are all over the same semiring $R = (M, \oplus, \odot)$.

3.1 Simple Nested Expressions

Theorem 1: For $i \in [m + n]$, let $T^{(i)}$ be an n_i-th order tensor with index strings $\boldsymbol{s_i} \in S^{n_i}$. Let $\boldsymbol{s_u}, \boldsymbol{s_v}$ be index strings. Let

$$U := (\boldsymbol{s_{m+1}}, \dots, \boldsymbol{s_{m+n}} \to \boldsymbol{s_u}, T^{(m+1)}, \dots, T^{(m+n)})$$

and

$$V := (\boldsymbol{s_1}, \dots, \boldsymbol{s_m}, \boldsymbol{s_u} \to \boldsymbol{s_v}, T^{(1)}, \dots, T^{(m)}, U)$$

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

$$V = (\boldsymbol{s_1}, \dots, \boldsymbol{s_{m+n}} \to \boldsymbol{s_v}, T^{(1)}, \dots, T^{(m+n)})$$

Proof. Let B, B', F, F' be the bound and free symbols of the second and first 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

$$V = (\boldsymbol{s_1}, \ldots, \boldsymbol{s_m}, \boldsymbol{s_u} \to \boldsymbol{s_v}, T^{(1)}, \ldots, T^{(m)}, U)$$

$$\Longleftrightarrow \forall I \in \mathcal{I} : V_{I:\boldsymbol{s_v}} = \bigoplus_{J \in \mathcal{J}} \bigodot_{i=1}^{m} T^{(i)}_{IJ:\boldsymbol{s_i}} \odot U_{IJ:\boldsymbol{s_u}}$$

$$= \bigoplus_{J \in \mathcal{J}} \bigodot_{i=1}^{m} T^{(i)}_{IJ:\boldsymbol{s_i}} \odot \bigoplus_{J' \in \mathcal{J}'} \bigodot_{i'=m+1}^{m+n} T^{(i')}_{IJJ':\boldsymbol{s_{i'}}}$$

$$= \bigoplus_{J \in \mathcal{J}} \bigoplus_{J' \in \mathcal{J}'} \bigodot_{i=1}^{m} T^{(i)}_{IJ:\boldsymbol{s_i}} \odot \bigodot_{i=m+1}^{m+n} T^{(i)}_{IJJ':\boldsymbol{s_{i'}}}$$

$$= \bigoplus_{J \in \mathcal{J} \times \mathcal{J}'} \bigodot_{i=1}^{m+n} T^{(i)}_{IJ:\boldsymbol{s_i}}$$

$$\Longleftrightarrow V = (\boldsymbol{s_1}, \ldots, \boldsymbol{s_{m+n}} \to \boldsymbol{s_v}, T^{(1)}, \ldots, T^{(m+n)})$$

where the third equality follows from

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

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

Compressing these nested Einsum expressions is already helpful when the output string of the inner expression is exactly the same as the input string of the outer expression, e.g. for $A \in \mathbb{R}^{m \times n}, v \in \mathbb{R}^n$:

$$|A \cdot v|_2^2 = (i, i \to, (ij, j \to i, A, v), (ij, j \to i, A, v))$$
$$= (ij, j, ij, j \to, A, v, A, v)$$

But sometimes, we need to access a different multi-index set than the one we computed, e.g. for $A \in \mathbb{R}^{m \times n}, B \in \mathbb{R}^{n \times m}, v \in \mathbb{R}^n$:

$$\text{trace}(A \cdot B) = (ii \to, (ik, kj \to ij, A, B))$$

or

$$A \cdot \text{diag}(v) = (ik, kj \to ij, A, (i \to ii, v)).$$

For this, we need more general ways of compressing nested Einsum expressions.

3.2 Introducing Duplications

In the following theorem, we explore a way of compressing the expression

$$(ij, jjj \to i, A, (kl, lo \to kko, B, C))$$

for $A \in \mathbb{R}^{a \times b}, B \in \mathbb{R}^{b \times c}, C \in \mathbb{R}^{c \times b}$. Note that, for the theorem, we use disjoined sets of symbols for the inner and outer expression. This helps in the proof, and is not a real constraint in practice, because we can just rename the symbols in different scopes. E.g. we could also write the above expression as

$$(ij, jjj \to i, A, (ik, kj \to iij, B, C)).$$

Theorem 2: For $i \in [m + n]$, let $T^{(i)}$ be an n_i-th order tensor with index strings $\boldsymbol{s_i} \in S^{n_i}$. Let $\boldsymbol{s_u}$ be an index string for the n_u-th order tensor U, which is defined as follows:

$$U := (\boldsymbol{s_{m+1}}, \dots, \boldsymbol{s_{m+n}} \to \boldsymbol{s_u}, T^{(m+1)}, \dots, T^{(m+n)})$$

Also let $\boldsymbol{\hat{s}_u}$ be alternative index strings for U with $s_{uj} = s_{uj'} \implies \hat{s}_{uj} = \hat{s}_{uj'}$ for all $j, j' \in [n_u]$, which means that $\boldsymbol{\hat{s}_u}$ can only introduce new symbol duplications, and cannot remove any.

In our example, $\boldsymbol{s_u} = kko$ and $\boldsymbol{\hat{s}_u} = jjj$. This does not break the symbol duplication of the first and second index, and introduces a new duplication on the third index.

Let s_v be an index string and

$$V := (\boldsymbol{s_1}, \dots, \boldsymbol{s_m}, \boldsymbol{\hat{s}_u} \to \boldsymbol{s_v}, T^{(1)}, \dots, T^{(m)}, U)$$

such that the first and second Einsum expression share no symbols. Then these nested Einsum expressions can also be compressed into a single Einsum expression.

In contrast to Theorem 1, we cannot just replace the input index string $\boldsymbol{\hat{s}_u}$ by all the input index strings in the inner Einsum expression $\boldsymbol{s_{m+1}}, \dots, \boldsymbol{s_{m+n}}$. Instead, we first need to apply a symbol map. Let $\nu : S \to S$ such that

$$\nu(s) := \begin{cases} \hat{s}_{uj} & \text{if } \exists j \in [n_u] : s_{uj} = s \\ s & \text{else} \end{cases}$$

which maps symbols in $\boldsymbol{s_u}$ to the symbol at the same index in $\boldsymbol{\hat{s}_u}$ and all other symbols to themselves.

This symbol map holds information about which symbols will be iterated over at the same time in the outer expression. In our example, the interesting parts of the map are $\nu(k) = j$ and $\nu(o) = j$, which means that k and j will be iterated over at the same time.

ν can be extended, such that it maps entire index strings instead of just symbols, by setting $\nu(\boldsymbol{s_i}) \in S^{n_i}, \nu(\boldsymbol{s_i})_j := \nu(s_{ij})$. Then we can write the substituted index strings by setting $\hat{\boldsymbol{s}}_{\boldsymbol{i}} := \nu(\boldsymbol{s_i})$ for $i \in [m+1, m+n]$.

Then the compressed Einsum expression is the following:

$$ V = (\boldsymbol{s_1}, \ldots, \boldsymbol{s_m}, \hat{\boldsymbol{s}}_{\boldsymbol{m+1}}, \ldots, \hat{\boldsymbol{s}}_{\boldsymbol{m+n}} \to \boldsymbol{s_v}, T^{(1)}, \ldots, T^{(m+n)}) $$

which helps us to compress the example:

$$ (ij, jjj \to i, A, (kl, lo \to kko, B, C)) = (ij, jl, lj \to i, A, B, C) $$

Proof. The fundamental idea behind this theorem is, that by using the index string $\hat{\boldsymbol{s}}_{\boldsymbol{u}}$, we only iterate over a sub-space of the indices that we defined for the computation of U. To formulate this, we need some idea of which multi-indices we iterate over. Therefore, let $\mathcal{M} : \boldsymbol{s} := \{M : \boldsymbol{s} \mid M \in \mathcal{M}\}$ for an index string $\boldsymbol{s}$ and a multi-index space $\mathcal{M}$.

Let $\mathcal{K} = \prod_{s \in \sigma(\hat{s}_u)}[d_s]$ be the multi-index space in the input for the computation of V, and let $\mathcal{K}' = \prod_{s \in \sigma(s_u)}[d_s]$ be the multi-index space in the output for the computation of U. Then $\mathcal{K} : \hat{\boldsymbol{s}}_{\boldsymbol{u}} \subseteq \mathcal{K}' : \boldsymbol{s_u}$, because $d_{s_{uj}} = d_{\hat{s}_{uj}}$ per the definition of einsum, and because the amount of axes contributing to $\mathcal{K}$ ($|\sigma(\hat{\boldsymbol{s}}_{\boldsymbol{u}})|$) has to be smaller or equal to the amount of axes contributing to $\mathcal{K}'$ ($|\sigma(\boldsymbol{s_u})|$). This last fact follows from the constraint $s_{uj} = s_{uj'} \implies \hat{s}_{uj} = \hat{s}_{uj'}$.

Then

$$ \forall K' \in \mathcal{K}' : U_{K':\boldsymbol{s_u}} = \bigoplus_{J' \in \mathcal{J}'} \bigodot_{i=m+1}^{m+n} T^{(i)}_{K'J':\boldsymbol{s_i}} $$

and therefore

$$ \forall K \in \mathcal{I}' : U_{K:\hat{\boldsymbol{s}}_{\boldsymbol{u}}} = \bigoplus_{J' \in \mathcal{J}'} \bigodot_{i=m+1}^{m+n} T^{(i)}_{KJ':\hat{\boldsymbol{s}}_{\boldsymbol{i}}} $$

because of the previous observation, and because the free symbols of the expression, which are used in J', are not changed by the symbol map ν.

Therefore

$$ V = (\boldsymbol{s_1}, \ldots, \boldsymbol{s_m}, \hat{\boldsymbol{s}}_{\boldsymbol{u}} \to \boldsymbol{s_v}, T^{(1)}, \ldots, T^{(m)}, U) $$

$$ \iff \forall I \in \mathcal{I} : V_{I:\boldsymbol{s_v}} = \bigoplus_{J \in \mathcal{J}} \bigodot_{i=1}^{m} T^{(i)}_{IJ:\boldsymbol{s_i}} \odot U_{IJ:\hat{\boldsymbol{s}}_{\boldsymbol{u}}} $$

$$ = \bigoplus_{J \in \mathcal{J}} \bigodot_{i=1}^{m} T^{(i)}_{IJ:\boldsymbol{s_i}} \odot \bigoplus_{J' \in \mathcal{J}'} \bigodot_{i'=m+1}^{m+n} T^{(i')}_{IJJ':\hat{\boldsymbol{s}}_{\boldsymbol{i'}}} $$

$$ = \bigoplus_{J \in \mathcal{J} \times \mathcal{J}'} \bigodot_{i=1}^{m} T^{(i)}_{IJ:\boldsymbol{s_i}} \odot \bigodot_{i=m+1}^{m+n} T^{(i)}_{IJ:\hat{\boldsymbol{s}}_{\boldsymbol{i}}} $$

$$ \iff V = (\boldsymbol{s_1}, \ldots, \boldsymbol{s_m}, \hat{\boldsymbol{s}}_{\boldsymbol{m+1}}, \ldots, \hat{\boldsymbol{s}}_{\boldsymbol{m+n}} \to \boldsymbol{s_v}, T^{(1)}, \ldots, T^{(m+n)}) $$

where the third equality holds because we only iterate over a sub-space of the indices that we defined for the computation of U, and because the first and second einsum expression share no symbols. The rest of the steps are the same as in Theorem 1. $\square$

With this theorem we can prove a property of the trace in a relatively simple manner, namely that for $A \in \mathbb{R}^{m \times n}, B \in \mathbb{R}^{n \times m}$, it holds that

$$\text{trace}(A \cdot B) = \text{trace}(B \cdot A).$$

Proof.

$$
\begin{aligned}
\text{trace}(A \cdot B) &= (ii \rightarrow, (ik, kj \rightarrow ij, A, B)) \\
&= (ik, ki \rightarrow, A, B) \\
&= (ki, ik \rightarrow, A, B) \\
&= (ik, ki \rightarrow, B, A) \\
&= (ii \rightarrow, (ik, kj \rightarrow ij, B, A)) \\
&= \text{trace}(B \cdot A)
\end{aligned}
$$

where the second equality holds because of Theorem 2, the third equality is just a renaming of the indices, and the fourth equality holds because of the commutivity in the used semiring. □

This is already a useful tool for compressing nested expressions, but there are still some naturally occuring expressions we cannot compress with this, e.g. for $A \in \mathbb{R}^{m \times n}, v \in \mathbb{R}^n$:

$$A \cdot \text{diag}(v) = (ik, kj \rightarrow ij, A, (i \rightarrow ii, v))$$

This is because we use more indices than the ones we computed by breaking the symbol duplication ii with the index string kj.

3.3 Removing Duplications

In the following theorem, we explore a way of compressing the expression

$$(ijk, jk \rightarrow ijk, A, (l \rightarrow ll, v))$$

for $A \in \mathbb{R}^{a \times b}, v \in \mathbb{R}^b$. Again, we use disjoined sets of symbols for the inner and outer expression to help us in the formulation and the proof.

Theorem 3: For $i \in [m + n]$, let $T^{(i)}$ be an n_i-th order tensor with index strings $\boldsymbol{s_i} \in S^{n_i}$. Let $\boldsymbol{s_u}$ be an index string for the n_u-th order tensor U, which is defined as follows:

$$U := (\boldsymbol{s_{m+1}}, \ldots, \boldsymbol{s_{m+n}} \rightarrow \boldsymbol{s_u}, T^{(m+1)}, \ldots, T^{(m+n)})$$

Also let $\hat{\boldsymbol{s}}_{\boldsymbol{u}}$ be alternative index strings for U with $s_{uj} \neq s_{uj'} \implies \hat{s}_{uj} \neq \hat{s}_{uj'}$ for all $j, j' \in [n_u]$, which means that $\hat{\boldsymbol{s}}_{\boldsymbol{u}}$ can only remove symbol duplications, and cannot introduce any. Note that this is the converse of the constraint in Theorem 2.

In our example, $\boldsymbol{s_u} = ll$ and $\hat{\boldsymbol{s}}_{\boldsymbol{u}} = jk$. This removes the symbol duplication of the first and second index.

Let s_v be an index string and

$$V := (\boldsymbol{s_1}, \ldots, \boldsymbol{s_m}, \hat{\boldsymbol{s}}_{\boldsymbol{u}} \to \boldsymbol{s_v}, T^{(1)}, \ldots, T^{(m)}, U)$$

where the first and second Einsum expression share no symbols. Then these nested Einsum expressions can also be compressed into a single Einsum expression.

As in Theorem 3, we need to apply a symbol map before substituting $\hat{\boldsymbol{s}}_{\boldsymbol{u}}$. Interestingly, the symbol map is not applied to the index strings in the computation of U ($\boldsymbol{s_{m+1}}, \ldots, \boldsymbol{s_{m+n}}$), but to the index strings in the computation of V ($\boldsymbol{s_1}, \ldots, \boldsymbol{s_m}$). Similarly, it does not map $\boldsymbol{s_u}$ to $\hat{\boldsymbol{s}}_{\boldsymbol{u}}$, but $\hat{\boldsymbol{s}}_{\boldsymbol{u}}$ to $\boldsymbol{s_u}$.

Let $\mu : S \to S$ such that

$$\mu(s) := \begin{cases} s_{uj} & \text{if } \exists j \in [n_u] : \hat{s}_{uj} = s \\ s & \text{else} \end{cases}$$

μ can be extended in a similar way as ν to map entire index strings.

Let $\hat{\boldsymbol{s}}_{\boldsymbol{i}} := \mu(\boldsymbol{s_i})$ for $i \in [m]$, $\hat{\boldsymbol{s}}_{\boldsymbol{v}} := \mu(\boldsymbol{s_v})$, then the compressed Einsum expression is the following:

$$V = (\hat{\boldsymbol{s}}_{\boldsymbol{1}}, \ldots, \hat{\boldsymbol{s}}_{\boldsymbol{m}}, \boldsymbol{s_{m+1}}, \ldots, \boldsymbol{s_{m+n}} \to \hat{\boldsymbol{s}}_{\boldsymbol{v}}, T^{(1)}, \ldots, T^{(m+n)})$$

which helps us to compress the example:

$$(ijk, jk \to ijk, A, (l \to ll, v)) = (ill, l \to ill, A, v)$$

Note how even the index string for the output $\boldsymbol{s_v}$ was changed into $\hat{\boldsymbol{s}}_{\boldsymbol{v}}$. This will become apparent in the proof.

Proof. The key idea behind this proof, is that the entries of U, which were not defined in the computation, are set to the additive neutral element $\mathbb{0}$. This is useful, because in a semiring over some set M, the additive neutral element *annihilates* M. This means, that for any $a \in M$, $a \cdot \mathbb{0} = \mathbb{0} \cdot a = \mathbb{0}$. Therefore, for any multiindex where U is set to $\mathbb{0}$, V is also set to $\mathbb{0}$. This means, that in the computation of V, only the indices which follow the duplications in $\boldsymbol{s_u}$ are defined.

Let $\mathcal{I}, \mathcal{J}$ be the appropriate multi-index spaces for the computation of V. Then

$$U_{IJ:\hat{\boldsymbol{s}}_{\boldsymbol{u}}} = \mathbb{0}$$

for all $IJ \in \mathcal{I} \times \mathcal{J}$ with   □

With these theorems, we can write some more complex expressions as Einsum.

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

$$\begin{aligned} |A \cdot v|_2^2 &= (i, i \to, (ij, j \to i, A, v), (ij, j \to i, A, v)) \\ &= (ij, j, ij, j \to, A, v, A, v) \end{aligned}$$

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

$$
\begin{aligned}
\text{trace}(A \cdot B) &= (ii \rightarrow, (ik, kj \rightarrow ij, A, B)) \\
&= (ik, ki \rightarrow, A, B)
\end{aligned}
$$

- The theorem for this still has to be shown ...: matrix multiplication with a diagonal matrix: Let $A \in \mathbb{R}^{m \times n}, v \in \mathbb{R}^n$. Then

$$
\begin{aligned}
A \cdot \text{diag}(v) &= (ik, kj \rightarrow ij, A, (i \rightarrow ii, v)) \\
&= (ij, j \rightarrow ij, A, v)
\end{aligned}
$$

3.4 General Nested Expressions

In the final generalisation of compressing nested Einsum expressions, all duplication breaking is allowed. This has no application for linear algebra, as all the previous theorems had, because this first comes into play with third order tensors. This is because, with two or less axes, there is no possibility of simultaniously breaking a duplication and introducing a new one. Nevertheless, it serves as a useful tool for compressing all kinds of nested Einsum expressions.

Theorem 4: For $i \in [m+n]$, let $T^{(i)}$ be an n_i-th order tensor with index strings $\boldsymbol{s_i} \in S^{n_i}$. Let $\boldsymbol{s_u}$ be an index string for the n_u-th order tensor U, which is defined as follows:
$$
U := (\boldsymbol{s_{m+1}}, \ldots, \boldsymbol{s_{m+n}} \rightarrow \boldsymbol{s_u}, T^{(m+1)}, \ldots, T^{(m+n)})
$$
Also let $\boldsymbol{\hat{s}_u}$ be alternative index strings for U.

Let s_v be an index string and
$$
V := (\boldsymbol{s_1}, \ldots, \boldsymbol{s_m}, \boldsymbol{\hat{s}_u} \rightarrow \boldsymbol{s_v}, T^{(1)}, \ldots, T^{(m)}, U)
$$

where the first and second Einsum expression share no symbols. Then these nested Einsum expressions can also be compressed into a single Einsum expression.

Once again, a map $\omega : S \rightarrow S$ has to be applied to the index strings before substituting index strings. The definition of the map this time is somewhat more complex. As in the previous two theorems, this map holds information about which symbols are essentially used together as one index.

For the definition of the map ω, we first construct an undirected graph $G = (V, E)$, in which the nodes $V = \sigma(\boldsymbol{s_v}) \cup \sigma(\boldsymbol{s_u}) \cup \sigma(\boldsymbol{\hat{s}_u}) \cup \bigcup_{i \in [m+n]} \sigma(\boldsymbol{s_i})$ consist of all symbols from both expressions. Now the edges of this graph are $E = \{\{s_{uj}, \hat{s}_{uj}\} \mid \exists j \in [n_u] : s_{uj} \neq \hat{s}_{uj}\}$, which connects all symbols from $\boldsymbol{s_u}$ and $\boldsymbol{\hat{s}_u}$ that share an index.

In this graph, if two symbols are connected, then they to be iterated over at the same time in the compressed expression, because they are essentially the same index.

Therefore, it makes sense assigning a symbol $s_C \in S \setminus V$ to each of the graphs components C. Then we can define ω as follows:

$$\omega(s) := \begin{cases} s_C & \text{if } s \in C \\ s & \text{else} \end{cases}$$

ω can be extended in a similar way as μ, ν to map entire index strings. In this general form, the this map is applied to all index strings from both expressions before the substitution. Let $\hat{\boldsymbol{s}}_{\boldsymbol{i}} := \omega(\boldsymbol{s_i})$ for $i \in [m+n]$, $\hat{\boldsymbol{s}}_{\boldsymbol{v}} := \omega(\boldsymbol{s_v})$, then the compressed Einsum expression is the following:

$$V = (\hat{\boldsymbol{s}}_{\boldsymbol{1}}, \dots, \hat{\boldsymbol{s}}_{\boldsymbol{m+n}} \to \hat{\boldsymbol{s}}_{\boldsymbol{v}}, T^{(1)}, \dots, T^{(m+n)})$$

Proof. Wird spannend. $\square$

4 Methods

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5 Results

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6 Discussion

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7 Conclusion

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Proofs

1 Exponential Blow-Up

Given: fully connected neural network with two 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:

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

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):

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

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

Now if we want to avoid switching semirings, we need to apply the distributive law

a bunch of times.

$$z = A_+^{(1)} \max(A_+^{(0)} x + b^{(0)}, A_-^{(0)} x)$$

$$z_i = \bigodot_{j=1}^{m} \left(b_j^{(0)} \odot \bigodot_{k=1}^{n} x_k^{\odot A_{jk+}^{(0)}} \oplus \bigodot_{k=1}^{n} x_k^{\odot A_{jk-}^{(0)}} \right)^{\odot A_{ij+}^{(1)}}$$

$$= \bigodot_{j=1}^{m} \left(\left(b_j^{(0)} \right)^{\odot A_{ij+}^{(1)}} \odot \bigodot_{k=1}^{n} x_k^{\odot \left(A_{ij+}^{(1)} + A_{jk+}^{(0)} \right)} \oplus \bigodot_{k=1}^{n} x_k^{\odot \left(A_{ij+}^{(1)} + A_{jk-}^{(0)} \right)} \right)$$

$$= \bigoplus_{J \in 2^{[m]}} \bigodot_{j \in J} \left[\left(b_j^{(0)} \right)^{\odot A_{ij+}^{(1)}} \odot \bigodot_{k=1}^{n} x_k^{\odot \left(A_{ij+}^{(1)} + A_{jk+}^{(0)} \right)} \right] \odot \bigodot_{j \in [n] \setminus J} \left[\bigodot_{k=1}^{n} x_k^{\odot \left(A_{ij+}^{(1)} + A_{jk-}^{(0)} \right)} \right]$$

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.

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 $x \in \mathbb{R}^n$

- (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

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

Attention with einsum:

$$(QK^\top)_{ij} = \sum_k Q_{ik} K_{jk}$$

$$QK^\top = (ik, jk \to ij, Q, K)$$

$$\text{softmax}(X)_{ij} = \frac{\exp(X_{ij})}{\sum_{j'} \exp(X_{ij'})}$$

$$= \exp(X_{ij}) \cdot \sum_{j'} \exp(-X_{ij'})$$

$$\text{softmax}(X) = (ij, i \to ij, \exp(X), (ij \to i, \exp(-X)))$$

$$(XV)_{ij} = \sum_k X_{ik} V_{kj}$$

$$XV = (ik, kj \to ij, X, V)$$

$$\text{Attention}(Q, K, V) = \text{softmax}\left(\frac{QK^\top}{\sqrt{d_K}}\right) V$$

$$= (ik, kj \to ij, (ij, i \to ij, \exp(\frac{1}{\sqrt{d_k}} \cdot (ik, jk \to ij, Q, K)),$$

$$(ij \to i, \exp(-\frac{1}{\sqrt{d_k}} \cdot (ik, jk \to ij, Q, K)))), V)$$

$$= (ik, i, kj \to ij, \exp(\frac{1}{\sqrt{d_k}} \cdot (ik, jk \to ij, Q, K)),$$

$$(ij \to i, \exp(-\frac{1}{\sqrt{d_k}} \cdot (ik, jk \to ij, Q, K))), V)$$

$$= (ik, ij, kj \to ij, \exp(\frac{1}{\sqrt{d_k}} \cdot (ik, jk \to ij, Q, K)),$$

$$\exp(-\frac{1}{\sqrt{d_k}} \cdot (ik, jk \to ij, Q, K)), V)$$

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Jena, 01.06.2023