



Exploring Einsum as a Universal Inference Language

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Abstract

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1 Introduction

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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:

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

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

Definition 1. Einsum expressions specify how several input tensors are combined into a single output tensor. Let $T^{(1)}, \dots, T^{(n)}$ 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 $\mathbf{s}_i \in S^{n_i}$, composed of symbols $s_{ij} \in S$ for $j \in [n_i]$. The index string that is right of the arrow (\rightarrow) belongs to the output tensor T and is referred to as output string \mathbf{s}_t .

In our example this could be $S = \{i, j, k\}$. The tensor $T^{(1)} = A$ has the index string $\mathbf{s}_1 = ijk$, $T^{(2)} = B$ has $\mathbf{s}_2 = iik$, $T^{(3)} = v$ has $\mathbf{s}_3 = j$, and the output string is $\mathbf{s}_t = ij$. The individual symbols are $s_{11} = i$, $s_{12} = j$, $s_{13} = k$, $s_{21} = i$, $s_{22} = i$, $s_{23} = k$, $s_{31} = j$, $s_{t1} = i$, $s_{t2} = j$.

The next step in the definition is to speak about 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 second axis of A and the first axis of v have to have the same size, which happens to be four. Let us express this formally.

Let $d_{ij} \in \mathbb{N}$ denote the size of the j -th axis of $T^{(i)}$ 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 be assigned the same symbol. For instance a square matrix could have index strings $\mathbf{s} = (i, i)$ or $\mathbf{s} = (i, j)$.

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 $\sigma(\mathbf{s})$ denote the set with all symbols used in an index string \mathbf{s} . That is, in our example $\sigma(\mathbf{s}_2) = \sigma(iik) = \{i, k\}$.

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 $F = \sigma(\mathbf{s}_t)$. All other symbols used in the expression are called *bound* symbols $B = \bigcup_{i \in [n]} \sigma(\mathbf{s}_i) \setminus \sigma(\mathbf{s}_t)$. 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 $\mathcal{F} = \prod_{s \in F} [d_s]$ and the multi-index space we sum over is $\mathcal{B} = \prod_{s \in B} [d_s]$. 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{F} , it follows that d_s has to be defined for all symbols $s \in F$. This means we have to add the constraint $\sigma(\mathbf{s}_t) \subseteq \bigcup_{i \in [n]} \sigma(\mathbf{s}_i)$.

However, we do not use every symbol in the multi-index spaces to index every input tensor. Instead, we use the index strings \mathbf{s} to index the tensor. To formally express this, we need a projection from a multi-index $(\mathbf{f}, \mathbf{b}) \in \mathcal{F} \times \mathcal{B}$ ¹ to another multi-index, which includes only the indices, that are represented by the symbols used in \mathbf{s} , in the same order as present in \mathbf{s} . We denote this as $(\mathbf{f}, \mathbf{b}) : \mathbf{s}$. Notice how this still allows duplication of indices given in (\mathbf{f}, \mathbf{b}) . This is needed, as can be seen in our example for B_{iik} , where a multi-index, e.g. $(i = 1, j = 4, k = 2) \in \mathcal{F} \times \mathcal{B}$, is projected onto a different multi-index, by the index string iik . With this index string, the index that is represented by the symbol i is projected onto the first and second position, and the index that is represented by the symbol k is projected onto the third position. Therefore, the resulting multi-index is $(i = 1, j = 4, k = 2) : iik = (1, 1, 2)$.

¹Here, we use (\mathbf{f}, \mathbf{b}) as the notation for concatenating the tuples \mathbf{f} and \mathbf{b} . This means, (\mathbf{f}, \mathbf{b}) is not a tuple of multi-indices, but another multi-index.

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

$$T := (\mathbf{s}_1, \dots, \mathbf{s}_n \rightarrow \mathbf{s}_t, T^{(1)}, \dots, T^{(n)})_R$$

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

$$\forall \mathbf{f} \in \mathcal{F} : T_{\mathbf{f}:\mathbf{s}_t} = \bigoplus_{\mathbf{b} \in \mathcal{B}} \bigodot_{i=1}^n T_{(\mathbf{f}, \mathbf{b}):\mathbf{s}_i}^{(i)}.$$

Because we also project the indices \mathbf{f} with the output string \mathbf{s}_t , we allow to iterate over duplicate indices, e.g. $\text{diag}(v) = (j \rightarrow jj, v)$. 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 later.

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

The careful reader might have noticed two potential problems that could arise in the above definition. The first potential problem could arise when one of the input tensors is a scalar, which is a 0-th order tensor. This would mean that the index string \mathbf{s} for that input tensor has to be the empty string ϵ . Now when the multi-index (\mathbf{f}, \mathbf{b}) is projected by this empty index string, then the resulting multi-index can only be the empty multi-index $\lambda := ()$. One might expect that this leads to a problem, because we can not access any entries of a tensor with an empty multi-index. But for scalars, it makes sense to define the empty multi-index in such a way, that it accesses precisely the only entry that is stored in the scalar, i.e. $T_\lambda := T$ for a scalar T . This way, we can easily support scalars with empty index strings in Einsum.

The second potential problem could arise when either the free symbols F or the bound symbols B are empty, because the universal quantor over an empty multi-index space \mathcal{F} is always trivially true, and the sum over an empty multi-index space \mathcal{B} is always trivially zero. But in fact, this leads to no problem, because the induced multi-index spaces of empty F or B are not empty themselves. They contain one element, namely the set including only the empty multi-index $\{\lambda\}$. In the following, we will explain why this is the case, and how this solves any problems with empty F or B .

Notice the definition of the product we use for to sets M, N :

$$M \times N = \{(m, n) \mid m \in M, n \in N\}.$$

This looks like an ordinary cartesian product, but the hidden difference lies in the meaning of (m, n) . Namely, if m and n are multi-indices $\mathbf{m} = (m_1, \dots, m_{k_1})$ and

$\mathbf{n} = (n_1, \dots, n_{k_2})$ for $k_1, k_2 \in \mathbb{N}$, then we defined (\mathbf{m}, \mathbf{n}) to be the concatenation of the multi-indices:

$$(\mathbf{m}, \mathbf{n}) = (m_1, \dots, m_{k_1}, n_1, \dots, n_{k_2}),$$

which is one tuple with the entries of \mathbf{m} and \mathbf{n} , instead of the tuple of tuples

$$((m_1, \dots, m_{k_1}), (n_1, \dots, n_{k_2})).$$

Therefore we can name a neutral element for concatenation, which is the empty multi-index λ with $(\mathbf{i}, \lambda) = \mathbf{i}$ for any multi-index \mathbf{i} . From this, we can derive a neutral element for our product of multi-index spaces, which is the set including only the empty multi-index $\{\lambda\}$ with $\mathcal{I} \times \{\lambda\} = \mathcal{I}$ for any multi-index space \mathcal{I} .

Now, because it makes sense to define an operation over an empty set of operands as the neutral element of said operation, we can safely define

$$\prod_{s \in \emptyset} [d_s] := \{\lambda\}.$$

Therefore, if $F = \emptyset$, then

$$T := (\mathbf{s}_1, \dots, \mathbf{s}_n \rightarrow \mathbf{s}_t, T^{(1)}, \dots, T^{(n)})_R$$

results in the computation of a $|\mathbf{s}_t|$ -th order tensor T with

$$\begin{aligned} \forall \mathbf{f} \in \mathcal{F} : T_{\mathbf{f}:\mathbf{s}_t} &= \sum_{\mathbf{b} \in \{\lambda\}} \bigodot_{i=1}^n T_{(\mathbf{f}, \mathbf{b}):\mathbf{s}_i}^{(i)} \\ \iff \forall \mathbf{f} \in \mathcal{F} : T_{\mathbf{f}:\mathbf{s}_t} &= \bigodot_{i=1}^n T_{\mathbf{f}:\mathbf{s}_i}^{(i)}. \end{aligned}$$

And if $B = \emptyset$, then

$$T := (\mathbf{s}_1, \dots, \mathbf{s}_n \rightarrow, T^{(1)}, \dots, T^{(n)})_R$$

results in the computation of a scalar T with

$$\begin{aligned} \forall \mathbf{f} \in \{\lambda\} : T_{\mathbf{f}:\epsilon} &= \bigoplus_{\mathbf{b} \in \mathcal{B}} \bigodot_{i=1}^n T_{(\mathbf{f}, \mathbf{b}):\mathbf{s}_i}^{(i)} \\ \iff T &= \bigoplus_{\mathbf{b} \in \mathcal{B}} \bigodot_{i=1}^n T_{\mathbf{b}:\mathbf{s}_i}^{(i)}. \end{aligned}$$

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

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

- 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 $|A \cdot v|_2^2 = (i, i \rightarrow, (ij, j \rightarrow i, A, v), (ij, j \rightarrow i, A, v))$. This expression dictates the order of evaluating the expression. In the example of the norm, the expression $(ij, j \rightarrow i, A, v)$ 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:

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

which is clearly worse than the optimal contraction order

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

for $A \in \mathbb{R}^{m \times r}, B \in \mathbb{R}^{r \times n}, v \in \mathbb{R}^n$. Another limitation of nested Einsum strings is that we can not fully benefit from the computational advantages that come with the optimization of single Einsum expressions.

But fortunately, all nested Einsum expressions can be compressed into a single Einsum expression, if they are computed over the same semiring. For instance,

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

and

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

This leaves the path of contraction up to the implementation, and lets us benefit from all the computational advantages mentioned in [Chapter 2](#). In the following theorems, we assume that the computations are all over the same semiring $R = (M, \oplus, \odot)$.

3.1 Simple Nested Expressions

In the following, we will explore how to compress such expressions as

$$\underbrace{(ij, j \rightarrow i, \overbrace{(ik, kj \rightarrow ij, A, B)}^{\text{inner expression}}, v)}_{\text{outer expression}}$$

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

Theorem 1: For $i \in [m+n]$, let $T^{(i)}$ be an n_i -th order tensor with index string $\mathbf{s}_i \in S^{n_i}$. Let $\mathbf{s}_u, \mathbf{s}_v$ be index strings. Let

$$U := (\mathbf{s}_{m+1}, \dots, \mathbf{s}_{m+n} \rightarrow \mathbf{s}_u, T^{(m+1)}, \dots, T^{(m+n)})$$

and

$$V := (\mathbf{s}_1, \dots, \mathbf{s}_m, \mathbf{s}_u \rightarrow \mathbf{s}_v, T^{(1)}, \dots, T^{(m)}, U)$$

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

$$V = (\mathbf{s}_1, \dots, \mathbf{s}_{m+n} \rightarrow \mathbf{s}_v, T^{(1)}, \dots, T^{(m+n)})$$

Proof. Let F, F', B, B' be the free and bound symbols of the outer and inner Einsum expression respectively. W.l.o.g. they are all non-empty. From them we can derive the multi-index spaces $\mathcal{F}, \mathcal{F}', \mathcal{B}, \mathcal{B}'$ as in the definition. Then

$$\begin{aligned} V &= (\mathbf{s}_1, \dots, \mathbf{s}_m, \mathbf{s}_u \rightarrow \mathbf{s}_v, T^{(1)}, \dots, T^{(m)}, U) \\ \iff \forall \mathbf{f} \in \mathcal{F} : V_{\mathbf{f}:\mathbf{s}_v} &= \bigoplus_{\mathbf{b} \in \mathcal{B}} \bigodot_{i=1}^m T_{(\mathbf{f}, \mathbf{b}):\mathbf{s}_i}^{(i)} \odot U_{(\mathbf{f}, \mathbf{b}):\mathbf{s}_u} \\ &= \bigoplus_{\mathbf{b} \in \mathcal{B}} \bigodot_{i=1}^m T_{(\mathbf{f}, \mathbf{b}):\mathbf{s}_i}^{(i)} \odot \left[\bigoplus_{\mathbf{b}' \in \mathcal{B}'} \bigodot_{i'=m+1}^{m+n} T_{(\mathbf{f}, \mathbf{b}, \mathbf{b}'):\mathbf{s}_{i'}}^{(i')} \right] \\ &= \bigoplus_{\mathbf{b} \in \mathcal{B}} \bigoplus_{\mathbf{b}' \in \mathcal{B}'} \bigodot_{i=1}^m T_{(\mathbf{f}, \mathbf{b}):\mathbf{s}_i}^{(i)} \odot \bigodot_{i=m+1}^{m+n} T_{(\mathbf{f}, \mathbf{b}, \mathbf{b}'):\mathbf{s}_i}^{(i)} \\ &= \bigoplus_{\mathbf{b} \in \mathcal{B} \times \mathcal{B}'} \bigodot_{i=1}^{m+n} T_{(\mathbf{f}, \mathbf{b}):\mathbf{s}_i}^{(i)} \\ \iff V &= (\mathbf{s}_1, \dots, \mathbf{s}_{m+n} \rightarrow \mathbf{s}_v, T^{(1)}, \dots, T^{(m+n)}) \end{aligned}$$

where the third equality follows from the definition of U :

$$\forall \mathbf{f}' \in \mathcal{F}' : U_{\mathbf{f}':\mathbf{s}_u} = \bigoplus_{\mathbf{b}' \in \mathcal{B}'} \bigodot_{i'=m+1}^{m+n} T_{(\mathbf{f}', \mathbf{b}'):\mathbf{s}_{i'}}^{(i')}$$

and from the fact, that the symbols in \mathbf{s}_u are used in the outer expression as an input string, and in the inner expression as the output string, and therefore $F' \subseteq B \cup F$. Additionally, because of the stated requirement $(B \cup F) \cap B' = \emptyset$, the symbols representing \mathbf{b}' do not clash with the symbols representing (\mathbf{f}, \mathbf{b}) , and therefore $(\mathbf{f}, \mathbf{b}, \mathbf{b}') : \mathbf{s}_{i'}$ is well-defined and projects on the same indices as $(\mathbf{f}', \mathbf{b}') : \mathbf{s}_{i'}$. The fourth equality follows from the distributivity in a semiring. \square

This means that we can compress all nested Einsum expressions, where the output string of the inner expression, which is used to compute U , is exactly the same as the respective input string in the outer expression, where U is used as an input tensor. This is already helpful for some naturally occurring expressions in linear algebra, e.g.

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

for $A \in \mathbb{R}^{m \times n}$, $v \in \mathbb{R}^n$, or

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

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

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

or

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

for $A \in \mathbb{R}^{m \times n}$, $B \in \mathbb{R}^{n \times m}$, $v \in \mathbb{R}^n$. For this, we need more general ways of compressing nested Einsum expressions.

3.2 General Nested Expressions

The following example is an expression, which we cannot compress with the previous theorem:

$$(a, b, c, d, e, abbcd \rightarrow bc, v^{(1)}, v^{(2)}, v^{(3)}, v^{(4)}, v^{(5)}, (i, j, k, l \rightarrow iijkk, v^{(6)}, v^{(7)}, v^{(8)}, v^{(9)}))$$

for $v^{(i)} \in \mathbb{R}^{d_{vi}}$ with $i \in [9]$, where $d_{vi} \in \mathbb{N}$ are appropriate dimensions. This is because the output string $\mathbf{s}_u = iijkk$ and the input string $\hat{\mathbf{s}}_u = abbde$ are not the same. In the following, we will explore how to compress such expressions. Note that, for the theorem, we use disjoint 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. For example, we could also write the above expression as

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

because the scope of each symbol does not reach into nested expressions, and therefore the j used in the outer expression and the j used in the inner expression are treated as different symbols.

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

$$U := (\mathbf{s}_{m+1}, \dots, \mathbf{s}_{m+n} \rightarrow \mathbf{s}_u, T^{(m+1)}, \dots, T^{(m+n)})$$

Also let $\hat{\mathbf{s}}_u$ be alternative index strings for U .

Let s_v be an index string and

$$V := (\mathbf{s}_1, \dots, \mathbf{s}_m, \hat{\mathbf{s}}_u \rightarrow \mathbf{s}_v, T^{(1)}, \dots, T^{(m)}, U)$$

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

Let us clarify that the index string \mathbf{s}_u corresponds to the output string of the inner expression, and the index string $\hat{\mathbf{s}}_u$ corresponds to the input string that is used for the input tensor U in the outer expression. In our example, these are \mathbf{s}_u and $\hat{\mathbf{s}}_u$:

$$(a, b, c, d, e, \overbrace{abcde}^{\hat{\mathbf{s}}_u} \rightarrow bc, v^{(1)}, v^{(2)}, v^{(3)}, v^{(4)}, v^{(5)}, (i, j, k, l \rightarrow \overbrace{ijkl}^{\mathbf{s}_u}, v^{(6)}, v^{(7)}, v^{(8)}, v^{(9)})).$$

In contrast to [Theorem 1](#), we cannot just replace the input index string $\hat{\mathbf{s}}_u$ by all the input index strings in the inner Einsum expression $\mathbf{s}_{m+1}, \dots, \mathbf{s}_{m+n}$. Instead, we first need to apply a symbol map $\nu : S \rightarrow S$ to each of the index strings. This symbol map holds information about which symbols are effectively the used for the same index.

For the definition of the map ν , we first construct an undirected graph $G = (V, E)$ that we call *symbol graph*. In the symbol graph, the nodes consist of all symbols from \mathbf{s}_u and $\hat{\mathbf{s}}_u$. The edges are $E = \{\{s_{uj}, \hat{s}_{uj}\} \mid j \in [n_u]\}$, which connects all symbols from \mathbf{s}_u and $\hat{\mathbf{s}}_u$ that share an index. The symbol graph for our example is illustrated in [Figure 3.1](#).

In the symbol graph, if two symbols are connected, then they are effectively 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 ν as follows:

$$\nu(s) := \begin{cases} s_C & \text{if } \exists C : C \text{ is a component of } G \text{ and } s \in C \\ s & \text{else} \end{cases}.$$

In our example, the components are $\{a, b, i, j\}$, $\{c, d, k\}$, and $\{e, l\}$. Therefore we

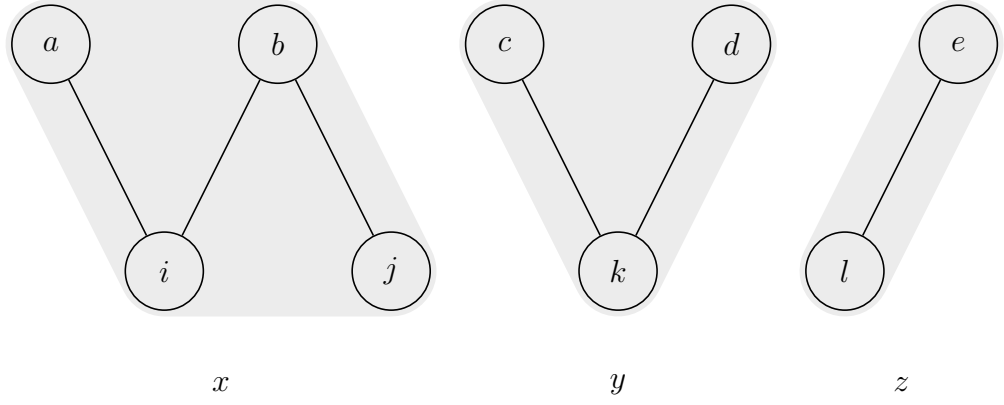


Figure 3.1: Symbol graph for the example

could use

$$\nu(s) := \begin{cases} x & \text{if } s \in \{a, b, i, j\} \\ y & \text{if } s \in \{c, d, k\} \\ z & \text{if } s \in \{e, l\} \\ s & \text{else} \end{cases}.$$

The symbol map ν can be extended, such that it maps entire index strings instead of just symbols, by setting $\nu(\mathbf{s}_i) \in S^{n_i}$, $\nu(\mathbf{s}_i)_j := \nu(s_{ij})$. Then we can write the substituted index strings by setting $\hat{\mathbf{s}}_i := \nu(\mathbf{s}_i)$ for $i \in [m+n]$ and $\hat{\mathbf{s}}_t = \nu(\mathbf{s}_t)$. With these index strings, the compressed Einsum expression is the following:

$$V = (\hat{\mathbf{s}}_1, \dots, \hat{\mathbf{s}}_{m+n} \rightarrow \hat{\mathbf{s}}_v, T^{(1)}, \dots, T^{(m+n)})$$

which helps us to compress the example:

$$\begin{aligned} & (a, b, c, d, e, abbde \rightarrow bc, v^{(1)}, v^{(2)}, v^{(3)}, v^{(4)}, v^{(5)}, (i, j, k, l \rightarrow iijkl, v^{(6)}, v^{(7)}, v^{(8)}, v^{(9)})) \\ & = (x, x, y, y, z, x, x, y, z \rightarrow xy, v^{(1)}, v^{(2)}, v^{(3)}, v^{(4)}, v^{(5)}, v^{(6)}, v^{(7)}, v^{(8)}, v^{(9)}). \end{aligned}$$

For the proof of this theorem, we first need three lemmata, which essentially boil down to one intuitive thought: The effective equality of two symbols can be expressed by multiplication with the unity matrix $\mathbb{1}_d$:

$$(\mathbb{1}_d)_{ij} := \begin{cases} 1 & \text{if } i = j \\ 0 & \text{else} \end{cases},$$

for $i, j \in [d]$, where 0 and 1 indicate the neutral element of addition and multiplication in the given semiring respectively.

Lemma 3: For $i \in [n]$, let $T^{(i)}$ be an n_i -th order tensor with index string $\mathbf{s}_i \in S^{n_i}$. Let \mathbf{s}_t be the index string for T with

$$T = (\mathbf{s}_1, \dots, \mathbf{s}_n \rightarrow \mathbf{s}_t, T^{(1)}, \dots, T^{(n)}).$$

Let F and B be the free and bound symbols of this expression. Let $k \in [n]$ and $j \in [n_k]$, then we can replace the j -th symbol of the k -th index string with a new symbol $s_{\text{new}} \in S \setminus (F \cup B)$ by adding the unity matrix $\mathbb{1}_{d_{kj}}$ as an input tensor in the following way:

Let \mathbf{s}'_k be a new index string such that

$$s'_{ki} := \begin{cases} s_{\text{new}} & \text{if } i = j \\ s_{ki} & \text{else} \end{cases}$$

for $i \in [n_k]$. Let $\mathbf{s}_1 = (s_{kj}, s_{\text{new}})$. Then

$$T = (\mathbf{s}_1, \dots, \mathbf{s}'_k, \dots, \mathbf{s}_n, \mathbf{s}_1 \rightarrow \mathbf{s}_t, T^{(1)}, \dots, T^{(n)}, \mathbb{1}_{d_{kj}}).$$

Proof. Let \mathcal{F} and \mathcal{B} be the induces multi-index spaces for the free and bound symbols of the Einsum expression. Then

$$\begin{aligned} T &= (\mathbf{s}_1, \dots, \mathbf{s}_n \rightarrow \mathbf{s}_t, T^{(1)}, \dots, T^{(n)}) \\ \iff \forall \mathbf{f} \in \mathcal{F} : T_{\mathbf{f}:\mathbf{s}_t} &= \bigoplus_{\mathbf{b} \in \mathcal{B}} \bigodot_{i \in [n]} T_{(\mathbf{f}, \mathbf{b}):s_i}^{(i)} \\ &= \bigoplus_{\mathbf{b} \in \mathcal{B} \times [d_{kj}]} \bigodot_{1 \leq i < k} T_{(\mathbf{f}, \mathbf{b}):s_i}^{(i)} \odot T_{(\mathbf{f}, \mathbf{b}):s'_k}^{(k)} \odot \bigodot_{k < i \leq n} T_{(\mathbf{f}, \mathbf{b}):s_i}^{(i)} \\ &\quad \odot \begin{cases} 1 & \text{if } (\mathbf{f}, \mathbf{b}) : s_{kj} = (\mathbf{f}, \mathbf{b}) : s_{\text{new}} \\ 0 & \text{else} \end{cases} \\ &= \bigoplus_{\mathbf{b} \in \mathcal{B} \times [d_{kj}]} \bigodot_{1 \leq i < k} T_{(\mathbf{f}, \mathbf{b}):s_i}^{(i)} \odot T_{(\mathbf{f}, \mathbf{b}):s'_k}^{(k)} \odot \bigodot_{k < i \leq n} T_{(\mathbf{f}, \mathbf{b}):s_i}^{(i)} \\ &\quad \odot (\mathbb{1}_{d_{kj}})_{(\mathbf{f}, \mathbf{b}):s_1} \\ \iff T &= (\mathbf{s}_1, \dots, \mathbf{s}'_k, \dots, \mathbf{s}_n, \mathbf{s}_1 \rightarrow \mathbf{s}_t, T^{(1)}, \dots, T^{(n)}, \mathbb{1}_{d_{kj}}) \end{aligned}$$

where the third equality holds because in the summation over $\mathcal{B} \times [d_{kj}]$, exactly those summands get selected by the condition, which are also valid summands in the previous summation over \mathcal{B} . All other summands are disregarded because they are multiplied by $\mathbb{0}$, which is the additive neutral element in the semiring and *annihilates* every element, which means $a \odot \mathbb{0} = \mathbb{0}$ for every $a \in M$. \square

This lemma intuitively means that we can replace any symbol in an index string of an input tensor of our choice with a new symbol by introducing the unity matrix with an appropriate index string as a factor. Now the same holds for the index string of the output tensor \mathbf{s}_t , which will be the content of the next lemma.

Lemma 4: For $i \in [n]$, let $T^{(i)}$ be an n_i -th order tensor with index string $\mathbf{s}_i \in S^{n_i}$. Let \mathbf{s}_t be the index string for T with

$$T = (\mathbf{s}_1, \dots, \mathbf{s}_n \rightarrow \mathbf{s}_t, T^{(1)}, \dots, T^{(n)}).$$

Let F and B be the free and bound symbols of this expression. Let $n_t := |\mathbf{s}_t|$, $j \in [n_t]$, and $d_{tj} := d_{s_{tj}}$, then we can replace the j -th symbol of the output string with a new symbol $s_{\text{new}} \in S \setminus (F \cup B)$ by adding the unity matrix $\mathbb{1}_{d_{tj}}$ as an input tensor in the following way:

Let \mathbf{s}'_t be a new index string such that

$$s'_{ti} := \begin{cases} s_{\text{new}} & \text{if } i = j \\ s_{ti} & \text{else} \end{cases}$$

for $i \in [n_t]$. Let $\mathbf{s}_1 = (s_{tj}, s_{\text{new}})$. Then

$$T = (\mathbf{s}_1, \dots, \mathbf{s}_n, \mathbf{s}_1 \rightarrow \mathbf{s}'_t, T^{(1)}, \dots, T^{(n)}, \mathbb{1}_{d_{kj}}).$$

Proof. Let \mathcal{F} and \mathcal{B} be the induces multi-index spaces for the free and bound symbols of the Einsum expression. If s_{tj} occurs in \mathbf{s}_t even after replacing it with s_{new} , then

$$\begin{aligned} T &= (\mathbf{s}_1, \dots, \mathbf{s}_n \rightarrow \mathbf{s}_t, T^{(1)}, \dots, T^{(n)}) \\ \iff \forall \mathbf{f} \in \mathcal{F} : T_{\mathbf{f}:\mathbf{s}_t} &= \bigoplus_{\mathbf{b} \in \mathcal{B}} \bigodot_{i \in [n]} T_{(\mathbf{f}, \mathbf{b}):\mathbf{s}_i}^{(i)} \\ \iff \forall \mathbf{f} \in \mathcal{F} \times [d_{tj}] : T_{\mathbf{f}:\mathbf{s}'_t} &= \bigoplus_{\mathbf{b} \in \mathcal{B}} \bigodot_{i \in [n]} T_{(\mathbf{f}, \mathbf{b}):\mathbf{s}_i}^{(i)} \odot \begin{cases} \mathbb{1} & \text{if } \mathbf{f} : s_{tj} = \mathbf{f} : s_{\text{new}} \\ \mathbb{0} & \text{else} \end{cases} \\ &= \bigoplus_{\mathbf{b} \in \mathcal{B}} \bigodot_{i \in [n]} T_{(\mathbf{f}, \mathbf{b}):\mathbf{s}_i}^{(i)} \odot (\mathbb{1}_{d_{tj}})_{(\mathbf{f}, \mathbf{b}):\mathbf{s}_1} \\ \iff T &= (\mathbf{s}_1, \dots, \mathbf{s}_n, \mathbf{s}_1 \rightarrow \mathbf{s}'_t, T^{(1)}, \dots, T^{(n)}, \mathbb{1}_{d_{tj}}) \end{aligned}$$

where the third equality holds because exactly those indices get selected by the condition, where T was originally defined. If s_{tj} no longer occurs in \mathbf{s}_t after replacing it with s_{new} , then s_{tj} turns into a bound symbol. Therefore we have to define $\mathcal{F}' = \prod_{s \in \mathbf{s}'_t} [d_s]$. Then

$$\begin{aligned} T &= (\mathbf{s}_1, \dots, \mathbf{s}_n \rightarrow \mathbf{s}_t, T^{(1)}, \dots, T^{(n)}) \\ \iff \forall \mathbf{f} \in \mathcal{F} : T_{\mathbf{f}:\mathbf{s}_t} &= \bigoplus_{\mathbf{b} \in \mathcal{B}} \bigodot_{i \in [n]} T_{(\mathbf{f}, \mathbf{b}):\mathbf{s}_i}^{(i)} \\ \iff \forall \mathbf{f} \in \mathcal{F}' : T_{\mathbf{f}:\mathbf{s}'_t} &= \bigoplus_{\mathbf{b} \in \mathcal{B} \times [d_{tj}]} \bigodot_{i \in [n]} T_{(\mathbf{f}, \mathbf{b}):\mathbf{s}_i}^{(i)} \odot \begin{cases} \mathbb{1} & \text{if } (\mathbf{f}, \mathbf{b}) : s_{tj} = (\mathbf{f}, \mathbf{b}) : s_{\text{new}} \\ \mathbb{0} & \text{else} \end{cases} \\ &= \bigoplus_{\mathbf{b} \in \mathcal{B} \times [d_{tj}]} \bigodot_{i \in [n]} T_{(\mathbf{f}, \mathbf{b}):\mathbf{s}_i}^{(i)} \odot (\mathbb{1}_{d_{tj}})_{(\mathbf{f}, \mathbf{b}):\mathbf{s}_1} \\ \iff T &= (\mathbf{s}_1, \dots, \mathbf{s}_n, \mathbf{s}_1 \rightarrow \mathbf{s}'_t, T^{(1)}, \dots, T^{(n)}, \mathbb{1}_{d_{tj}}) \end{aligned}$$

where the third equality holds because exactly those summands get selected by the condition, where $(\mathbf{f}, \mathbf{b}) : \mathbf{s}_t$ could also get used as an index for T . All others are annihilated. \square

Now with these two lemmata, we can replace any symbol in any index string,

regardless if it is an input string or the output string by introducing the unity matrix with an appropriate index string as a factor. In the following lemma, we will show that any unity matrix factors can be removed again, by renaming certain symbols in all other index strings in the Einsum expression.

Lemma 5: For $i \in [n]$, let $T^{(i)}$ be an n_i -th order tensor with index string $\mathbf{s}_i \in S^{n_i}$, where $T^{(n)} = \mathbb{1}_m$ for some $m \in \mathbb{N}$. Let \mathbf{s}_t be the index string for T with

$$T = (\mathbf{s}_1, \dots, \mathbf{s}_n \rightarrow \mathbf{s}_t, T^{(1)}, \dots, T^{(n)}).$$

Let F and B be the free and bound symbols of this expression. Then we can introduce a symbol map $\mu : S \rightarrow S$, which maps both symbols in \mathbf{s}_n to the same symbol $s_{\text{new}} \in S \setminus (F \cup B)$:

$$\mu(s) := \begin{cases} s_{\text{new}} & \text{if } s \in \{s_{n1}, s_{n2}\} \\ s & \text{else} \end{cases}$$

The symbol map μ can be extended, such that it maps entire index strings instead of just symbols, by setting $\mu(\mathbf{s}_i) \in S^{n_i}$, $\mu(\mathbf{s}_i)_j := \mu(s_{ij})$. Then we can write the substituted index strings by setting $\mathbf{s}'_i := \mu(\mathbf{s}_i)$ for $i \in [n]$ and $\mathbf{s}'_t = \mu(\mathbf{s}_t)$. With these index strings, the following holds:

$$T = (\mathbf{s}'_1, \dots, \mathbf{s}'_{n-1} \rightarrow \mathbf{s}'_t, T^{(1)}, \dots, T^{(n-1)}).$$

Proof. For this proof, we provide the following example of an Einsum expression on which we demonstrate the given arguments for better understanding:

$$(ij, kl, mn, ij, kl, mn \rightarrow imn, A, B, C, \mathbb{1}_a, \mathbb{1}_b, \mathbb{1}_c)$$

for $A \in \mathbb{R}^{a \times a}$, $B \in \mathbb{R}^{b \times b}$, $C \in \mathbb{R}^{c \times c}$ and some $a, b, c \in \mathbb{N}$.

We need to consider three cases for the symbols used in the index string $\mathbf{s}_n = (s_{n1}, s_{n2})$:

- s_{n1} and s_{n2} are both free symbols,
- s_{n1} and s_{n2} are both bound symbols,
- one symbol of s_{n1} and s_{n2} is a free symbol, the other is a bound symbol.

Every one of these cases leads to the same result, but in a slightly different way.

First let us consider the case where both symbols are free. In this case, both symbols can be replaced by a single symbol, because T is $\mathbb{0}$ for all entries with a multi-index, where the indices projected by the symbols are not equal.

In our example, this is equivalent to the following:

$$\begin{aligned}
\forall i, m, n : T_{imn} &= \bigoplus_{j,k,l} A_{ij} B_{kl} C_{mn} (\mathbb{1}_a)_{ij} (\mathbb{1}_b)_{kl} (\mathbb{1}_c)_{mn} \\
&= \begin{cases} \bigoplus_{j,k,l} A_{ij} B_{kl} C_{mn} (\mathbb{1}_a)_{ij} (\mathbb{1}_b)_{kl} & \text{if } m = n \\ \mathbb{0} & \text{else} \end{cases} \\
\iff \forall i, z : T_{izz} &= \bigoplus_{j,k,l} A_{ij} B_{kl} C_{zz} (\mathbb{1}_a)_{ij} (\mathbb{1}_b)_{kl}.
\end{aligned}$$

Next let us consider the case where both symbols are bound. In this case, those summands are multiplied with $\mathbb{0}$, which have a multi-index where the projected indices are not equal. Therefore, those summands are annihilated and left out from the summation. This means that both symbols can be replaced by a single symbol.

In our example, this is equivalent to the following:

$$\begin{aligned}
\forall i, z : T_{izz} &= \bigoplus_{j,k,l} A_{ij} B_{kl} C_{zz} (\mathbb{1}_a)_{ij} (\mathbb{1}_b)_{kl} \\
&= \bigoplus_{j,k,l} A_{ij} B_{kl} C_{zz} (\mathbb{1}_a)_{ij} \odot \begin{cases} 1 & \text{if } k = l \\ \mathbb{0} & \text{else} \end{cases} \\
&= \bigoplus_{j,y} A_{ij} B_{yy} C_{zz} (\mathbb{1}_a)_{ij}.
\end{aligned}$$

Next let us consider the case where one symbol is free and one symbol is bound. W.l.o.g. we consider the case where s_{n1} is free and s_{n2} is bound. In this case, those summands are multiplied with $\mathbb{0}$, which have a multi-index where the index projected by the bound symbol s_{n2} is not the same as the index projected by the free symbol s_{n1} . Therefore those summands are annihilated and left out from the summation, and the symbol s_{n2} can be replaced by the symbol s_{n1} . Additionally, we can rename the s_{n1} to some new symbol.

In our example, this is equivalent to the following:

$$\begin{aligned}
\forall i, z : T_{izz} &= \bigoplus_{j,y} A_{ij} B_{yy} C_{zz} (\mathbb{1}_a)_{ij} \\
&= \bigoplus_{j,y} A_{ij} B_{yy} C_{zz} \odot \begin{cases} 1 & \text{if } i = j \\ \mathbb{0} & \text{else} \end{cases} \\
&= \bigoplus_y A_{ii} B_{yy} C_{zz} \\
\iff \forall x, z : T_{xzz} &= \bigoplus_y A_{xx} B_{yy} C_{zz}.
\end{aligned}$$

Therefore, in all three cases, the symbols, that are used in an index string for a unity matrix, can simply be replaced by a single symbol. \square

From these three lemmata, [Theorem 2](#) follows with the following procedure:

1. Apply [Lemma 3](#) to all of the symbols in the input string \hat{s}_u and therefore replace it with a new index string $s'_u \in S^{n_u}$ where s'_u contains no duplicate symbols.
2. Apply [Lemma 4](#) to all of the symbols in the output string s_u and therefore replace it with the same new index string s'_u .
3. Apply [Theorem 1](#) to the nested expression and therefore compress the nested expression into a single expression with lots of unity matrices. This is possible because the input string and output string for U are both s'_u now.
4. Apply [Lemma 5](#) to remove unity matrices from the compressed expression until there are no more of those unity matrices left, which were introduced in step one and two.

Proof. For the proof, we again demonstrate the arguments on the example used in [Theorem 2](#) for better understanding:

$$(a, b, c, d, e, abbcde \rightarrow bc, v^{(1)}, v^{(2)}, v^{(3)}, v^{(4)}, v^{(5)}, (i, j, k, l \rightarrow iijkl, v^{(6)}, v^{(7)}, v^{(8)}, v^{(9)}))$$

Applying step one and two to this example results in the following Einsum expression if $s'_u = s_1 s_2 s_3 s_4 s_5 s_6$:

$$\begin{aligned} &(a, b, c, d, e, s_1 s_2 s_3 s_4 s_5 s_6, as_1, bs_2, bs_3, cs_4, ds_5, es_6 \rightarrow bc, \\ &\quad v^{(1)}, v^{(2)}, v^{(3)}, v^{(4)}, v^{(5)}, 1, 1, 1, 1, 1, 1, \\ &\quad (i, j, k, l, is_1, is_2, js_3, ks_4, ks_5, ls_6 \rightarrow s_1 s_2 s_3 s_4 s_5 s_6, \\ &\quad v^{(6)}, v^{(7)}, v^{(8)}, v^{(9)}, 1, 1, 1, 1, 1, 1)), \end{aligned}$$

where we used 1 to indicate unity matrices of different sizes, because the sizes can be derived from the context and are not important for better understanding. Applying step three results in the following compressed expression:

$$\begin{aligned} &(a, b, c, d, e, i, j, k, l, is_1, is_2, js_3, ks_4, ks_5, ls_6, as_1, bs_2, bs_3, cs_4, ds_5, es_6 \rightarrow bc, \\ &\quad v^{(1)}, v^{(2)}, v^{(3)}, v^{(4)}, v^{(5)}, v^{(6)}, v^{(7)}, v^{(8)}, v^{(9)}, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1) \end{aligned}$$

The only fact that remains to be understood is why the removal the unity matrices in step four leads to the transformation described in [Theorem 2](#). For this, we construct another undirected graph $G' = (V', E')$ that we call *extended symbol graph*. In the symbol graph, the nodes consist of all symbols from s_u , s'_u , and \hat{s}_u . An edge $\{u, v\}$ exists precisely when the compressed expression contains a unity matrix with index string uv , that was introduced in step one or step two. The extended symbol graph for our example is illustrated in [Figure 3.2](#).

Now, every newly introduced unity matrix is represented by an edge in the extended symbol graph. If a unity matrix is removed with [Lemma 5](#), the symbols connected by the representing edge collapse into one symbol, and the rest of the extended symbol graph stays the same. An example of this collapse is illustrated in [Figure 3.3](#).

Therefore, after repeatedly applying [Lemma 5](#), all nodes that are part of the same component in the extended symbol graph will collapse into one symbol. Now the only

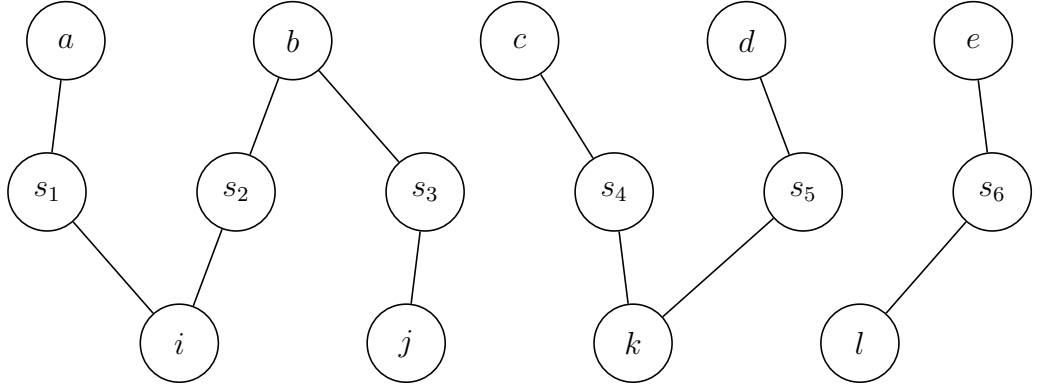


Figure 3.2: Extended symbol graph for the example

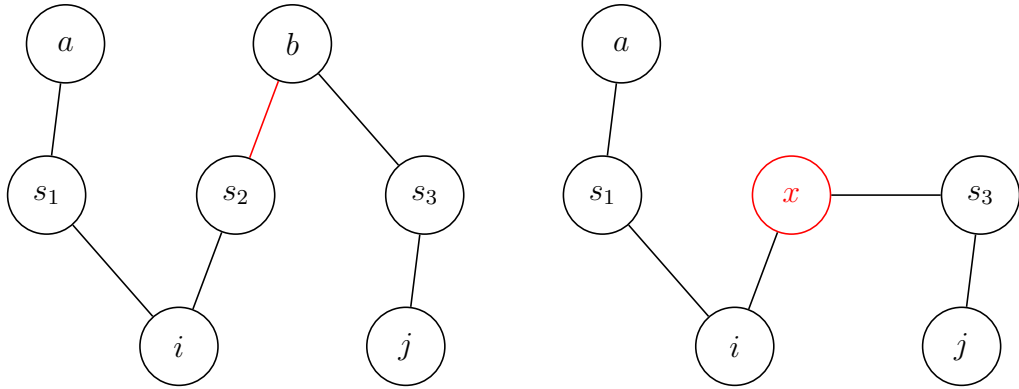


Figure 3.3: First component of the extended symbol graph after removing the unity matrix represented by the edge $\{b, s_2\}$

thing left to show is that two nodes are connected in G exactly if they are also connected in G' . This can be seen by understanding the edges of G and G' . In G , two symbols s_{ui} and \hat{s}_{uj} share an edge if they share a position $i = j$. In G' , two symbols s_{ui} and \hat{s}_{uj} share a neighbour s'_{uk} if both were replaced by s'_{uk} in step one and step two, which happens exactly if they share a position $i = j = k$. Therefore every edge in G is represented by a shared neighbour in G' . Now, because every s'_{uk} has exactly two neighbours, and because there are no direct edges between any symbols of \mathbf{s}_u and $\hat{\mathbf{s}}_u$, there are no more edges in G' other than the ones that contribute to a shared neighbour s'_{uk} . Then, because sharing an edge in G is the same as sharing a neighbour in G' , two symbols are in the same component in G precisely when they are also in the same component in G' .

Therefore collapsing every edge in the extended symbol graph leads to the symbol map defined in [Theorem 2](#). \square

From this general theorem we can derive two more specific theorems, which make the process of compressing simpler for a subset of nested expressions.

3.3 Duplications

The following two theorems revolve around duplicated symbols in index strings and the way these duplications are *broken*. We speak of a broken duplication in \mathbf{s}_u , if the symbols s_{ui} and s_{uj} at two positions $i, j \in [n_u]$ are the same, meaning $s_{ui} = s_{uj}$, but symbols at the same positions in $\hat{\mathbf{s}}_u$, \hat{s}_{ui} and \hat{s}_{uj} are different, meaning $\hat{s}_{ui} \neq \hat{s}_{uj}$. In the same way, duplications in $\hat{\mathbf{s}}_u$ can be broken by \mathbf{s}_u .

Because \mathbf{s}_u and $\hat{\mathbf{s}}_u$ are easily confused, we can also use a different terminology that does not include these similar variable names. If \mathbf{s}_u breaks duplications in $\hat{\mathbf{s}}_u$, we say that the outer expression *introduces* duplications to the inner expression, because the outer expression uses duplications in the input string for the inner expression, that were not used in the output string of the inner expression. If $\hat{\mathbf{s}}_u$ breaks duplications in \mathbf{s}_u , we say that the outer expression *removes* duplications from the inner expression, because the outer expression uses different symbols in the input string for the inner expression, where there was originally a duplication in the output string of the inner expression.

3.3.1 Introducing Duplications

The first duplication theorem handles all nested expressions, where the outer expression can only introduce duplications and cannot remove any. This means that if two positions hold the same symbol in \mathbf{s}_u , these positions also have to hold the same symbol in $\hat{\mathbf{s}}_u$. This brings the advantage, that the symbol map is much simpler and only has to be applied to the inner expression.

The following example is an expression, which respects this condition:

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

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

Theorem 6: For $i \in [m+n]$, let $T^{(i)}$ be an n_i -th order tensor with index strings $\mathbf{s}_i \in S^{n_i}$. Let \mathbf{s}_u be an index string for the n_u -th order tensor U , which is defined as follows:

$$U := (\mathbf{s}_{m+1}, \dots, \mathbf{s}_{m+n} \rightarrow \mathbf{s}_u, T^{(m+1)}, \dots, T^{(m+n)})$$

Also let $\hat{\mathbf{s}}_u$ 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 the outer expression can only introduce new symbol duplications, and cannot remove any.

Let \mathbf{s}_v be an index string and

$$V := (\mathbf{s}_1, \dots, \mathbf{s}_m, \hat{\mathbf{s}}_u \rightarrow \mathbf{s}_v, T^{(1)}, \dots, T^{(m)}, U)$$

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.

As in [Theorem 2](#), we need to apply a symbol map in order to compress the nested expression. Let $\nu : S \rightarrow S$ 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 \mathbf{s}_u to the symbol at the same index in $\hat{\mathbf{s}}_u$ and all other symbols to themselves.

In our example, we have the following symbols on the same positions:

- $s_{u1} = k$ and $\hat{s}_{u1} = j$,
- $s_{u2} = k$ and $\hat{s}_{u2} = j$,
- $s_{u3} = o$ and $\hat{s}_{u3} = j$.

Therefore these are the important mappings:

$$\begin{aligned} k &\rightarrow j, \\ o &\rightarrow j. \end{aligned}$$

The symbol map ν can be extended, such that it maps entire index strings instead of just symbols as in [Theorem 2](#). Then we can write the substituted index strings by setting $\hat{\mathbf{s}}_i := \nu(\mathbf{s}_i)$ for $i \in [m+1, m+n]$. With these index strings, the compressed Einsum expression is the following:

$$V = (\mathbf{s}_1, \dots, \mathbf{s}_m, \hat{\mathbf{s}}_{m+1}, \dots, \hat{\mathbf{s}}_{m+n} \rightarrow \mathbf{s}_v, T^{(1)}, \dots, T^{(m+n)})$$

which helps us to compress the example:

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

Proof. Because $s_{uj} = s_{uj'} \implies \hat{s}_{uj} = \hat{s}_{uj'}$ for all $j, j' \in [n_u]$, each symbol in \mathbf{s}_u only has one neighbour in the symbol graph. This is illustrated for our example in [Figure 3.4](#). Therefore each symbol in $\hat{\mathbf{s}}_u$ defines its own component, and can be used as the symbol in the symbol map, that replaces all symbols in their component. Therefore the symbols in $\hat{\mathbf{s}}_u$ are not changed by applying the symbol map, which are the only symbols in the outer expression that could have been changed by the map. Therefore the symbol map only has to be applied to the inner expression. □

This theorem suffices to 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

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

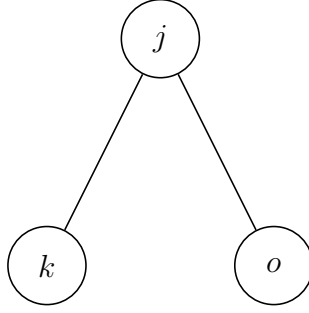


Figure 3.4: Symbol graph for the example

Proof.

$$\begin{aligned}
 \text{trace}(A \cdot B) &= (ll \rightarrow, (ik, kj \rightarrow ij, A, B)) \\
 &= (lk, kl \rightarrow, A, B) \\
 &= (kl, lk \rightarrow, B, A) \\
 &= (kk \rightarrow, (il, lj \rightarrow ij, B, A)) \\
 &= \text{trace}(B \cdot A)
 \end{aligned}$$

where the second and fourth equality hold because of [Theorem 6](#), and the third equality holds because of the commutativity of multiplication in the standard semiring. \square

3.4 Removing Duplications

The second duplication theorem handles all nested expressions, where the outer expression can only remove duplications and cannot remove any. This means that if two positions hold the same symbol in $\hat{\mathbf{s}}_{\mathbf{u}}$, these positions also have to hold the same symbol in $\mathbf{s}_{\mathbf{u}}$. This brings the advantage, that the symbol map is much simpler and only has to be applied to the outer expression.

The following example is an expression, which respects this condition:

$$(ij, kl, mn, ijklmn \rightarrow ijk, A, B, C, (abc \rightarrow aabbcc, D))$$

for $A \in \mathbb{R}^{x \times x}$, $B \in \mathbb{R}^{y \times y}$, $C \in \mathbb{R}^{z \times z}$, $D \in \mathbb{R}^{x \times y \times z}$. This is because duplications aa , bb , and cc in the output string $\mathbf{s}_{\mathbf{u}}$ are broken by ij , kl , mn indicate the input string $\hat{\mathbf{s}}_{\mathbf{u}} = ijklmn$, and no new duplications are introduced by the output string. Again, we use disjoint sets of symbols for the inner and outer expression to help us in the formulation and the proof.

Theorem 7: For $i \in [m + n]$, let $T^{(i)}$ be an n_i -th order tensor with index strings $\mathbf{s}_i \in S^{n_i}$. Let $\mathbf{s}_{\mathbf{u}}$ be an index string for the $n_{\mathbf{u}}$ -th order tensor U , which is defined as follows:

$$U := (\mathbf{s}_{m+1}, \dots, \mathbf{s}_{m+n} \rightarrow \mathbf{s}_{\mathbf{u}}, T^{(m+1)}, \dots, T^{(m+n)})$$

Also let $\hat{\mathbf{s}}_{\mathbf{u}}$ 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 $\hat{\mathbf{s}}_{\mathbf{u}}$ can only remove symbol duplications, and cannot introduce any. Note that this is the converse of the constraint in [Theorem 6](#).

Let s_v be an index string and

$$V := (\mathbf{s}_1, \dots, \mathbf{s}_m, \hat{\mathbf{s}}_{\mathbf{u}} \rightarrow \mathbf{s}_v, T^{(1)}, \dots, T^{(m)}, U)$$

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 2](#), we need to apply a symbol map in order to compress the nested expression. Let $\nu : S \rightarrow S$ such that

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

which can be extended to map entire index strings as in [Theorem 2](#). In our example, these are the important mappings:

$$\begin{array}{lll} i \rightarrow a, & k \rightarrow b, & m \rightarrow c, \\ j \rightarrow a, & l \rightarrow b, & n \rightarrow c. \end{array}$$

This means that i and j will be iterated over at the same time, k and l will be iterated over at the same time, and m and n will be iterated over at the same time.

We can write the substituted index strings by setting $\hat{\mathbf{s}}_i := \nu(\mathbf{s}_i)$ for $i \in [m]$, $\hat{\mathbf{s}}_v := \nu(\mathbf{s}_v)$. With these index strings, the compressed Einsum expression is the following:

$$V = (\hat{\mathbf{s}}_1, \dots, \hat{\mathbf{s}}_m, \mathbf{s}_{m+1}, \dots, \mathbf{s}_{m+n} \rightarrow \hat{\mathbf{s}}_v, T^{(1)}, \dots, T^{(m+n)})$$

which helps us to compress the example:

$$\begin{aligned} & (ij, kl, mn, ijklmn \rightarrow ijk, A, B, C, (abc \rightarrow aabbcc, D)) \\ & = (aa, bb, cc, abc \rightarrow aab, A, B, C, D). \end{aligned}$$

Proof. Because $\hat{s}_{uj} = \hat{s}_{uj'} \implies s_{uj} = s_{uj'}$ for all $j, j' \in [n_u]$, each symbol in $\hat{\mathbf{s}}_{\mathbf{u}}$ only has one neighbour in the symbol graph. This is illustrated for our example in [Figure 3.5](#). Therefore each symbol in $\mathbf{s}_{\mathbf{u}}$ defines its own component, and can be used as the symbol in the symbol map, that replaces all symbols in their component. Therefore the symbols in $\mathbf{s}_{\mathbf{u}}$ are not changed by applying the symbol map, which are the only symbols in the inner expression that could have been changed by the map. Therefore the symbol map only has to be applied to the outer expression. □

With these two more specific theorems, we can write every naturally occurring complex expression from linear algebra as a single Einsum expression. The reason

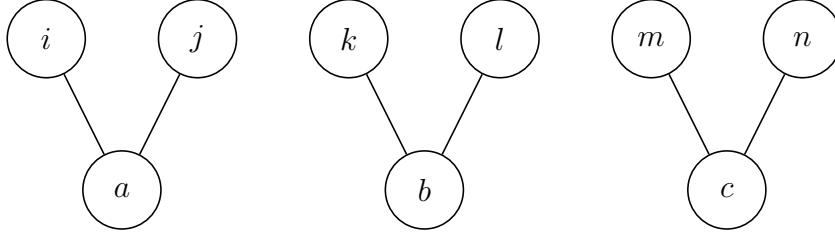


Figure 3.5: Symbol graph for the example

for this is, that in linear algebra, only up to two indices are used for a single tensor, which means that with two index strings, it cannot happen that a duplication is removed and another duplication is introduced simultaneously. Here are some more complex expressions as examples:

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

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

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

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

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

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

But to write every expression from linear algebra as a single Einsum expression respectively was already possible before (TODO: cite Julien). With these theorems, we just derived a different way of achieving that. For this, we can state a simple procedure. First, every function is translated to their respective Einsum expression, which results in a nested Einsum expression. Then, the nested expressions are compressed from the bottom up.

Now, with [Theorem 2](#), this procedure allows us to write every computation, where the single steps can be translated to Einsum, as one big Einsum expression that does not blow up in size with levels of nesting.

4 Naturally Occuring Einsum Expressions

4.1 Discrete Fourier Transform

Let T be an n -th order tensor where all axes have size m . Then the Discrete Fourier Transform $\text{DFT}(T)$ is the n -th order tensor where all axes have size m with:

$$\text{DFT}(T)_{x_1, \dots, x_n} = \sum_{y_1, \dots, y_n \in [m]} T_{y_1, \dots, y_n} \cdot \prod_{j+k \leq n+1} \exp \left(-i2\pi \frac{(x_j - 1)(y_k - 1)}{m^{n-j-k+2}} \right)$$

for $x_1, \dots, x_n \in [m]$. This formulation of the DFT is slightly rewritten form of the formulation by [?].

To write the DFT as an Einsum expression, we need to define $\binom{n+1}{2}$ matrices $T^{(j,k)} \in \mathbb{C}^{m \times m}$ for $j+k \leq n+1$ in the following way:

$$T_{x_j y_k}^{(j,k)} := \exp \left(-i2\pi \frac{(x_j - 1)(y_k - 1)}{m^{n-j-k+2}} \right)$$

for $x_j, y_k \in [m]$. Then

$$\text{DFT}(T)_{x_1, \dots, x_n} = \sum_{y_1, \dots, y_n \in [m]} T_{y_1, \dots, y_n} \cdot \prod_{j+k \leq n+1} T_{x_j y_k}^{(j,k)}$$

for $x_1, \dots, x_n \in [m]$. Therefore the DFT can be written as an Einsum expression with index strings consisting of symbols s_{x_i} and s_{y_j} for $j, k \in [n]$:

- $\mathbf{s}_x = s_{x1} \dots s_{xn}$
- $\mathbf{s}_y = s_{y1} \dots s_{yn}$
- $\mathbf{s}_{j,k} = s_{x_j} s_{y_k}$ for $j, k \in [n]$

With these index strings, the Einsum expression for a general DFT over any number of dimensions is the following:

$$\text{DFT}(T) = (\mathbf{s}_y, \mathbf{s}_{1,1}, \dots, \mathbf{s}_{1,n}, \mathbf{s}_{2,1}, \dots, \mathbf{s}_{2,n-1}, \dots, \mathbf{s}_{n,1} \rightarrow \mathbf{s}_x, T, T^{(1,1)}, \dots, T^{(1,n)}, T^{(2,1)}, \dots, T^{(2,n-1)}, \dots, T^{(n,1)})$$

Because this notation is hard to read, we will explore an example of the DFT of a third-order tensor with axes of size 32. In this example, we have to define 6 matrices $T^{(1,1)}$, $T^{(1,2)}$, $T^{(1,3)}$, $T^{(2,1)}$, $T^{(2,2)}$, and $T^{(3,1)}$. We will use a, b, c as symbols for the indices of T , and x, y, z as the symbols for the indices of $\text{DFT}(T)$. Then the matrices are defined in the following way:

$$\begin{aligned} T_{xa}^{(1,1)} &= \exp\left(-i2\pi \frac{(x-1)(a-1)}{32^3}\right) & T_{xc}^{(1,3)} &= \exp\left(-i2\pi \frac{(x-1)(c-1)}{32}\right) \\ T_{xb}^{(1,2)} &= \exp\left(-i2\pi \frac{(x-1)(b-1)}{32^2}\right) & T_{yb}^{(2,2)} &= \exp\left(-i2\pi \frac{(y-1)(b-1)}{32}\right) \\ T_{ya}^{(2,1)} &= \exp\left(-i2\pi \frac{(y-1)(a-1)}{32^2}\right) & T_{za}^{(3,1)} &= \exp\left(-i2\pi \frac{(z-1)(a-1)}{32}\right) \end{aligned}$$

for $x, y, z, a, b, c \in [32]$. Then the Einsum expression is the following:

$$\begin{aligned} \text{DFT}(T) &= (abc, xa, xb, xc, ya, yb, za \rightarrow xyz, \\ &\quad T, T^{(1,1)}, T^{(1,2)}, T^{(1,3)}, T^{(2,1)}, T^{(2,2)}, T^{(3,1)}) \end{aligned}$$

The inverse transform is analogue with

$$\hat{T}_{x_j y_k}^{(j,k)} := \exp\left(i2\pi \frac{(x_j-1)(y_k-1)}{m^{n-j-k+2}}\right).$$

4.2 Hadamard Transform

Let T be an n -th order tensor where all axes have size m . Then the Hadamard Transform $H(T)$ is the n -th order tensor where all axes have size m with:

$$H(T)_{x_1 \dots x_n} = \sum_{y_1, \dots, y_n \in [m]} T_{y_1 \dots y_n} (-1)^{x_1 y_1 + \dots + x_n y_n}$$

for $x_1, \dots, x_n \in [m]$.

Then we can define n matrices $T^{(i)} \in \mathbb{R}^{m \times m}$ for $i \in [n]$:

$$T_{x_i y_i}^{(i)} = (-1)^{x_i y_i}$$

for $x_i, y_i \in [m]$. Then

$$H(T)_{x_1 \dots x_n} = \sum_{y_1 \dots y_n \in [m]} T_{y_1 \dots y_n} \cdot \prod_{i \in [n]} T_{x_i y_i}^{(i)}$$

for $x_1, \dots, x_n \in [m]$. Therefore the Hadamard Transform can be written as an Einsum expression with index strings consisting of symbols s_{x_i} and s_{y_j} for $j, k \in [n]$:

- $\mathbf{s}_x = s_{x1} \dots s_{xn}$
- $\mathbf{s}_y = s_{y1} \dots s_{yn}$
- $\mathbf{s}_i = s_{xi}s_{yi}$ for $i \in [n]$

Then

$$H(T) = (\mathbf{s}_y, \mathbf{s}_1, \dots, \mathbf{s}_n \rightarrow \mathbf{s}_x, T, T^{(1)}, \dots, T^{(n)}).$$

5 Deep Learning

5.1 Fully Connected Feed-Forward Net

A single layer of a fully connected Feed-Forward Neural Net with ReLU activations can be expressed as a nested Einsum expression, with the use of multiple semirings. For this, let

- $R_{(+,\cdot)}$ be the standard semiring $(\mathbb{R}, +, \cdot)$,
- $R_{(\max,+)}$ be the tropical semiring $(\mathbb{R} \cup \{-\infty\}, \max, +)$,
- $R_{(\min,\max)}$ be the minimax semiring $(\mathbb{R} \cup \{-\infty, +\infty\}, \min, \max)$.

Let $\nu : \mathbb{R}^n \rightarrow \mathbb{R}^m$ be the function that computes the output of the layer for a given input vector $x \in \mathbb{R}^n$, with weights $A \in \mathbb{R}^{m \times n}$ and biases $b \in \mathbb{R}^m$. Then

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

A multi-layer network can be achieved by nesting the respective Einsum expressions of each layer.

Because each level of nesting needs a different semiring, we can not use the theorems from [Chapter 3](#) to compress the expression. But if we could find a way of compressing the massively nested expressions of deeper neural networks despite of that, then we could benefit from the advantages mentioned in [Chapter 2](#) such as the optimisation of contraction paths. Unfortunately, it is unlikely that this is possible, because we found that expanding the matrix multiplication, that transforms the outputs of another layer, results in an exponentially big term.

To see this, we use the tropical semiring $(\mathbb{R}, \oplus, \odot)$, where $a \oplus b = \max(a, b)$ and $a \odot b = a + b$. We do this because tropical semiring can naturally express all the operations used in a fully connected neural network. For this we need to define the tropical power:

$$a^{\odot n} = \underbrace{a \odot a \odot \dots \odot a}_{n \text{ times}}$$

for $n \in \mathbb{N}$. The following property of the tropical power is also needed:

$$(a^{\odot b})^{\odot c} = a^{\odot(b+c)}.$$

The tropical semiring also allows us to use the distributive law of maximization and addition

$$a \odot (b \oplus c) = a \odot b \oplus a \odot c,$$

as well as the distributive law of addition and multiplication

$$(a \odot b)^{\odot n} = a^{\odot n} \odot b^{\odot n},$$

and the distributive law of maximization and multiplication, which is restricted on natural numbers

$$(a \oplus b)^{\odot n} = a^{\odot n} \oplus b^{\odot n}.$$

Let $\nu : \mathbb{R}^n \rightarrow \mathbb{R}^l$ be the function that computes the output of a two-layer fully connected neural network ($n \rightarrow m \rightarrow l$ neurons) with ReLU activations, which maps inputs $x \in \mathbb{R}^n$ to outputs $\nu(y) \in \mathbb{R}^l$, 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:

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

In order to reasonably work with matrix multiplication in the tropical semiring, we can only view matrices with positive integer entries. This is not a limitation, because making the entries integers does not impact the strength of the neural network [see ? , sec. 4].

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

$$\begin{aligned} \max(Ax + b, 0) &= \max(A_+x - A_-x + b, A_-x - A_-x) \\ &= \max(A_+x + b, A_-x) - A_-x \end{aligned}$$

where $A_+ = \max(A, 0)$, $A_- = \max(-A, 0)$ and therefore $A = A_+ - A_-$. This turns the network output into a tropical rational function [see ? , sec. 5]:

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

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

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

multiple times.

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

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 of standard addition and multiplication and the distributive law of maximization and multiplication, and the last equality follows from the distributive law of maximization and addition.

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.

5.2 Attention

For $Q \in \mathbb{R}^{d_v \times d_k}$, $K \in \mathbb{R}^{d_v \times d_k}$, $V \in \mathbb{R}^{d_v \times d_v}$, the attention mechanism is the following:

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

It is comprised of multiple steps, which can all be expressed with Einsum expressions and element-wise operations:

- matrix multiplication QK^\top :

$$\begin{aligned}
(QK^\top)_{ij} &= \sum_{k \in [d_k]} Q_{ik} K_{jk} \\
QK^\top &= (ik, jk \rightarrow ij, Q, K)
\end{aligned}$$

- scaling by $\sqrt{d_k}$ (no Einsum needed)
- normalizing with softmax: Let $X \in \mathbb{R}^{m \times n}$, then

$$\text{softmax}(X)_{ij} := \frac{\exp(X_{ij})}{\omega_i}$$

where

$$\omega_i := \sum_{j \in [n]} \exp(X_{ij}).$$

Therefore

$$\text{softmax}(X) = (ij, i \rightarrow ij, \exp(X), 1/(ij \rightarrow i, \exp(X)))$$

- another matrix multiplication with V . Let $X \in \mathbb{R}^{d_v \times d_v}$:

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

Then the whole attention mechanism can be expressed with Einsum expressions and the use of element-wise operations:

$$\begin{aligned} \text{Attention}(Q, K, V) &= \text{softmax} \left(\frac{QK^\top}{\sqrt{d_K}} \right) V \\ &= (ik, kj \rightarrow ij, (ij, i \rightarrow ij, \exp(\frac{1}{\sqrt{d_k}} \cdot (ik, jk \rightarrow ij, Q, K)), \\ &\quad 1/(ij \rightarrow i, \exp(\frac{1}{\sqrt{d_k}} \cdot (ik, jk \rightarrow ij, Q, K))))), V) \\ &= (ik, kj, k \rightarrow ij, \exp(\frac{1}{\sqrt{d_k}} \cdot (ik, jk \rightarrow ij, Q, K)) \\ &\quad 1/(ij \rightarrow i, \exp(\frac{1}{\sqrt{d_k}} \cdot (ik, jk \rightarrow ij, Q, K))))), V) \end{aligned}$$

5.3 Batch Norm

Let $x^{(1)}, \dots, x^{(m)}$ be m 4th-order tensors. Let X be the 5th-order tensor that consists of all those tensors combined along a new axis. Then the Batch Norm with parameters $\gamma, \beta \in \mathbb{R}$ over this *mini-batch* of tensors is defined in the following way:

$$\text{BN}_{\gamma, \beta}(X)_i = \frac{x_i - \mathbb{E}_j[x_j]}{\sqrt{\text{Var}_j[x_j] + \epsilon}} \cdot \gamma + \beta$$

for $i \in [m]$, where ϵ is some constant added for numerical stability [?]. This computation is comprised of multiple steps, which can all be expressed with Einsum expressions and element-wise operations:

- mini-batch mean:

$$\begin{aligned} \mu_{abcd} &= \frac{1}{m} \sum_{i=1}^m x_{abcd}^{(i)} \\ \mu &= \frac{1}{m} (abcdi \rightarrow abcd, X) \end{aligned}$$

- centralize:

$$\begin{aligned}\bar{x}_{abcd}^{(i)} &= x_{abcd}^{(i)} - \mu_{abcd} \\ \bar{X} &= (abcdi, abcd \rightarrow abcd, X, -\mu)_{R_{(\max,+)}}\end{aligned}$$

- mini-batch variance:

$$\begin{aligned}\sigma_{abcd}^2 &= \frac{1}{m} \sum_{i=1}^m \left(\bar{x}_{abcd}^{(i)} \right)^2 \\ \sigma^2 &= \frac{1}{m} (abcdi, abcdi \rightarrow abcd, \bar{X})\end{aligned}$$

- normalize:

$$\begin{aligned}\hat{x}_{abcd}^{(i)} &= \frac{\bar{x}_{abcd}^{(i)}}{\sqrt{\sigma_{abcd}^2 + \epsilon}} \\ \hat{X} &= (abcdi, abcd \rightarrow abcd, \bar{X}, (\sigma^2 + \epsilon)^{-\frac{1}{2}})\end{aligned}$$

- scale and shift:

$$\begin{aligned}y_{abcd}^{(i)} &= \gamma \hat{x}_{abcd}^{(i)} + \beta \\ Y &= \gamma \hat{X} + \beta\end{aligned}$$

Therefore the whole attention mechanism can be expressed with Einsum expressions and the use of element-wise operations:

$$\begin{aligned}\text{BN}_{\gamma, \beta}(X) &= (abcdi, abcd \rightarrow abcd, \\ &\quad (abcdi, abcd \rightarrow abcd, X, -\frac{1}{m}(abcdi \rightarrow abcd, X))_{R_{(\max,+)}} , \\ &\quad (\frac{1}{m}(abcdi, abcdi \rightarrow abcd, \\ &\quad \quad (abcdi, abcd \rightarrow abcd, X, -\frac{1}{m}(abcdi \rightarrow abcd, X))_{R_{(\max,+)}} \\ &\quad \quad) + \epsilon)^{-\frac{1}{2}} \\ &\quad) \cdot \gamma + \beta\end{aligned}$$

5.4 Convolution

Let F and G be two n -th order tensors where all axes of F have size d_F and all axes of G have size d_G with $d_F < d_G$. Let $d_O = d_G - d_F + 1$. Then the convolution $F * G$

is defined in the following way:

$$(F * G)_x := \sum_{y \in [d_F]^n} F_y \cdot G_{x+d_F-y}$$

for all $x \in [d_O]^n$, where $x + d_F - y$ indicates the element-wise addition $(x + d_F - y)_i = x_i + d_F - y_i$ for $i \in [n]$. Let

$$G'_{(x,y)} := G_{x+d_F-y}$$

for $x \in [d_O]^n, y \in [d_F]^n$. Then

$$(F * G)_x = \sum_{y \in [d_G]^n} F_y G'_{(x,y)}$$

for $x \in [d_O]^n$. Let

$$P_{(x,y,z)} := \begin{cases} 1 & \text{if } z = x + d_F - y \\ 0 & \text{else} \end{cases}$$

for $x \in [d_O]^n, y \in [d_F]^n, z \in [d_G]^n$. Then

$$G'_{(x,y)} = \sum_{z \in [d_G]^n} P_{(x,y,z)} G_z$$

for $x \in [d_O]^n, y \in [d_F]^n$. Therefore, convolution can be expressed as an Einsum expression:

$$(F * G) = ((\mathbf{s}_x, \mathbf{s}_y, \mathbf{s}_z), \mathbf{s}_y, \mathbf{s}_z \rightarrow \mathbf{s}_x, P, F, G)$$

where $\mathbf{s}_x, \mathbf{s}_y, \mathbf{s}_z \in S^n$ use distinct symbols.

The manual computation of the design tensor¹ P is quite expensive, and therefore this expression could be inefficient. It could lead to a more efficient computation, if this design tensor could be expressed as an *outer product* of 2 or more smaller tensors. Sadly, this is not possible.

Proof. To prove this, we will first show that, if P can be expressed as an outer product, then the factors also have to be scaled design tensors. Then we will give an example of a convolution, where P can not be expressed as an outer product of design tensors.

Let U be an m -th order tensor, and V an $(3n - m)$ -th order tensor for $1 \leq m < 3n$. Let $\mathbf{s}_u \in S^m$ be the index string for U , and let $\mathbf{s}_v \in S^{3n-m}$ be the index string for V such that \mathbf{s}_u and \mathbf{s}_v use distinct symbols. Then P being the outer product of U and V means

$$P = (\mathbf{s}_u, \mathbf{s}_v \rightarrow (\mathbf{s}_u, \mathbf{s}_v), U, V)$$

up to reordering of axes.

Let u and v be entries of U and V respectively, and let \mathbf{i}_u and \mathbf{i}_v be a multi-index of U and V respectively, where this value occurs. Then the value $u \cdot v$ occurs in P at the multi-index

¹A design tensor is a tensor that is filled only with the additive and multiplicative neutral element of the used semiring.

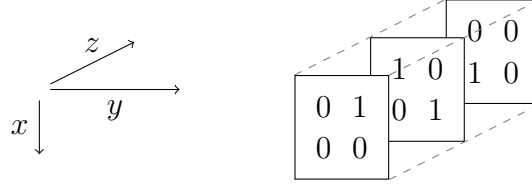


Figure 5.1: P for $F \in \mathbb{R}^2$ and $G \in \mathbb{R}^3$

$(\mathbf{i}_u, \mathbf{i}_v)$. Therefore, if the sets of values contained in U and V are not of the form $\{0, c\}$ and $\{0, \frac{1}{c}\}$ for some $c \in \mathbb{R}$, then we can produce more values than 0 and 1 in P . Therefore U and V must be design tensors that were scaled by c and $\frac{1}{c}$ respectively for some $c \in \mathbb{R}$.

W.l.o.g. we now assume that U and V are both unscaled design tensors, because if

$$P = (\mathbf{s}_u, \mathbf{s}_v \rightarrow (\mathbf{s}_u, \mathbf{s}_v), cU, \frac{1}{c}V)$$

then

$$\begin{aligned} P &= c \cdot \frac{1}{c} \cdot (\mathbf{s}_u, \mathbf{s}_v \rightarrow (\mathbf{s}_u, \mathbf{s}_v), U, V) \\ &= (\mathbf{s}_u, \mathbf{s}_v \rightarrow (\mathbf{s}_u, \mathbf{s}_v), U, V). \end{aligned}$$

Consider a convolution $F * G$ of vectors $F \in \mathbb{R}^2$ and $G \in \mathbb{R}^3$. Then

$$(F * G)_x = \sum_{y \in [2]} F_y G_{x+2-y}$$

for $x \in [2]$, and

$$P_{(x,y,z)} = \begin{cases} 1 & \text{if } z = x + 2 - y \\ 0 & \text{else} \end{cases}$$

for $x \in [2], y \in [2], z \in [3]$. This is illustrated in [Figure 5.1](#).

Now, the only two possibilities for m are $m = 1$ and $m = 2$, because $n = 1$ and therefore $1 \leq m < 3$. This means, U and V are a matrix and a vector. W.l.o.g. we assume that U is a matrix and V is a vector. Then for U to be a matrix and a factor of P , there are only three possibilities:

$$\begin{aligned} P_{xyz} &= U_{xy} V_z, \\ P_{xyz} &= U_{xz} V_y, \\ P_{xyz} &= U_{yz} V_x. \end{aligned}$$

In the first case, it has to hold that $U_{xy} = 1$ where $P_{xyz} = 1$ for any $z \in [3]$, because otherwise, no design tensor V could produce the entry $P_{xyz} = 1$. For the other two cases, the analogous fact holds: all the entries, where missing index exists such that $P_{xyz} = 1$, have to hold one as well. And unless V is full of zeros (which it cannot be), the converse is true as well, meaning if all entries of the missing index hold $P_{xyz} = 0$, then the entry in U also has to hold zero. Therefore there is only possibility for U for each of the cases, which

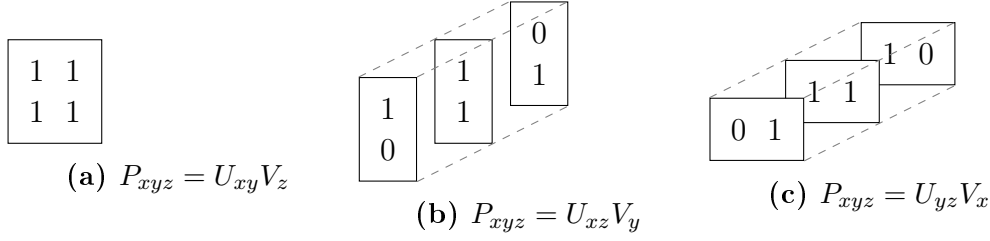


Figure 5.2: Possibilities for U in the factorization of P

are illustrated in Figure 5.2:

$$\begin{aligned}
 P_{xyz} &= U_{xy}V_z & U &= \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \\
 P_{xyz} &= U_{xz}V_y & U &= \begin{pmatrix} 1 & 1 & 0 \\ 0 & 1 & 1 \end{pmatrix} \\
 P_{xyz} &= U_{yz}V_x & U &= \begin{pmatrix} 0 & 1 & 1 \\ 1 & 1 & 0 \end{pmatrix}
 \end{aligned}$$

Therefore, the multiplication with V has to spread out the ones across different values of the missing index, which is not possible, because depending on the entries of V on the missing index:

- if V is one at a value of the missing index, then P is a copy of U at this value of the missing index, and
- if V is zero at a value of the missing index, then P is zero at this value of the missing index.

Therefore, there is no factorization of P when $F \in \mathbb{R}^2$ and $G \in \mathbb{R}^3$, which means P can not generally be expressed as an outer product of two lower-order tensors. \square

5.5 Max-Pooling

Let T be an n -th order tensor where all axes have size m . Let $p \in \mathbb{N}$ be the *pool size* such that $m = k \cdot p$ for $k \in \mathbb{N}$. Then the max-pooling of T is defined in the following way:

$$M(T)_x := \max_{y \in [p]^n} T_{p(x-1)+y}$$

for $x \in [k]^n$, where $x - 1$ indicates the element-wise subtraction $(x - 1)_i = x_i - 1$ for $i \in [n]$. Let

$$T'_{(x,y)} = T_{p(x-1)+y}$$

for $x \in [k]^n, y \in [p]^n$. Then

$$M(T)_x = \max_{y \in [p]^n} T'_{(x,y)}$$

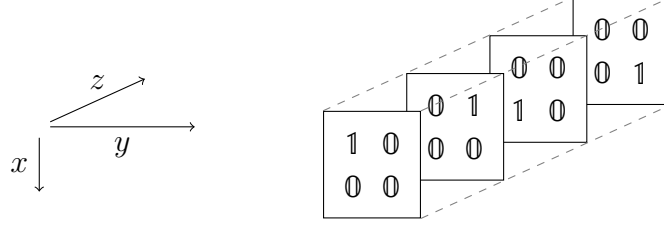


Figure 5.3: P for $F \in \mathbb{R}^2$ and $G \in \mathbb{R}^3$

for $x \in [k]^n$. Let

$$P_{(x,y,z)} := \begin{cases} 0 & \text{if } z = p(x-1) + y \\ -\infty & \text{else} \end{cases}$$

for $x \in [k]^n, y \in [p]^n, z \in [m]^n$. Then

$$T'_{(x,y)} = \max_{z \in [m]^n} P_{(x,y,z)} + T_z$$

for $x \in [k]^n, y \in [p]^n$. Therefore, Max-Pooling can be expressed as an Einsum expression:

$$M(T) = ((s_x, s_y, s_z), s_z \rightarrow s_x, P, T)_{R_{(\max,+)}}$$

where $s_x, s_y, s_z \in S^n$ use distinct symbols and $R_{(\max,+)}$ denotes the tropical semiring $(\mathbb{R} \cup \{-\infty\}, \max, +)$.

As in [Section 5.4](#), the efficiency of the computation could benefit from decomposition of the design tensor P into an outer product of lower-order design tensors. But yet again, this is not possible.

Proof. Because $-\infty$ and 0 are the additive neutral and multiplicative neutral element of the used semiring respectively, the argument in [Section 5.4](#), that the factors have to be scaled design tensors, holds here as well.

Therefore, w.l.o.g. we assume that U and V are design tensors of order one or higher. Consider max-pooling where $n = 1, m = 4, p = 2$, and $k = 2$. Then

$$P_{(x,y,z)} := \begin{cases} 0 & \text{if } z = 2(x-1) + y \\ -\infty & \text{else} \end{cases}$$

for $x \in [2], y \in [2], z \in [4]$. This is illustrated in [Figure 5.3](#), where 0 and 1 were used to indicate the additive and multiplicative neutral element of the tropical semiring, $-\infty$ and 0.

The rest of the proof is analogous to the proof in [Section 5.4](#), where the key argument is, that the multiplicative neutral element cannot be distributed with an outer product in such a way, that there are no copied slices in P . \square

5.6 Discussion

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6 Conclusion

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Selbstständigkeitserklärung

Ich erkläre, dass ich die vorliegende Arbeit selbstständig und nur unter Verwendung der angegebenen Quellen und Hilfsmittel angefertigt habe. Seitens des Verfassers bestehen keine Einwände die vorliegende Bachelorarbeit für die öffentliche Benutzung im Universitätsarchiv zur Verfügung zu stellen.

A handwritten signature in black ink, appearing to read 'Wenig', with a long, sweeping horizontal stroke extending to the right.

Jena, 23.07.2023