Exploring Einsum as a Universal Inference Language

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Abstract

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Contents

Abstract iii

1 Introduction 1

2 Einsum 3
- 2.1 Syntax and Semantics . . . 3
- 2.2 Simple Examples From Linear Algebra . . . 6
- 2.3 Computational Benefits . . . 7

3 Nested Expressions 9
- 3.1 Simple Nested Expressions . . . 10
- 3.2 General Nested Expressions . . . 11

4 Naturally Occuring Einsum Expressions 19
- 4.1 Discrete Fourier Transform . . . 19
- 4.2 Hadamard Transform . . . 20

5 Deep Learning 23
- 5.1 Fully Connected Feed-Forward Net . . . 23
- 5.2 Attention . . . 25
- 5.3 Batch Norm . . . 26
- 5.4 Convolution . . . 27
- 5.5 Max-Pooling . . . 30

6 Practical Results 33

7 Discussion 35

8 Conclusion 37

Selbständigkeitserklärung 45

1 Introduction

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2 Einsum

Given two third-order tensors $A \in \mathbb{R}^{3\times4\times5}$ and $B \in \mathbb{R}^{3\times3\times5}$, and a vector $v \in \mathbb{R}^4$. Consider the following computation resulting in a matrix $C \in \mathbb{R}^{3\times3}$:

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

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 is the result of a general Einsum expression.

2.1 Syntax and Semantics

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 $S = \{i, j, k\}$. The tensor $T^{(1)} = A$ has the index string $\boldsymbol{s_1} = ijk$, $T^{(2)} = B$ has $\boldsymbol{s_2} = iik$, $T^{(3)} = v$ has $\boldsymbol{s_3} = j$, and the output string is $\boldsymbol{s_t} = ij$. The individual symbols are $s_{11} = i$, $s_{12} = j$, $s_{13} = k$, $s_{12} = i$, $s_{22} = i$, $s_{23} = k$, $s_{31} = j$, $s_{t1} = i$, $s_{t2} = j$.

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 $\boldsymbol{s} = (i, i)$ 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 $\mathcal{F} = \prod_{s \in F} [d_s]$ 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 $\sigma(\boldsymbol{s_t}) \subseteq \bigcup_{i \in [n]} \sigma(\boldsymbol{s_i})$.

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 $(\boldsymbol{f}, \boldsymbol{b}) \in \mathcal{F} \times \mathcal{B}$ [1] to another multi-index, which includes only the indices, that are represented by the symbols used in $\boldsymbol{s}$, in the same order as present in $\boldsymbol{s}$. We denote this as $(\boldsymbol{f}, \boldsymbol{b}) : \boldsymbol{s}$. Notice how this still allows duplication of indices given in $(\boldsymbol{f}, \boldsymbol{b})$. 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

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

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 $(i = 1, j = 4, k = 2) : iik = (1, 1, 2)$.

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

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

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

$$\forall \boldsymbol{f} \in \mathcal{F} : T_{\boldsymbol{f}:\boldsymbol{s_t}} = \bigoplus_{\boldsymbol{b} \in \mathcal{B}} \bigodot_{i=1}^{n} T^{(i)}_{(\boldsymbol{f},\boldsymbol{b}):\boldsymbol{s_i}}.$$

Because we also project the indices $\boldsymbol{f}$ with 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 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 $\boldsymbol{s}$ for that input tensor has to be the empty string ϵ. Now when the multi-index $(\boldsymbol{f}, \boldsymbol{b})$ 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 $\boldsymbol{m} = (m_1, \ldots, m_{k_1})$ and $\boldsymbol{n} = (n_1, \ldots, n_{k_2})$ for $k_1, k_2 \in \mathbb{N}$, then we defined $(\boldsymbol{m}, \boldsymbol{n})$ to be the concatenation of the multi-indices:

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

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

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

Therefore we can name a neutral element for concatenation, which is the empty multi-index λ with $(\boldsymbol{i}, \lambda) = \boldsymbol{i}$ for any multi-index $\boldsymbol{i}$. 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

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

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

$$\begin{aligned} &\forall \boldsymbol{f} \in \mathcal{F} : T_{\boldsymbol{f}:\boldsymbol{s_t}} = \sum_{\boldsymbol{b} \in \{\lambda\}} \bigodot_{i=1}^{n} T^{(i)}_{(\boldsymbol{f},\boldsymbol{b}):\boldsymbol{s_i}} \\ \iff &\forall \boldsymbol{f} \in \mathcal{F} : T_{\boldsymbol{f}:\boldsymbol{s_t}} = \bigodot_{i=1}^{n} T^{(i)}_{\boldsymbol{f}:\boldsymbol{s_i}}. \end{aligned}$$

And if $B = \emptyset$, then

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

results in the computation of a scalar T with

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

2.2 Simple Examples From Linear Algebra

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

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

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

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

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

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

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

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

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

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

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

2.3 Computational Benefits

Query Language, faster inference, stuff like that. How can it be faster? - we can optimize contraction path - high parallelism allows for a lot of optimization with the use of vectorization - intermediate steps in optimal contraction path can be optimized with pipelining - we can optimize hardware specifically for computing Einsum expressions, which is pretty much just tensor operations.

By mapping a lot of problems to Einsum, we can spare time in trying to find efficient solutions for new problems, and focus on optimizing the computation of Einsum expressions. This reduces the effort of finding an efficient solution for a problem to finding a mapping of the problem to einsum.

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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 of a single Einsum string, that were stated in Section 2.3.

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

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

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 $\boldsymbol{s_i} \in S^{n_i}$. 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 bound 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 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

$$\begin{aligned}
V \quad & = (\boldsymbol{s_1}, \dots, \boldsymbol{s_m}, \boldsymbol{s_u} \to \boldsymbol{s_v}, T^{(1)}, \dots, T^{(m)}, U) \\
\iff \forall \boldsymbol{f} \in \mathcal{F} : V_{\boldsymbol{f}:\boldsymbol{s_v}} & = \bigoplus_{\boldsymbol{b} \in \mathcal{B}} \bigodot_{i=1}^{m} T^{(i)}_{(\boldsymbol{f},\boldsymbol{b}):\boldsymbol{s_k}} \odot U_{(\boldsymbol{f},\boldsymbol{b}):\boldsymbol{s_u}} \\
& = \bigoplus_{\boldsymbol{b} \in \mathcal{B}} \bigodot_{i=1}^{m} T^{(i)}_{(\boldsymbol{f},\boldsymbol{b}):\boldsymbol{s_i}} \odot \left[\bigoplus_{\boldsymbol{b'} \in \mathcal{B}'} \bigodot_{i'=m+1}^{m+n} T^{(i')}_{(\boldsymbol{f},\boldsymbol{b},\boldsymbol{b'}):\boldsymbol{s_{i'}}} \right] \\
& = \bigoplus_{\boldsymbol{b} \in \mathcal{B}} \bigoplus_{\boldsymbol{b'} \in \mathcal{B}'} \bigodot_{i=1}^{m} T^{(i)}_{(\boldsymbol{f},\boldsymbol{b}):\boldsymbol{s_i}} \odot \bigodot_{i=m+1}^{m+n} T^{(i)}_{(\boldsymbol{f},\boldsymbol{b},\boldsymbol{b'}):\boldsymbol{s_i}} \\
& = \bigoplus_{\boldsymbol{b} \in \mathcal{B} \times \mathcal{B}'} \bigodot_{i=1}^{m+n} T^{(i)}_{(\boldsymbol{f},\boldsymbol{b}):\boldsymbol{s_i}} \\
\iff V \quad & = (\boldsymbol{s_1}, \dots, \boldsymbol{s_{m+n}} \to \boldsymbol{s_v}, T^{(1)}, \dots, T^{(m+n)})
\end{aligned}$$

where the third equality follows from the definition of U:

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

and from the fact, that the symbols in $\boldsymbol{s_u}$ 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 $\boldsymbol{b'}$ do not clash with the symbols representing $(\boldsymbol{f}, \boldsymbol{b})$, and therefore $(\boldsymbol{f}, \boldsymbol{b}, \boldsymbol{b'}) : \boldsymbol{s_{i'}}$ is well-defined and projects on the same indices as $(\boldsymbol{f'}, \boldsymbol{b'}) : \boldsymbol{s_{i'}}$. The fourth equality follows from the distributivity in a semiring. □

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 occuring expressions in linear algebra, e.g.

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

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

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

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.

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

or

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

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:

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

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 $\boldsymbol{s_u} = iijkkl$ and the input string $\boldsymbol{\hat{s}_u} = abbde$ 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

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

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 $\boldsymbol{s_i} \in S^{n_i}$. Let $\boldsymbol{s_u}$ be an index string for the n_u-th order tensor U, which is defined as follows:

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

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

Let s_v be an index string and

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

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

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 $\boldsymbol{s_{m+1}}, \ldots, \boldsymbol{s_{m+n}}$. Instead, we first need to apply a symbol map $\nu : S \to S$ 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 both expressions. The edges are $E = \{\{s_{uj}, \hat{s}_{uj}\} \mid j \in [n_u]\}$, which connects all symbols from $\boldsymbol{s_u}$ and $\boldsymbol{\hat{s}_u}$ that share an index. The symbol graph for our example is illustrated in Figure 3.1.

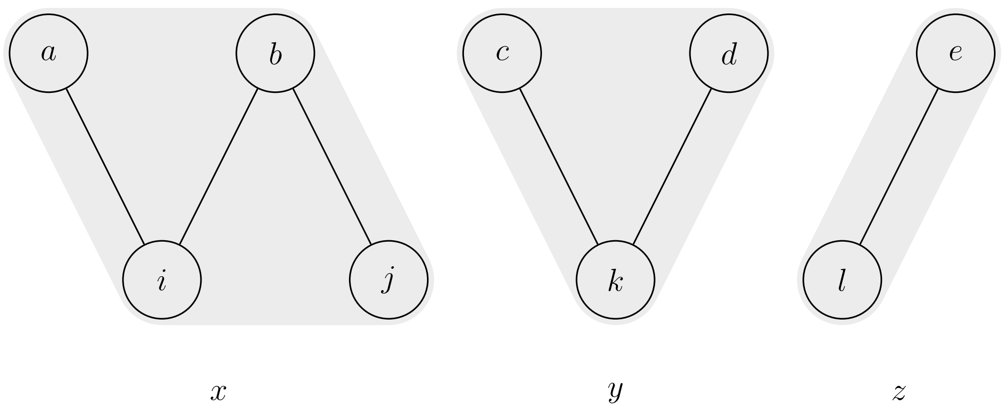


Figure 3.1: Symbol graph for the example

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:

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

In our example, the components are $\{a, b, i, j\}$, $\{c, d, k\}$, and $\{e, l\}$. Therefore we 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 $\nu(\boldsymbol{s_i}) \in S^{n_i}, \nu(\boldsymbol{s_i})_j := \nu(s_{ij})$. Then we can write the substituted index strings by setting $\boldsymbol{\hat{s}_i} := \nu(\boldsymbol{s_i})$ for $i \in [m+n]$ and $\boldsymbol{\hat{s}_t} = \nu(\boldsymbol{s_t})$. With these index strings, the compressed Einsum expression is the following:

$$V = (\boldsymbol{\hat{s}_1}, \ldots, \boldsymbol{\hat{s}_{m+n}} \to \boldsymbol{\hat{s}_v}, T^{(1)}, \ldots, T^{(m+n)})$$

which helps us to compress the example:

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

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 $\mathbb{1}_d$:

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

for $i, j \in [d]$, where $\mathbb{0}$ and $\mathbb{1}$ 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 $\boldsymbol{s_i} \in S^{n_i}$. Let $\boldsymbol{s_t}$ be the index string for T with

$$T = (\boldsymbol{s_1}, \ldots, \boldsymbol{s_n} \to \boldsymbol{s_t}, T^{(1)}, \ldots, T^{(n)}).$$

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 $\boldsymbol{s'_k}$ 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 $\boldsymbol{s}_{\mathbb{1}} = (s_{kj}, s_{\text{new}})$. Then

$$T = (\boldsymbol{s_1}, \ldots, \boldsymbol{s'_k}, \ldots, \boldsymbol{s_n}, \boldsymbol{s}_{\mathbb{1}} \to \boldsymbol{s_t}, T^{(1)}, \ldots, T^{(n)}, \mathbb{1}_{d_{kj}}).$$

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

$$\begin{aligned}
& T = (\boldsymbol{s_1}, \ldots, \boldsymbol{s_n} \to \boldsymbol{s_t}, T^{(1)}, \ldots, T^{(n)}) \\
\iff & \forall \boldsymbol{f} \in \mathcal{F} : T_{\boldsymbol{f}:\boldsymbol{s_t}} = \bigoplus_{\boldsymbol{b} \in \mathcal{B}} \bigodot_{i \in [n]} T^{(i)}_{(\boldsymbol{f},\boldsymbol{b}):\boldsymbol{s_i}} \\
& = \bigoplus_{\boldsymbol{b} \in \mathcal{B} \times [d_{kj}]} \bigodot_{1 \le i < k} T^{(i)}_{(\boldsymbol{f},\boldsymbol{b}):\boldsymbol{s_i}} \odot T^{(k)}_{(\boldsymbol{f},\boldsymbol{b}):\boldsymbol{s'_k}} \odot \bigodot_{k < i \le n} T^{(i)}_{(\boldsymbol{f},\boldsymbol{b}):\boldsymbol{s_i}} \\
& \qquad \odot \begin{cases} \mathbb{1} & \text{if } (\boldsymbol{f},\boldsymbol{b}) : s_{kj} = (\boldsymbol{f},\boldsymbol{b}) : s_{\text{new}} \\ \mathbb{0} & \text{else} \end{cases} \\
& = \bigoplus_{\boldsymbol{b} \in \mathcal{B} \times [d_{kj}]} \bigodot_{1 \le i < k} T^{(i)}_{(\boldsymbol{f},\boldsymbol{b}):\boldsymbol{s_i}} \odot T^{(k)}_{(\boldsymbol{f},\boldsymbol{b}):\boldsymbol{s'_k}} \odot \bigodot_{k < i \le n} T^{(i)}_{(\boldsymbol{f},\boldsymbol{b}):\boldsymbol{s_i}} \\
& \qquad \odot \left(\mathbb{1}_{d_{kj}}\right)_{(\boldsymbol{f},\boldsymbol{b}):\boldsymbol{s}_{\mathbb{1}}} \\
\iff & T = (\boldsymbol{s_1}, \ldots, \boldsymbol{s'_k}, \ldots, \boldsymbol{s_n}, \boldsymbol{s}_{\mathbb{1}} \to \boldsymbol{s_t}, T^{(1)}, \ldots, T^{(n)}, \mathbb{1}_{d_{kj}})
\end{aligned}$$

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 $a \in M$. □

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 $\boldsymbol{s_t}$, 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 $\boldsymbol{s_i} \in S^{n_i}$. Let $\boldsymbol{s_t}$ be the index string for T with

$$T = (\boldsymbol{s_1}, \ldots, \boldsymbol{s_n} \to \boldsymbol{s_t}, T^{(1)}, \ldots, T^{(n)}).$$

Let F and B be the free and bound symbols of this expression. Let $n_t := |\boldsymbol{s_t}|$, $j \in [n_t]$, 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 $\boldsymbol{s'_t}$ 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 $\boldsymbol{s_{\mathbb{1}}} = (s_{tj}, s_{\text{new}})$. Then

$$T = (\boldsymbol{s_1}, \ldots, \boldsymbol{s_n}, \boldsymbol{s_{\mathbb{1}}} \to \boldsymbol{s_t'}, T^{(1)}, \ldots, T^{(n)}, \mathbb{1}_{d_{kj}}).$$

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 $\boldsymbol{s_t}$ even after replacing it with s_{new}, then

$$\begin{aligned}
& T = (\boldsymbol{s_1}, \ldots, \boldsymbol{s_n} \to \boldsymbol{s_t}, T^{(1)}, \ldots, T^{(n)}) \\
\iff & \forall \boldsymbol{f} \in \mathcal{F} : T_{\boldsymbol{f}:\boldsymbol{s_t}} = \bigoplus_{\boldsymbol{b}\in\mathcal{B}} \bigodot_{i\in[n]} T^{(i)}_{(\boldsymbol{f},\boldsymbol{b}):\boldsymbol{s_i}} \\
\iff & \forall \boldsymbol{f} \in \mathcal{F} \times [d_{tj}] : T_{\boldsymbol{f}:\boldsymbol{s_t'}} = \bigoplus_{\boldsymbol{b}\in\mathcal{B}} \bigodot_{i\in[n]} T^{(i)}_{(\boldsymbol{f},\boldsymbol{b}):\boldsymbol{s_i}} \odot \begin{cases} \mathbb{1} & \text{if } \boldsymbol{f} : s_{tj} = \boldsymbol{f} : s_{\text{new}} \\ \mathbb{0} & \text{else} \end{cases} \\
& = \bigoplus_{\boldsymbol{b}\in\mathcal{B}} \bigodot_{i\in[n]} T^{(i)}_{(\boldsymbol{f},\boldsymbol{b}):\boldsymbol{s_i}} \odot \left(\mathbb{1}_{d_{tj}}\right)_{(\boldsymbol{f},\boldsymbol{b}):\boldsymbol{s_{\mathbb{1}}}} \\
\iff & T = (\boldsymbol{s_1}, \ldots, \boldsymbol{s_n}, \boldsymbol{s_{\mathbb{1}}} \to \boldsymbol{s_t'}, T^{(1)}, \ldots, T^{(n)}, \mathbb{1}_{d_{tj}})
\end{aligned}$$

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 $\boldsymbol{s_t}$ after replacing it with s_{new}, then s_{tj} turns into a bound symbol. Therefore we have to define $\mathcal{F}' = \prod_{s\in\boldsymbol{s_t'}} [d_s]$. Then

$$\begin{aligned}
& T = (\boldsymbol{s_1}, \ldots, \boldsymbol{s_n} \to \boldsymbol{s_t}, T^{(1)}, \ldots, T^{(n)}) \\
\iff & \forall \boldsymbol{f} \in \mathcal{F} : T_{\boldsymbol{f}:\boldsymbol{s_t}} = \bigoplus_{\boldsymbol{b}\in\mathcal{B}} \bigodot_{i\in[n]} T^{(i)}_{(\boldsymbol{f},\boldsymbol{b}):\boldsymbol{s_i}} \\
\iff & \forall \boldsymbol{f} \in \mathcal{F}' : T_{\boldsymbol{f}:\boldsymbol{s_t'}} = \bigoplus_{\boldsymbol{b}\in\mathcal{B}\times[d_{tj}]} \bigodot_{i\in[n]} T^{(i)}_{(\boldsymbol{f},\boldsymbol{b}):\boldsymbol{s_i}} \odot \begin{cases} \mathbb{1} & \text{if } (\boldsymbol{f},\boldsymbol{b}) : s_{tj} = (\boldsymbol{f},\boldsymbol{b}) : s_{\text{new}} \\ \mathbb{0} & \text{else} \end{cases} \\
& = \bigoplus_{\boldsymbol{b}\in\mathcal{B}\times[d_{tj}]} \bigodot_{i\in[n]} T^{(i)}_{(\boldsymbol{f},\boldsymbol{b}):\boldsymbol{s_i}} \odot \left(\mathbb{1}_{d_{tj}}\right)_{(\boldsymbol{f},\boldsymbol{b}):\boldsymbol{s_{\mathbb{1}}}} \\
\iff & T = (\boldsymbol{s_1}, \ldots, \boldsymbol{s_n}, \boldsymbol{s_{\mathbb{1}}} \to \boldsymbol{s_t'}, T^{(1)}, \ldots, T^{(n)}, \mathbb{1}_{d_{tj}})
\end{aligned}$$

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

Now with these two lemmata, we can replace any symbol in any index string, regardless if it is and 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 $\boldsymbol{s_i} \in S^{n_i}$, where $T^{(n)} = \mathbb{1}_m$ for some $m \in \mathbb{N}$. Let $\boldsymbol{s_t}$ be the index string for T with

$$T = (\boldsymbol{s_1}, \ldots, \boldsymbol{s_n} \to \boldsymbol{s_t}, T^{(1)}, \ldots, T^{(n)}).$$

Let F and B be the free and bound symbols of this expression. Then we can introduce a symbol map $\mu : S \to S$, which maps both symbols in $\boldsymbol{s_n}$ 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 $\mu(\boldsymbol{s_i}) \in S^{n_i}, \mu(\boldsymbol{s_i})_j := \mu(s_{ij})$. Then we can write the substituted index strings by setting $\boldsymbol{s'_i} := \mu(\boldsymbol{s_i})$ for $i \in [n]$ and $\boldsymbol{s'_t} = \mu(\boldsymbol{s_t})$. With these index strings, the following holds:

$$T = (\boldsymbol{s'_1}, \ldots, \boldsymbol{s'_{n-1}} \to \boldsymbol{s'_t}, T^{(1)}, \ldots, T^{(n-1)}).$$

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

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

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 $\boldsymbol{s_n} = (s_{n1}, s_{n2})$:

- 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:

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

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:

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

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:

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

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. $\square$

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 $\mathrm{DFT}(T)$ is the n-th order tensor where all axes have size m with:

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

for $x_1, \ldots, x_n \in [m]$. This formulation of the DFT is slightly rewritten form of the formulation by Aji [1].

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:

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

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

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

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

- $\boldsymbol{s_x} = s_{x1} \ldots s_{xn}$
- $\boldsymbol{s_y} = s_{y1} \ldots s_{yn}$
- $\boldsymbol{s_{j,k}} = s_{xj} s_{yk}$ for $j, k \in [n]$

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

$$\begin{aligned}\mathrm{DFT}(T) = (&\boldsymbol{s_y}, \boldsymbol{s_{1,1}}, \ldots, \boldsymbol{s_{1,n}}, \boldsymbol{s_{2,1}}, \ldots, \boldsymbol{s_{2,n-1}}, \ldots, \boldsymbol{s_{n,1}} \to \boldsymbol{s_x}, \\ &T, T^{(1,1)}, \ldots, T^{(1,n)}, T^{(2,1)}, \ldots, T^{(2,n-1)}, \ldots, T^{(n,1)})\end{aligned}$$

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 $\mathrm{DFT}(T)$. Then the matrices are defined in the following way:

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

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

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

The inverse transform is anologue with

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

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:

$$H(T)_{x_1\dots x_n} = \sum_{y_1,\dots,y_n\in[m]} T_{y_1\dots y_n}(-1)^{x_1y_1+\dots+x_ny_n}$$

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

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

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

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

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

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_{xi} and s_{yj} for $j, k \in [n]$:

- $\boldsymbol{s_x} = s_{x1} \dots s_{xn}$
- $\boldsymbol{s_y} = s_{y1} \dots s_{yn}$
- $\boldsymbol{s_i} = s_{xi} s_{yi}$ for $i \in [n]$

Then
$$H(T) = (\boldsymbol{s_y}, \boldsymbol{s_1}, \dots, \boldsymbol{s_n} \rightarrow \boldsymbol{s_x}, T, T^{(1)}, \dots, T^{(n)}).$$

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 $\nu : \mathbb{R}^n \to \mathbb{R}^m$ 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

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

A multi-layer network can the 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:

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

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

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

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

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

In order to reasonably work with matrix multiplication in the tropcial 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 2, 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 2, sec. 5]:

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

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

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

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

Where the second equality is just the first equality written with the operations of the tropical semiring, the third equality follows from the distributive law 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^T:

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

- 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

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

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

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

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

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

5.3 Batch Norm

Let $x^{(1)}, \ldots, x^{(m)}$ 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:

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

for $i \in [m]$, where ϵ is some constant added for numerical stability [3]. This computation is comprised of multiple steps, which can all be expressed with Einsum expressions and element-wise operations:

- mini-batch mean:

$$\mu_{abcd} = \frac{1}{m} \sum_{i=1}^{m} x^{(i)}_{abcd}$$

$$\mu = \frac{1}{m}(abcdi \to abcd, X)$$

- centralize:

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

- mini-batch variance:

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

- normalize:

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

- scale and shift:

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

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

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

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:

$$(F * G) = ((\boldsymbol{s_x}, \boldsymbol{s_y}, \boldsymbol{s_z}), \boldsymbol{s_y}, \boldsymbol{s_z} \to \boldsymbol{s_x}, P, F, G)$$

where $\boldsymbol{s_x}, \boldsymbol{s_y}, \boldsymbol{s_z} \in S^n$ use distinct symbols.

The manual computation of the design tensor[1] 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 $\boldsymbol{s_u} \in S^m$ be the index string for U, and let $\boldsymbol{s_v} \in S^{3n-m}$ be the index string for V such that $\boldsymbol{s_u}$ and $\boldsymbol{s_v}$ use distinct symbols. Then P being the outer product of U and V means

$$P = (\boldsymbol{s_u}, \boldsymbol{s_v} \to (\boldsymbol{s_u}, \boldsymbol{s_v}), U, V)$$

up to reordering of axes.

Let u and v be entries of U and V respectively, and let $\boldsymbol{i_u}$ and $\boldsymbol{i_v}$ 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

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

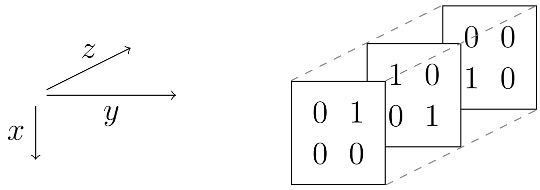


Figure 5.1: P for $F \in \mathbb{R}^2$ and $G \in \mathbb{R}^3$

$(\boldsymbol{i_u}, \boldsymbol{i_v})$. 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

$$P = (\boldsymbol{s_u}, \boldsymbol{s_v} \to (\boldsymbol{s_u}, \boldsymbol{s_v}), cU, \frac{1}{c}V)$$

then

$$\begin{aligned} P &= c \cdot \frac{1}{c} \cdot (\boldsymbol{s_u}, \boldsymbol{s_v} \to (\boldsymbol{s_u}, \boldsymbol{s_v}), U, V) \\ &= (\boldsymbol{s_u}, \boldsymbol{s_v} \to (\boldsymbol{s_u}, \boldsymbol{s_v}), U, V). \end{aligned}$$

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

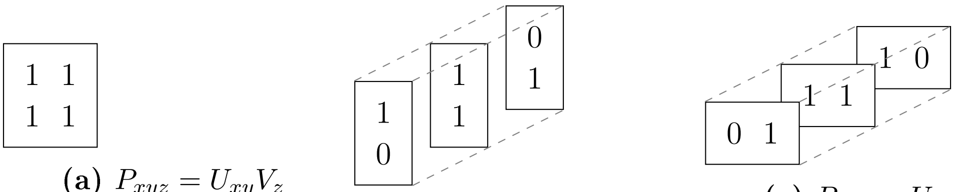
$$P_{(x,y,z)} = \begin{cases} 1 & \text{if } z = x + 2 - y \\ 0 & \text{else} \end{cases}$$

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



(a) $P_{xyz} = U_{xy}V_z$ (b) $P_{xyz} = U_{xz}V_y$ (c) $P_{xyz} = U_{yz}V_x$

Figure 5.2: Possiblities for U in the factorization of P

are illustrated in Figure 5.2:

$$P_{xyz} = U_{xy}V_z \qquad U = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$$

$$P_{xyz} = U_{xz}V_y \qquad U = \begin{pmatrix} 1 & 1 & 0 \\ 0 & 1 & 1 \end{pmatrix}$$

$$P_{xyz} = U_{yz}V_x \qquad U = \begin{pmatrix} 0 & 1 & 1 \\ 1 & 1 & 0 \end{pmatrix}$$

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 substraction $(x-1)_i = x_i - 1$ for $i \in [n]$. Let

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

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

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

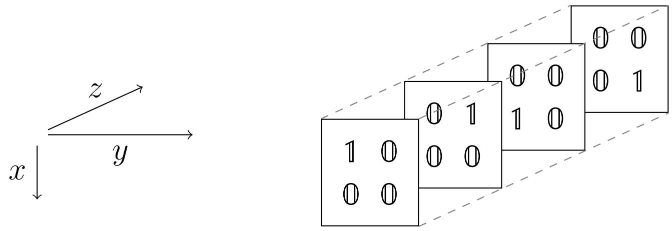


Figure 5.3: P for $F \in \mathbb{R}^2$ and $G \in \mathbb{R}^3$

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:

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

where $\boldsymbol{s_x}, \boldsymbol{s_y}, \boldsymbol{s_z} \in S^n$ 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 $\mathbb{0}$ and $\mathbb{1}$ 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. $\square$

6 Practical Results

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7 Discussion

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8 Conclusion

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List of Figures

3.1 Symbol graph for the example 12

5.1 P for $F \in \mathbb{R}^2$ and $G \in \mathbb{R}^3$ 29
5.2 Possiblities for U in the factorization of P 30
5.3 P for $F \in \mathbb{R}^2$ and $G \in \mathbb{R}^3$ 31

List of Tables

Selbständigkeitserklärung

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.

Jena, 21.07.2023