Convolutions Through the Lens of Tensor Networks

Felix Dangel

December 01, 2023

Convolutions ~~Through the Lens of Tensor Networks~~ as `einsum`

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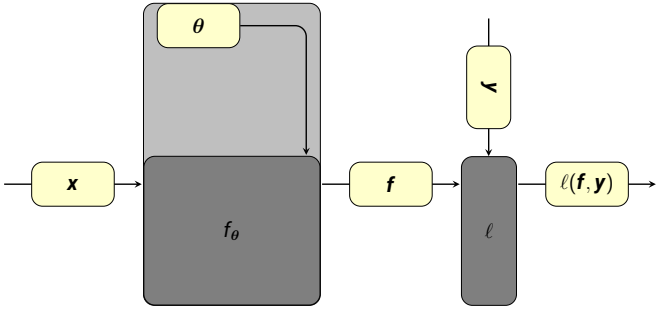
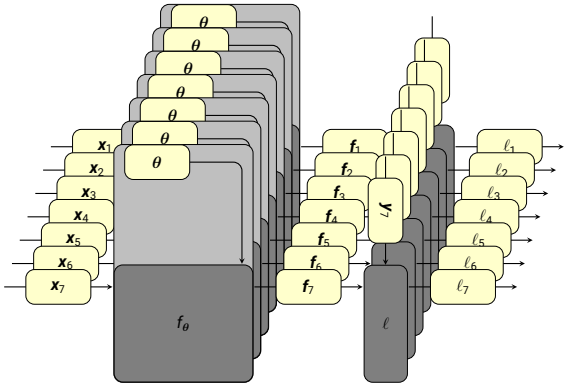
The Broader Picture

Supervised Deep Learning in a Nutshell (Math)



$$\ell(\boldsymbol{f}_{\boldsymbol{\theta}}(\boldsymbol{x}\ ), \boldsymbol{y}\ )$$

Supervised Deep Learning in a Nutshell (Math)



Minimize $\mathcal{L}_{\mathbb{D}}(\boldsymbol{\theta})$ with

$$\mathcal{L}_{\mathbb{D}}(\boldsymbol{\theta}) = \frac{1}{|\mathbb{D}|} \sum_{(\boldsymbol{x}_n, \boldsymbol{y}_n) \in \mathbb{D}} \ell(f_{\boldsymbol{\theta}}(\boldsymbol{x}_n), \boldsymbol{y}_n)$$

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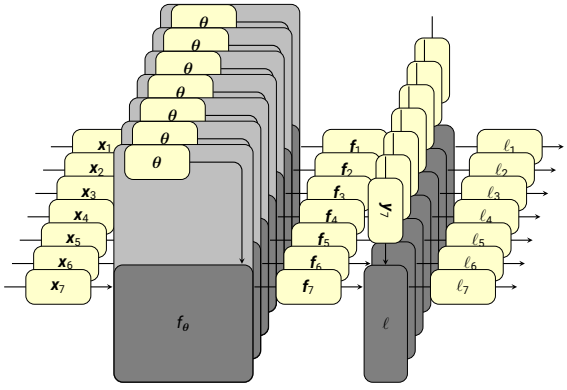

Minimize $\mathcal{L}_{\mathbb{D}}(\boldsymbol{\theta})$ with

$$\mathcal{L}_{\mathbb{B}}(\boldsymbol{\theta}) = \frac{1}{|\mathbb{B}|} \sum_{(\boldsymbol{x}_n, \boldsymbol{y}_n) \in \mathbb{B}} \ell(f_{\boldsymbol{\theta}}(\boldsymbol{x}_n), \boldsymbol{y}_n) \qquad \text{where} \qquad \mathbb{B} \sim \mathbb{D}\,,$$

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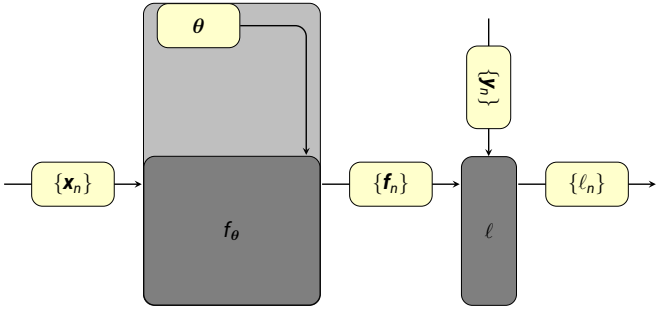

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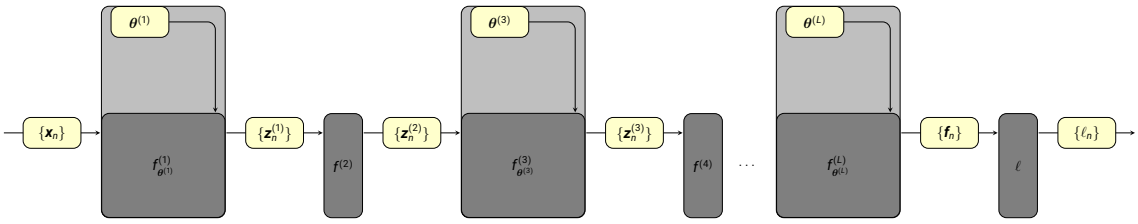

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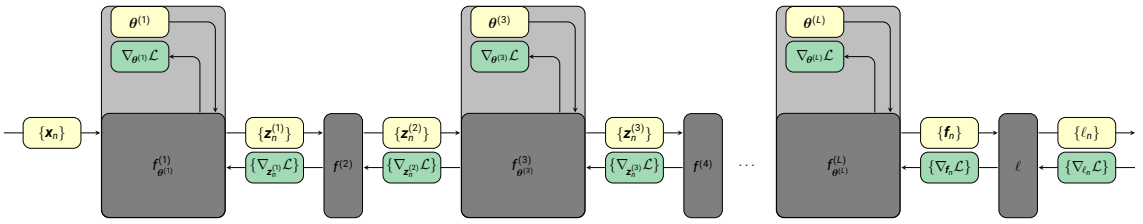
$$\mathbb{B} \sim \mathbb{D}\,,$$
$$\boldsymbol{f}_{\boldsymbol{\theta}} = f^{(L)}_{\boldsymbol{\theta}^{(L)}} \circ f^{(L-1)}_{\boldsymbol{\theta}^{(L-1)}} \circ \ldots \circ f^{(1)}_{\boldsymbol{\theta}^{(1)}}\,.$$

Supervised Deep Learning in a Nutshell (Math)



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Goal: Make Richer Information More Accessible

$$\nabla_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{\theta})$$

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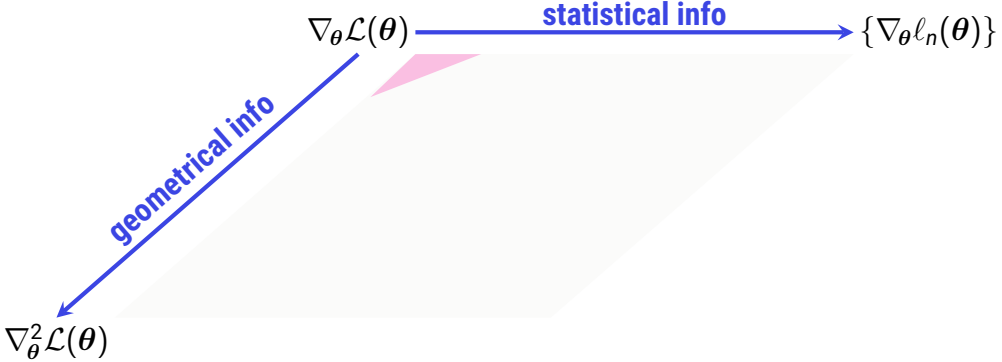
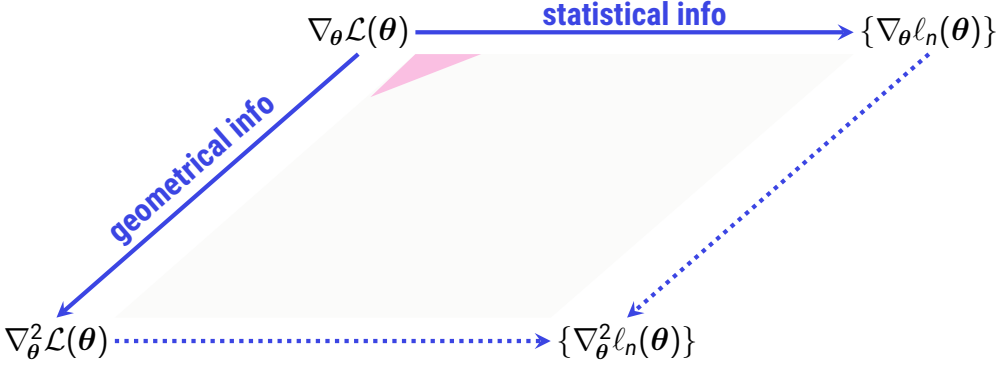


Goal: Make Richer Information More Accessible



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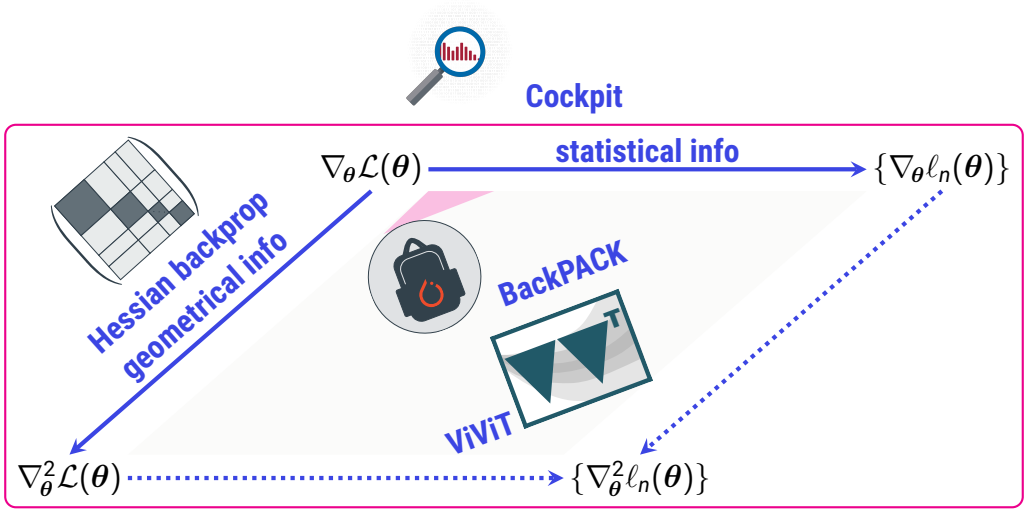
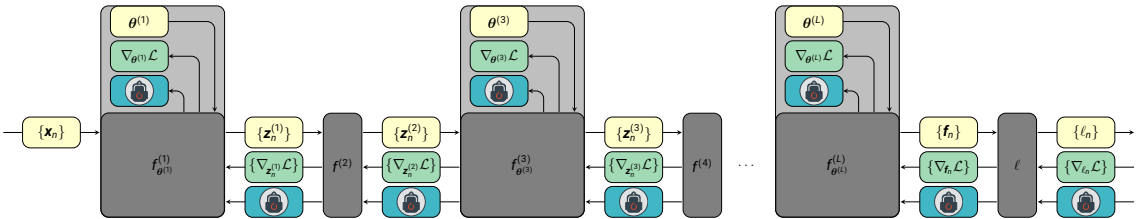


Customized Backpropagation

1. What to backpropagate
2. How to backpropagate
3. How to extract target quantity



Convolutions Are More Tedious than Linear Layers

- Personal example: Vector-Jacobian products (VJPs)

```python
def _weight_jac_t_mat_prod(
    self,
    module: Linear,
    g_inp: Tuple[Tensor],
    g_out: Tuple[Tensor],
    mat: Tensor,
    sum_batch: int = True,
    subsampling: List[int] = None,
) -> Tensor:
    """Batch-apply transposed Jacobian of the output w.r.t. the weight.

    Args:
        module: Linear layer.
        g_inp: Gradients w.r.t. module input. Not required by the implementation.
        g_out: Gradients w.r.t. module output. Not required by the implementation.
        mat: Batch of ``V`` vectors of same shape as the layer output
            (``[N, *, out_features]``) to which the transposed output-input Jacobian
            is applied. Has shape ``[V, N, *, out_features]`` if subsampling is not
            used, otherwise ``N`` must be ``len(subsampling)`` instead.
        sum_batch: Sum the result's batch axis. Default: ``True``.
        subsampling: Indices of samples along the output's batch dimension that
            should be considered. Defaults to ``None`` (use all samples).

    Returns:
        Batched transposed Jacobian vector products. Has shape
        ``[V, N, *module.weight.shape]`` when ``sum_batch`` is ``False``. With
        ``sum_batch=True``, has shape ``[V, *module.weight.shape]``. If sub-
        sampling is used, ``N`` must be ``len(subsampling)`` instead.
    """
    d_weight = subsample(module.input0, subsampling=subsampling)

    equation = f"vn...o,n...i->v{'' if sum_batch else 'n'}oi"
    return einsum(equation, mat, d_weight)
```

Convolutions Are More Tedious than Linear Layers

- Personal example: Vector-Jacobian products (VJPs)
- Other algorithmic & theoretical ideas

Concept	**for MLPs**	**for CNNs**
Approximate Hessian diagonal	1989	2023
Kronecker-factored curvature (KFAC, KFRA, KFLR)	2015, 2017, 2017	2016, 2020, 2020
Kronecker-factored quasi-Newton methods (KBFGS)	2021	2022
Neural tangent kernel (NTK)	2018	2019
Hessian rank	2021	2023

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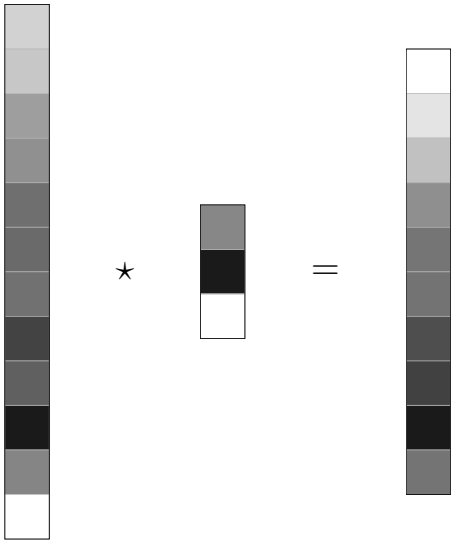
This talk: A simplifying perspective of convolutions through tensor networks

Convolutions — A Visual Walkthrough

A Simple Convolution

$\mathbf{Y} = \mathbf{X} \star \mathbf{W}$ with

- $\mathbf{X} \in \mathbb{R}^I$
- $\mathbf{W} \in \mathbb{R}^K$
- $\mathbf{Y} \in \mathbb{R}^O$



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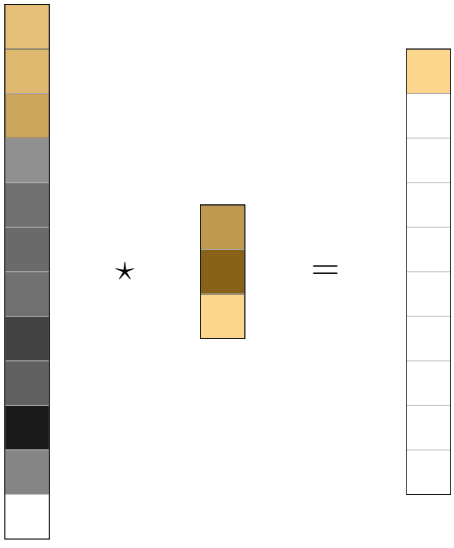

S is for Stride

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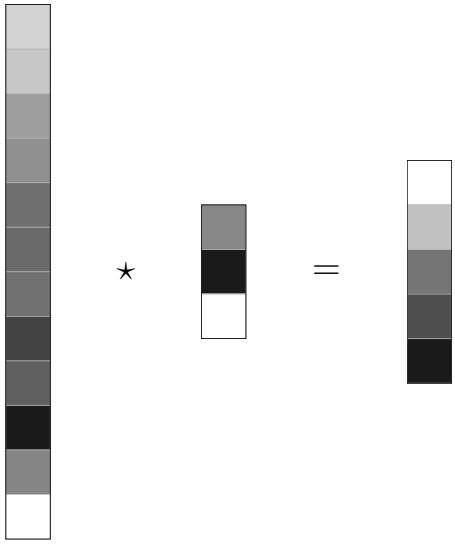

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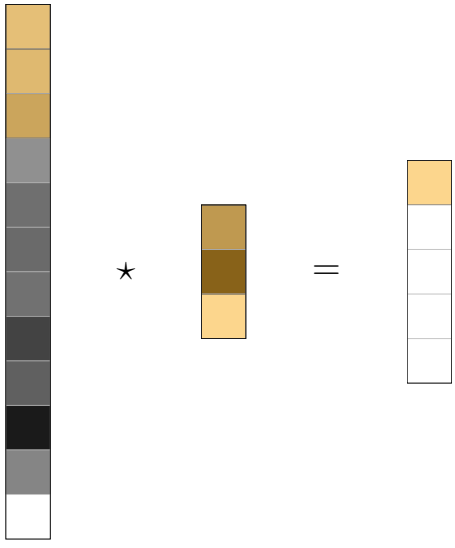

P is for Padding

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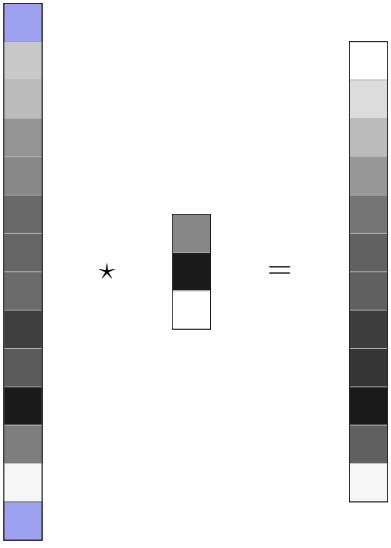

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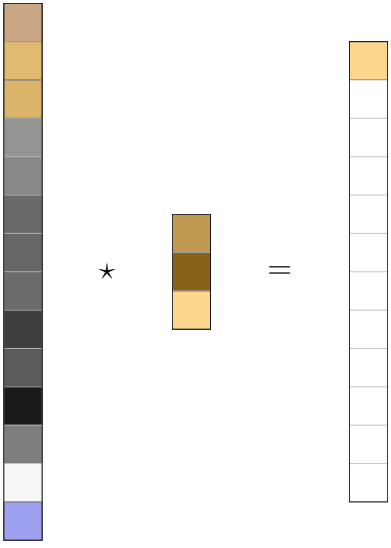

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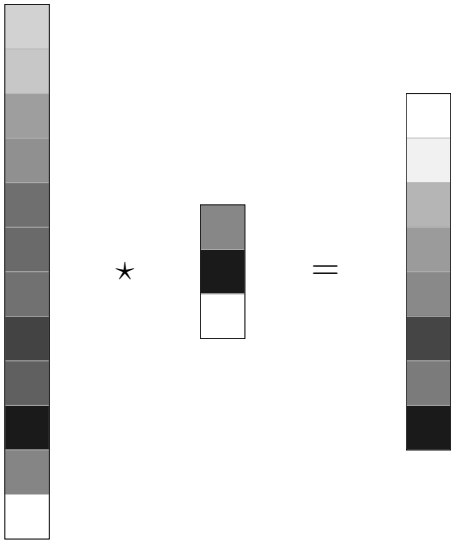

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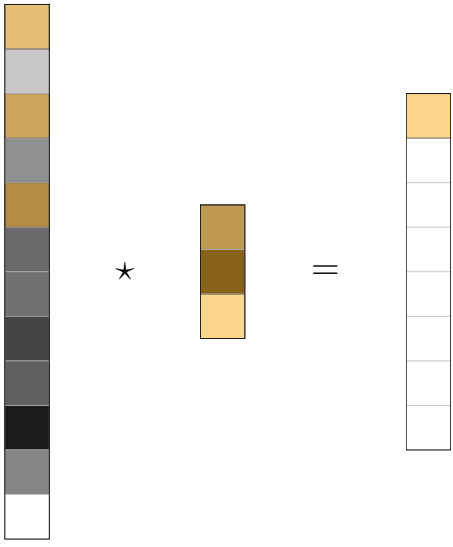

C_{in} is for Input Channels

$\mathbf{Y} = \mathbf{X} \star \mathbf{W}$ with

- $\mathbf{X} \in \mathbb{R}^{C_{\text{in}} \times I}$
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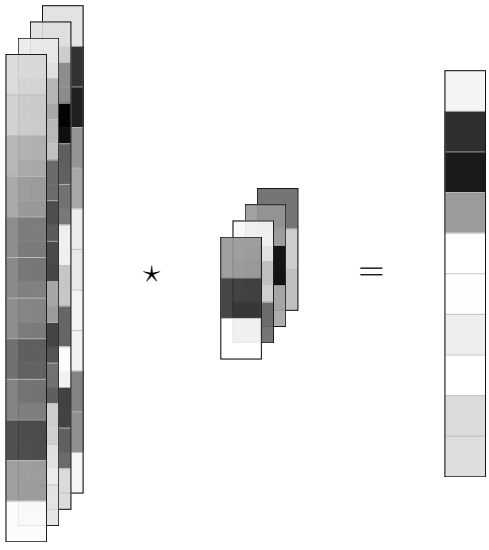

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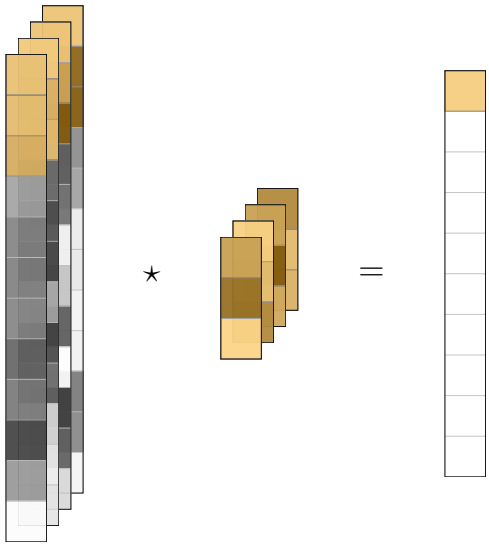

C_{out} is for Output Channels

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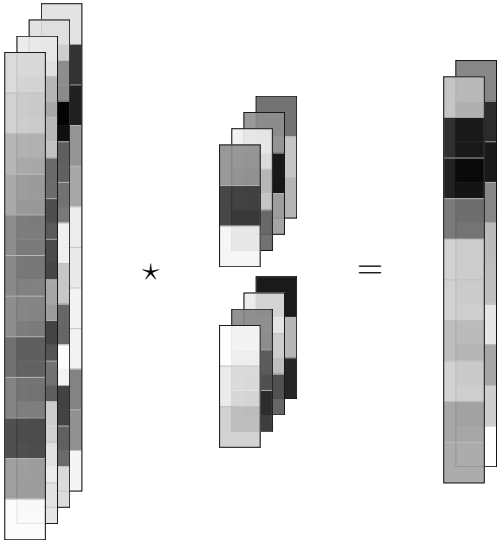

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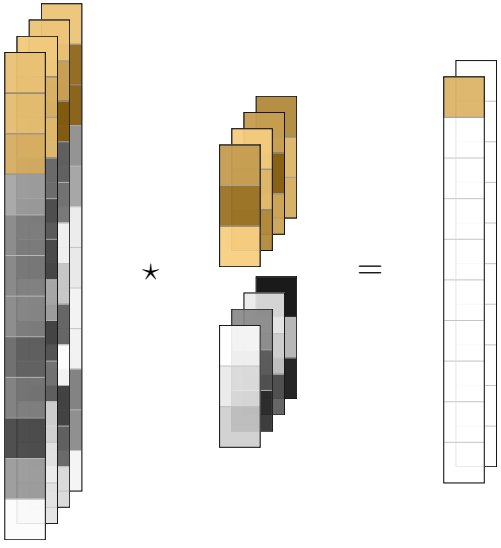

G is for Groups

$\mathbf{Y} = \mathbf{X} \star \mathbf{W}$ with

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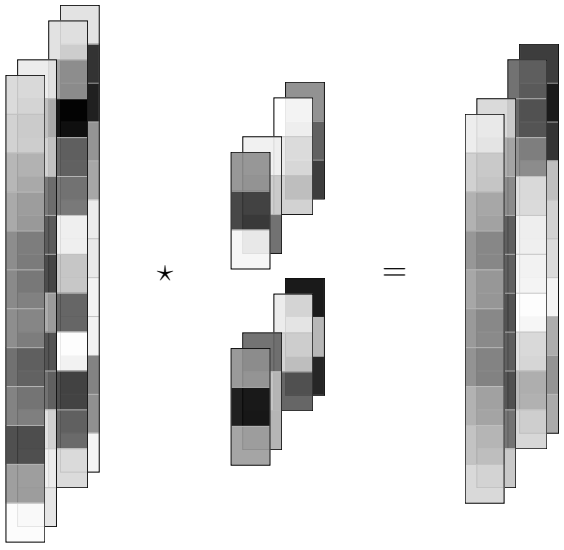

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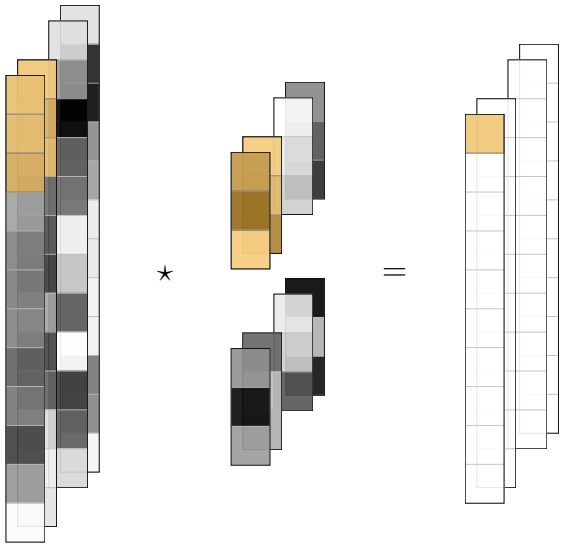

N is for Batch Size

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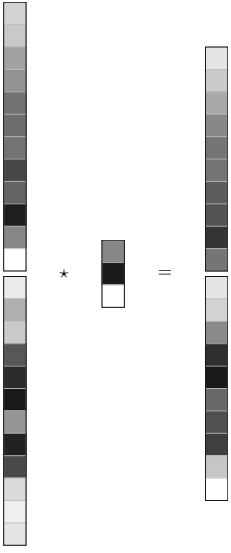

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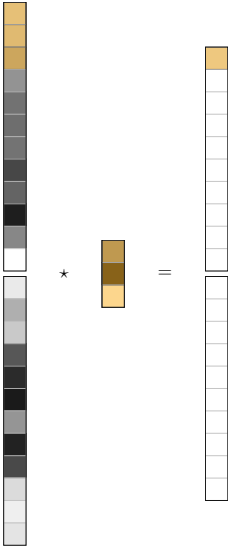

Putting Everything Together in One Dimension...

$\mathbf{Y} = \mathbf{X} \star \mathbf{W}$ with

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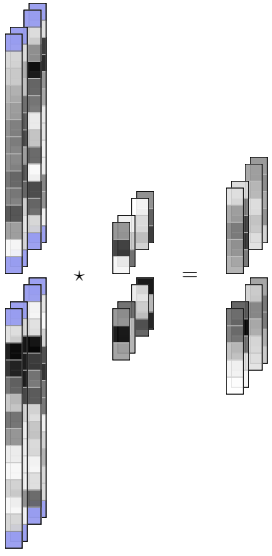

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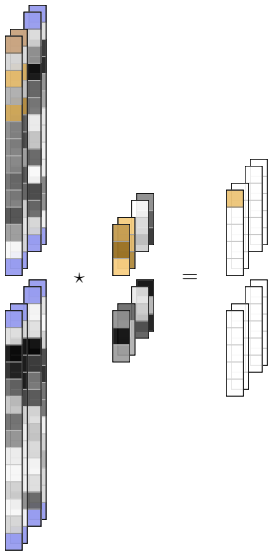
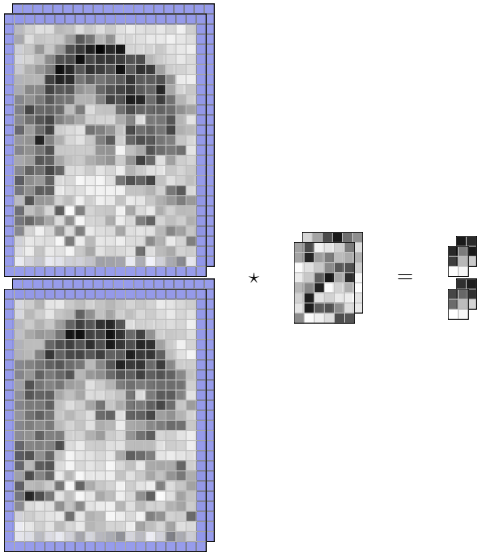


. . . and in Two Dimensions

$\mathbf{Y} = \mathbf{X} \star \mathbf{W}$ with

- $\mathbf{X} \in \mathbb{R}^{N \times C_{\text{in}} \times I_1 \times I_2}$
- $\mathbf{W} \in \mathbb{R}^{C_{\text{out}} \times C_{\text{in}}/G \times K_1 \times K_2}$
- $\mathbf{Y} \in \mathbb{R}^{N \times C_{\text{out}} \times O_1 \times O_2}$



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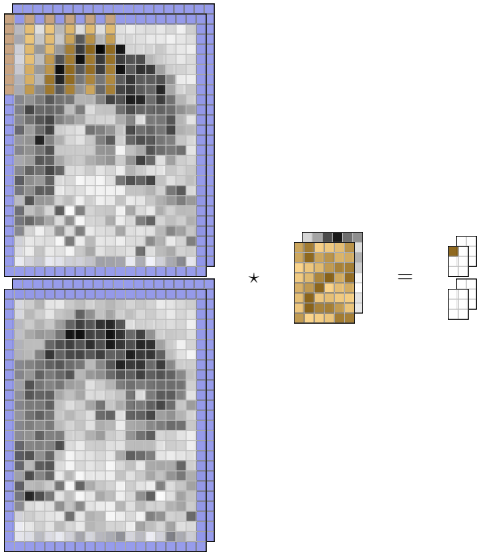

Tensor Multiplication & Tensor Networks

Tensor Multiplication Unifies Vector & Matrix Multiplications

(Disclaimer: Tensor = multi-dimensional array; sorry)

Tensor Multiplication Unifies Vector & Matrix Multiplications

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Consider two vectors $\boldsymbol{a}, \boldsymbol{b}$

Product	**Notation**
Inner	$c = \boldsymbol{a}^\top \boldsymbol{b}$
Element-wise	$\boldsymbol{c} = \boldsymbol{a} \odot \boldsymbol{b}$
Outer/Kronecker	$\boldsymbol{C} = \boldsymbol{a}\boldsymbol{b}^\top = \boldsymbol{a} \otimes \boldsymbol{b}^\top$

Tensor Multiplication Unifies Vector & Matrix Multiplications

(Disclaimer: Tensor = multi-dimensional array; sorry)

Consider two vectors $\boldsymbol{a}, \boldsymbol{b}$

Product	**Notation**	**Index notation**
Inner	$c = \boldsymbol{a}^\top \boldsymbol{b}$	$c = \sum_i a_i b_i$
Element-wise	$\boldsymbol{c} = \boldsymbol{a} \odot \boldsymbol{b}$	$c_i = a_i b_i$
Outer/Kronecker	$\boldsymbol{C} = \boldsymbol{a}\boldsymbol{b}^\top = \boldsymbol{a} \otimes \boldsymbol{b}^\top$	$C_{i,j} = a_i b_j$

Tensor Multiplication Unifies Vector & Matrix Multiplications

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Consider two vectors $\boldsymbol{a}, \boldsymbol{b}$ and two matrices $\boldsymbol{A}, \boldsymbol{B}$

Product	**Notation**	**Index notation**
Inner	$c = \boldsymbol{a}^\top \boldsymbol{b}$	$c = \sum_i a_i b_i$
Element-wise	$\boldsymbol{c} = \boldsymbol{a} \odot \boldsymbol{b}$	$c_i = a_i b_i$
Outer/Kronecker	$\boldsymbol{C} = \boldsymbol{a}\boldsymbol{b}^\top = \boldsymbol{a} \otimes \boldsymbol{b}^\top$	$C_{i,j} = a_i b_j$
Inner	$\boldsymbol{C} = \boldsymbol{A}\boldsymbol{B}$	
Element-wise	$\boldsymbol{C} = \boldsymbol{A} \odot \boldsymbol{B}$	
Kronecker	$\boldsymbol{C} = \boldsymbol{A} \otimes \boldsymbol{B}$	

Tensor Multiplication Unifies Vector & Matrix Multiplications

(Disclaimer: Tensor = multi-dimensional array; sorry)

Consider two vectors $\boldsymbol{a}, \boldsymbol{b}$ and two matrices $\boldsymbol{A}, \boldsymbol{B}$

Product	**Notation**	**Index notation**
Inner	$c = \boldsymbol{a}^\top \boldsymbol{b}$	$c = \sum_i a_i b_i$
Element-wise	$\boldsymbol{c} = \boldsymbol{a} \odot \boldsymbol{b}$	$c_i = a_i b_i$
Outer/Kronecker	$\boldsymbol{C} = \boldsymbol{a}\boldsymbol{b}^\top = \boldsymbol{a} \otimes \boldsymbol{b}^\top$	$C_{i,j} = a_i b_j$
Inner	$\boldsymbol{C} = \boldsymbol{A}\boldsymbol{B}$	$C_{i,k} = \sum_j A_{i,j} B_{j,k}$
Element-wise	$\boldsymbol{C} = \boldsymbol{A} \odot \boldsymbol{B}$	$C_{i,j} = A_{i,j} B_{i,j}$
Kronecker	$\boldsymbol{C} = \boldsymbol{A} \otimes \boldsymbol{B}$	$C_{(i,k),(j,l)} = A_{i,j} B_{k,l}$

Tensor Multiplication Unifies Vector & Matrix Multiplications

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Consider two vectors $\boldsymbol{a}, \boldsymbol{b}$ and two matrices $\boldsymbol{A}, \boldsymbol{B}$

Product	**Notation**	**Index notation**	**In**	**Out**
Inner	$c = \boldsymbol{a}^\top \boldsymbol{b}$	$c = \sum_i a_i b_i$	$(i), (i)$	$()$
Element-wise	$\boldsymbol{c} = \boldsymbol{a} \odot \boldsymbol{b}$	$c_i = a_i b_i$	$(i), (i)$	(i)
Outer/Kronecker	$\boldsymbol{C} = \boldsymbol{a}\boldsymbol{b}^\top = \boldsymbol{a} \otimes \boldsymbol{b}^\top$	$C_{i,j} = a_i b_j$	$(i), (j)$	(i,j)
Inner	$\boldsymbol{C} = \boldsymbol{A}\boldsymbol{B}$	$C_{i,k} = \sum_j A_{i,j} B_{j,k}$	$(i,j), (j,k)$	(i,k)
Element-wise	$\boldsymbol{C} = \boldsymbol{A} \odot \boldsymbol{B}$	$C_{i,j} = A_{i,j} B_{i,j}$	$(i,j), (i,j)$	(i,j)
Kronecker	$\boldsymbol{C} = \boldsymbol{A} \otimes \boldsymbol{B}$	$C_{(i,k),(j,l)} = A_{i,j} B_{k,l}$	$(i,j), (k,l)$	$((i,k),(j,l))$

We can infer the summations given the index signature

A Mathematical Definition of Tensor Multiplication [e.g. Laue et al., 2020]

Given two tensors $\mathbf{A}, \mathbf{B}$ with index tuples $S_\mathbf{A}, S_\mathbf{B}$

$$\mathbf{C} := *_{(S_\mathbf{A}, S_\mathbf{B}, S_\mathbf{C})}(\mathbf{A}, \mathbf{B}) \quad \Leftrightarrow \quad [\mathbf{C}]_{S_\mathbf{C}} = \sum_{(S_\mathbf{A} \cup S_\mathbf{B}) \setminus S_\mathbf{C}} [\mathbf{A}]_{S_\mathbf{A}} [\mathbf{B}]_{S_\mathbf{B}} \,,$$

indices not present in the output are summed out; $S_\mathbf{C}$ satisfies $S_\mathbf{C} \subseteq S_\mathbf{A} \cup S_\mathbf{B}$.

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[Example] Matrix-matrix multiplication $\boldsymbol{C} = \boldsymbol{AB}$ as tensor multiplication

$$\begin{aligned} S_A &= (i, j) \\ S_B &= (j, k) \\ S_C &= (i, k) \end{aligned}$$

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$$\Longrightarrow \boldsymbol{C} = *_{((i,j),(j,k),(i,k))}(\boldsymbol{A}, \boldsymbol{B}), \qquad \text{or} \qquad \texttt{C = einsum("ij,jk->ik", A, B).}$$

Many libraries provide $*_{(\ldots)}(\ldots)$ as `einsum`.

A Mathematical Definition of Tensor Multiplication [e.g. Laue et al., 2020]

General case: Given N tensors $\mathbf{A}_1, \ldots, \mathbf{A}_N$ with index tuples $S_{\mathbf{A}_1}, \ldots, S_{\mathbf{A}_N}$

$$\mathbf{C} := *_{(S_{\mathbf{A}_1}, \ldots, S_{\mathbf{A}_N}, S_{\mathbf{C}})}(\mathbf{A}_1, \ldots, \mathbf{A}_N) \quad \Leftrightarrow \quad [\mathbf{C}]_{S_{\mathbf{C}}} = \sum_{(S_{\mathbf{A}_1} \cup \cdots \cup S_{\mathbf{A}_N}) \setminus S_{\mathbf{C}}} [\mathbf{A}_1]_{S_{\mathbf{A}_1}} \cdots [\mathbf{A}_N]_{S_{\mathbf{A}_N}},$$

indices not present in the output are summed out; $S_{\mathbf{C}}$ satisfies $S_{\mathbf{C}} \subseteq S_{\mathbf{A}_1} \cup \cdots \cup S_{\mathbf{A}_N}$.

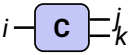
[Example] Matrix-matrix multiplication $\boldsymbol{C} = \boldsymbol{AB}$ as tensor multiplication

$$\begin{aligned} S_{\boldsymbol{A}} &= (i,j) \\ S_{\boldsymbol{B}} &= (j,k) \\ S_{\boldsymbol{C}} &= (i,k) \end{aligned} \quad \Longrightarrow \quad (S_{\boldsymbol{A}} \cup S_{\boldsymbol{B}}) \setminus S_{\boldsymbol{C}} = (i,j,k) \setminus (i,k) = (j)$$

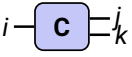
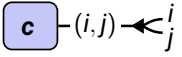
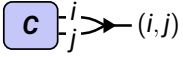
$\Longrightarrow \boldsymbol{C} = *_{((i,j),(j,k),(i,k))}(\boldsymbol{A}, \boldsymbol{B})$, or `C = einsum("ij,jk->ik", A, B).`

Many libraries provide $*_{(\ldots)}(\ldots)$ as `einsum`.

Tensor Networks: Graphical Notation for Tensor Multiplications

Operation	Diagram
Scalar	
Vector	
Matrix	
Tensor	

Tensor Networks: Graphical Notation for Tensor Multiplications

Operation	Diagram
Scalar	
Vector	
Matrix	
Tensor	
Matricize	
Flatten	

Tensor Networks: Graphical Notation for Tensor Multiplications

Operation	Diagram
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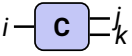
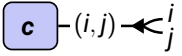
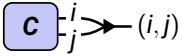
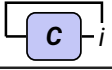
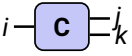
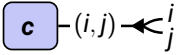
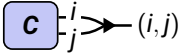
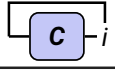
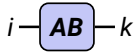
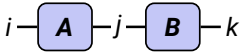
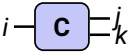
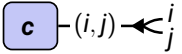
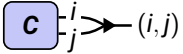
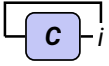
Vector	
Matrix	
Tensor	
Matricize	
Flatten	
Trace	

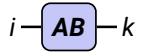
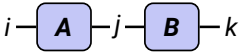
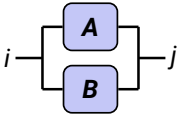
Tensor Networks: Graphical Notation for Tensor Multiplications

Operation	Diagram
Scalar	
Vector	
Matrix	
Tensor	
Matricize	
Flatten	
Trace	

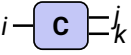
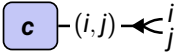
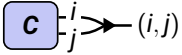
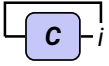
Operation	Diagram
	

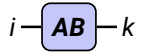
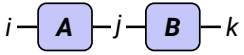
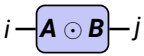
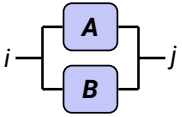
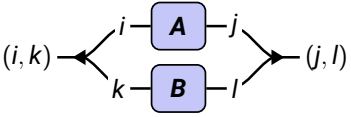
Tensor Networks: Graphical Notation for Tensor Multiplications

Operation	Diagram
Scalar	
Vector	
Matrix	
Tensor	
Matricize	
Flatten	
Trace	

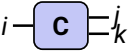
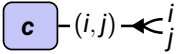
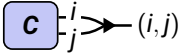
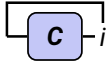
Operation	Diagram
	
	

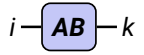
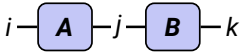
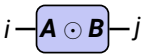
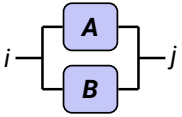
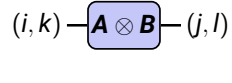
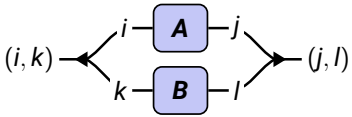
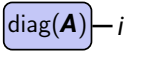
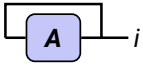
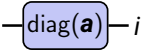
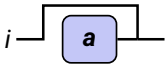
Tensor Networks: Graphical Notation for Tensor Multiplications

Operation	Diagram
Scalar	
Vector	
Matrix	
Tensor	
Matricize	
Flatten	
Trace	

Operation	Diagram
	
	
	

Tensor Networks: Graphical Notation for Tensor Multiplications

Operation	Diagram
Scalar	
Vector	
Matrix	
Tensor	
Matricize	
Flatten	
Trace	

Operation	Diagram
	
	
	
	
	

Benefits of TN/`einsum` Abstraction

Improved `einsum` Syntax: `einops` [Rogozhnikov, 2022, ICLR]

Powerful syntax extensions: multi-letter indices, index (un-)grouping, . . .

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[Example] Batched matrix-matrix multiplication

Given $\{\boldsymbol{A}_n\}_{n=1}^N$, $\{\boldsymbol{B}_n\}_{n=1}^N$, compute $\{\boldsymbol{C}_n\}_{n=1}^N = \{\boldsymbol{A}_n\boldsymbol{B}_n\}_{n=1}^N$

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C = einsum(A, B, "batch i j, batch j k -> batch i k")
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```
C = einsum(A, B, "batch i j, batch j k -> batch i k")
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[Example] Improved readability (from an ICLR 2024 submission)

```
x = x.unfold(2, kernel_size[0], stride[0])
x = x.unfold(3, kernel_size[1], stride[1])
x = x.transpose_(1, 2).transpose_(2, 3)
return torch.mean(
    x.reshape((x.size(0), x.size(1), x.size(2), groups, -1, x.size(4), x.size(5))),
    3,
).view(x.size(0), x.size(1), x.size(2), -1)
```

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```
C = einsum(A, B, "batch i j, batch j k -> batch i k")
```

[Example] Improved readability (from an ICLR 2024 submission)

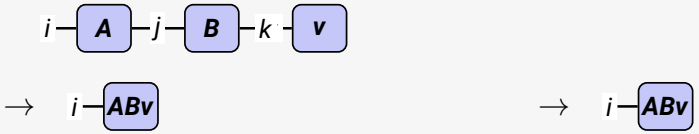
```
# average channel groups
x = rearrange(x, "b (g c_in) i1 i2 -> b g c_in i1 i2", g=groups)
x = reduce(x, "b g c_in i1 i2 -> b c_in i1 i2", "mean")

x_unfold = F.unfold(x, kernel_size, dilation=dilation, padding=padding, stride=stride)
return rearrange(x_unfold, "b c_in_k1_k2 o1_o2 -> b o1_o2 c_in_k1_k2")
```

Contraction Path Optimization (e.g. `opt_einsum` [Smith and Gray, 2018])

[Example] Matrix-matrix-vector-product

Consider $\boldsymbol{A}, \boldsymbol{B} \in \mathbb{R}^{3.000 \times 3.000}$ and $\boldsymbol{v} \in \mathbb{R}^{3.000}$.



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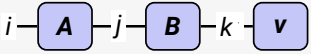

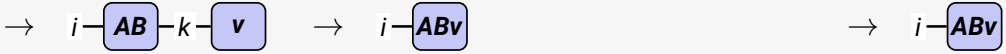

Schedule 1:

```
A @ B @ v
```

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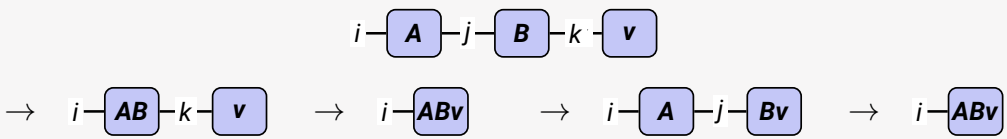

Schedule 1:

```
A @ B @ v
```

Schedule 2:

```
A @ (B @ v)
```

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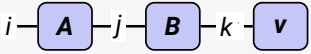

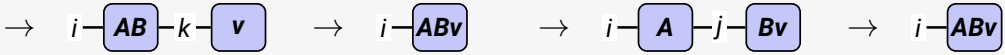

Schedule 1: **1.1 s**

```
A @ B @ v
```

Schedule 2: **2.2 ms**

```
A @ (B @ v)
```

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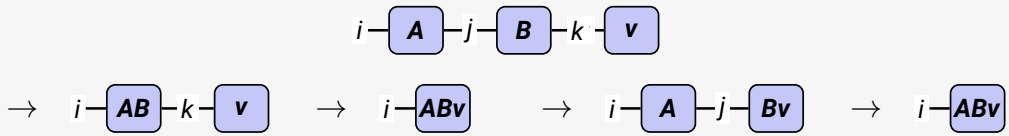

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```
A @ B @ v
```

Schedule 2: **2.2 ms**

```
A @ (B @ v)
```

```
einsum("ij,jk,k->i", A, B, v)
```

Contraction Path Optimization (e.g. `opt_einsum` [Smith and Gray, 2018])

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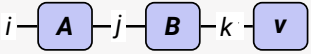

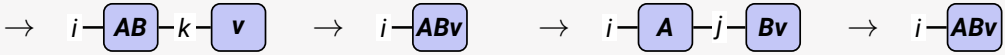

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```

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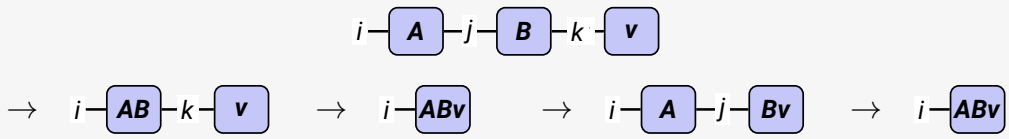

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Schedule 2: **2.2 ms**

```
A @ (B @ v)
```

PyTorch: **1.1 s**

with update + `pip install opt_einsum`, **2.3 ms**

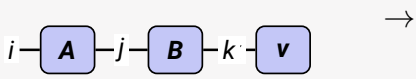
```
einsum("ij,jk,k->i", A, B, v)
```

Order matters; `einsum` automatically finds a 'good' schedule.

Function Transformations with Tensor Networks

[Example] Batching/`vmap`-ing: adding legs

$$(\boldsymbol{A}, \boldsymbol{B}, \boldsymbol{v}) \mapsto \boldsymbol{ABv}$$

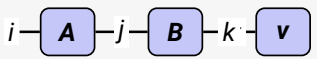


$\rightarrow$

Function Transformations with Tensor Networks

[Example] Batching/`vmap`-ing: adding legs

$$(\boldsymbol{A}, \boldsymbol{B}, \boldsymbol{v}) \mapsto \boldsymbol{A}\boldsymbol{B}\boldsymbol{v} \qquad \{(\boldsymbol{A}_n, \boldsymbol{B}_n, \boldsymbol{v}_n)\}_{n=1}^{N} \mapsto \{\boldsymbol{A}_n \boldsymbol{B}_n \boldsymbol{v}_n\}_{n=1}^{N}$$



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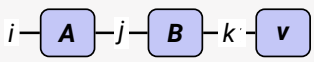

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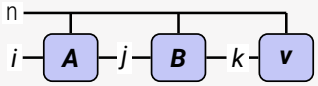

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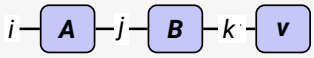

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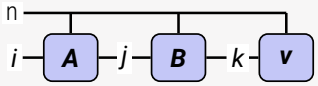
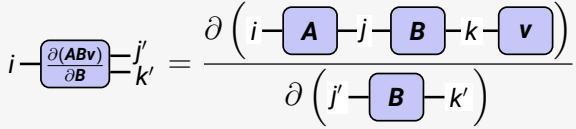


[Example] Differentiation: removing arguments



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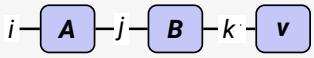

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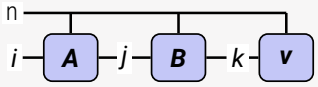

[Example] Differentiation: removing arguments

$$\boldsymbol{i} \text{ — } \boxed{\frac{\partial(\boldsymbol{ABv})}{\partial \boldsymbol{B}}} \text{ — } \begin{matrix} j' \\ k' \end{matrix} = \frac{\partial \left(\boldsymbol{i} \text{ — } \boxed{\boldsymbol{A}} \text{ — } \boldsymbol{j} \text{ — } \boxed{\boldsymbol{B}} \text{ — } \boldsymbol{k} \text{ — } \boxed{\boldsymbol{v}} \right)}{\partial \left(\boldsymbol{j}' \text{ — } \boxed{\boldsymbol{B}} \text{ — } \boldsymbol{k}' \right)} = \boldsymbol{i} \text{ — } \boxed{\boldsymbol{A}} \text{ — } \boldsymbol{j}' \qquad \boldsymbol{k}' \text{ — } \boxed{\boldsymbol{v}}$$

Function Transformations with Tensor Networks

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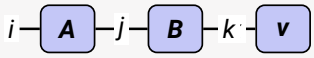

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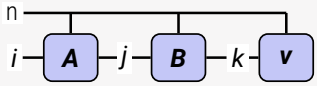

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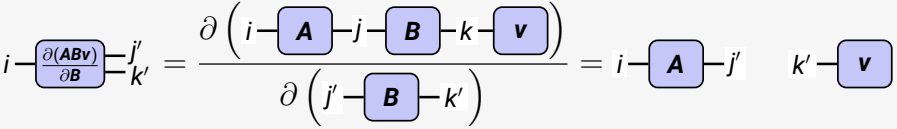

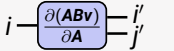

Function Transformations with Tensor Networks

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$$i \;\boxed{\frac{\partial(\boldsymbol{ABv})}{\partial \boldsymbol{B}}}\; \begin{matrix} j' \\ k' \end{matrix} = \frac{\partial \left(i \;\boxed{\boldsymbol{A}}\; j \;\boxed{\boldsymbol{B}}\; k \;\boxed{\boldsymbol{v}} \right)}{\partial \left(j' \;\boxed{\boldsymbol{B}}\; k' \right)} = i \;\boxed{\boldsymbol{A}}\; j' \qquad k' \;\boxed{\boldsymbol{v}}$$

$$i \;\boxed{\frac{\partial(\boldsymbol{ABv})}{\partial \boldsymbol{A}}}\; \begin{matrix} i' \\ j' \end{matrix} = \frac{\partial \left(i \;\boxed{\boldsymbol{I}}\; I \;\boxed{\boldsymbol{A}}\; j \;\boxed{\boldsymbol{Bv}} \right)}{\partial \left(i' \;\boxed{\boldsymbol{A}}\; j' \right)}$$

Function Transformations with Tensor Networks

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$$i \boxed{\frac{\partial(\boldsymbol{ABv})}{\partial \boldsymbol{B}}} j' \\ \qquad\quad k' = \frac{\partial\left(i \boxed{\boldsymbol{A}} j \boxed{\boldsymbol{B}} k \boxed{\boldsymbol{v}}\right)}{\partial\left(j' \boxed{\boldsymbol{B}} k'\right)} = i \boxed{\boldsymbol{A}} j' \qquad k' \boxed{\boldsymbol{v}}$$

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- Randomized/Approximate evaluation (somebody should do this!)

Also (regarding tensor networks)

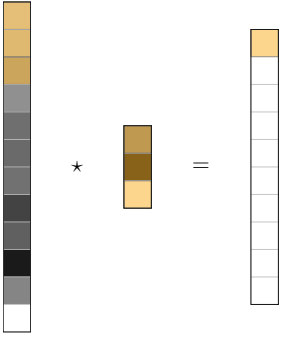
- Drawing diagrams is more fun
- Simplifications/Transformations via graphical manipulations

Convolutions as Tensor Networks

Convolution as Matrix Multiplication

$$\mathbf{X} \in \mathbb{R}^{C_{\text{in}} \times I}$$
$$\mathbf{Y} \in \mathbb{R}^{C_{\text{out}} \times O}$$
$$\mathbf{W} \in \mathbb{R}^{C_{\text{out}} \times C_{\text{in}} \times K}$$

$$\mathbf{Y} = \mathbf{X} \star \mathbf{W}$$

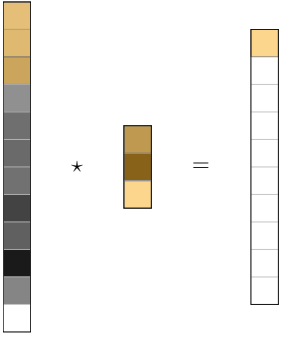


$$\boldsymbol{Y} = \boldsymbol{W}[\![\boldsymbol{X}]\!]$$

Convolution as Matrix Multiplication

$$\begin{aligned} \mathbf{X} &\in \mathbb{R}^{C_{\text{in}} \times I} \\ \mathbf{Y} &\in \mathbb{R}^{C_{\text{out}} \times O} \\ \mathbf{W} &\in \mathbb{R}^{C_{\text{out}} \times C_{\text{in}} \times K} \end{aligned}$$

$$\mathbf{Y} = \mathbf{X} \star \mathbf{W}$$



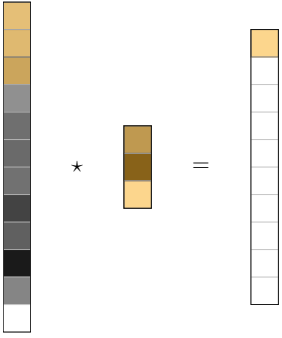
$$\begin{aligned} [\![\mathbf{X}]\!] &\in \mathbb{R}^{C_{\text{in}} K \times O} \\ \mathbf{Y} &\in \mathbb{R}^{C_{\text{out}} \times O} \\ \boldsymbol{W} &\in \mathbb{R}^{C_{\text{out}} \times C_{\text{in}} K} \end{aligned}$$

$$\boldsymbol{Y} = \boldsymbol{W}[\![\boldsymbol{X}]\!]$$

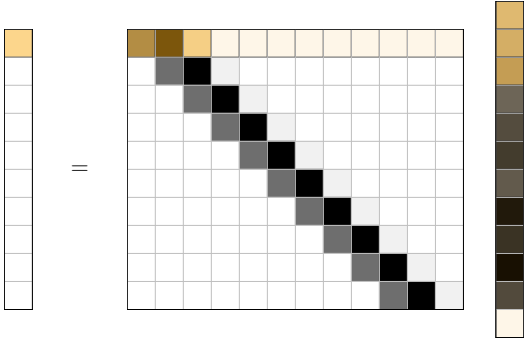
Convolution as Structured Matrix Multiplication

$$\mathbf{X} \in \mathbb{R}^{C_{\text{in}} \times I}$$
$$\mathbf{Y} \in \mathbb{R}^{C_{\text{out}} \times O}$$
$$\mathbf{W} \in \mathbb{R}^{C_{\text{out}} \times C_{\text{in}} \times K}$$

$$\mathbf{Y} = \mathbf{X} \star \mathbf{W}$$



$$\boldsymbol{y} = \boldsymbol{A}(\mathbf{W})\boldsymbol{x}$$



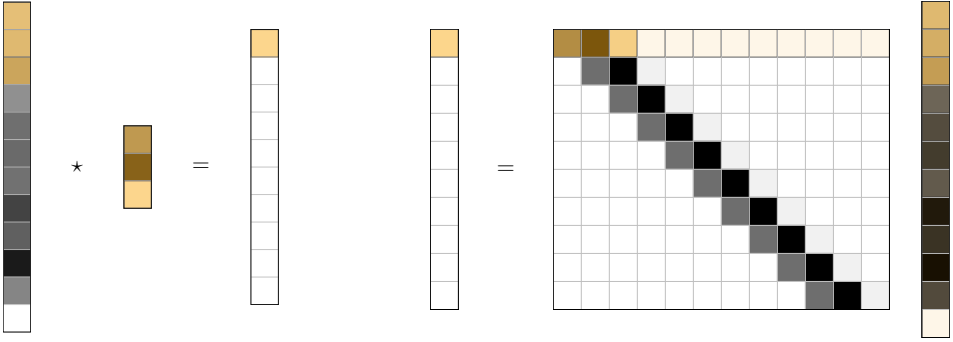
Convolution as Structured Matrix Multiplication

$$\mathbf{X} \in \mathbb{R}^{C_{\text{in}} \times I}$$
$$\mathbf{Y} \in \mathbb{R}^{C_{\text{out}} \times O}$$
$$\mathbf{W} \in \mathbb{R}^{C_{\text{out}} \times C_{\text{in}} \times K}$$

$$\boldsymbol{x} \in \mathbb{R}^{C_{\text{in}} I}$$
$$\boldsymbol{y} \in \mathbb{R}^{C_{\text{out}} O}$$
$$\boldsymbol{A}(\mathbf{W}) \in \mathbb{R}^{C_{\text{out}} O \times C_{\text{in}} I}$$

$$\mathbf{Y} = \mathbf{X} \star \mathbf{W}$$

$$\boldsymbol{y} = \boldsymbol{A}(\mathbf{W})\boldsymbol{x}$$



Convolution as Tensor Network [Hayashi et al., 2019]

$$Y_{c_{\text{out}},o} = \sum_{c_{\text{in}},k} X_{c_{\text{in}},i} \qquad W_{c_{\text{out}},c_{\text{in}},k}$$

Convolution as Tensor Network [Hayashi et al., 2019]

$$Y_{c_{\text{out}},o} = \sum_{c_{\text{in}},k} X_{c_{\text{in}},i(k,o)} W_{c_{\text{out}},c_{\text{in}},k}$$

Convolution as Tensor Network [Hayashi et al., 2019]

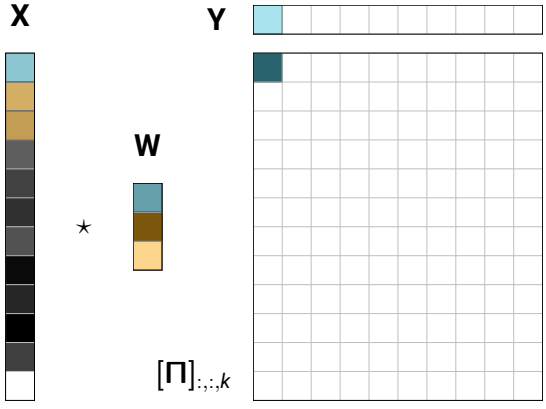
Index pattern $\Pi(I, K, S, P, D)$ captures the convolution's connectivity

$$
\begin{aligned}
Y_{c_{\text{out}},o} &= \sum_{c_{\text{in}},k} X_{c_{\text{in}},i(k,o)} W_{c_{\text{out}},c_{\text{in}},k} \\
&= \sum_{c_{\text{in}},k} \sum_{i} X_{c_{\text{in}},i} \Pi_{i,o,k} W_{c_{\text{out}},c_{\text{in}},k}
\end{aligned}
$$

Convolution as Tensor Network [Hayashi et al., 2019]

Index pattern $\Pi(I, K, S, P, D)$ captures the convolution's connectivity

$$Y_{c_{\text{out}},o} = \sum_{c_{\text{in}},k} X_{c_{\text{in}},i(k,o)} W_{c_{\text{out}},c_{\text{in}},k}$$
$$= \sum_{c_{\text{in}},k} \sum_{i} X_{c_{\text{in}},i} \Pi_{i,o,k} W_{c_{\text{out}},c_{\text{in}},k}$$

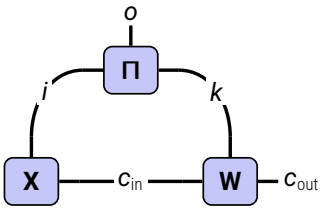


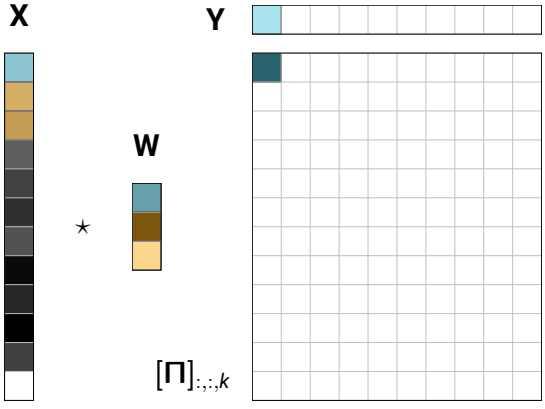
Convolution as Tensor Network [Hayashi et al., 2019]

Index pattern $\Pi(I, K, S, P, D)$ captures the convolution's connectivity

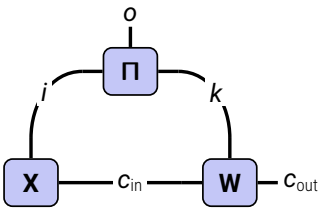
$$Y_{c_{\text{out}},o} = \sum_{c_{\text{in}},k} X_{c_{\text{in}},i(k,o)} W_{c_{\text{out}},c_{\text{in}},k}$$

$$= \sum_{c_{\text{in}},k} \sum_{i} X_{c_{\text{in}},i} \Pi_{i,o,k} W_{c_{\text{out}},c_{\text{in}},k}$$



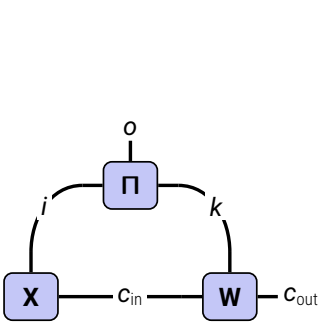


Higher-dimensional Convolutions [Hayashi et al., 2019]

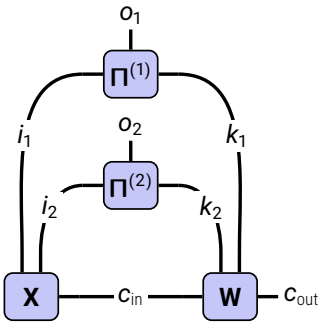


1d

Higher-dimensional Convolutions [Hayashi et al., 2019]

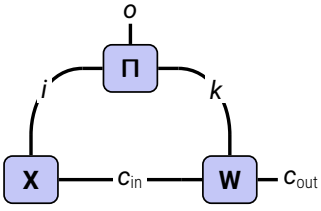


1d

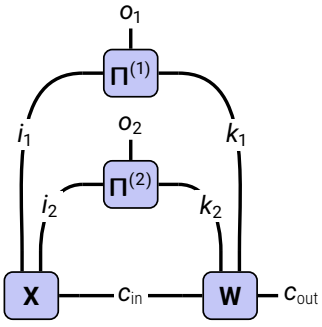


2d

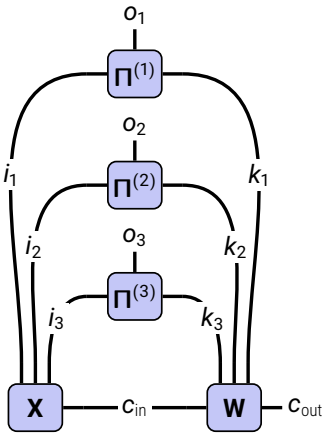
Higher-dimensional Convolutions [Hayashi et al., 2019]



1d

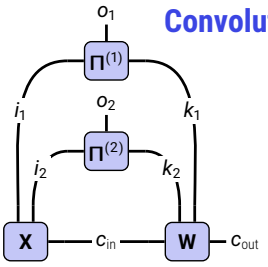


2d



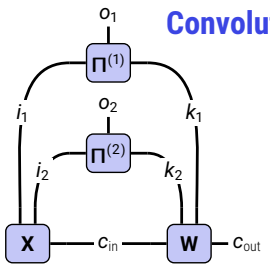
3d

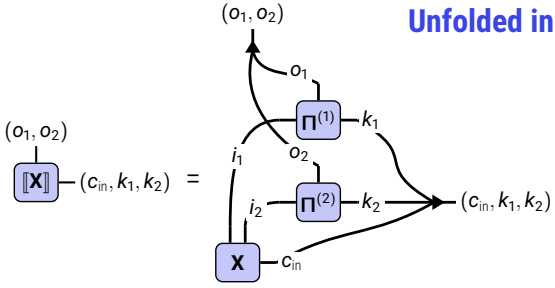
Connection to Matrix-multiplication Perspective



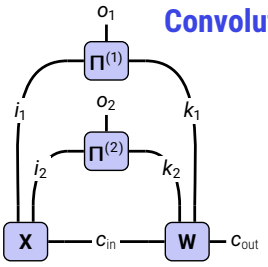
Convolution

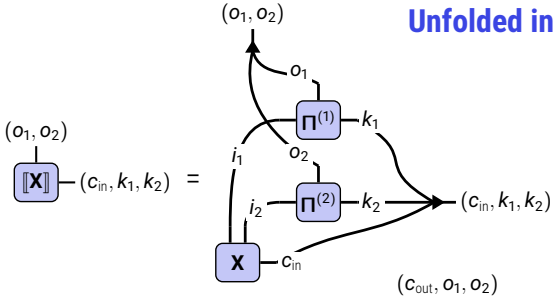
Connection to Matrix-multiplication Perspective

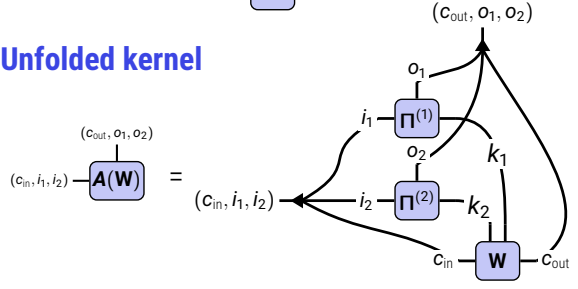




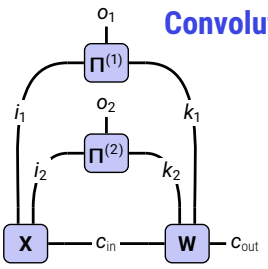
Connection to Matrix-multiplication Perspective

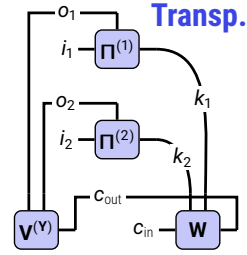


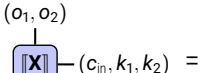




Connection to Matrix-multiplication Perspective







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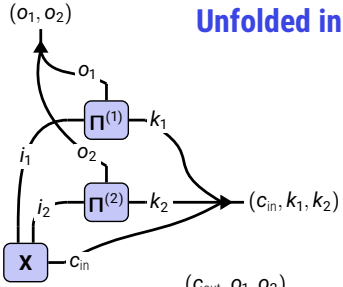

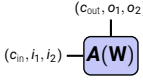

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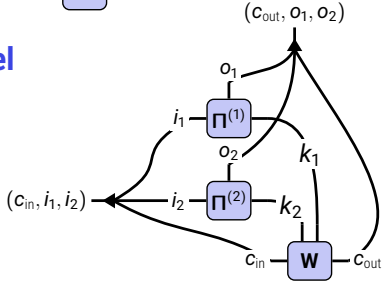
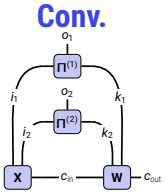
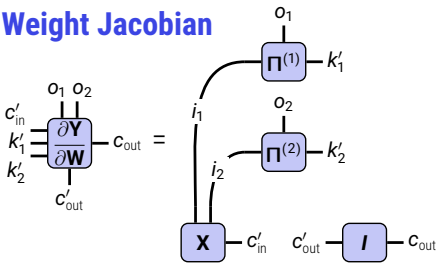


Derivatives & Autodiff Routines

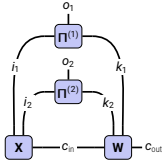


Derivatives & Autodiff Routines

Weight Jacobian

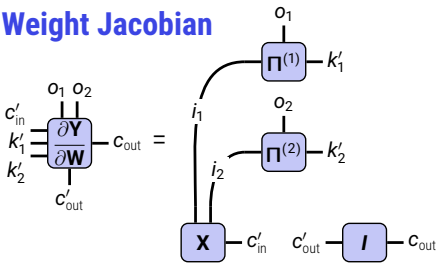


Conv.

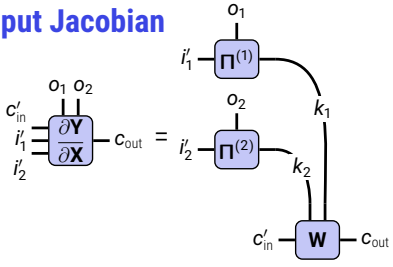


Derivatives & Autodiff Routines

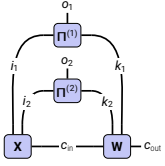
Weight Jacobian



Input Jacobian

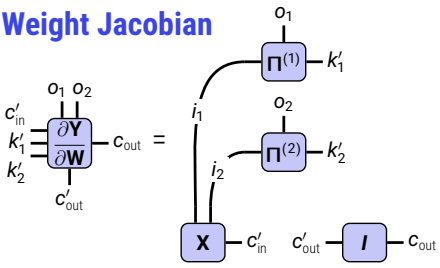


Conv.

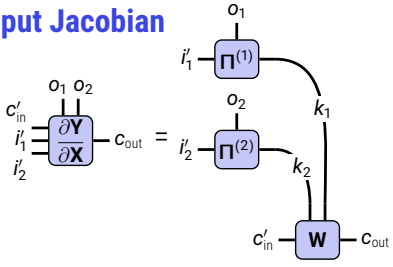


Derivatives & Autodiff Routines

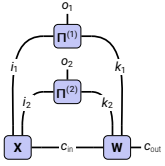
Weight Jacobian



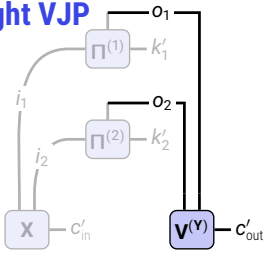
Input Jacobian



Conv.

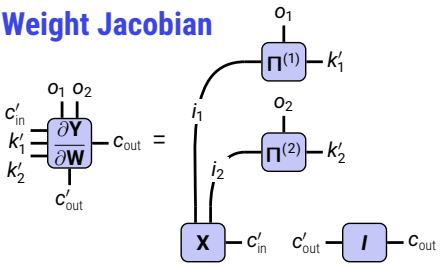


Weight VJP

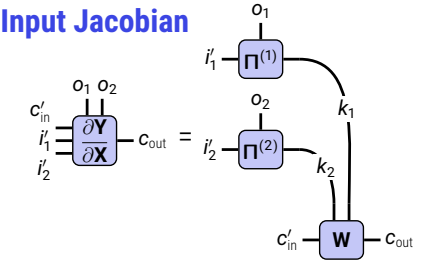


Derivatives & Autodiff Routines

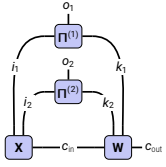
Weight Jacobian



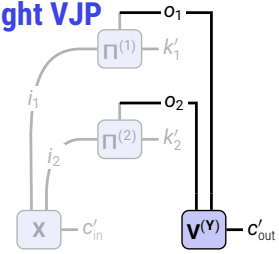
Input Jacobian



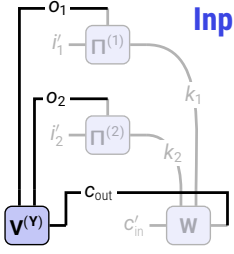
Conv.



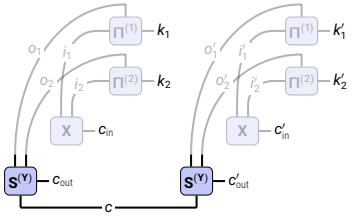
Weight VJP



Input VJP

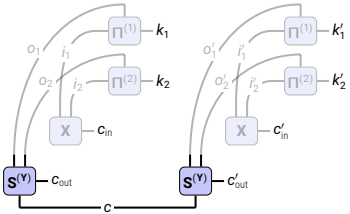


Fisher/GGN block

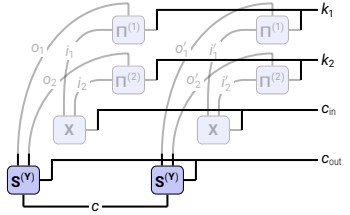


Higher-order Derivatives & Approximations

Fisher/GGN block

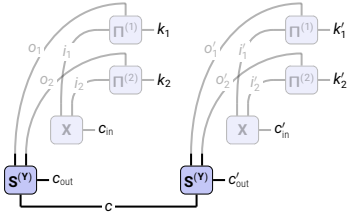


Fisher/GGN diagonal

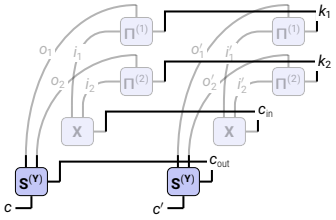


Higher-order Derivatives & Approximations

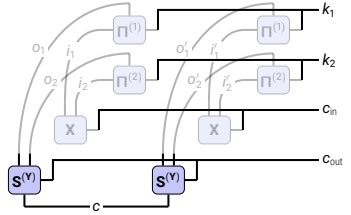
Fisher/GGN block



GGN Gram/Empirical NTK matrix

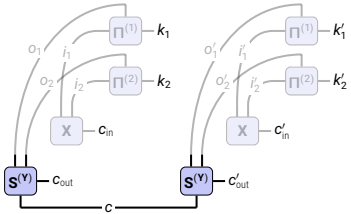


Fisher/GGN diagonal

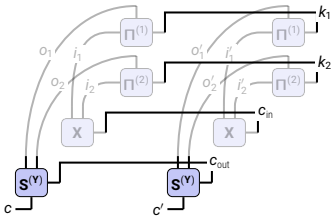


Higher-order Derivatives & Approximations

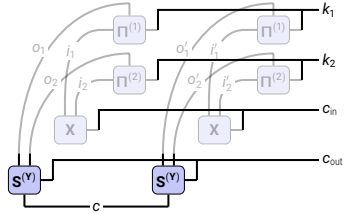
Fisher/GGN block



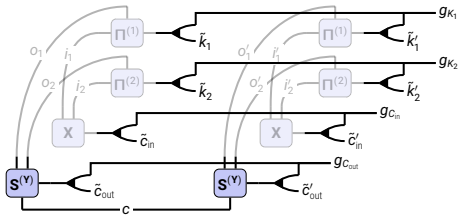
GGN Gram/Empirical NTK matrix



Fisher/GGN diagonal

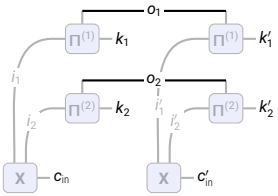


Fisher/GGN mini-block diagonal

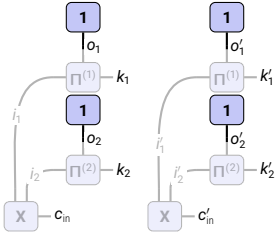


... and More!

KFC/KFAC-expand

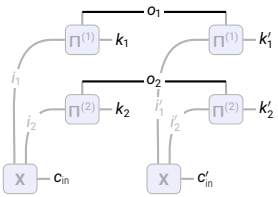


KFAC-reduce

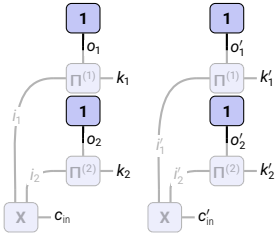


... and More!

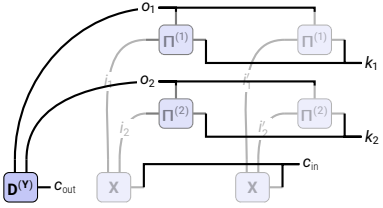
KFC/KFAC-expand



KFAC-reduce



Approximate Hessian diagonal



Check out the table in the paper's appendix!

Example & Conclusion

Improving KFAC-reduce [Eschenhagen et al., 2023, NeurIPS]

State of the art

x

Improving KFAC-reduce [Eschenhagen et al., 2023, NeurIPS]

State of the art

$\mathbf{X}$

$\rightarrow [\![\mathbf{X}]\!]$

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$\rightarrow [\![\mathbf{X}]\!]$

$\rightarrow \mathbf{1}^\top [\![\mathbf{X}]\!]$

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$$
\begin{aligned}
&\mathbf{X} \\
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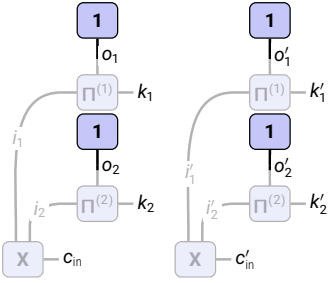
\end{aligned}
$$

Tensor Network



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\end{aligned}
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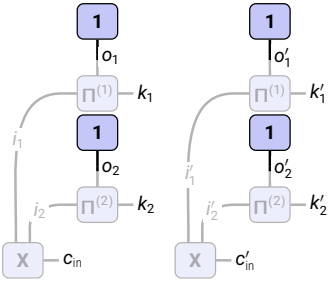
Time: **9.87 ms**

Tensor Network



Time: **2.69 ms (3.7 x)**

(`features.1.0.block.0` convolution of ConvNeXt-base with (32, 3, 256, 256) input)

Improving KFAC-reduce [Eschenhagen et al., 2023, NeurIPS]

Non-conventional operations can be much cheaper with tensor networks

State of the art

$$
\begin{aligned}
&\mathbf{X} \\
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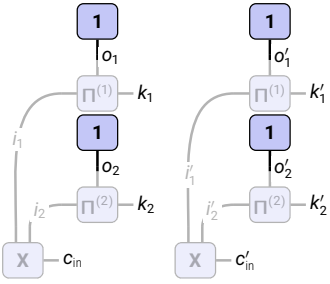
\end{aligned}
$$

Time: **9.87 ms**
Extra memory: **3.07 GiB**

Tensor Network



Time: **2.69 ms (3.7 x)**
Extra memory: **0 MiB**

(`features.1.0.block.0` convolution of ConvNeXt-base with (32, 3, 256, 256) input)

Convolutions and More as `einsum`

- TN perspective simplifies the transfer of algorithmic ideas
- Enables flexible/faster implementations of black box routines
- Relies on automatically efficient evaluation inside `einsum`

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Try it out!

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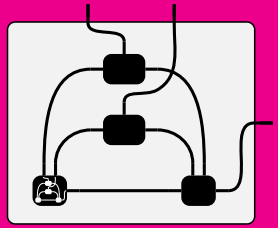
from einconv.expressions import kfac_reduce
from torch import einsum

# create the tensor network
equation, operands, shape = kfac_reduce.
    einsum_expression(..., simplify=True)
# evaluate it
einsum(equation, *operands).reshape(shape)
```



pip install einconv

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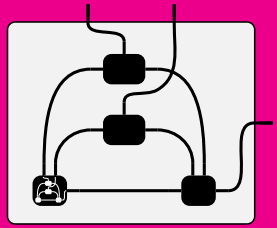

pip install einconv

Paper: arxiv/2307.02275

Code: github.com/f-dangel/einconv

Thank you 🙏 questions?

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Convolution-specific Simplifications

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$\rightarrow$ even better performance

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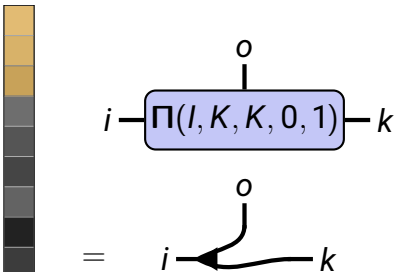

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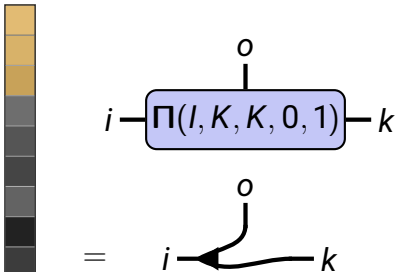
Dense convolution ($K = S$)



Down-sampling convolution ($S > K$)

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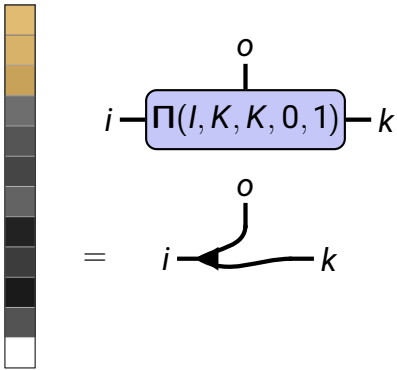
Dense convolution ($K = S$)



Down-sampling convolution ($S > K$)