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Convolutional Neural Networks

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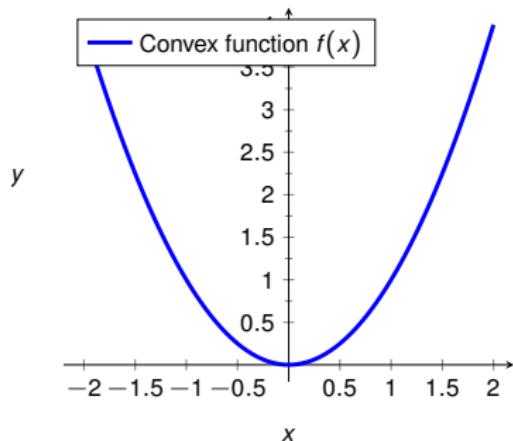
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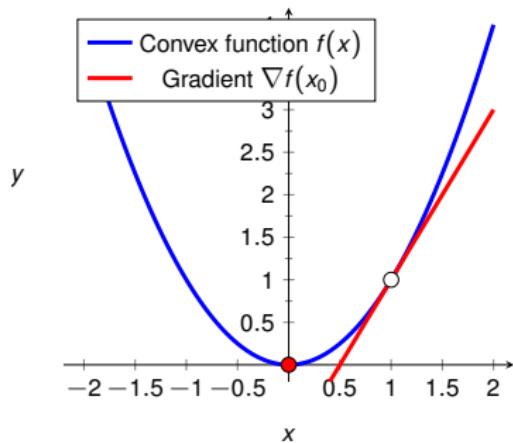
Initializers



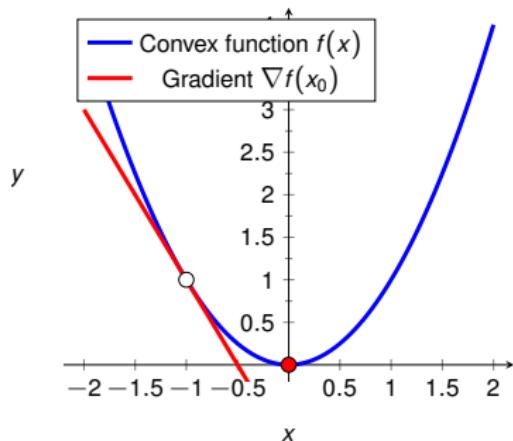
Does initialization matter?



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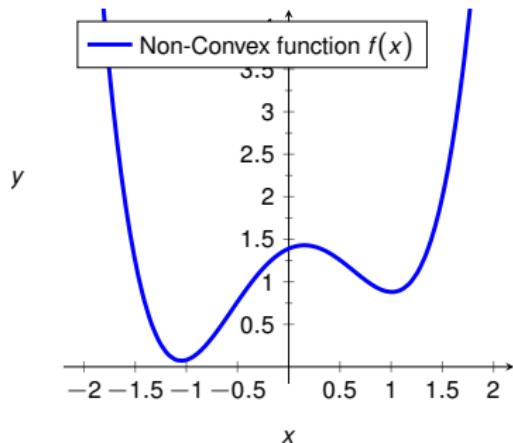


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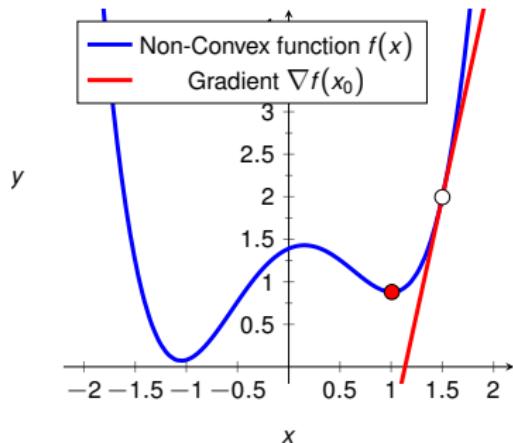
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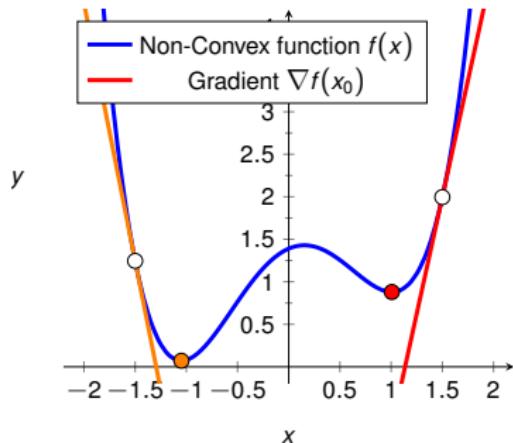
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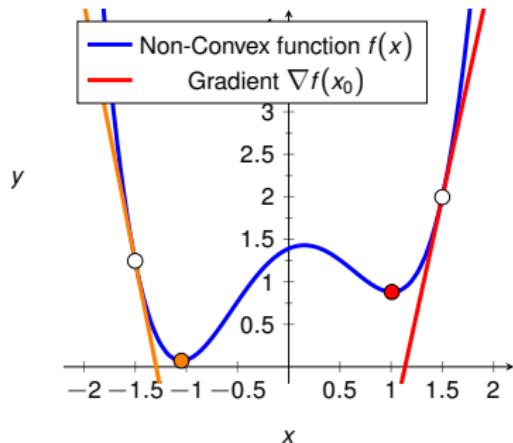
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- No it doesn't for **convex** optimization problems
- But it **does** for every **non-convex** one
- Neural Networks with a non-linearity are in general **non-convex**

Initializer objects

- **Goal:** Be flexible and allow different initialization strategies
- **Solution:** Every layer with weights will get **initializer objects**:
One object for the **bias** and one for the other **weights**
- We have to refactor the code:
 - The **FullyConnected** layer to accept initializers
 - And the **NeuralNetwork** class to distribute them

Simple initialization schemes

Uniform

- Usually in the range $[0, 1]$
- Same as before

Constant

- With a given value
- Default to 0.1
- **Very bad** for weights
- Typically for **biases**
- . . . in conjunction with **ReLUs**

Initializers: Nomenclature

The number of **inputs** and **outputs** to a layer are often used for initializing weights

- For **fully connected** layers:
 - “fan_in”: **input** dimension of the weights
 - “fan_out”: **output** dimension of the weights
- For **convolutional** layers:
 - “fan_in”: [**# input channels** \times **kernel height** \times **kernel width**]
 - “fan_out”: [**# output channels** \times **kernel height** \times **kernel width**]

Xavier/Glorot

- Typically for **weights**
- Normalizes weights with respect to number of units
- Zero-mean Gaussian: $\mathcal{N}(0, \sigma)$
- $$\sigma = \sqrt{\frac{2}{\text{fan_out} + \text{fan_in}}}$$

“fan_in” and “fan_out” as defined previously

He

- Derived from Xavier initialization
- He initialization: Standard deviation of weights determined by size of previous layer only
- $\sigma = \sqrt{\frac{2}{\text{fan_in}}}$
- Weights initialized by zero-mean Gaussian: $\mathcal{N}(0, \sigma)$



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Advanced Optimizers



Momentum

- Parameter update based on current and past gradients:

$$\mathbf{v}^{(k)} = \underbrace{\mu}_{\text{momentum}} \mathbf{v}^{(k-1)} - \eta \underbrace{\nabla L(\mathbf{w}^{(k)})}_{\text{Gradient}}$$
$$\mathbf{w}^{(k+1)} = \mathbf{w}^{(k)} + \mathbf{v}^{(k)}$$

- commonly: $\mu = \{0.9, 0.95, 0.99\}$

Where to save intermediate values?

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- Possibilities:
 - Make a cache and every layer identifiable
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- Our solution: Make the bias and weights of every layer have a copy of the optimizer
- This means each set of weights **could** have a different optimizer

ADAM

- Parameter update based on current and past gradients:

$$\mathbf{g}^{(k)} = \nabla L(\mathbf{w}^{(k)})$$

$$\mathbf{v}^{(k)} = \mu \mathbf{v}^{(k-1)} + (1 - \mu) \mathbf{g}^{(k)}$$

$$\mathbf{r}^{(k)} = \rho \mathbf{r}^{(k-1)} + (1 - \rho) \mathbf{g}^{(k)} \odot \mathbf{g}^{(k)}$$

$$\mathbf{w}^{(k+1)} = \mathbf{w}^{(k)} - \eta \frac{\hat{\mathbf{v}}^{(k)}}{\sqrt{\hat{\mathbf{r}}^{(k)}} + \epsilon}$$

- commonly: $\mu = 0.9, \rho = 0.999, \eta = 0.001$

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Bias correction: $\hat{\mathbf{v}}^{(k)} = \frac{\mathbf{v}^{(k)}}{1 - \mu^k}$ $\hat{\mathbf{r}}^{(k)} = \frac{\mathbf{r}^{(k)}}{1 - \rho^k}$

$$\mathbf{w}^{(k+1)} = \mathbf{w}^{(k)} - \eta \frac{\hat{\mathbf{v}}^{(k)}}{\sqrt{\hat{\mathbf{r}}^{(k)}} + \epsilon}$$

- commonly: $\mu = 0.9$, $\rho = 0.999$, $\eta = 0.001$
- The k is actually an exponent, not an iteration-index!



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Convolution layer



Vectors versus Images

- So far we only considered **batches** of abstract **input vectors**
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Vectors versus Images

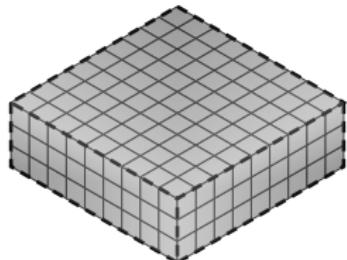
- So far we only considered **batches** of abstract **input vectors**
- This has been intuitive when Neural Networks were considered classifiers
- For feature learning, we have to consider **spatial** layout again
- Convolution layers therefore have to consider the spatial dimensions
- Keep in mind: We can also convolve 1-D signals!

Forward pass

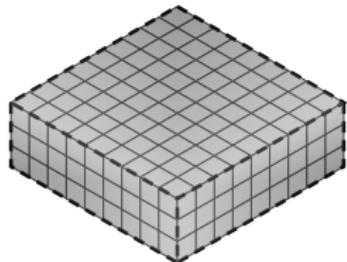
Figure: Convolution

Source: https://github.com/vdumoulin/conv_arithmetic

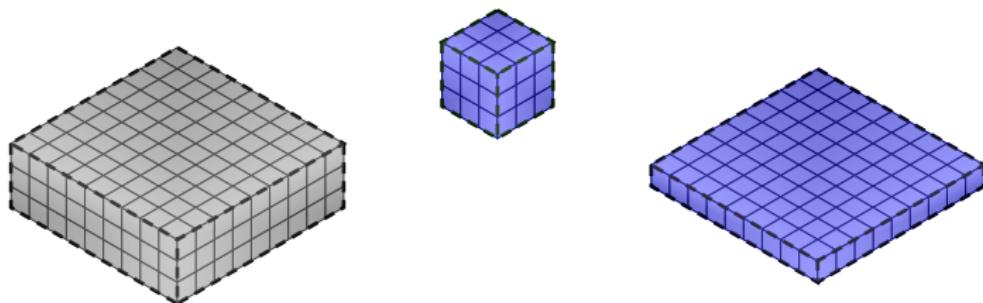
Forward pass, Multi channel, Multi output maps



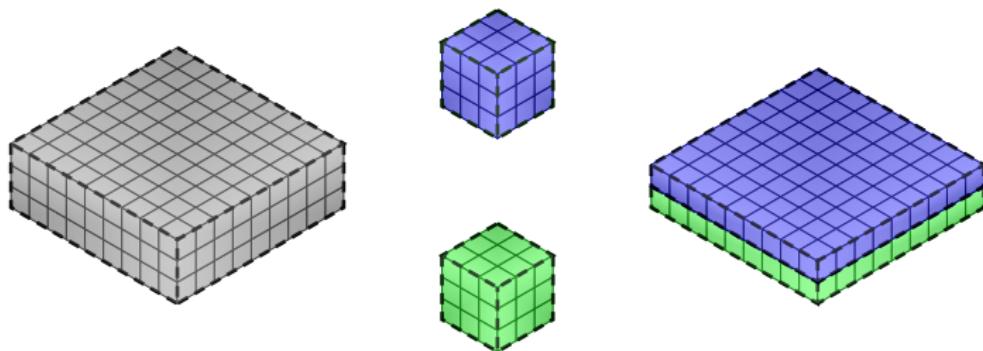
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Forward pass, Multi channel, Multi output maps



Forward pass

size of output = size of input - K + 1

Convolution implementation

- Run a loop for every element of the **batch**
- The “depth” dimension S is **identical** for **kernel** and **image**
 - fully connected across channels
 - 3D convolution with no padding across channels
- The number of kernels H determines the output “depth”
- **Bias** is an element-wise addition of a scalar value for every kernel
- Important! We have a ‘same’ convolution across the image plane axes and a ‘valid’ convolution across the channel axis
- Even kernel sizes are allowed
 - This requires asymmetric padding at the boundaries to result in the correct dimension.

Forward pass

Matrix implementation

- Convolution is a linear operator → it has a matrix representation
- Reshape the kernel to the correct matrix before performing the convolution

Backward pass

Matrix implementation

- We can use the same formulas as in a fully connected layer!
- $\mathbf{E}_{n-1} = \mathbf{W}^T \mathbf{E}_n$
- $\nabla \mathbf{W} = \mathbf{E}_n \mathbf{X}^T$
- **Needs a lot of rearranging to create the right weights and error matrices!**

Convolution implementation

Backward pass

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Convolution implementation

- Backward pass is also a convolution but with spatially-flipped filters
- Instead of flipping filters, cross correlation (CC) can be used...
- ... and vice versa, we can use CC in the forward and convolution in the backward pass

Backward pass

Why to flip the filters in the backward pass?

- Lets consider the 1D case:
- We have an input $[a, b, c]$ and a filter $[x, y]$. Including padding this will lead to an output $[ay \ ax + by \ bx + cy \ cx]$.
- For the backward pass we want to calculate the derivative:

$$\frac{\partial E}{\partial I} = \frac{\partial E}{\partial O} \frac{\partial O}{\partial I} \quad (1)$$

- The important part now is $\frac{\partial O}{\partial I}$.
- E.g. if we calculate $\frac{\partial O}{\partial b} \rightarrow [0 \ y \ x \ 0] \rightarrow$ the kernel is flipped.
- Also for a and c we will get a flipped kernel.

Convolution versus cross correlation

- Convolution:

$$(f * g)(x) := \int_{-\infty}^{\infty} f(\tau)g(x - \tau)d\tau \quad (2)$$

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- Often cross correlation is used in the **forward pass**, because the **weights** are random anyway. This means convolution is then used if you want to flip the kernel

Backward pass

How to handle the bias on backward pass

- The bias in the backward pass can be handled by:

$$\frac{\partial L}{\partial b} = \sum_{b,w,h}^{B,W,H} E_{b,w,h} \quad (4)$$

Backward pass

How does a pixel of the input contribute to the pixels of the output?

Figure: Convolution

Backward pass

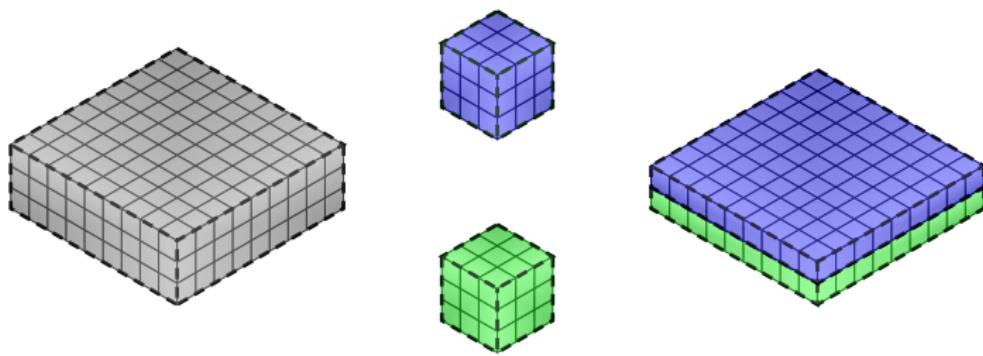
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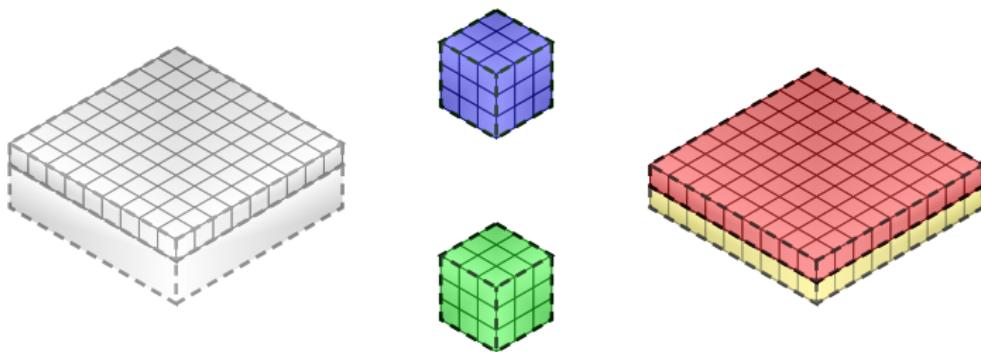
Convolution implementation

- The gradient with respect to the bias is simply sums over \mathbf{E}_n
- Filters need to be **flipped** (rotated 180°)
- What about the channels?
 - If we had H kernels with S channels
 - We obviously need S kernels in the backward pass → rearrange weights

Backward pass - Gradient with respect to lower layers

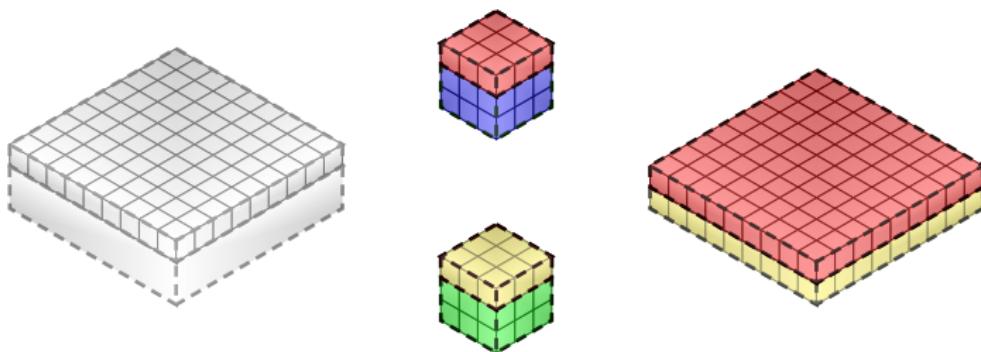


Backward pass - Gradient with respect to lower layers



- Channel h of \mathbf{E}_{n-1} **depends only** on the H kernels $\mathbf{K}_{s,N,M}$, where $h = s$

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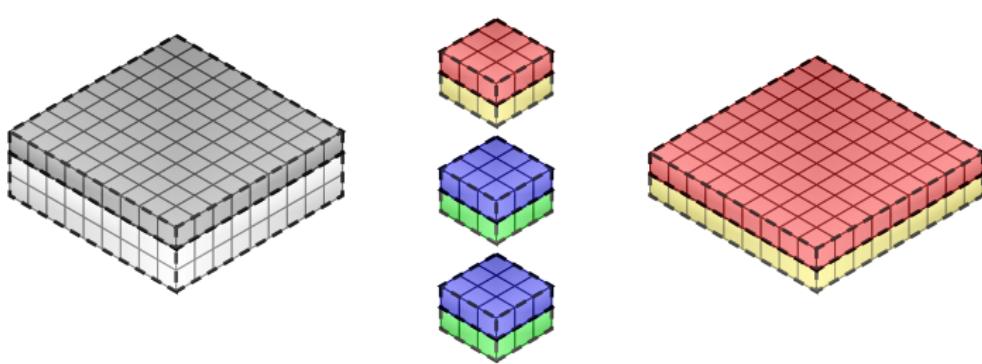
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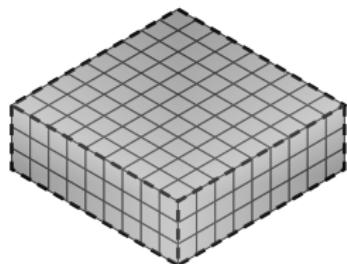
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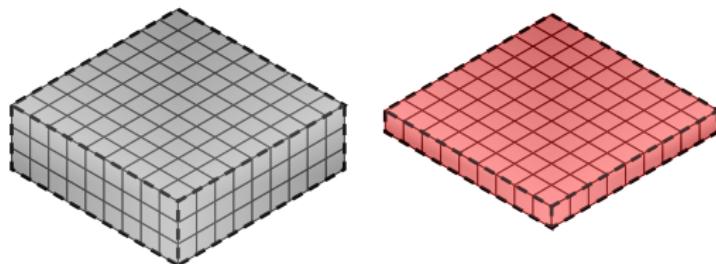


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- We have to **combine the channels** of the H kernels to S new kernels
- Using 3D operations is possible if you include the channel dimension
- If a 3D-cross-correlation was used in the forward pass and 3D-convolution in the backward, the channel dimension needs to be flipped once more!
- If cross-correlation and convolution were 2D, e.g. you looped over the channels, no additional channel flipping is needed.

Backward pass - Gradient with respect to the weights

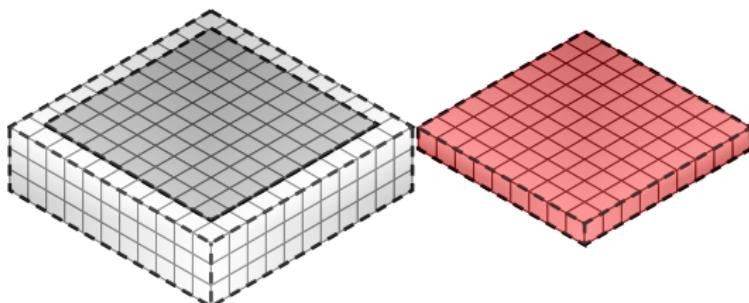


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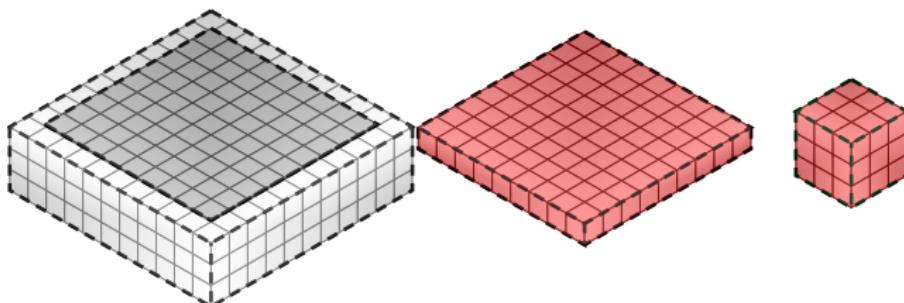
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Backward pass - Gradient with respect to the weights



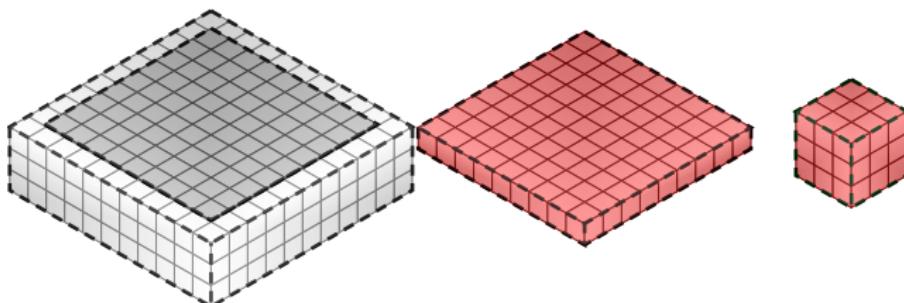
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- Pad \mathbf{X} with half the kernels' width

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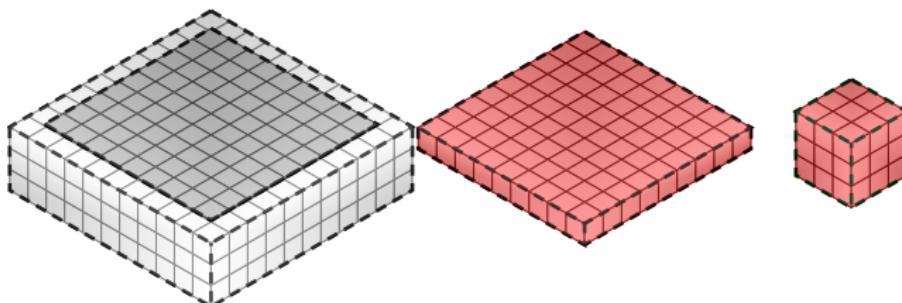
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- Compute for $s \in [1 \cdots S]$: $\mathbf{X}_s \star \mathbf{E}_{\underline{h},n}$ to receive the kernel $\nabla K_{\underline{h},S,N,M}$

Backward pass - Gradient with respect to the weights



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Backward pass - Gradient with respect to the weights



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- If correlation is used in the forward pass we directly receive the correct gradient in the backward pass
- If convolution is used in the forward pass, we have to manually rotate the x, y -plane by 180° of the kernels

Stride

Figure: Strided convolution

Source: https://github.com/vdumoulin/conv_arithmetic

Stride

- Stride is often used to **reduce the dimension** of the input

Stride

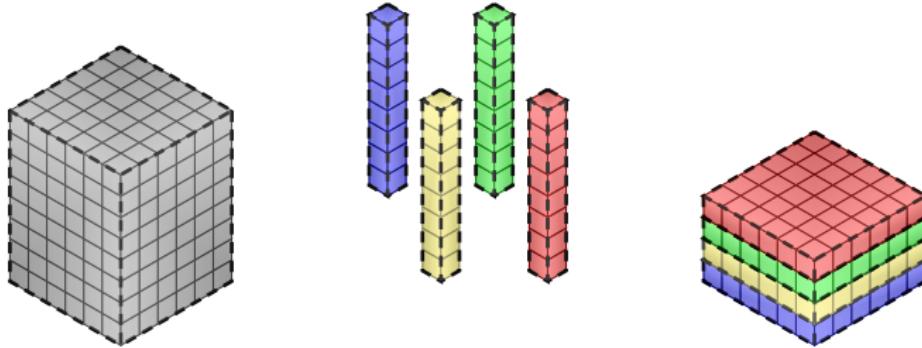
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- Similarly the backward pass can be calculated by **upsampling followed by convolution/correlation**

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- Stride is often used to **reduce the dimension** of the input
- More mathematically stride can be seen as **correlation/convolution followed by subsampling**
- Similarly the backward pass can be calculated by **upsampling followed by convolution/correlation**
- Stride is not provided by any scipy/numpy convolution

1x1 Convolutions

- Important special case
- Equal to applying a **fully connected layer along the channels**



Overview tensor shapes

The following table shows exemplary tensor shapes for forward and backward pass for an input image of size (S, X, Y) . The batch size is neglected. Be aware that the tensor of the input column still needs to be padded to achieve the desired output shape.

	Input tensor	Convolve/correlate with	Output tensor
Forward pass	(S, X, Y)	$H \times (S, N, M)$	(H, X, Y)
Gradient w.r.t weights	(S, X, Y)	$H \times (X, Y)$	(H, S, N, M)
Gradient w.r.t. lower layers	(H, X, Y)	$S \times (H, N, M)$	(S, X, Y)



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Pooling layer



Forward pass max-pooling

Figure: Max-pooling

Source: https://github.com/vdumoulin/conv_arithmetic

Forward pass max-pooling

- **Stride** is crucial now and controls amount of **downsampling**
- . . . and **typically as big** as the **kernel size**
- We need to **store the locations** of the **maxima**

Backward pass max-pooling



Backward pass max-pooling

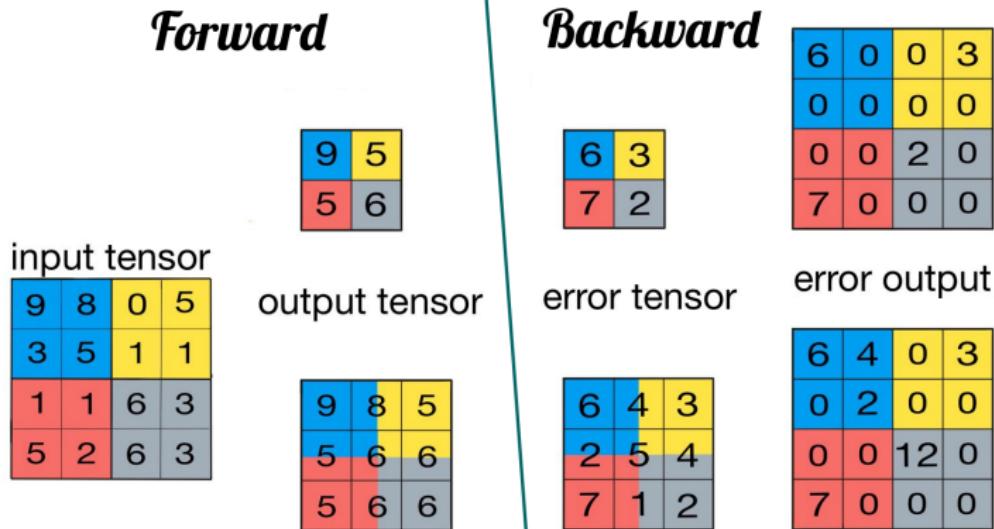


"THE WINNER
TAKES IT ALL"
- En hyllning till ABBA

Backward pass max-pooling

- A **subgradient** is given by the colloquial rule “**Winner takes it all**”
- Layer has no trainable parameters, hence only gradient with respect to input required
- We need the stored maxima locations
- The error is routed towards these locations and is zero for all other pixels
- In cases where the stride is smaller than the kernel size the error might be routed multiple times to the same location and therefore has to be summed up

Pooling with/without stride





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Flatten layer



Flatten layer

What does it do?

- **Input:** batch of multi-dimensional arrays (spatial + channels)
- **Output:** batch of one dimensional feature vectors
- “Linearizes” each element in a batch

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Why flatten?

- Enables connecting convolution/pooling and fully connected layers
- Modularity - flatten as a separate layer provides flexibility
- Alternatives include global pooling layers

Thanks for listening.
Any questions?