Convolutional Neural Networks

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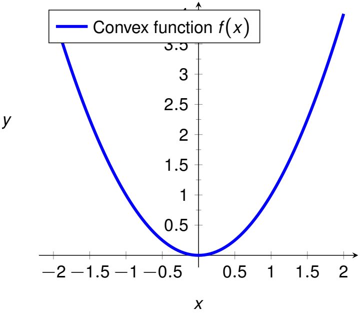
Initializers

Does initialization matter?



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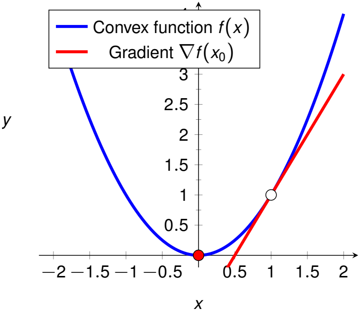

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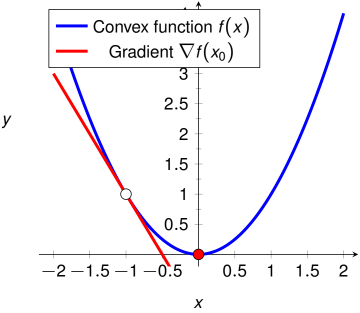

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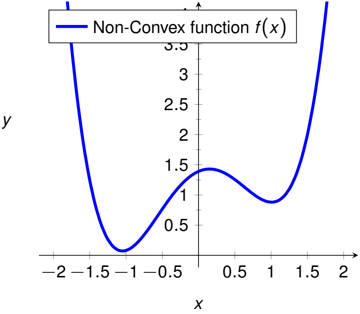

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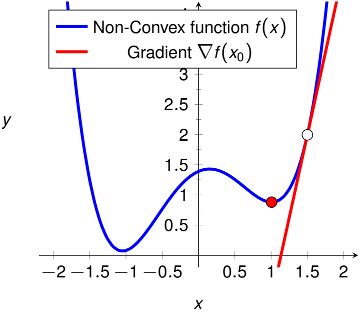

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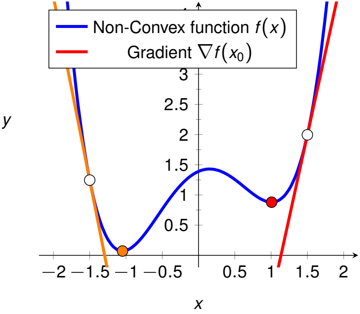

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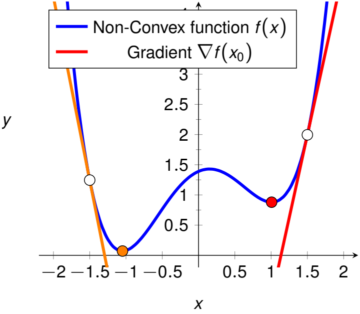

- No it doesn't for **convex** optimization problems
- But it **does** for every **non-convex** one
- Neural Networks with a non-linearity are in general **non-convex**

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**
- $\cdots$ in conjunction with **ReLU**s

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

$\rightarrow$ 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: $\mathcal{N}(0, \sigma)$

Advanced Optimizers

Momentum

- Parameter update based on current and past gradients:

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

$$\mathbf{w}^{(k+1)} = \mathbf{w}^{(k)} + \mathbf{v}^{(k)}$$

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

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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:

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

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

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$$\text{Bias correction: } \hat{\mathbf{v}}^{(k)} = \frac{\mathbf{v}^{(k)}}{1-\mu^{k}} \quad \hat{\mathbf{r}}^{(k)} = \frac{\mathbf{r}^{(k)}}{1-\rho^{k}}$$
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- commonly: $\mu = 0.9, \rho = 0.999, \eta = 0.001$
- The k is actually an **exponent**, not an iteration-index!

Convolution layer

Vectors versus Images

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

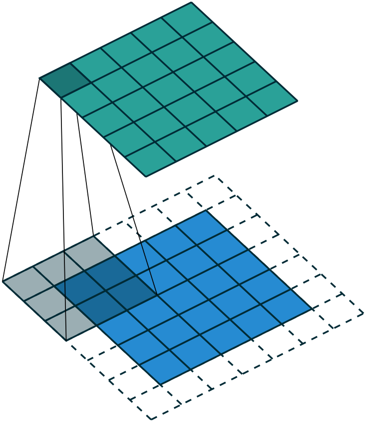
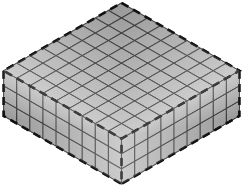


Figure: Convolution

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

Forward pass, Multi channel, Multi output maps



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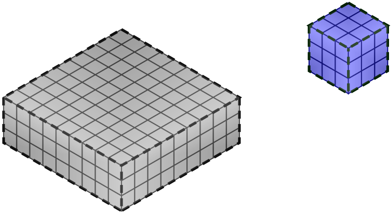

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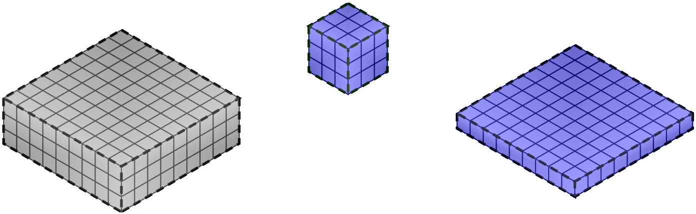

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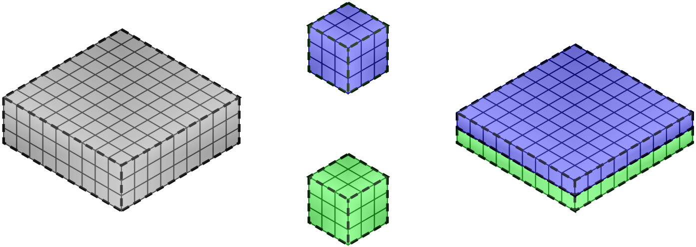

Forward pass

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 $\rightarrow$ 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!
- $\mathbf{E}_{n-1} = \mathbf{W}^{\mathbf{T}}\mathbf{E}_n$
- $\nabla\mathbf{W} = \mathbf{E_n}\mathbf{X}^T$
- **Needs a lot of rearranging to create the right weights and error matrices!**

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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:

$$\frac{\partial \mathrm{E}}{\partial \mathrm{I}} = \frac{\partial \mathrm{E}}{\partial \mathrm{O}} \frac{\partial \mathrm{O}}{\partial \mathrm{I}} \tag{1}$$

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

Convolution versus cross correlation

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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:

$$\frac{\partial \mathrm{L}}{\partial \mathrm{b}} = \sum_{b,w,h}^{B,W,H} \mathrm{E}_{b,w,h} \tag{4}$$

Backward pass

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

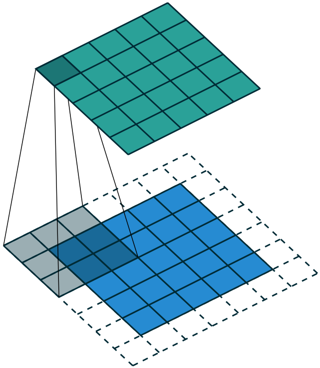

Figure: Convolution

Backward pass

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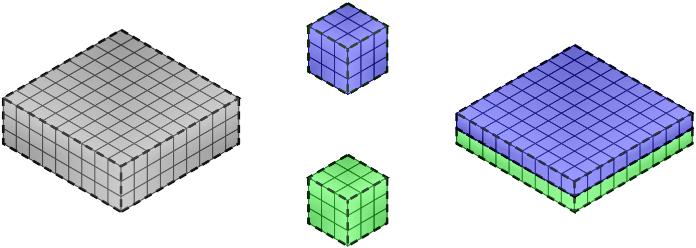
Convolution implementation

- 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 $\rightarrow$ rearrange weights

Backward pass - Gradient with respect to lower layers



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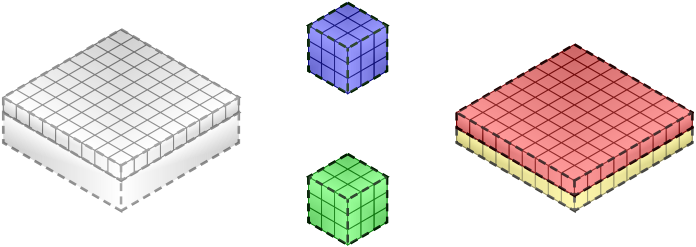

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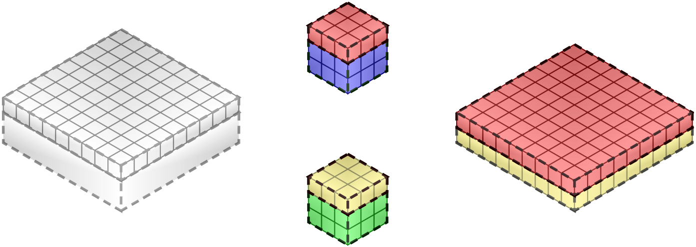

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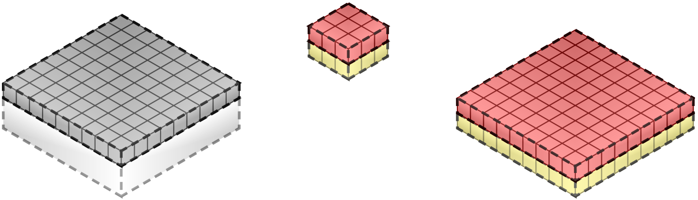

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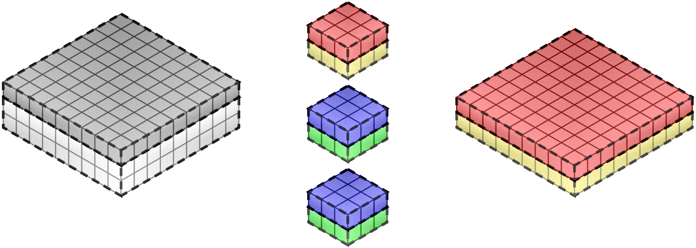

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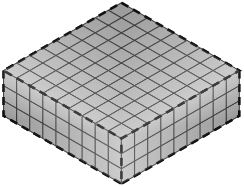
- We have to **combine the channels** of the H kernels to S new kernels
- Using 3D operations is possible if you include the channel dimension
- If a 3D-cross-correlation was used in the forward pass and 3D-convolution in the backward, the channel dimension needs to be flipped once more!
- If cross-correlation 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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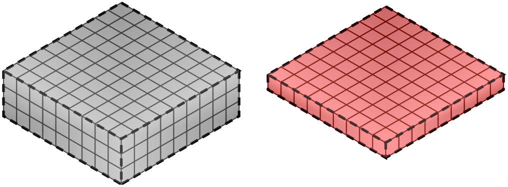

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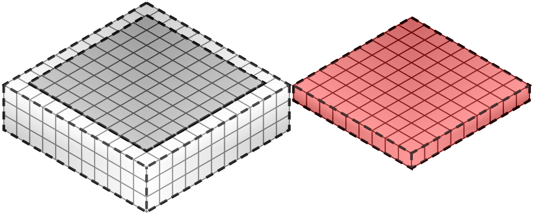

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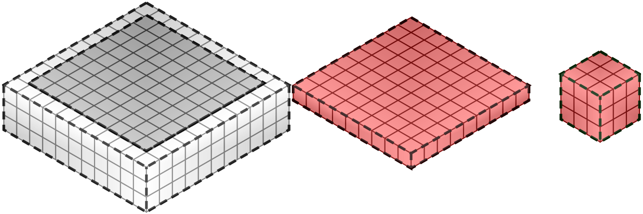

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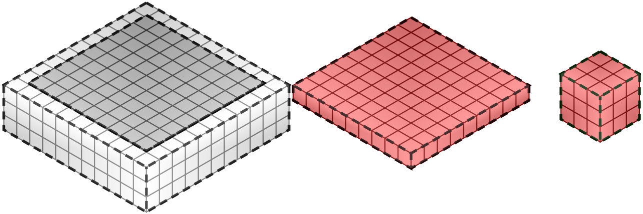

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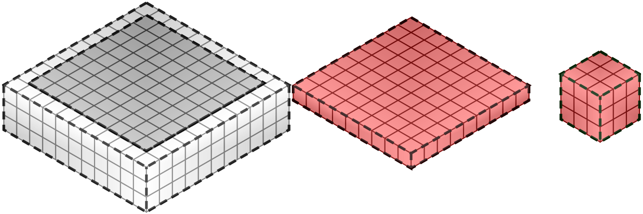

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- If correlation is used in the forward pass we directly receive the correct gradient in the backward pass
- If convolution is used in the forward pass, we have to manually rotate the x, y-plane by 180° of the kernels

Stride

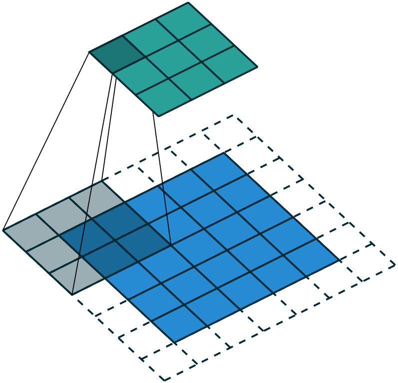

Figure: Strided convolution

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

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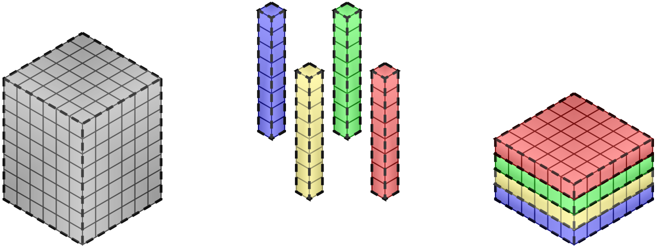
- Similarly the backward pass can be calculated by **upsampling followed by convolution/correlation**
- Stride is not provided by any scipy/numpy convolution

1x1 Convolutions

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



Overview tensor shapes

The following table shows examplatory 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)

Pooling layer

Forward pass max-pooling

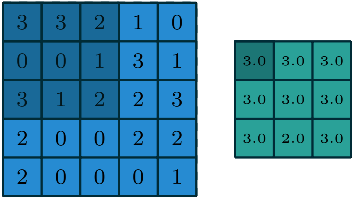


Figure: Max-pooling

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Forward pass max-pooling

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

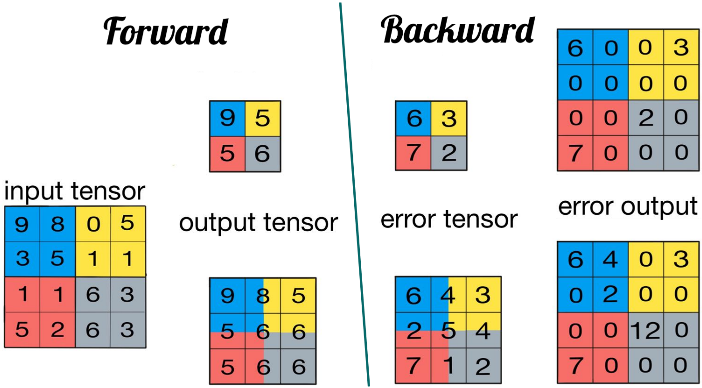
Backward pass max-pooling

Backward pass max-pooling

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



Flatten layer

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- **Input**: batch of multi-dimensional arrays (spatial + channels)
- **Output**: batch of one dimensional feature vectors
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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?