Convolutional Neural Networks

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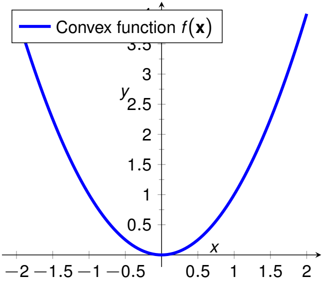
May 9, 2021

Initializers

Does initialization matter?



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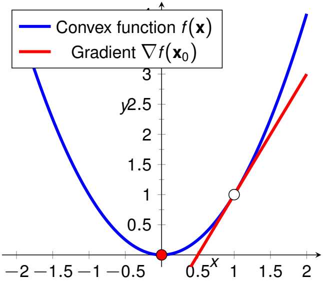

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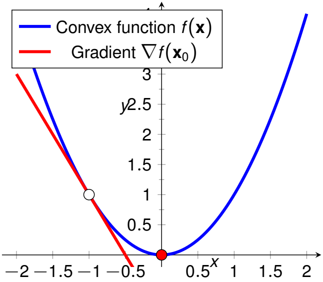

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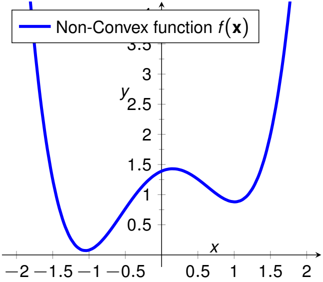

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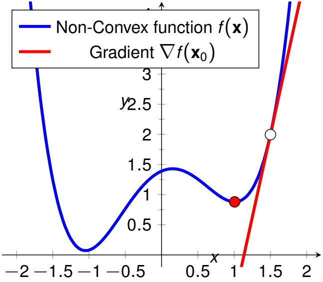

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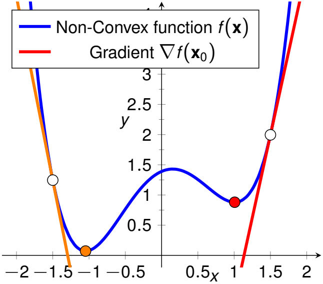

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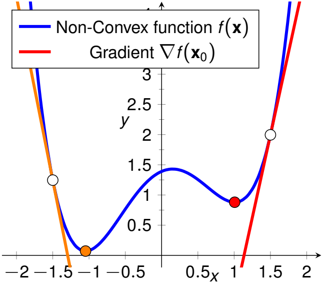

- No it doesn't for **convex** optimization problems
- But it **does** for every **non-convex** one
- Neural Networks with a non-linearity are in general **non-convex**

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 **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

$\rightarrow$ 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:

$$\mathbf{g}^{(k)} = \nabla L(\mathbf{w}^{(k)})$$
$$\mathbf{v}^{(k)} = \mu \mathbf{v}^{(k-1)} + (1-\mu)\mathbf{g}^{(k)}$$
$$\mathbf{r}^{(k)} = \rho \mathbf{r}^{(k-1)} + (1-\rho)\mathbf{g}^{(k)} \odot \mathbf{g}^{(k)}$$

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

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

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

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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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- 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

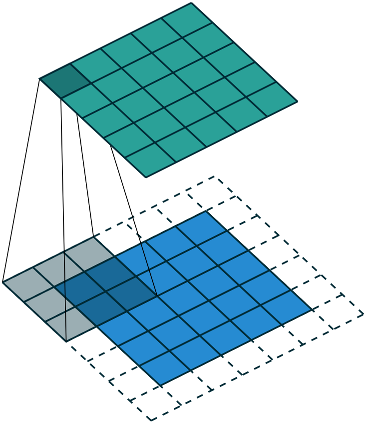
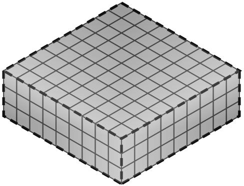


Figure: Convolution

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

Forward pass, Multi channel, Multi output maps



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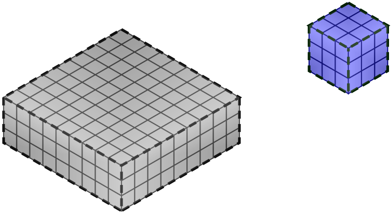

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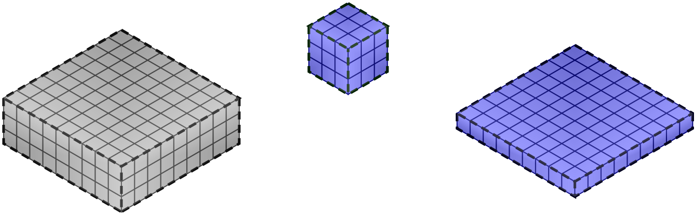

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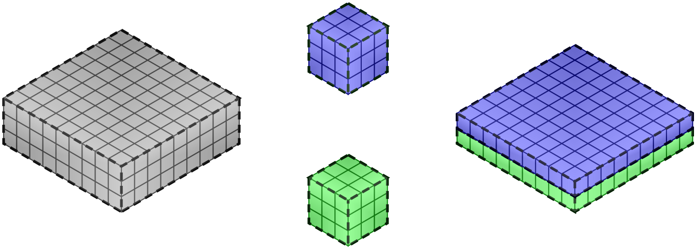

Forward pass

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.

Forward pass

Matrix implementation

- Convolution is a linear operator $\longrightarrow$ it has a matrix representation
- Reshape the kernel to the correct matrix 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

Convolution versus cross correlation

- Convolution:

$$(f * g)(x) := \int_{-\infty}^{\infty} f(\tau)g(x - \tau)\mathrm{d}\tau \tag{1}$$

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

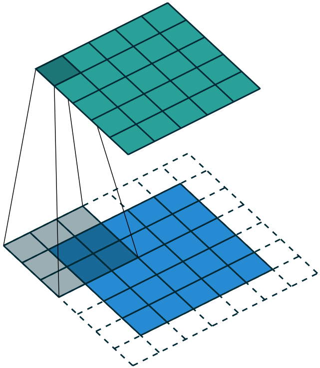

Figure: Convolution

Backward pass

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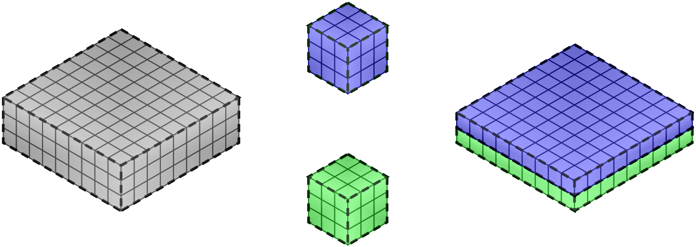
Convolution implementation

- 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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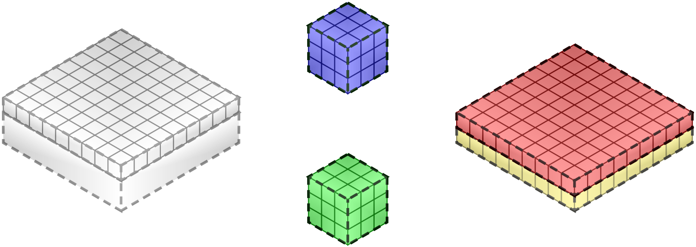

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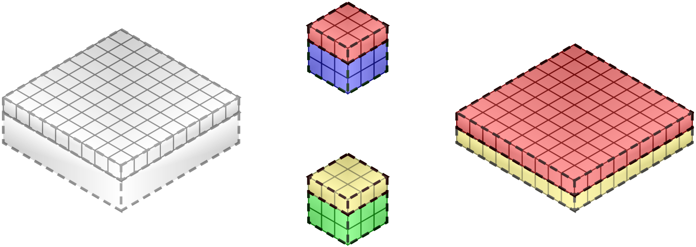

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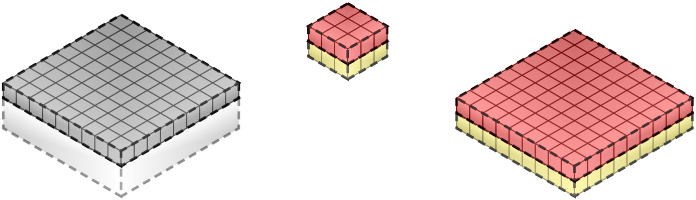

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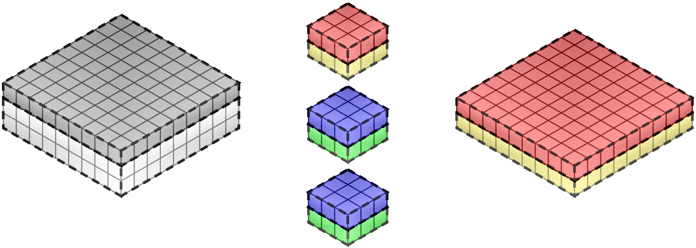

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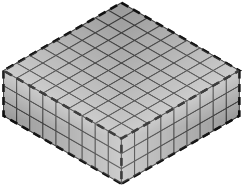
- We have to **combine the channels** of the H kernels to S new kernels
- Using 3D operations is possible if you include the channel dimension
- If a 3D-cross-correlation was used in the forward pass and 3D-convolution in the backward, the channel dimension needs to be flipped once more!
- If cross-correlation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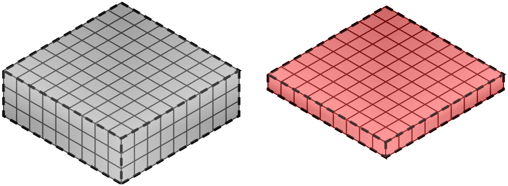

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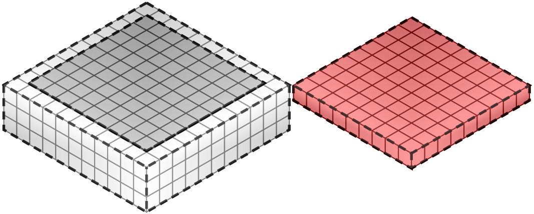

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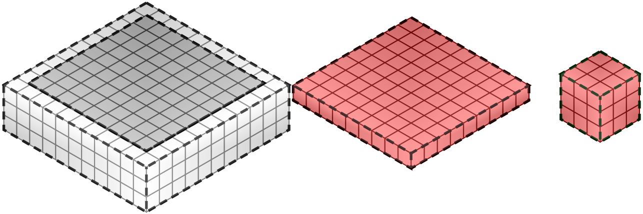

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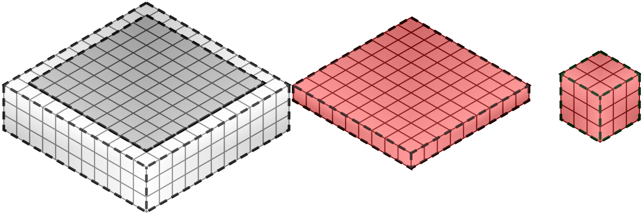

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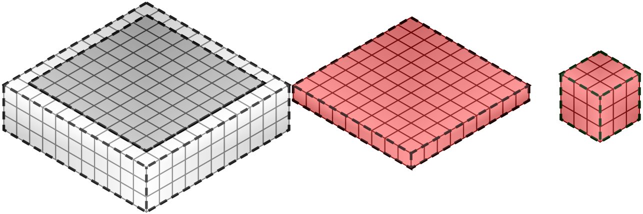

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- If correlation is used in the forward pass we directly receive the correct gradient in the backward pass
- If convolution is used in the forward pass, we have to manually rotate the x,y-plane by 180° of the kernels

Stride

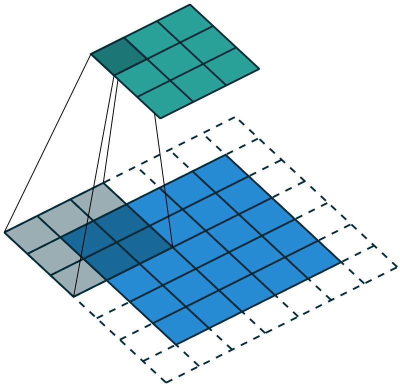

Figure: Strided convolution

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

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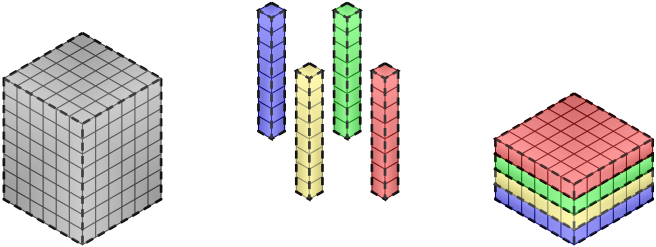
- More mathematically stride can be seen as **convolution followed by subsampling**
- Similarly the backward pass can be calculated by **upsampling followed by transposed convolution**
- Stride is not provided by any scipy/numpy convolution

1x1 Convolutions

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



Pooling layer

Forward pass max-pooling

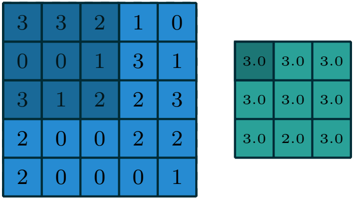


Figure: Max-pooling

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

Forward pass max-pooling

- **Stride** is crucial now and controls amount of downsampling
- $\cdots$ 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

Flatten layer

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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?