Convolutional Neural Networks

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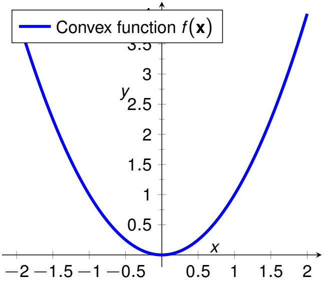
Exercise Schedule

Week	Task
18.10.-24.10.	Presentation Exercise 0: Numpy Tutorial
28.10.-01.11.	Presentation Exercise 1: Fully Connected
11.11.-15.11	**Deadline Exercise 0, 1**
18.11.-22.11.	Presentation Exercise 2: CNN
09.12.-13.12	**Deadline Exercise 2**

Initializers

Does initialization matter?



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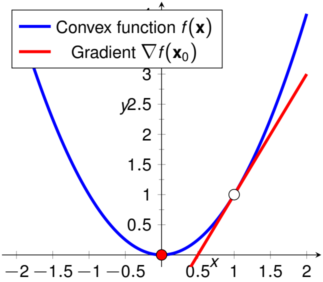

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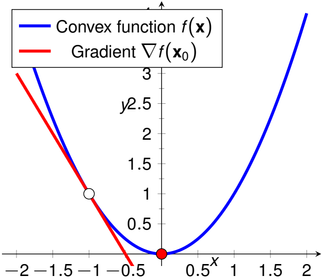

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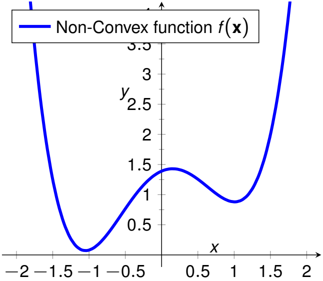

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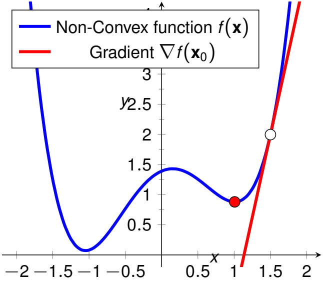

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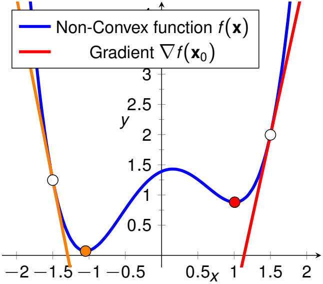

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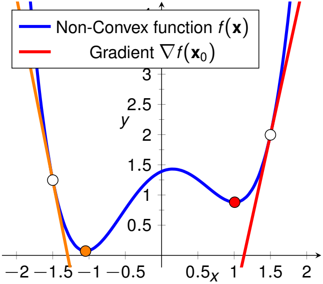

- No it doesn't for **convex** optimization problems
- But it **does** for every **non-convex** one
- Neural Networks with a non-linearity are in general **non-convex**

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
- Xavier assumes linear activation function - but **ReLU** is not

→ 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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  - ➔ Make a cache and every layer identifiable
  - ➔ Enable every layer to have a customizable cache
- 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:

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

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

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

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$$

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

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

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

Convolution layer

Vectors versus Images

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

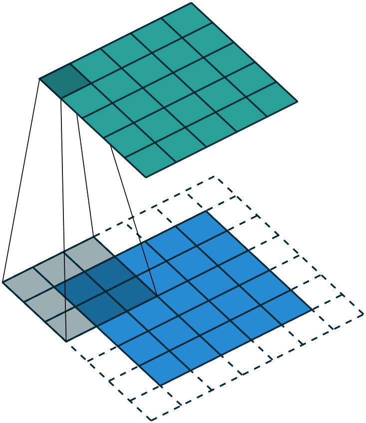
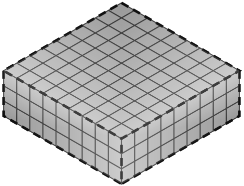


Figure: Convolution

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

Forward pass, Multi channel, Multi output maps



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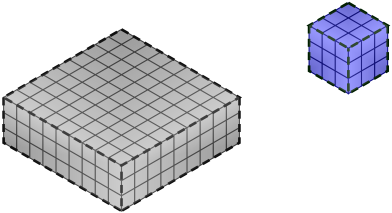

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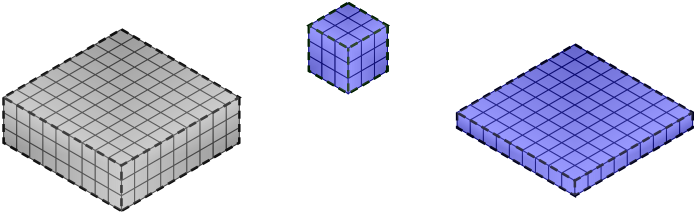

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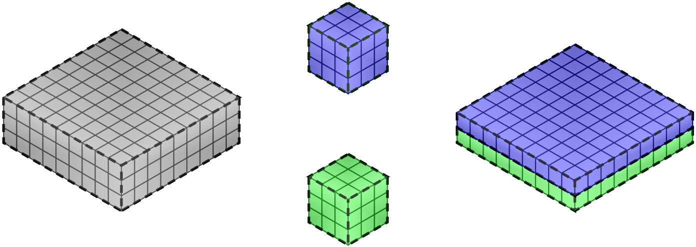

Forward pass

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 requieres 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!
- $\mathbf{E}_{n-1} = \mathbf{W}^{\mathbf{T}}\mathbf{E}_n$
- $\nabla \mathbf{W} = \mathbf{E_n}\mathbf{X}^T$

Convolution implementation

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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

Backward pass

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

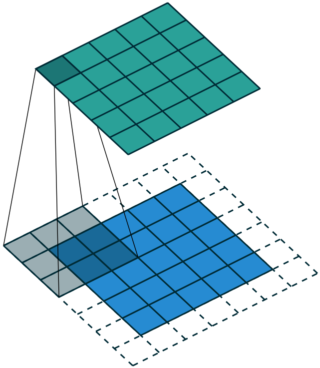

Figure: Convolution

Backward pass

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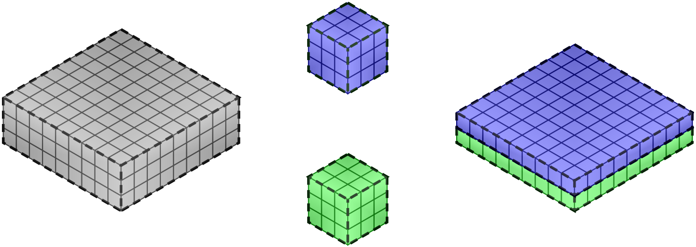
Convolution implementation

- The gradient with respect to the bias is simply sums over $\mathbf{E}_n$ (attention: w)
- 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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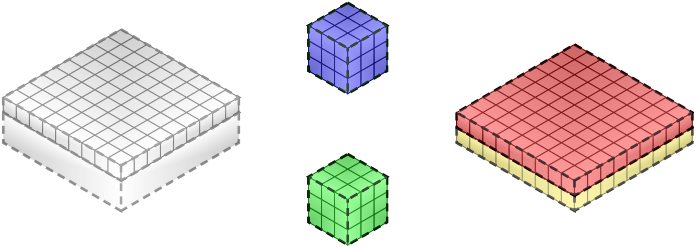

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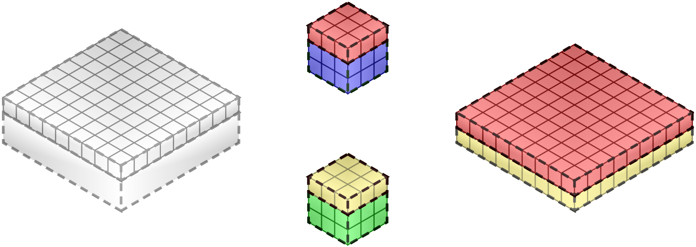

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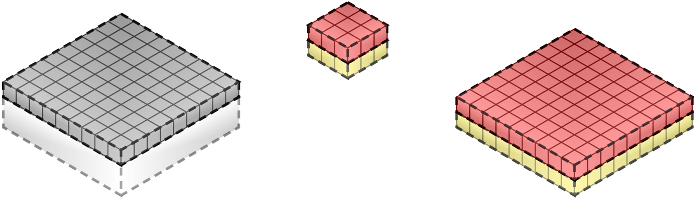

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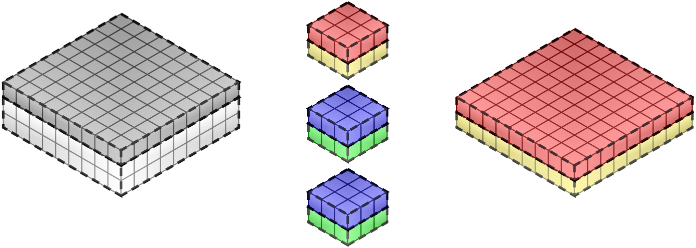

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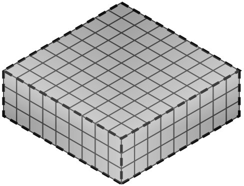
- We have to **combine the channels** of the H kernels to S new kernels
- If a 3D-cross-correlation was used in the forward pass and 3D-convolution in the backward, only the channel dimension needs to be flipped!
- If cross-correlation and convolution were 2D, no channel flipping is needed.

Backward pass - Gradient with respect to the weights



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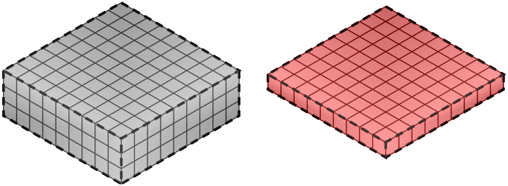

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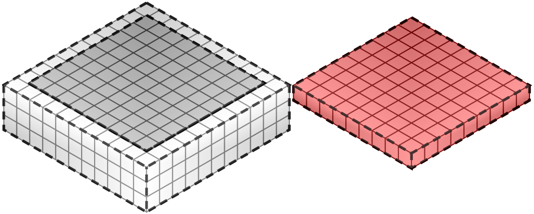

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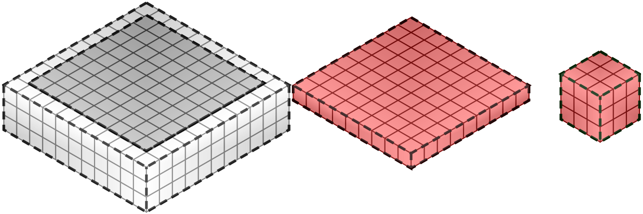

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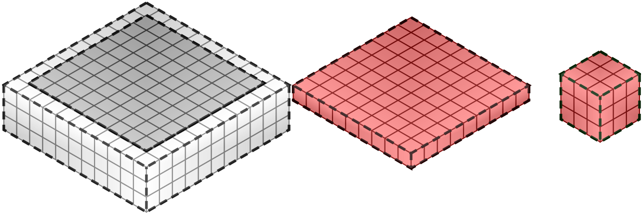

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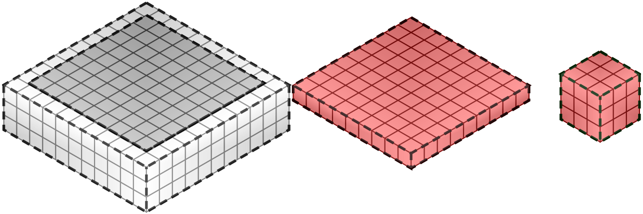

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- If convolution is used in the forward pass, we have to manually rotate the x,y-plane by 180° of the kernels

Stride

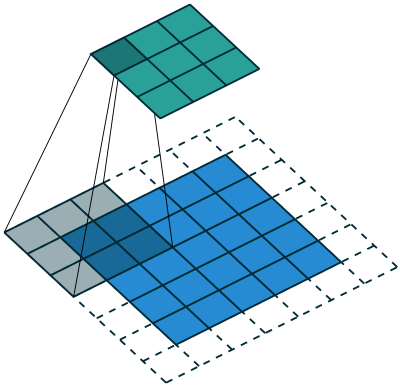

Figure: Strided convolution

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

Stride

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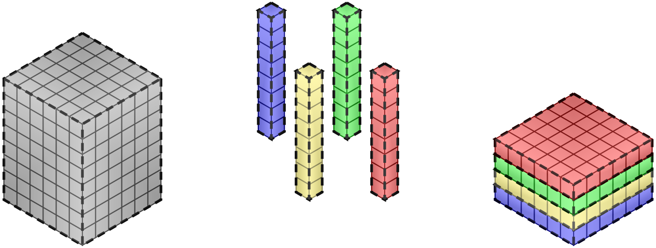
- More mathematically stride can be seen as **convolution followed by subsampling**
- Similarly the backward pass can be calculated by **upsampling followed by transposed convolution**
- Stride is not provided by any scipy/numpy convolution

1x1 Convolutions

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



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Pooling layer

Forward pass max-pooling

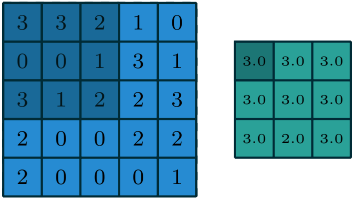

Figure: Max-pooling

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

Forward pass max-pooling

- **Stride** is crucial now and controls amount of downsampling
- $\cdots$ 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
- And summed if the stride is smaller than the kernel size

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?