Convolution in Neural Networks

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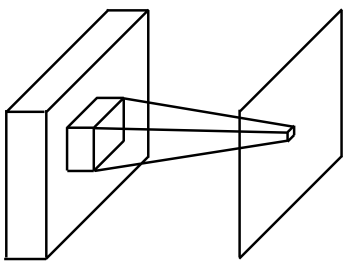
Many pictures used here are from https://github.com/vdumoulin/conv_arithmetic

Receptive Fields

- We saw from the lecture on neuroanatomy that parts of the visual system consist spatially local connections being fed into the neurons
    - In such a scenario, we can think about the Receptive Field (RF) of a neuron



Equivariance

- A function $f(x)$ is **equivariant** to a function g if $f(g(x)) = g(f(x))$
  - If the input changes, the output changes the **same** way

Translation Equivariance

- Consider what would happen if you had grids of neurons with their own receptive fields, but with **shared weights**.
  - Each neuron would respond in the same way to a given stimulus within its RF
  - If an input stimulus were moved over the grid, then the outputs of the neurons would *move* in the same way
    - This is **translational equivariance** and this is the key property of a ‘Convolutional Layer’ in a network

Signal Processing: Convolution and Cross-Correlation

- Convolution is an element-wise multiplication in the Fourier domain (*c.f. Convolution Theorem*)
  - *f* ∗ *g* = ifft(fft(*f*) . fft(*g*))
  - Whilst *f* and *g* might only contain real numbers, the FFTs are complex (*real* + *imag*j)
    - Need to do **complex multiplication**!

$$\boxed{(x+yi)(u+vi) = (xu - yv) + (xv + yu)i}$$

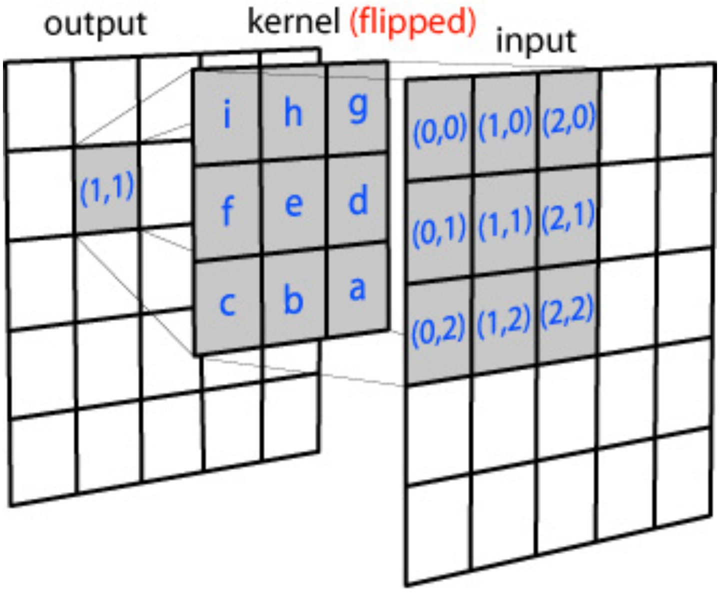
Template Convolution

- In the time domain, convolution is:

$$\begin{aligned}(f * g)(t) &\stackrel{\text{def}}{=} \int_{-\infty}^{\infty} f(\tau)\, g(t-\tau)\, d\tau \\ &= \int_{-\infty}^{\infty} f(t-\tau)\, g(\tau)\, d\tau.\end{aligned}$$

- **Notice that the image or kernel is “flipped” in time**
  - Also notice that the is no normalisation or similar

Template Convolution

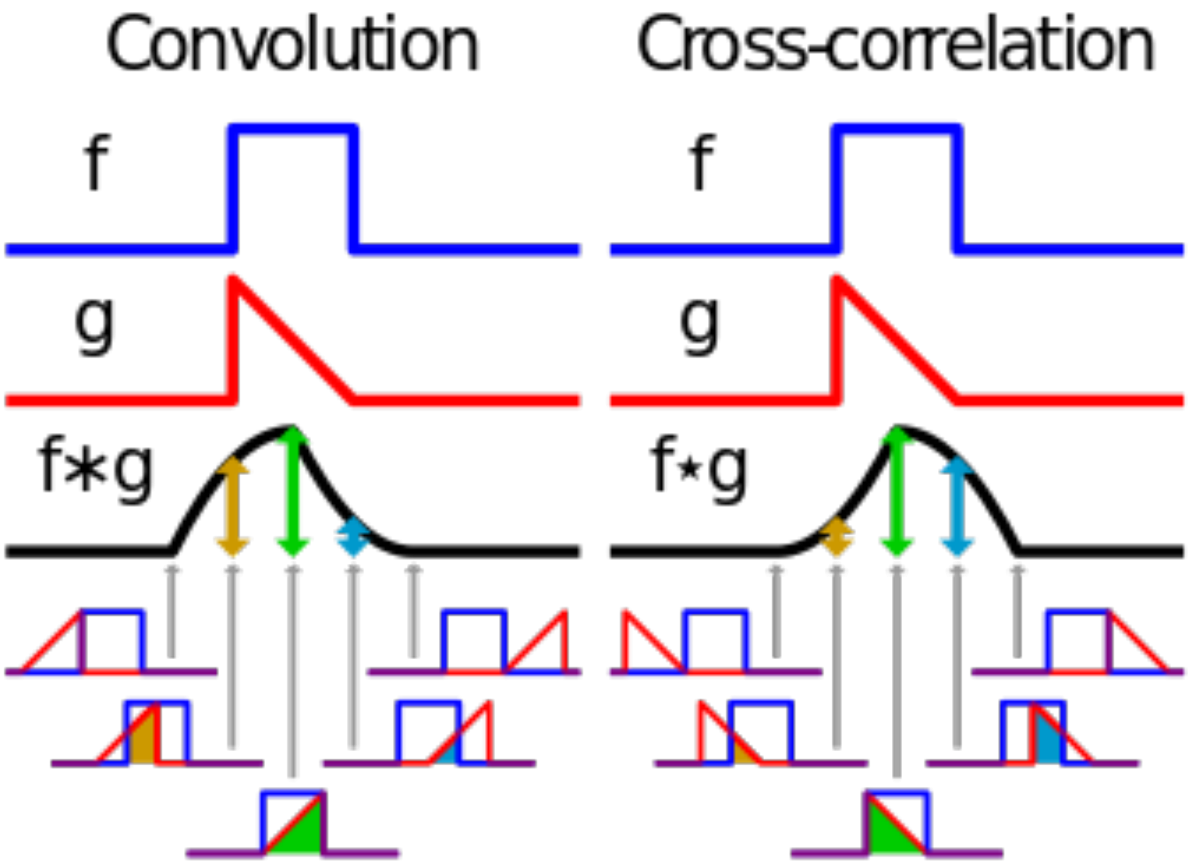


What if you don't flip the kernel?

- Obviously if the kernel is symmetric there is no difference
- However, you're actually not computing convolution, but another operation called cross-correlation

$$(f \star g)(\tau) \stackrel{\mathrm{def}}{=} \int_{-\infty}^{\infty} f^*(t)\; g(t+\tau)\, dt,$$

- * represents the complex conjugate
- (you can compute this with the multiplication of the FFTs just like convolution: iFFT(FFT(f)* . FFT(g))



"Convolution" in Neural Networks

- "Convolution" in the neural network literature almost always refers to an operation akin cross-correlation
    - An element-wise multiplication of learned weights across a receptive field, which is repeated at various positions across the input.
    - Normally, we also add an additional *bias term*
        - Most often a single one (for each *kernel*), but could be one for each spatial position.
    - There are also other parameters of these "convolutions"…

Convolutional Layers

- In a convolutional layer, we have multiple kernels or filters which are learnt (plus the biases)
  - Each filter produces a single "Response Map" or "Feature Map" which are stacked together as "channels" of the resultant output tensor

Efficient Computation of Convolutions

- Classical theory would suggest that the most efficient way to compute convolution (or cross-correlation) is via the Fourier transform if the kernels are larger
  - Or via direct spatial-domain implementation for small kernels
- In neural networks we need to be able to compute many convolutions on a single input as quickly as possible
  - We have specialised multi-core hardware to help though…

Convolution as a Matrix Multiplication

- The convolution operation can be expressed as a matrix multiplication if either the kernel or the signal is manipulated into a form known as a Toeplitz matrix:

$$y = h * x = \begin{bmatrix} h_1 & 0 & \ldots & 0 & 0 \\ h_2 & h_1 & \ldots & \vdots & \vdots \\ h_3 & h_2 & \ldots & 0 & 0 \\ \vdots & h_3 & \ldots & h_1 & 0 \\ h_{m-1} & \vdots & \ldots & h_2 & h_1 \\ h_m & h_{m-1} & \vdots & \vdots & h_2 \\ 0 & h_m & \ldots & h_{m-2} & \vdots \\ 0 & 0 & \ldots & h_{m-1} & h_{m-2} \\ \vdots & \vdots & \vdots & h_m & h_{m-1} \\ 0 & 0 & 0 & \ldots & h_m \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_n \end{bmatrix}$$

  - For 2D convolution one would use a “doubly block circulate matrix”

GEMM

- Efficient numeric computing tools have a long heritage
  - BLAS is a standard interface for high performance computing
    - The GEneral Matrix Multiply (GEMM) defined in the interface for matrix-matrix multiplications
  - Matrix-Matrix multiplication has many ways in which it can be optimised, including with multiple cores (like on a GPU!)

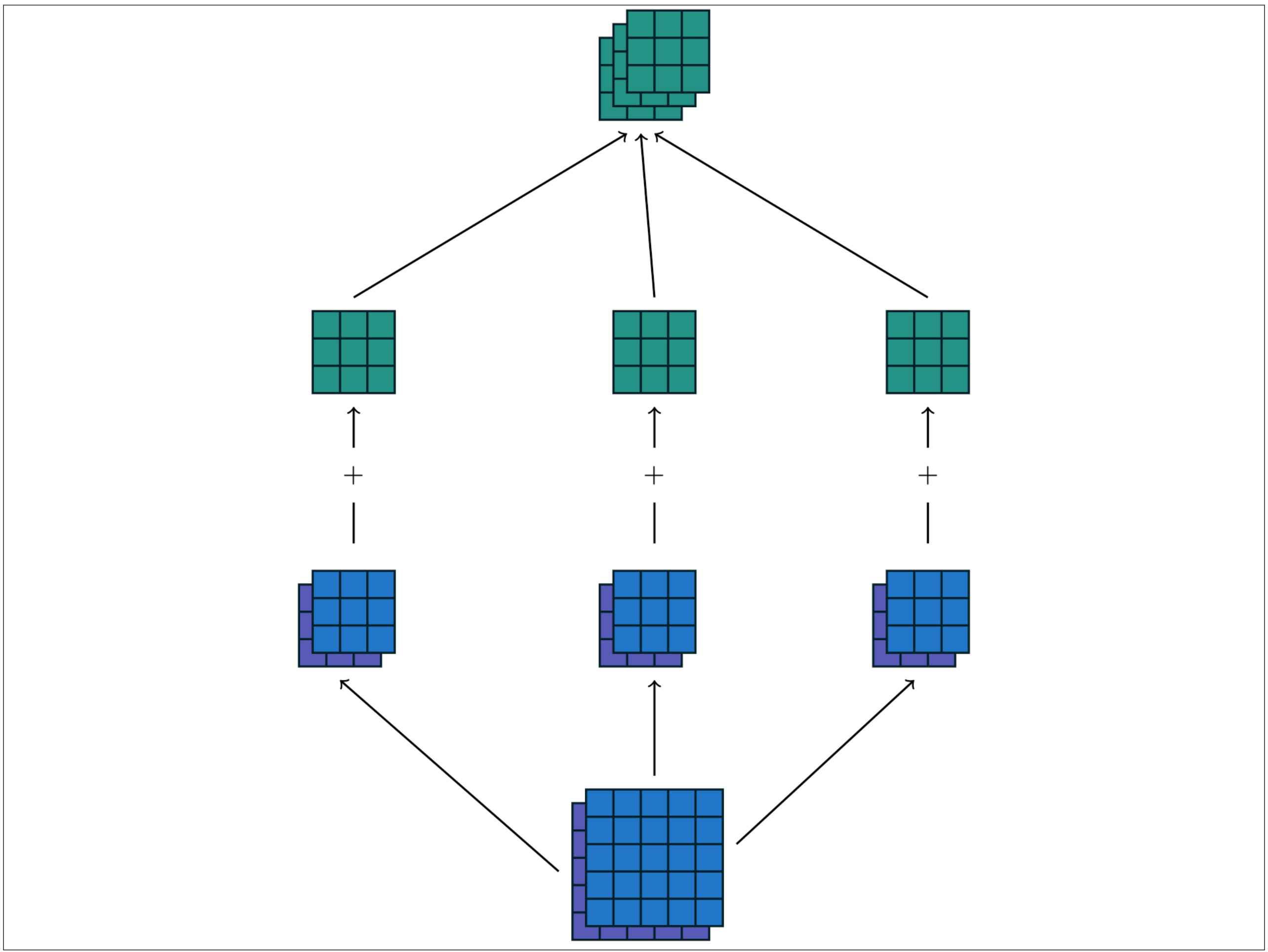
N-d Tensor Convolution

- In neural networks we want to expand our use of convolutions to work with tensors of any number of dimensions
  - If the input is say N x P x Q, where N is the "channels" dimension and P & Q are the spatial dimensions, we would define a convolutional kernel of size N x K x L

N-d Tensor Convolution

- We also don't typically want a single kernel, but rather many
  - Each one acting as a feature detector producing "feature maps"
  - We can just add another dimension to the kernel tensor to incorporate convolution with all kernels in one operation:

$$Z_{i,j,k} = \sum_{l,m,n} V_{l,j+m-1,k+n-1} K_{i,l,m,n}$$



Data Types

- Convolutions are applied to many dimensionalities and types of data - for example:

	Single Channel	**Multichannel**
1-D	Audio	Multiple sensor data over time
2-D	Audio data preprocessed into a spectrogram; greyscale images	Colour image data (e.g. RGB)
3-D	Volumetric data, e.g. CT scans	Colour video data

Convolutional Layer Parameters

- The core parameters of a convolution are:
  - The dimensionality (is it 1-D, 2-D, 3-D in the spatial sense?)
  - The spatial extent of the kernel(s)
  - The number of kernels (or output channels)

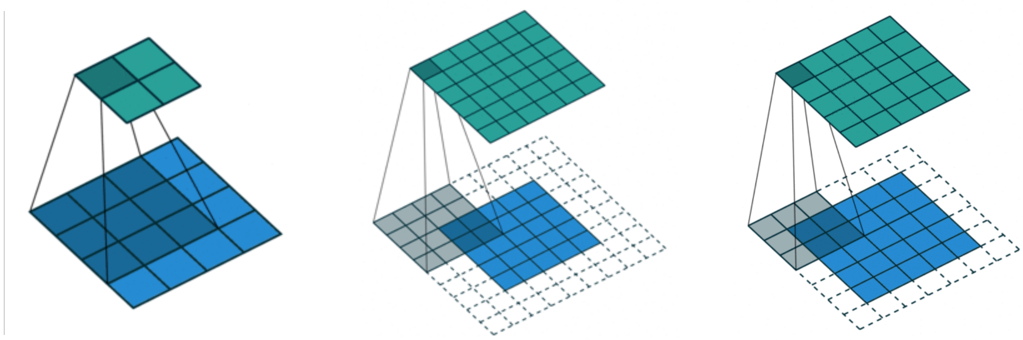
2d convolutions, kernel size=(1,1)

- 1x1 convolutions are a common place operation, but might seem non-sensical at first
  - They do not capture any local spatial information
  - They are used to change the number of feature maps without affecting the spatial resolution

Padding

- What happens to a convolution at the edges of its spatial extent?
  - In signal processing, using the Fourier transform the "image" wraps around, so the output is the same size as the input
  - In spatial convolution if we do nothing, the output will be smaller…
    - So, we often use zero-padding to retain the size

Arbitrary padding

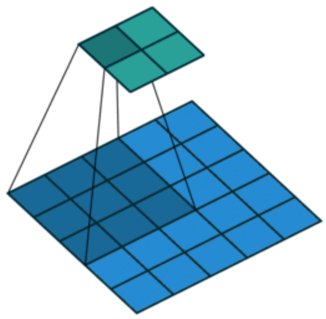


No padding

"same" padding

Striding

- Convolution is expensive… could we make it cheaper by skipping over positions?

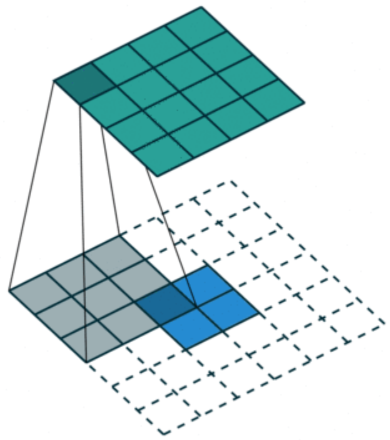


Stride=(2,2)

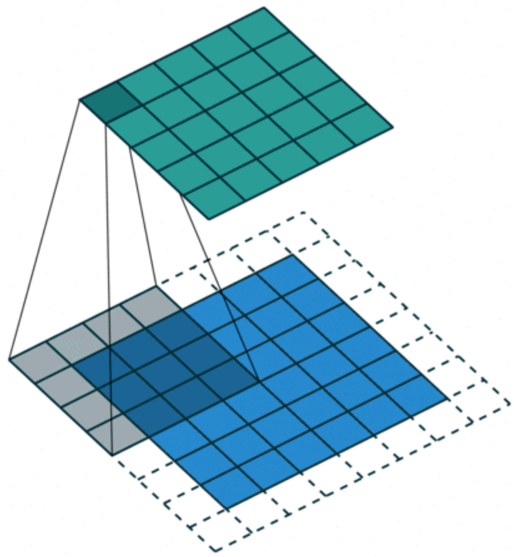
Fractional Striding/Transpose Convolution

- What if we consider *fractional* strides between 0 and 1?
  - Intuitively, if bigger strides subsample, then fractional strides should upsample
  - This is equivalent to “expanding” the input by padding and performing convolution
    - And potentially also striding by adding zeros around all the values

Transpose convolution, stride=1

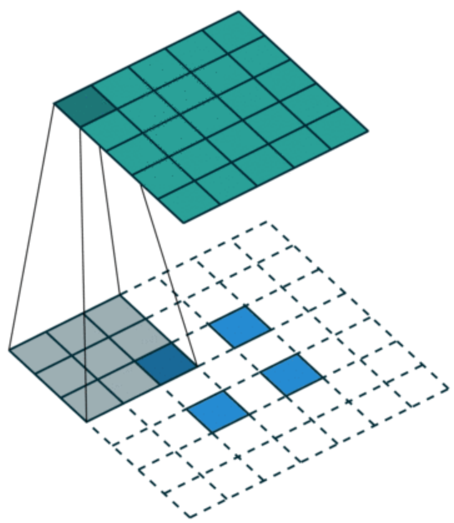


No padding

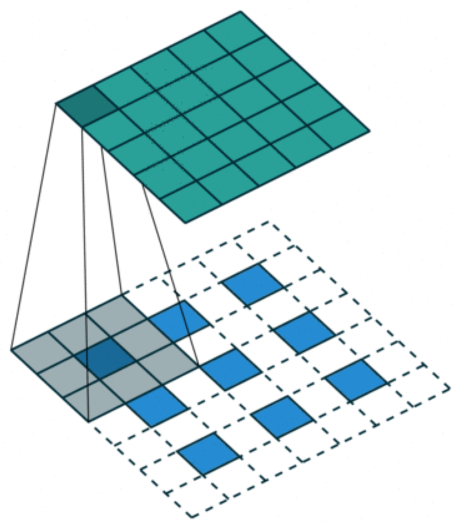


Arbitrary padding

Transpose convolution, stride=2



No padding



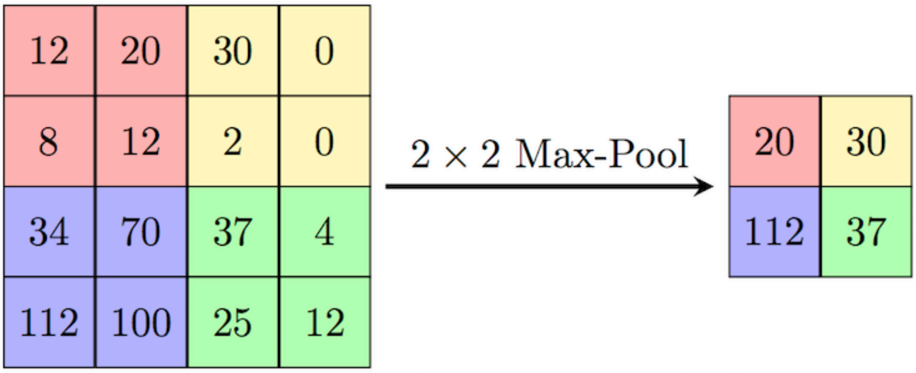
Padding

- You'll often find fractionally stride convolutions described as "transposed convolutions"
  - That's because they can be implemented by transposing the kernel's Toeplitz matrix before the multiply
- Some literature also refers to this as "deconvolution"
  - *Please don't do that!!*
- Also note that this might not be the best way of upsampling (see https://distill.pub/2016/deconv-checkerboard/)

Pooling

- Striding is a popular way to reduce spatial dimensionality in modern networks
  - before striding was devised, **pooling**, was the defacto way of reducing dimensionality

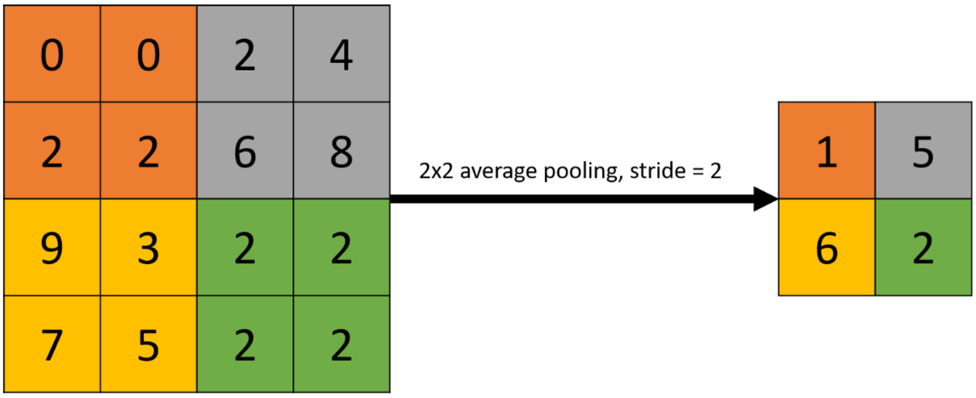
Max Pooling, 2x2, stride=2



Max Pooling Gradients

- The gradient of the max pooling operation is 1 everywhere a max value was selected, and zero elsewhere
  - This means that implementations not only need to record the max values in the forward-pass, but also keep track of the positions of those maximums for the backward pass

Average Pooling



Local Versus Global Pooling

- The pooling operations on the previous slides are local
    - They result in a feature map reducing in spatial size
- Global pooling reduces a feature map to a scalar
    - So a tensor of many feature maps would be reduced to a single feature vector
    - Often used near the end of networks to flatten feature maps into feature vectors that can be fed into an MLP

Dilated Convolutions

- Sometimes we want to have larger receptive fields in our networks
  - We can increase the kernel size to achieve this, but this introduces more weights
  - We can downsample/pool the input, but this decreases spatial resolution
  - Or we could 'pad' the kernel with zeros throughout to increase the effective size without increasing the number of parameters