Convolutional Neural Networks

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Mostly based on Thomas Hofmann's lecture in ETH

https://zhims.github.io/datascience.html

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Integral Operators

Definition 1 (Integral operator)

A transform T expressible with the kernel H and $t_1, t_2 \in \mathbb{R} \bigcup \{-\infty, \infty\}$ such that for any function f (for with Tf exists)

$$(Tf)(u) = \int_{t_1}^{t_2} H(u,t) f(t) dt \tag{1}$$

is called an integral operator.

Example 1 (Fourier transform)

$$(\mathcal{F}f)(u) \triangleq \int_{-\infty}^{\infty} e^{-2\pi i t u} f(t)\, dt \tag{2}$$

Definition 2 (Convolution)

Given two functions f, h, their convolution is defined as

$$(f * h)(u) \triangleq \int_{-\infty}^{\infty} h(u-t)\, f(t)\, dt = \int_{-\infty}^{\infty} f(u-t)\, h(t)\, dt \tag{3}$$

Remark 1

1. *integral operator with kernel* $H(u,t) = h(u-t)$
2. *shift-invariant as* $H(u-s, t-s) = h(u-t) = H(u,t) \quad (\forall s)$
3. *convolution operator is commutative*
4. *existence depends on properties of* f, h
5. *typical use* $f =$ *signal,* $h =$ *fast decaying kernel function*

Linear Time-Invariant Transforms

Definition 3 (Linear transform)

T is linear, if for all functions f, g and the scalars α, β,

$$T(\alpha f + \beta g) = \alpha T f + \beta T g \tag{4}$$

Definition 4 (Translation invariant transform)

T is translation (or shift) invariant, if for any f and scalar τ,

$$f_\tau(t) \triangleq f(t+\tau), \quad (T f_\tau)(t) \triangleq (Tf)(t+\tau) \tag{5}$$

Theorem 1

Any linear, translation-invariant transformation T can be written as convolution with a suitable h.

Signal Processing with Neural Networks

1. Transforms in deep networks: linear $+$ simple non-linearity
2. Many signals (audio, image, etc.) obey translation invariance $\Rightarrow$ invariant feature maps: shift in input $=$ shift in feature map

1 $+$ 2 in above:

1. $\Rightarrow$ learn convolutions, not (full connectivity) weight matrices
2. $\Rightarrow$ convolutional layers for signal processing

Discrete Convolutions

For all practical purposes: signal are sampled, i.e. discrete.

Definition 5 (Discrete convolution (1-D))

For $f, h : \mathbb{Z} \to \mathbb{R}$, we can define the discrete convolution via

$$(f * h)[u] \triangleq \sum_{t=-\infty}^{\infty} f[t]\, h[u-t] \tag{6}$$

Remark 2

1. *use of rectangular brackets to suggest "arrays"*
2. *2D case:*

$$\textit{content}\ldots \tag{7}$$

3. *typical: h with finite support (window size)*

Discrete Convolutions: Example

Example 2

Small Gaussian kernel with support $[-2:2] \subset \mathbb{Z}$

$$h[t] = \frac{1}{16} \begin{cases} 6 & t = 0 \\ 4 & |t| = 1 \\ 1 & |t| = 2 \\ 0 & \textit{otherwise} \end{cases} \tag{8}$$

Consequence: convolution sum can be truncated:

$$\begin{aligned} (f * h)[u] &= \sum_{t=u-2}^{u+2} f[t]\, h[u-t] = \sum_{t=-2}^{2} h[t]\, f[u-t] \\ &= \frac{6f[u] \; + 4f[u-1] + 4f[u+1] + f[u-2] + f[u+2]}{16} \end{aligned} \tag{9}$$

Discrete Cross-Correlation

Definition 6 (Discrete cross-correlation)

Let $f, h : \mathbb{Z} \to \mathbb{R}$, then

$$(h \otimes f)[u] \triangleq \sum_{t=-\infty}^{\infty} h[t] f[u+t] \tag{10}$$

Discrete Cross-Correlation

Remark 3

1. *Def. 6 also called a "sliding inner product", $u + t$ instead of $u - t$*
2. *note that cross-correlation and convolution are closely related:*

$$
\begin{aligned}
(h \otimes f)[u] &= \sum_{t=-\infty}^{\infty} h[t] f[u+t] \\
&= \sum_{t=-\infty}^{\infty} h[-t] f[u-t] \\
&= \left(\overline{h} * f\right)[u] \\
&= \left(f * \overline{h}\right)[u]
\end{aligned}
\tag{11}
$$

where $\overline{h}[t] \triangleq h[-t]$.

Only difference: kernel flipped over, but not non-commutative.

Convolution via Matrices

1. In practice: signal f and kernel h have finite support
2. Without loss of generality (w.l.o.g) $f[t] = 0$ for $t \notin [1:n]$, $h[t] = 0$ for $t \notin [1:m]$
3. We can think of f and h as vectors and define:

$$\underbrace{\begin{bmatrix} h_1 & 0 & 0 & \cdots & 0 & 0 & \cdots & \cdots & \cdots & \cdots \\ h_2 & h_1 & 0 & \cdots & 0 & 0 & \vdots & \vdots & \vdots & \vdots \\ h_3 & h_2 & h_1 & \cdots & 0 & 0 & \vdots & \vdots & \vdots & \vdots \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ h_m & h_{m-1} & h_{m-2} & \cdots & h_1 & 0 & \vdots & \vdots & \vdots & \vdots \\ 0 & h_m & h_{m-1} & \cdots & h_2 & h_1 & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & h_m & \cdots & h_3 & h_2 & \cdots & \cdots & \cdots & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & h_m & h_{m-1} & \cdots & \cdots & \cdots \\ \vdots & \vdots & \vdots & \cdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 & h_m \end{bmatrix}}_{\triangleq H_n^h \in \mathbb{R}^{(m+n-1)\times n}} \begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ \vdots \\ f_{m-1} \\ f_m \\ \vdots \\ \vdots \\ f_{n-2} \\ f_{n-1} \\ f_n \end{bmatrix} \tag{12}$$

Toeplitz Matrix

Definition 7 (Toeplitz matrix)

A matrix $H \in \mathbb{R}^{k \times n}$ is a Toeplitz matrix, if there exists $n + k - 1$ numbers c_l $(l \in [-(n-1) : (k-1)] \subset \mathbb{Z})$ such that

$$H_{ij} = c_{i-j} \tag{13}$$

Remark 4

1. *in plain English, all NW-SE diagonals are constant*
2. *if $m \ll n$: additional sparseness (band matrix of width m)*
3. *H_n^h has only m degrees of freedom*
4. *locality (sparseness $m \ll n$) and weight sharing (kernel)*

Sparse Connectivity

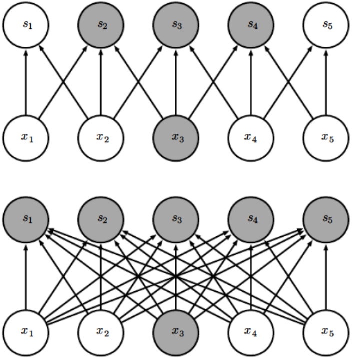


Figure 1: Sparse vs dense connectivity

Convolutions in Higher Dimensions

Generalize concept of convolution to:

1. 2D: e.g. images, spectograms
2. 3D: e.g. color or multi-spectral images, voxel images, video
3. or even higher dimensions

Replace vector by:

1. matrices or fields (e.g. in discrete case)

$$(F * G)[i, j] = \sum_{k=-\infty}^{\infty} \sum_{l=-\infty}^{\infty} F[i-k, j-l] \cdot G[k, l] \tag{14}$$

2. tensors: for 3D and higher

Different options for border handling:

1. our definition: padding with zeros = same padding
2. only retain values from windows fully contained in support of signal f = valid padding

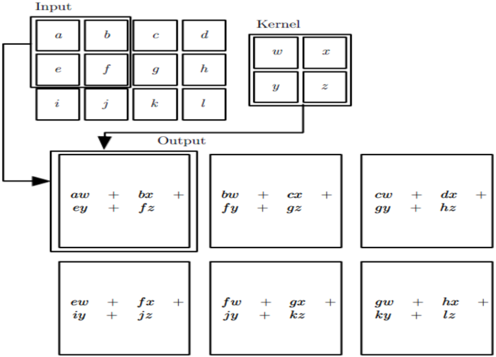


Figure 2:

Convolutional Layers: Layout

1. Convolved signal inherits topology of original signal
2. Hence: units in a convolutional layer are typically arranged on the same grid (1D, 2D, 3D,...)

Convolutional Layers: Backpropagation

Exploit structural sparseness in computing $\frac{\partial x_i^l}{\partial x_j^{l-1}}$:

1. receptive filed of x_i^l : $\mathcal{I}_i^l \triangleq \left\{ j : W_{ij}^l \neq 0 \right\}$, where W^l is the Toeplitz matrix of the convolution
2. obviously $\frac{\partial x_i^l}{\partial x_j^{l-1}} = 0$ for $j \notin \mathcal{I}_i^l$

Weight sharing in computing $\frac{\partial \mathcal{R}}{\partial h_j^l}$, where h_j^l is a kernel weight

$$\frac{\partial \mathcal{R}}{\partial h_j^l} = \sum_i \frac{\partial \mathcal{R}}{\partial x_i^l} \frac{\partial x_i^l}{\partial h_j^l} \tag{15}$$

Weight is re-used for every unit within target layer $\Rightarrow$ additive combination of derivatives in chain rule.

Efficient Computations of Convolutional Activities

FFT (Fast Fourier Transform): compute convolutions fast(er).

1. Fourier transform of signal $f \to (\mathcal{F}f)$ and kernel $h \to (\mathcal{F}h)$
2. pointwise multiplication and inverse Fourier transform:

$$(f * h) = \mathcal{F}^{-1}((\mathcal{F}f) \cdot (\mathcal{F}h)) \tag{16}$$

3. FFT: signal of length n, can be done in $O(n \ \mathrm{log} n)$
4. pays off, if many channels (amortizes computation of $\mathcal{F}f$)
5. small kernels ($m < \log n$): favor time / space domain

Convolutional Layers: Stages

1. Non-linearites: detector stage. As always: scalar non-linearities (activation function)
2. Pooling stage: locally combine activities

Pooling

Most frequently used pooling function: max pooling.

Definition 8 (Max Pooling)

Define window size r (e.g. 3 or 3×3), then

$$\begin{aligned} 1D: \quad & x_i^{\max} = \max\left\{x_{i+k} : 0 \leqslant k < r\right\}, \\ 2D: \quad & x_{ij}^{\max} = \max\left\{x_{i+k,j+l} : 0 \leqslant k, l < r\right\} \end{aligned} \tag{17}$$

Remark 5

1. *maximum over a small patch of units*
2. *other functions are possible: average, soft-maximization*

Max-pooling

Max-pooling: invariance

1. set of invertible transformations $\mathcal{T}$: group w.r.t composition
2. $\mathcal{T}-$invariance through maximization $f_{\mathcal{T}}(x) \triangleq \max_{\tau \in \mathcal{T}} f(\tau x)$

Proposition 1

$f_{\mathcal{T}}$ is invariant under $\tau \in \mathcal{T}$.

Proof.

$$f_{\mathcal{T}}(\tau x) = \max_{\rho \in \mathcal{T}} f(\rho(\tau x)) = \max_{\rho \in \mathcal{T}} (f(\rho \circ \tau) x) = \max_{\sigma \in \mathcal{T}} f(\sigma x) \tag{18}$$

as $\forall \sigma, \sigma = \rho \circ \tau$ with $\rho = \sigma \circ \tau^{-1}$. $\square$

Sub-Sampling(also known as (aka) Strides)

1. often, it is desirable to reduce the size of feature maps
2. sub-sampling: reduce temporal/spatial resolution. Often: combined with (max-)pooling (aka. stride)
3. example: max-pool, filter 2×2, stride 2×2
4. disadvantage: loss of information

Channels

Learn multiple convolution kernel (or filters) = multiple channels:

1. typically: all channels use same window size
2. channels form additional dimension for next layer (e.g. 2D signal $\times$ channels = 3D tensor)
3. number of channels: design parameter

Convolutional Layers: Animation

http://cs231n.github.io/assets/conv-demo/index.html

Convolutional Layers for Vision

Note that kernels (across channels) form a linear map:

$$h : \mathbb{R}^{r^2 \times d} \to \mathbb{R}^k \tag{19}$$

where $r \times r$ is the window size and d is the depth.

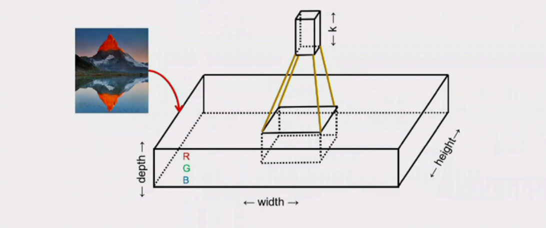


Figure 3: convolutional layers for vision

Convolutional Networks: ConvNets

Convolutional networks: multiple, stacked feature maps

$$\underbrace{y[r]}_{r-th\ channel}[s,t] = \sum_u \sum_{\Delta s, \Delta t} \underbrace{w[r,u][\Delta s, \Delta t]}_{parameters} \underbrace{x[u]}_{u-th\ channel}[s+\Delta s, t+\Delta t] \tag{20}$$

1. x, y tensor, 3-rd order
2. number of parameters:

$$\underbrace{\#r \cdot \#u}_{fully\ connected} \cdot \underbrace{\#\Delta s \cdot \#\Delta t}_{window\ size} \tag{21}$$

3. pointwise non-linearities (e.g. ReLU)
4. interleaved with: pooling (e.g. max, average)
5. optionally: downsampling (use of strides)

Convolutional Pyramid

Typical use of convolution in vision: sequence of convolutions that

1. reduce spatial dimensions (sub-sampling)
2. increase number of channels

$\Rightarrow$ smaller, but more feature maps.

LeNet5

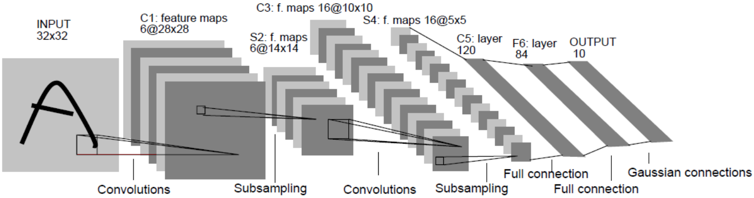


Figure 4: Architecture of LeNet-5, a convolutional neural network, here for digits recognition. Each plan is a feature map, i.e. a set of units whose weights are constrained to be identical.

1. C1/S2: 6 channels, 5×5 kernels, 2×2 sub (4704 units)
2. C3/S4: 16 channels,6×6 kernels, 2×2 sub (1600 units)
3. C5: 120 channels, F6: fully-connected
4. output: Gaussian noise model (squared loss)

AlexNet

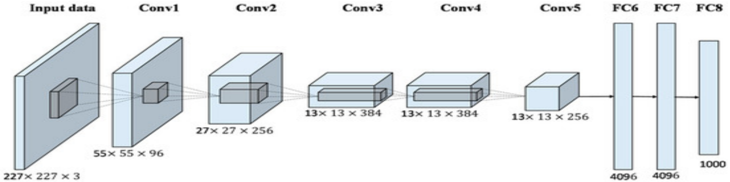


Figure 5: AlexNet architecture

1. Pyramidal architecture: reduce spatial resolution, increase channels with depth
2. Challenge: many channels (width) + large windows + depth
3. Number of parameters
    1. 384 to 384 channels with 3×3 windows: > 1.3 M
    2. $13 \times 13 \times 384$ tensor to 4096, fully connected: > 265 M

Deep ConvNets: Key Challenges

1. avoid blow-up of model size (e.g. # parameters)
2. preserve computational efficiency of learning (e.g. gradients)
3. allow for large depth (as it is known to be a plus)
4. allow for sufficient width (as it is known to be a plus, too)

Very Deep Convolutional Networks: VGG

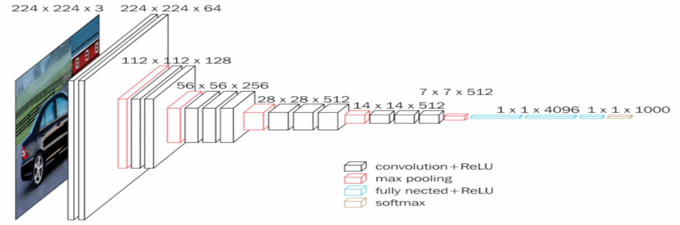


Figure 6: VGG 16

1. use very small receptive fields (maximally 3×3)
2. avoid downsampling/pooling
3. stacking small receptive fields: more depth, fewer parameters
4. example: $3 \cdot (3 \times 3) = 27 < 49 (7 \times 7)$

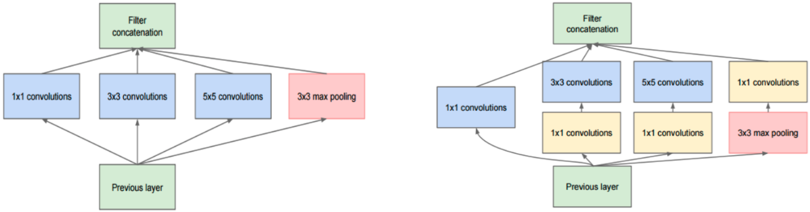
Inception Module: 1×1 Convolution

Many channels needed for high accuracy, typically $k \sim 200 - 1000$ (e.g. AlexNet: 2×192).
Observation (motivated by Arora et al, 2013): when convolving, dimension reduction across channels may be acceptable.
Dimension reduction: m channels of a $1 \times 1 \times k$ convolution $m \leq k$:

$$x_{ij}^{+} = \sigma\left(W x_{ij}\right), \quad W \in \mathbb{R}^{m \times k} \tag{22}$$

1. 1×1 convolution $=$ no convolution
2. inception module (Szegedy et al.)
3. network within a network (Lin et al.)
4. i.e. W is shared for all (i, j) (translation invariance)

Inception Module: Mixing



(a) naive version (b)

Figure 7: Inception Module

Instead of fixed window size convolution: mix 1×1 with 3×3 and 5×5, max-polling. Use 1×1 convolutions for dimension reduction before convolving with large kernels.

Google Inception Network

Very deep network: many inception modules (green boxes: concatenation points). Additional trick: connect softmax layer (and loss) at intermediate stages (yellow boxes) $\Rightarrow$ gradient shortcuts.

Google Inception Network

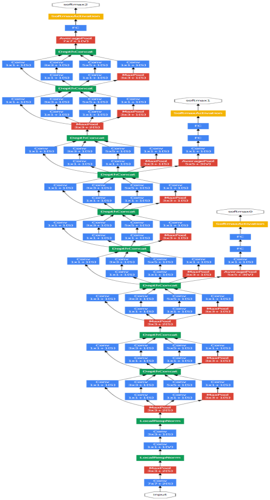


Figure 8: Google inception networks

Residual Networks: ResNets

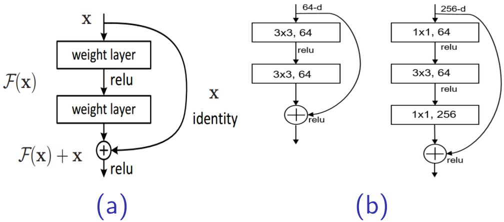


Figure 9: Residual Networks module

1. learn changes to the identity map (aka. shortcut connections)
2. use small filters (VGG), use dimension reduction (inception)
3. reach depth of 100 + layers (+ increase accuracy + trainable)

Thank you all of you! –Yao