Lecture 1: Convolutional Neural Networks

Lecturer: Thomas Hofmann

Scribes: Yao Zhang

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Definition 1.1 (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)

$$(Tf)(u) = \int_{t_1}^{t_2} H(u,t) f(t) dt$$
(1.1)

is called an integral operator.

Example 1.1 (Fourier transform).

$$\left(\mathcal{F}f\right)\left(u\right) \triangleq \int_{-\infty}^{\infty} e^{-2\pi i t u} f\left(t\right) dt \tag{1.2}$$

Definition 1.2 (Convolution). Given two functions f, h, their convolution is defined as

$$(f*h)(u) \triangleq \int_{-\infty}^{\infty} h(u-t) f(t) dt = \int_{-\infty}^{\infty} f(u-t) h(t) dt$$
(1.3)

Remark 1.1.

- 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) ($\forall s$)

Proof. content...

3. convolution operator is commutative

Proof. content...

- 4. existence depends on properties of f, h
- 5. typical use f = signal, h = fast decaying kernel function

Definition 1.3 (Linear transform). T is linear, if for all functions f, g and the scalars α, β ,

$$T\left(\alpha f + \beta g\right) = \alpha T f + \beta T g \tag{1.4}$$

Definition 1.4 (Translation invariant transform). *T* is translation (or shift) invariant, if for any *f* and scalar τ ,

$$f_{\tau}(t) \triangleq f(t+\tau), \quad (Tf_{\tau})(t) \triangleq (Tf)(t+\tau)$$
(1.5)

Remark 1.2. content...

Theorem 1.1. Any linear, translation-invariant transformation T can be written as convolution with a suitable h.

Proof. content...

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

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

Definition 1.5 (Discrete convolution (1-D)). For $f, h : \mathbb{Z} \to \mathbb{R}$, we can define the discrete convolution via

$$(f * h) [u] \triangleq \sum_{t=-\infty}^{\infty} f[t] h [u-t]$$
(1.6)

Remark 1.3.

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

- content... (1.7)
- 3. typical: h with finite support (window size)

Example 1.2. Small Gaussian kernel with support $[-2:2] \subset \mathbb{Z}$

$$h[t] = \frac{1}{16} \begin{cases} 6 & t = 0\\ 4 & |t| = 1\\ 1 & |t| = 2\\ 0 & otherwise \end{cases}$$
(1.8)

Consequence: convolution sum can be truncated:

$$(f*h)[u] = \sum_{t=u-2}^{u+2} f[t]h[u-t] = \sum_{t=-2}^{2} h[t]f[u-t]$$

=
$$\frac{6f[u] + 4f[u-1] + 4f[u+1] + f[u-2] + f[u+2]}{16}$$
(1.9)

Remark 1.4. content...

Definition 1.6 (Discrete cross-correlation). Let $f, h : \mathbb{Z} \to \mathbb{R}$, then

$$(h \otimes f) [u] \triangleq \sum_{t=-\infty}^{\infty} h [t] f [u+t]$$
(1.10)

Remark 1.5.

- 1. Def. 1.6 also called a "sliding inner product", u + t instead of u t
- 2. note that cross-correlation and convolution are closely related:

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

=
$$\sum_{t=-\infty}^{\infty} h[-t] f[u-t]$$

=
$$(\overline{h} * f) [u]$$

=
$$(f * \overline{h}) [u]$$

(1.11)

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:

 $\triangleq H_n^h \in \mathbb{R}^{(m+n-1) \times n}$

Remark 1.6. content...

(1.12)

Definition 1.7 (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

$$H_{ij} = c_{i-j} \tag{1.13}$$

Remark 1.7.

- 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)



Figure 1.1: 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)

$$(F * G)[i, j] = \sum_{k=-\infty}^{\infty} \sum_{l=-\infty}^{\infty} F[i - k, j - l] \cdot G[k, l]$$
(1.14)

2. tensors: for 3D and higher

Different options for border handling:

1. our definition: padding with zeros = same padding



Figure 1.2

2. only retain values from windows fully contained in support of signal f = valid padding 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,...)

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

1. receptive filed of $x_i^l : \mathcal{I}_i^l \triangleq \{j : W_{ij}^l \neq 0\}$, 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 $\frac{\partial \mathcal{R}}{\partial h_i^l}$, where h_j^l is a kernel weight

$$\frac{\partial \mathcal{R}}{\partial h_j^l} = \sum_i \frac{\partial \mathcal{R}}{\partial x_i^l} \frac{\partial x_i^l}{\partial h_j^l} \tag{1.15}$$

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

$$(f * h) = \mathcal{F}^{-1} \left((\mathcal{F}f) \cdot (\mathcal{F}h) \right) \tag{1.16}$$



Figure 1.3

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

Remark 1.8. content...

Stages:

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

Most frequently used pooling function:max pooling.

Definition 1.8 (Max Pooling). Define window size r (e.g. 3 or 3×3), then

$$1D: \quad x_i^{\max} = \max \left\{ x_{i+k} : 0 \le k < r \right\},
2D: \quad x_{ij}^{\max} = \max \left\{ x_{i+k,j+l} : 0 \le k, l < r \right\}$$
(1.17)

Remark 1.9.

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

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

Proof.

$$f_{\mathcal{T}}(\tau x) = \max_{\rho \in \mathcal{T}} f(\rho(\tau x)) = \max_{\rho \in \mathcal{T}} \left(f(\rho \circ \tau) x \right) = \max_{\sigma \in \mathcal{T}} f(\sigma x)$$
(1.18)

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

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

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

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

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

$$h: \mathbb{R}^{r^2 \times d} \to \mathbb{R}^k \tag{1.19}$$

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



Figure 1.4: convolutional layers for vision

Convolutional networks: multiple, stacked feature maps

$$\underbrace{y[r]}_{r-th\ channel}[s,t] = \sum_{u} \sum_{\Delta s,\Delta t} \underbrace{w[r,u][\Delta s,\Delta t]}_{parameters} \underbrace{x[u]}_{u-th\ channel}[s+\Delta s,t+\Delta t]$$
(1.20)

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

$$\underbrace{\#r \cdot \#u}_{fully \ connected} \quad \cdot \quad \underbrace{\#\Delta s \cdot \#\Delta t}_{window \ size} \tag{1.21}$$

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.



Figure 1.5: 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. [2]

LeNet5 [1,2]

- 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[3]

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



Figure 1.6: AlexNet architecture





Figure 1.7: 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: $3 \cdot (3 \times 3) = 27 < 49(7 \times 7)$

Many channels needed for high accuracy, typically $k \sim 200 - 1000$ (e.g. AlexNet: 2×192).

Observation (motivated by Arora et al, 2013 [5]): when convolving, dimension reduction across channels may be acceptable.

Dimension reduction: *m* channels of a $1 \times 1 \times k$ convolution $m \leq k$:

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

$$(1.22)$$

- 1. 1×1 convolution = no convolution
- 2. inception module (Szegedy et al. [6])
- 3. network within a network (Lin et al, [7])
- 4. i.e. W is shared for all (i, j) (translation invariance)

Inception module: mixing



Figure 1.8: Inception module [8]

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 networks [6]



Figure 1.9: Google inception networks

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.

Residual networks: ResNets [9]



(b)

Figure 1.10: Residual Networks module [9]

- 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)

Models for sequences:

- 1. many relevant application deal with sequences, e.g. time series(speech, sensors), sequences of symbols (language, biology)
- 2. vector-valued sequences: $x^t \in \mathbb{R}^d, t = 0, 1, 2, \dots$
- 3. symbol sequences: $\omega^t \in \Omega, t = 0, 1, 2, \dots$ with Ω : alphabet
 - (a) variable length sequences, how to represent?
 - (b) translation invariance, how to incorporate?

From symbols to vectors: DNNs operate on real-valued vectors. How can we process (and learn with) symbol sequences? The answer is: via embeddings.

Definition 1.9 (symbol Embedding). A *d*-dimensional symbol embedding is a mapping $z : \Omega \to \mathbb{R}^d$, which maps every symbol to a vector representation.

Definition 1.10 (Sequence Matrix). Given a symbol sequence $\omega^1, ..., \omega^s$ and an embedding z, the sequence matrix Z is defined via

$$Z = \left| z \left(\omega^1 \right) \cdots z \left(\omega^s \right) \right| \in \mathbb{R}^{d \times s}$$
(1.23)

DNN terminology: embedding "layer" = look-up layer. Shortcut $z_i \triangleq z(\omega_i)$.

Learnable symbol representations:

- 1. embedding are not fixed, but are learned from data!
- 2. gradient-based updates via backpropagation, compute $\nabla_{Z_i} l$
- 3. which embeddings are updated depends on which symbols occurred (and how often)
- 4. learn (just) embeddings in self-supervised learning (a.k.a representation learning), e.g. word embeddings (word2vec, skipgram, GloVe)

CNNs for natural language processing: multi-Channel CNNs for NLP

Classical CNN architecture [10]:

- 1. look-up layers for words and (optionally) linguistic feature
- 2. 1-d multi-channel convolution
- 3. polling over time (e.g. max)
- 4. fully connected layers
- 5. softmax classifier (e.g.)



Figure 1.11: A general deep NN architecture for NLP, in [10]

Deep CNNs for sentence modeling: single-channel cross-pooling CNNs for NLP, alternative modern CNN architecture in [11]:

- 1. embedding layers
- 2. (wide) one-channel convolutions

- 3. max-k polling (order preserving)
- 4. "dynamic" = k based on data
- 5. cross-channel interactions via folding (parameter free)



Figure 1.12: A DCNN for the seven word input sentence., in [11]

Other work on CNNs for NLP: themes and variants found in the recent literature

- 1. Pham et al [12], convoluctional neural network language model: avoid max pooling, use batch normalization, (almost) competitive language model.
- 2. Severyn & Moschitti [13], sentiment prediction for tweets.

Next topic is recurrent networks

Reading List

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