Lecture 4

Representation Learning with Convolutions

Part 1: Representation Learning

Machine Learning for Structured Data

Vlad Niculae · LTL, UvA · `https://vene.ro/mlsd`

Representation Learning with Convolutions

Representation Learning

So far, we have used hand-crafted representations $\boldsymbol{h}(x)$.

Starting today, we explore deep learning methods that can generate representations of structured data.

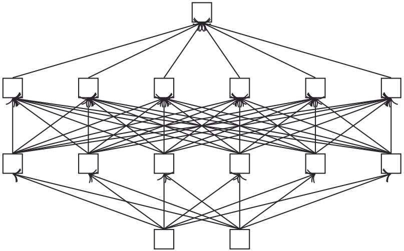
Fully-connected feed-forward layers.

For unstructured data, where we can represent each data point as a fixed-dim vector $\boldsymbol{z}_0 = \boldsymbol{h}_0(\boldsymbol{x}) \in \mathbb{R}^d$, feed-forward network.

The last hidden layer $\boldsymbol{z}_m$ can be seen as a richer vector representation of the data point.

How to handle structured inputs? Often of different sizes?

We will explore architectures that can handle sequences, grids, graphs of different dimensions.



$f(x)$

$\boldsymbol{z}_2 = \phi(\boldsymbol{W}_2\boldsymbol{z}_1 + \boldsymbol{b}_2)$

$\boldsymbol{z}_1 = \phi(\boldsymbol{W}_1\boldsymbol{z}_0 + \boldsymbol{b}_1)$

$\boldsymbol{z}_0 = \boldsymbol{h}_0(x)$

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Part 2: 1-d convolutions

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Convolutions

When applying a dense linear layer $\boldsymbol{W}\boldsymbol{z} + \boldsymbol{b}$,
the *input* and *output* dimensions must be fixed, because

$$\text{shape}(\boldsymbol{W}) = (d_{\text{out}}, d_{\text{in}})$$

Convolutions

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the *input* and *output* dimensions must be fixed, because

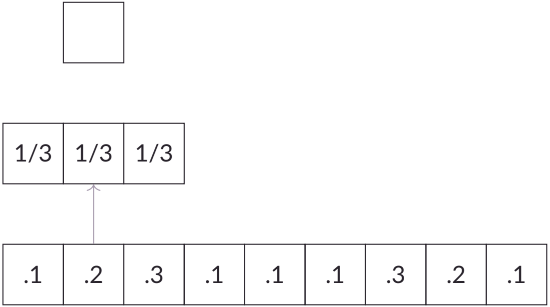
$$\text{shape}(\boldsymbol{W}) = (d_{\text{out}}, d_{\text{in}})$$

Convolutions: what if we learned small linear layers
that we **slide** along an input of variable size.

1-d, single-channel convolution

Simplest case: z_0 is just a sequence of numbers.

(Example: audio signal processing, time series...)



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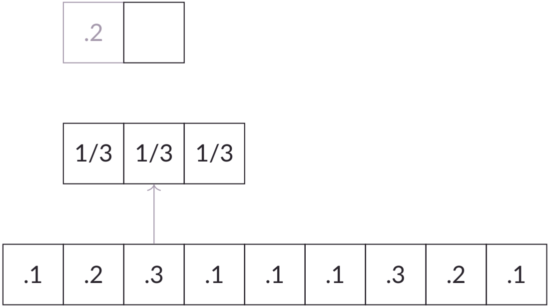

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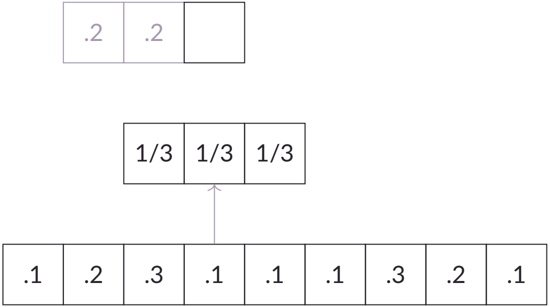

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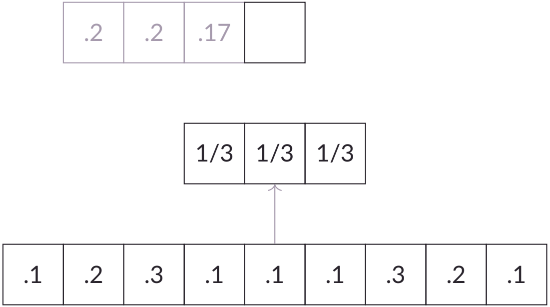

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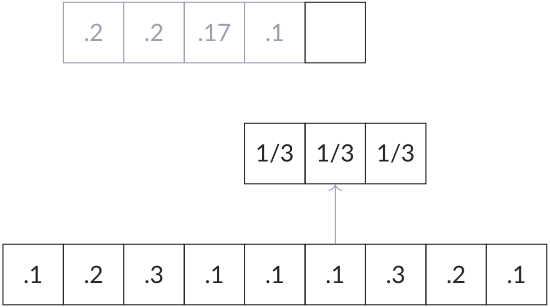

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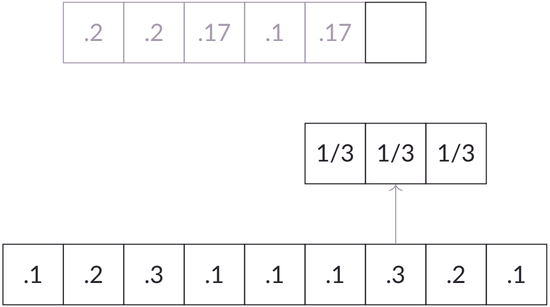

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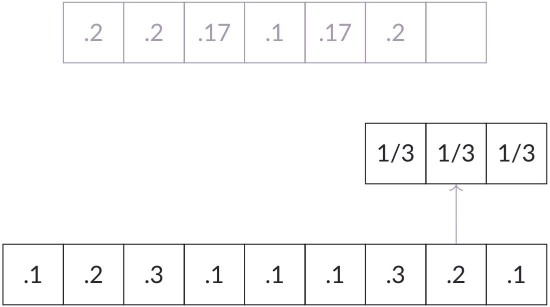

1-d, single-channel convolution

Simplest case: z_0 is just a sequence of numbers.

(Example: audio signal processing, time series…)

.2	.2	.17	.1	.17	.2	.2

.1	.2	.3	.1	.1	.1	.3	.2	.1

1-d, single-channel convolution

Simplest case: z_0 is just a sequence of numbers.

(Example: audio signal processing, time series…)

.2	.2	.17	.1	.17	.2	.2

.1	.2	.3	.1	.1	.1	.3	.2	.1

- Only k parameters, but can apply to seq. of any length.
- Filters are **activated** by patches that match them.
- Since we slide, the **position** of the matching patch doesn't matter. ("translation equivariance")
- Maps an input sequence to an output sequence of (almost) the same length. To make it the same length, we can assume zero padding.

1-d, single-channel convolution

Simplest case: z_0 is just a sequence of numbers.

(Example: audio signal processing, time series…)

.1	.2	.2	.17	.1	.17	.2	.2	.1

0	.1	.2	.3	.1	.1	.1	.3	.2	.1	0

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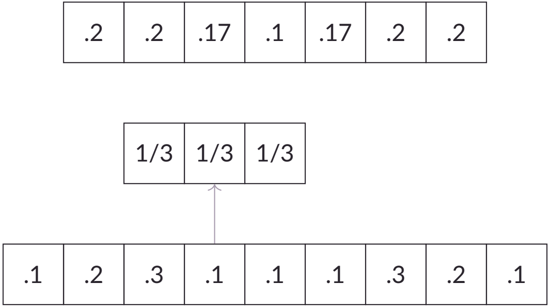
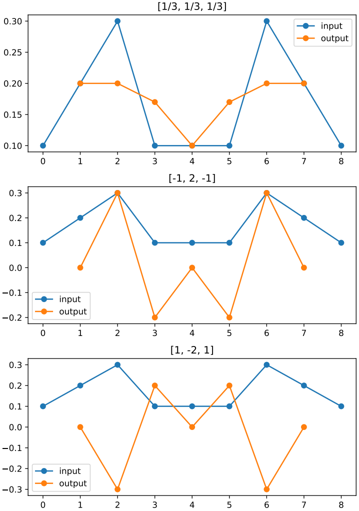
Effects of different convolutional filters





Convolution is sparkling matrix multiplication

- Turns out, convolution is multiplication with a “special” matrix, $\boldsymbol{z}_1 = \boldsymbol{W}\boldsymbol{z}_0$.
- But this $\boldsymbol{W}$ has a very special form that allows it to “stretch” to any size!
- This happens implicitly: such a matrix is never actually built in memory.

$$\begin{bmatrix} .1 \\ .2 \\ .2 \\ .17 \\ .1 \\ .17 \\ .2 \\ .2 \\ .1 \end{bmatrix} = \boldsymbol{W} \begin{bmatrix} .1 \\ .2 \\ .3 \\ .1 \\ .1 \\ .1 \\ .3 \\ .2 \\ .1 \end{bmatrix}$$

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$$
\begin{bmatrix} .1 \\ .2 \\ .2 \\ .17 \\ .1 \\ .17 \\ .2 \\ .2 \\ .1 \end{bmatrix}
=
\begin{bmatrix}
1/3 & 1/3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1/3 & 1/3 & 1/3 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1/3 & 1/3 & 1/3 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1/3 & 1/3 & 1/3 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1/3 & 1/3 & 1/3 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1/3 & 1/3 & 1/3 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1/3 & 1/3 & 1/3 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1/3 & 1/3 & 1/3 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1/3 & 1/3
\end{bmatrix}
\begin{bmatrix} .1 \\ .2 \\ .3 \\ .1 \\ .1 \\ .1 \\ .3 \\ .2 \\ .1 \end{bmatrix}
$$

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Part 3: Embedding Discrete Data

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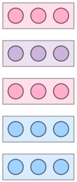
Embeddings of Discrete Tokens

Neural networks perform continuous operations.

For sequential **discrete** data, (language, DNA, etc), we must first represent each token as a continuous “embedding” vector.

$$\underbrace{\begin{bmatrix} 3 \\ 2 \\ 3 \\ 1 \\ 1 \end{bmatrix}}_{\in \mathbb{R}^{L}} \rightarrow \underbrace{\begin{bmatrix} \boldsymbol{e}(3) \\ \boldsymbol{e}(2) \\ \boldsymbol{e}(3) \\ \boldsymbol{e}(1) \\ \boldsymbol{e}(1) \end{bmatrix}}_{\in \mathbb{R}^{L \times d}}$$



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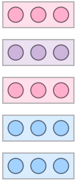
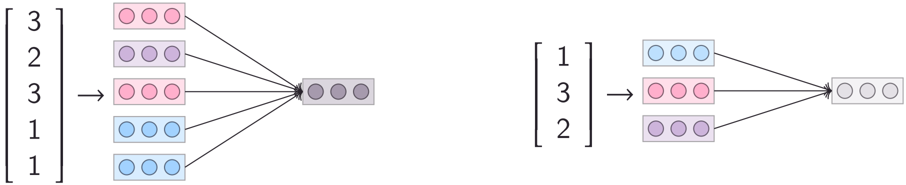


The function $\boldsymbol{e}(i)$ retrieves the ith row from an *embedding matrix* $\mathbf{E} \in \mathbb{R}^{|V| \times d}$.

The embeddings could be fixed or learned as model parameters.

Continuous Bag Of Words

Different-length sequences can be encoded by pooling their embeddings.



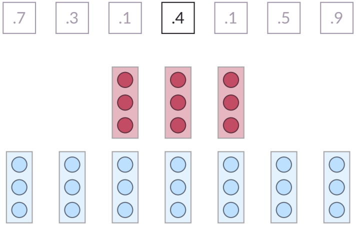
- average pooling: $\boldsymbol{z} = \frac{1}{L}(\boldsymbol{z}_1 + \ldots + \boldsymbol{z}_L)$
- max pooling: $[\boldsymbol{z}]_j = \max([\boldsymbol{z}_1]_j, \ldots, [\boldsymbol{z}_L]_j$ (coordinate-wise)

Just like in the standard bag of words, word order doesn't matter.

Sequence convolutions

aka 1-d convolution with *d* channels

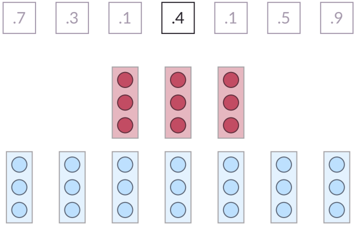
- Denote L=sequence length, d=embedding size, k=window size.



To reduce visual noise on slides, we now use the same color for all words, even if they're different words in general.

Sequence convolutions

aka 1-d convolution with d channels



- Denote L=sequence length, d=embedding size, k=window size.
- In the single-channel case, a filter was a dim-k vector. Now, a filter is a $d \times k$ matrix.

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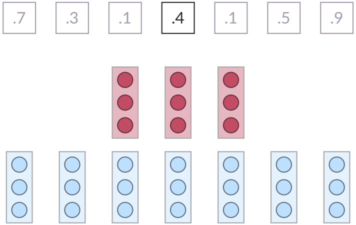

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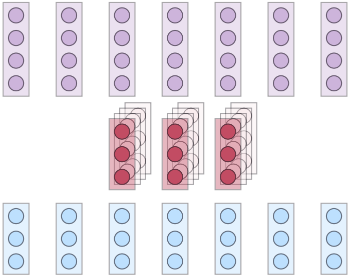

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- Apply m filters in parallel: output is a dim-m vector per window:

  a “layer” maps $(L, d) \rightarrow (L, m)$, for any L.

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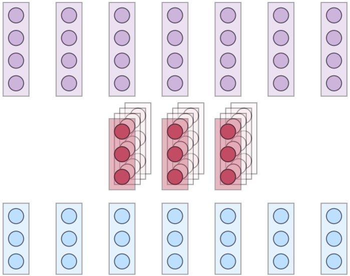

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  a "layer" maps $(L, d) \to (L, m)$, for any L.
- Kind of like "continuous" n-grams!

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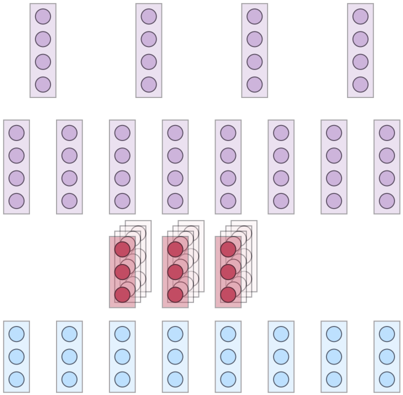
Stacking convolutions



- Many different architectures are possible.
- One successful idea: (also in your assignment 1)
  alternate convolutions with (max-)pooling over small windows: hidden representations go from finer (local) to coarser (more global).
- Each (conv + max-pool) layer reduces sequence length by the size of the pooling window.
- After enough layers, pool globally to get a d_{out}-dimensional representation independent of L.

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Part 4: 2-d convolution

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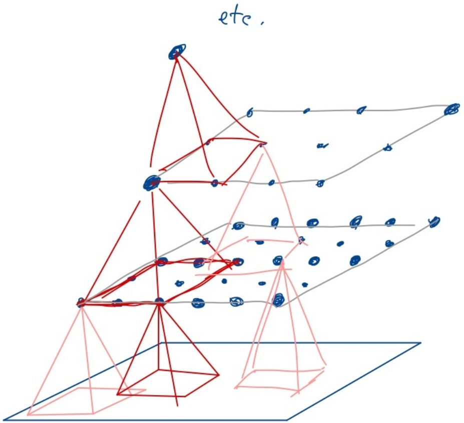
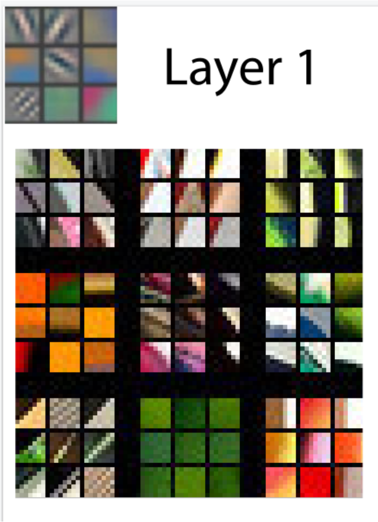
Representation Learning with Convolutions

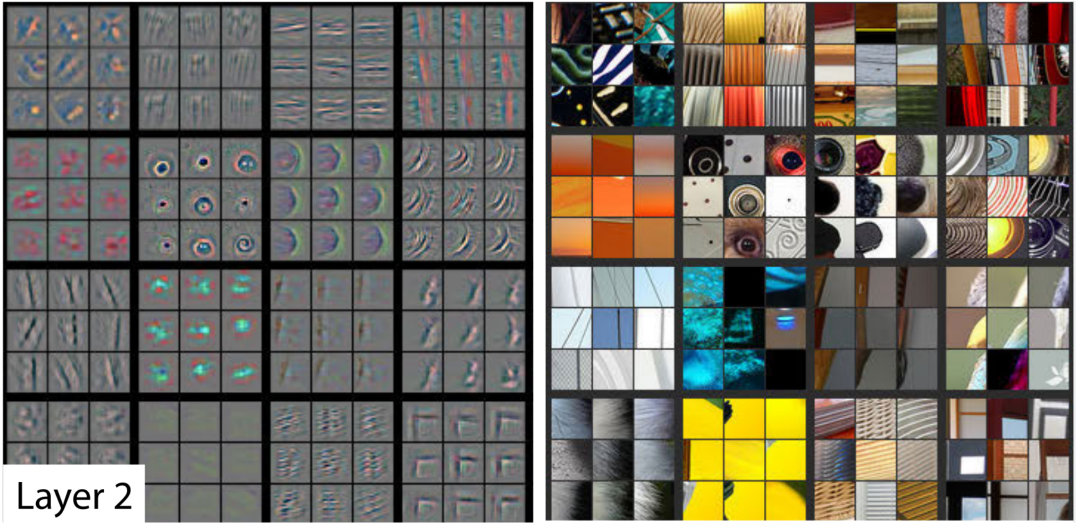
Convolutions for images: 2-d convolution



- Instead of just left-to-right, we slide the filter left-to-right top-to-bottom.
- As we go deeper, learned filters become more global/abstract.



From Zeiler and Fergus (2014), “Visualizing and Understanding Convolutional Networks”. ECCV, ©Springer.



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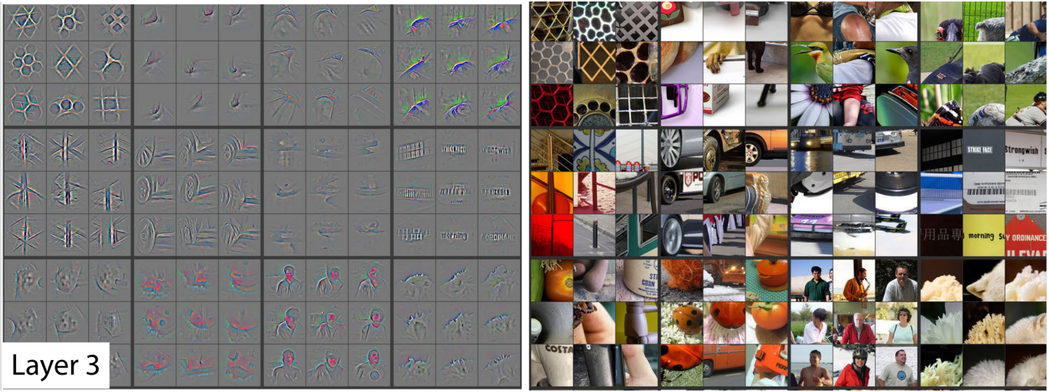

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Some more practical considerations of convolutions

- Convolutions work great when the phenomenon of interest is fairly local.
- *Strided* convolution: when sliding, skip over a few positions.
  (As long as stride $<$ kernel size $/$ 2, no input positions are ignored.)
- If we want to compute representations of every position (word/pixel) rather than a global representation, there are two options:
  1. no pooling and no striding,
  2. down-sample and then up-sample again ("transpose convolutions"), e.g. "U-net" (Ronneberger et al, 2015).

Convolutions:

1. Representation Learning
2. 1-d convolutions
3. Embedding Discrete Data
4. 2-d convolution