Popular NN Architectures

…and a little bit on the No Free Lunch theorems

Machine Learning and Data Mining, 2020

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Side note: No Free Lunch

A question from an IQ test

- Given the following pattern of numbers:

$$1, \qquad 8, \qquad 27, \qquad ?, \qquad 125, \qquad 216$$

what is the missing number?

a) 36
b) 45
c) 46
d) 64
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$$X_{\text{test}} = (4,)$$

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Prior knowledge

- No free lunch theorem (roughly speaking): without prior knowledge all solutions are equally good (or bad)

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- Generalization performance:

$$\text{gP}(\mathcal{A}, D_{train}) = \frac{1}{|D_{\text{test}}|} \sum_{x,y \in D_{\text{test}}} \mathbb{I}[A(D_{\text{train}})(x) = y] - \frac{1}{2}$$

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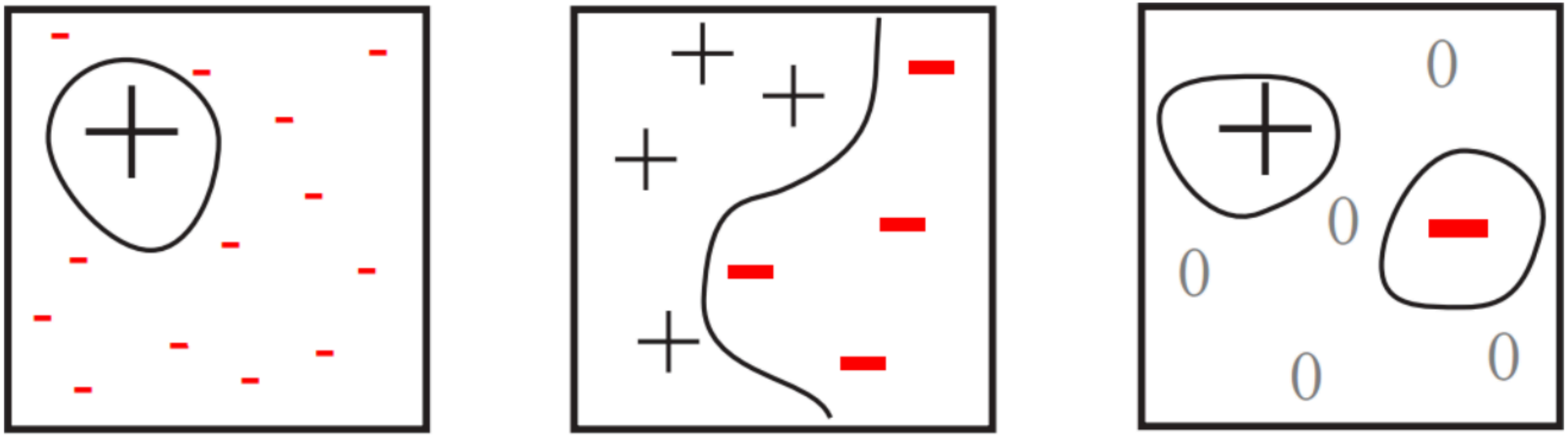
- Theorem statement:

$$\boxed{\sum_{f, D_{train}} \text{gP}(\mathcal{A}, D_{train}) = 0}$$

In the problem space



- Possible performance of learning algorithms:
  - Worse than average (–)
  - Better than average (+)

Back to the IQ test problem

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- To solve the test one must think like the authors of the test
- To solve a real world ML problem one must think like… the real world.

NFL theorem: critique

- Not all problems are equally likely (in the real world):
  - continuity;
  - human bias: e.g. feature preselection
  - prior knowledge of the problem at hand
- E.g. memorization + interpolation becomes an effective strategy for continuous data
- The following still holds though:

To improve the performance on one class of problems one must sacrifice the performance on others.

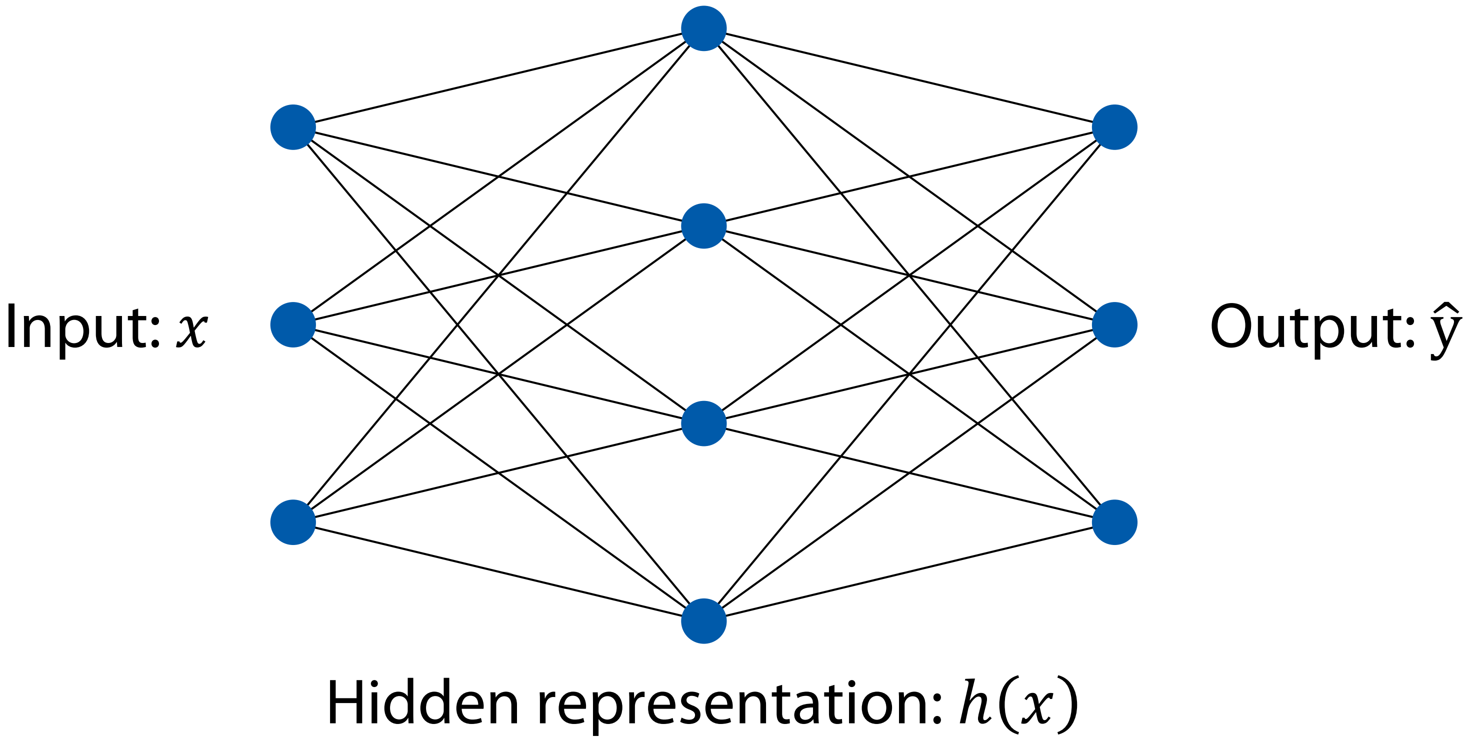
The role of data scientist

- Identify the suitable learning algorithm using the prior knowledge:
  - continuity;
  - structure of the data;
  - quality of the data;
  - domain knowledge;
  - size of the dataset;
  - common sense;
  - etc.
- In the context of deep learning: **find a suitable architecture**

NN architecure: simple examples

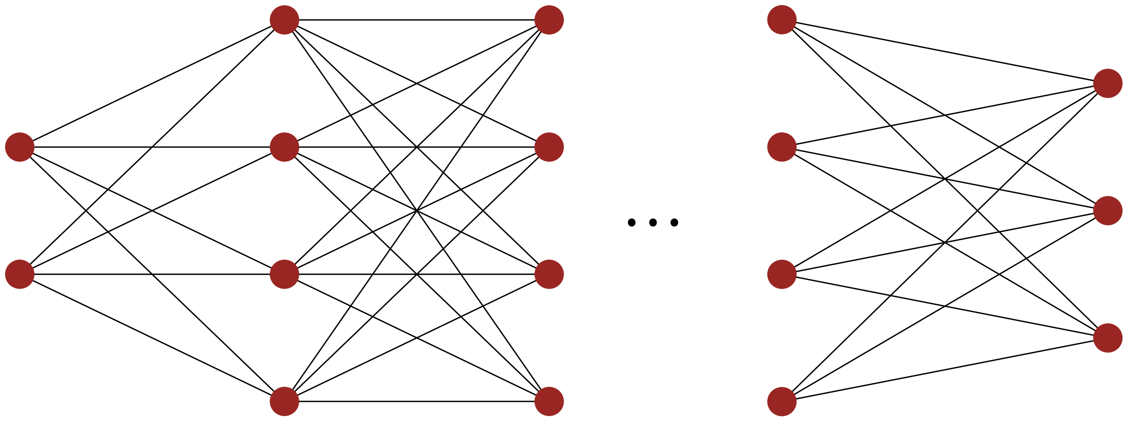
Single hidden layer fully-connected network

- Universal approximator
- May reqire infeasibly large hidden representation for more complex dependencies



Deep fully-connected network

- May use smaller representations
- Suitable for many real-world problems
- Harder to optimize
  - Typically becomes quite challenging for 10+ layers



- **An initial point for other architectures.**

Convolution

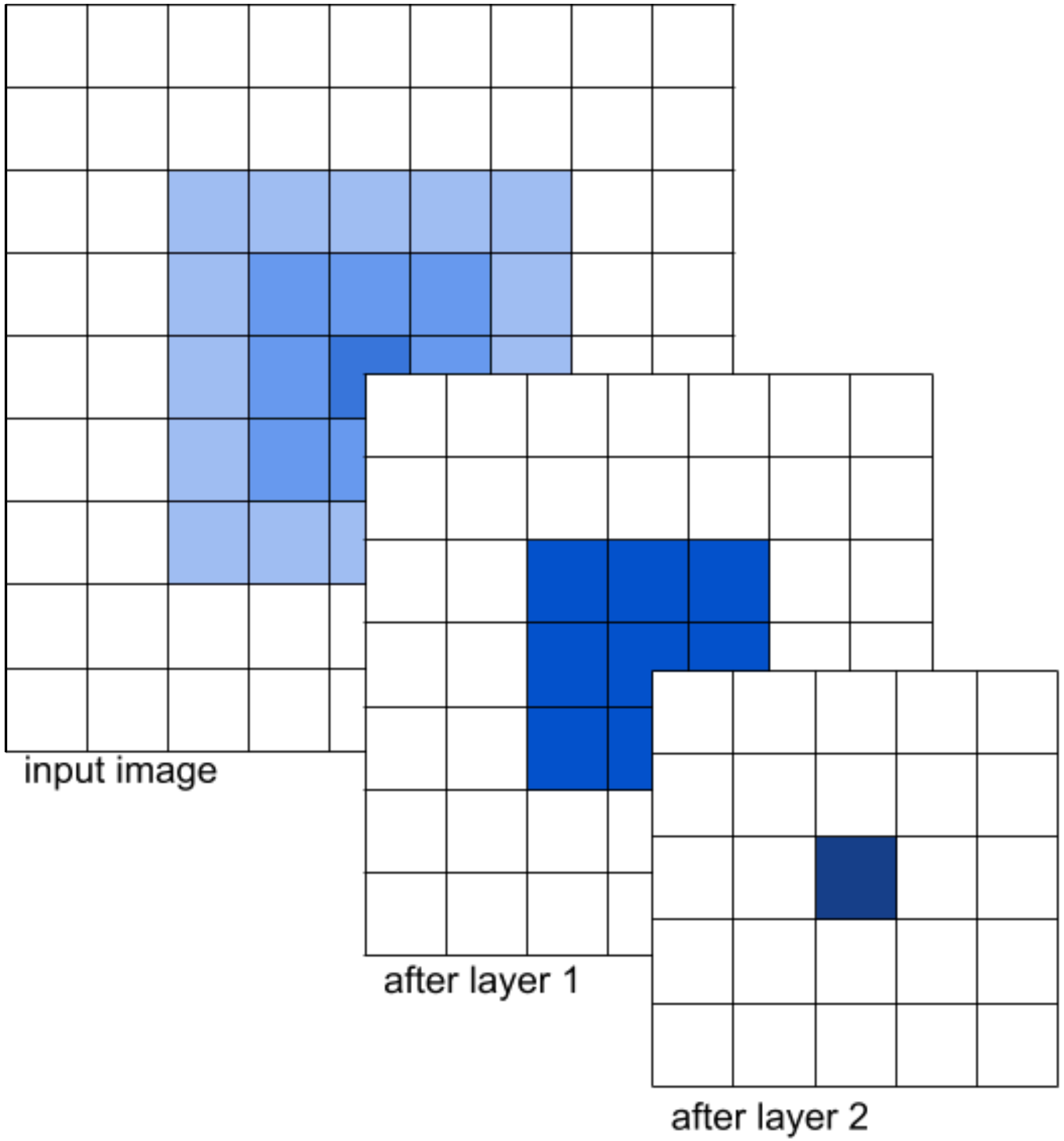
- Spacial/temporal structure of the data
- Can be described in terms of a fully connected layer
- Uses much less parameters
  - Re-uses weights in a sliding window

2D convolution as a matrix multiplication

$$\underbrace{\begin{bmatrix} a & b & c \\ d & e & f \\ g & h & i \end{bmatrix}}_{\text{Input}} \quad \underbrace{\begin{bmatrix} x & y \\ z & w \end{bmatrix}}_{\text{Kernel}} \quad \underbrace{\begin{bmatrix} ax+by+dz+ew & bx+cy+ez+fw \\ dx+ey+gz+hw & ex+fy+hz+iw \end{bmatrix}}_{\text{Output}}$$

$$\begin{bmatrix} ax+by+dz+ew \\ dx+ey+gz+hw \\ bx+cy+ez+fw \\ ex+fy+hz+iw \end{bmatrix} = \begin{bmatrix} x & y & 0 & z & w & 0 & 0 & 0 & 0 \\ 0 & x & y & 0 & z & w & 0 & 0 & 0 \\ 0 & 0 & 0 & x & y & 0 & z & w & 0 \\ 0 & 0 & 0 & 0 & x & y & 0 & z & w \end{bmatrix} \times \begin{bmatrix} a \\ b \\ c \\ d \\ e \\ f \\ g \\ h \\ i \end{bmatrix}$$

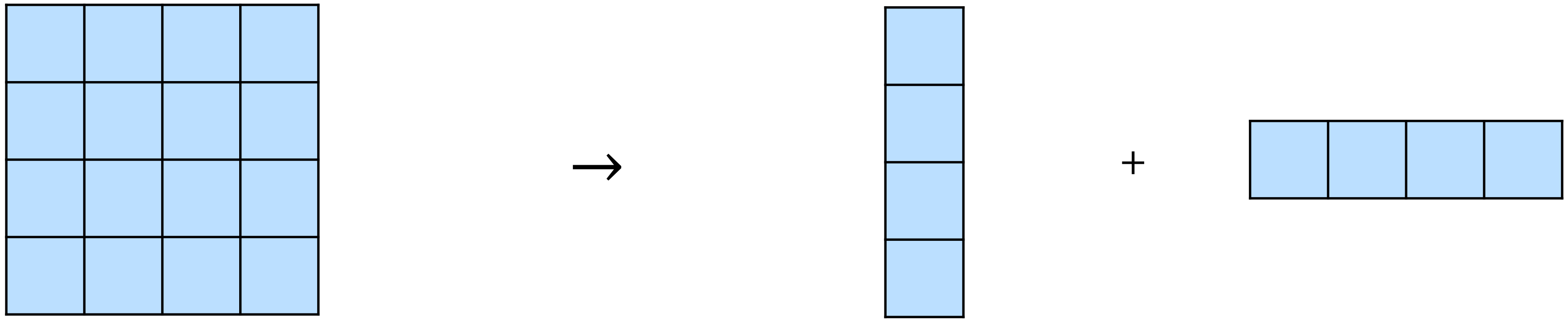
Receptive field



Img from: https://www.learnopencv.com/cnn-receptive-field-computation-using-backprop/

Combining simpler convolutions

- Replacing a $n \times n$ convolution with two subsequent convolutions with kernels $n \times 1$ and $1 \times n$:



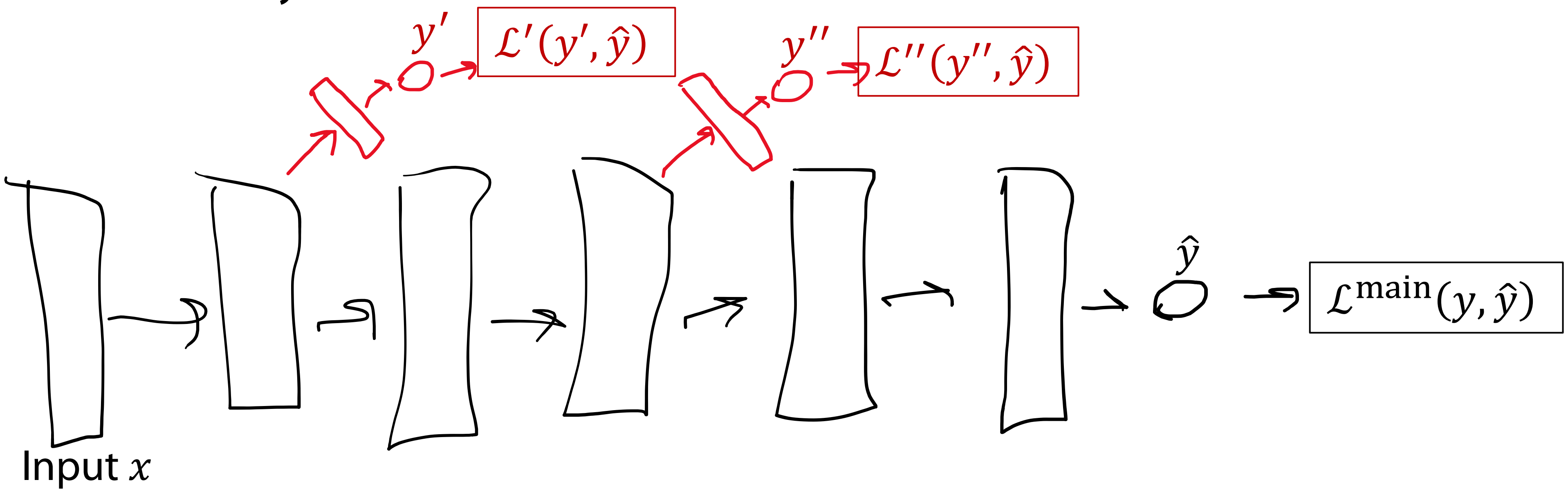
$n \times n$ convolution $\quad$ $n \times 1$ convolution $\quad$ $1 \times n$ convolution

- Same receptive field, fewer parameters

Deeply supervised architectures

Main idea

- Hard to optimize deep network due to vanishing gradients
- Encourage good gradients by introducing additional "heads" from the intermediate layers



$$\mathcal{L}^{\text{total}} = \mathcal{L}^{\text{main}} + \alpha' \mathcal{L}' + \alpha'' \mathcal{L}''$$

- Typically does not lead to good hidden representations
  – Makes sense to decay α' and α'' to 0 during training

Auxiliary tasks

- Introduce multiheaded models to solve similar tasks
  - E.g. when detecing images of people in glasses
  - add a head to predict the color of their hair
- The multiple heads may share common features and lead to a better result for the main task

Transfer learning and fine-tuning

- Assume your problem provides a dataset too little to train a full-scale model from scratch
- Yet there exists a similar or a more general large dataset with a trained model that solves it well enough
- Transfer learning:
  - take first N layers of the trained model and freeze them
  - attach a new untrained head
  - train the whole thing (with only the head parameters being trainable)
- Fine-tuning:
  - After having trained the head, release the frozen weights and train the whole model further (with very small learning rate)

Residual connections

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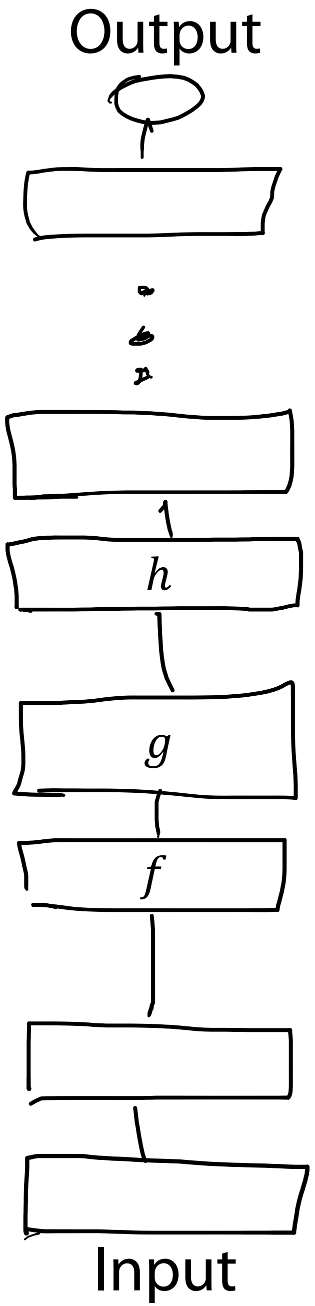
- Vanishing gradients: the derivative wrt early layer's parameters accumulates the product of derivatives for further layers (chain rule)



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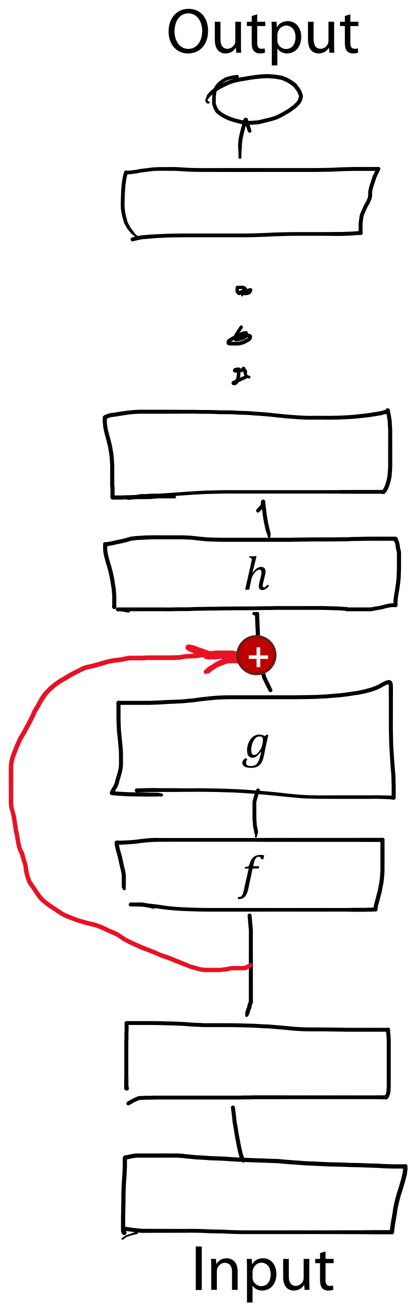

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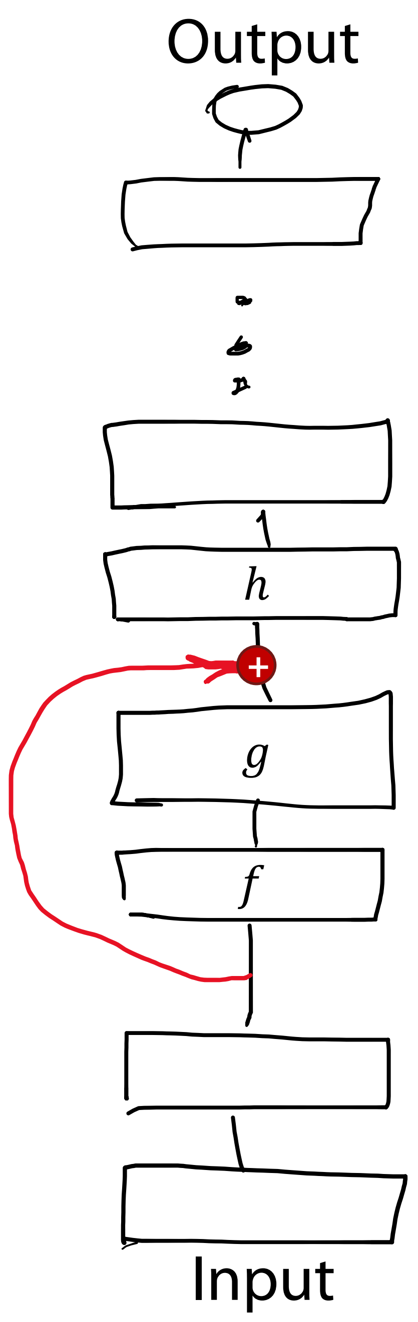

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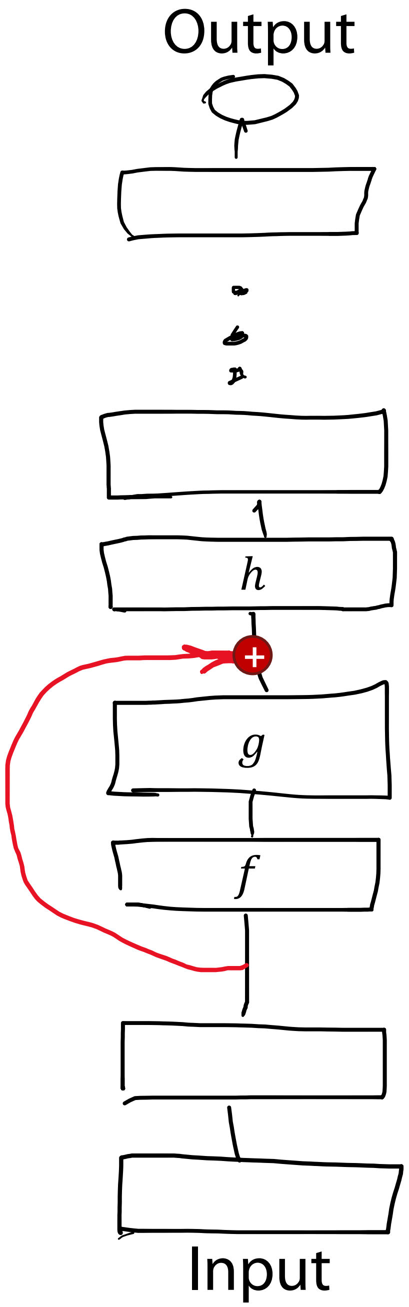
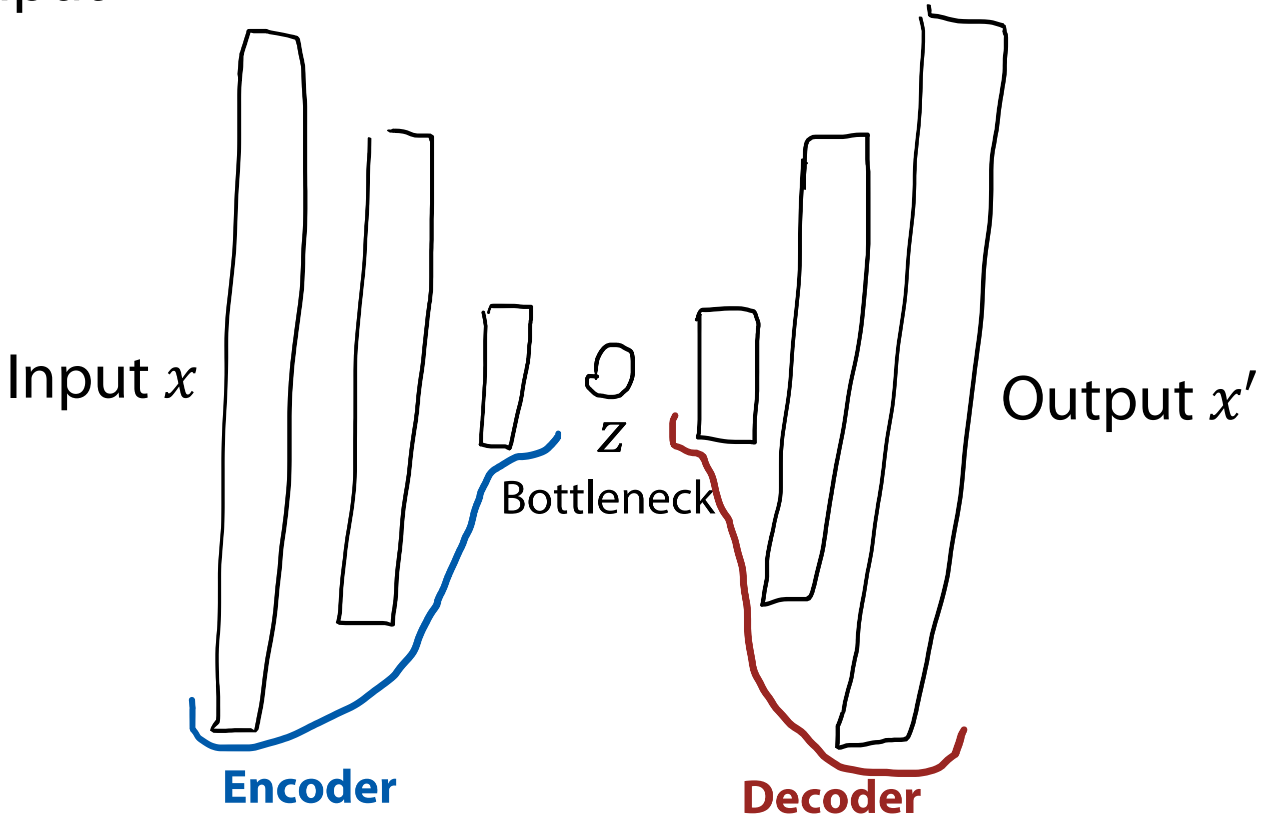
- Note: is this always possible to do?



Autoencoders

Autoencoders

- A network that reconstructs its own input
- Has a ‘bottleneck’ representation
- Common use cases:
  - Dimensionality reduction
  - Anomaly detection
  - Denoising
  - Pretraining
  - Auxiliary loss, regularization



Semi-supervised learning with AE

- Note that training an AE doesn't require any targets!
- Imagine a situation having a small labelled dataset and large unlabelled
- Semi-supervised approach:
  - train an AE on the unlabelled dataset
  - then train a classification head on top of a hidden representation from the AE
  - may also train both models simultaneously

U-net

- Problems involving image to image transformation or image segmentation

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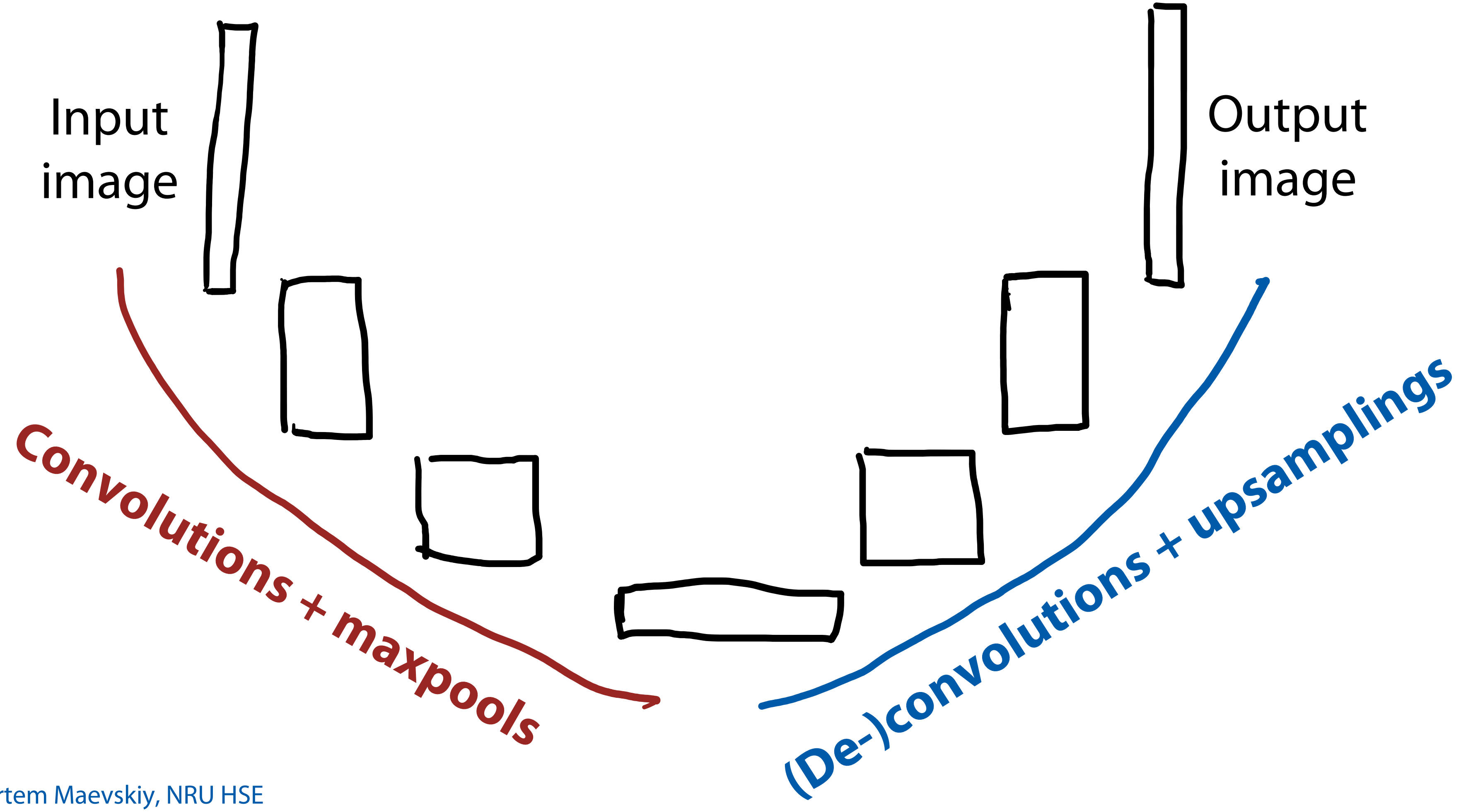

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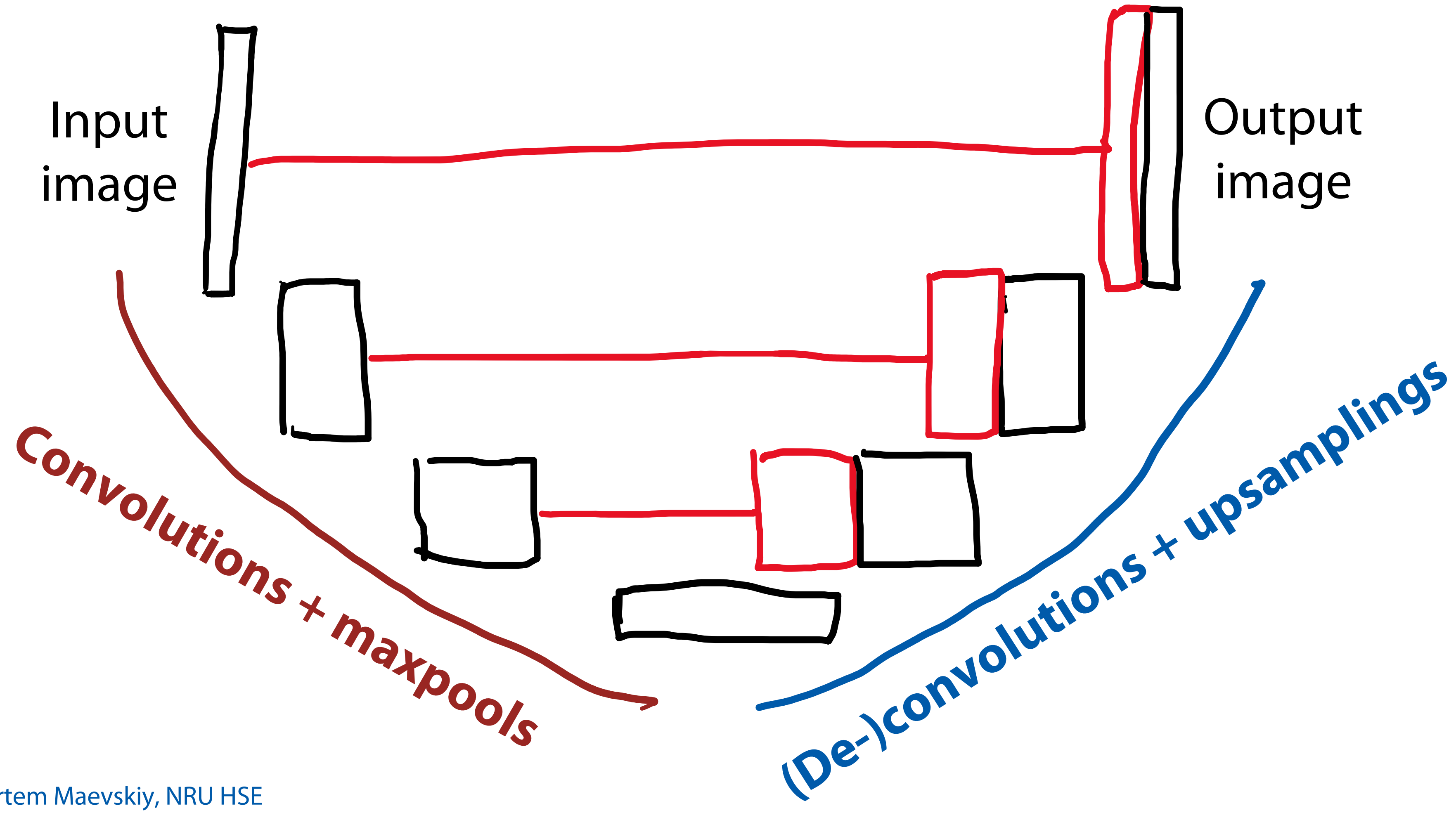

Typical approach: autoencoder-like architecture

Additional detail: skip-connections (typically concatenated)

- this combines low- and high-level information in the "decoder" branch

Summary

- According to the no-free-lunch theorem, all learning algorithms are equally useless
- It's the goal of the data scientist to make them useful leveraging the prior knowledge about the problem
- In the context of deep learning this typically involves finding (inventing) a suitable architecture
- As you can see, neural networks are extremely flexible
  - Finding a good architecture may require some creativity
- The list of shown architectures is by no means comprehensive
  - Countless other architectures and tricks

Thank you!

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