Popular NN Architectures

…and a little bit on the No Free Lunch theorems

Machine Learning and Data Mining, 2025

Majid Sohrabi
National Research University Higher School of Economics

November 19, 2025

Side note: No Free Lunch

A question from an IQ test

Given the following pattern of numbers:

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

what is the missing number?

a) 36
b) 45
c) 46
d) 64
e) 99

A question from an IQ test

Given the following pattern of numbers:

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

what is the missing number?

a) 36

b) 45

c) 46

d) 64

e) 99

X_{train}	1	2	3	5	6
y_{train}	1	8	27	125	216

$$X_{\text{test}} = (4,)$$

Solution:

$$f(x) = \frac{1}{12}(35x^5 - 595x^4 + 3757x^3 - 10745x^2 + 13860x - 6300)$$

A question from an IQ test

Given the following pattern of numbers:

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

what is the missing number?

a) 36

b) 45

c) 46

d) 64

e) $\boxed{99}$

X_{train}	1	2	3	5	6
y_{train}	1	8	27	125	216

$$X_{\text{test}} = (4,)$$

Solution:

$$f(x) = \frac{1}{12}(35x^5 - 595x^4 + 3757x^3 - 10745x^2 + 13860x - 6300)$$

Answer: $f(4) = 99$

A question from an IQ test

Given the following pattern of numbers:

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

what is the missing number?

a) 36

b) 45

c) 46

d) 64

e) ~~99~~

$f(x) = x^3$

X_{train}	1	2	3	5	6
y_{train}	1	8	27	125	216

$X_{\text{test}} = (4,)$

~~Solution:~~

$$\cancel{f(x) = \frac{1}{12}(35x^5 - 595x^4 + 3757x^3 - 10745x^2 + 13860x - 6300)}$$

~~Answer:~~ $\cancel{f(4) = 99}$

Discussion

Why $f(x) = x^3$ is better than

$f(x) = \frac{1}{12}(35x^5 - 595x^4 + 3757x^3 - 10745x^2 + 13860x - 6300)$?

Discussion

Why $f(x) = x^3$ is better than

$$f(x) = \frac{1}{12}(35x^5 - 595x^4 + 3757x^3 - 10745x^2 + 13860x - 6300)?$$

First one is more suitable **in the context of an IQ test**

Discussion

Why $f(x) = x^3$ is better than

$f(x) = \frac{1}{12}(35x^5 - 595x^4 + 3757x^3 - 10745x^2 + 13860x - 6300)$?

First one is more suitable **in the context of an IQ test**

Prior knowledge

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

No Free Lunch Theorem

True (deterministic) mapping: $f: y = f(x), \quad x \in \mathcal{X}, \quad y \in \mathcal{Y}$

No Free Lunch Theorem

True (deterministic) mapping: $f: y = f(x), \quad x \in \mathcal{X}, \quad y \in \mathcal{Y}$

Dataset: $D = (X, y) \subseteq \mathcal{X} \times \mathcal{Y}$

No Free Lunch Theorem

True (deterministic) mapping: $f: y = f(x), \quad x \in \mathcal{X}, \quad y \in \mathcal{Y}$

Dataset: $D = (X, y) \subseteq \mathcal{X} \times \mathcal{Y}$

ML algorithm: $\mathcal{A}(D_{\text{train}}) = \hat{f}, \quad \hat{f}: \mathcal{X} \rightarrow \mathcal{Y}$

No Free Lunch Theorem

True (deterministic) mapping: $f: y = f(x), \quad x \in \mathcal{X}, \quad y \in \mathcal{Y}$

Dataset: $D = (X, y) \subseteq \mathcal{X} \times \mathcal{Y}$

ML algorithm: $\mathcal{A}(D_{\text{train}}) = \hat{f}, \quad \hat{f}: \mathcal{X} \to \mathcal{Y}$

Binary features and targets: $\mathcal{X} = \{0, 1\}^m, \quad \mathcal{Y} = \{0, 1\}$

No Free Lunch Theorem

True (deterministic) mapping: $f: y = f(x), \quad x \in \mathcal{X}, \quad y \in \mathcal{Y}$

Dataset: $D = (X, y) \subseteq \mathcal{X} \times \mathcal{Y}$

ML algorithm: $\mathcal{A}(D_{\text{train}}) = \hat{f}, \quad \hat{f}: \mathcal{X} \to \mathcal{Y}$

Binary features and targets: $\mathcal{X} = \{0, 1\}^m, \quad \mathcal{Y} = \{0, 1\}$

Training dataset of fixed size: $|D_{\text{train}}| = n$

No Free Lunch Theorem

True (deterministic) mapping: $f: y = f(x), \quad x \in \mathcal{X}, \quad y \in \mathcal{Y}$

Dataset: $D = (X, y) \subseteq \mathcal{X} \times \mathcal{Y}$

ML algorithm: $\mathcal{A}(D_{\text{train}}) = \hat{f}, \quad \hat{f}: \mathcal{X} \to \mathcal{Y}$

Binary features and targets: $\mathcal{X} = \{0, 1\}^m, \quad \mathcal{Y} = \{0, 1\}$

Training dataset of fixed size: $|D_{\text{train}}| = n$

Test set: $D_{\text{test}}: X_{test} = \mathcal{X} \setminus X_{\text{train}}$

No Free Lunch Theorem

True (deterministic) mapping: $f\colon y = f(x), \quad x \in \mathcal{X}, \quad y \in \mathcal{Y}$

Dataset: $D = (X, y) \subseteq \mathcal{X} \times \mathcal{Y}$

ML algorithm: $\mathcal{A}(D_{\text{train}}) = \hat{f}, \quad \hat{f}\colon \mathcal{X} \to \mathcal{Y}$

Binary features and targets: $\mathcal{X} = \{0,1\}^m, \quad \mathcal{Y} = \{0,1\}$

Training dataset of fixed size: $|D_{\text{train}}| = n$

Test set: $D_{\text{test}}\colon X_{test} = \mathcal{X} \setminus X_{\text{train}}$

Generalization performance:

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

No Free Lunch Theorem

True (deterministic) mapping: $f : y = f(x), \quad x \in \mathcal{X}, \quad y \in \mathcal{Y}$

Dataset: $D = (X, y) \subseteq \mathcal{X} \times \mathcal{Y}$

ML algorithm: $\mathcal{A}(D_{\text{train}}) = \hat{f}, \quad \hat{f} : \mathcal{X} \to \mathcal{Y}$

Binary features and targets: $\mathcal{X} = \{0, 1\}^m, \quad \mathcal{Y} = \{0, 1\}$

Training dataset of fixed size: $|D_{\text{train}}| = n$

Test set: $D_{\text{test}} : X_{test} = \mathcal{X} \setminus X_{\text{train}}$

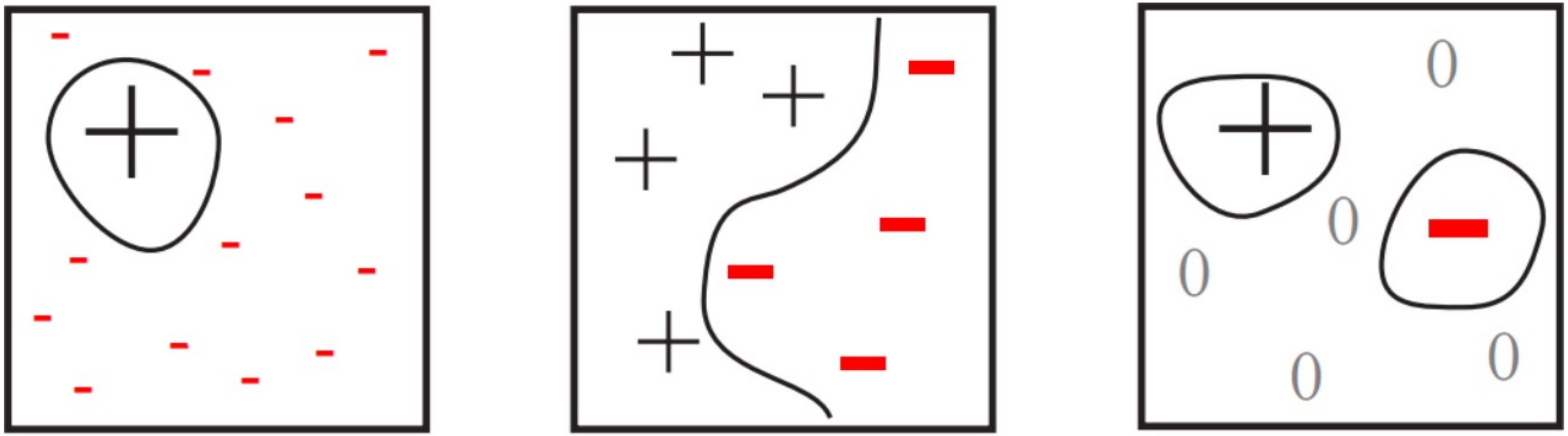
Generalization performance:

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

Theorem statement:

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

In the problem space



Possible performance of learning algorithms:

- Worse than average (–)
- Better than average (**+**)

Back to the IQ test problem

Without our prior knowledge about IQ tests any solution is equally likely

- We know that the authors of the test don't expect people to fit 5^{th} degree polynomials in their head

Back to the IQ test problem

Without our prior knowledge about IQ tests any solution is equally likely

- We know that the authors of the test don't expect people to fit 5th degree polynomials in their head

To solve the test one must think like the authors of the test

Back to the IQ test problem

- Without our prior knowledge about IQ tests any solution is equally likely
  - We know that the authors of the test don't expect people to fit 5^{th} degree polynomials in their head
- 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**

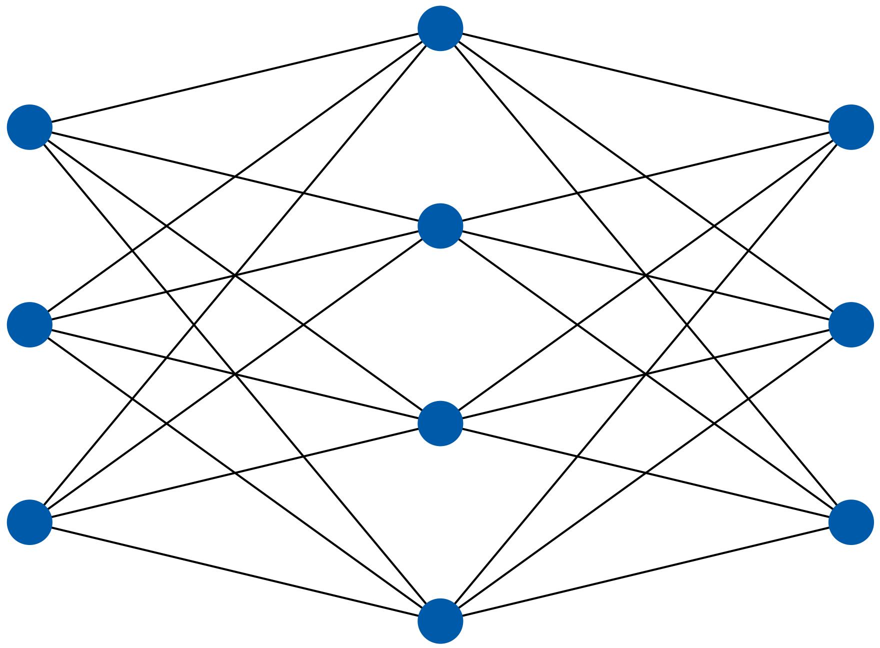
NN architecure: simple examples

Single hidden layer fully-connected network

Universal approximator

May reqire infeasibly large hidden representation for more complex dependencies

Input: x



Output: $\hat{y}$

Hidden representation: $h(x)$

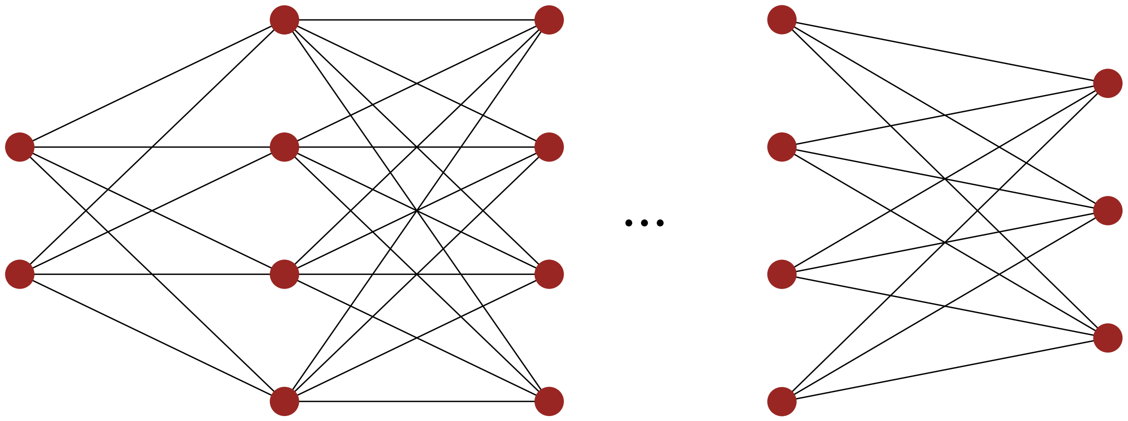
Deep fully-connected network

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

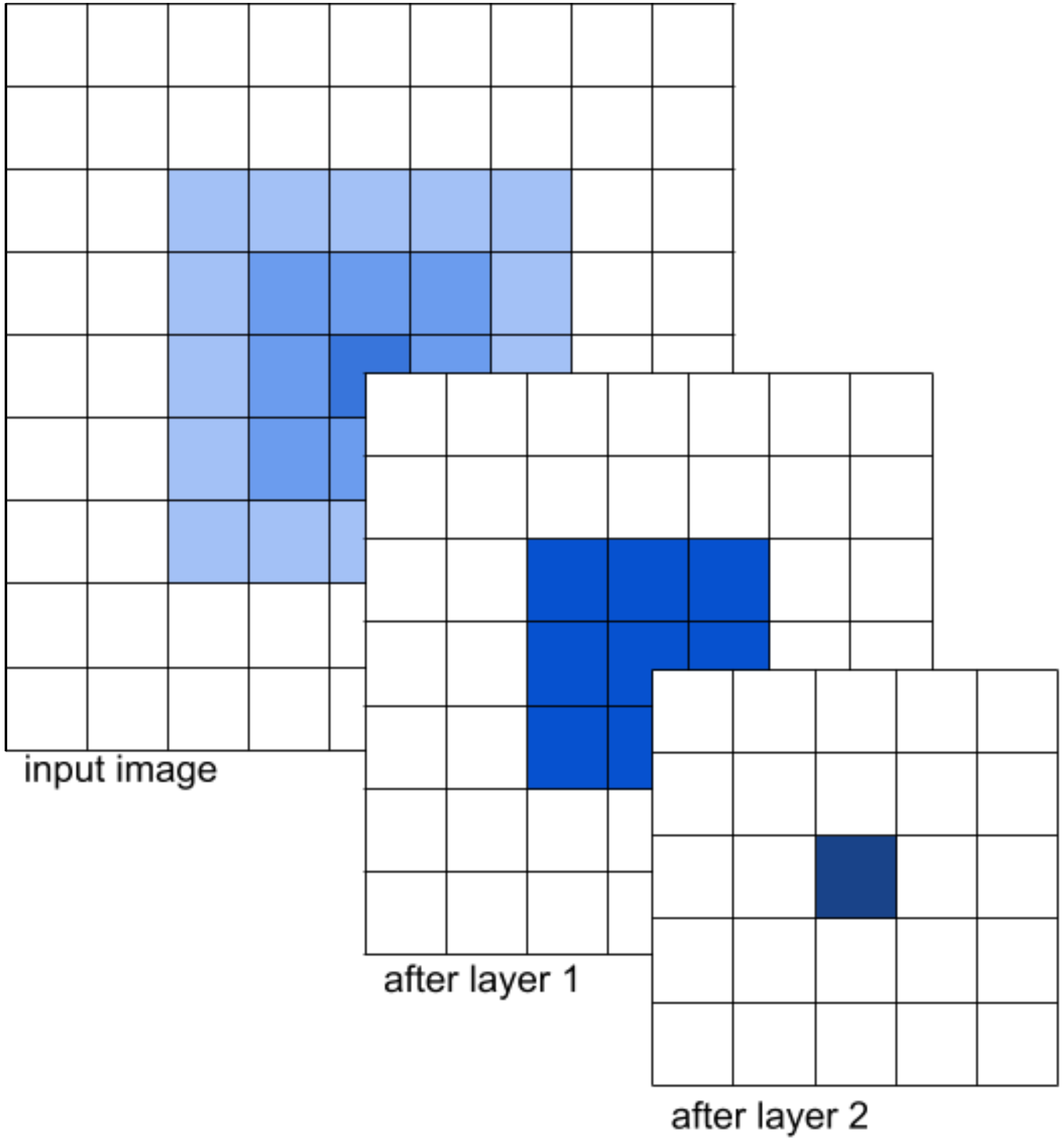
- Re-uses weights in a sliding window

2D convolution as a matrix multiplication

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

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

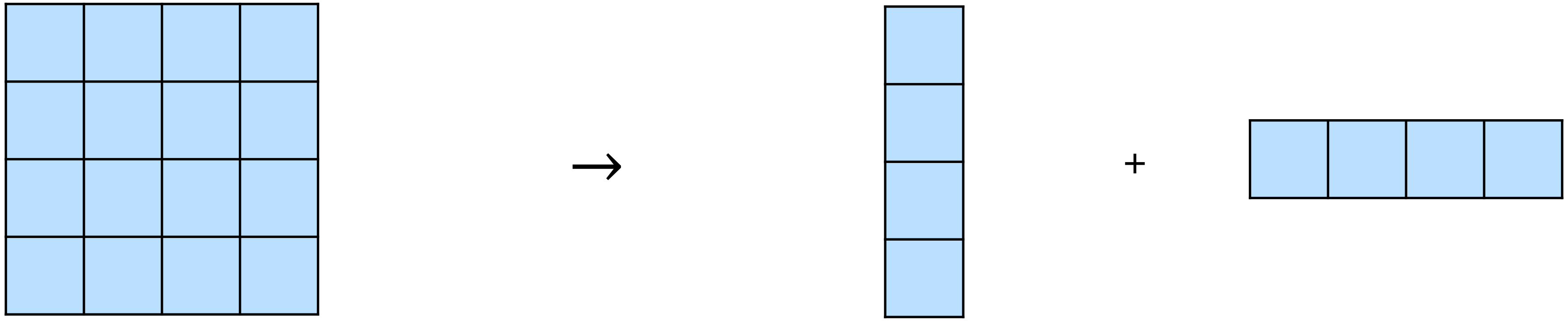
Receptive field



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

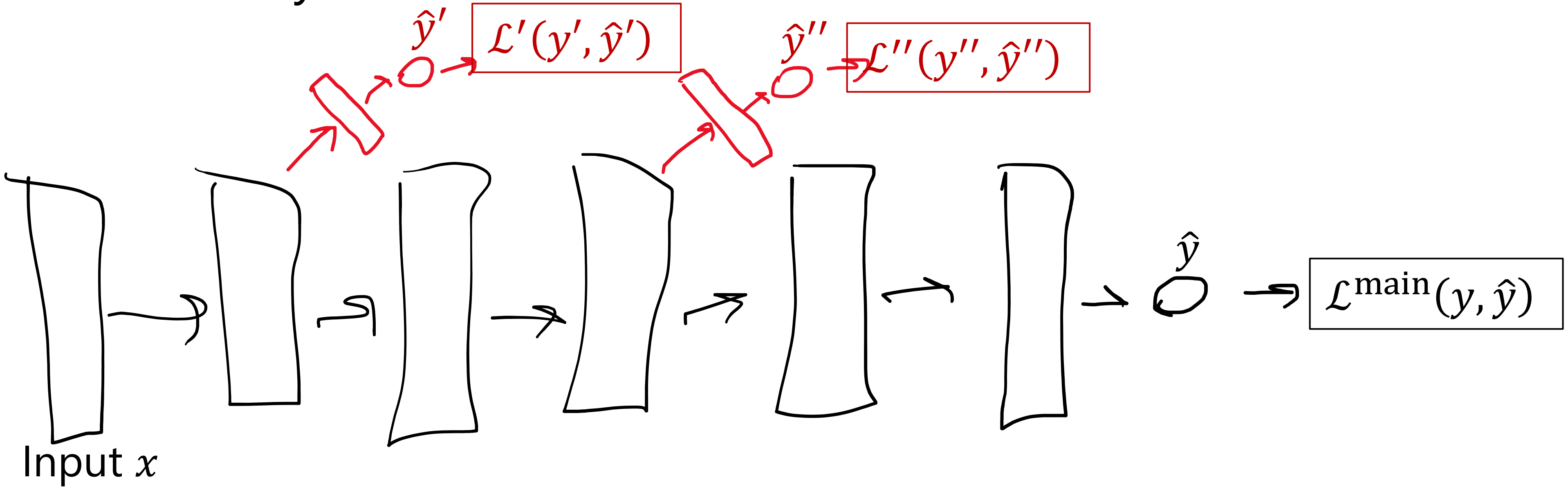
Same receptive field, fewer parameters

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)

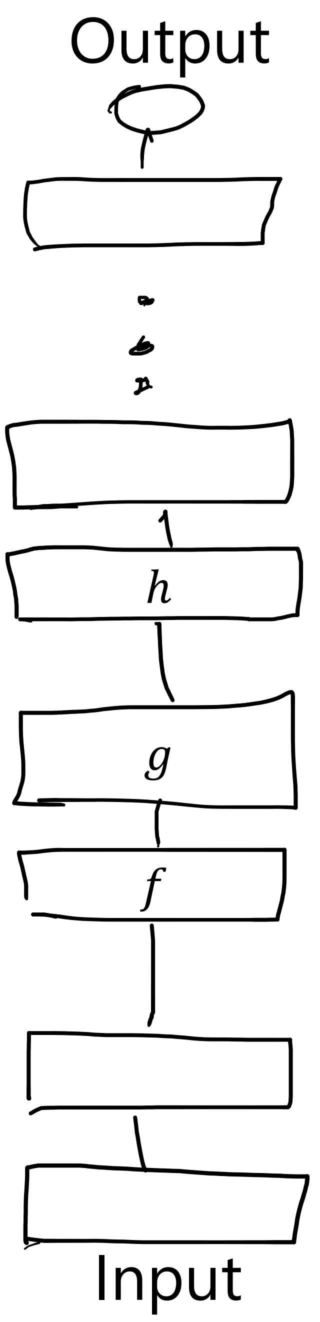
Fine-tuning:

- After having trained the head, release the frozen weights and train the whole model further (with very small learning rate)

Residual connections

Residual connections

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

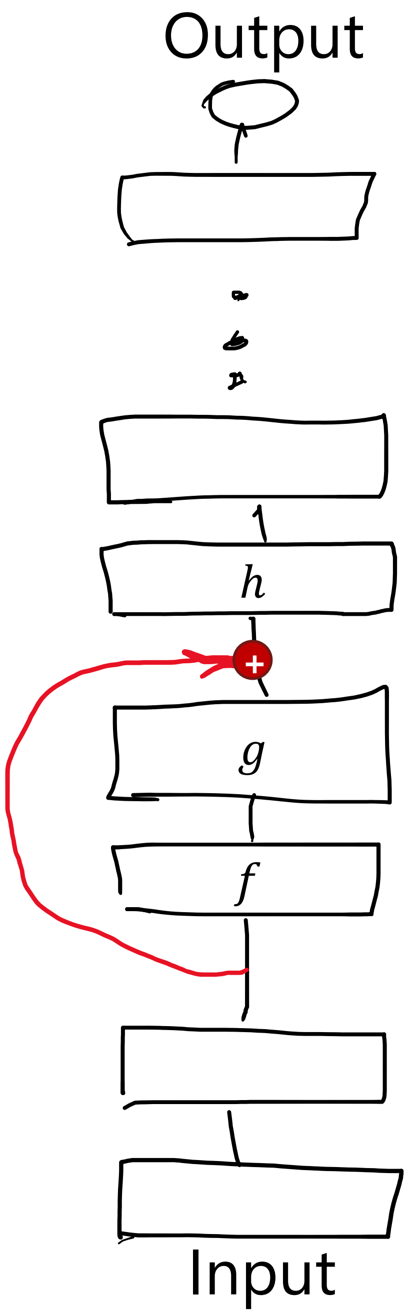


Residual connections

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

Solution: add resiudal connections (skip-connections)

$$h\Big(g\big(f(\tilde{x})\big)\Big) \to h\Big(\tilde{x} + g\big(f(\tilde{x})\big)\Big)$$



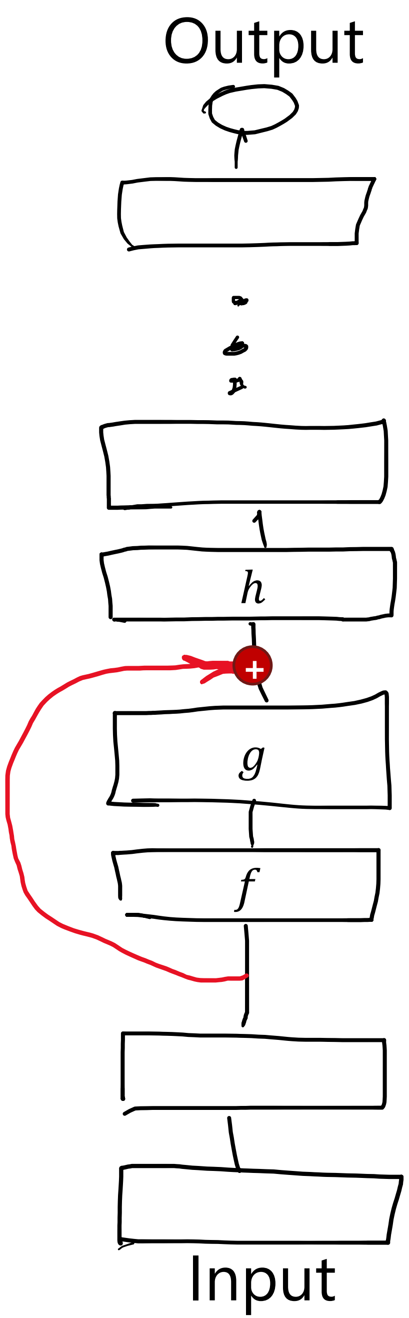
Residual connections

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

Solution: add resiudal connections (skip-connections)

$$h\Big(g\big(f(\tilde{x})\big)\Big) \rightarrow h\Big(\tilde{x} + g\big(f(\tilde{x})\big)\Big)$$

Allows extremely deep networks to be trained (like, 1000 layers!)



Residual connections

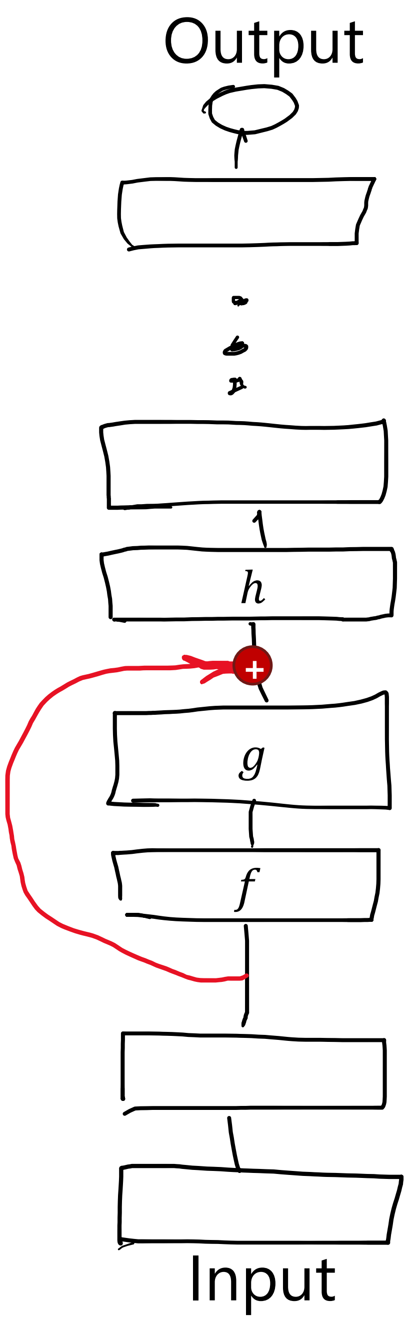
Vanishing gradients: the derivative wrt early layer's parameters accumulates the product of derivatives for further layers (chain rule)

Solution: add resiudal connections (skip-connections)

$$h\left(g\left(f\left(\tilde{x}\right)\right)\right) \to h\left(\tilde{x} + g\left(f\left(\tilde{x}\right)\right)\right)$$

Allows extremely deep networks to be trained (like, 1000 layers!)

Note: is this always possible to do?



Autoencoders

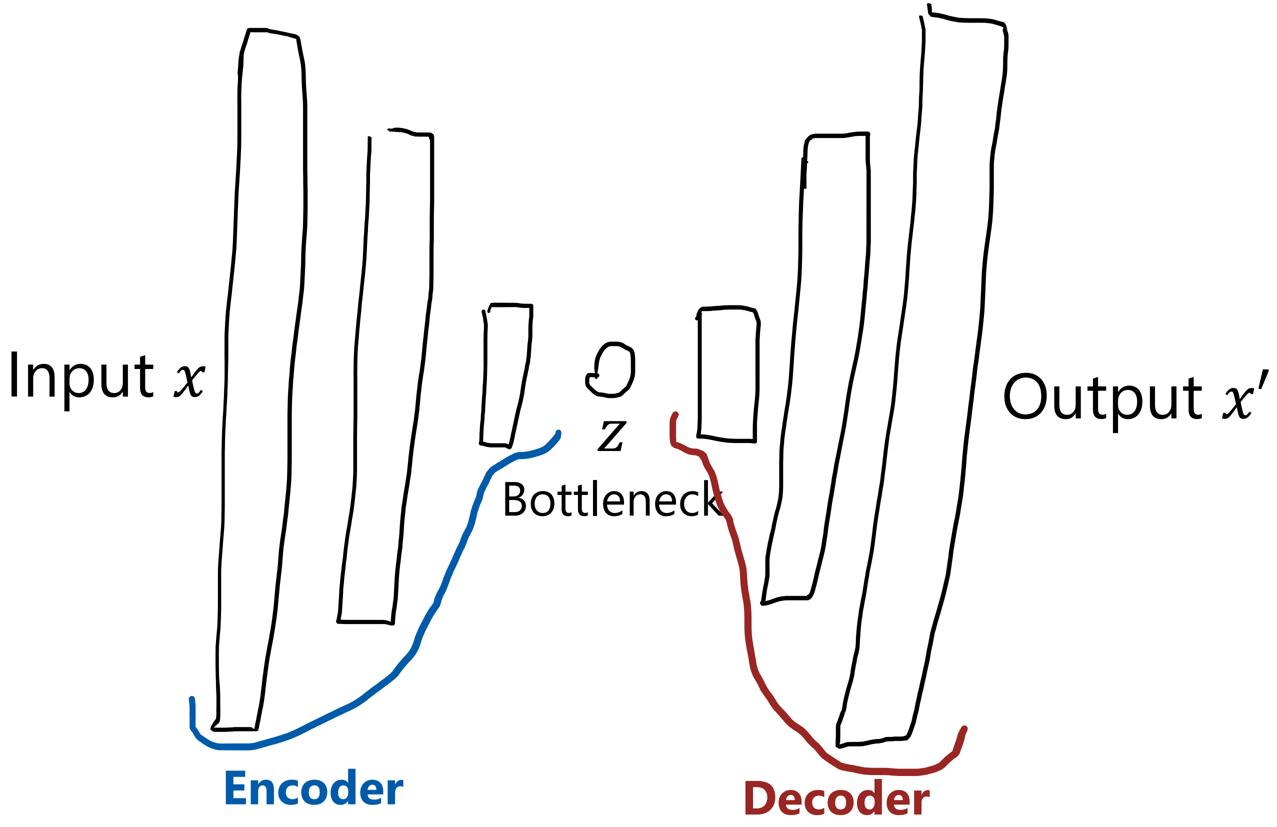
Autoencoders

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:

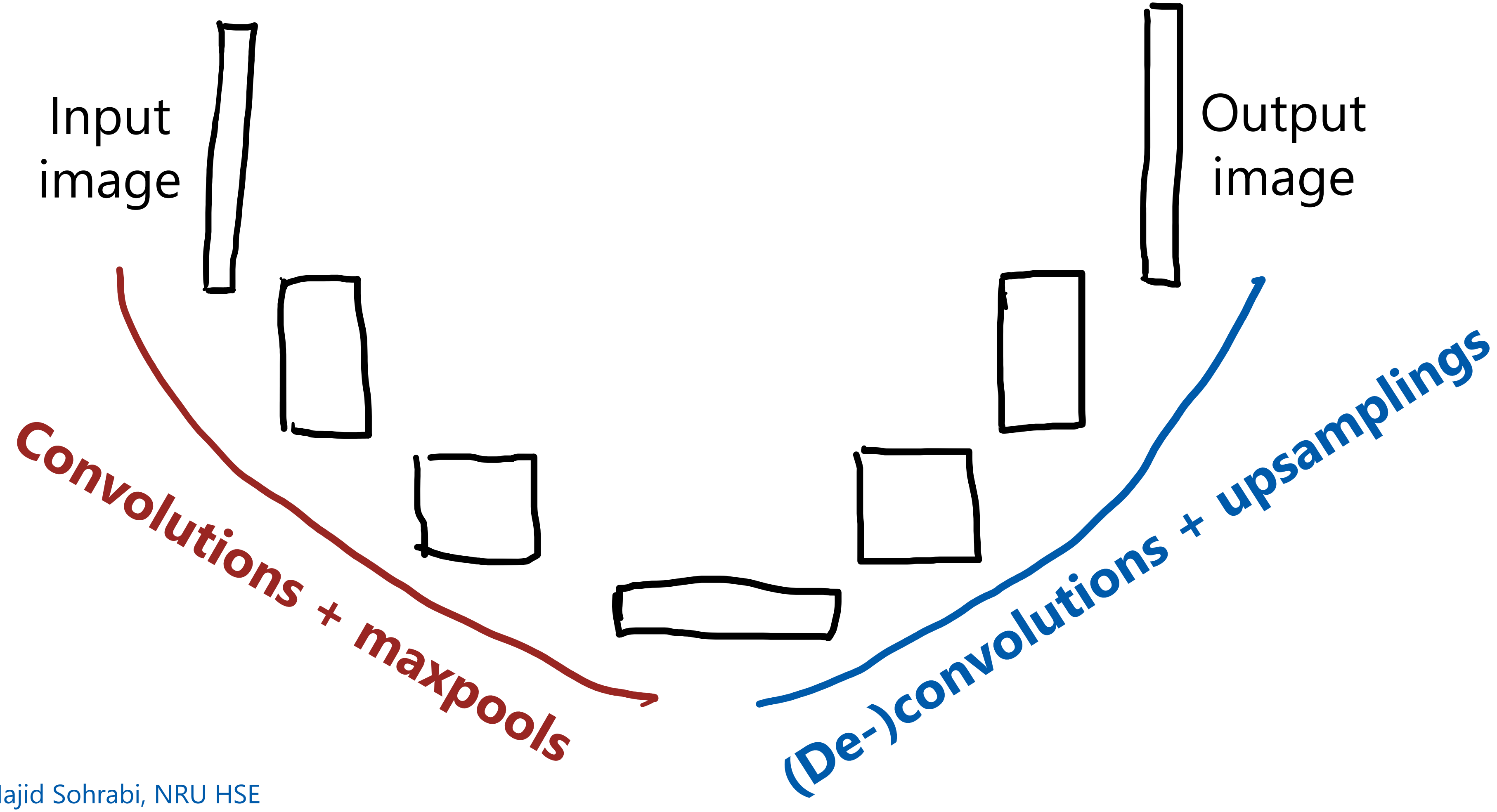
- train an AE on the unlabelled dataset
- then train a classification head on top of a hidden representation from the AE
- may also train both models simultaneously

U-net

Problems involving image to image transformation or image segmentation

U-net

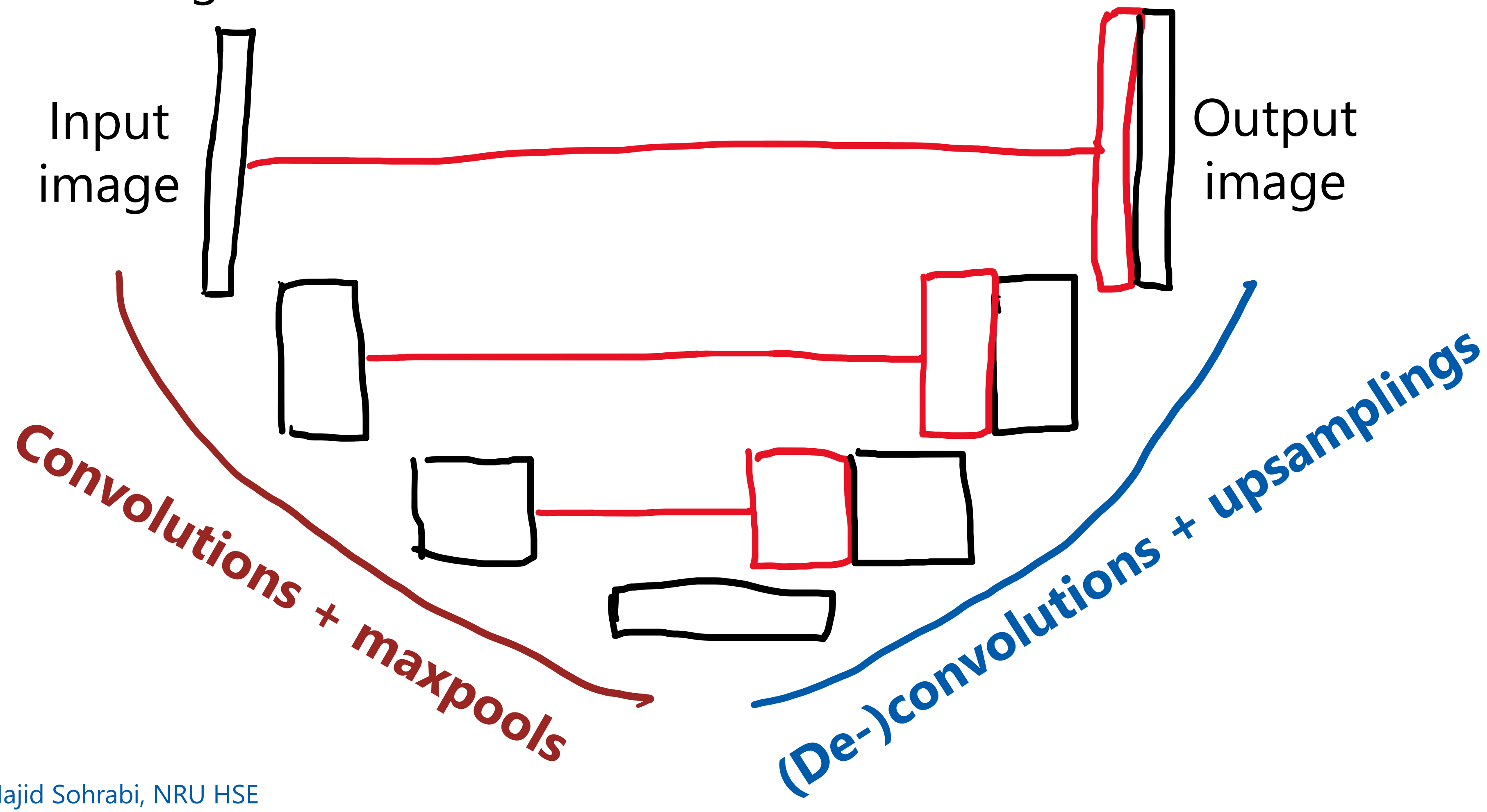
Problems involving image to image transformation or image segmentation



Typical approach: autoencoder-like architecture

U-net

Problems involving image to image transformation or image segmentation



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!

Majid Sohrabi

msohrabi@hse.ru