Algorithms

Deep learning

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UNIVERSITÀ DI ROMA

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Models for describing the data

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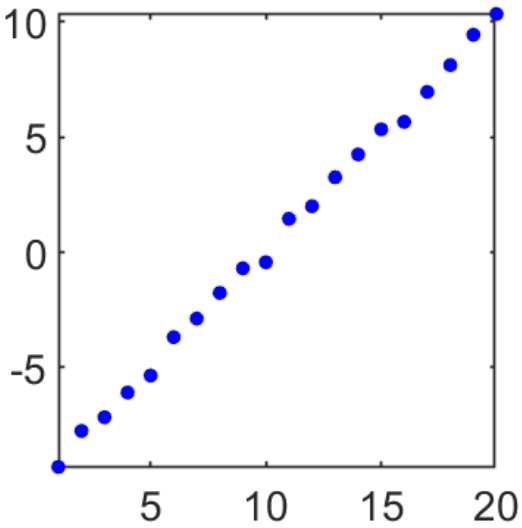

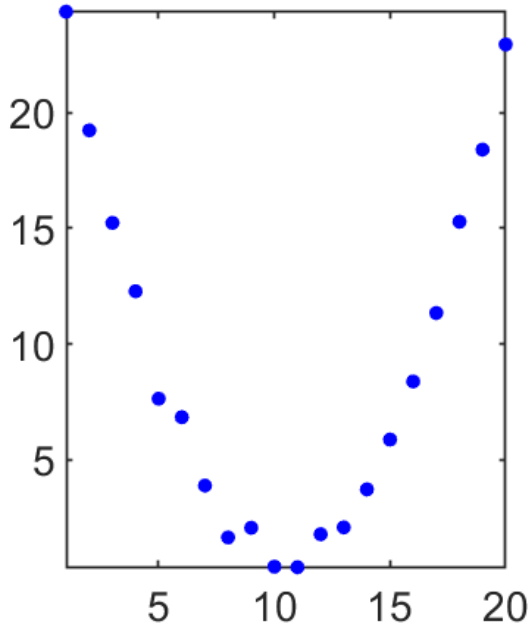

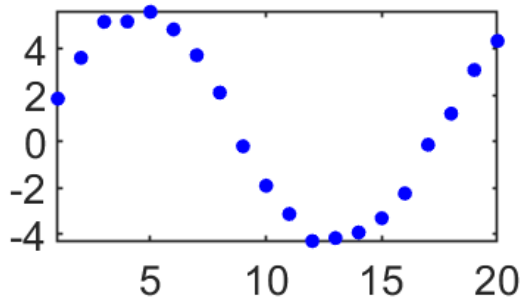

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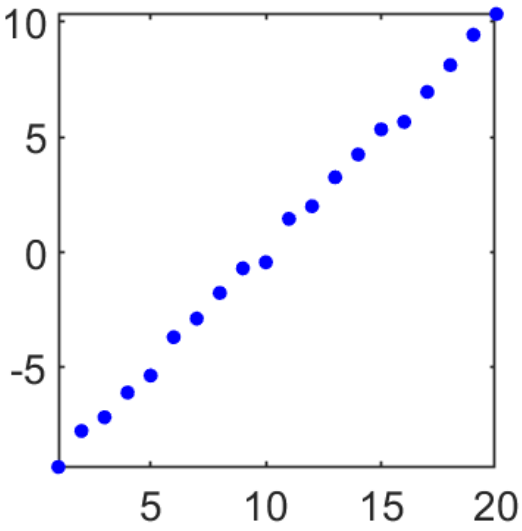
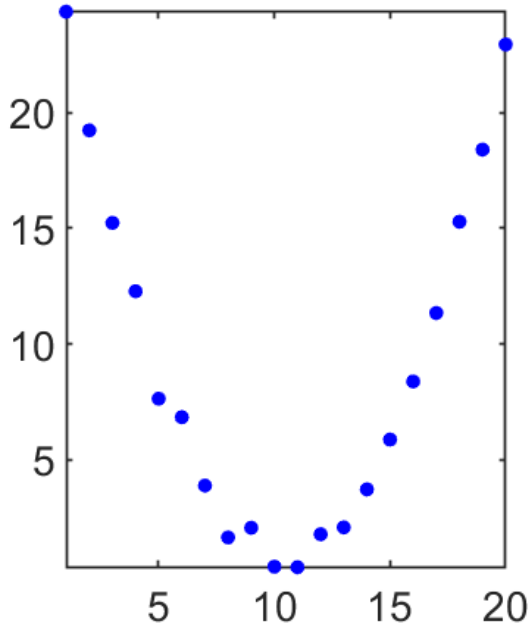


$y = ax + b$



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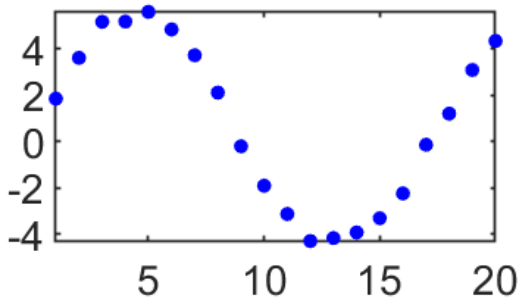

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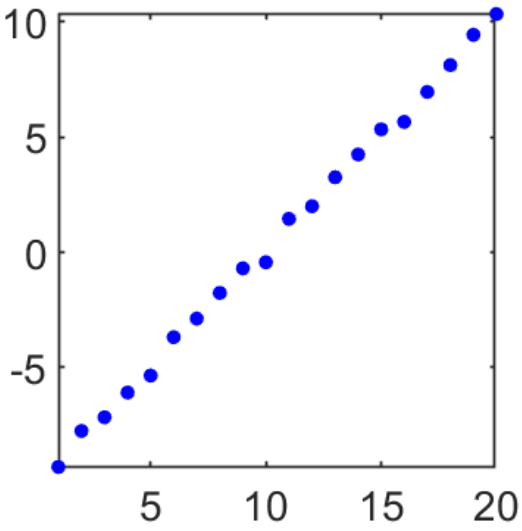

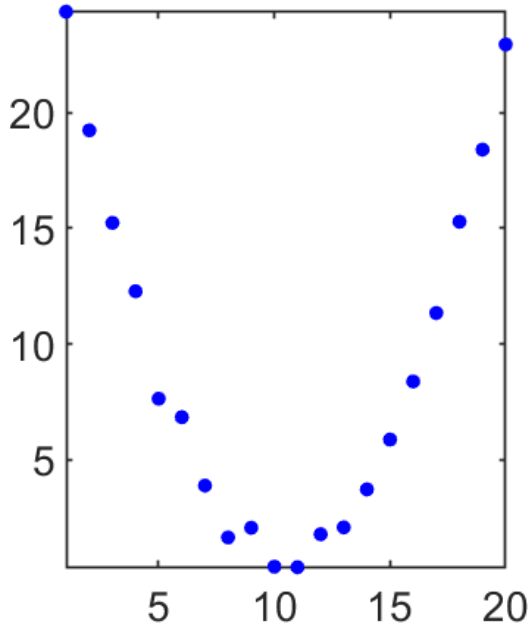

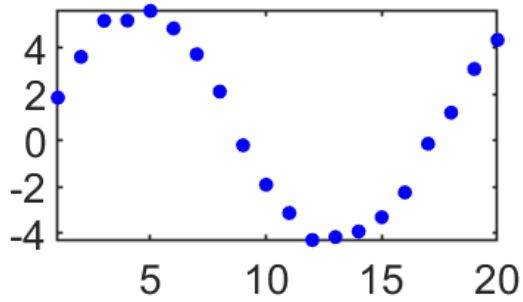

$y = ax + b$ $y = ax^2 + bx + c$ $y = a\sin(x) + bx + c$

Our model might use prior knowledge on the data.

For example, in the third plot, we might know *a priori* that the data actually comes from a periodic process.

Modeling prior knowledge

Main idea: Look at the world, identify what knowledge we have about it, and use this knowledge to construct our model.

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Some forms of prior knowledge:

- Data distribution
- Energy function
- Constraints
- Invariances
- Input-output examples (data prior)

All these encode, to different extents, some expected behavior.

Explaining the data

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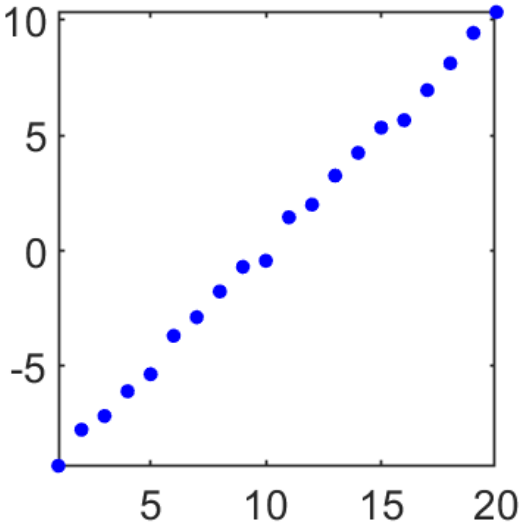

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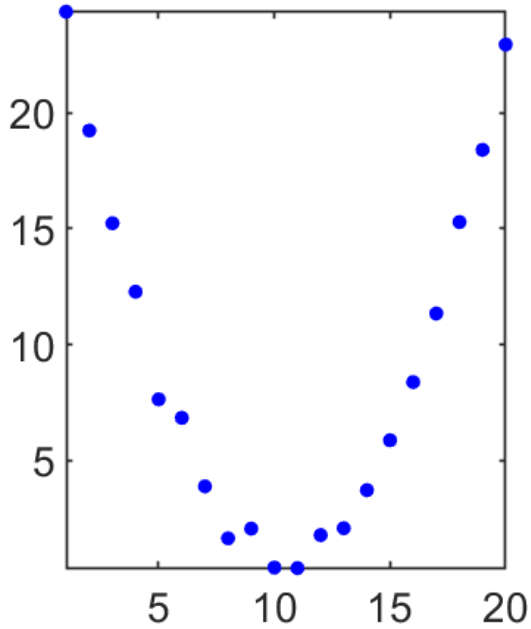

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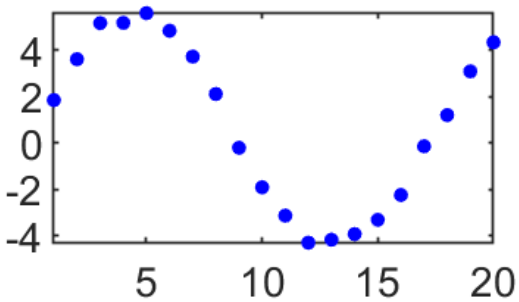

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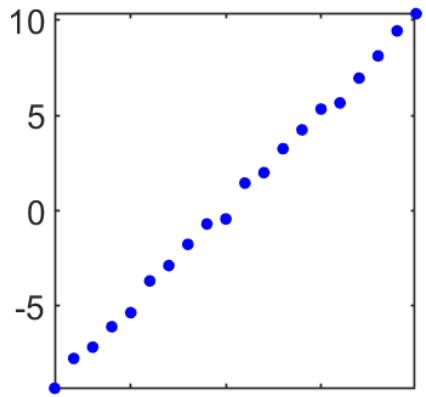
This structure is almost never captured by a simple expression.



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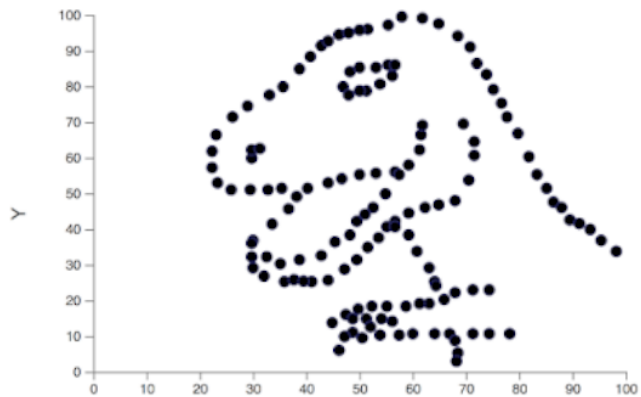

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Of course, data can have more than 1 or 2 dimensions.

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For example, a $w \times h$ image has wh dimensions, i.e., it is a point in a wh-dimensional space. A dataset of such images is a point cloud in $\mathbb{R}^{wh}$.

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Are all those dimensions significant?

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There is only one dimension; each image is a point along one axis.

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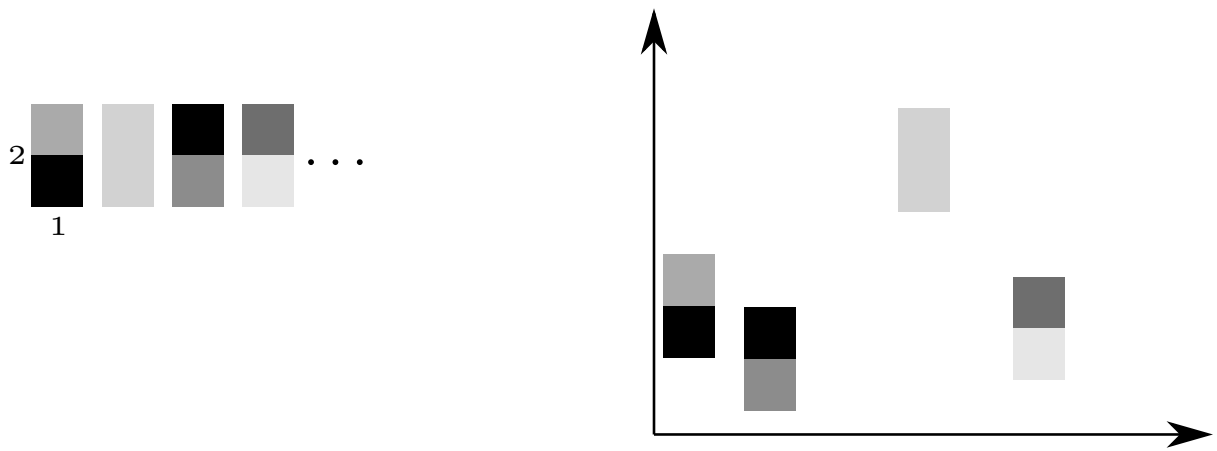

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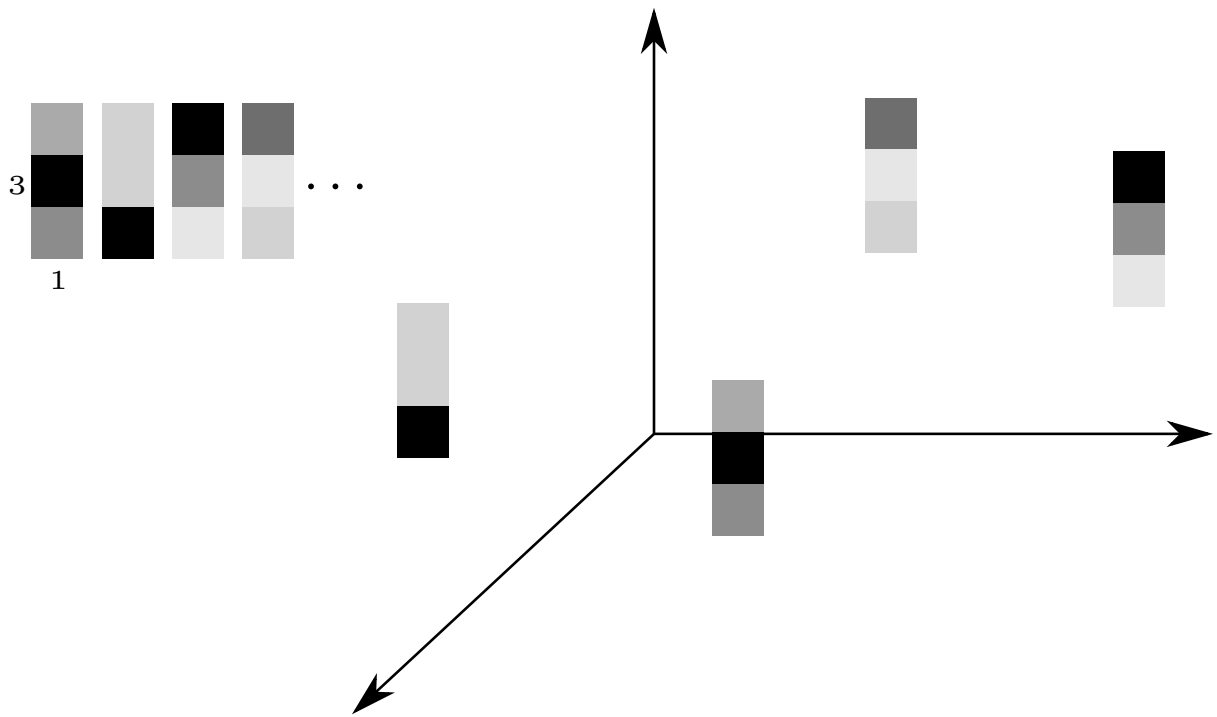

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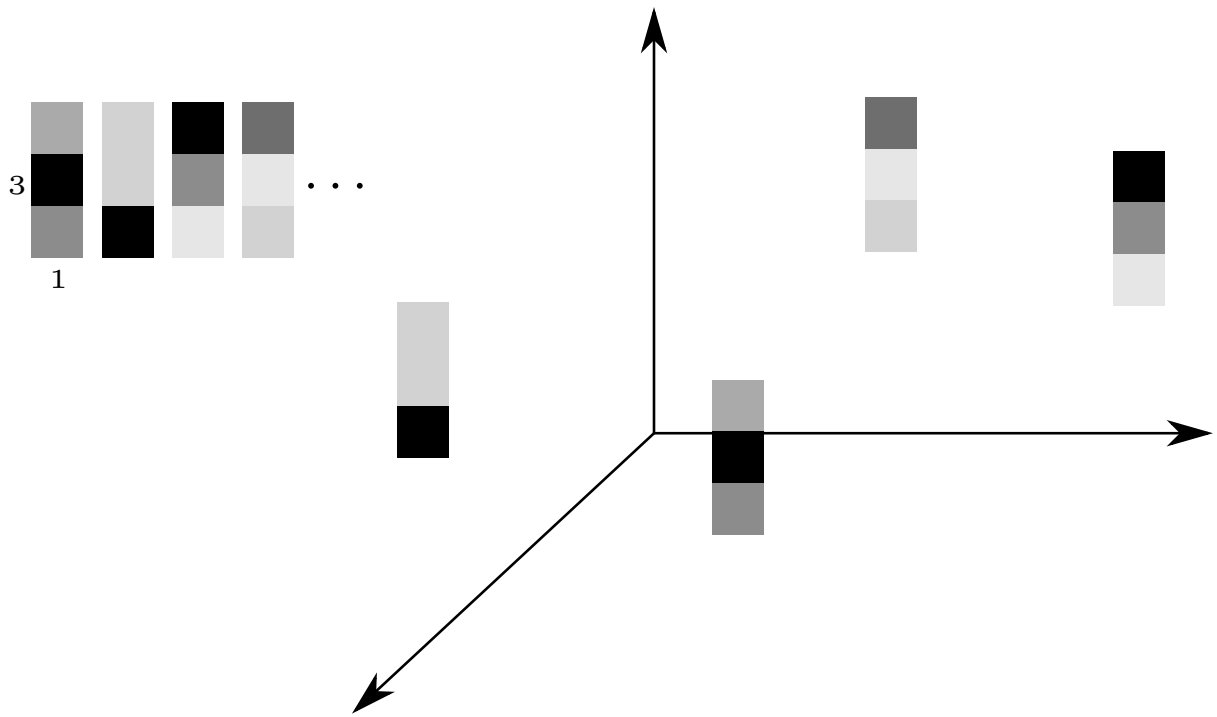

Each new dimension increases sparsity of the point cloud.

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then n^d data points are required for d-dimensional images.

More data points make interesting structures emerge

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Two options:

1. **Increase** the dataset
2. **Decrease** the dimensions

Features

Assume each data point $x \in \mathcal{D} \subset \mathbb{R}^n$ is the result of a synthesis process:

$$\sigma : F \mapsto x$$

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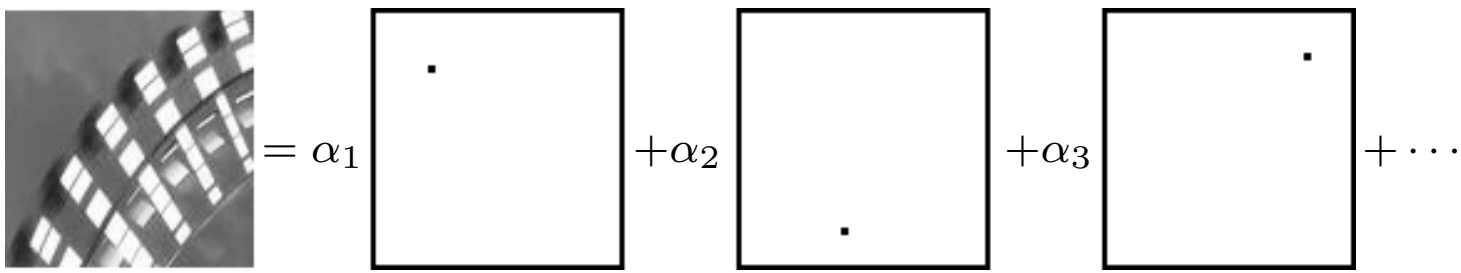

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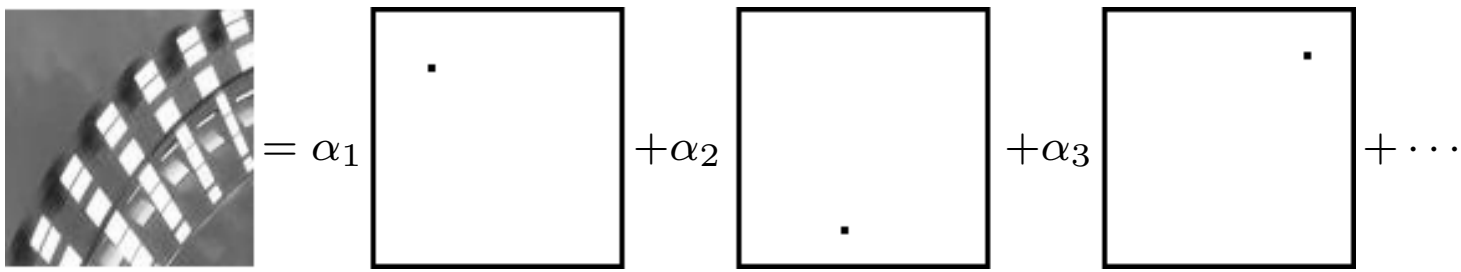

In this case, the feature space F is spanned by individual pixels.

Each feature (each pixel) represents a dimension.

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In this **particular case**, the feature space is a vector space and σ is linear.

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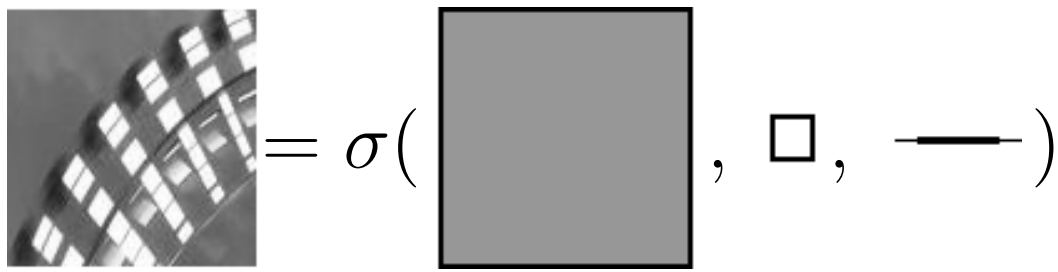

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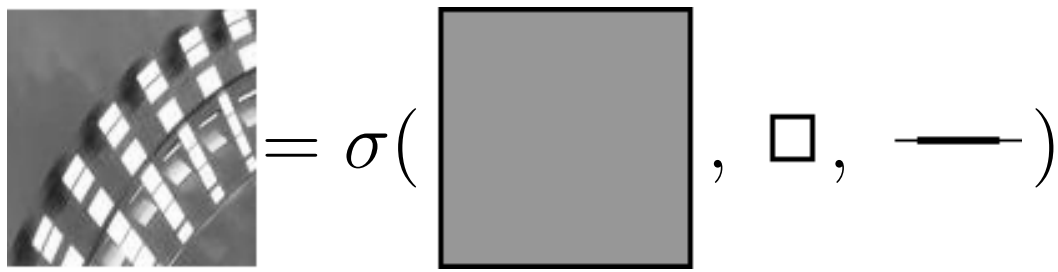

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The output of σ is called an embedding of the data point.
For the data point $x \in \mathcal{D} \subset \mathbb{R}^n$, the embedding space is $\mathbb{R}^n$.

Intrinsic invariances

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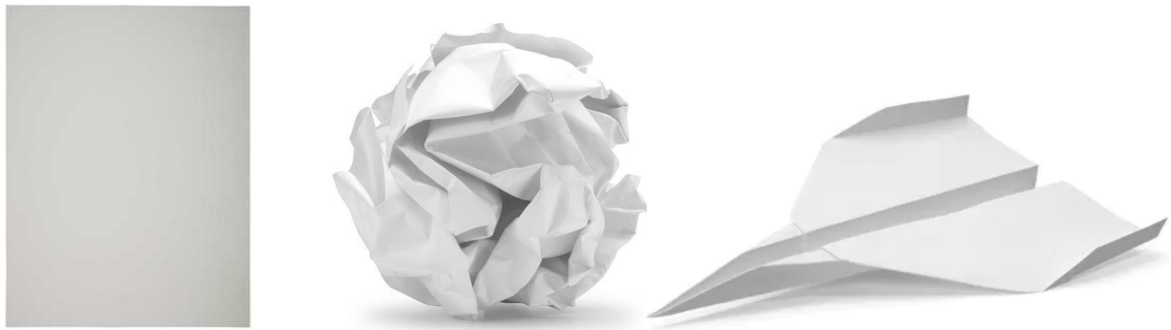

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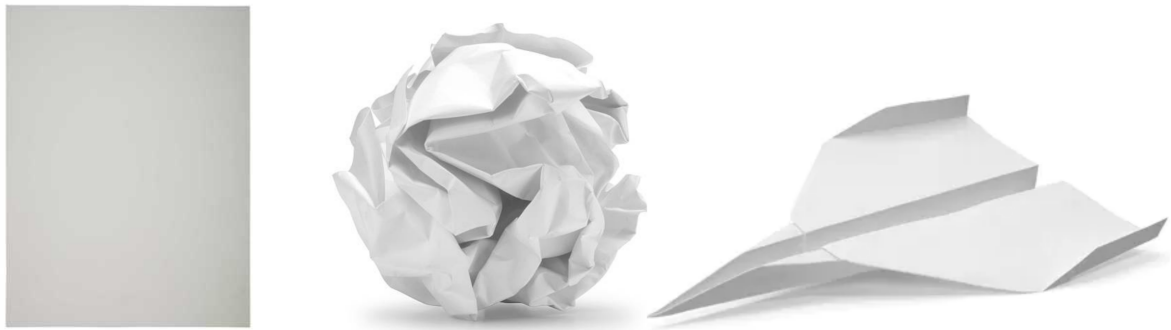

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(distances are preserved in all the embeddings)

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Challenge: discover what intrinsic properties are preserved; these properties characterize the data.

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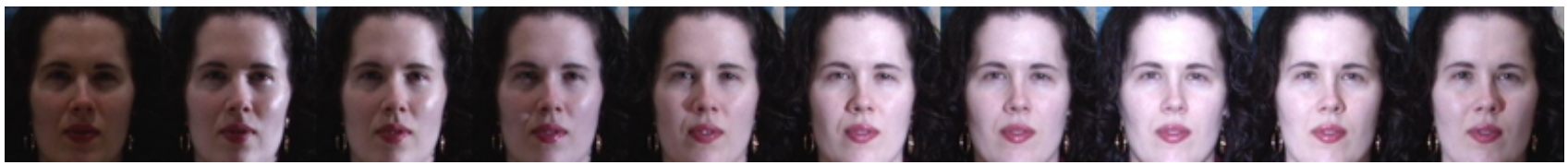

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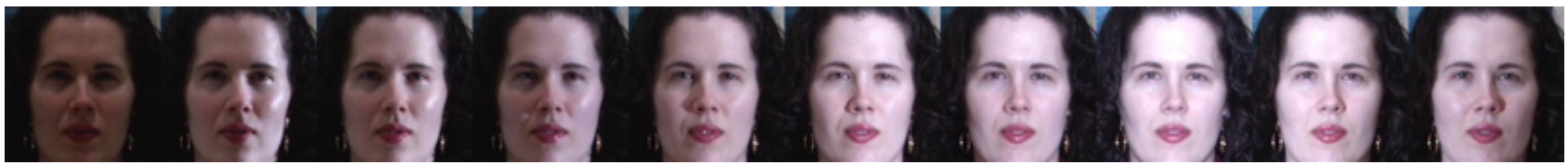

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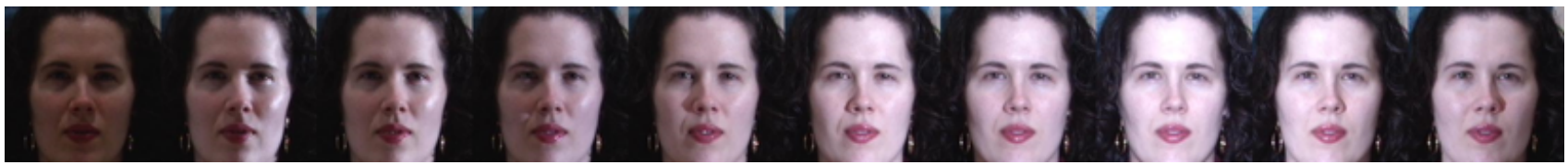

Latent feature: directional illumination

3 params for the light source position + **1** param for light intensity

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Discovering latent features involves discovering:

the "true" embedding space for the data
+
the transformation between the two spaces

We want to discard the non-informative dimensions from the data.

The manifold hypothesis

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Is color important?

Rank, suit, and color are generic features, but specific problems determine what features are important for that task.

What counts in spades, does not count in poker.

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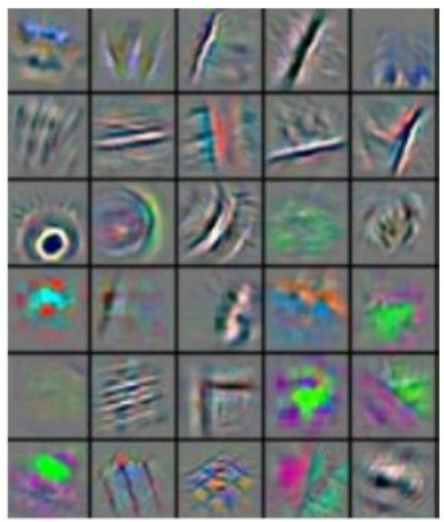
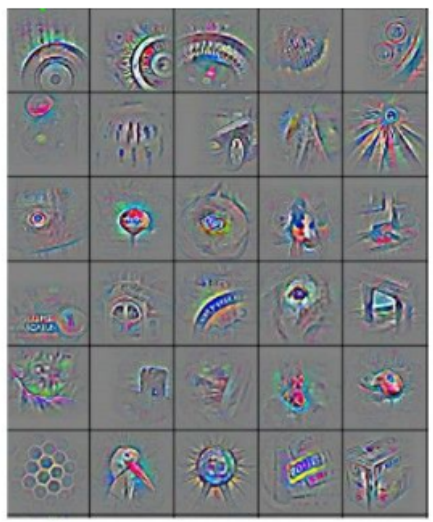
However, features are not always the focus of deep learning; rather, they are instrumental for the given task and drive the decision.

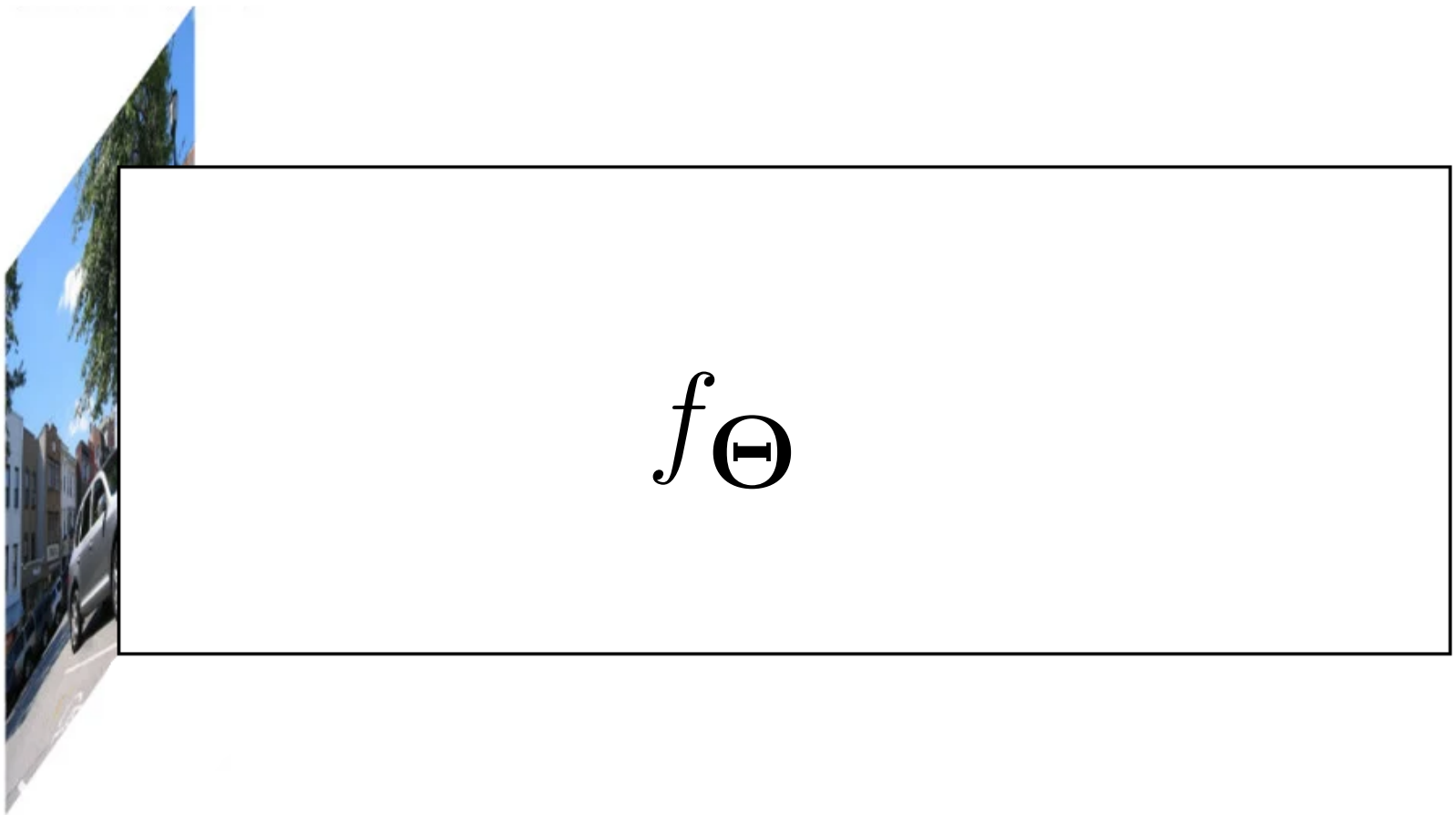
Example: Visual classification


→ low-level features → mid-level features → hi-level features → "car"

A glimpse into neural networks

In deep learning, we deal with highly parametrized models called deep neural networks:



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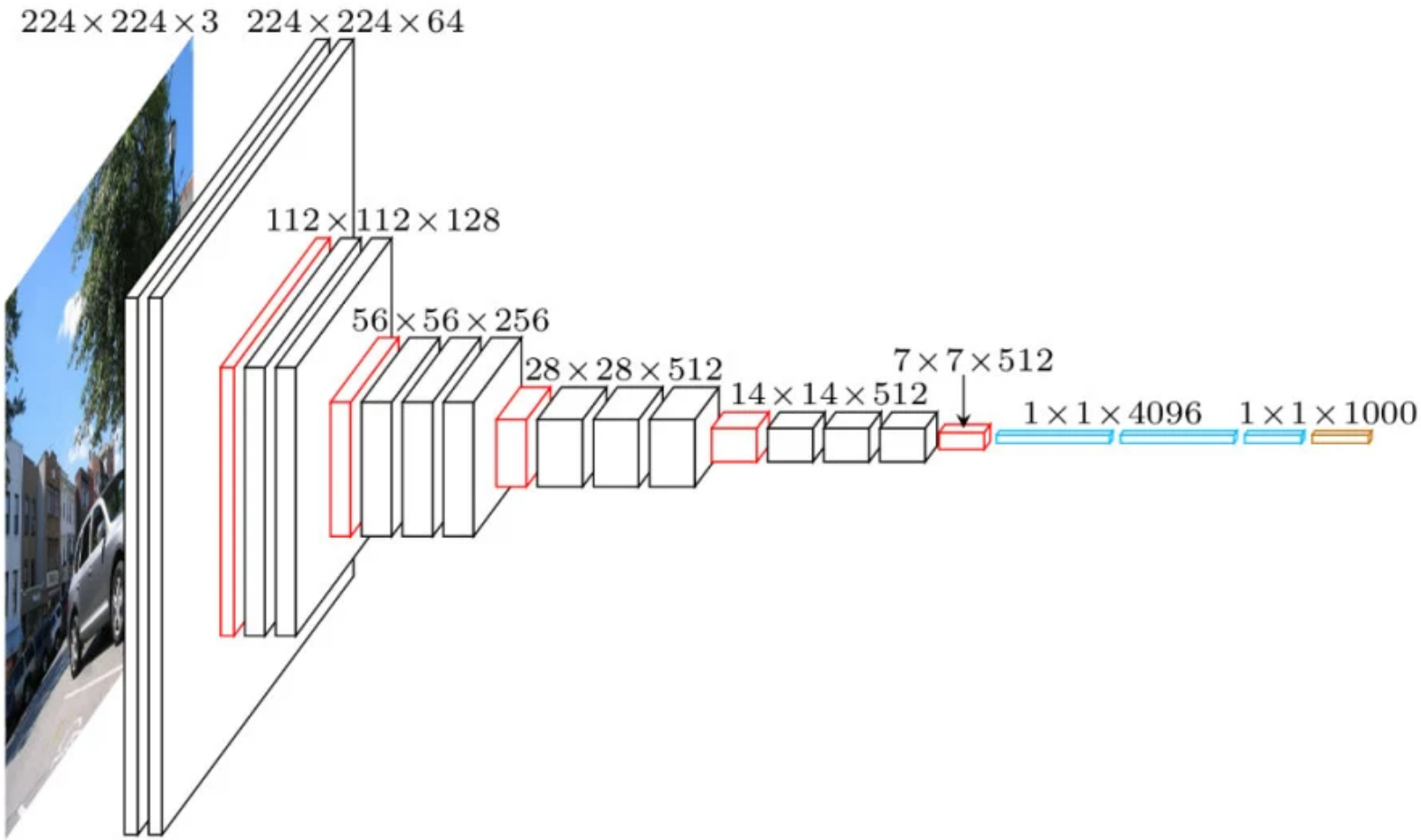

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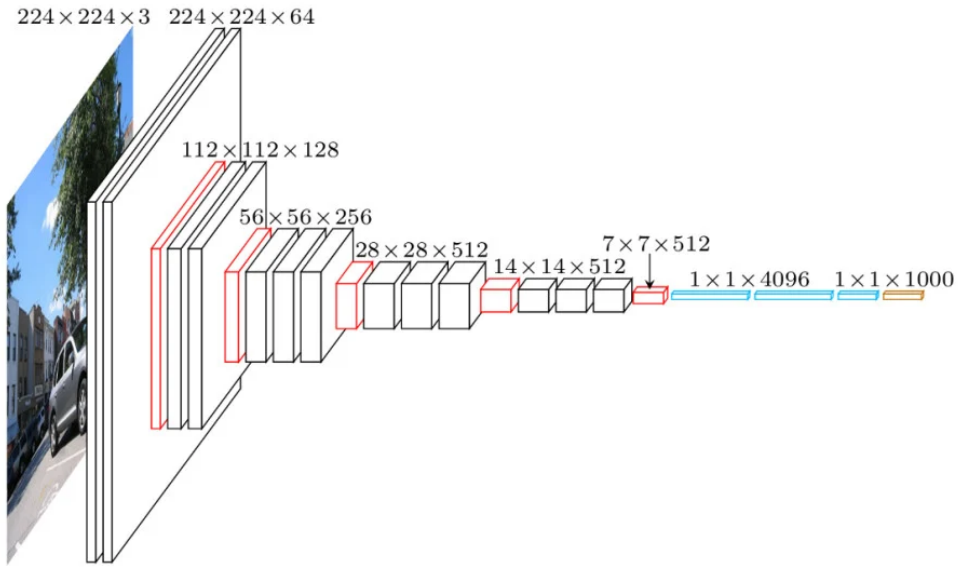

- Each block has a predefined structure (e.g., a linear map)

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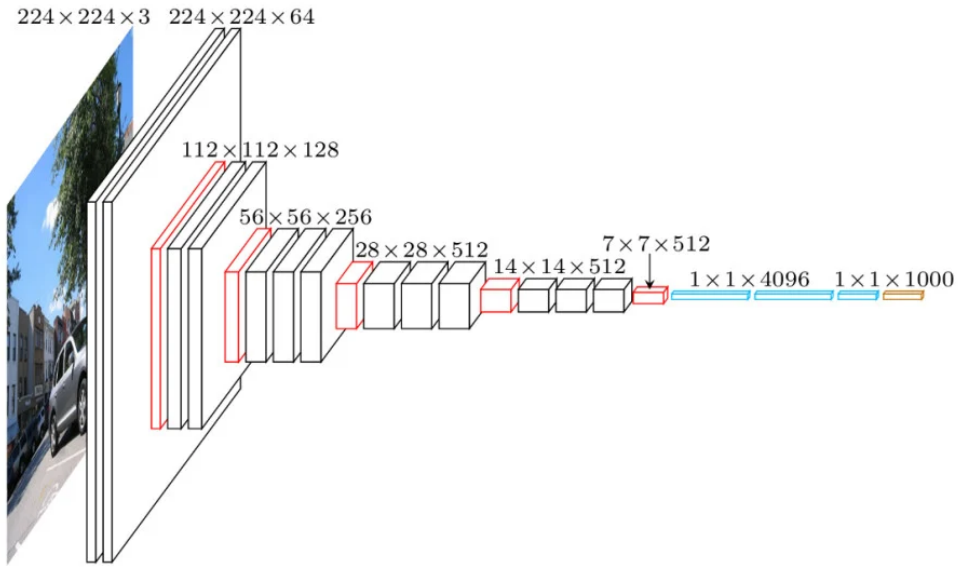

- Each block has a predefined structure (e.g., a linear map)
- Each block is defined in terms of unknown parameters θ

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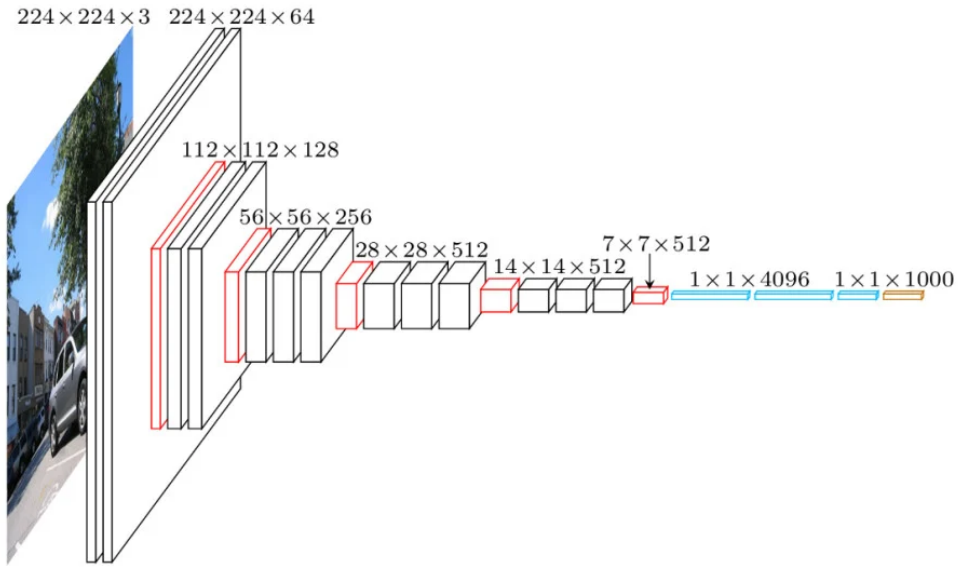

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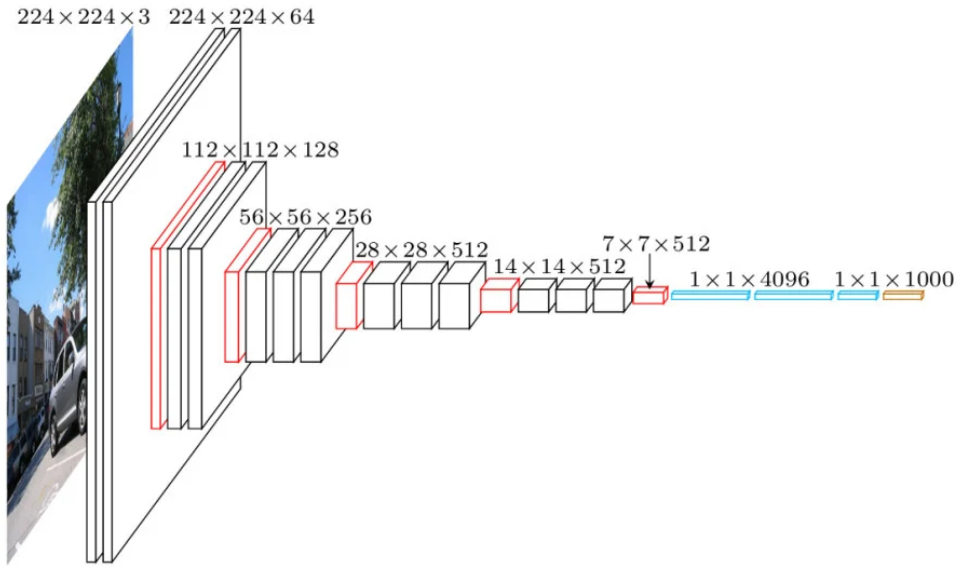

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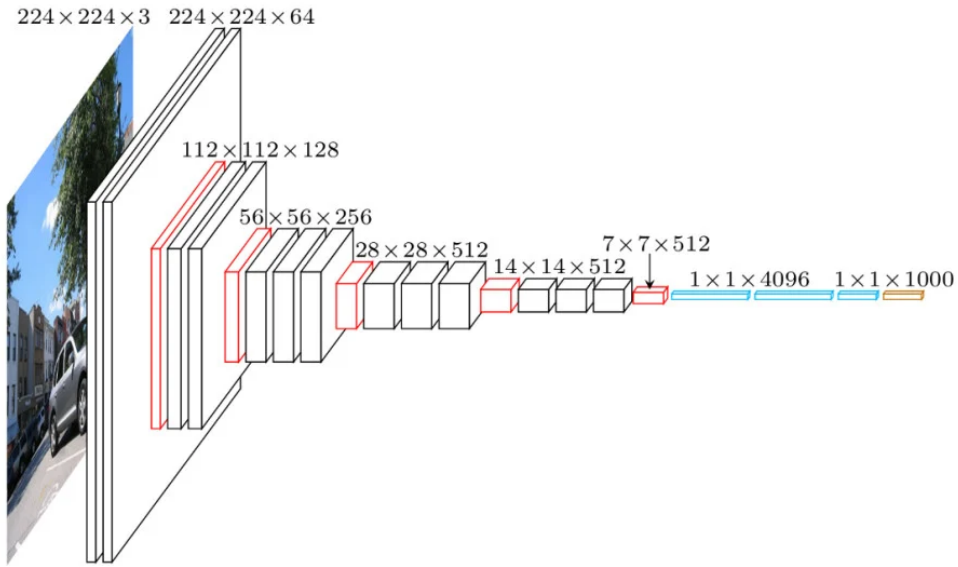

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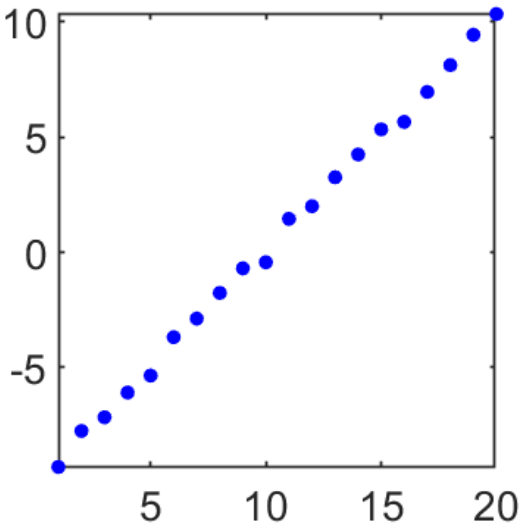
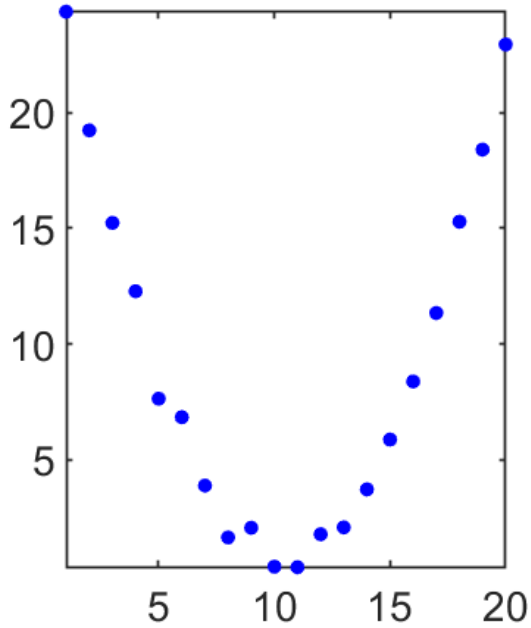
- ...which is done by minimizing a function called loss
- Minimization requires computing gradients, called backpropagation

Parametrized models

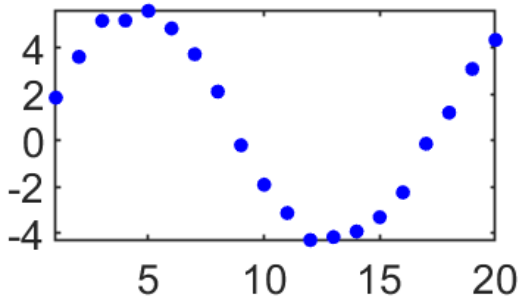
The parameters describe the behavior of the network, and must be solved for.



$y = ax + b$



$y = ax^2 + bx + c$



$y = a\sin(x) + bx + c$

Parametrized models

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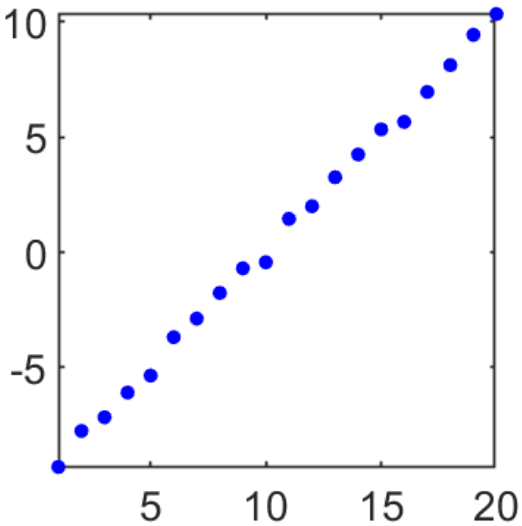

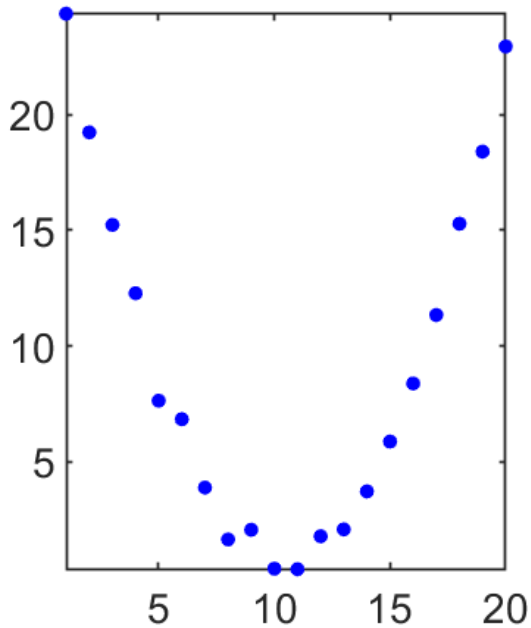

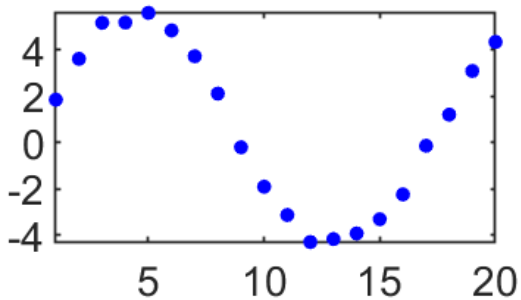

$$f_{a,b}(x) = ax + b$$

Parametrized models

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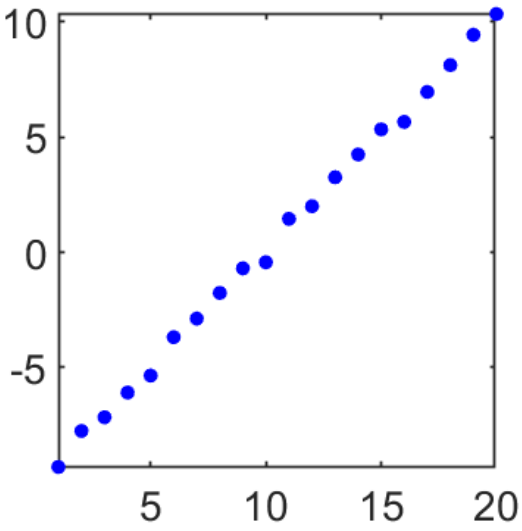
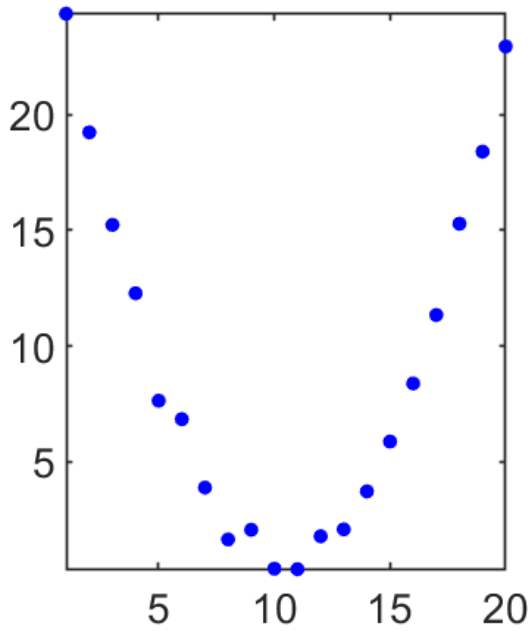
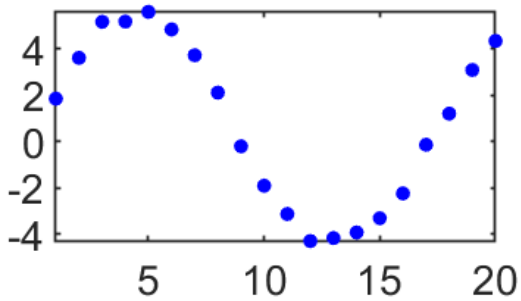


$f_{\Theta_f}(x)$

$\Theta_f \equiv \{a, b\}$



$g_{\Theta_g}(x)$

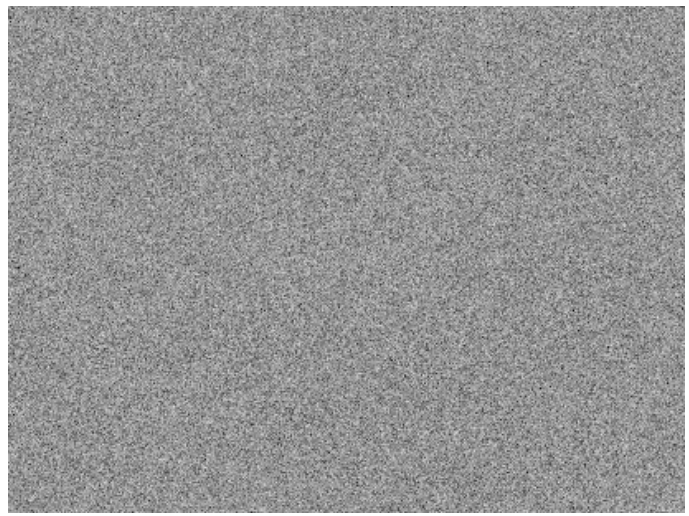


$h_{\Theta_h}(x)$

From a technical standpoint, our task is to determine the parameters Θ.

Structure as a strong prior

Key insight: Data often carries structural priors in terms of repeating patterns, compositionality, locality, ...



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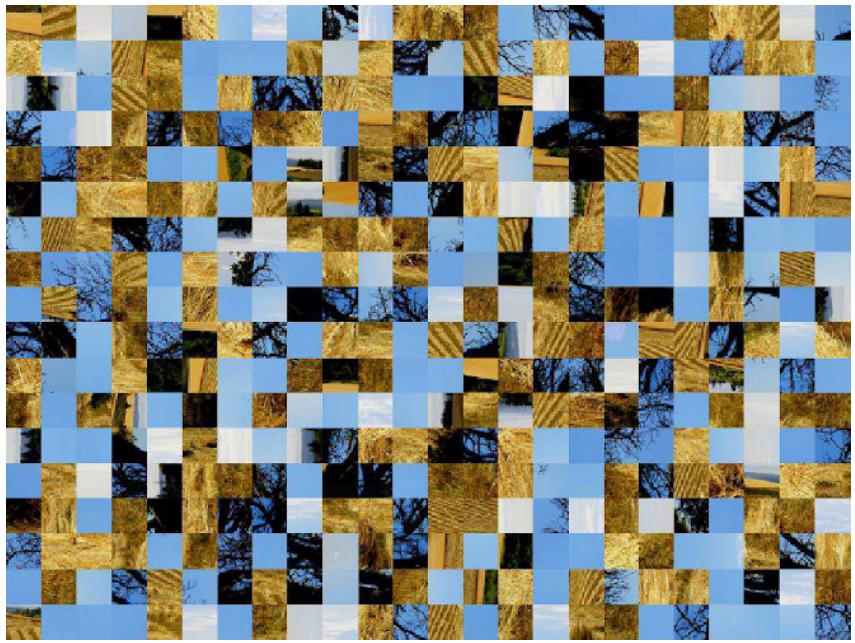

Son et al, "Solving Small-piece Jigsaw Puzzles by Growing Consensus", CVPR 2016

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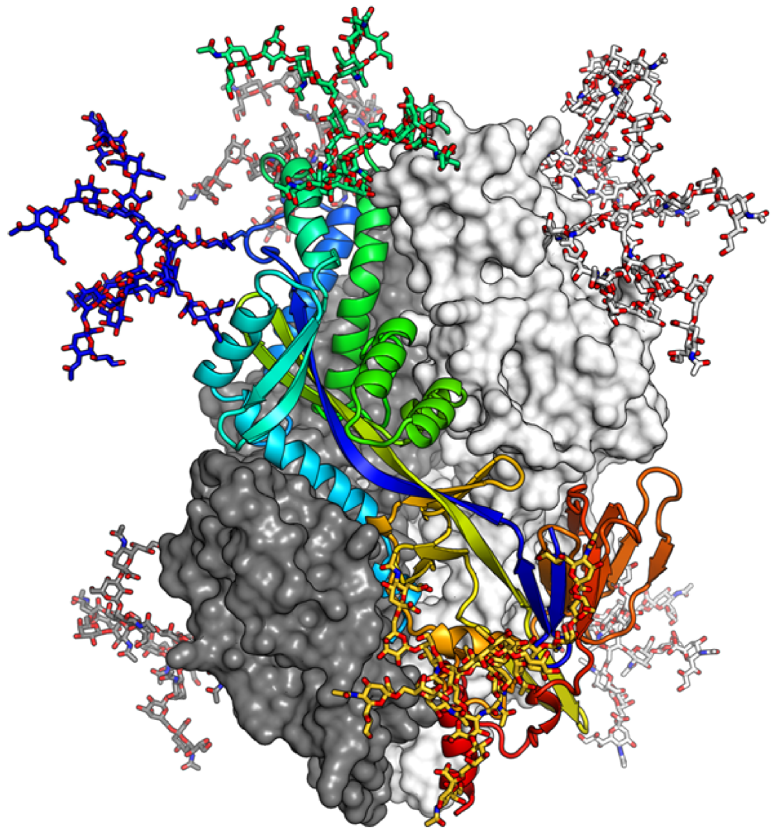

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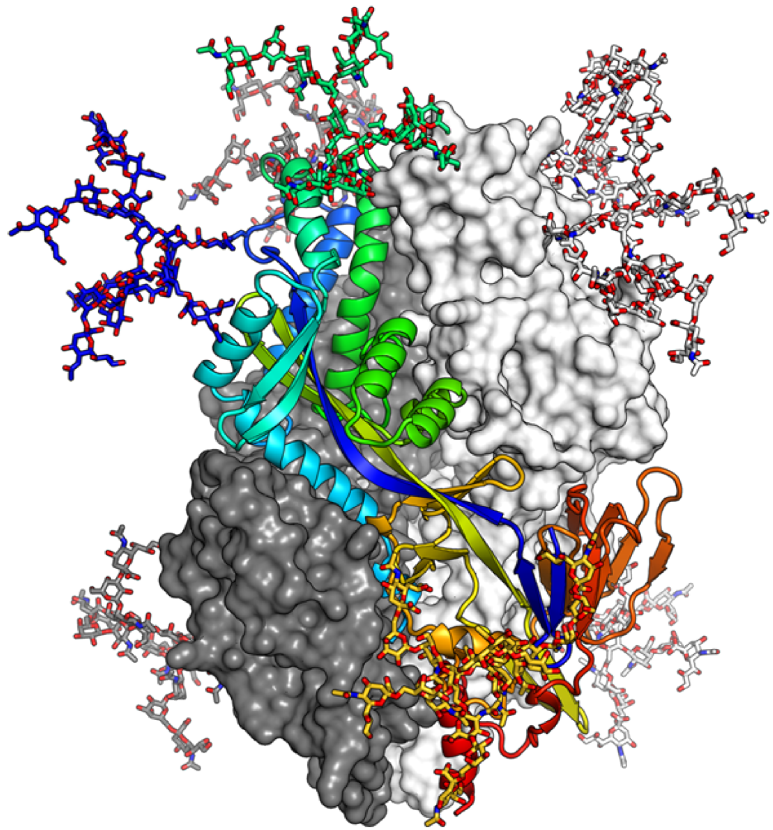
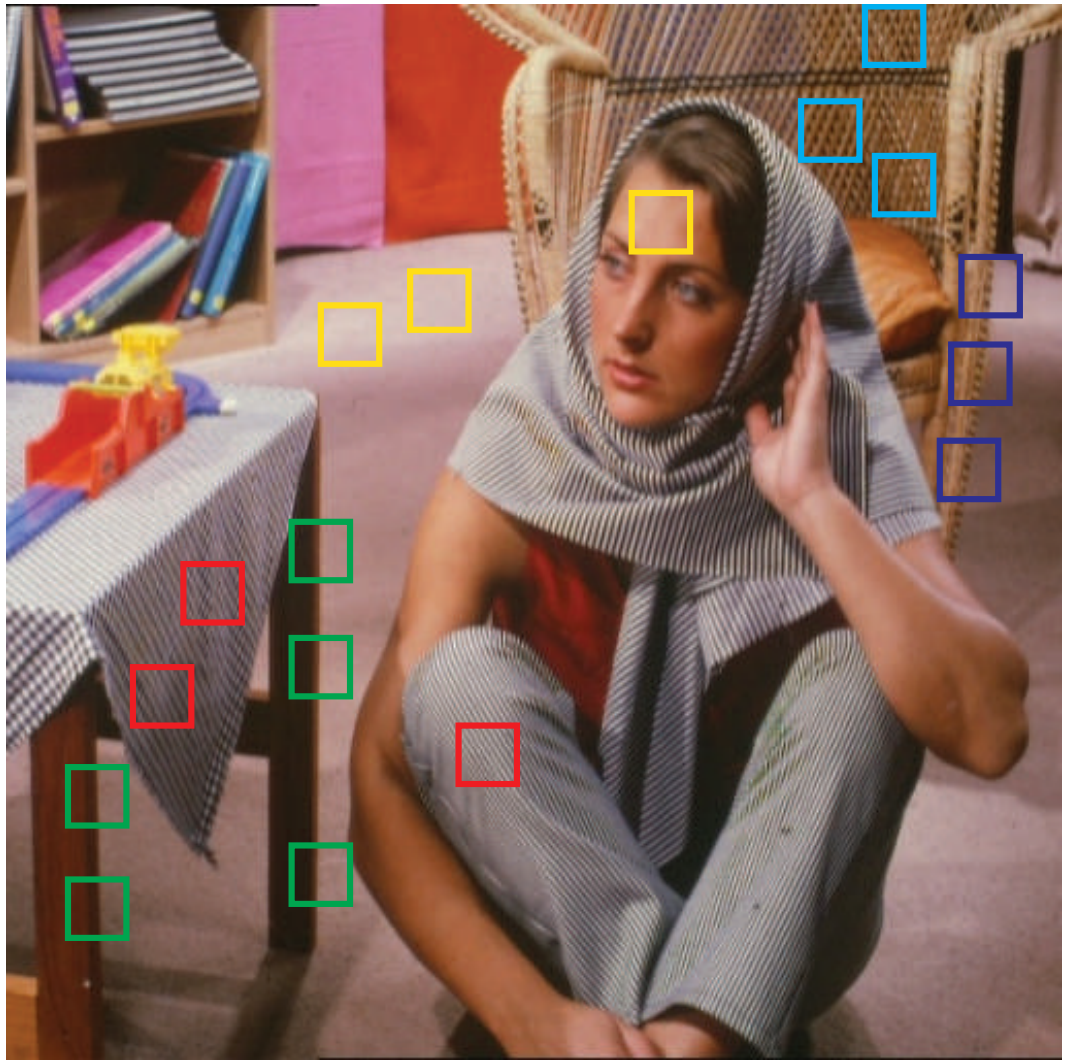


Take advantage of the structure of the data.

Self-similarity

Data tends to be self-similar across the domain:



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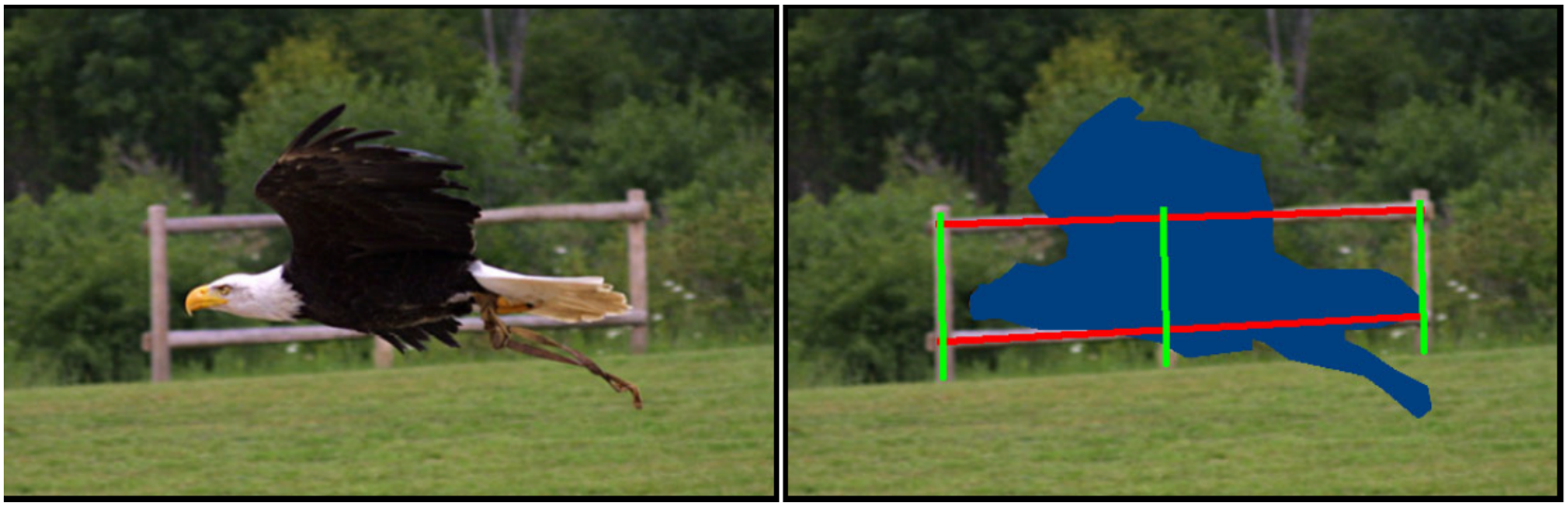

Barnes et al, "PatchMatch: A Randomized Correspondence Algorithm for Structural Image Editing", TOG 2009

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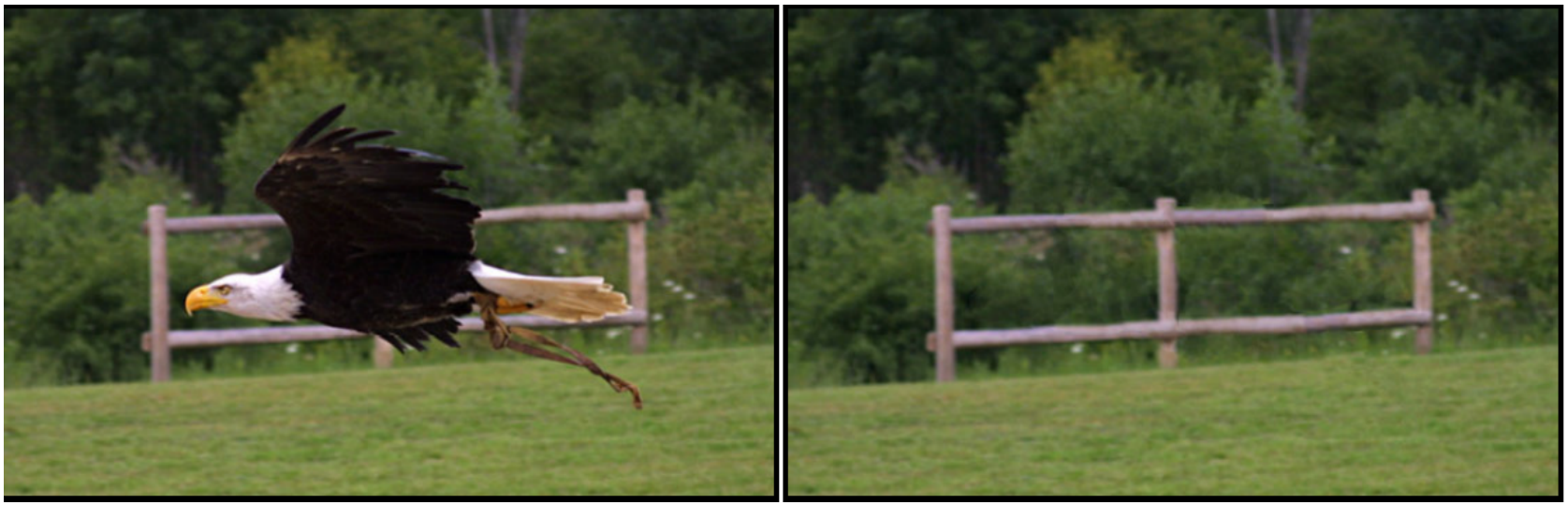

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Convolutional neural networks (CNN)

Data is often composed of hierarchical, local, shift-invariant patterns.

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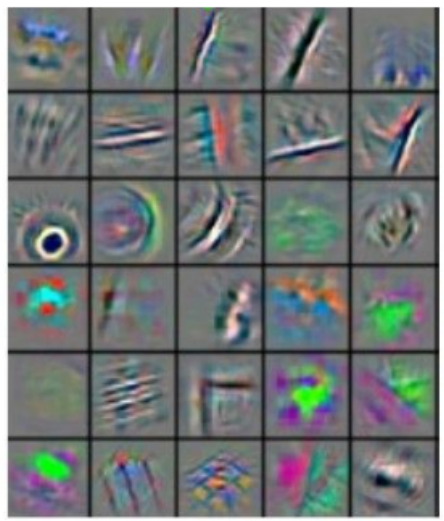
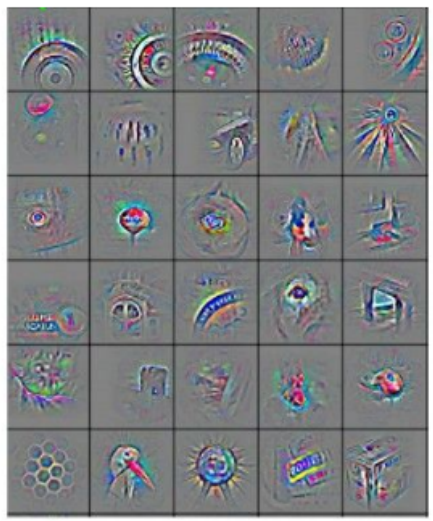
CNNs directly exploit this fact as a prior.

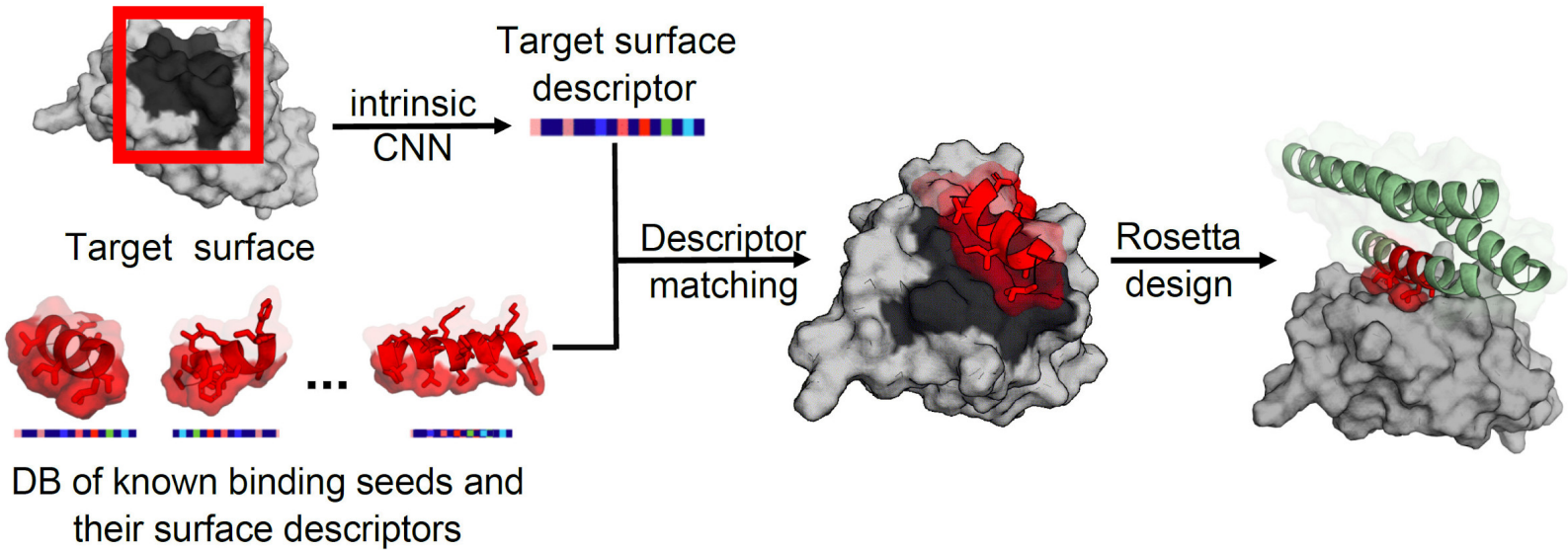
Learned features

→ low-level features → mid-level features → hi-level features → “car”





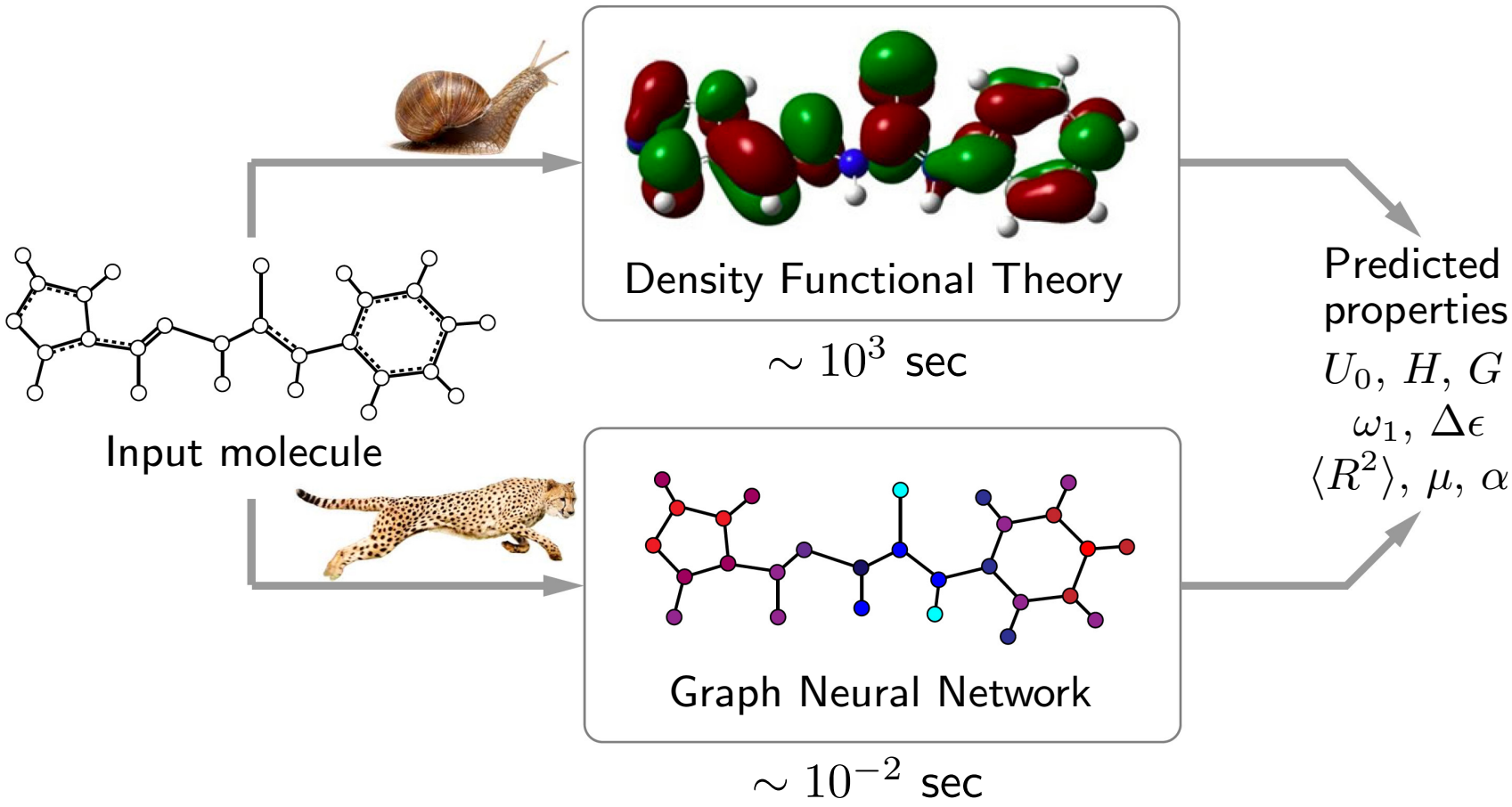
Application: Protein-Protein Interaction



Designing protein binder for the PD-L1 protein target

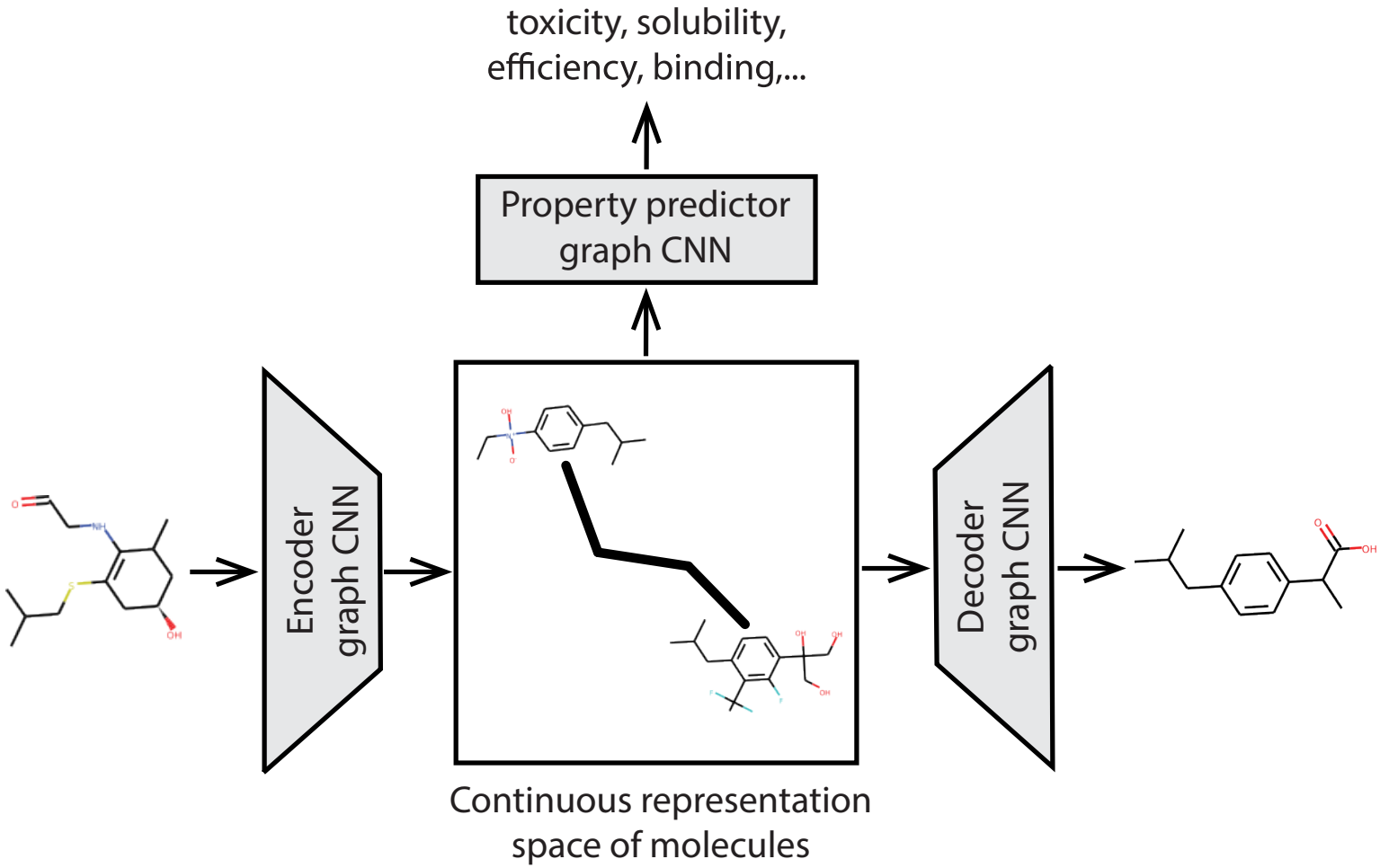
Gainza et al, "Deciphering interaction fingerprints from protein molecular surfaces using geometric deep learning", Nature Methods 2020

Molecule property prediction

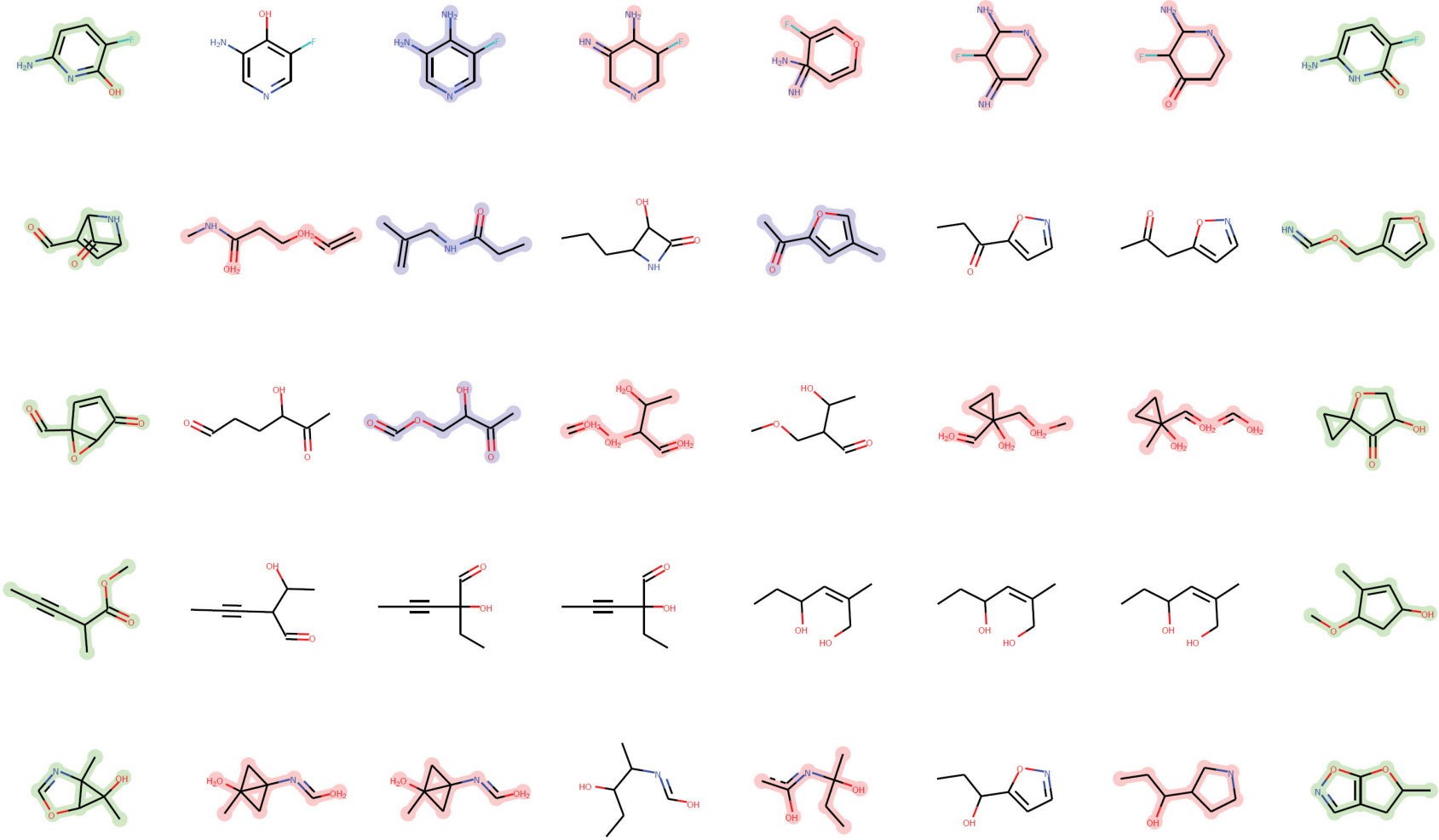


Duvenaud et al, "Convolutional Networks on Graphs for Learning Molecular Fingerprints", NIPS 2015; Gomez-Bombarelli et al, "Automatic chemical design using a data-driven continuous representation of molecules", ACS Cent. Sci. 2018

Generative models



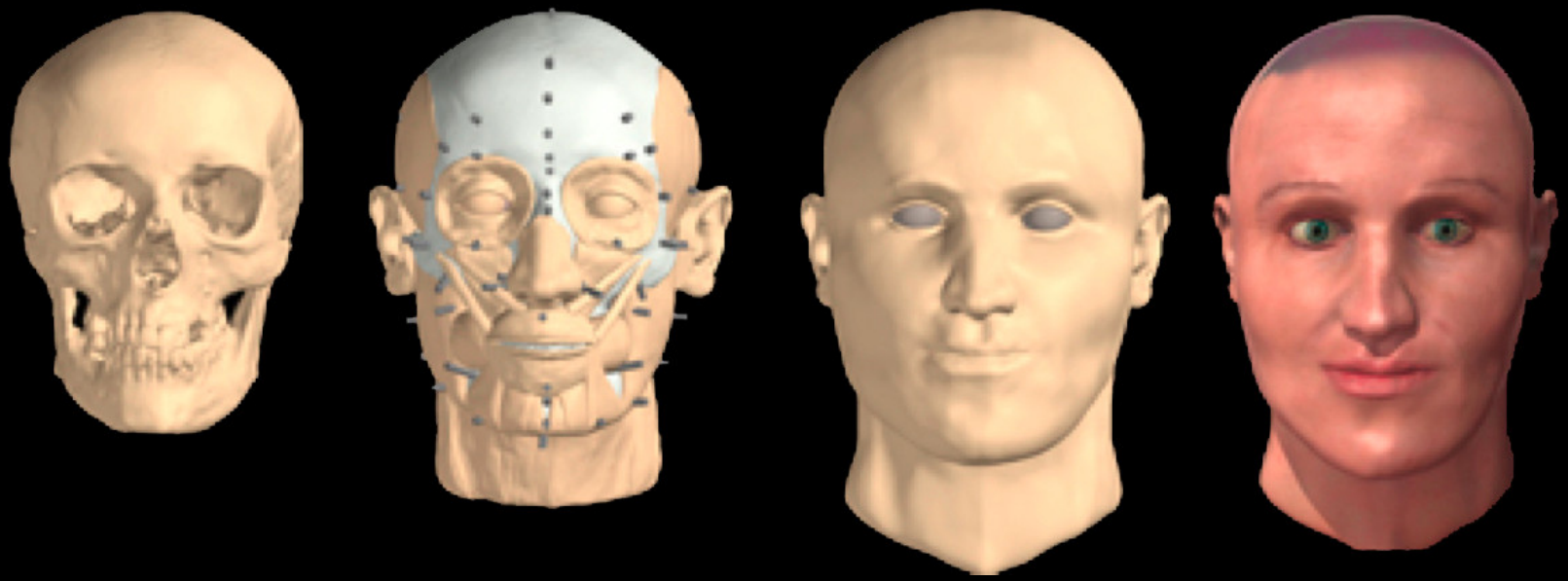
Molecule generation



Molecules generated with a graph VAE

Simonovsky and Komodakis, "Graphvae: Towards generation of small graphs using variational autoencoders", 2017; De Cao and Kipf, "MolGAN: An implicit generative model for small molecular graphs", 2018

Face from DNA



Claes et al, “Facial recognition from DNA using face-to-DNA classifiers”, Nature Communications 2019

Suggested reading

If you are curious, my course on Deep Learning (Computer Science):

`https://erodola.github.io/DLAI-s2-2021/`

`https://www.youtube.com/playlist?list=PL53MAHEGhXqLNzg-8ue8li2SU6ORE2rCl`