Introduction to Machine Learning in Data Assimilation

Eviatar Bach

10 June 2025

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    - Train and test error, cross-validation

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- Using a learned forecast model in DA
- Learning the assimilation step, or the forecast + assimilation step jointly.

Inverse Problems and Data Assimilation: A Machine Learning Approach

Eviatar Bach [♯♮], Ricardo Baptista [♯], Daniel Sanz-Alonso [♭], Andrew Stuart [♯]

https://www.arxiv.org/abs/2410.10523

Types of machine learning

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- **Supervised learning**: data is given "labelled", objective is to learn relationship to predict on new data.
- **Unsupervised learning**: data is unlabelled, and objective is to learn some patterns in the data.

Supervised learning

Supervised learning

Assume we have a dataset of N pairs of points

$$\{(\mathbf{x}_n, \mathbf{y}_n)\}_{n=1}^{N},$$

that is, $(\mathbf{x}_1, \mathbf{y}_1), \ldots, (\mathbf{x}_N, \mathbf{y}_N)$.

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Labels: the $\mathbf{x}_n$ are inputs, $\mathbf{y}_n$ are outputs.

We assume that the $\mathbf{y}_n$ are related to the $\mathbf{x}_n$ through some possibly noisy function, i.e.,

$$\mathbf{y}_n = f(\mathbf{x}_n; \theta) + \text{noise}.$$

The objective is to learn the parameters θ for some specific form of $\mathbf{f}$.

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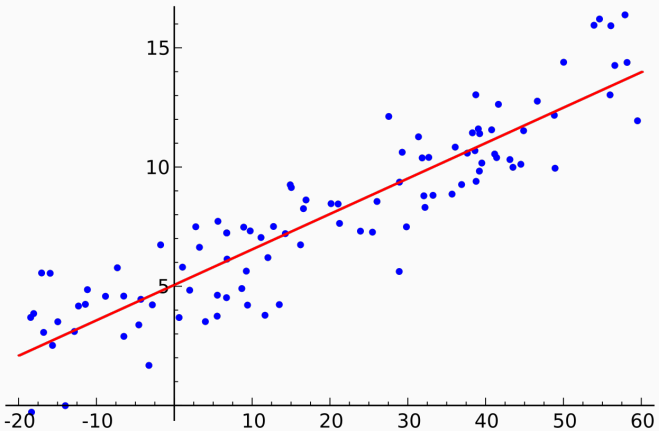
Example: in linear regression,

$$\mathbf{y}_n = \boldsymbol{\beta}^\top \mathbf{x}_n + \text{noise}.$$

In this case, $\boldsymbol{\theta} = \boldsymbol{\beta}$.



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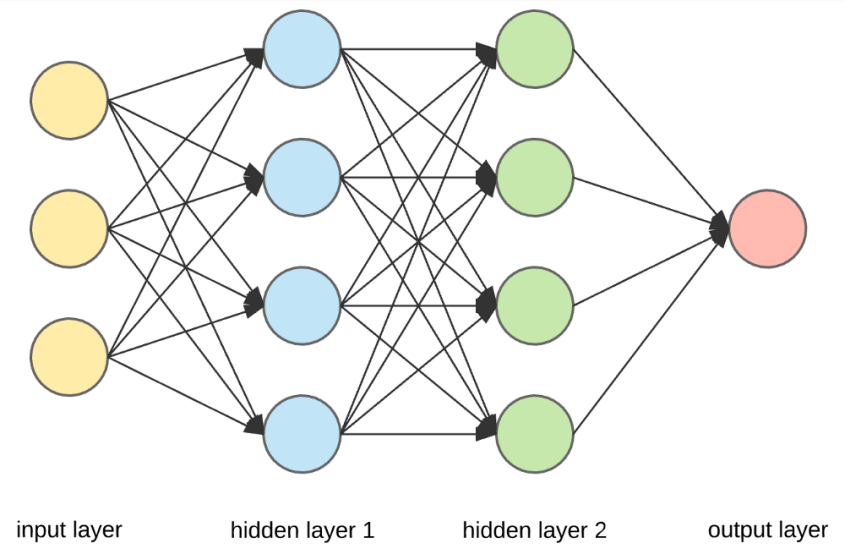
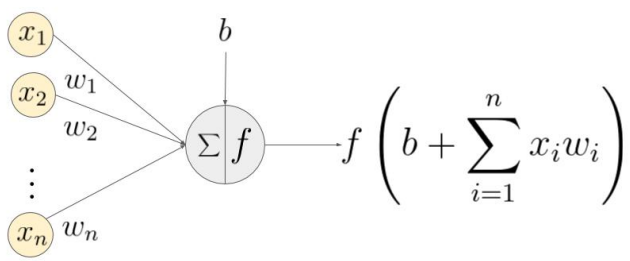
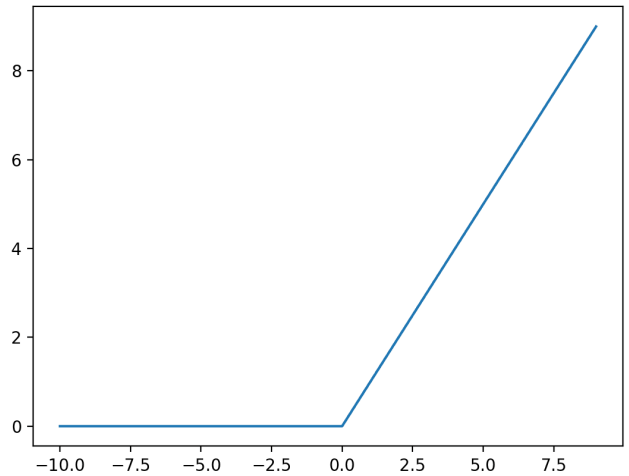
Example: neural networks.

Neural networks





An example of a neuron showing the input (x_1 - x_n), their corresponding weights (w_1 - w_n), a bias (b) and the activation function f applied to the weighted sum of the inputs.



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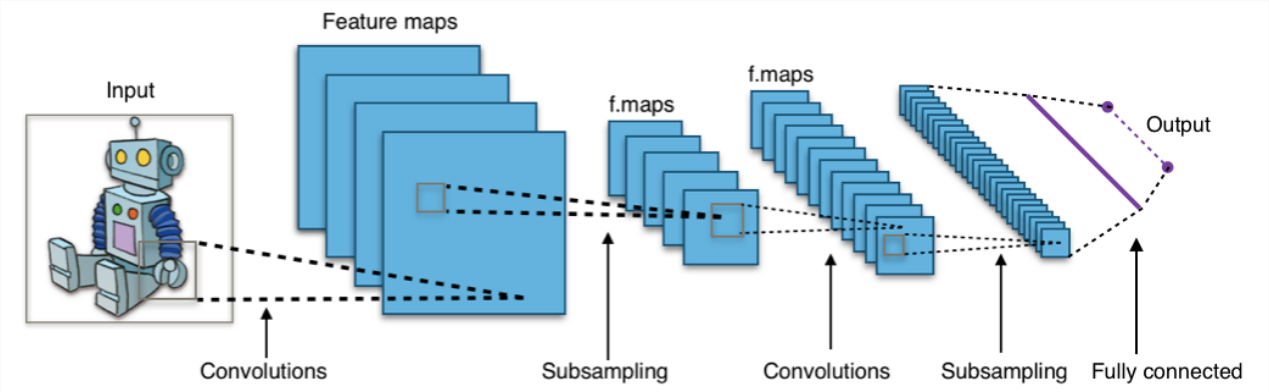
Can build in spatial structure: convolutional neural networks.



Time-series forecasting

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or memory can be incorporated as

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where τ is the amount of memory. If $\mathbf{x}$ includes all the relevant variables, memory will in general not be needed. If there are unobserved variables it can be useful.

Classification

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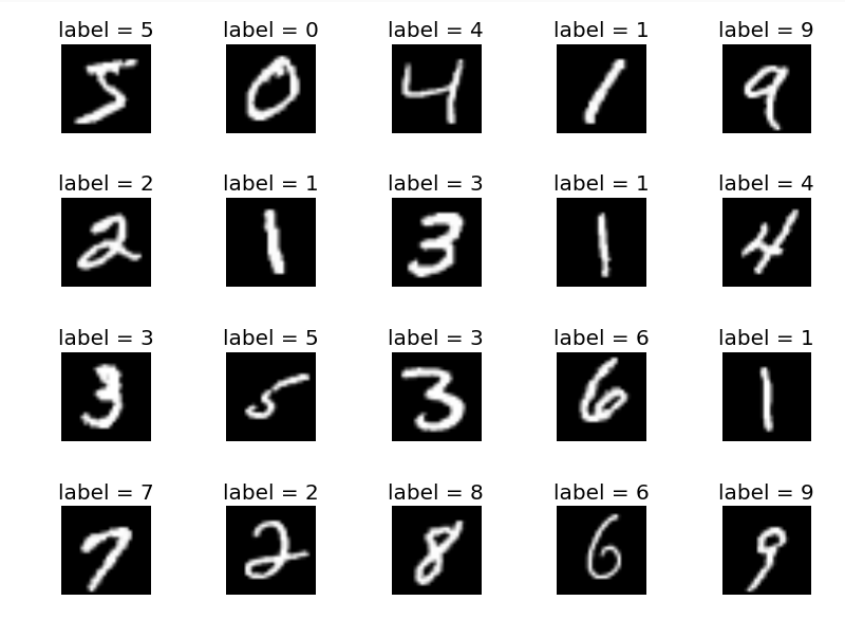
Example: MNIST



Unsupervised learning

Generative models

Suppose we have a dataset

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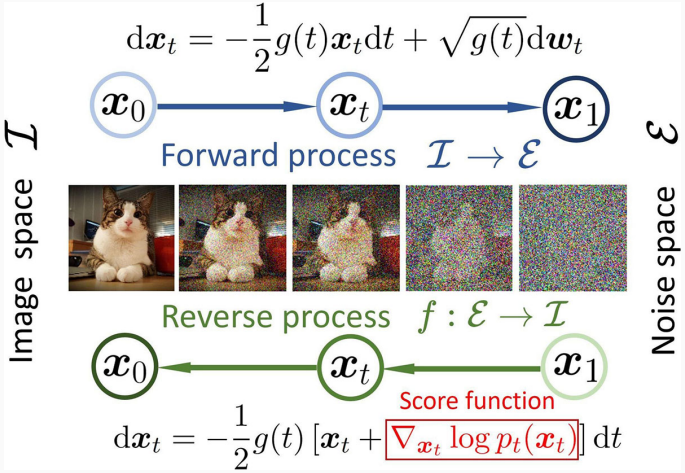
Example: diffusion models

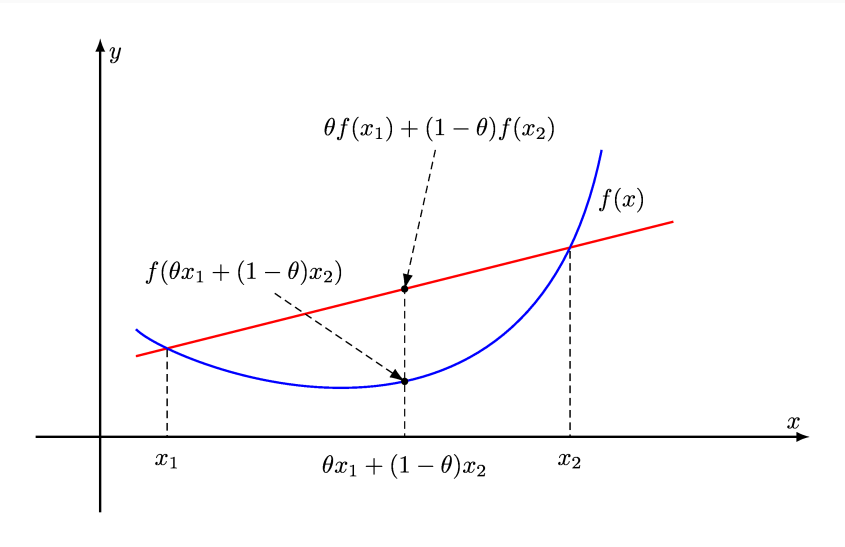


Optimisation

Convexity

A function $f : \mathbb{R}^d \to \mathbb{R}$ is called *convex* if, for all s_1, s_2 and for all $\theta \in [0, 1]$, we have that

$$f(\theta s_1 + (1 - \theta)s_2) \leq \theta f(s_1) + (1 - \theta)f(s_2).$$



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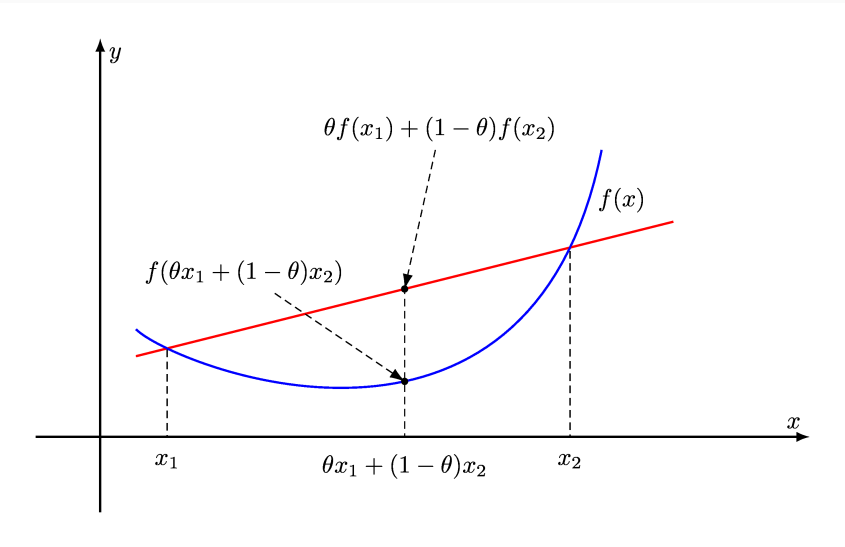

A function is called *strictly convex* if the inequality is strict for $s_1 \neq s_2$.

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Positive definite Hessian (positive second derivative) $\implies$ strictly convex, and positive semidefinite Hessian (nonnegative second derivative) $\iff$ convex.

Gradient descent

Given $f : \mathbb{R}^d \to \mathbb{R}$, gradient descent is computed from a sequence of step-sizes $\{\alpha_j\}_{j \in \mathbb{Z}^+}$ by picking an $x_0 \in \mathbb{R}^d$ and then iterating as follows:

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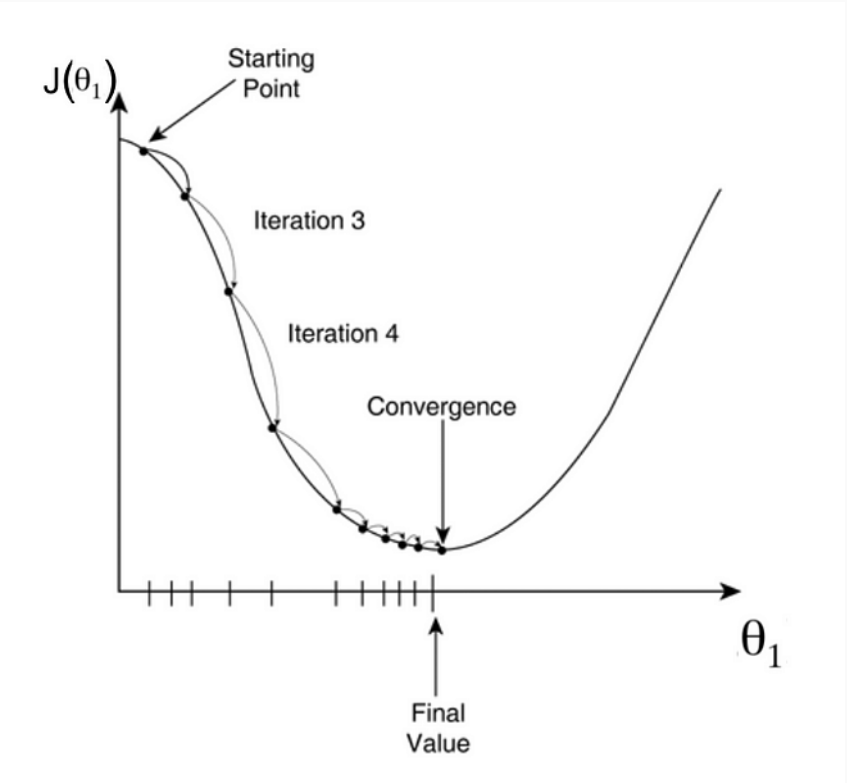

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Optimisation algorithms for nonconvex functions try to balance *exploration* and *exploitation*:

- Exploitation: pursue the most promising current avenue (e.g., gradient descent)
- Exploration: venture out to find new avenues in the hope of finding a more promising avenue (e.g., stochasticity)

Stochastic gradient descent (SGD)

Suppose the cost function can be written as a mean over data points, e.g., recall

$$J(\boldsymbol{\theta}) = \frac{1}{N} \sum_{n=1}^{N} (f(x_n; \boldsymbol{\theta}) - y_n)^2.$$

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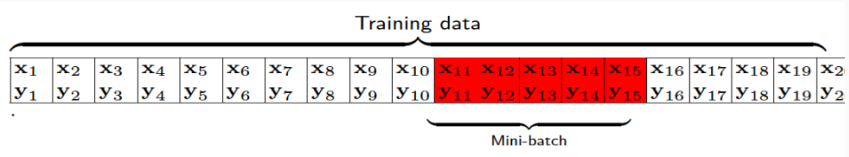
Stochastic gradient descent (SGD) instead computes the gradient with respect to a random subset: a *mini-batch*.



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Popular optimisation methods used in ML (e.g., ADAM) are variants of stochastic gradient descent.

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This can allow differentiation through model states (adjoint), model parameters, and DA algorithms, and enable use of gradient-based optimization.

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We assume the implementation of f in computer code is made up of n elementary operations $f_i : \mathbb{R}^{d_{i-1}} \to \mathbb{R}^{d_i}$ (for instance, addition, multiplication, logarithms, etc.), such that

$$f(x) = f_n \circ f_{n-1} \circ \cdots \circ f_1(x), \tag{1}$$

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Writing the partial evaluations up to $i \leq n$ as

$$g_i = (f_i \circ \cdots \circ f_1)(x),$$

by the chain rule we have that

$$D_x f(x) = (D_{g_{n-1}} f_n(g_{n-1})) \cdots (D_{g_1} f_2(g_1))(D_x f_1(x)). \tag{2}$$

Automatic differentiation

This suggests the following algorithm (*forward mode* automatic differentiation):

1: **Input**: The functions $\{f_i(\cdot)\}_{i=1}^n$, their corresponding Jacobians $\{Df_i(\cdot)\}_{i=1}^n$, and the function input x.
2: Set $g_1 = f_1(x)$ and $J_1 = Df_1(x)$.
3: For $i = 2, \ldots, n$: set $g_i = f_i(g_{i-1})$ and $J_i = (Df_i(g_{i-1}))J_{i-1}$.
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Reverse mode autodiff requires a backwards pass to compute the derivative, and is more efficient when $d_0 \gg d_n$ (many inputs), whereas forward mode is more efficient when $d_n \gg d_0$ (many outputs).

Generalisation

Under- and over-fitting

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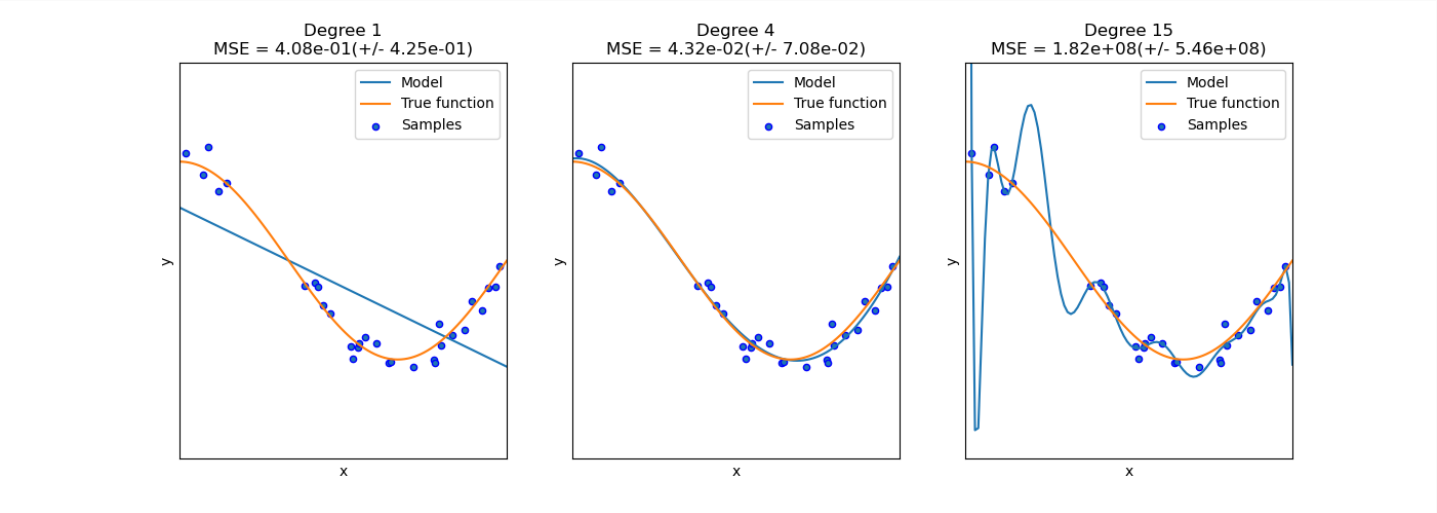

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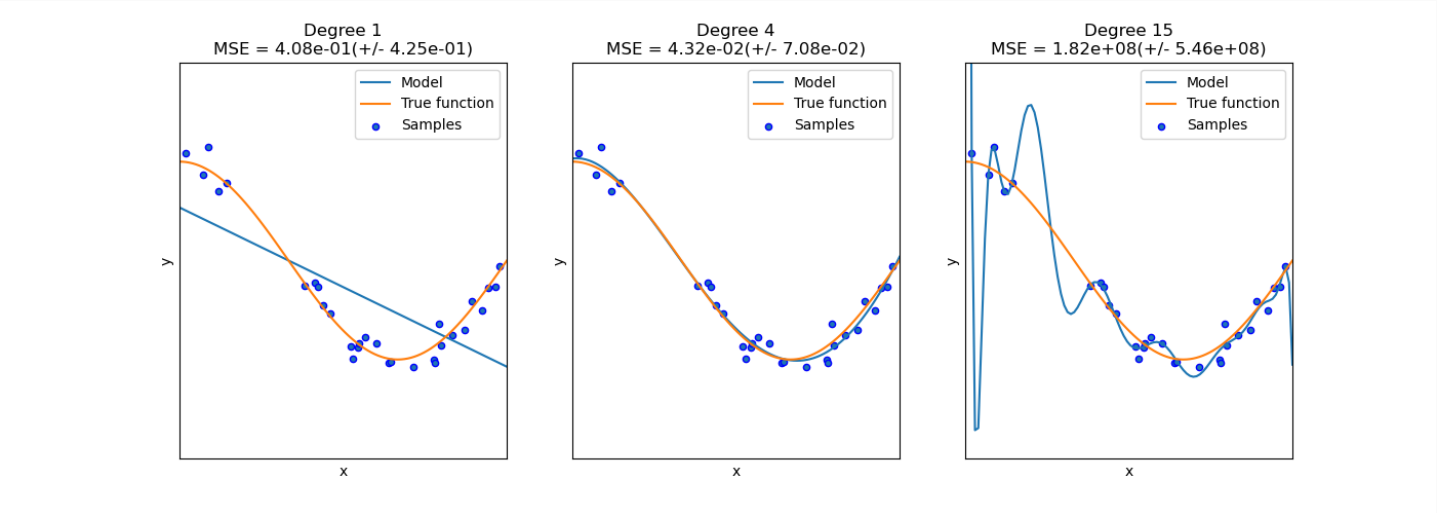

This failure to generalise is called *overfitting*. The performance on the training set is misleading.

Train and test set

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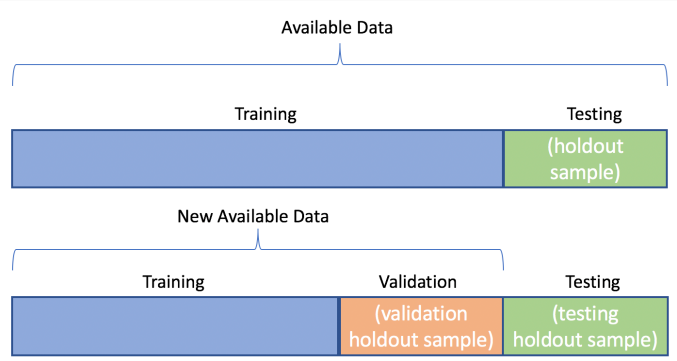
How to choose hyperparameters? Split data again, and validate performance on a *validation set*.



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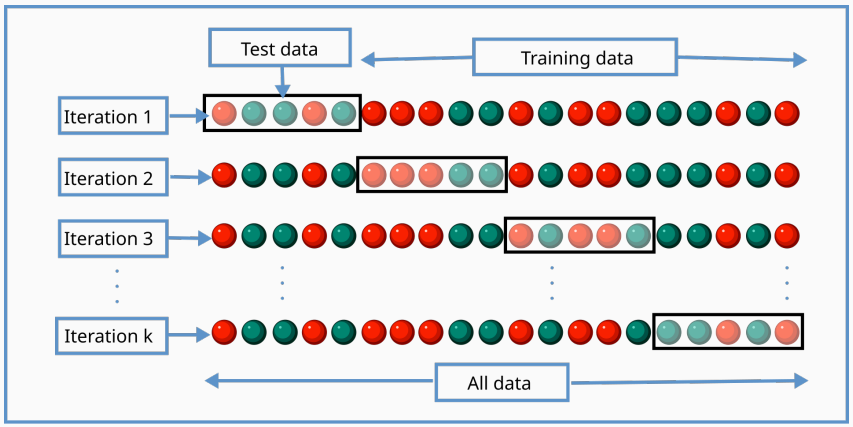

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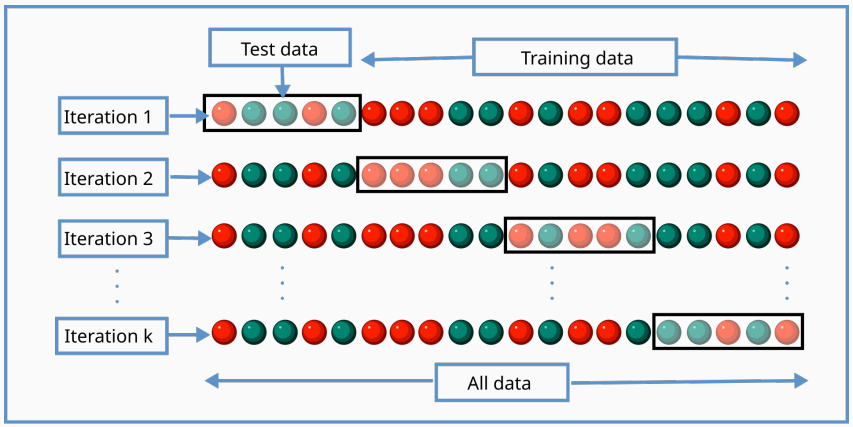

With k splits, called *k-fold* cross-validation.

References i