Lecture 07
Machine Learning 1:
regression

2024-10-02

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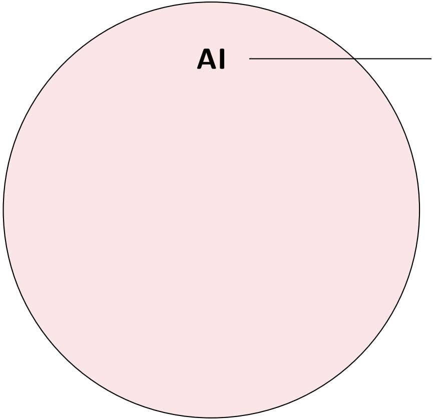
Introduction



Artificial Intelligence

broad concept, whereby machine mimics human behaviour

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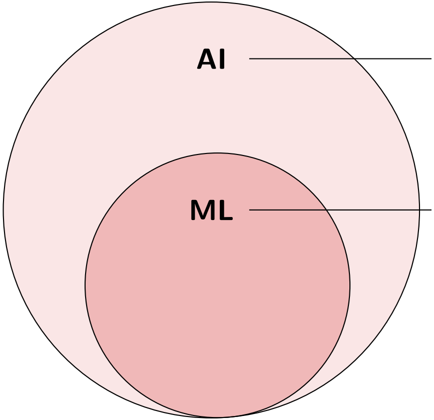

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subset of AI which uses **statistical** methods

(features are designed by the user)

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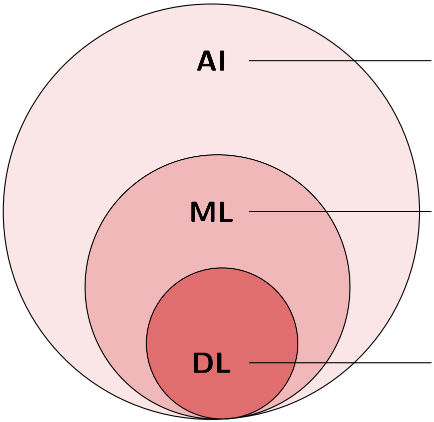

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subset of ML, which uses **multi-layered neural networks**
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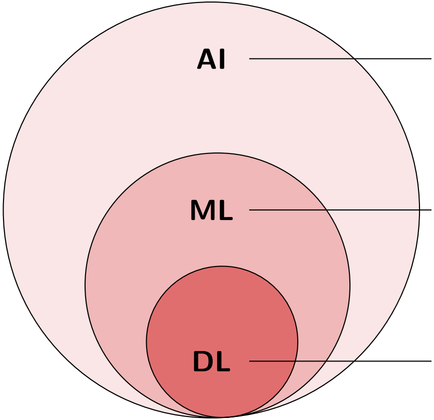

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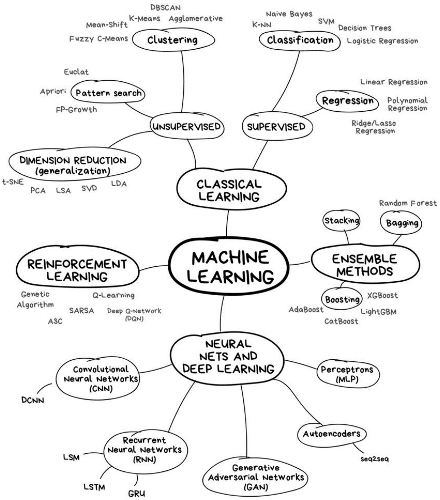
ML: lectures 07 (today), 08, 09, 10
DL: lectures 11, 12, 13

Introduction

Machine Learning is a huge (and growing) field!



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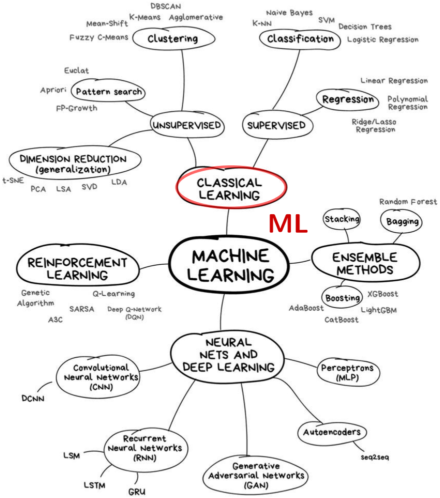

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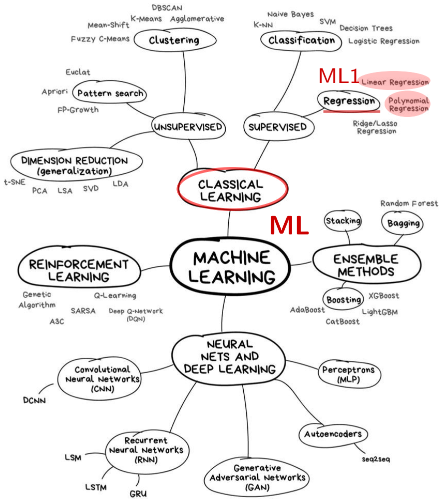

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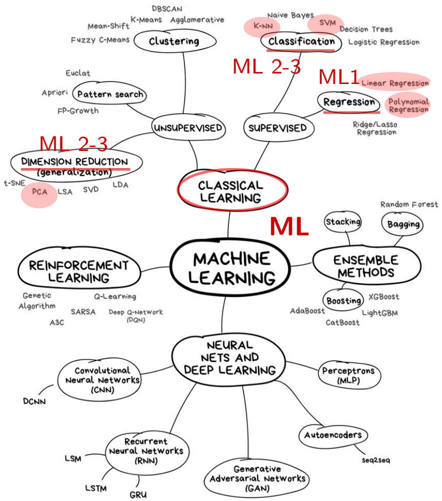

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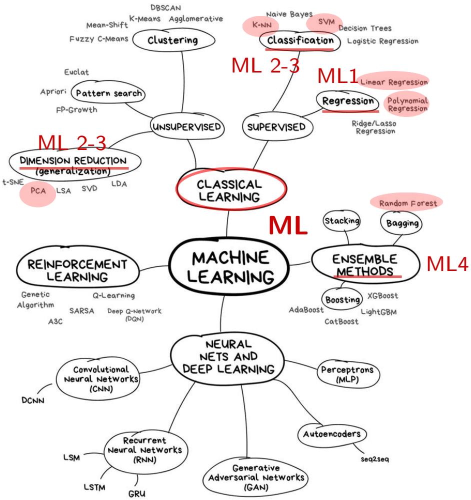

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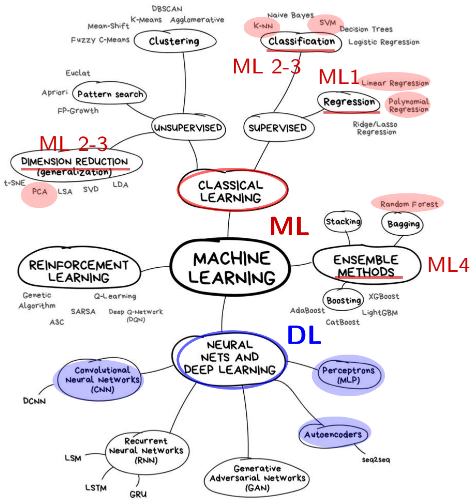

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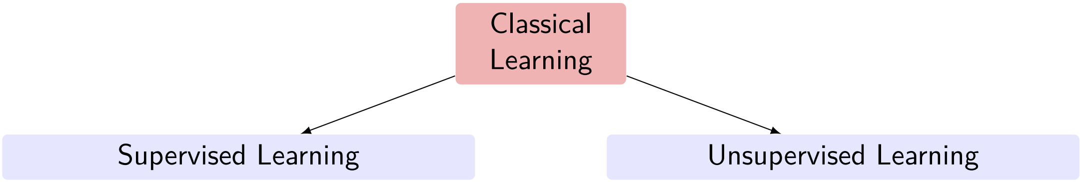

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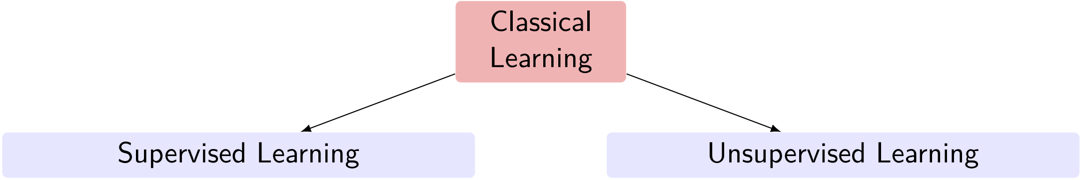

- Learning algorithm is presented inputs and desired outputs:
  training data $D = (in, out)$
- Goal: learn a general rule f that maps inputs to outputs
  $f(in) = out$

⇒ **Regression task**: *out* is a *continuous* number
e.g. linear regression, polynomial regression

⇒ **Classification task**: *out* is a *nominal* number (class label)
e.g. kNN, SVM, Logistic Regression

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Classical Learning

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Unsupervised Learning

- No training data is given to the learning algorithm
- Goal: find structure data, discover hidden patterns, learn features

⇒ **Dimension reduction**
e.g. PCA ($\rightarrow$ also used to craft features)

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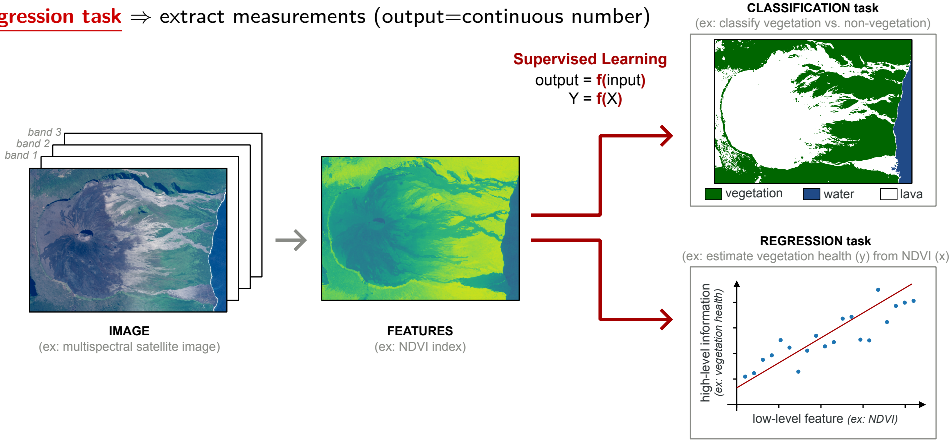
Goal of supervised learning

⇒ learn a function f which maps low-level image features (X) to high-level image information (Y):

- → **classification task** ⇒ extract semantic classes (output=nominal number)
- → **regression task** ⇒ extract measurements (output=continuous number)



*the term "feature" is here used in a broad sense, referring to any information extracted from the image

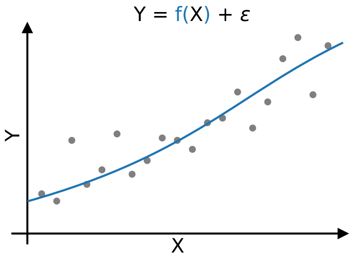
Regression model

⇒ we assume that two variables X & Y are ideally related by a function f:

$$Y = f(X) + \epsilon$$

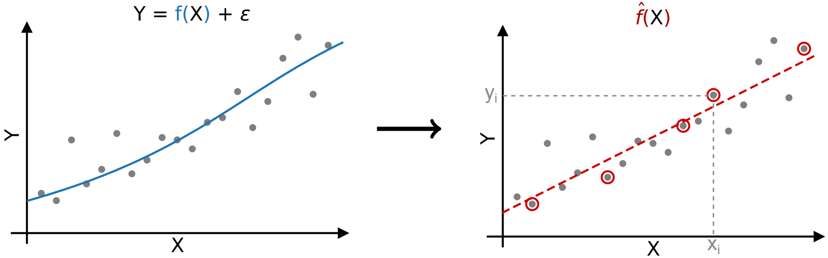
where:

- X = *input variable* (a.k.a. *independent variable*, or *feature*)
- Y = *output variable* (a.k.a. *dependent variable*, or *target variable*)
- ϵ = *random error* (intrinsic dataset error)



Regression model

⇒ goal: learn the **prediction function $\hat{f}$** using a set of **training samples** (i.e. pairs of (x_i, y_i))



⇒ how: minimize a criterion (a.k.a. the **prediction error** or **cost function**), which measures how well the predicted function f fits our training samples

→ for regression models, this metric is typically the **Mean Squared Error (MSE)**:

$$MSE(\hat{f}) = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{f}(x_i))^2$$

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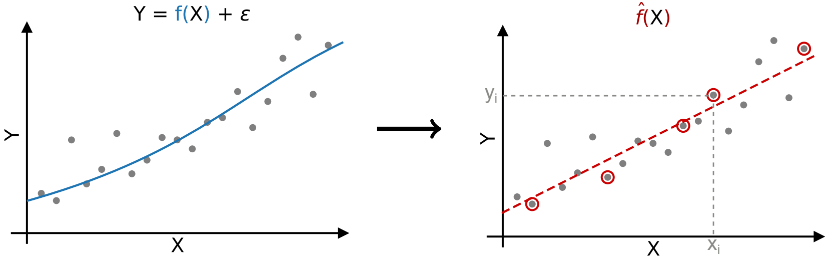

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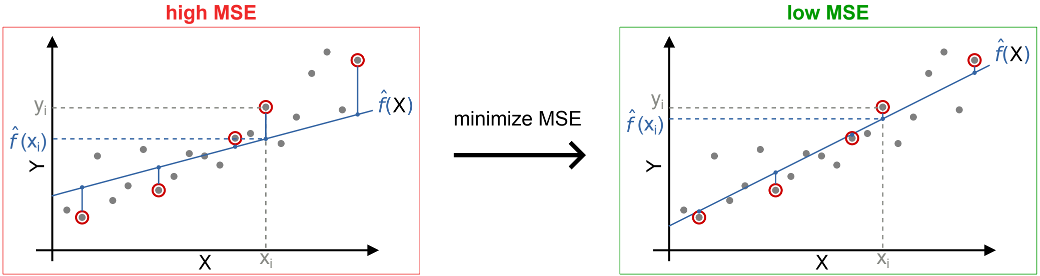
Regression model

⇒ minimizing the MSE means finding function $\hat{f}$ that best fits the training samples

$$MSE(\hat{f}) = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{f}(x_i))^2$$

$$\hat{f} = \text{argmin}_{f\in\mathcal{M}} MSE(f)$$



** the expression $\text{argmin}_{f\in\mathcal{M}}$ is mathematical notation for "the argument of the minimum", indicating we are trying to find the function f from a set of possible functions $\mathcal{M}$ that minimizes the MSE*

Parametric method: linear regression

⇒ parametric supervised learning means *we assume that $\hat{f}$ takes a specific form*, for example a linear relationship between X and Y:

$$\hat{f}(x) = \alpha x + \beta$$

⇒ the prediction error $MSE(\hat{f})$ therefore depends on 2 parameters (α, β) which need to be determined:

$$E(\alpha, \beta) = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{f}(x_i))^2$$
$$= \frac{1}{n}\sum_{i=1}^{n}(y_i - (\alpha x_i + \beta))^2$$

⇒ solution: solving for $dE/d\alpha = 0$ and $dE/d\beta = 0$ allows for an analytical solution of $(\hat{\alpha}, \hat{\beta})$:

$$\hat{\alpha} = \frac{\sum_i (x_i - \bar{x})(y_i - \bar{y})}{\sum_i (x_i - \bar{x})^2} = \frac{(X - \bar{X}) \cdot (Y - \bar{Y})}{(X - \bar{X}) \cdot (X - \bar{X})} = \frac{cov(X, Y)}{var(X)}$$

$$\hat{\beta} = \bar{y} - \hat{\alpha}\bar{x}$$

where $\bar{x}$ and $\bar{y}$ are the mean of x and y: $\bar{x} = \frac{1}{n}\sum_{i=1}^{n} x_i$ and $\bar{y} = \frac{1}{n}\sum_{i=1}^{n} y_i$

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2.3. parametric method: linear regression

The analytical solutions for $(\alpha,\ \beta)$ can be found using the *normal equation*:

$\Rightarrow$ the linear equation for a dataset with n observations is written as:

$$Y = \alpha X + \beta$$

where:

- $X = \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix}$ = nx1 vector of observed values x_i; $Y = \begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix}$ = nx1 vector of observed values y_i
- α = slope of the line
- β = intercept

$\Rightarrow$ the linear equation can be written in matrix form:

$$Y = X\theta$$

where:

- $X = \begin{pmatrix} 1 & x_1 \\ \vdots & \vdots \\ 1 & x_n \end{pmatrix}$ = nx2 matrix of ones & values of x_i; $Y = \begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix}$ = nx1 vector of values y_i

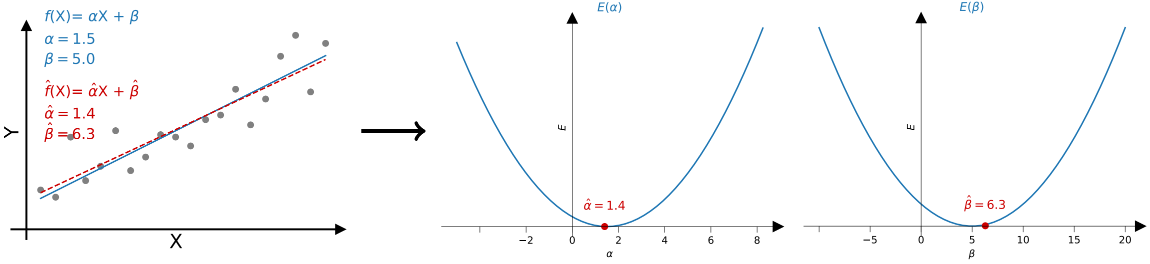
  NB: the first column in X are all ones to account for the intercept β
- $\theta = \begin{pmatrix} \beta \\ \alpha \end{pmatrix}$ = 2x1 vector of coefficients $(\beta,\ \alpha)$

$\Rightarrow$ now $\hat{\theta} = (\hat{\beta}, \hat{\alpha})$ is estimated by minimizing the least squares error, which results in the following solution:

$$\hat{\theta} = (X^T X)^{-1} X^T Y$$

2.3. parametric method: linear regression

⇒ **Error surface** of the coefficients (α, β) and estimated values $(\hat{\alpha}, \hat{\beta})$:



⇒ Note: the error surface is *convex*, which means a unique minimum exists

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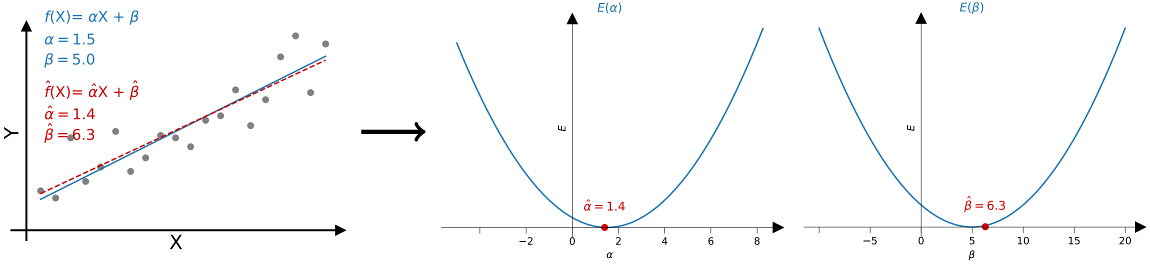

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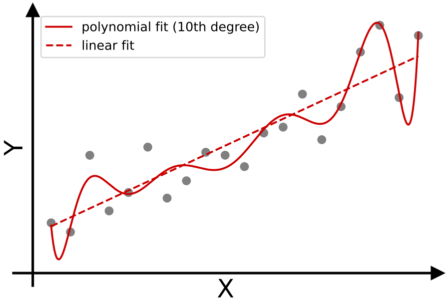
What if linear regression is not enough?

⇒ **polynomial regression** is a form of linear regression, where the relationship between the independent variable X and the dependent variable Y is modeled as an n^{th} degree polynomial:

$$\hat{f}(x) = \alpha_0 + \alpha_1 x^1 + \alpha_2 x^2 + \ldots + \alpha_n x^n$$



Polynomial regression as a linear model

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→ we are effectively mapping the feature x in a higher dimensional feature space $x' = (x, ..., x^n)$

→ if we treat x^n as a *new features*, we can think of this as a linear equation in the transformed feature space:

$$y = \alpha_0 + \alpha_1 \cdot (\textit{new\_feature\_1}) + ... + \alpha_n \cdot (\textit{new\_feature\_n})$$

→ this allows us to use linear regression to fit the polynomial model!

Polynomial regression as a linear model

$\Rightarrow$ linearity *in terms of coefficients* allows us to use *linear regression to fit polynomial data of degree d*:

$\rightarrow$ the equation is **non-linear with respect to x** because of the higher-order terms $(x^2, \ldots, x^d)$
$\Rightarrow$ *the model can capture non-linear relationships between X and Y*

$\rightarrow$ however, the equation is **linear with respect to the coefficients** $(\alpha_0, \ldots, \alpha_d)$
$\Rightarrow$ *the model can be solved using linear regression (coefficients found analytically using the normal equation)*:

$$\hat{\theta} = (X^T X)^{-1} X^T Y$$

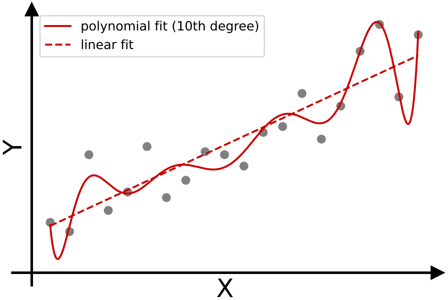
where:

- $X = \begin{pmatrix} 1 & x_1 & x_1^2 & \cdots & x_1^d \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_n & x_n^2 & \cdots & x_n^d \end{pmatrix} = n \times (d+1)$ matrix of ones and powers of x_i
- $Y = \begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix} = n \times 1$ vector of values y_i
- $\hat{\theta} = \begin{pmatrix} \alpha_0 \\ \vdots \\ \alpha_d \end{pmatrix} = (d+1) \times 1$ vector of coefficients α_i

Polynomial regression as a linear model

⇒ advantages: can model non-linear relationships, more flexible than linear regression

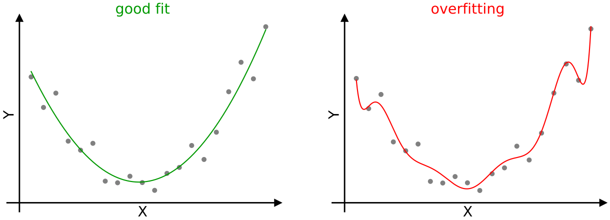
⇒ drawbacks: more complex, more prone to **overfitting**



What is overfitting & underfitting?

overfitting ⇒ model is too complex

→ captures the noise in the training data
→ does not generalize well to new data



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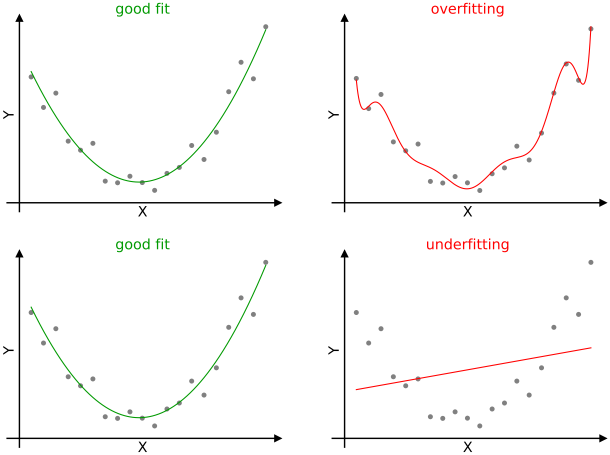
underfitting $\Rightarrow$ model is too simple

$\rightarrow$ does not capture the underlying structure of the data



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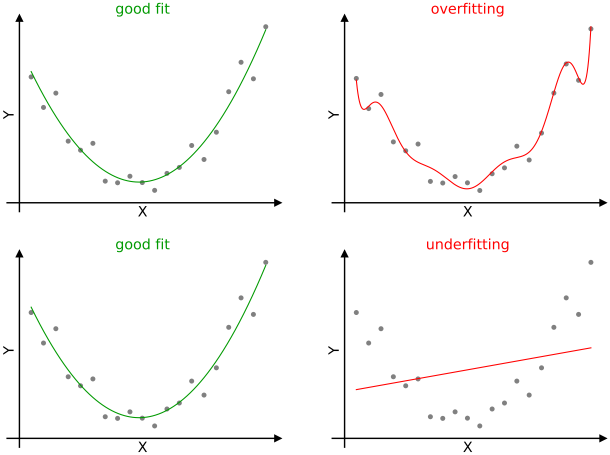

$\Rightarrow$ optimal model complexity & ability to generalize to unseen data?

Bias-variance trade-off

A model's generalization error can be expressed as the sum of three different errors:

- irreducible error: error due to the noisiness of the data itself

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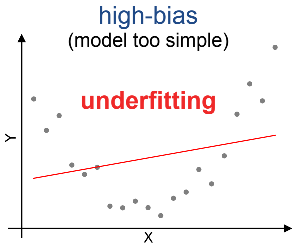
- **bias**: error due to overly simplistic assumptions in the model
  - → *high-bias* model ⇒ model is too simple (e.g., linear model for quadratic data), prone to *underfitting*



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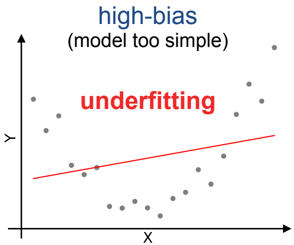
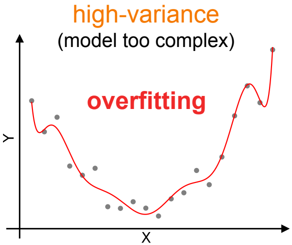
- **bias**: error due to overly simplistic assumptions in the model
  → *high-bias* model ⇒ model is too simple (e.g., linear model for quadratic data), prone to *underfitting*
- **variance**: error due to excessive sensitivity to small fluctuations in the training data
  → *high-variance* model ⇒ model with many degrees of freedom (e.g. high-deg. polynomial), prone to *overfitting*

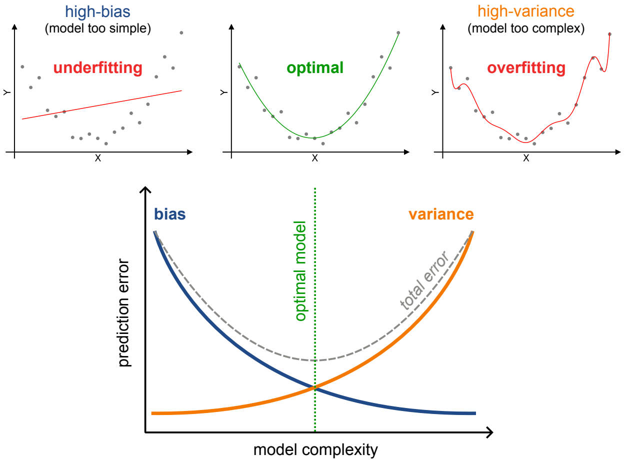




Bias-variance trade-off

⇒ *as the model complexity increases, bias decreases but variance increases*

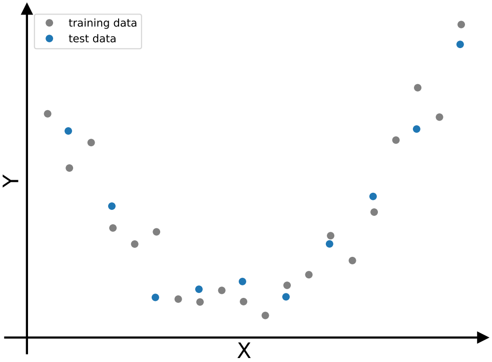
⇒ the optimal model complexity results from a trade-off between bias and variance:

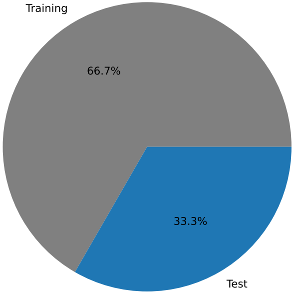


How can we evaluate the model capability to generalize?

⇒ we divide the dataset into 2 subsets *(sometimes more, we'll see that later)*:

- **training set**: used to train the model (i.e. estimate the coefficients)
- **test set**: used to evaluate the model's performance on unseen data





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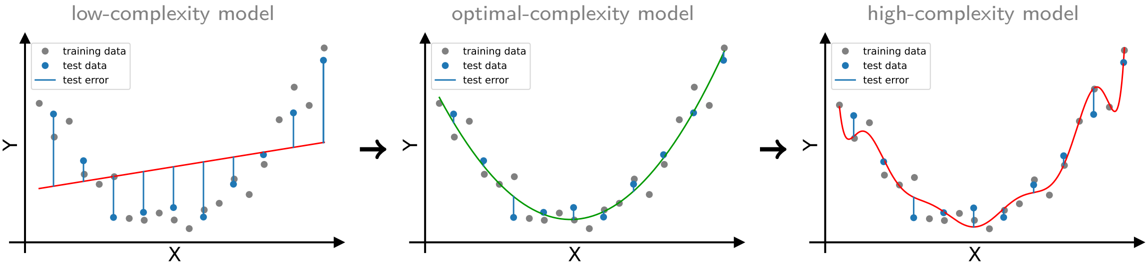

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