Big Data Computing

Master's Degree in Computer Science

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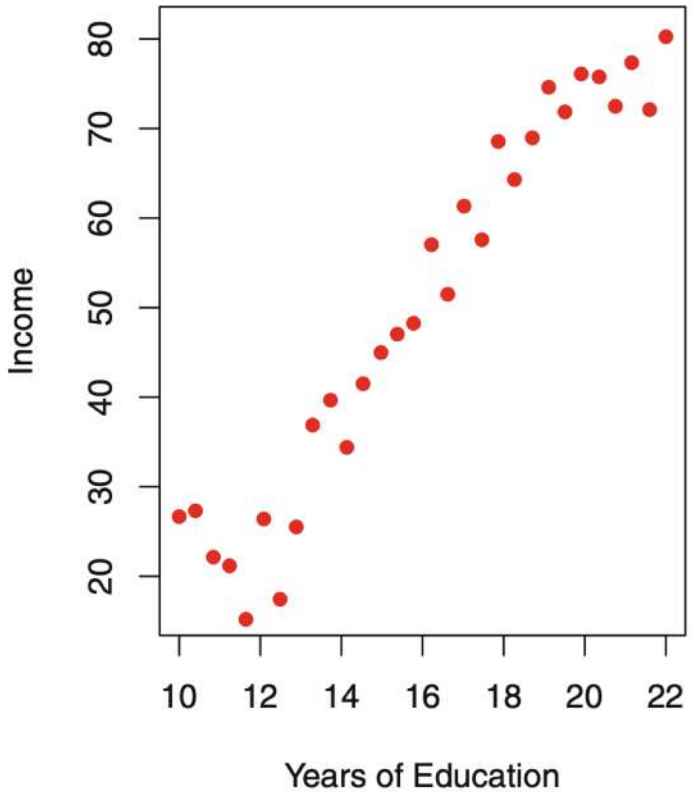
UNIVERSITÀ DI ROMA

Recap from Last Lecture

- Supervised Learning as an optimization problem
  - Hypothesis space (assumption)
  - Loss Function (objective)
  - Learning Algorithm (optimizer)
- Regression vs. Classification
- Bias-Variance Tradeoff
- Model selection vs. Model evaluation

LINEAR REGRESSION

Example: Y=Income vs. X=Education



Observations
(simulated)

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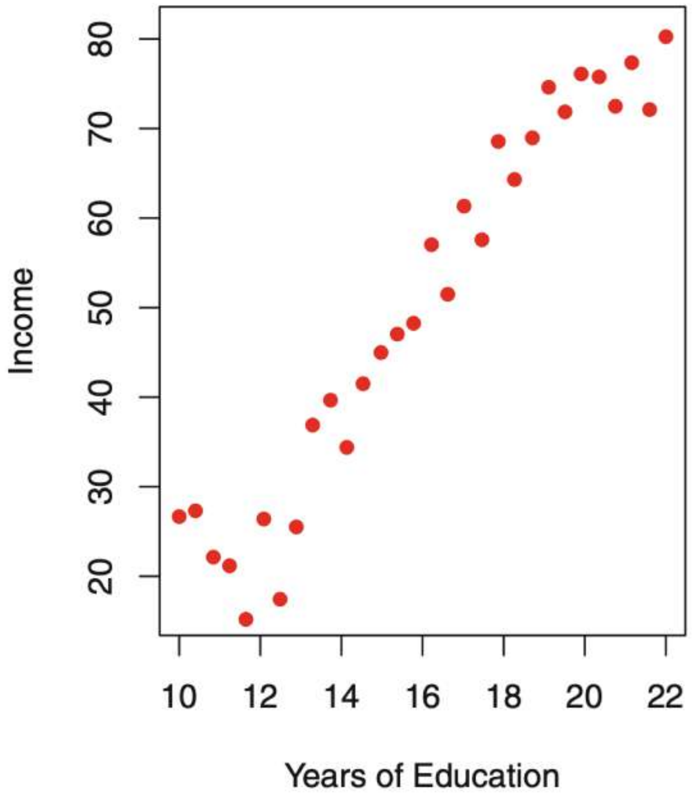

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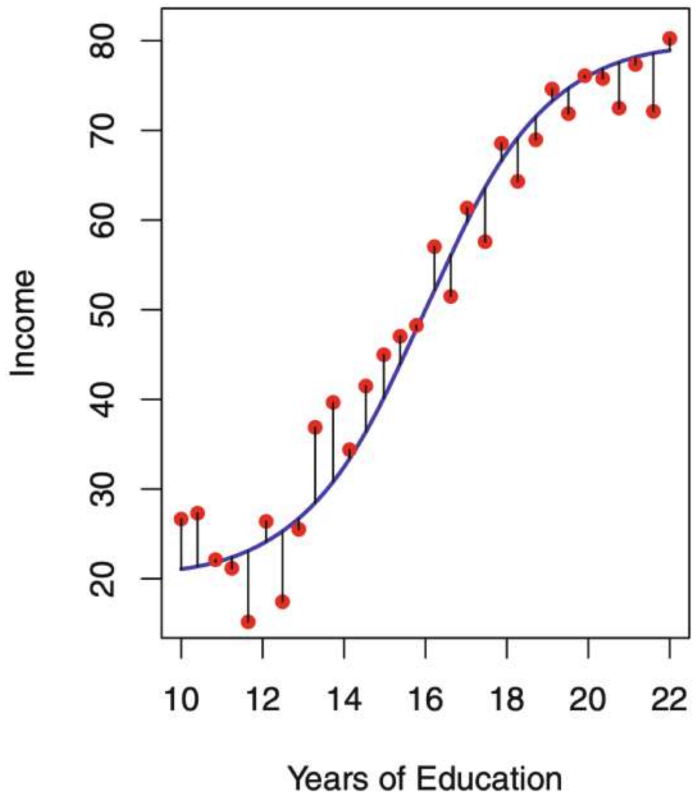

True yet unknown relationship
between X and Y

$$\boxed{Y = f(X) + \varepsilon}$$

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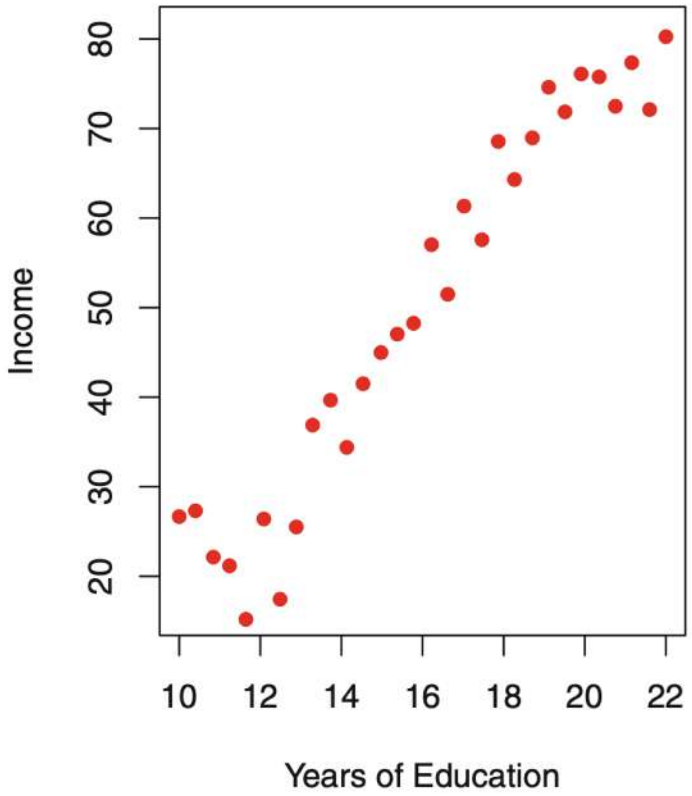

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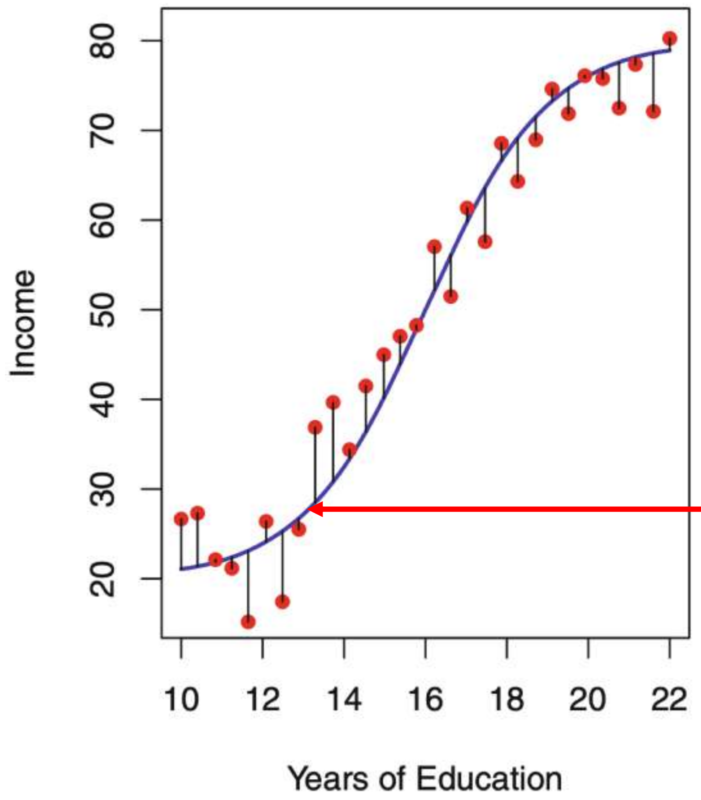

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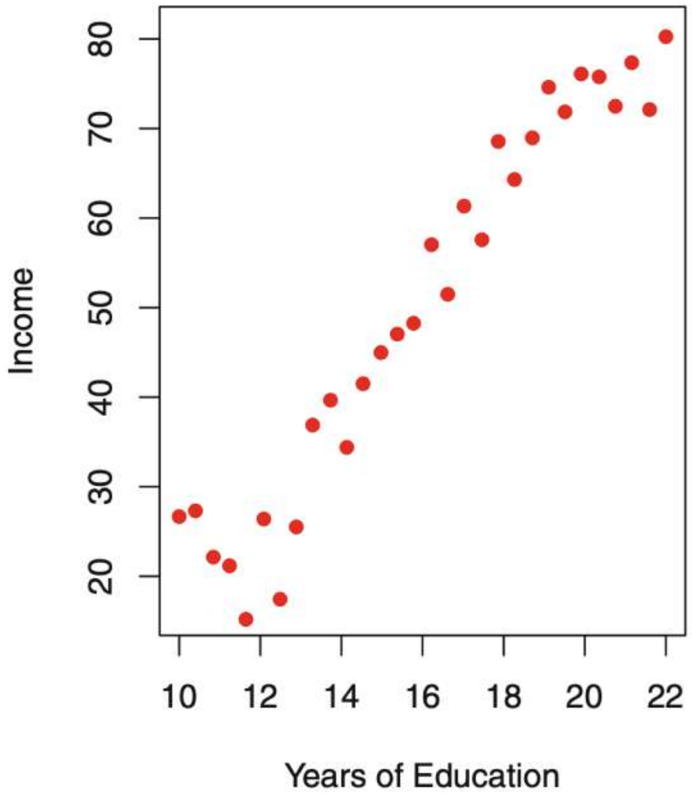

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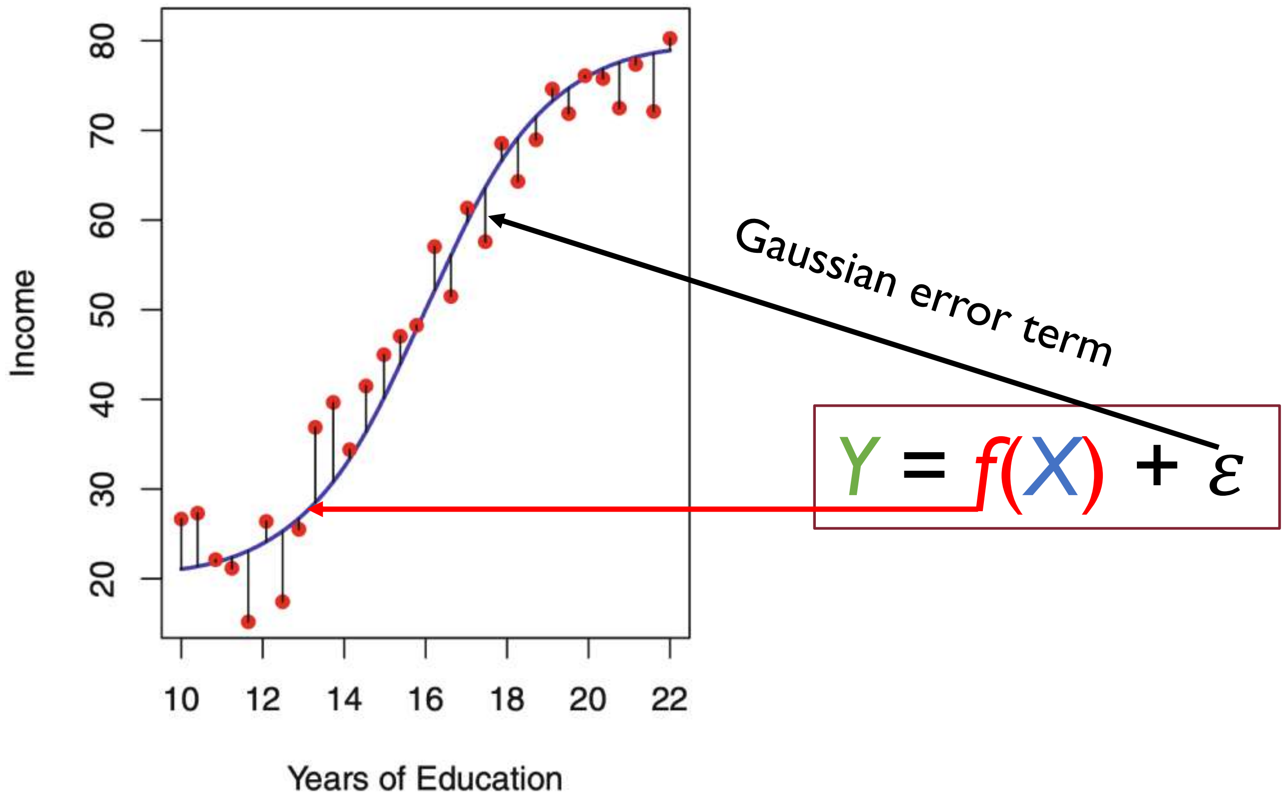

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- There exists a relationship between X (features) and Y (values)

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Means that epsilon does not depends on the magnitude of X

- ε is a random error term, which is independent of X and has 0-mean

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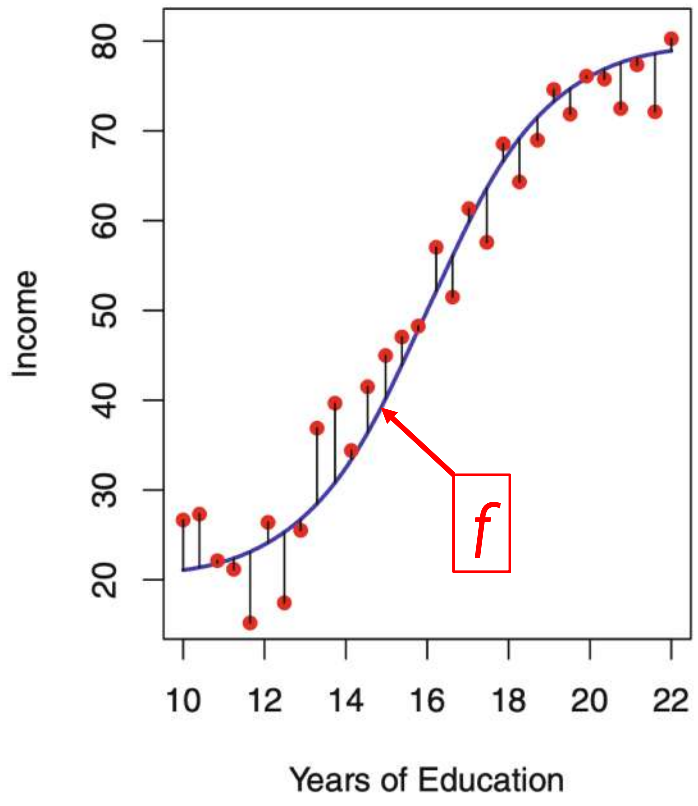
$$\mathcal{Y} = f(\mathcal{X}) + \epsilon$$

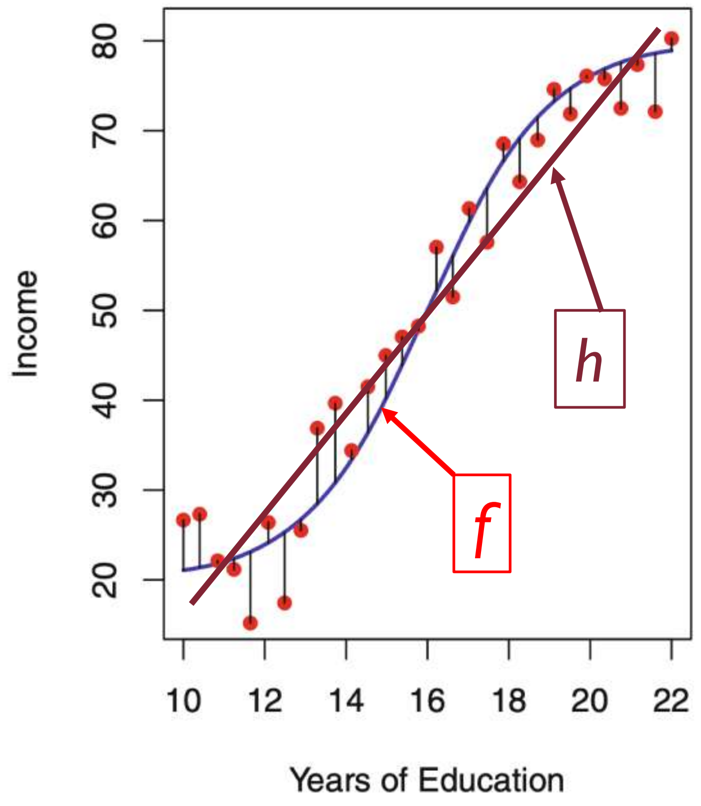
- f is some fixed but unknown function of X
- ε is a random error term, which is independent of X and has 0-mean
- In this formulation, f represents the systematic information that X provides about Y

Goal



Income
20
30
40
50
60
70
80
10
12
14
16
18
20
22
Years of Education
f

Goal



- Find an approximation *h* of the true relationship *f*

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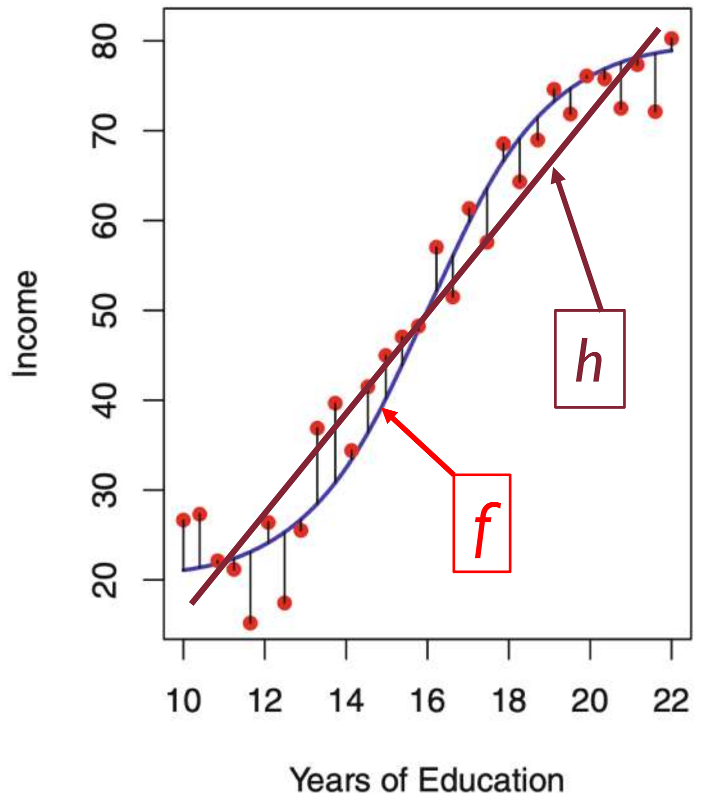

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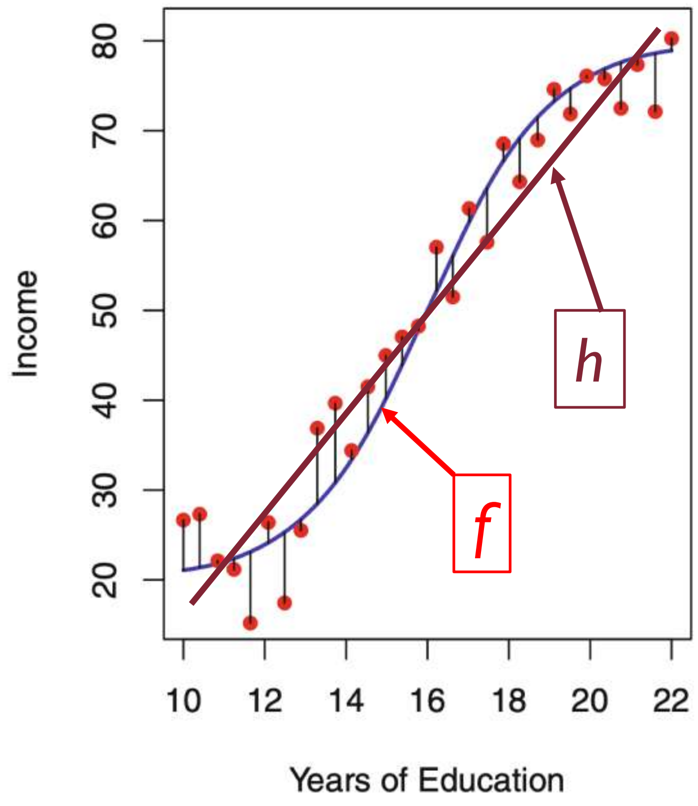

- Find an approximation *h* of the true relationship *f*
- Choose *h* from a specific hypothesis space *H* (i.e., linear functions)
- Use a dataset *D* of observations to learn *h*

$$\boxed{h(X) \sim f(X)}$$

Recap of Notation

$\mathcal{X} \subseteq \mathbb{R}^n$	input feature space
$\mathcal{Y}$	output space
$\mathcal{Y} \in \mathbb{R}$	real-value label of the *i*-th instance (regression)
$(\mathbf{x}_i, y_i)$	*i*-th labeled instance
$\mathbf{x}_i = (x_{i,1}, \ldots, x_{i,n}) \in \mathcal{X}$	*n*-dimensional feature vector of the *i*-th instance
$y_i \in \mathcal{Y}$	label of the *i*-th instance
$\mathcal{D} = \{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_m, y_m)\}$	dataset of *m* i.i.d. labeled instances

The Hypothesis Space *H*

The hypothesis space is defined as follows:

$$\mathcal{H} = \{h_{\boldsymbol{\theta}} : \mathcal{X} \mapsto \mathcal{Y} \mid h_{\boldsymbol{\theta}}(\mathbf{x}) = \theta_0 x_0 + \theta_1 x_1 + \ldots + \theta_n x_n\}$$

Intercept of the function

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Among all the possible instantiations of θ the learning algorithm selects θ^* as the one which minimizes a **loss function** measured on *D*

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$y_i = f(\mathbf{x}_i) + \epsilon_i$ *i*-th observation

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$$\boxed{\mathrm{RSS}(h_{\boldsymbol{\theta}}, \mathcal{D}) = \sum_{i=1}^{m} e_i^2 = \sum_{i=1}^{m} (\hat{y}_i - y_i)^2 = \sum_{i=1}^{m} (h_{\boldsymbol{\theta}}(\mathbf{x}_i) - y_i)^2}$$

Ordinary Least Squares (OLS)

- Remember that the supervised learning problem can be generally defined as the following optimization problem

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$$\boxed{h^* = h_{\boldsymbol{\theta}^*} = \mathrm{argmin}_{\boldsymbol{\theta}} L(h_{\boldsymbol{\theta}}, \mathcal{D})}$$

The Loss Function *L*: Mean Squared Error

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- OLS uses **Mean Squared Error** as the loss function to minimize
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$$\mathrm{MSE}(h_{\boldsymbol{\theta}}, \mathcal{D}) = \frac{1}{m}\mathrm{RSS}(h_{\boldsymbol{\theta}}, \mathcal{D}) = $$

$$= \frac{1}{m}\sum_{i=1}^{m}(h_{\boldsymbol{\theta}}(\mathbf{x}_i) - y_i)^2$$

The OLS Learning Algorithm

OLS aims at solving the following optimization problem:

$$h^* = h_{\boldsymbol{\theta}^*} = \text{argmin}_{\boldsymbol{\theta}} \text{MSE}(h_{\boldsymbol{\theta}}, \mathcal{D}) =$$

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How do we solve that?

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- Any local minimum (maximum) of a convex (concave) function is also a global minimum (maximum)

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- If the function is convex (concave) finding the minimum (maximum) can be done just by computing the first derivative and set it to 0
- In the case of a multivariate function, this generalizes to compute the gradient (∇) of the function and set it to 0

The Gradient ∇

The gradient of an *n*-variable function is the *n*-dimensional vector of the **partial derivatives** of the function w.r.t. each of its variable

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Solving $\nabla f = \mathbf{0}$ means finding the n-dimensional vector **x** such that:

$$\nabla f = \left(\frac{\partial f}{\partial x_1}, \frac{\partial f}{\partial x_2}, \ldots, \frac{\partial f}{\partial x_n} \right) = \underbrace{(0, 0, \ldots, 0)}_{n} = \mathbf{0}$$

Solving the Optimization Problem

$$\text{argmin}_{\boldsymbol{\theta}} \left[\frac{1}{m} \sum_{i=1}^{m} (h_{\boldsymbol{\theta}}(\mathbf{x}_i) - y_i)^2 \right]$$

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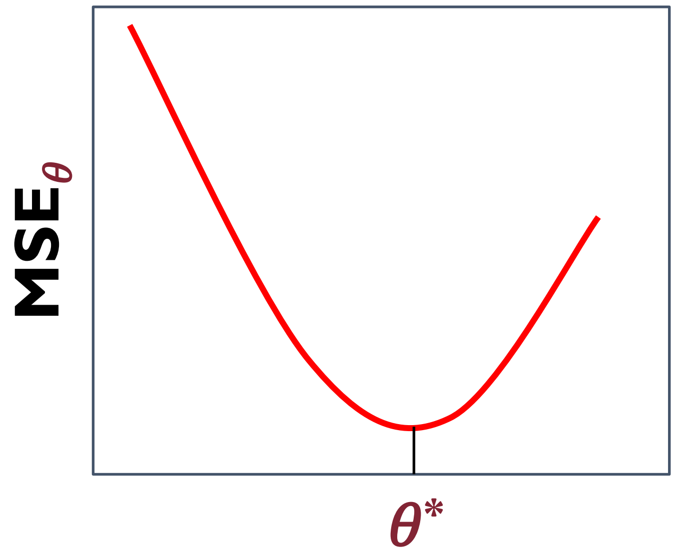

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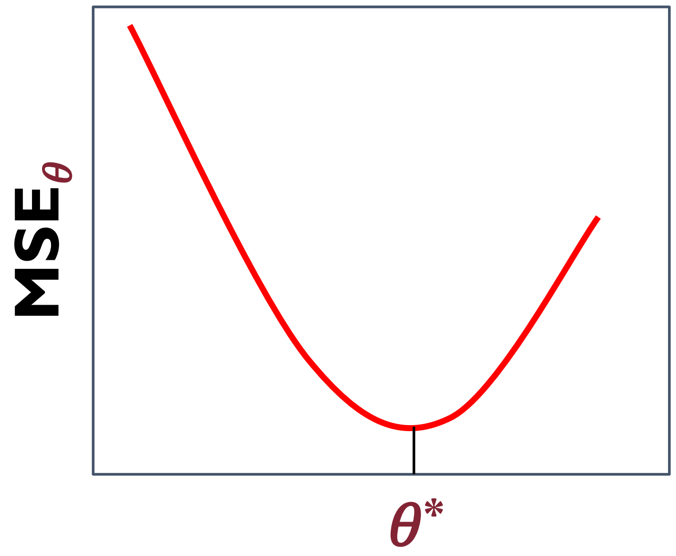

Linear functions are convex and so do sum of those

Convex functions have a **unique local minimum**, which therefore happens to be the **global minimum**

Computing the Gradient of MSE

$$\nabla \mathrm{MSE}(h_{\boldsymbol{\theta}}, \mathcal{D}) = \nabla \left[\frac{1}{m} \sum_{i=1}^{m} (h_{\boldsymbol{\theta}}(\mathbf{x}_i) - y_i)^2 \right]$$

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$$\boxed{\frac{\partial f}{\partial t}(\alpha t) = \alpha \frac{\partial f}{\partial t}(t) \;\; \alpha \in \mathbb{R}, \text{constant}}$$

scalar multiple rule

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sum rule

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sum rule

$$\Downarrow$$

$$\nabla \mathrm{MSE}(h_{\boldsymbol{\theta}}, \mathcal{D}) = \frac{1}{m} \left[\sum_{i=1}^{m} \nabla (h_{\boldsymbol{\theta}}(\mathbf{x}_i) - y_i)^2 \right]$$

Computing the Gradient of MSE (1 instance)

To make things easier, let's assume the dataset D contains a single instance ($\mathbf{x}$, y)

$$\nabla \mathrm{MSE}(h_{\boldsymbol{\theta}}, \mathcal{D}) = \nabla (h_{\boldsymbol{\theta}}(\mathbf{x}) - y)^2$$

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$$2(h_{\boldsymbol{\theta}}(\mathbf{x}) - y)\nabla(h_{\boldsymbol{\theta}}(\mathbf{x}) - y)$$

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$$\nabla \mathrm{MSE}(h_{\boldsymbol{\theta}}, \mathcal{D}) = \underbrace{2(h_{\boldsymbol{\theta}}(\mathbf{x}) - y)}_{\text{scalar}} \cdot \overbrace{\mathbf{x}}^{}$$

$(n+1)$-dimensional vector

Vectorized Notation

$$\nabla \text{MSE}(h_{\boldsymbol{\theta}}, \mathcal{D}) = \underbrace{2(h_{\boldsymbol{\theta}}(\mathbf{x}) - y)}_{\text{scalar}} \cdot \underbrace{\mathbf{x}}_{(n+1)\text{-dimensional vector}}$$

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x_0 = 1 by definition

Vectorized Notation

$$\nabla \mathrm{MSE}(h_{\boldsymbol{\theta}}, \mathcal{D}) = 2(\boldsymbol{\theta}^T \cdot \mathbf{x} - y)\mathbf{x}$$

$$= \begin{bmatrix} 2(\boldsymbol{\theta}^T \cdot \mathbf{x} - y)x_0 \\ 2(\boldsymbol{\theta}^T \cdot \mathbf{x} - y)x_1 \\ \vdots \\ 2(\boldsymbol{\theta}^T \cdot \mathbf{x} - y)x_n \end{bmatrix} = \begin{bmatrix} 2(\boldsymbol{\theta}^T \cdot \mathbf{x} - y) \\ 2(\boldsymbol{\theta}^T \cdot \mathbf{x} - y)x_1 \\ \vdots \\ 2(\boldsymbol{\theta}^T \cdot \mathbf{x} - y)x_n \end{bmatrix}$$

x_0 = 1 by definition

The resulting gradient is an *(n+1)*-dimensional vector as expected!

Setting the Gradient Equal to Zero

$$\nabla \mathrm{MSE}(h_{\boldsymbol{\theta}}, \mathcal{D}) = \begin{bmatrix} 2(\boldsymbol{\theta}^T \cdot \mathbf{x} - y) \\ 2(\boldsymbol{\theta}^T \cdot \mathbf{x} - y)x_1 \\ \vdots \\ 2(\boldsymbol{\theta}^T \cdot \mathbf{x} - y)x_n \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix} = \mathbf{0}$$

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We need to solve a system of *n+1* linear equations with *n+1* variables

$$2(\boldsymbol{\theta}^T \cdot \mathbf{x} - y)x_j = 0 \ \forall j \in \{0, 1, \ldots, n\}$$

Computing the Gradient of MSE (*m* instances)

In the general case where the dataset *D* contains a *m* instances

$$\nabla \mathrm{MSE}(h_{\boldsymbol{\theta}}, \mathcal{D}) = \frac{2}{m}\left[\sum_{i=1}^{m}\Big(h_{\boldsymbol{\theta}}(\mathbf{x}_i) - y_i\Big)\nabla\Big(h_{\boldsymbol{\theta}}(\mathbf{x}_i) - y_i\Big)\right]$$

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$$\nabla \mathrm{MSE}(h_{\boldsymbol{\theta}}, \mathcal{D}) = \begin{bmatrix} \frac{2}{m}(\boldsymbol{\theta}^T \cdot \mathbf{x}_1 - y_1)x_{1,0} + \ldots + \frac{2}{m}(\boldsymbol{\theta}^T \cdot \mathbf{x}_m - y_m)x_{m,0} \\ \frac{2}{m}(\boldsymbol{\theta}^T \cdot \mathbf{x}_1 - y_1)x_{1,1} + \ldots + \frac{2}{m}(\boldsymbol{\theta}^T \cdot \mathbf{x}_m - y_m)x_{m,1} \\ \vdots \\ \frac{2}{m}(\boldsymbol{\theta}^T \cdot \mathbf{x}_1 - y_1)x_{1,n} + \ldots + \frac{2}{m}(\boldsymbol{\theta}^T \cdot \mathbf{x}_m - y_m)x_{m,n} \end{bmatrix}$$

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$$\frac{2}{m}\left[(\boldsymbol{\theta}^T \cdot \mathbf{x}_1 - y_1)x_{1,j} + \ldots + (\boldsymbol{\theta}^T \cdot \mathbf{x}_m - y_m)x_{m,j}\right] = 0 \;\forall j \in \{0, \ldots, n\}$$

Matrix Notation

$$\mathbf{X} = \underbrace{\begin{bmatrix} x_{1,0} & x_{1,1} & \dots & x_{1,n} \\ x_{2,0} & x_{2,1} & \dots & x_{2,n} \\ \vdots & \vdots & \vdots & \vdots \\ x_{m,0} & x_{m,1} & \dots & x_{m,n} \end{bmatrix}}_{m \times n+1 \textbf{ feature matrix}} = \begin{bmatrix} -\mathbf{x}_1^T- \\ -\mathbf{x}_2^T- \\ \vdots \\ -\mathbf{x}_m^T- \end{bmatrix}$$

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Vectorized Form of the Optimization Problem

$$\boxed{h^* = h_{\boldsymbol{\theta}^*} = \operatorname{argmin}_{\boldsymbol{\theta}} \left[\underbrace{\frac{1}{m} ||\mathbf{X} \cdot \boldsymbol{\theta} - \mathbf{y}||^2}_{\mathrm{MSE}(h_{\boldsymbol{\theta}}, \mathcal{D})} \right]}$$

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$$\mathbf{X}^T \mathbf{X} \cdot \boldsymbol{\theta} = \mathbf{X}^T \cdot \mathbf{y}$$

$$\boxed{\boldsymbol{\theta} = \mathbf{X}^{\dagger} \cdot \mathbf{y}}$$

$\mathbf{X}^{\dagger} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T$ is the **pseudo-inverse** of $\mathbf{X}$

The Pseudo-Inverse of $\mathbf{X}$

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This gonna be likely equals to be the inverse matrix

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  - The chance of a randomly generated squared matrix is invertible approaches 1
  - To be non-invertible, the determinant must be 0 (linearly dependent columns)
- Typically, the number m of rows (instances) are way larger than the number n of columns (features)
  - $\mathbf{X}^T\mathbf{X}$ is smaller than $\mathbf{X}$

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- OLS is also known as one-step learning as there exists a closed-form (i.e., analytical) solution to the convex optimization problem

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- OLS is also known as one-step learning as there exists a closed-form (i.e., analytical) solution to the convex optimization problem
- However, other choices of loss functions (even if convex) may need an **iterative** approach to get to a (local) minimum
- Though in general $n << m$, computing the inverse of an n-by-n matrix is still a costly operation ($O(n^3)$ time complexity)

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Subtle yet important difference between **errors** and **residuals**

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MSE is computed from residuals, not unobservable errors!

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- Weak exogeneity → Predictor variables (i.e., features) can be treated as error-free constants

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- Weak exogeneity → Predictor variables (i.e., features) can be treated as error-free constants
- Linearity → Linear relationship between the features and the response
  - Only a restriction on the parameters; features themselves can be arbitrarily combined using non-linear transformations
- Error independence → Error terms ε_i are uncorrelated with each other
  - Knowing that ε_i is positive (negative) gives no information on the sign of ε_{i+1}

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  - In practice, this does not hold when the response varies over a wide scale

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- Homoscedasticity→ Different values of the response variable have the same variance in their errors, regardless of the feature values
  - In practice, this does not hold when the response varies over a wide scale
- No Multicollinearity → There must not be two or more features whose values are perfectly correlated with each other
  - The feature matrix $\mathbf{X}$ must have full column rank n
  - If $\mathbf{X}$ is full column rank n then $\mathbf{X}^T\mathbf{X}$ is always invertible
    - It can be shown that if $\mathbf{X}^T\mathbf{X}\mathbf{u} = \mathbf{0}$ for some vector $\mathbf{u}$, then $\mathbf{u} = \mathbf{0}$ (trivial solution)

Checking OLS Assumptions

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- A good way to assess the OLS assumptions hold is to use residual plots
- Plotting residuals against each feature and/or the predicted value may help spot:
  - Non-linearity
  - Correlation between error terms
  - Non-constant variance of error terms (i.e., heteroscedasticity)
  - …

Assessing the Quality of a Model

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R^2 statistic

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Recall that every observation of the target variable y_i is associated with an error term ε_i

$$y_i = \underbrace{\theta_0 x_{i,0} + \theta_1 x_{i,1} + \ldots + \theta_0 x_{i,n}}_{h_{\boldsymbol{\theta}}(\mathbf{x}_i) \;\approx\; f(\mathbf{x}_i)} + \epsilon_i$$

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Even if we were able to find the exact parameters of the true f, we would not be able to perfectly predict y_i from $\mathbf{x}_i$

Residual Standard Error (RSE)

$\boxed{\text{RSE is an estimate of the standard deviation of } \varepsilon}$

$$\mathrm{RSE}(h_{\boldsymbol{\theta}}, \mathcal{D}) = \sqrt{\frac{1}{\underbrace{m-n-1}_{\textbf{degrees of freedom}}} \underbrace{\sum_{i=1}^{m} (\hat{y}_i - y_i)^2}_{\mathrm{RSS}}}$$

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A measure of the **lack** of fit of the model to the data
the lower the better

Degrees of Freedom

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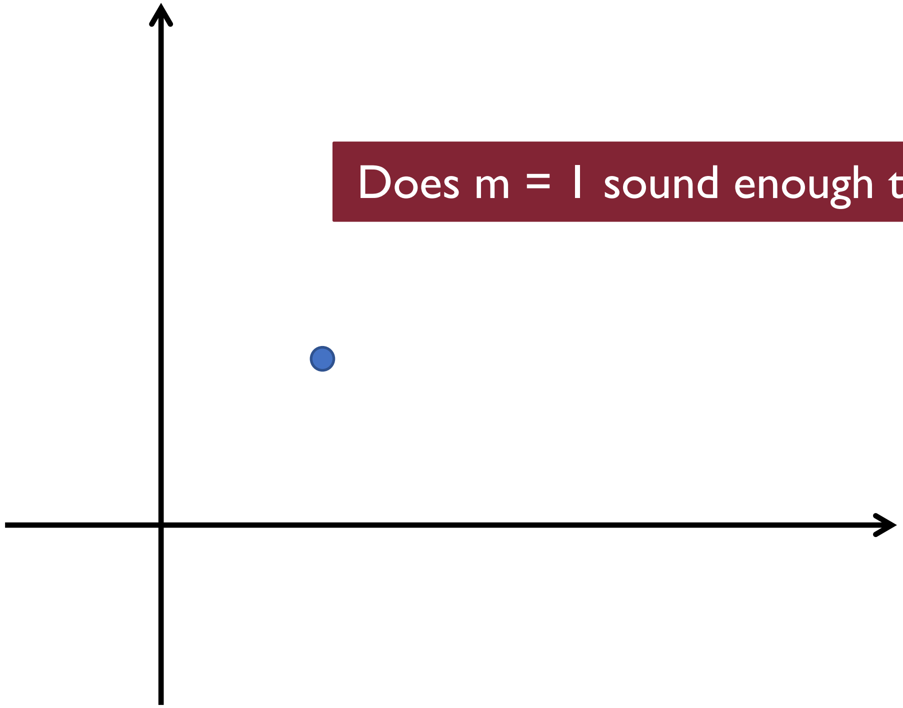
How many observations m do I need to estimate model's parameters?

Does m = 1 sound enough to fit a line?



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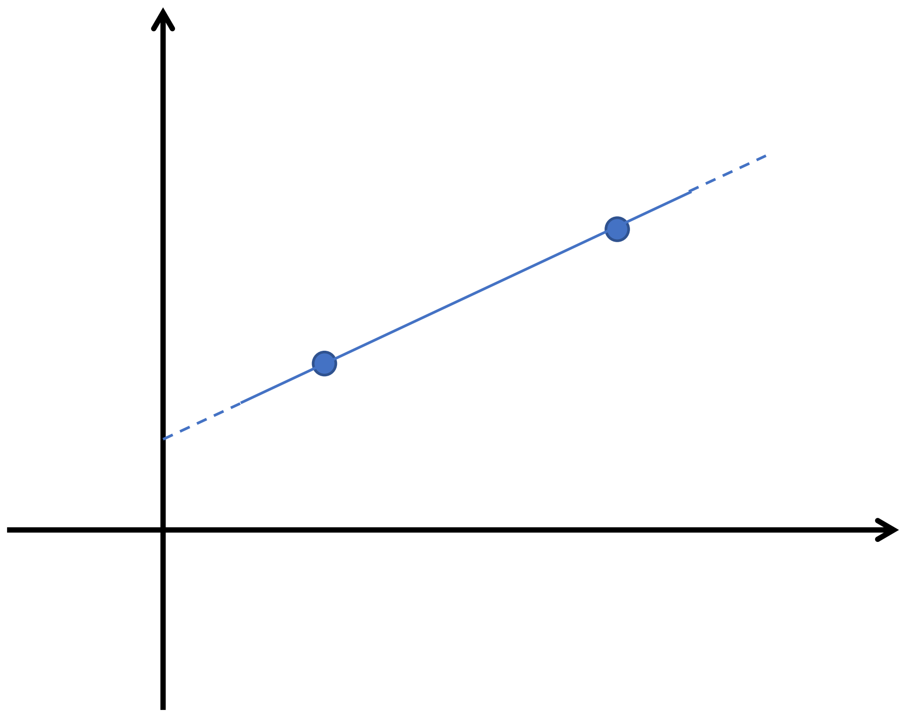

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With 2 data points I am always able to fit a perfect line

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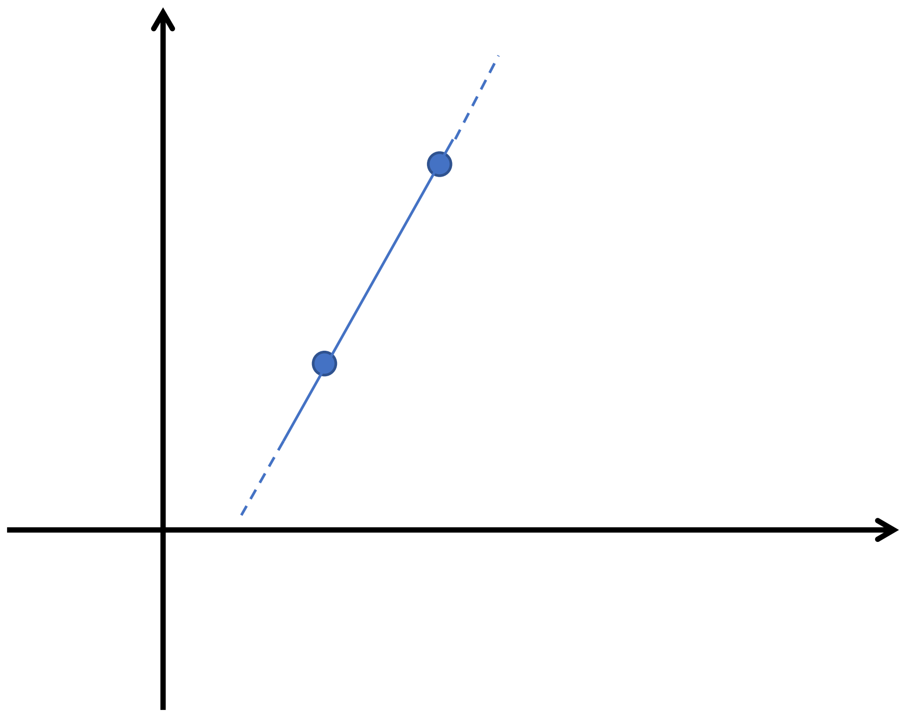

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Problem is that my fitted line may drastically change depending on where the second point is located!

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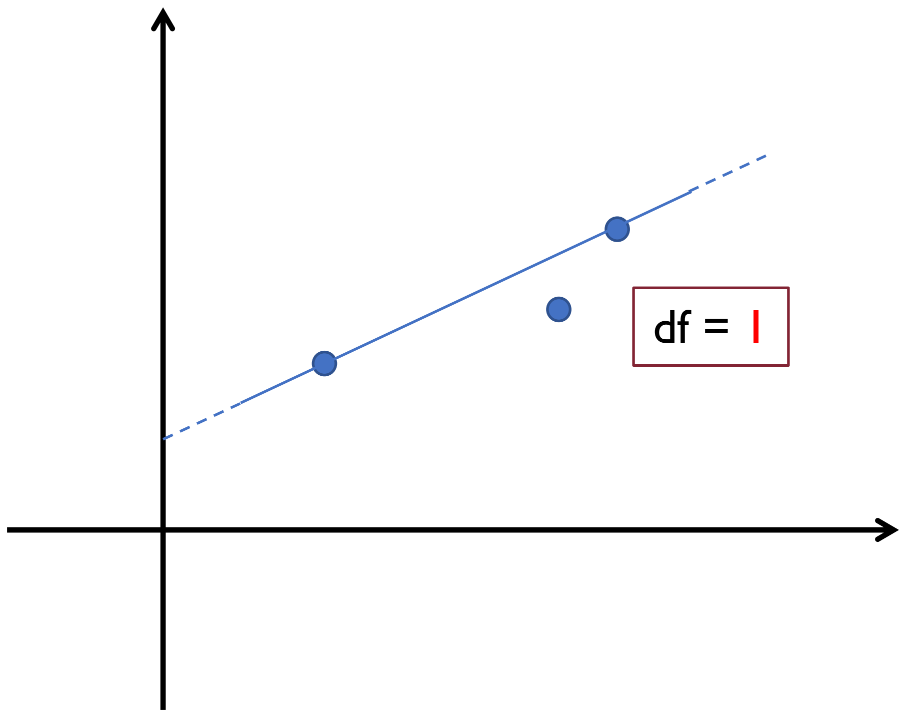

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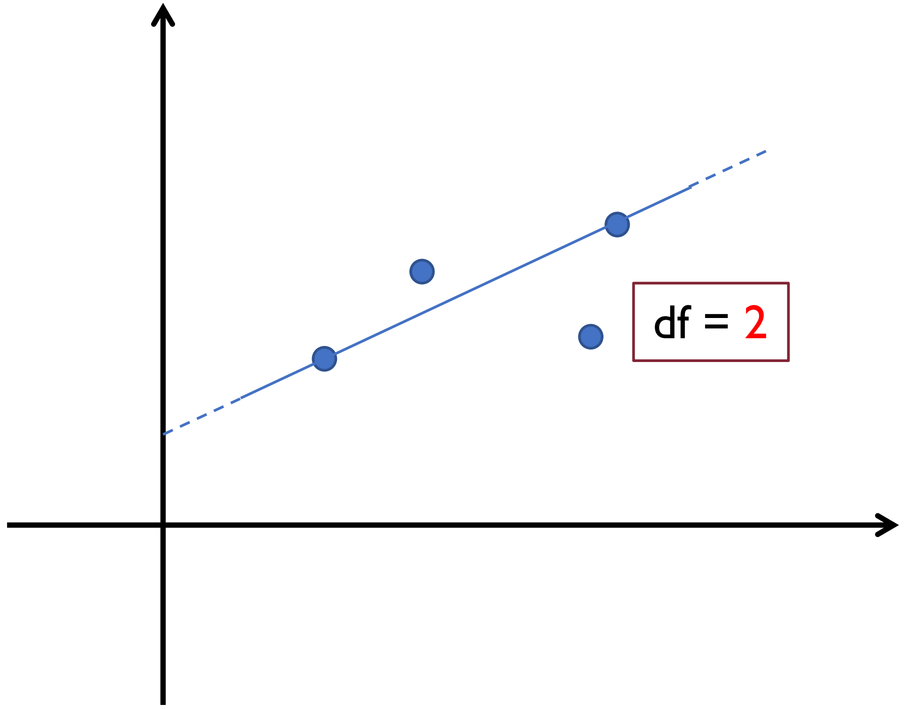

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$$\boxed{\mathrm{df} = \underbrace{m}_{\#\text{observations}} - \underbrace{n}_{\#\text{features}} - \underbrace{1}_{\text{intercept}}}$$

R^2 Statistic

$$R^2 = 1 - \frac{\text{RSS}}{\text{TSS}} = 1 - \frac{\sum_{i=1}^{m}(\hat{y}_i - y_i)^2}{\sum_{i=1}^{m}(y_i - \bar{y})^2}$$

TSS measures the total variance in the response Y before the regression takes place

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R^2 measures the proportion of variability in Y that can be explained using X

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- An R^2 statistic that is close to 1 indicates that a large proportion of the variability in the response has been explained by the regression
- The larger R^2 the better is the linear regression model
- R^2 is easier to interpret than RSE as it always ranges between 0 and 1

Adjusted R^2 Statistic

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- Fixing the sample size m, RSS decreases (or, at worst, it stays the same) as more variables are added to the fitted model
- R^2 always increases as more variables are added (as df decreases!)
- We need a way to adjust for that, otherwise we could get a better model by simply adding useless features to it!

$$R^2_{\text{adj}} = 1 - \frac{\frac{\text{RSS}}{m-n-1}}{\frac{\text{TSS}}{m-1}}$$

Adjusted R^2 Statistic

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- **Regularization** → Put some constraint on the optimization problem so as to limit the values of the learned parameters

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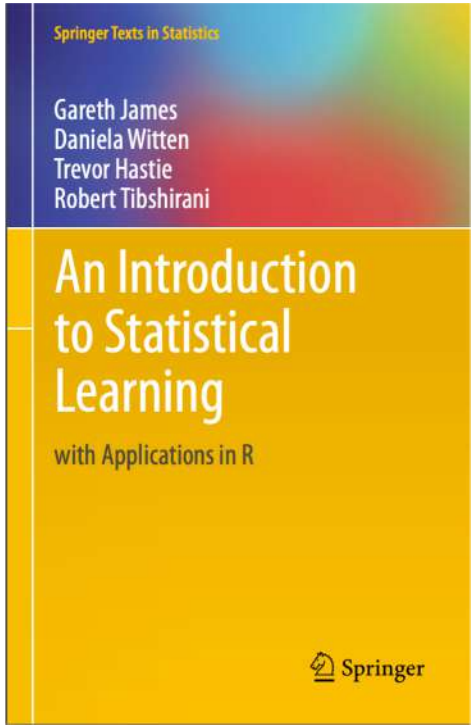
- Regularization to prevent overfitting: Elastic Net, LASSO, Ridge

Further Readings

An Introduction to Statistical Learning [Chapter 3]



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