Big Data Computing

Master's Degree in Computer Science

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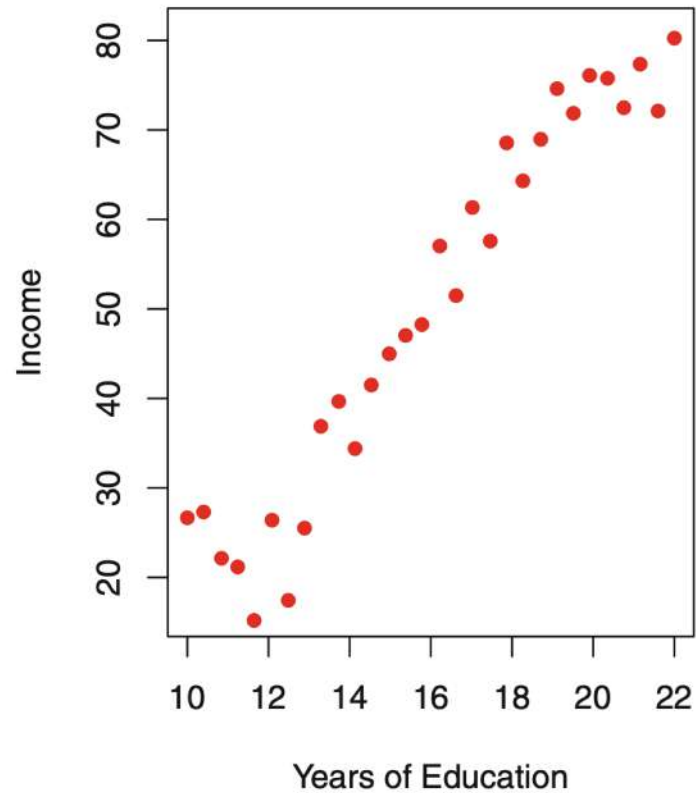
Recap from Last Lecture

- Supervised Learning as an optimization problem

  - Hypothesis space (assumption)

  - Loss Function (objective)

  - Learning Algorithm (optimizer)

- Regression vs. Classification

- Bias-Variance Tradeoff
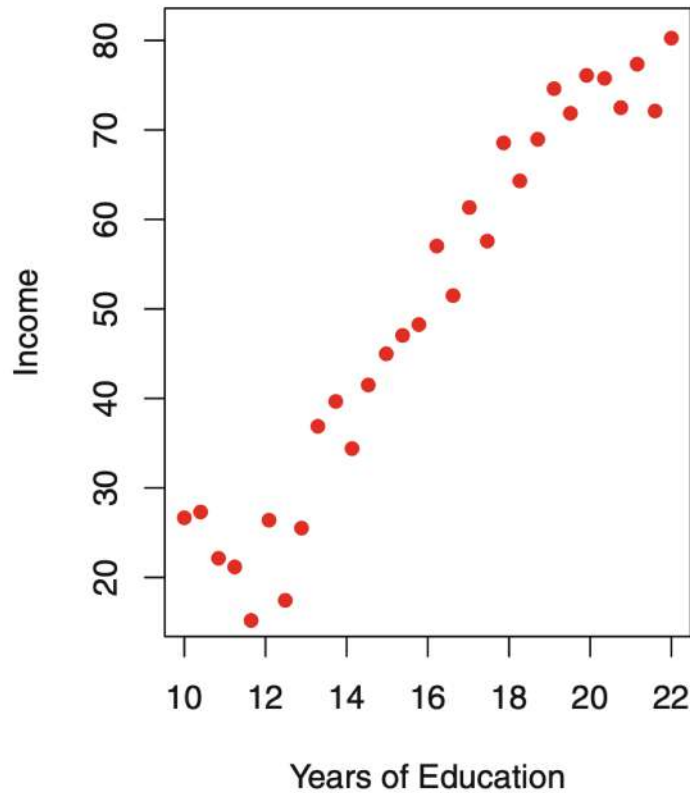
- Model selection vs. Model evaluation

LINEAR REGRESSION

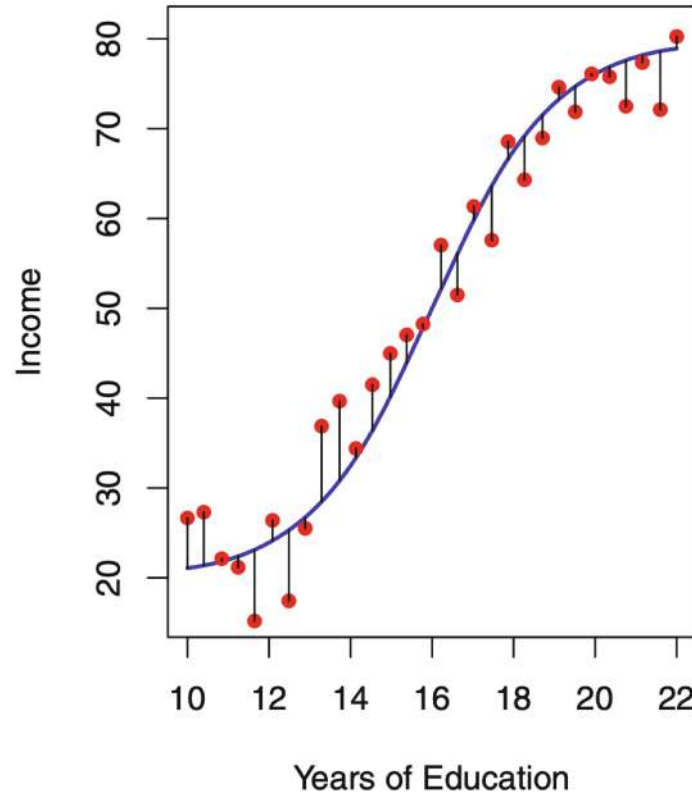# Example: Y=Income vs. X=Education

Observations
(simulated)

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True yet unknown relationship
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$$Y = f(X) + \varepsilon$$

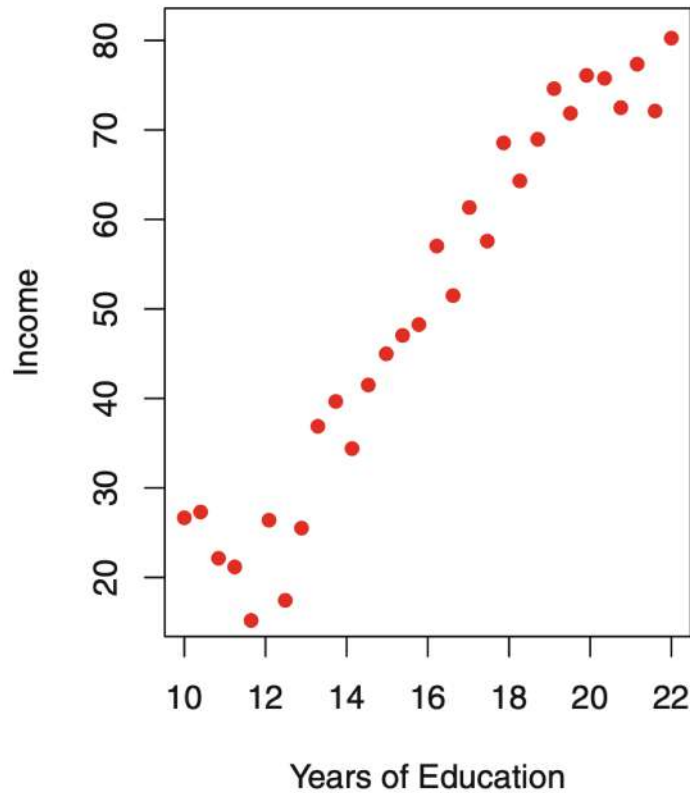# Example: Y=Income vs. X=Education

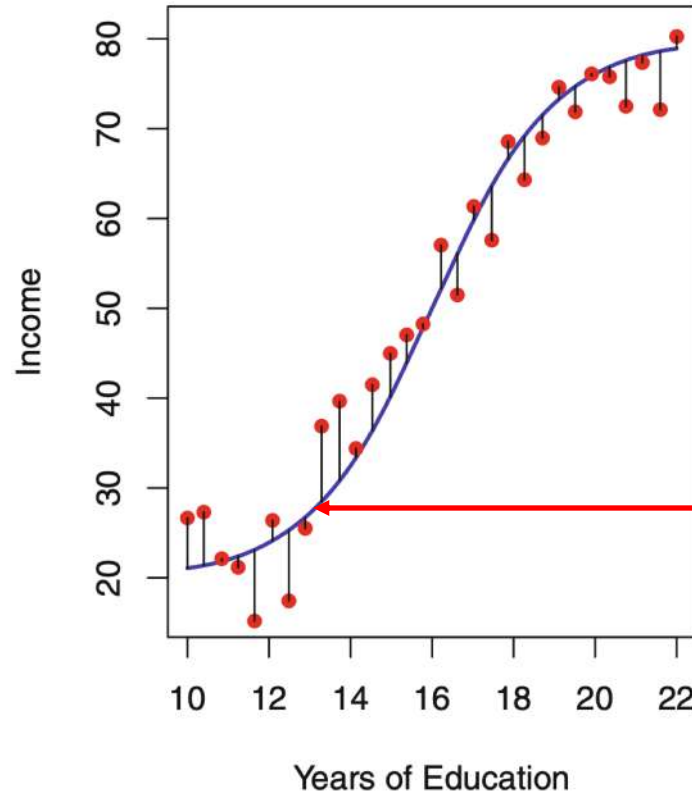

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Gaussian error term

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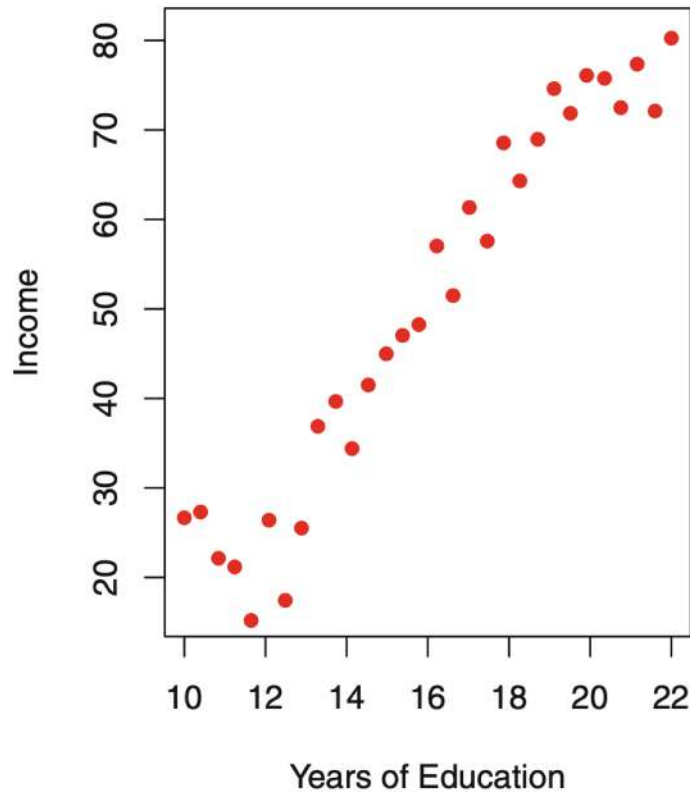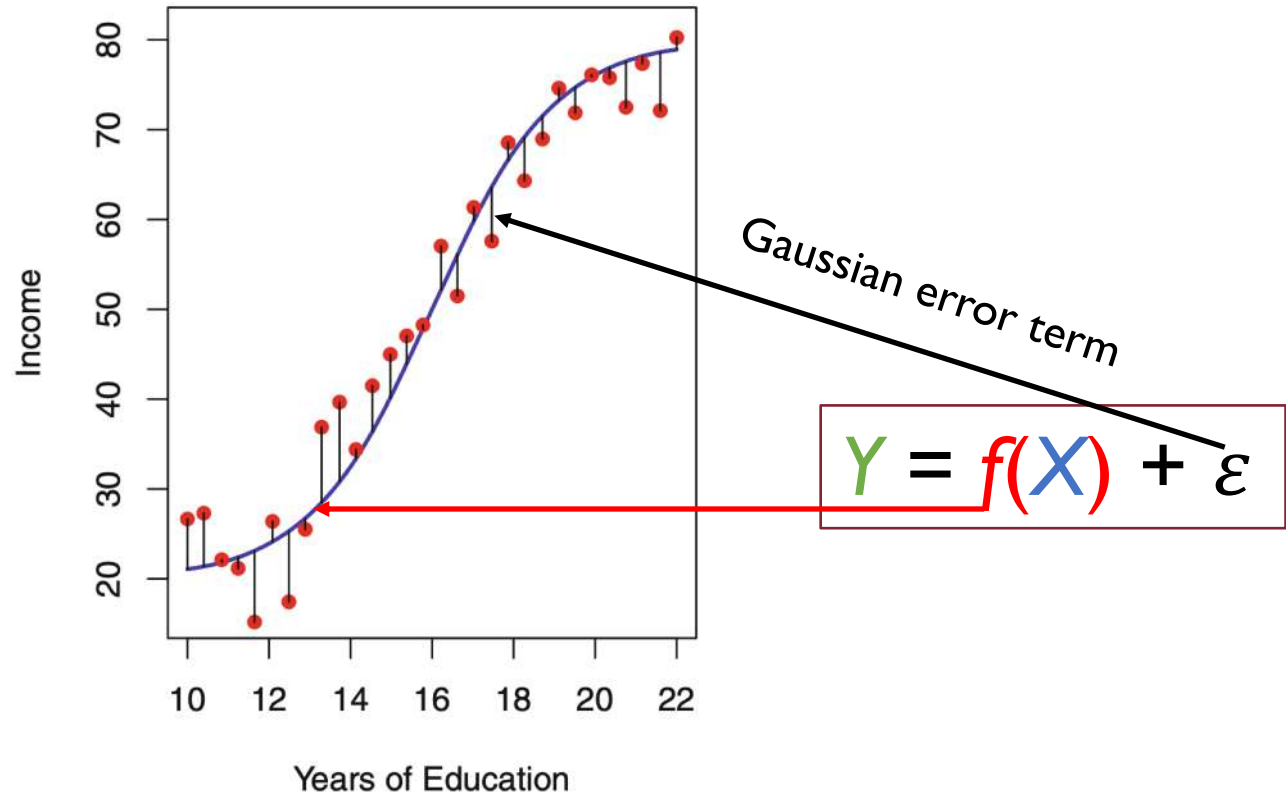
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- In this formulation, *f* represents the systematic information that X provides about Y

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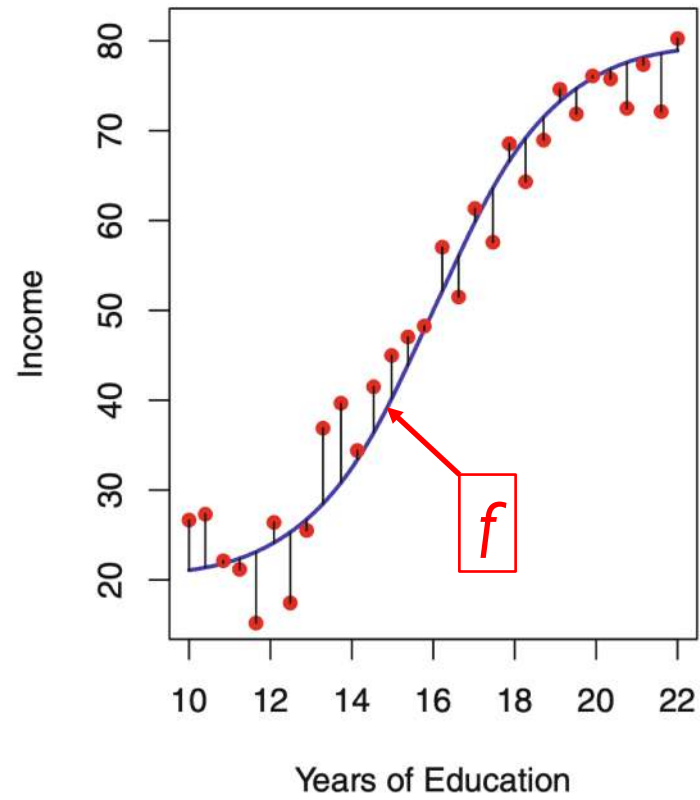
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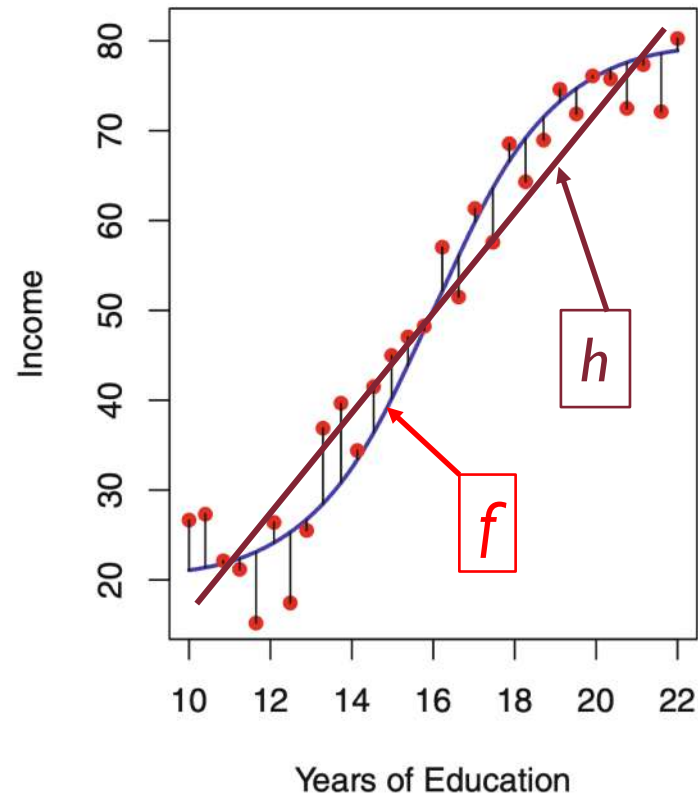
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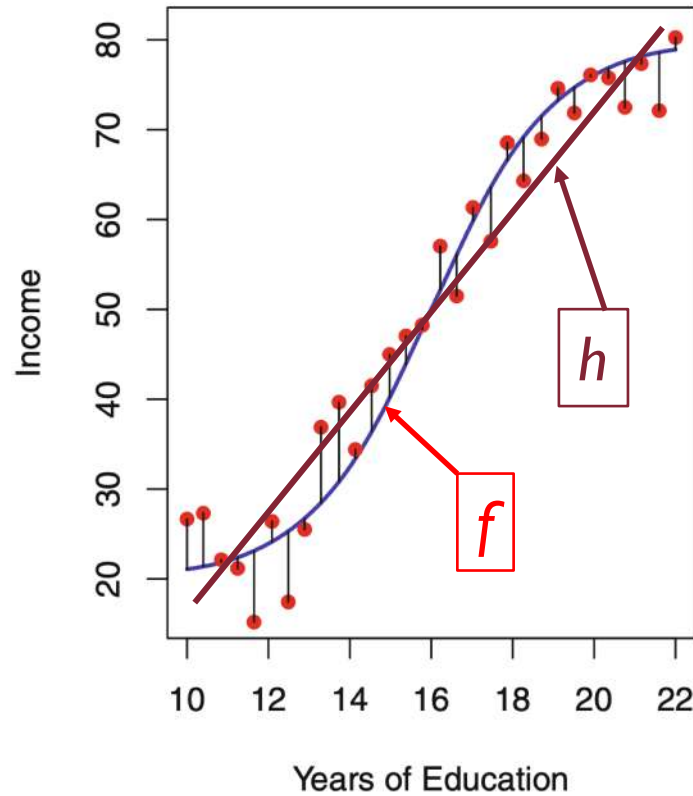
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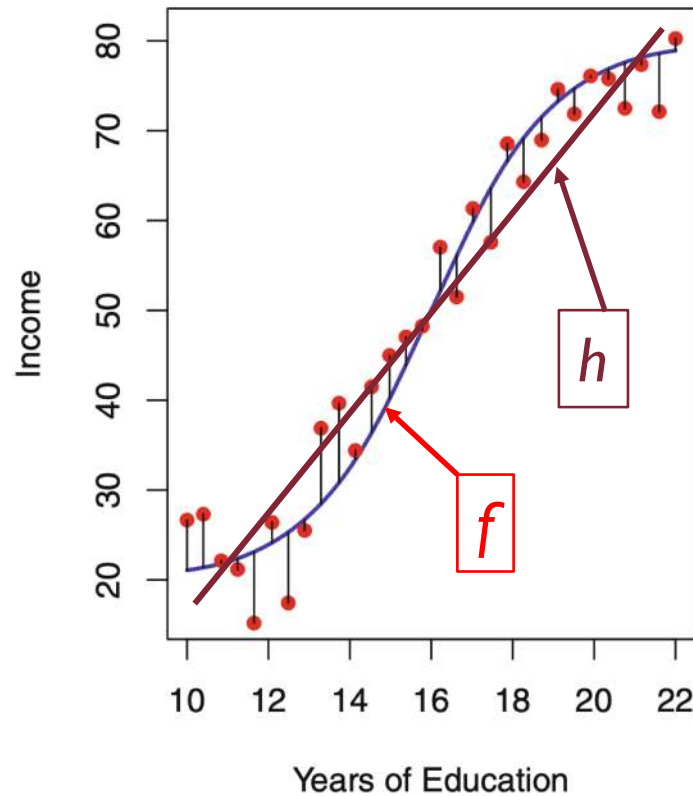
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- Use a dataset *D* of observations to learn *h*

$$h(X) \sim f(X)$$

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:

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

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

Ordinary Least Squares (OLS)

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

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$$\text{MSE}(h_{\boldsymbol{\theta}}, \mathcal{D}) = \frac{1}{m}\text{RSS}(h_{\boldsymbol{\theta}}, \mathcal{D}) =$$

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

The OLS Learning Algorithm

OLS aims at solving the following optimization problem:

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How do we solve that?

Min/Max of a Convex/Concave Function

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- 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 $\mathbf{x}$ 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

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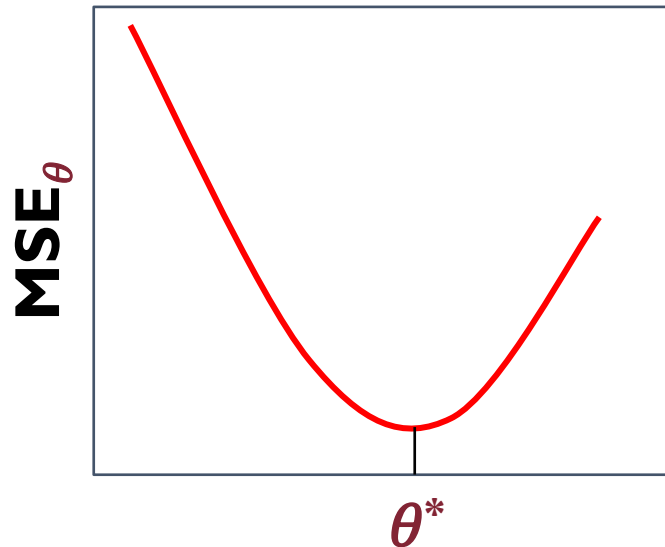Observations y_i and features $\mathbf{x}_i$ can be thought of as fixed constants

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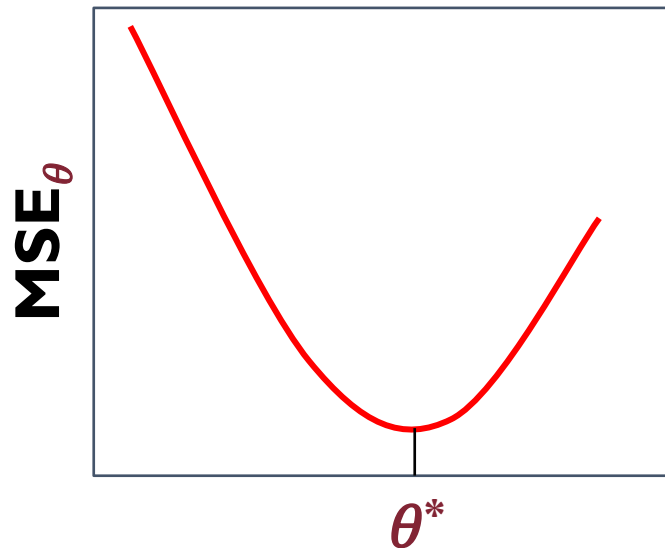
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Convex functions have a **unique local minimum**, which therefore happens to be the **global minimum**

MSE$_\theta$ plotted as a convex curve with minimum at θ^*

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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scalar multiple rule

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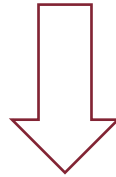
$$\nabla \mathrm{MSE}(h_{\boldsymbol{\theta}}, \mathcal{D}) = \frac{1}{m} \left[\sum_{i=1}^{m} \nabla (h_{\boldsymbol{\theta}}(\mathbf{x}_i) - y_i)^2 \right]$$

Computing the Gradient of MSE (1 instance)

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

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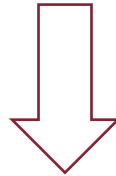To make things easier, let's assume the dataset D contains a single instance $(\mathbf{x}, y)$

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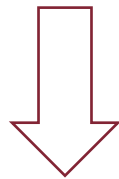
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The resulting gradient is an *(n+1)*-dimensional vector as expected!

Setting the Gradient Equal to Zero

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

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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

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

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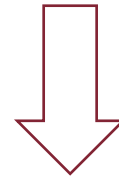$$\nabla \text{MSE}(h_{\boldsymbol{\theta}}, \mathcal{D}) = \frac{2}{m} \left[\sum_{i=1}^{m} \underbrace{\left(h_{\boldsymbol{\theta}}(\mathbf{x}_i) - y_i \right)}_{\text{scalar}} \underbrace{\mathbf{x}_i}_{n+1\text{-dimensional vector}} \right]$$

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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

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

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Vectorized Form of the Optimization Problem

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

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

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

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- Typically, the number *m* of rows (instances) are way larger than the number *n* of columns (features)

  - $\mathbf{X}^\mathsf{T}\mathbf{X}$ 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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- Though in general $n \ll m$, computing the inverse of an n-by-n matrix is still a costly operation ($O(n^3)$ time complexity)

OLS Assumptions

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- 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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- 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)

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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)

RSE is an estimate of the standard deviation of ε

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

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

R² Statistic

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

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- R^2 is easier to interpret than RSE as it always ranges between 0 and 1

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- R^2 always increases as more variables are added

- We need a way to adjust for that, otherwise we could get a better model by simply adding useless features to it!

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

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- We may need to increase the sample size *m* to compensate for the increasing of RSS due to the inclusion of more features *n*

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

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$\lambda > 0;\ \alpha = 0$ **Ridge** (L2-regularization only)

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

Further Readings

An Introduction to Statistical Learning [Chapter 3]
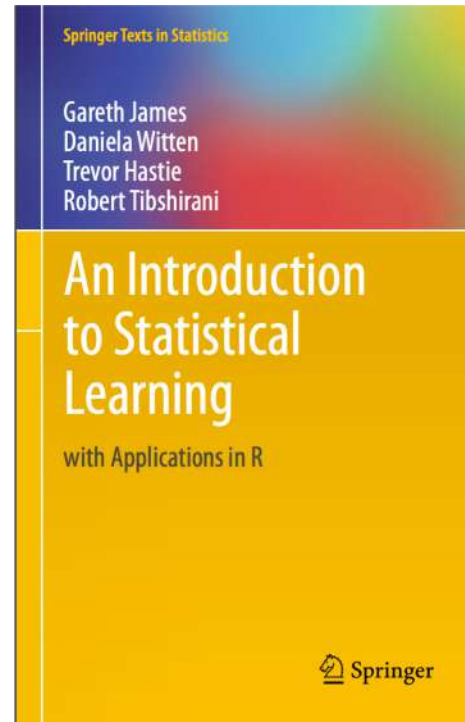
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