

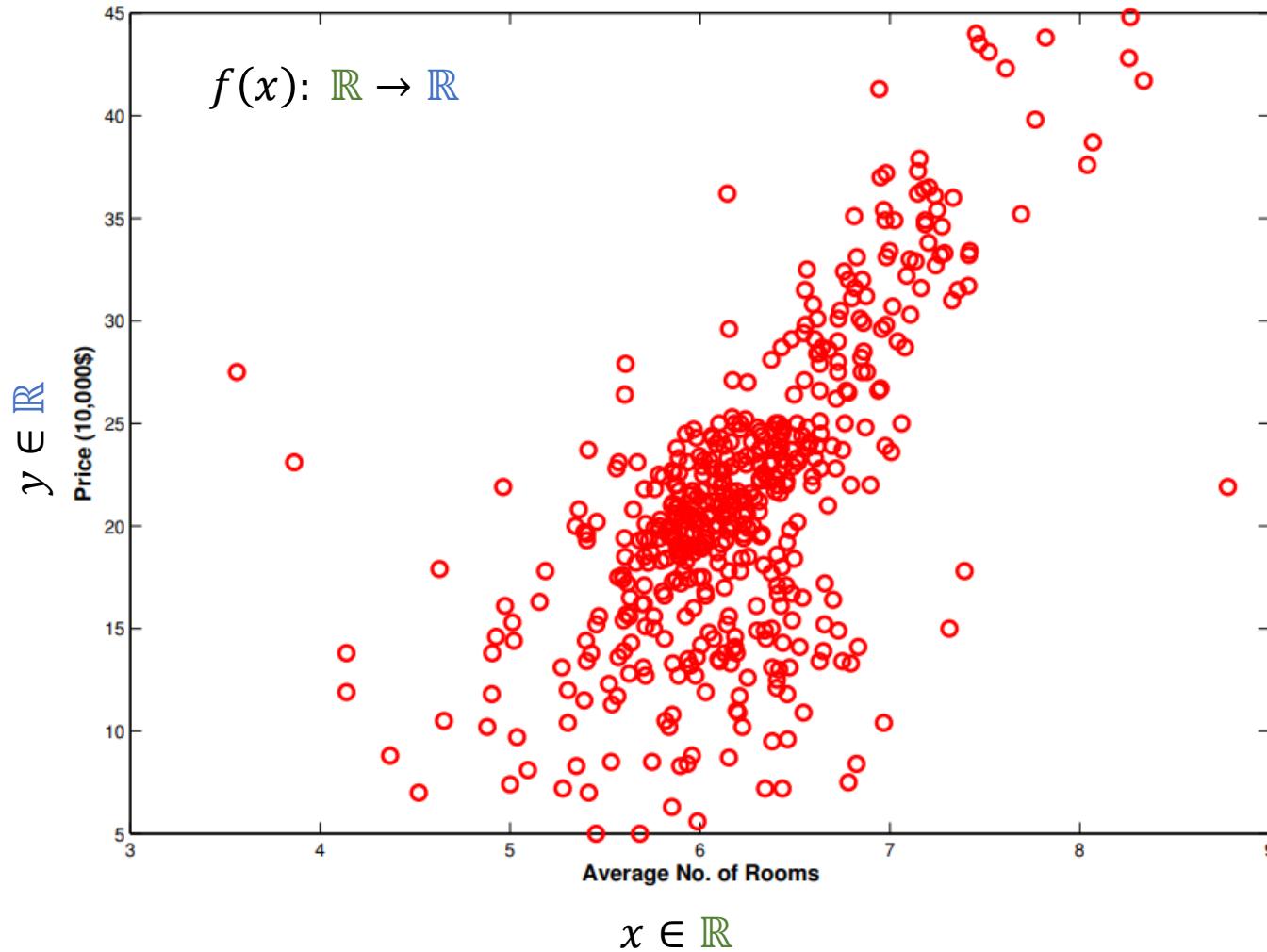
Linear Regression

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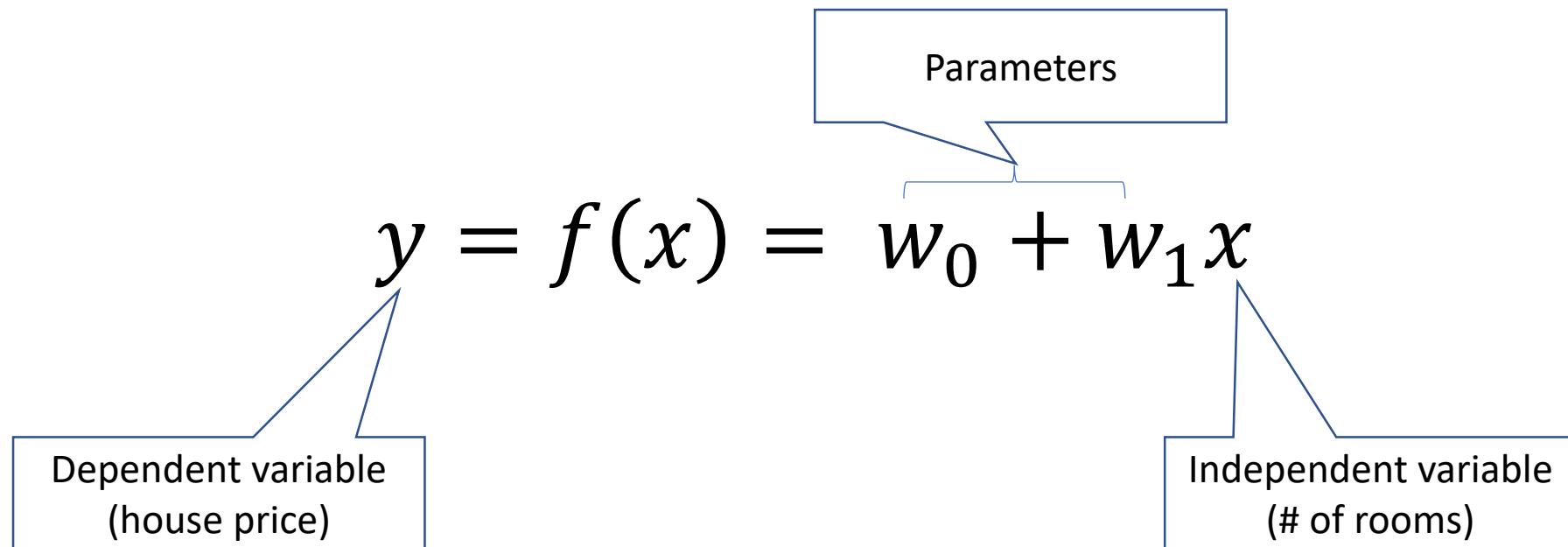
Agenda

- Regression formulation
- Assumptions, Implications, Diagnostics
- Analytic solution
- Iterative solution
- Pitfalls
- Ridge Regression

Example



A linear model



A linear model

$$y = f(x) = w_0 + w_1 x$$

$$y_1 = w_0 + w_1 x_1$$

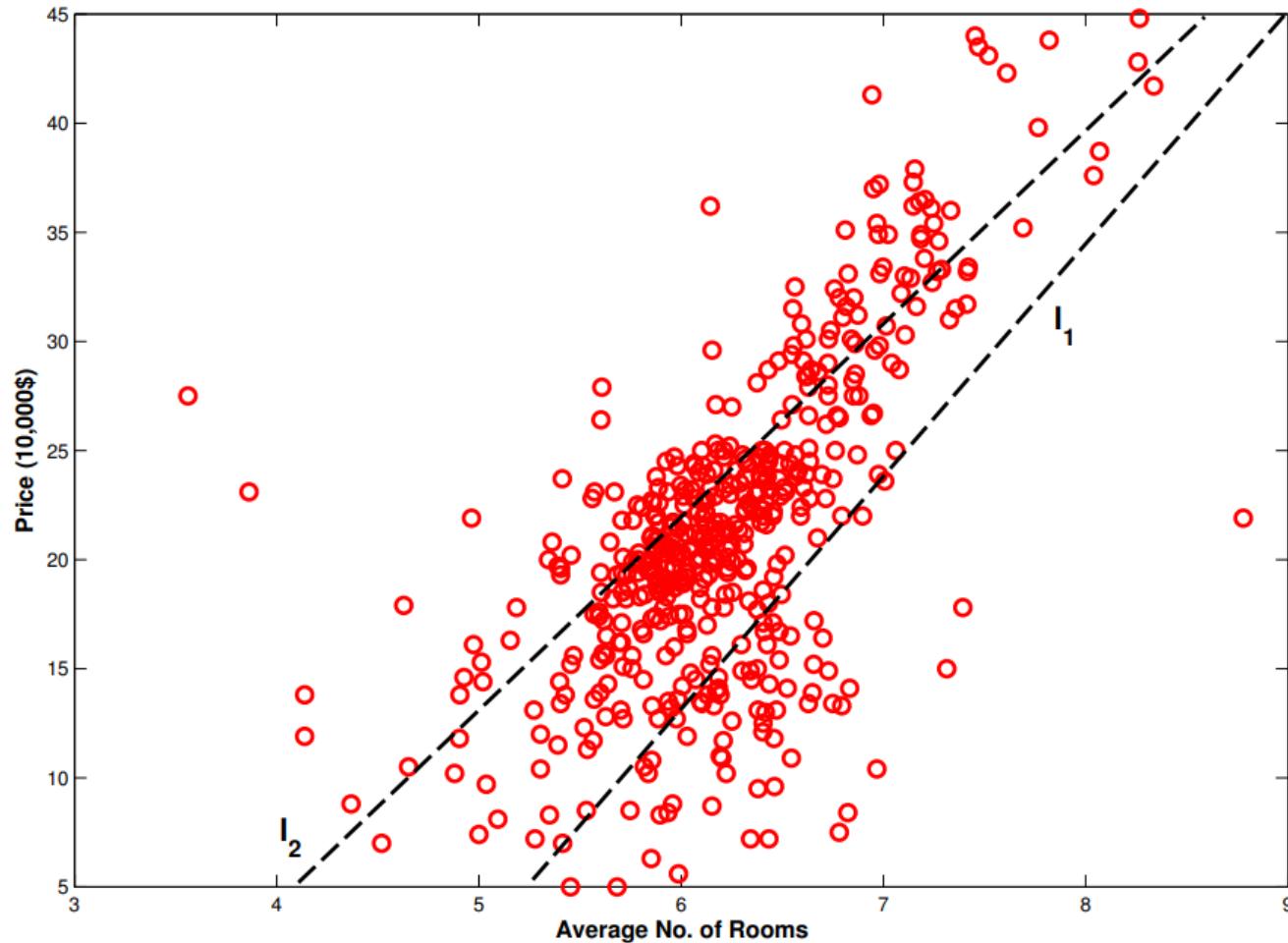
$$y_2 = w_0 + w_1 x_2$$

$$y_3 = w_0 + w_1 x_3$$

...

$$y_N = w_0 + w_1 x_N$$

A linear model



A linear model: multiple features

$$x_i \in \mathbb{R}^m$$

$$X = \begin{bmatrix} x_{11} & \cdots & x_{1m} \\ \vdots & \ddots & \vdots \\ x_{N1} & \cdots & x_{Nm} \end{bmatrix}$$

$$y_i \in \mathbb{R}^N$$

$$y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{bmatrix}$$

$$f(x) : \mathbb{R}^m \rightarrow \mathbb{R}$$

$$y = f_w(x) = w_0 + w_1 x_1 + w_2 x_2 + \dots + w_m x_m$$

A linear model: multiple features

$$f(x) : \mathbb{R}^{m+1} \rightarrow \mathbb{R}$$

$$y = f_w(x) = w_0 x_0 + w_1 x_1 + w_2 x_2 + \dots + w_m x_m$$

$$y = f_w(x) = \sum_{j=1}^m w_j x_j$$

A linear model: multiple features

$$y = f_w(x) = w_0 x_0 + w_1 x_1 + w_2 x_2 + \dots + w_m x_m$$

$$X = \begin{bmatrix} 1 & x_{11} & \cdots & x_{1m} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_{N1} & \cdots & x_{Nm} \end{bmatrix}$$

Assumptions

- Linearity
- IID
- Homoscedasticity
- Normality
- No Multicollinearity

The learning task

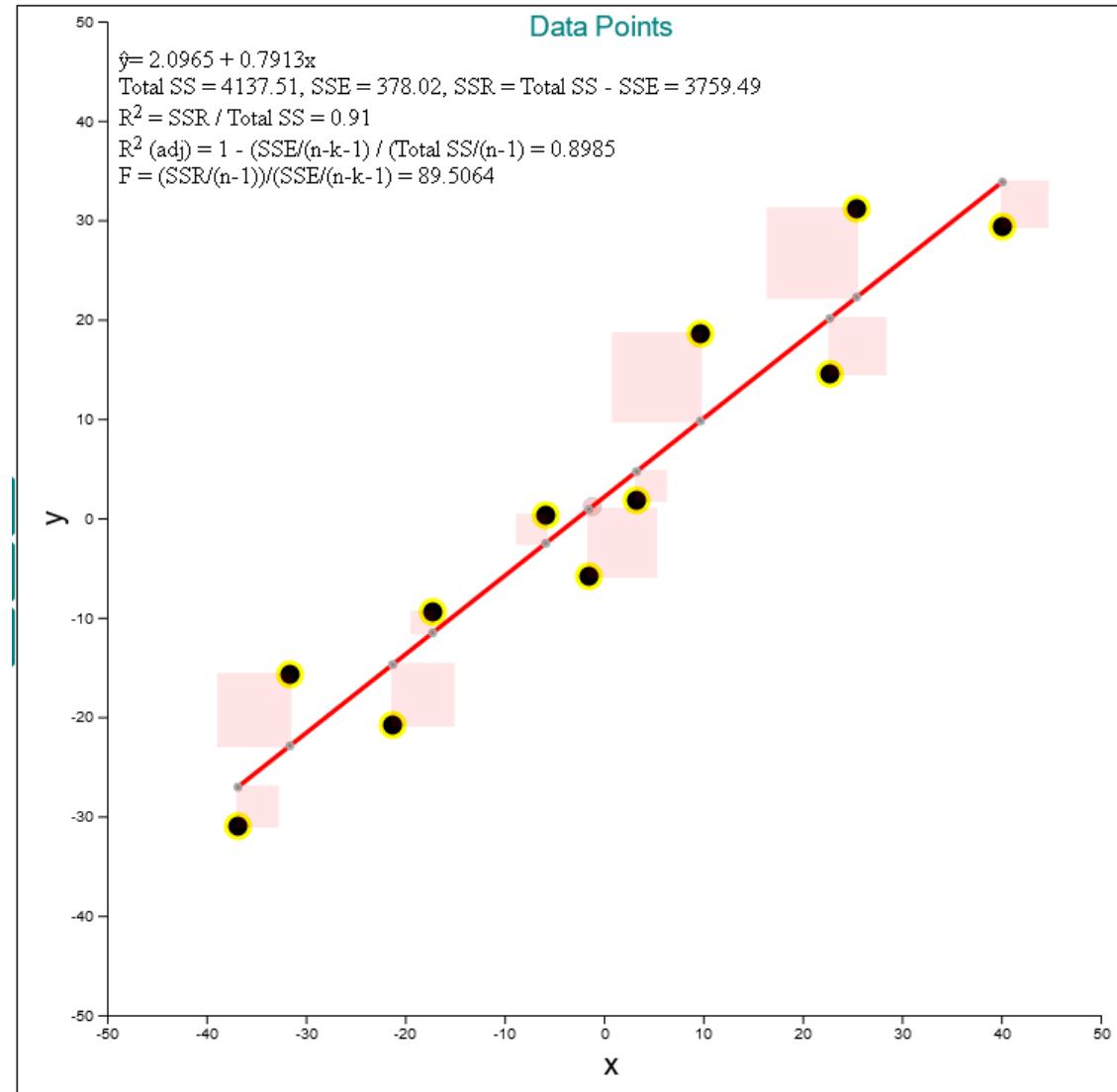
$$f(x) : \mathbb{R}^{m+1} \rightarrow \mathbb{R}$$

$$\hat{y} = f_w(x) = \sum_{j=1}^m w_j x_j$$

$$E(w_m) = \sum_{i=1}^N (\hat{y}_i - y_i)^2 = \sum_{i=1}^N \left(\sum_{j=1}^m w_j x_j - y_i \right)^2 = (Xw - y)^T (Xw - y)$$

$$\arg \min_w (Xw - y)^T (Xw - y)$$

Least Squares



Ordinary Least Squares

$$X = \begin{bmatrix} x_{11} & \cdots & x_{1m} \\ \vdots & \ddots & \vdots \\ x_{N1} & \cdots & x_{Nm} \end{bmatrix} \quad y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{bmatrix}$$

$$E = \begin{bmatrix} f_{\mathbf{w}}(\mathbf{x}_1) - y_1 \\ \dots \\ f_{\mathbf{w}}(\mathbf{x}_N) - y_N \end{bmatrix} = \begin{bmatrix} \mathbf{x}_1^T \mathbf{w} \\ \dots \\ \mathbf{x}_N^T \mathbf{w} \end{bmatrix} - \begin{bmatrix} y_1 \\ \dots \\ y_N \end{bmatrix} = X\mathbf{w} - \mathbf{y}$$

Ordinary Least Squares

$$J(w) = \frac{1}{2} \sum_{i=1}^N (f_w(\mathbf{x}_i) - y_i)^2 = \frac{1}{2} E^T E = \frac{1}{2} (\mathbf{X}\mathbf{w} - \mathbf{y})^T (\mathbf{X}\mathbf{w} - \mathbf{y})$$

$$\nabla_w J(\mathbf{w}) = \nabla_w \frac{1}{2} E^T E = \nabla_w \frac{1}{2} (\mathbf{X}\mathbf{w} - \mathbf{y})^T (\mathbf{X}\mathbf{w} - \mathbf{y})$$

$$= \mathbf{X}^T \mathbf{X} \mathbf{w} - \mathbf{X}^T \mathbf{y}$$

$$\hat{\mathbf{w}}_{OLS} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y}$$

Ordinary Least Squares

$$J(w) = \frac{1}{2} \sum_{i=1}^N (f_w(\mathbf{x}_i) - y_i)^2 = \frac{1}{2} E^T E = \frac{1}{2} (\mathbf{X}\mathbf{w} - \mathbf{y})^T (\mathbf{X}\mathbf{w} - \mathbf{y})$$

$$\nabla_w J(\mathbf{w}) = \frac{1}{2} (\mathbf{X}^T \mathbf{w}^T \mathbf{X} \mathbf{w} - \mathbf{X}^T \mathbf{w}^T \mathbf{y} - \mathbf{y}^T \mathbf{X} \mathbf{w} + \mathbf{y}^T \mathbf{y})$$

$$\nabla_w J(\mathbf{w}) = \frac{1}{2} (2\mathbf{X}^T \mathbf{X} \mathbf{w} - \mathbf{X}^T \mathbf{y} - \mathbf{y}^T \mathbf{X} + 0)$$

$$\nabla_w J(\mathbf{w}) = \frac{1}{2} (2\mathbf{X}^T \mathbf{X} \mathbf{w} - 2\mathbf{X}^T \mathbf{y}) = \frac{2}{2} (\mathbf{X}^T \mathbf{X} \mathbf{w} - \mathbf{X}^T \mathbf{y}) = \mathbf{X}^T \mathbf{X} \mathbf{w} - \mathbf{X}^T \mathbf{y}$$

$$\nabla_w J(\mathbf{w}) = \mathbf{X}^T \mathbf{X} \mathbf{w} - \mathbf{X}^T \mathbf{y} = 0$$

$$\nabla_w (\mathbf{X}^T \mathbf{w}^T \mathbf{X} \mathbf{w}) = 2\mathbf{X}^T \mathbf{X}$$

$$\nabla_w (\mathbf{X}^T \mathbf{w}^T \mathbf{y}) = \mathbf{X}^T \mathbf{y}$$

$$\nabla_w (\mathbf{y}^T \mathbf{X} \mathbf{w}) = \mathbf{y}^T \mathbf{X}$$

$$\nabla_w (\mathbf{y}^T \mathbf{y}) = 0$$

$$\boxed{\mathbf{w} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y}}$$

Iterative Least Squares

$$E(w_m) = \sum_{i=1}^N (\hat{y}_i - y_i)^2 = \sum_{i=1}^N \left(\sum_{j=1}^m w_j x_j - y_i \right)^2 = \sum_{i=1}^N (W^T x_i - y_i)^2$$

$$J = \frac{1}{2} \sum_{i=1}^N (W^T x_i - y_i)^2$$

$$\frac{\partial J}{\partial w_j} J = \frac{\partial J}{\partial w_j} \frac{1}{2} \sum_{i=1}^N (W^T x_i - y_i)^2$$

$$\frac{\partial J}{\partial w_j} J = \frac{1}{2} \frac{\partial J}{\partial w_j} \sum_{i=1}^N (W^T x_i - y_i)^2$$

$$\frac{\partial J}{\partial w_j} J = \frac{2}{2} \frac{\partial J}{\partial w_j} \sum_{i=1}^N (W^T x_i - y_i)^1 \cdot \frac{\partial J}{\partial w_j} (W^T x_i - y_i)$$

Iterative Least Squares

$$E(w_m) = \sum_{i=1}^N (\hat{y}_i - y_i)^2 = \sum_{i=1}^N \left(\sum_{j=1}^m w_j x_j - y_i \right)^2$$

$$\frac{\partial J}{\partial w_j} J = \frac{2}{2} \sum_{i=1}^N (W^T x_i - y_i)^1 \cdot \frac{\partial J}{\partial w_j} (W^T x_i - y_i)$$

$$\frac{\partial J}{\partial w_j} J = \sum_{i=1}^N (W^T x_i - y_i) \cdot \frac{\partial J}{\partial w_j} (W^T x_i - y_i)$$

$$\frac{\partial J}{\partial w_j} J = \sum_{i=1}^N (W^T x_i - y_i) \cdot (x_i)$$

Repeat until converged:

$$w_j^{(t+1)} = w_j^{(t)} - \eta \frac{\partial J}{\partial w_j}$$

Regression Challenges

- Function choice
 - Linear
 - Polynomial
- Generalizability
 - Overfitting
 - Cross validation
- Feature engineering
- Multicollinearity

