CS5489
Lecture 5.1: Regression

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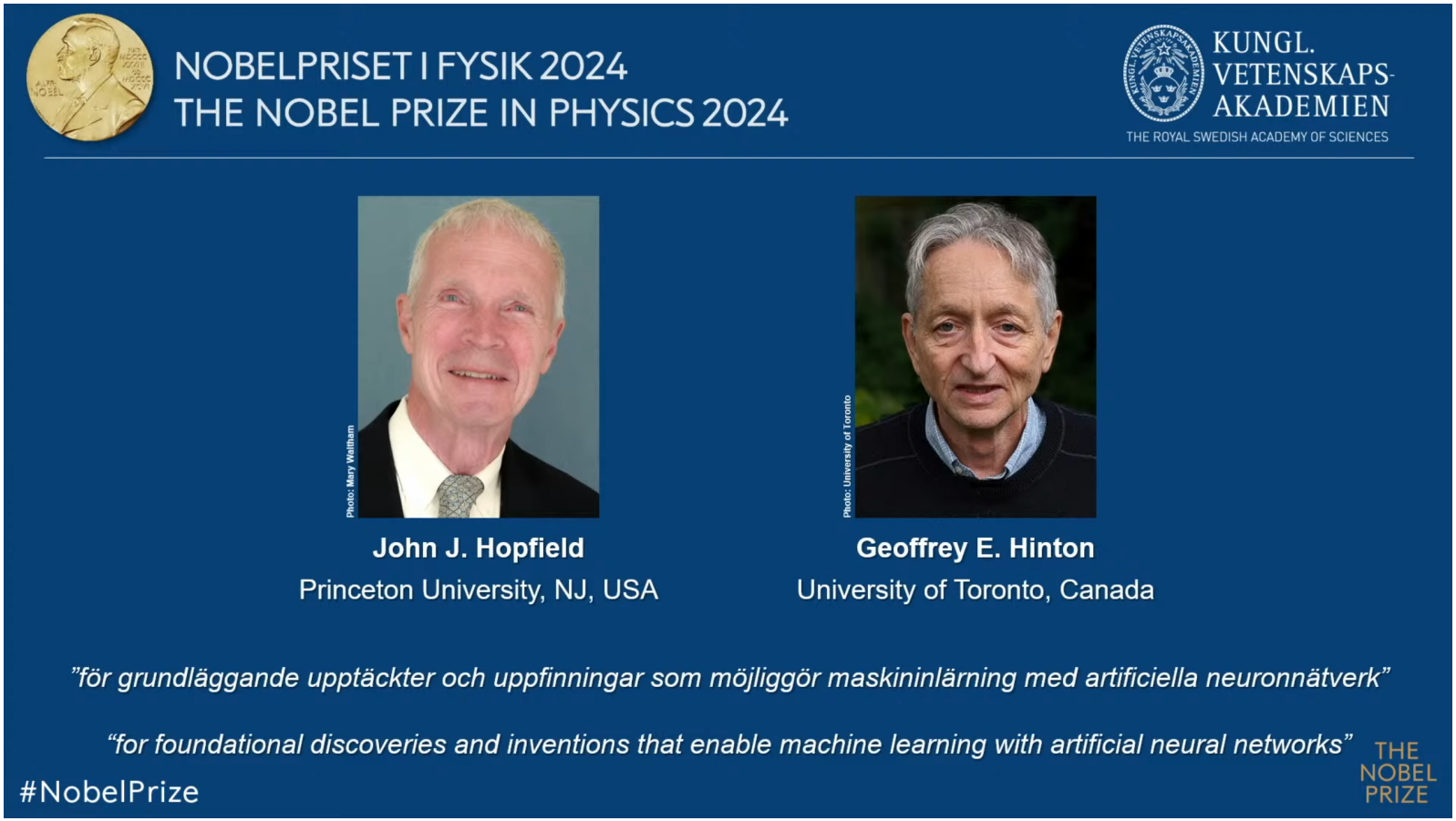
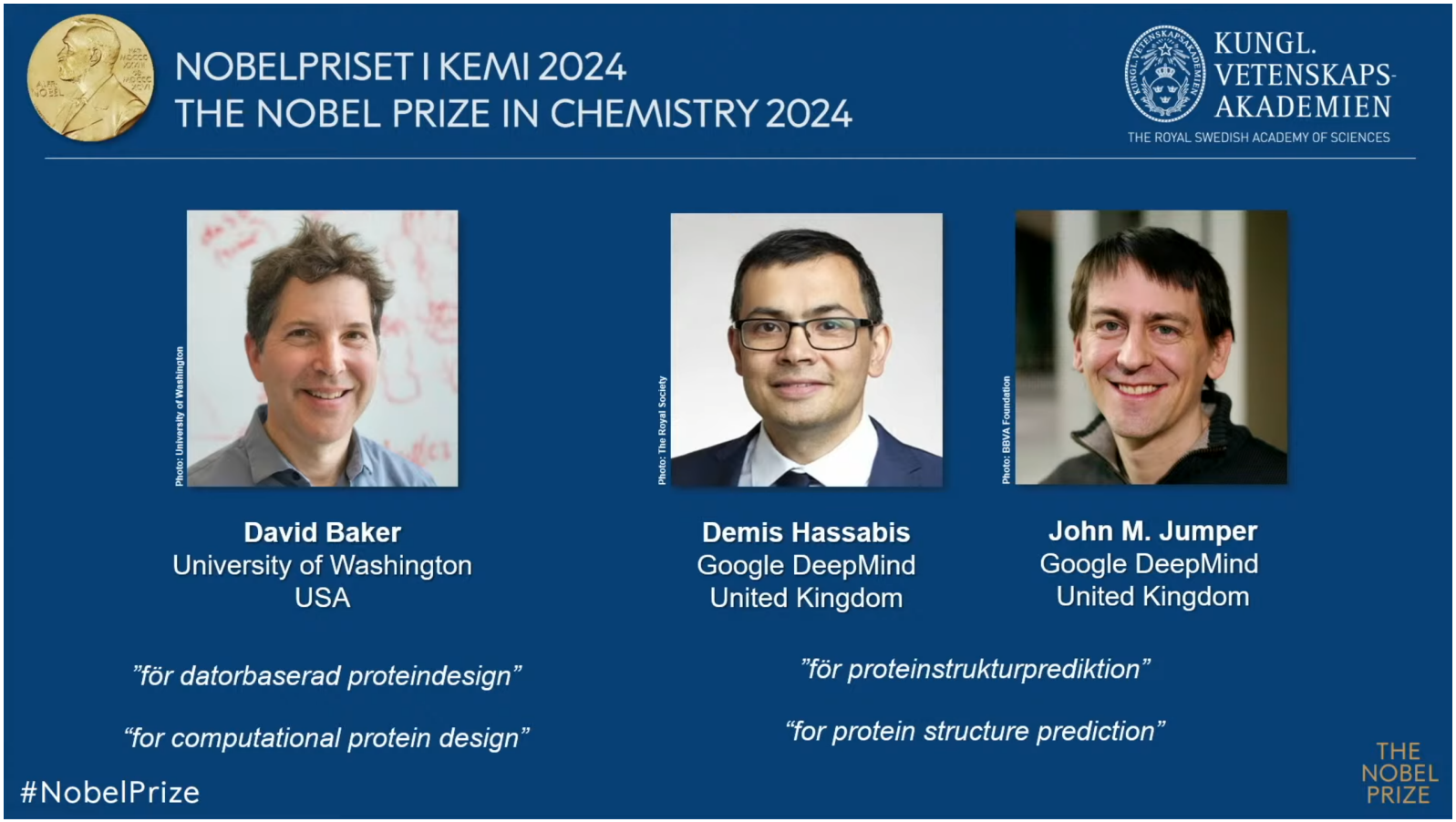
The Nobel Prize in Physics Awarded to ML



The Nobel Prize in Chemistry Awarded to ML

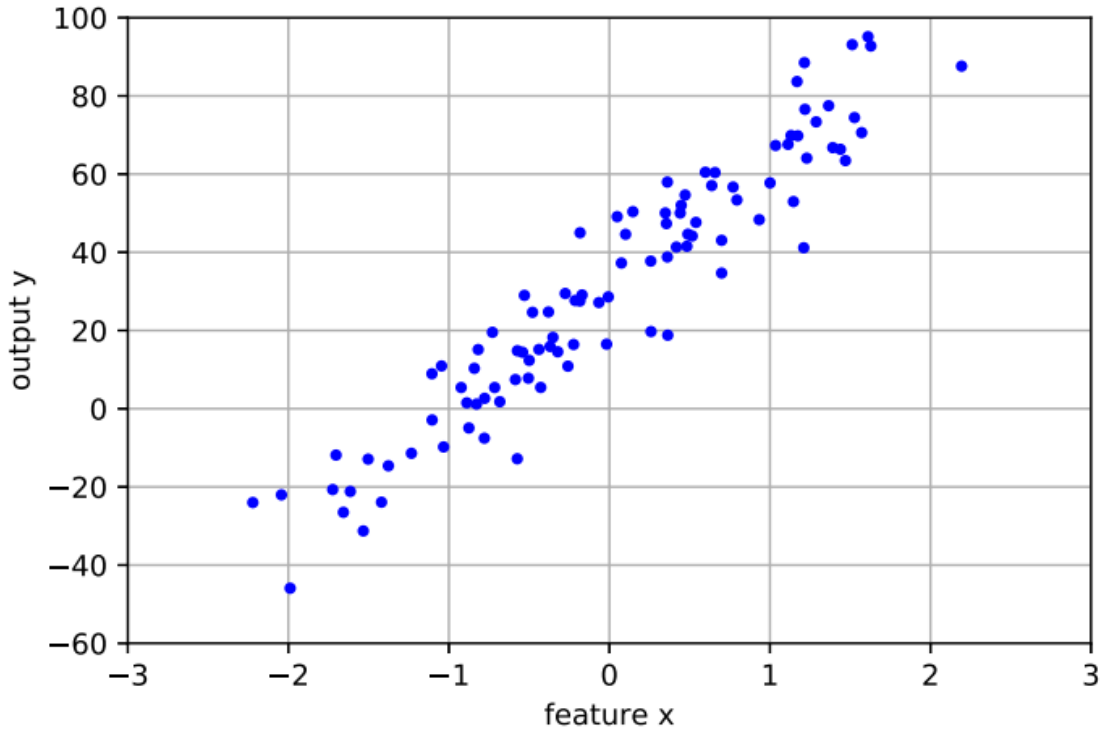


Outline

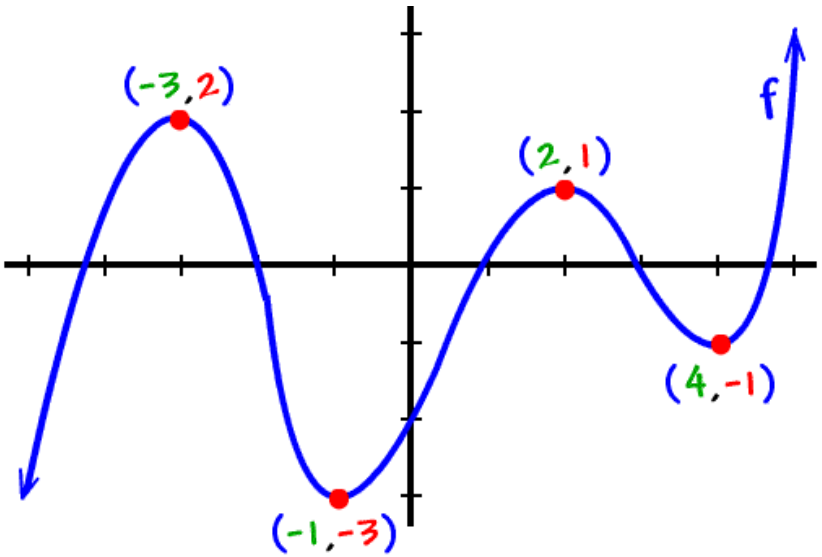
The Regression Task

Definition: The Regression Task

Given a feature vector $\mathbf{x} \in \mathbb{R}^N$, predict its corresponding output value $y \in \mathbb{R}$



Example: Curve Fitting



Given: M points sampled from some underlying curve (assuming no measurement noise)
Goal: Find that curve

- **Question 1**: Would a small handful of points work well, or the more the better?
- **Question 2**: Given the number of points fixed, do their locations matter?
- **Question 3**: Given a set of M points, is curve fitting unique?
- **Question 4**: Why you might be able to choose one "seemingly best" curve, from other possibilities?

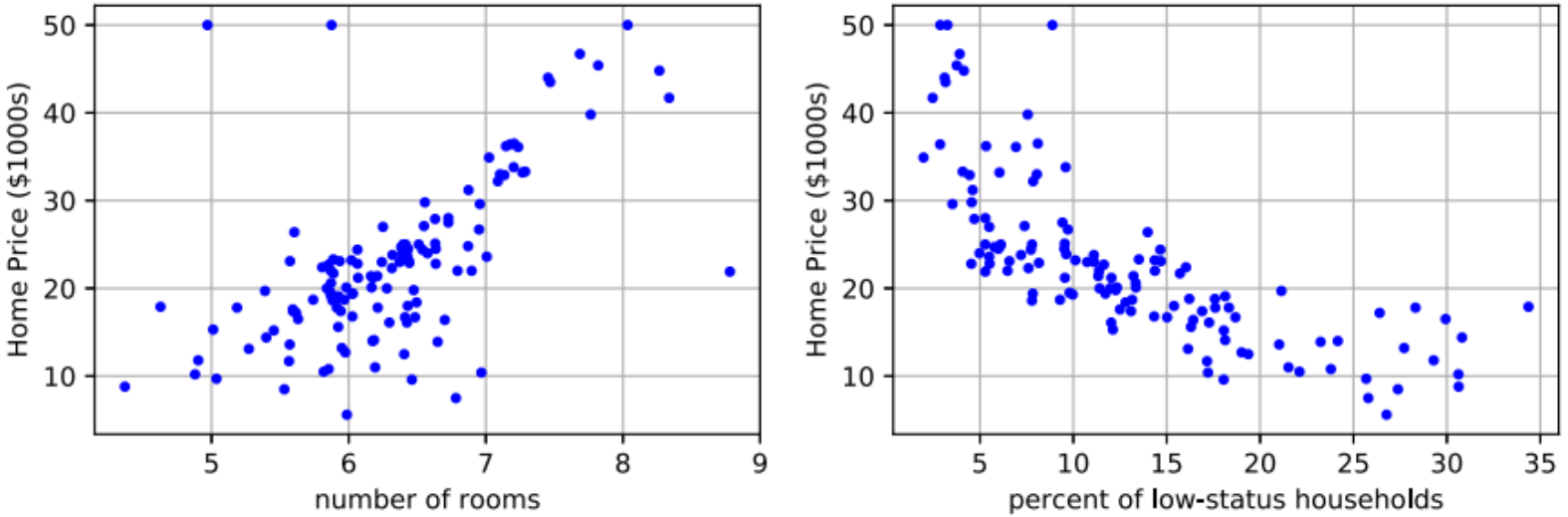
Example: Curve Fitting

- **Question 1**: Would a small handful of points work well, or the more the better?
- **Question 2**: Given the number of points fixed, do their locations matter?
- **Question 3**: Given a set of M points, is curve fitting unique?
- **Question 4**: Why you might be able to choose one "seemingly best" curve, from those infinite possibilities?

- We always like more samples, if possible
- Samples need be representative or informative
- Estimating continuous model from discrete data is an ill-posed problem and in most cases cannot be certain
- You need to have some criteria to choose your preferred model

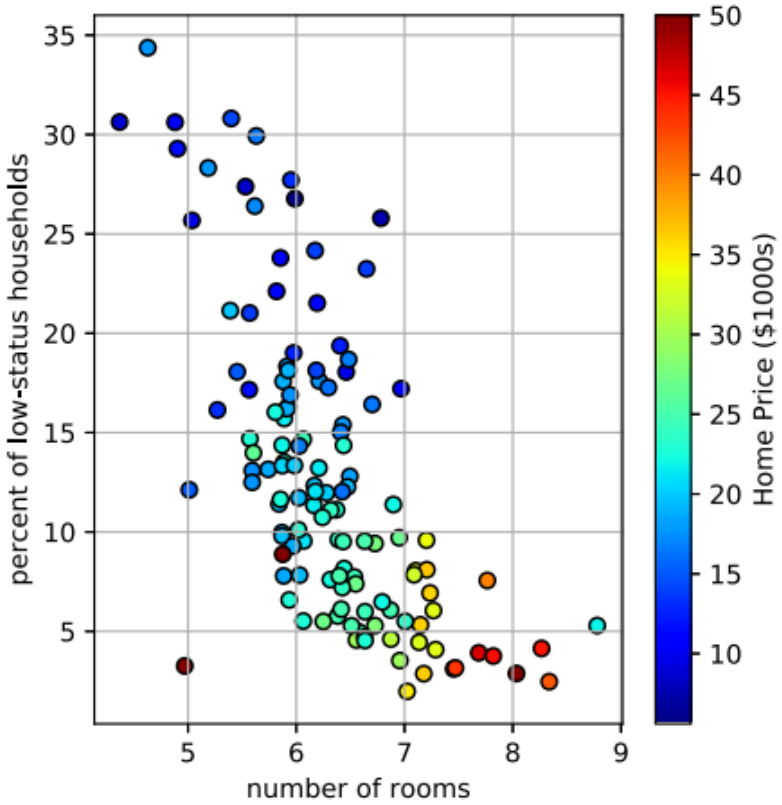
Example: House Price

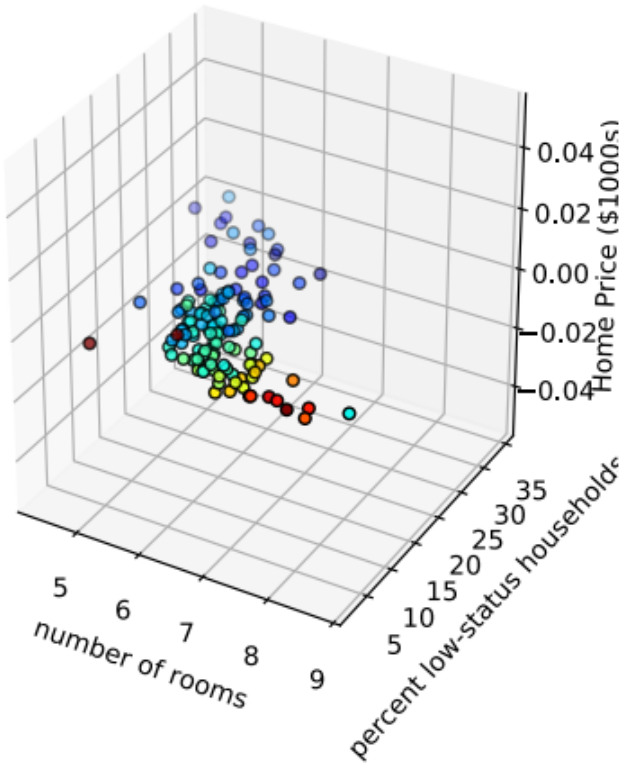
- Predict Boston house price from number of rooms, or percentage of low-status households in neighborhood



Example: House Price

- Predict from both features





The Regression Learning Problem

Definition: Regression Learning Problem

Given a data set of example pairs $\mathcal{D} = \{(\mathbf{x}^{(i)}, y^{(i)}), i = 1, \ldots, M\}$ where $\mathbf{x}^{(i)} \in \mathbb{R}^N$ is a feature vector and $y^{(i)} \in \mathbb{R}$ is the output, learn a function $f : \mathbb{R}^N \mapsto \mathbb{R}$ that accurately predicts y for any feature vector $\mathbf{x}$

Error Measure: Mean Squared Error (MSE)

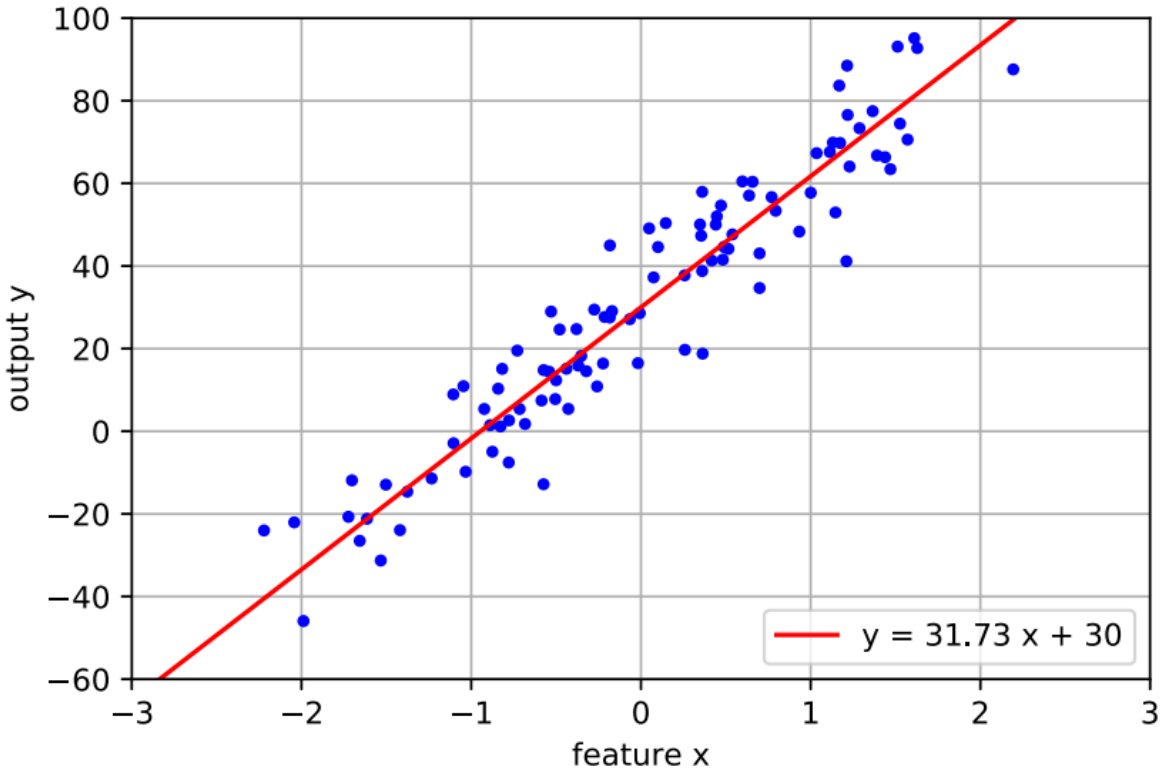
Given a data set of example pairs $\mathcal{D} = \{(\mathbf{x}^{(i)}, y^{(i)}), i = 1, \cdots, M\}$ and a function $f : \mathbb{R}^N \mapsto \mathbb{R}$, the MSE of f on $\mathcal{D}$ is

$$\text{MSE}(\mathcal{D}, f) = \frac{1}{M} \sum_{i=1}^{M} (y^{(i)} - f(\mathbf{x}^{(i)}))^2$$

Outline

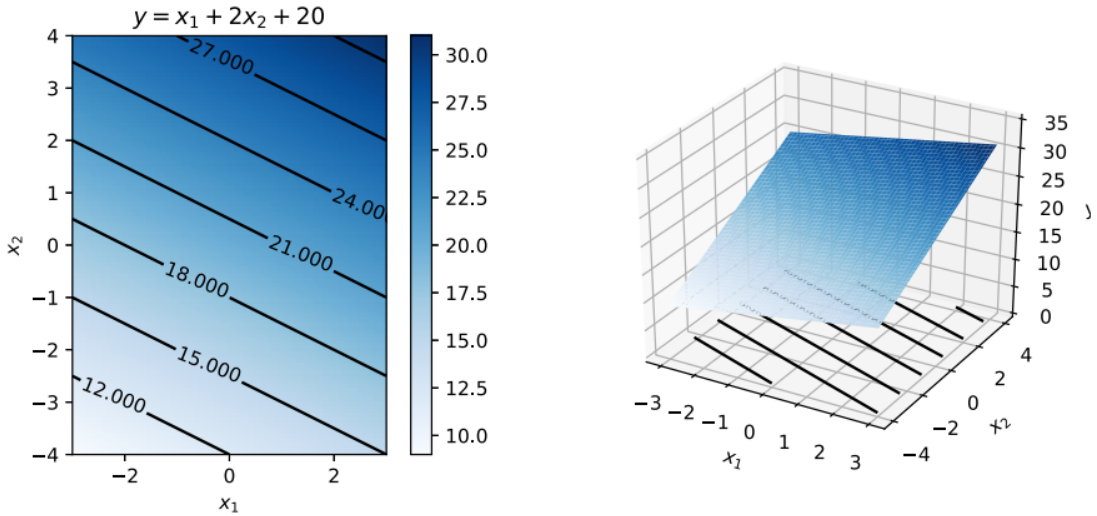
Linear Regression

- **1-D case**: the output y is a linear function of input feature x
  - $y = w \cdot x + b$
  - w is the slope, b is the intercept



Linear Regression

- **N-D case**: the output y is a linear combination of N input features $x_1, \ldots, x_N$:
  - $y = w_1 x_1 + w_2 x_2 + \cdots + w_N x_N + w_0$
- Equivalently,
  - $y = \mathbf{w}^T \mathbf{x} + w_0 = \sum_{j=1}^{N} w_j x_j + w_0 = \sum_{j=0}^{N} w_j x_j$, defining $x_0 = 1$
  - $\mathbf{x} \in \mathbb{R}^N$ is the vector of input values
  - $\mathbf{w} \in \mathbb{R}^N$ are the weights of the linear function and w_0 is the intercept (bias term)



Ordinary Least Squares (OLS)

- The linear function has form $f(\mathbf{x}) = \mathbf{w}^T\mathbf{x} + b$
- How to estimate the parameters $(\mathbf{w}, b)$ from the data?
- OLS selects the linear regression parameters to minimize the MSE on the training data set

$$\mathbf{w}^\star, b^\star = \arg\min_{\mathbf{w},b} \frac{1}{M}\sum_{i=1}^{M}(y^{(i)} - \mathbf{w}^T\mathbf{x}^{(i)} - b)^2$$

Solving OLS For One Feature

- Take the derivative of the objective w.r.t. w and set it to zero:

$$\frac{\partial}{\partial w}\frac{1}{M}\sum_{i=1}^{M}(y^{(i)} - wx^{(i)} - b)^2 = 0$$

$$2\frac{1}{M}\sum_{i=1}^{M}(y^{(i)} - wx^{(i)} - b)(-x^{(i)}) = 0$$

$$\left(\sum_{i=1}^{M}(x^{(i)})^2\right)w + \left(\sum_{i=1}^{M}x^{(i)}\right)b = \sum_{i=1}^{M}y^{(i)}x^{(i)}$$

Solving OLS For One Feature

- Take the derivative of the objective w.r.t. b and set it to zero:

$$\frac{\partial}{\partial b}\frac{1}{M}\sum_{i=1}^{M}(y^{(i)} - wx^{(i)} - b)^2 = 0$$

$$2\frac{1}{M}\sum_{i=1}^{M}(y^{(i)} - wx^{(i)} - b)(-1) = 0$$

$$\left(\sum_{i=1}^{M} x^{(i)}\right) w + Mb = \sum_{i=1}^{M} y^{(i)}$$

Solving OLS For One Feature

- Write the two equations in matrix form:

$$\begin{bmatrix} \sum_{i=1}^{M} (x^{(i)})^2 & \sum_{i=1}^{M} x^{(i)} \\ \sum_{i=1}^{M} x^{(i)} & M \end{bmatrix} \begin{bmatrix} w \\ b \end{bmatrix} = \begin{bmatrix} \sum_{i=1}^{M} y^{(i)} x^{(i)} \\ \sum_{i=1}^{M} y^{(i)} \end{bmatrix}$$

$$\begin{bmatrix} w \\ b \end{bmatrix} = \begin{bmatrix} \sum_{i=1}^{M} (x^{(i)})^2 & \sum_{i=1}^{M} x^{(i)} \\ \sum_{i=1}^{M} x^{(i)} & M \end{bmatrix}^{-1} \begin{bmatrix} \sum_{i=1}^{M} y^{(i)} x^{(i)} \\ \sum_{i=1}^{M} y^{(i)} \end{bmatrix}$$

General OLS Solution

- **Matrix notation**:
  - $\mathbf{x}^{(i)} \in \mathbb{R}^{N+1}$, where we have defined $x_0^{(i)} = 1$
  - $\mathbf{X} \in \mathbb{R}^{M \times (N+1)}$ with one data case $\mathbf{x}^{(i)} \in \mathbb{R}^{N+1}$ per row

$$\mathbf{X} = \begin{bmatrix} — & (\mathbf{x}^{(1)})^T & — \\ — & (\mathbf{x}^{(2)})^T & — \\ & \vdots & \\ — & (\mathbf{x}^{(M)})^T & — \end{bmatrix}$$

  - $\mathbf{y} \in \mathbb{R}^M$ is a column vector containing the corresponding outputs

$$\mathbf{y} = \begin{bmatrix} y^{(1)} \\ y^{(2)} \\ \vdots \\ y^{(M)} \end{bmatrix}$$

  - $\mathbf{w} \in \mathbb{R}^{N+1}$, where $w_0 = b$

General OLS Solution

- The general OLS solution for $\mathbf{w} \in \mathbb{R}^{N+1}$ is

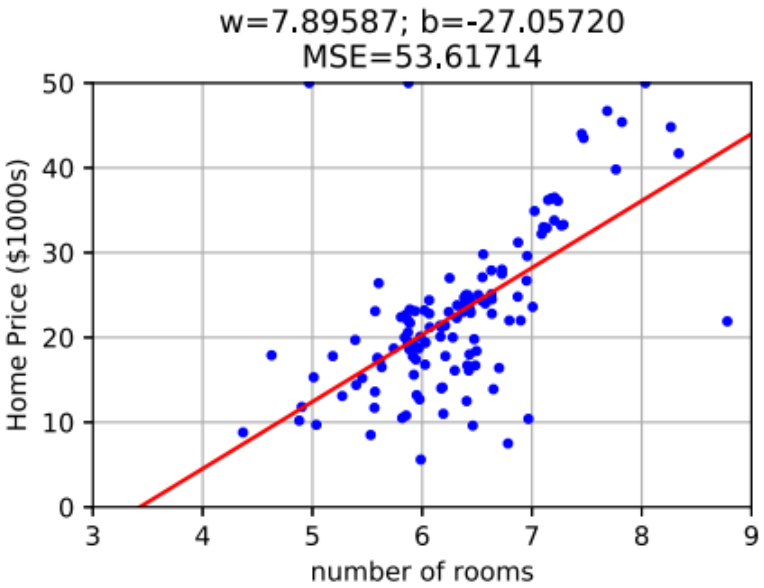
$$\begin{aligned}\mathbf{w}^\star &= \arg\min_{\mathbf{w}} \frac{1}{M} \sum_{i=1}^{M} (y^{(i)} - (\mathbf{x}^{(i)})^T \mathbf{w})^2 \\ &= \arg\min_{\mathbf{w}} \frac{1}{M} (\mathbf{y} - \mathbf{X}\mathbf{w})^T (\mathbf{y} - \mathbf{X}\mathbf{w})\end{aligned}$$

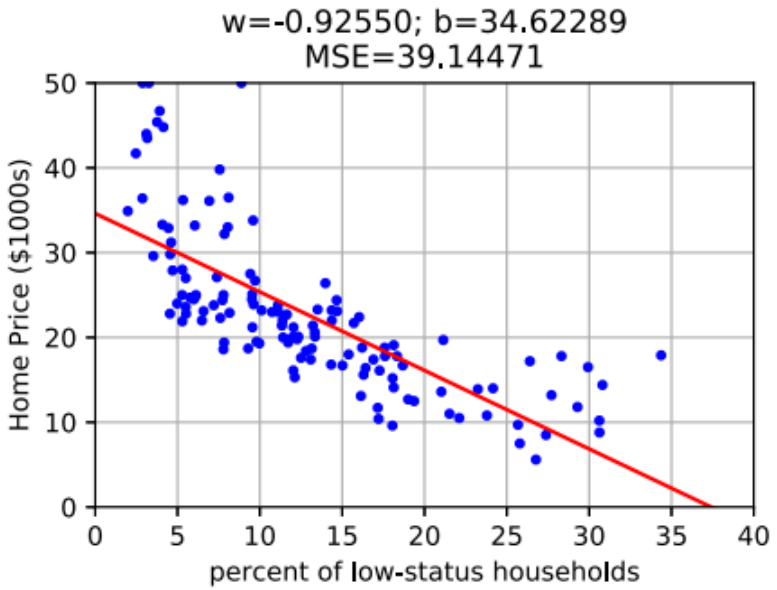
- Take the derivative w.r.t. $\mathbf{w}$ and set it to zero:

$$\begin{aligned}\frac{\partial}{\partial \mathbf{w}} \frac{1}{M} (\mathbf{y} - \mathbf{X}\mathbf{w})^T (\mathbf{y} - \mathbf{X}\mathbf{w}) &= 0 \\ \mathbf{X}^T (\mathbf{y} - \mathbf{X}\mathbf{w}) &= 0 \\ \mathbf{X}^T \mathbf{X}\mathbf{w} &= \mathbf{X}^T \mathbf{y} \\ \mathbf{w}^\star &= (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y}\end{aligned}$$

Boston Housing price (1-D)

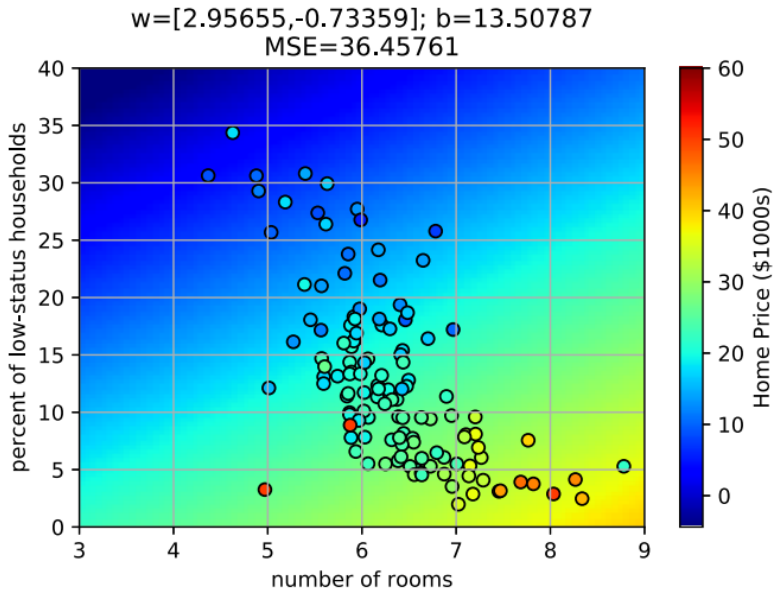
- Learn regression function for each feature separately





Boston Housing price (2-D)

- For both features together



- Interpretation from the linear model parameters
  - Each room increases home price by $\$2,956$ (w_1)
  - Each percentage of low-status households decreases home price by $\$733$ (w_2)
  - The "starting" price is $\$13,508$ (b)

Connection to Probabilistic Models

- The same solution can be derived as the MLE of the parameters under a conditional Gaussian model
- Assumption: the output (or the observation) $\mathbf{y}$ is from a deterministic function with additive Gaussian noise:

$$\mathbf{y} = \mathbf{X}\mathbf{w} + \boldsymbol{\epsilon}, \text{ where } p(\boldsymbol{\epsilon}; \sigma^2) = \mathcal{N}(\boldsymbol{\epsilon}; 0, \sigma^2\mathbf{I})$$

- This implies that

$$p(\mathbf{y}|\mathbf{X}; \mathbf{w}, \sigma^2) = p(\mathbf{y}-\mathbf{X}\mathbf{w}; \sigma^2) = \mathcal{N}(\mathbf{y}-\mathbf{X}\mathbf{w}; 0, \sigma^2\mathbf{I}) = \mathcal{N}(\mathbf{y}; \mathbf{X}\mathbf{w}, \sigma^2\mathbf{I})$$

- Equivalently,

$$p(\mathbf{y}|\mathbf{X}; \mathbf{w}, \sigma^2) = \frac{1}{\sqrt{(2\pi\sigma^2)^M}} \exp\left(-\frac{1}{2\sigma^2}(\mathbf{y} - \mathbf{X}\mathbf{w})^T(\mathbf{y} - \mathbf{X}\mathbf{w})\right)$$

Connection to Probabilistic Models

- Maximize the log likelihood:

$$\begin{aligned}
&\arg\max_{\mathbf{w},\sigma^2} \log p(\mathbf{y}|\mathbf{X};\mathbf{w},\sigma^2) \\
&= \arg\max_{\mathbf{w},\sigma^2} -\frac{M}{2}\log 2\pi - \frac{M}{2}\log\sigma^2 - \frac{1}{2\sigma^2}(\mathbf{y}-\mathbf{X}\mathbf{w})^T(\mathbf{y}-\mathbf{X}\mathbf{w}) \\
&= \arg\min_{\mathbf{w},\sigma^2} \frac{M}{2}\log\sigma^2 + \frac{1}{2\sigma^2}(\mathbf{y}-\mathbf{X}\mathbf{w})^T(\mathbf{y}-\mathbf{X}\mathbf{w})
\end{aligned}$$

- Note that solving for $\mathbf{w}$ is independent of σ^2:

$$\mathbf{w}^\star = \arg\min_{\mathbf{w}} \frac{1}{2}(\mathbf{y}-\mathbf{X}\mathbf{w})^T(\mathbf{y}-\mathbf{X}\mathbf{w})$$

More on Linear Regression

- Take a closer look at the closed-form solution

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

  - We call $\mathbf{X}^\dagger = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T$ pseudo-inverse (generalization of inverse to non-square matrix). See for a square invertible matrix $\mathbf{X}$, we have $\mathbf{X}^\dagger = \mathbf{X}^{-1}(\mathbf{X}^T)^{-1}\mathbf{X}^T = \mathbf{X}^{-1}$
  - What if $\mathbf{X}^T\mathbf{X} \in \mathbb{R}^{(N+1)\times(N+1)}$ is non-invertible?
    - If $M < N+1$, add more data or enforce regularization
    - If $M \geq N+1$, remove redundant features or enforce regularization
  - What if N is too large? Use gradient descent

$$\mathbf{w}^{(t+1)} = \mathbf{w}^{(t)} - \alpha\mathbf{X}^T(\mathbf{X}\mathbf{w}^{(t)} - \mathbf{y})$$

  - What if M is too large? Use mini-batch gradient descent

$$\mathbf{w}^{(t+1)} = \mathbf{w}^{(t)} - \alpha \sum_{(\mathbf{x},y)\in\mathcal{B}} \mathbf{x}(\mathbf{x}^T\mathbf{w}^{(t)} - y)$$