Lecture 5: 23 January, 2023

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Data Mining and Machine Learning
January–April 2024

Predicting numerical values

- Data about housing prices
- Predict house price from living area

Living area (feet^2)	Price (1000\$s)
2104	400
1600	330
2400	369
1416	232
3000	540
⋮	⋮

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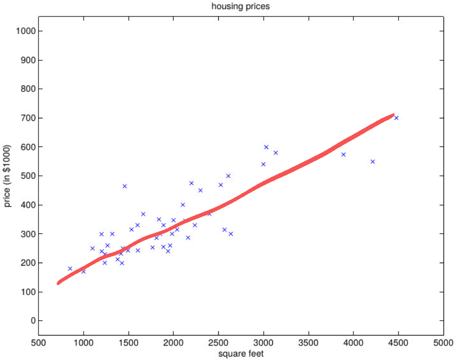
- Scatterplot corresponding to the data
- Fit a function to the points



Linear predictors

- A richer set of input data

Living area (feet^2)	#bedrooms	Price (1000\$s)
2104	3	400
1600	3	330
2400	3	369
1416	2	232
3000	4	540
$\vdots$	$\vdots$	$\vdots$

Linear predictors

- A richer set of input data
- Simplest case: fit a linear function with parameters $\theta = (\theta_0, \theta_1, \theta_2)$

  $h_\theta(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2$

x_1	x_2	$h(x_1, x_2)$
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- Input x may have k features $(x_1, x_2, \ldots, x_k)$
- By convention, add a dummy feature $x_0 = 1$
- For k input features

  $$h_\theta(x) = \sum_{i=0}^{k} \theta_i x_i$$

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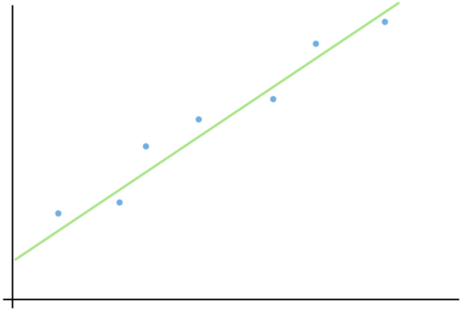
Finding the best fit line

- Training input is
  $\{(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)\}$
  - Each input x_i is a vector $(x_i^1, \ldots, x_i^k)$
  - Add $x_i^0 = 1$ by convention
  - y_i is actual output



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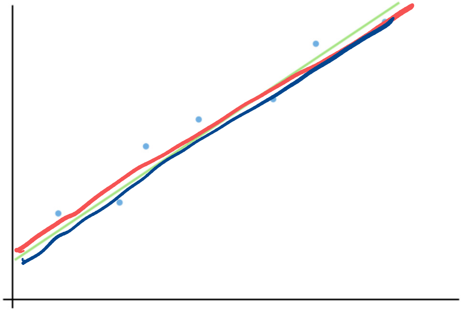

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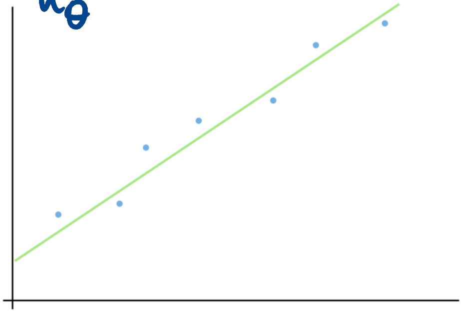
- Define a cost (loss) function

$$J(\theta) = \frac{1}{2}\sum_{i=1}^{n}(h_\theta(x_i) - y_i)^2$$

θ – unknown $(\theta_0, \theta_1, \ldots, \theta_k)$

h_θ



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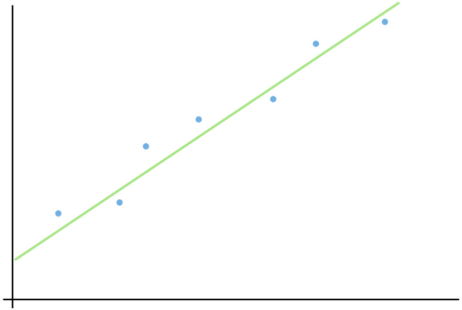
- Essentially, the sum squared error (SSE)



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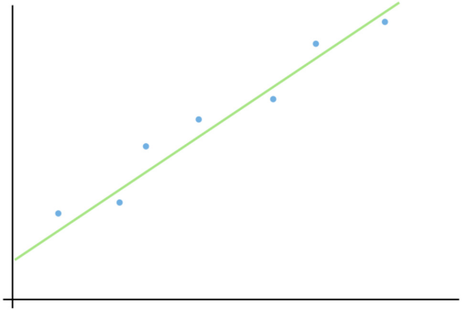
- Essentially, the sum squared error (SSE)
- Divide by n, mean squared error (MSE)



Minimizing SSE

- Write x_i as row vector $\begin{bmatrix} 1 & x_i^1 & \cdots & x_i^k \end{bmatrix}$

x_i^0 set to 1

Minimizing SSE

- Write x_i as row vector $\begin{bmatrix} 1 & x_i^1 & \cdots & x_i^k \end{bmatrix}$
- $X = \begin{bmatrix} 1 & x_1^1 & \cdots & x_1^k \\ 1 & x_2^1 & \cdots & x_2^k \\ & & \cdots & \\ 1 & x_i^1 & \cdots & x_i^k \\ & & \cdots & \\ 1 & x_n^1 & \cdots & x_n^k \end{bmatrix}, y = \begin{bmatrix} y_1 \\ y_2 \\ \cdots \\ y_i \\ \cdots \\ y_n \end{bmatrix}$
- Write θ as column vector, $\theta^T = \begin{bmatrix} \theta_0 & \theta_1 & \cdots & \theta_k \end{bmatrix}$

Minimizing SSE

- Write x_i as row vector $\left[\begin{array}{cccc} 1 & x_i^1 & \cdots & x_i^k \end{array}\right]$

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- Write θ as column vector, $\theta^T = \left[\begin{array}{cccc} \theta_0 & \theta_1 & \cdots & \theta_k \end{array}\right]$

- $J(\theta) = \dfrac{1}{2}\displaystyle\sum_{i=1}^{n}(h_\theta(x_i) - y_i)^2 = \dfrac{1}{2}(X\theta - y)^T(X\theta - y)$

$$X\theta = \begin{bmatrix} h(x_1) \\ \vdots \\ h(x_n) \end{bmatrix} \quad \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix}$$

$$\theta = \begin{bmatrix} \ \end{bmatrix}$$

Minimizing SSE

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- $J(\theta) = \dfrac{1}{2} \sum_{i=1}^{n} (h_\theta(x_i) - y_i)^2 = \dfrac{1}{2} (X\theta - y)^T (X\theta - y)$

- Minimize $J(\theta)$ — set $\nabla_\theta \, J(\theta) = 0$

Minimizing SSE

- $J(\theta) = \dfrac{1}{2}(X\theta - y)^T(X\theta - y)$
- $\nabla_\theta \; J(\theta) = \nabla_\theta \; \frac{1}{2}(X\theta - y)^T(X\theta - y)$
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- Expand, $\frac{1}{2}\nabla_\theta\ (\theta^T X^T X\theta - y^T X\theta - \theta^T X^T y + y^T y) = 0$

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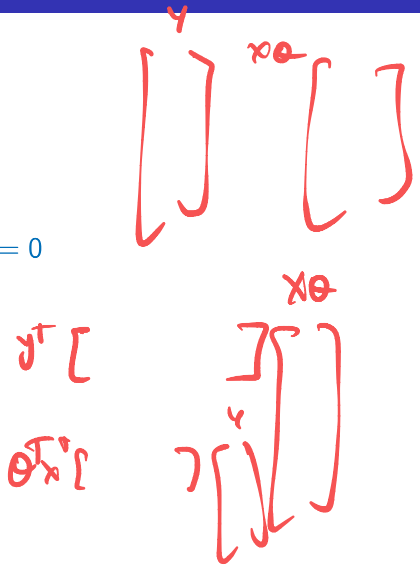
  - Check that $y^T X\theta = \theta^T X^T y = \sum_{i=1}^{n} h_\theta(x_i) \cdot y_i$



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- Combining terms, $\cancel{\frac{1}{2}}\nabla_\theta\, (\theta^T X^T X\theta - \cancel{2}\underline{\theta^T X^T y} + y^T y) = 0$
- After differentiating, $X^T X\theta - X^T y = 0$

$X^T X\theta^2$

$\cancel{2}X^T X\theta$

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- Combining terms, $\frac{1}{2}\nabla_\theta\ (\theta^T X^T X\theta - 2\theta^T X^T y + y^T y) = 0$
- After differentiating, $X^T X\theta - X^T y = 0$
- Solve to get normal equation, $\theta = (X^T X)^{-1} X^T y$

Minimizing SSE iteratively

- Normal equation $\theta = (X^T X)^{-1} X^T y$ is a closed form solution

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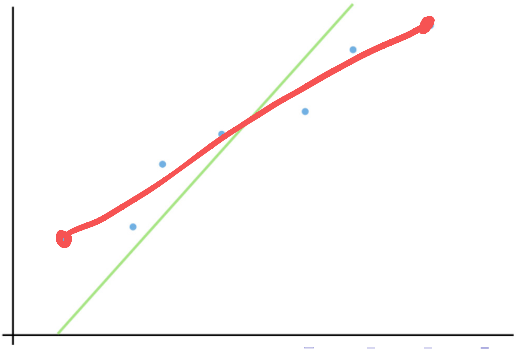
- Iterative approach, make an initial guess



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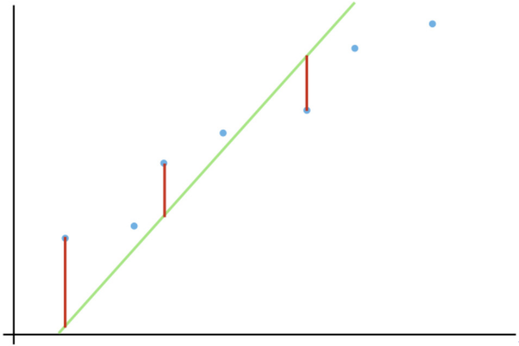

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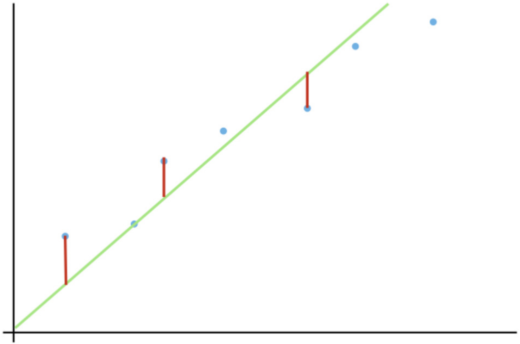
- Iterative approach, make an initial guess
- Keep adjusting the line to reduce SSE



Minimizing SSE iteratively

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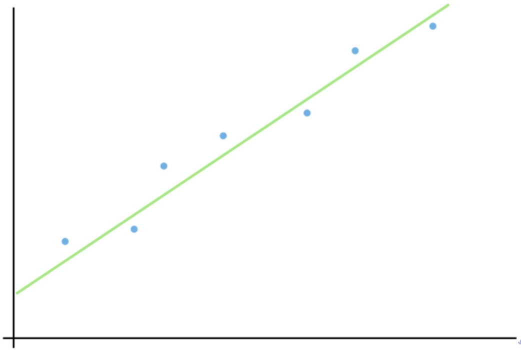
- Keep adjusting the line to reduce SSE
- Stop when we find the best fit line



Minimizing SSE iteratively

- Normal equation $\theta = (X^TX)^{-1}X^Ty$ is a closed form solution
- Computational challenges
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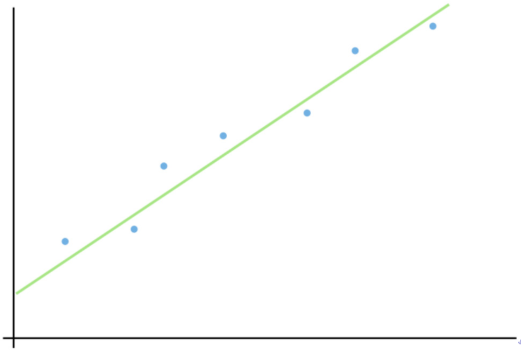
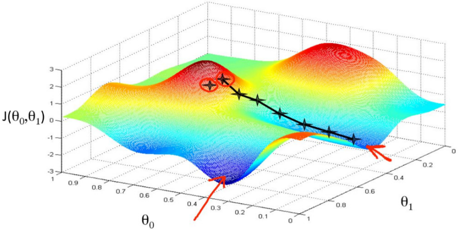
- Iterative approach, make an initial guess
- Keep adjusting the line to reduce SSE
- Stop when we find the best fit line
- How do we adjust the line?



Gradient descent

- How does cost vary with parameters $\theta = (\theta_0, \theta_1, \ldots, \theta_k)$?
  - Gradients $\dfrac{\partial}{\partial \theta_i} J(\theta)$



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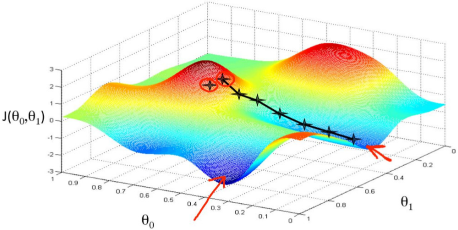
- Adjust each parameter against gradient
  - $\theta_i = \theta_i - \alpha \frac{\partial}{\partial \theta_i} J(\theta)$



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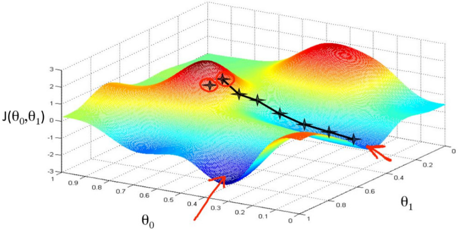
- For a single training sample (x, y)

$$\frac{\partial}{\partial \theta_i} J(\theta) = \frac{\partial}{\partial \theta_i} \frac{1}{2} (h_\theta(x) - y)^2$$



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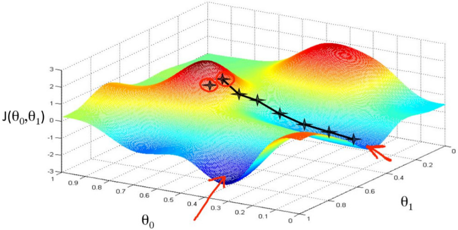
$$\begin{aligned}\frac{\partial}{\partial \theta_i} J(\theta) &= \frac{\partial}{\partial \theta_i} \frac{1}{2}(h_\theta(x) - y)^2 \\ &= 2 \cdot \frac{1}{2}(h_\theta(x) - y) \frac{\partial}{\partial \theta_i}(h_\theta(x) - y)\end{aligned}$$



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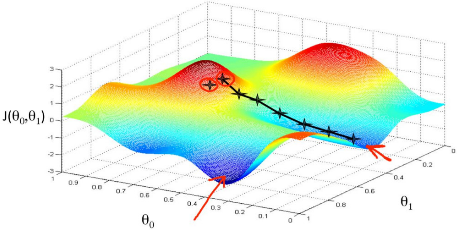
\frac{\partial}{\partial \theta_i} J(\theta) &= \frac{\partial}{\partial \theta_i} \frac{1}{2} (h_\theta(x) - y)^2 \\
&= 2 \cdot \frac{1}{2} (h_\theta(x) - y) \frac{\partial}{\partial \theta_i} (h_\theta(x) - y) \\
&= (h_\theta(x) - y) \frac{\partial}{\partial \theta_i} \left[\left(\sum_{j=0}^{k} \theta_j x_j \right) - y \right]
\end{aligned}$$



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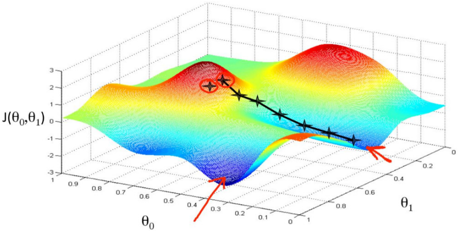

- For a single training sample (x, y)

$$\begin{aligned}
\frac{\partial}{\partial \theta_i} J(\theta) &= \frac{\partial}{\partial \theta_i} \frac{1}{2} (h_\theta(x) - y)^2 \\
&= 2 \cdot \frac{1}{2} (h_\theta(x) - y) \frac{\partial}{\partial \theta_i} (h_\theta(x) - y) \\
&= (h_\theta(x) - y) \frac{\partial}{\partial \theta_i} \left[\left(\sum_{j=0}^{k} \theta_j x_j \right) - y \right] \quad = \quad (h_\theta(x) - y) \cdot x_i
\end{aligned}$$

Gradient descent

- For a single training sample (x, y), $\dfrac{\partial}{\partial \theta_i} J(\theta) = (h_\theta(x) - y) \cdot x_i$

Gradient descent

- For a single training sample (x, y), $\dfrac{\partial}{\partial \theta_i} J(\theta) = (h_\theta(x) - y) \cdot x_i$
- Over the entire training set, $\dfrac{\partial}{\partial \theta_i} J(\theta) = \sum_{j=1}^{n} (h_\theta(x_j) - y_j) \cdot x_j^i$

Gradient descent

- For a single training sample (x, y), $\frac{\partial}{\partial \theta_i} J(\theta) = (h_\theta(x) - y) \cdot x_i$
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Batch gradient descent

- Compute $h_\theta(x_j)$ for entire training set $\{(x_1, y_1), \ldots, (x_n, y_n)\}$
- Adjust each parameter

$$\begin{aligned} \theta_i &= \theta_i - \alpha \frac{\partial}{\partial \theta_i} J(\theta) \\ &= \theta_i - \alpha \cdot \sum_{j=1}^{n} (h_\theta(x_j) - y_j) \cdot x_j^i \end{aligned}$$

- Repeat until convergence

Gradient descent

- For a single training sample (x, y), $\frac{\partial}{\partial \theta_i} J(\theta) = (h_\theta(x) - y) \cdot x_i$
- Over the entire training set, $\frac{\partial}{\partial \theta_i} J(\theta) = \sum_{j=1}^{n} (h_\theta(x_j) - y_j) \cdot x_j^i$

Batch gradient descent

- Compute $h_\theta(x_j)$ for entire training set $\{(x_1, y_1), \ldots, (x_n, y_n)\}$
- Adjust each parameter

$$\begin{aligned}\theta_i &= \theta_i - \alpha \frac{\partial}{\partial \theta_i} J(\theta) \\ &= \theta_i - \alpha \cdot \sum_{j=1}^{n} (h_\theta(x_j) - y_j) \cdot x_j^i\end{aligned}$$

- Repeat until convergence

Stochastic gradient descent

- For each input x_j, compute $h_\theta(x_j)$
- Adjust each parameter — $\theta_i = \theta_i - \alpha \cdot (h_\theta(x_j) - y) \cdot x_j^i$

Gradient descent

- For a single training sample (x, y), $\frac{\partial}{\partial \theta_i} J(\theta) = (h_\theta(x) - y) \cdot x_i$
- Over the entire training set, $\frac{\partial}{\partial \theta_i} J(\theta) = \sum_{j=1}^{n} (h_\theta(x_j) - y_j) \cdot x_j^i$

Batch gradient descent

- Compute $h_\theta(x_j)$ for entire training set $\{(x_1, y_1), \ldots, (x_n, y_n)\}$
- Adjust each parameter

$$\theta_i = \theta_i - \alpha \frac{\partial}{\partial \theta_i} J(\theta)$$

$$= \theta_i - \alpha \cdot \sum_{j=1}^{n} (h_\theta(x_j) - y_j) \cdot x_j^i$$

- Repeat until convergence

Stochastic gradient descent

- For each input x_j, compute $h_\theta(x_j)$
- Adjust each parameter —
  $\theta_i = \theta_i - \alpha \cdot (h_\theta(x_j) - y) \cdot x_j^i$

Pros and cons

Batch gradient descent

- Faster progress for large batch size
- May oscillate indefinitely