Lecture 7: 31 January, 2023

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Data Mining and Machine Learning
January–April 2023

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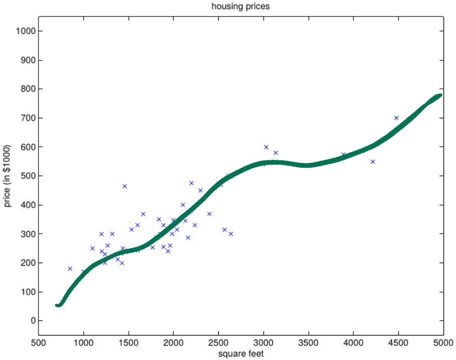
- Scatterplot corresponding to the data
- Fit a function to the points



Linear predictors

- A richer set of input data

Living area (feet^2)	#bedrooms	Price (1000\$s)
2104	3	400
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Linear predictors

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- Simplest case: fit a linear function with parameters $\theta = (\theta_0, \theta_1, \theta_2)$

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

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  $x = (x_1, x_2, \ldots, x_k)$
- 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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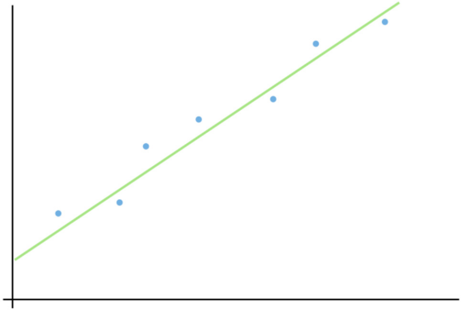
$\theta_0 \cdot x_0 = \theta_0 \cdot 1 = \theta_0$

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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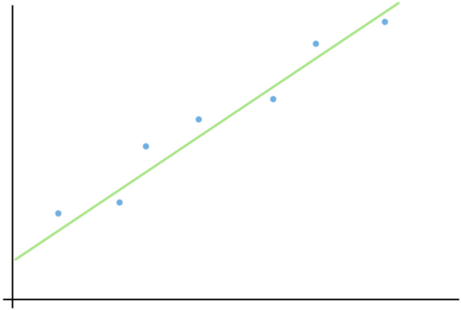

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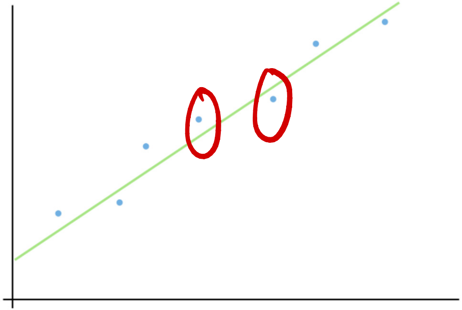
- Define a cost (loss) function

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

prediction actual



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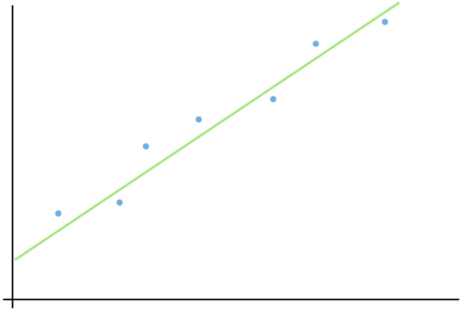
- Essentially, the sum squared error (SSE)



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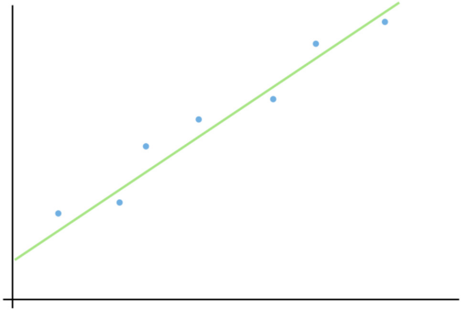
- Essentially, the sum squared error (SSE)
- Divide by n, mean squared error (MSE)



Minimizing SSE

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

Minimizing SSE

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

$$[1\ x_i^1 \cdots x_i^k]\begin{bmatrix} \theta_0 \\ \theta_1 \\ \vdots \\ \theta_k \end{bmatrix}$$

$$h_\theta(x_i) = \theta_0 \cdot 1 + \theta_1 \cdot x_i^1 \cdots + \theta_k x_i^k$$

Minimizing SSE

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

SSE

$X\theta = \begin{bmatrix} h_\theta(x_1) \\ h_\theta(x_2) \\ \vdots \\ h_\theta(x_n) \end{bmatrix}$

$[h_\theta(x_1) - y_1 \ \cdots \ h_\theta(x_n) - y_n]$

Minimizing SSE

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

$(X\theta)^T = \theta^T X^T$

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az^2

$2az$

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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, $\theta = (X^T X)^{-1} X^T y$

$X^T X\theta = X^T y$

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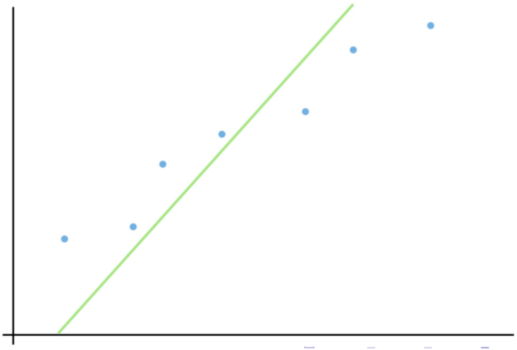

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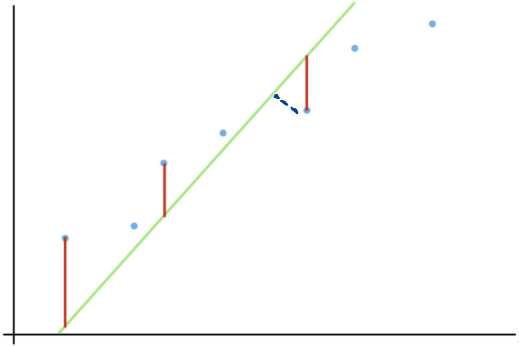

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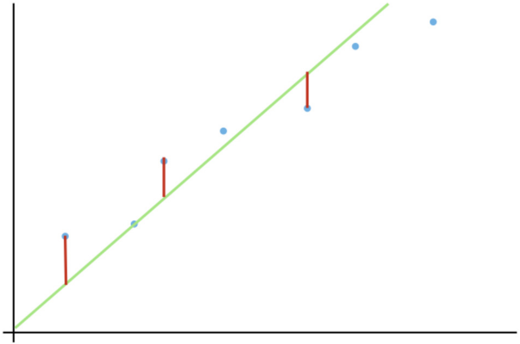
- Keep adjusting the line to reduce SSE



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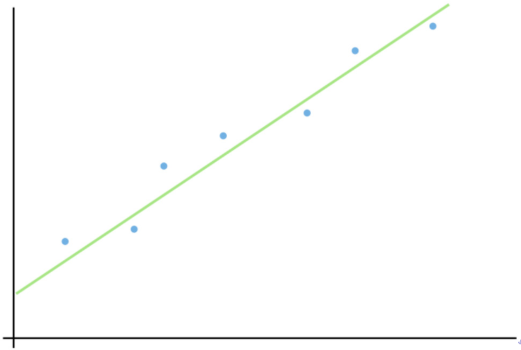
- Stop when we find the best fit line



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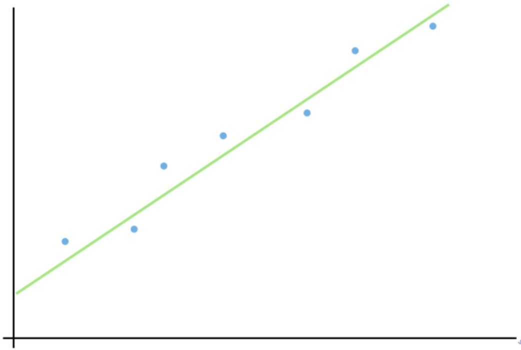
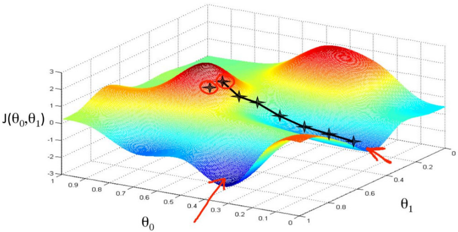
- Keep adjusting the line to reduce SSE
- Stop when we find the best fit line
- How do we adjust the line?



Gradient descent

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



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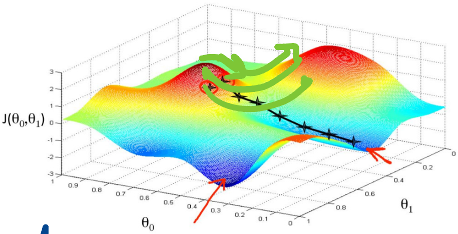
- Adjust each parameter against gradient
  - $\theta_i = \theta_i - \alpha \frac{\partial}{\partial \theta_i} J(\theta)$

user defined parameter



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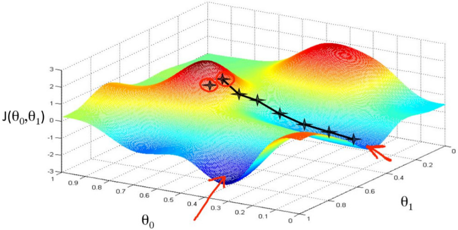
- For a single training sample (x, y)

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



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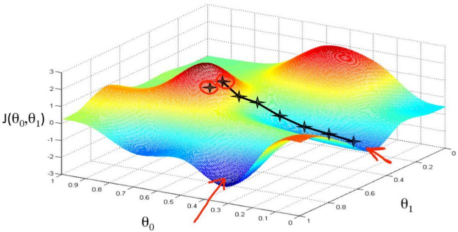
- For a single training sample (x, y)

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

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



$$\frac{d}{dx} f(x)^2 = 2 f(x) \frac{d}{dx} f(x)$$

Gradient descent

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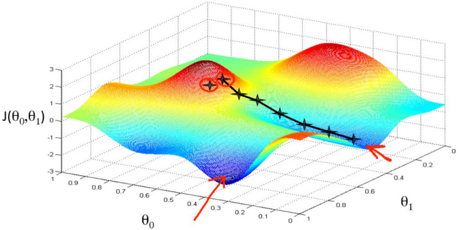

- For a single training sample (x, y)

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

$\theta_i \cdot x_i$

Gradient descent

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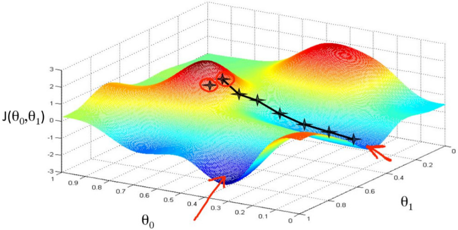

- For a single training sample (x, y)

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

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

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

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

- Repeat until convergence

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 $h_\theta(x_j)$
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Pros and cons

- Faster progress for large batch size
- May oscillate indefinitely

Regression and SSE loss

- Training input is $\{(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)\}$
  - Noisy outputs from a linear function
  - $y_i = \theta^T x_i + \epsilon$
  - $\epsilon \sim \mathcal{N}(0, \sigma^2)$: Gaussian noise, mean 0, fixed variance σ^2
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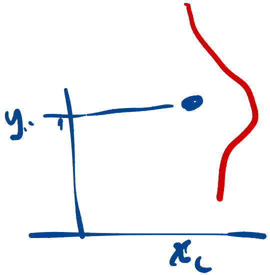

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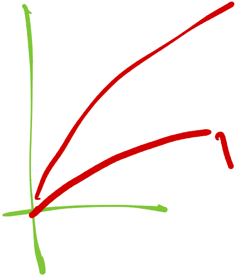

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$$\mathcal{L}(\theta) = \prod_{i=1}^{n} P(y_i \mid x_i; \theta)$$

- Instead, maximize log likelihood

$$\ell(\theta) = \log\left(\prod_{i=1}^{n} P(y_i \mid x_i; \theta)\right) = \sum_{i=1}^{n} \log(P(y_i \mid x_i; \theta))$$

Log likelihood and SSE loss

- $y_i = \mathcal{N}(\mu_i, \sigma^2)$, so $P(y_i \mid x_i; \theta) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(y-\mu_i)^2}{2\sigma^2}}$

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- Log likelihood (assuming natural logarithm)

$$\ell(\theta) = \sum_{i=1}^{n} \log\left(\frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(y-\theta^T x_i)^2}{2\sigma^2}}\right) = n \log\left(\frac{1}{\sqrt{2\pi\sigma^2}}\right) - \sum_{i=1}^{n} \frac{(y-\theta^T x_i)^2}{2\sigma^2}$$

ln

f · g

ln f + ln g

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- Assuming data points are generated by linear function and then perturbed by Gaussian noise, SSE is the “correct” loss function to maximize likelihood