Lecture 6: 27 January, 2026

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Data Mining and Machine Learning
January–April 2026

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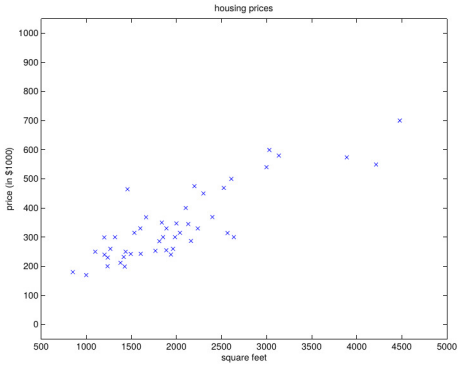
- Scatterplot corresponding to the data
- Fit a function to the points



Linear predictors

- A richer set of input data

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

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 $f(x_1, x_2)$

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$x = (x_1, x_2)$

Find best $\theta_0, \theta_1, \theta_2$

$ax_1 + bx_2 + c$

Linear predictors

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- Input x may have k features $(x_1, x_2, \ldots, x_k)$

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$\theta_0 \cdot x_0 = \theta_0 \cdot 1 = \theta_0$

Linear predictors

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

  $h_\theta(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2$
- Input x may have k features $(x_1, x_2, \ldots, x_k)$
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- For k input features

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

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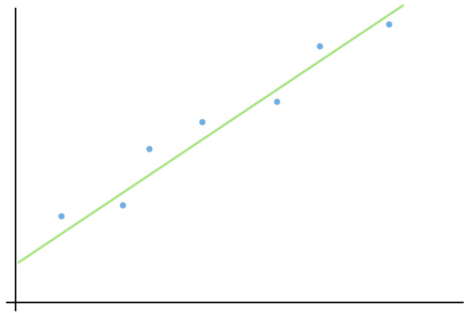
Finding the best fit line

- 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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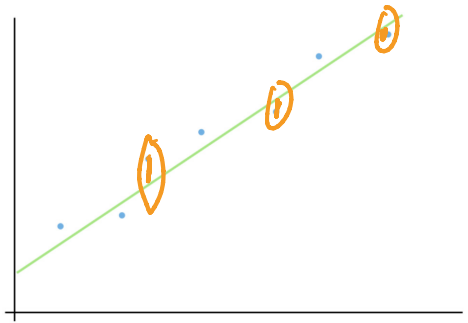

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- Define a cost (loss) function

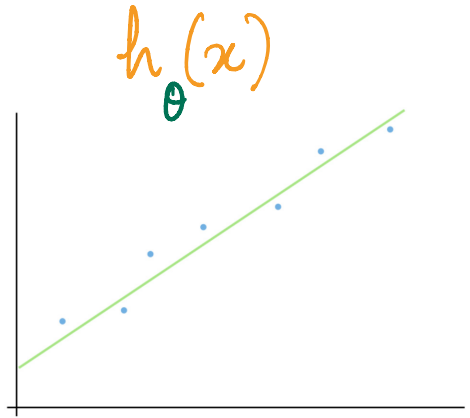
$$J(\theta) = \frac{1}{2} \sum_{i=1}^{n} (h_\theta(x_i) - y_i)^2$$

Technicality

difference

prediction

actual



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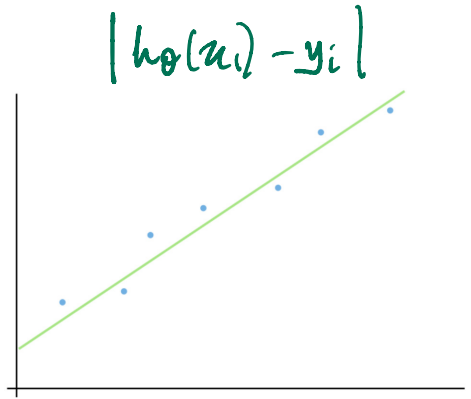
- Essentially, the sum squared error (SSE)



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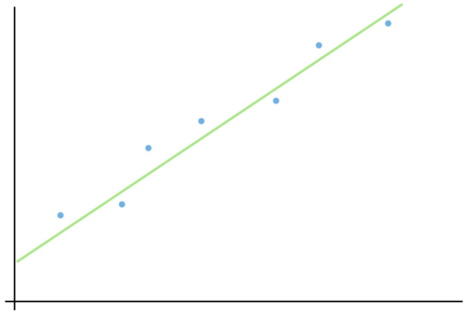
- Essentially, the sum squared error (SSE)
- Divide by n, mean squared error (MSE)



Minimizing SSE

Find θ to minimize $J(\theta)$

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

x_i^0

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

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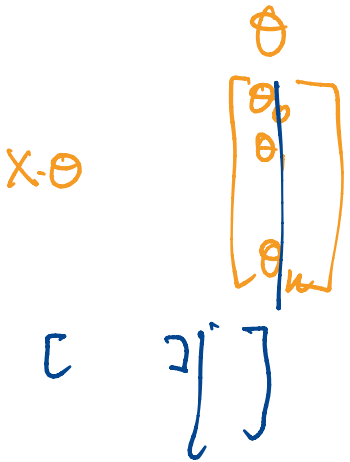
- $J(\theta) = \frac{1}{2}\sum_{i=1}^{n}(h_\theta(x_i) - y_i)^2 = \frac{1}{2}(X\theta - y)^T(X\theta - y)$



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

Minimizing SSE

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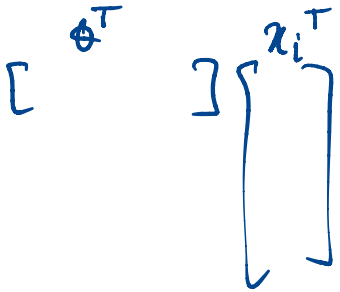
  - Check that $y^T X\theta = \theta^T X^T y = \sum_{i=1}^{n} h_\theta(x_i) \cdot y_i$



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- After differentiating, $X^T X\theta - X^T y = 0$

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

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

Minimizing SSE iteratively

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

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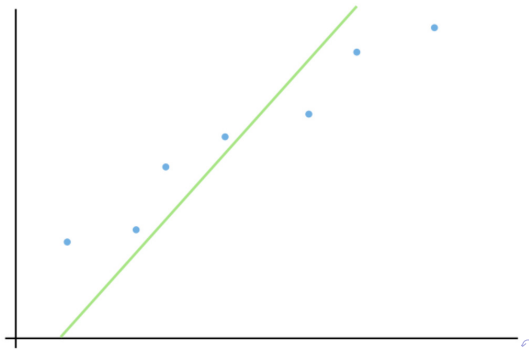

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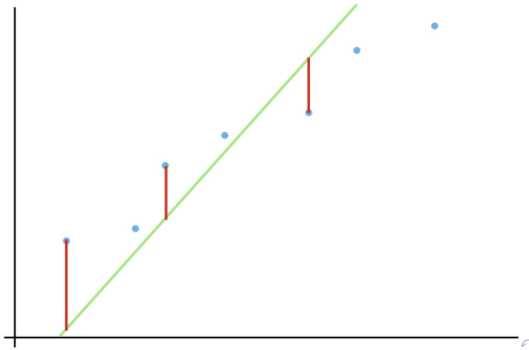

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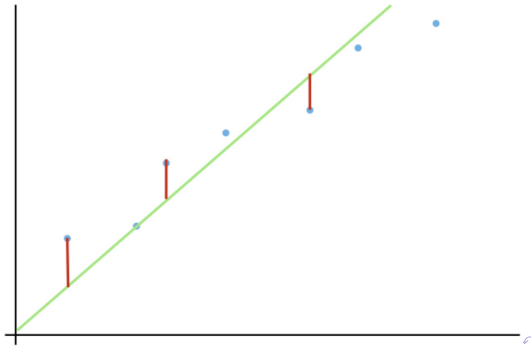
- Iterative approach, make an initial guess
- Keep adjusting the line to reduce SSE



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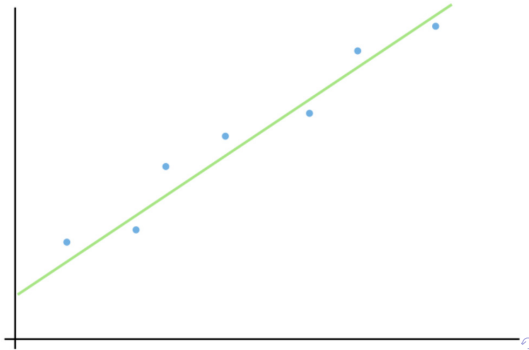
- Keep adjusting the line to reduce SSE
- Stop when we find the best fit line



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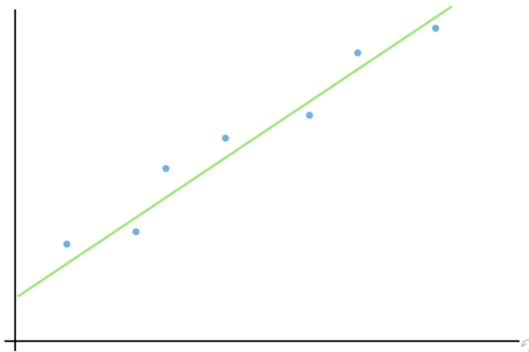
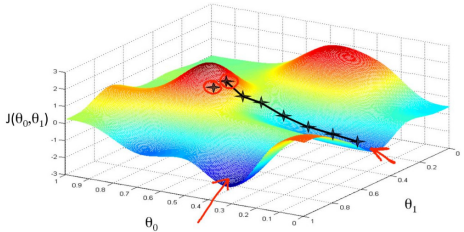
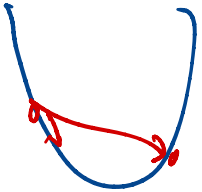
- Keep adjusting the line to reduce SSE
- Stop when we find the best fit line
- How do we adjust the line?



Gradient descent

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

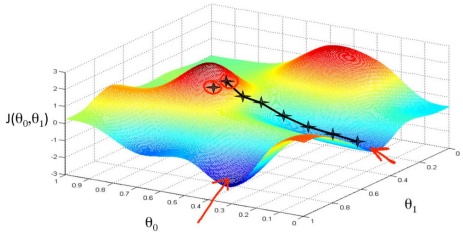




Gradient descent

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

step size



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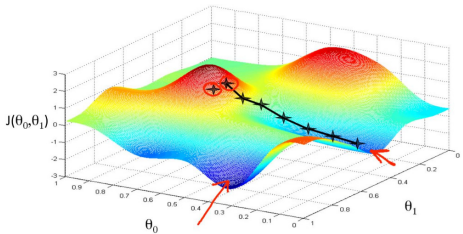
- For a single training sample (x, y)

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



$\theta_0 \cdot 1 + \theta_1 \cdot x$

Gradient descent

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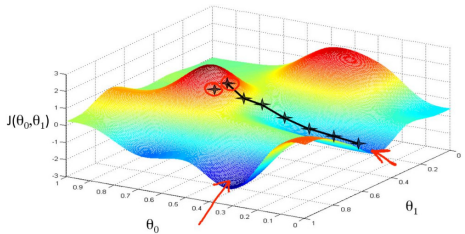
- For a single training sample (x, y)

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



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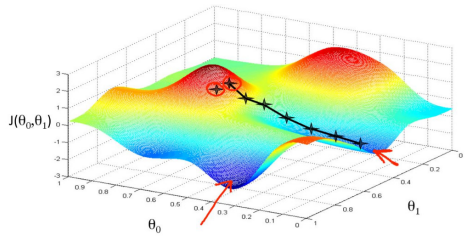
- For a single training sample (x, y)

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



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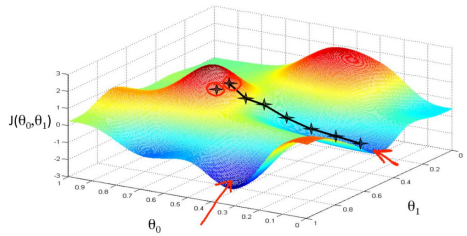
$$\begin{aligned}\frac{\partial}{\partial \theta_i} J(\theta) &= \frac{\partial}{\partial \theta_i} \frac{1}{2} (h_\theta(x) - y)^2 \\ &= 2 \cdot \frac{1}{2} (h_\theta(x) - y) \frac{\partial}{\partial \theta_i} (h_\theta(x) - y) \\ &= (h_\theta(x) - y) \frac{\partial}{\partial \theta_i} \left[\left(\sum_{j=0}^{k}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

input



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actual predictions

Batch gradient descent

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

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

Optimum or $< \varepsilon$-change

- Repeat until convergence

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Stochastic gradient descent

- For each input x_j, compute $h_\theta(x_j)$
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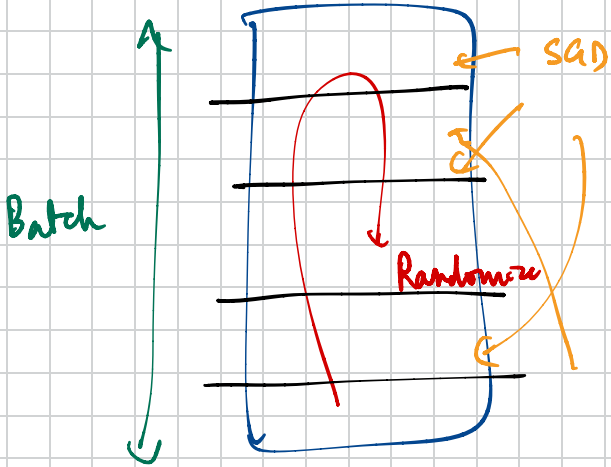
Pros and cons

- Faster progress for large batch size
- May oscillate indefinitely

Mini-batch stochastic gradient descent

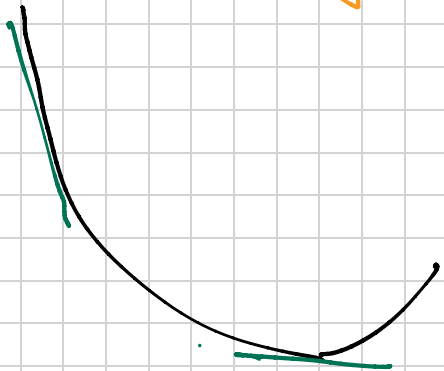


Choosing α?

Cannot be tuned via training data

"Hyperparameter"

Variable α – how?



Regression and SSE loss

- Training input is $\{(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)\}$
  - Outputs are noisy samples from a linear function
  - $y_i = \theta^T x_i + \epsilon$

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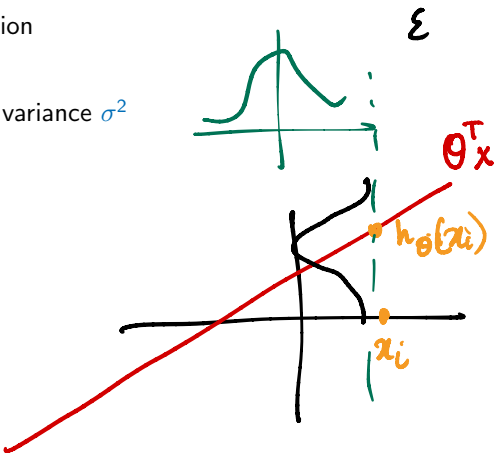

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- Likelihood — probability of current observation given θ

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

Estimating p(heads) for a coin

1000 tosses → 563 heads
437 tails

p(heads) ? = 0.563 Why ?

p

Suppose I had coins with different values of p

Given p → prob(563/1000 heads)

Maximum likelihood

Likelihood

- How good is our estimate?

Likelihood

- How good is our estimate?
- Want Maximum Likelihood Estimator (MLE)
  - Find θ that maximizes $\mathcal{L}(\theta) = \prod_{i=1}^{n} P(y_i \mid x_i; \theta)$

$\Rightarrow$ loss function choice