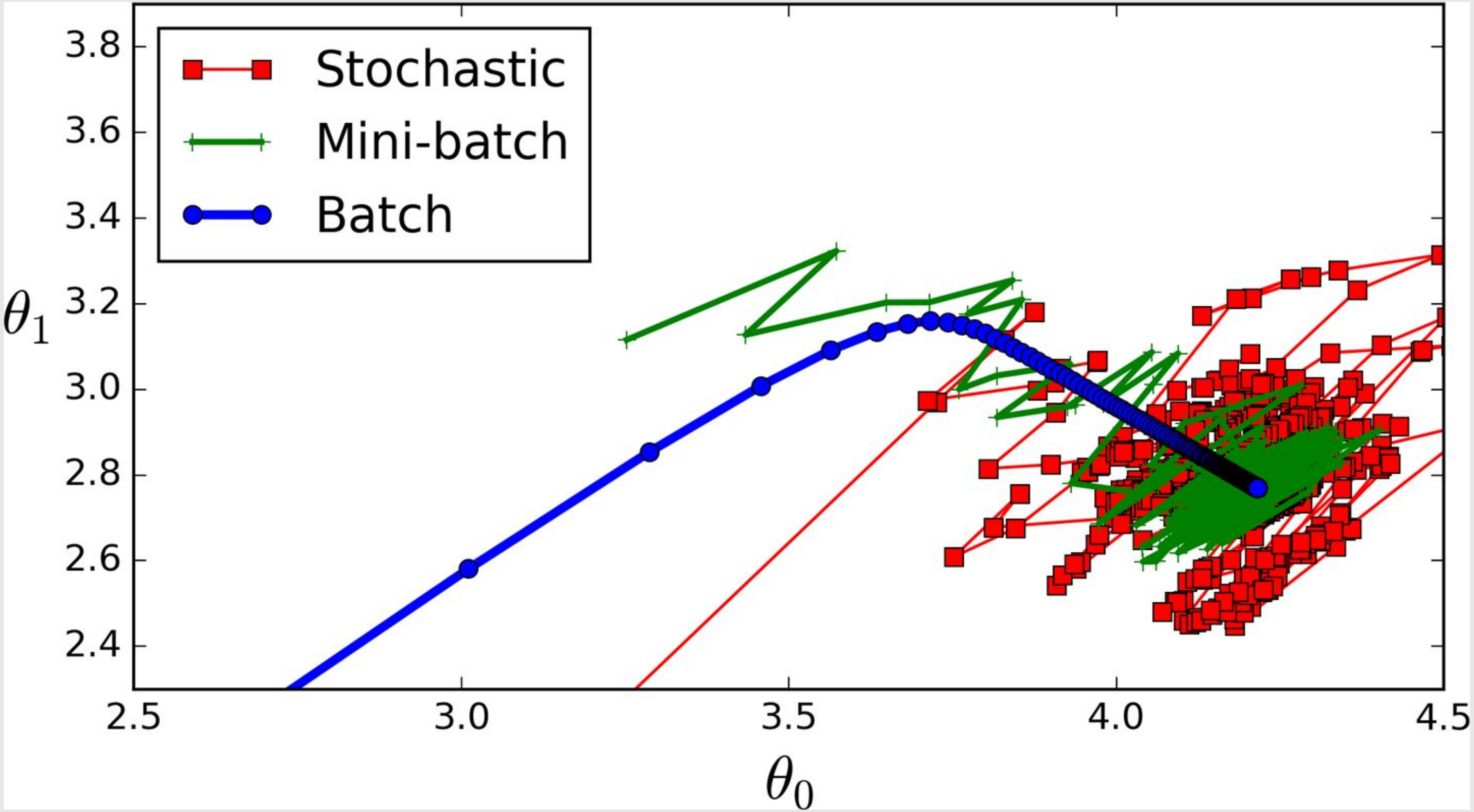
Recall from last time ...

Batch vs. Stochastic vs. Mini-batch



http://ruder.io/optimizing-gradient-descent

Sebastian Ruder

I'm a PhD student in Natural Language Processing and a research scientist at AYLIEN. I blog about Machine Learning, Deep Learning, NLP, and startups.

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- Papers
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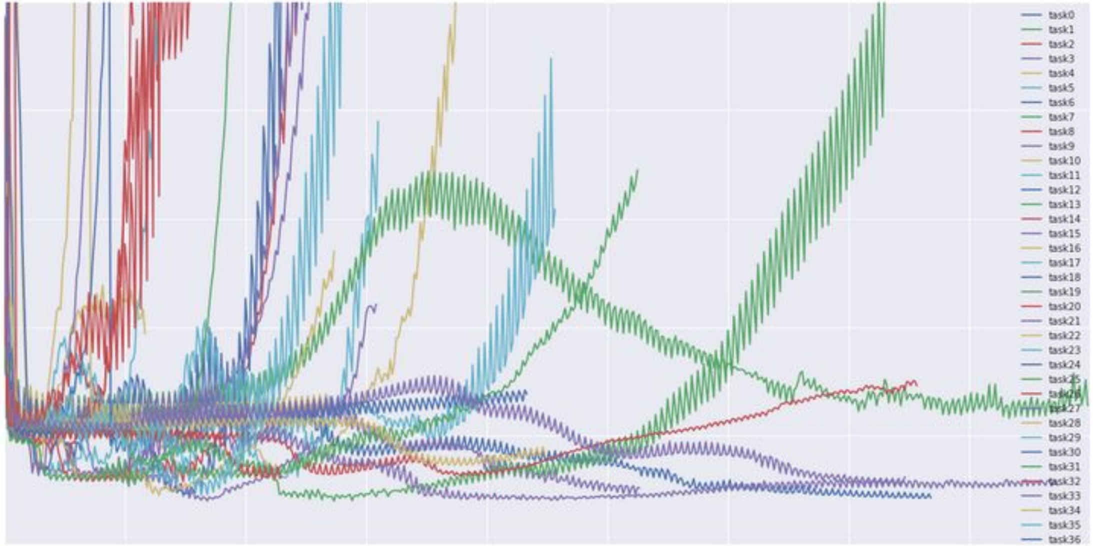
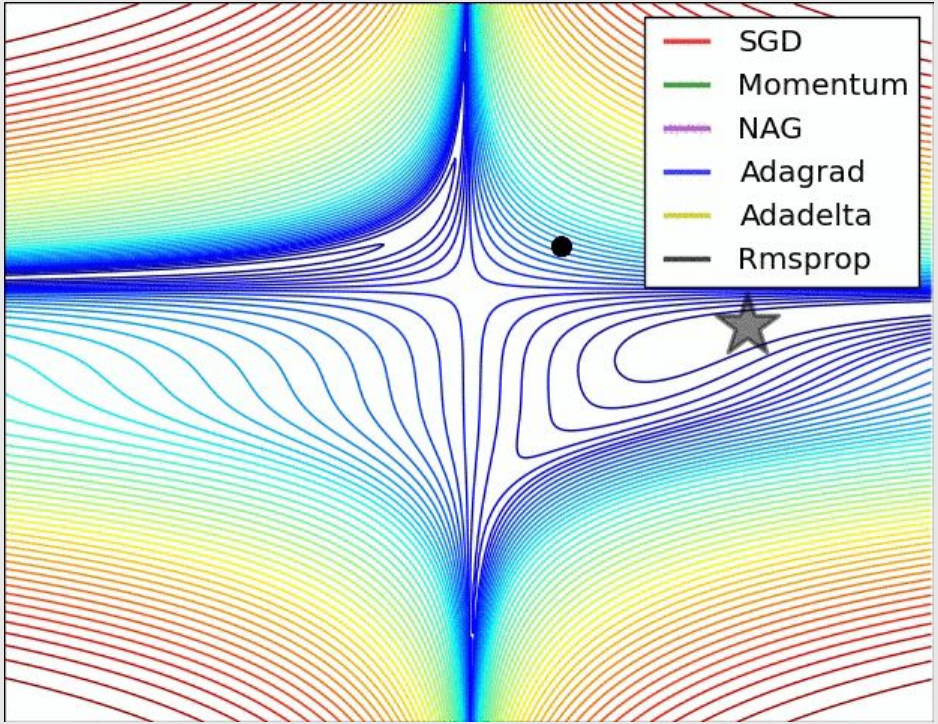
- Newsletter
- FAQ
- Progress

19 Jan 2016 in OPTIMIZATION DEEP LEARNING SGD ~ 25 min read.



An overview of gradient descent optimization algorithms



Credit: Alec Radford.

Linear Regression

Machine Learning and Pattern Recognition

(Largely based on slides from Andrew Ng)

Prof. Sandra Avila
Institute of Computing (IC/Unicamp)

MC886/MO444, August 16, 2018

Today's Agenda

- Linear Regression with One Variable
  - Model Representation
  - Cost Function
  - Gradient Descent
- Linear Regression with Multiple Variables
  - Gradient Descent for Multiple Variables
  - **Feature Scaling**
  - **Learning Rate**
  - **Features and Polynomial Regression**
  - **Normal Equation**

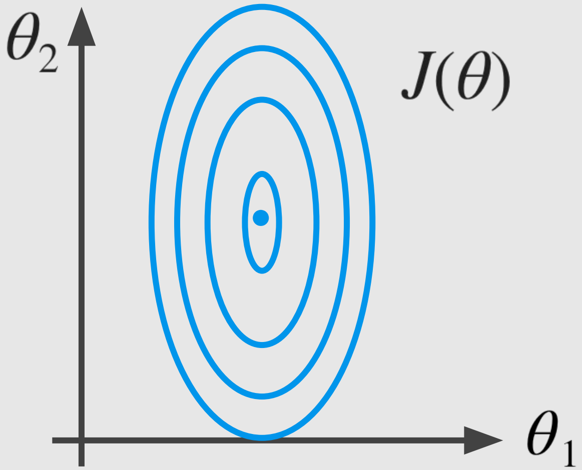
Feature Scaling

Feature Scaling

Idea: Make sure features are on similar scale.

E.g. x_1 = size (0–2000 feet^2)

x_2 = number of bedrooms (1–5)



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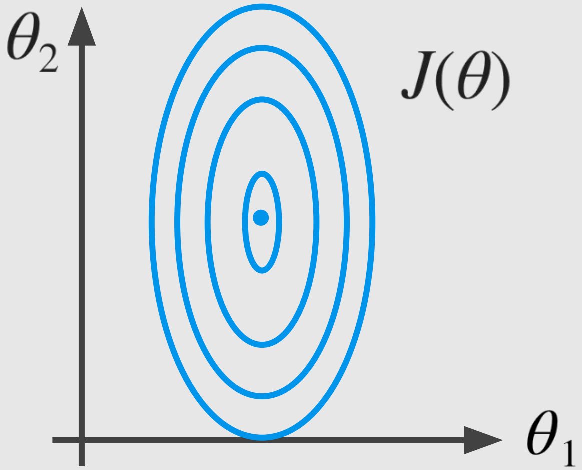

$$x_1 = \frac{\text{size (feet}^2\text{)}}{2000}$$

$$x_2 = \frac{\text{number of bedrooms}}{5}$$

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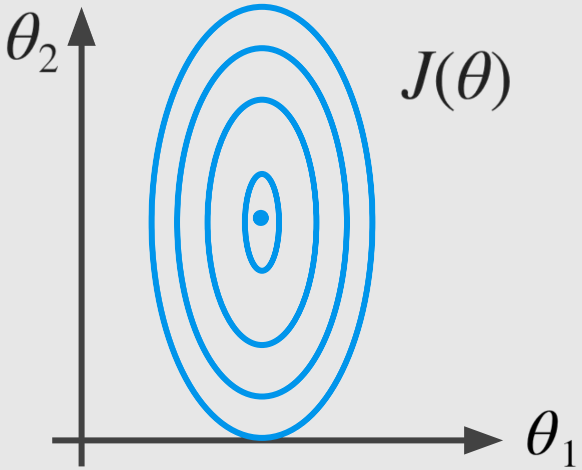

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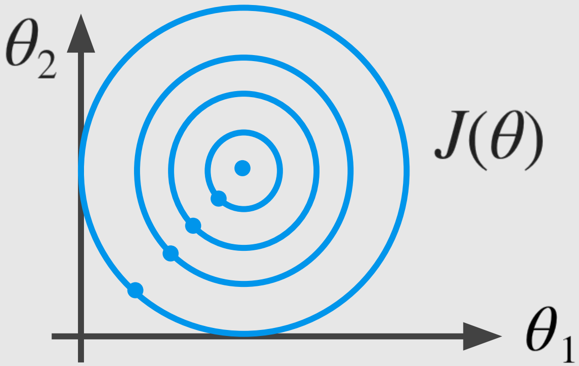

Feature Scaling

Get every feature into approximately a $-1 \leq x_i \leq 1$ range.

Mean Normalization

Replace x_i with $x_i - \mu_i$ to make features have approximately zero mean (do not apply to $x_0 = 1$).

E.g. $x_1 = \dfrac{\text{size} - 1000}{2000}$ ➡ $-0.5 \leq x_1 \leq 0.5$

$x_2 = \dfrac{\#\text{bedrooms} - 2.5}{5}$ ➡ $-0.5 \leq x_2 \leq 0.5$

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$x_2 = \dfrac{\text{\#bedrooms} - 2.5}{5}$ ➡ $-0.5 \leq x_2 \leq 0.5$

$$x_1 = \frac{x_1 - \mu_1}{s_1} \qquad x_2 = \frac{x_2 - \mu_2}{s_2}$$

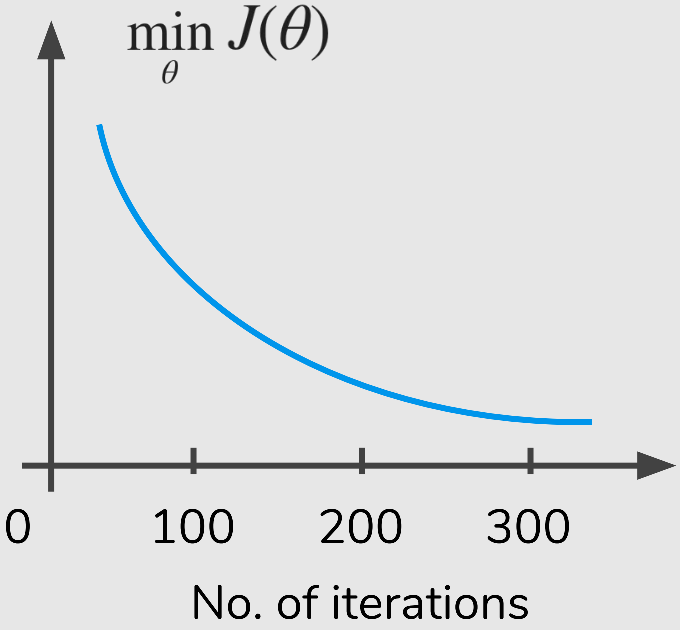
Learning Rate

Gradient Descent

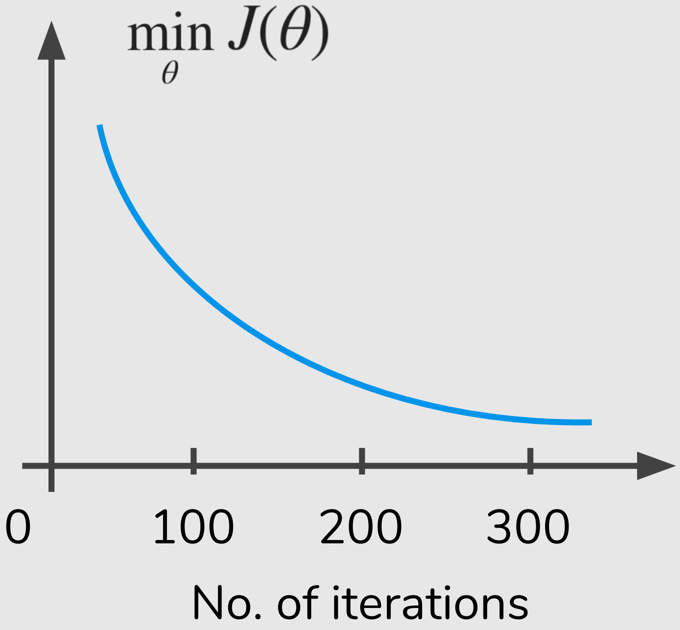
$$\theta_j := \theta_{\mathrm{j}} - \alpha \frac{\partial}{\partial \theta_j} J(\theta)$$

- “Debugging” : How to make sure gradient descent is working correctly.
- How to choose learning rate α.

Making sure gradient descent is working correctly.



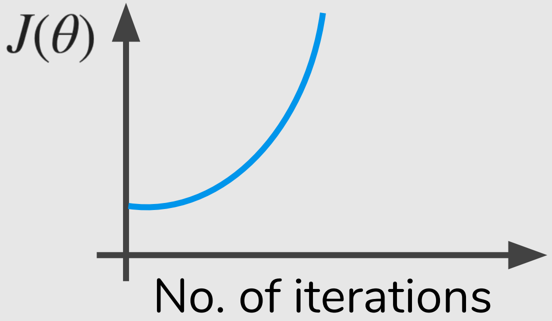
Making sure gradient descent is working correctly.



Example automatic convergence test:

Declare convergence if $J(\theta)$ decreases by less than 10^{-3} in one iteration.

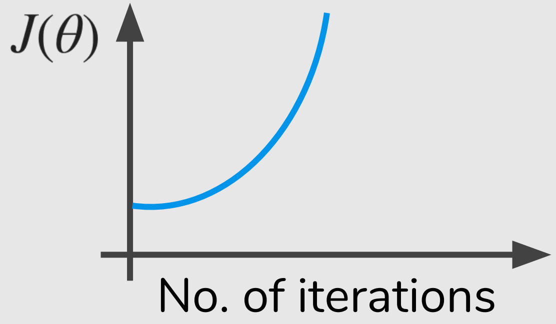
Making sure gradient descent is working correctly.



Gradient descent not working.

Use smaller α.

Making sure gradient descent is working correctly.



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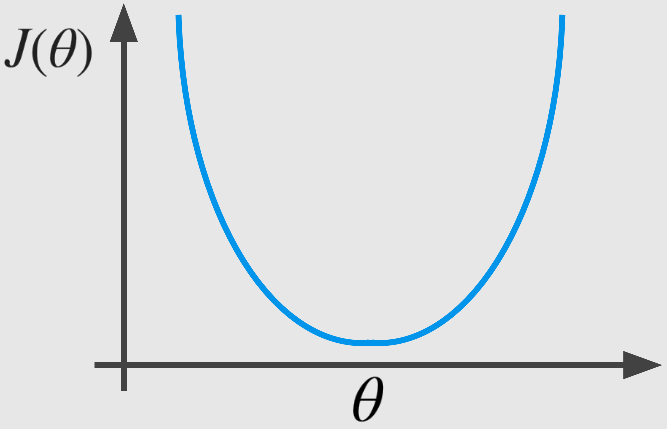

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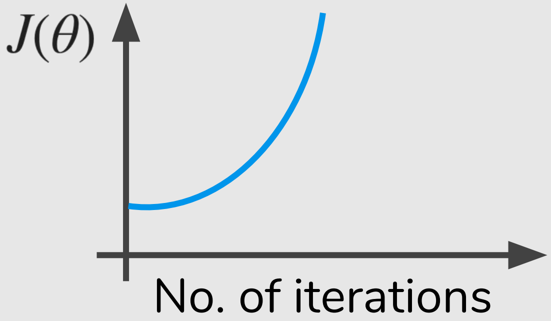

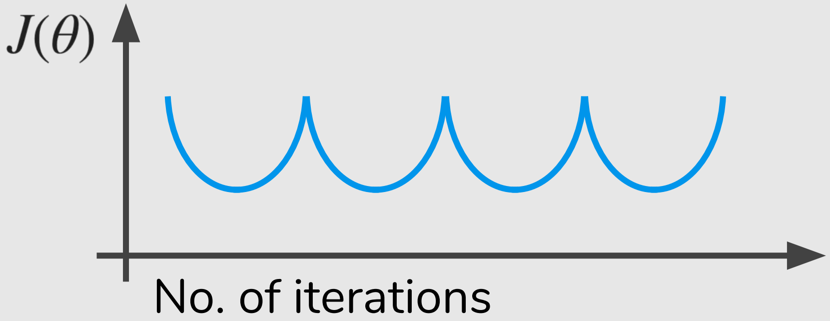

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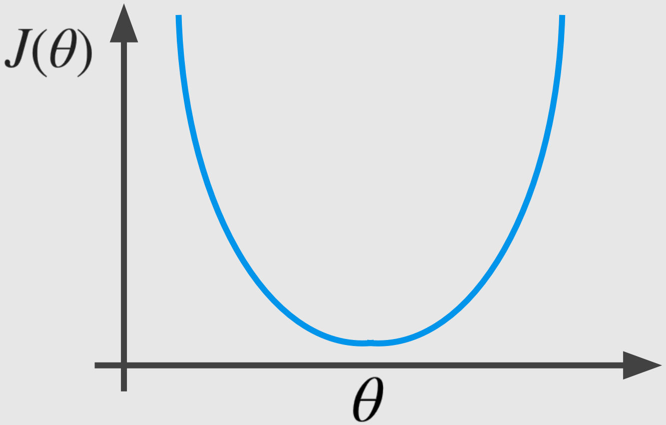

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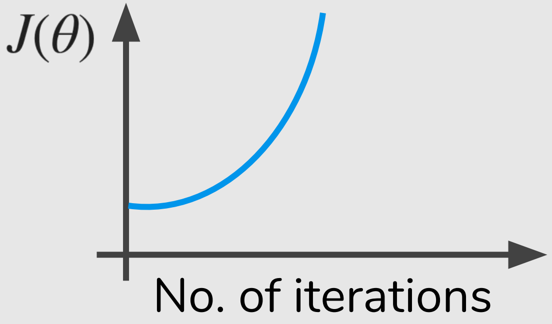

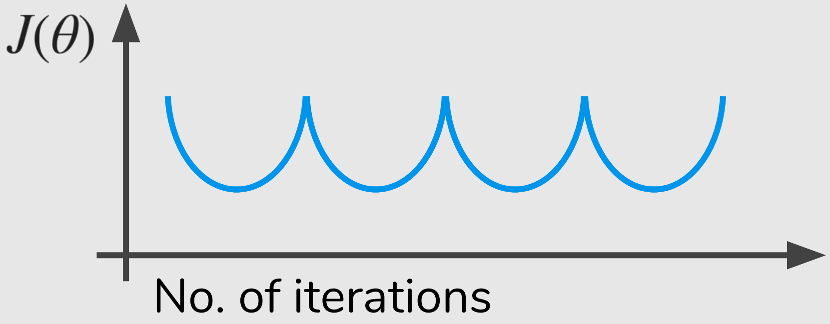

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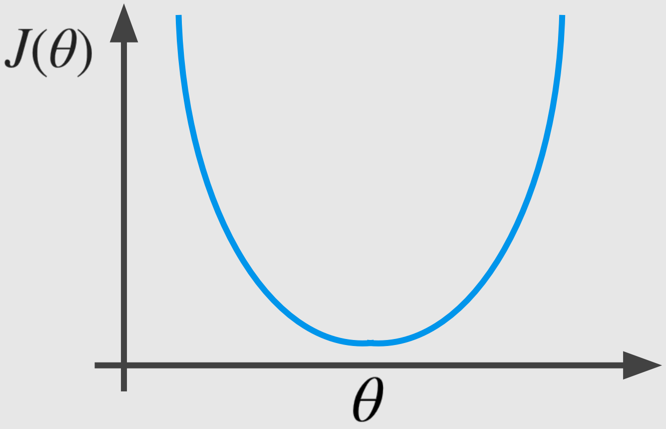

- For sufficiently small α, $J(\theta)$ should decrease on every iteration.
- But if α is too small, gradient descent can be slow to converge.

Summary

- If α is too small: slow convergence.
- If α is too large: $J(\theta)$ may not decrease on every iteration; may not converge.

To choose α, try

$$\dots, 0.001, \dots, 0.01, \dots, 0.1, \dots, 1, \dots$$

Features and Polynomial Regression

Housing prices prediction

$$h_\theta(x) = \theta_0 + \theta_1 \times \text{frontage} + \theta_2 \times \text{depth}$$

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Housing prices prediction

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$$x_1 \qquad\qquad x_2$$

Area $x = \text{frontage} \times \text{depth}$

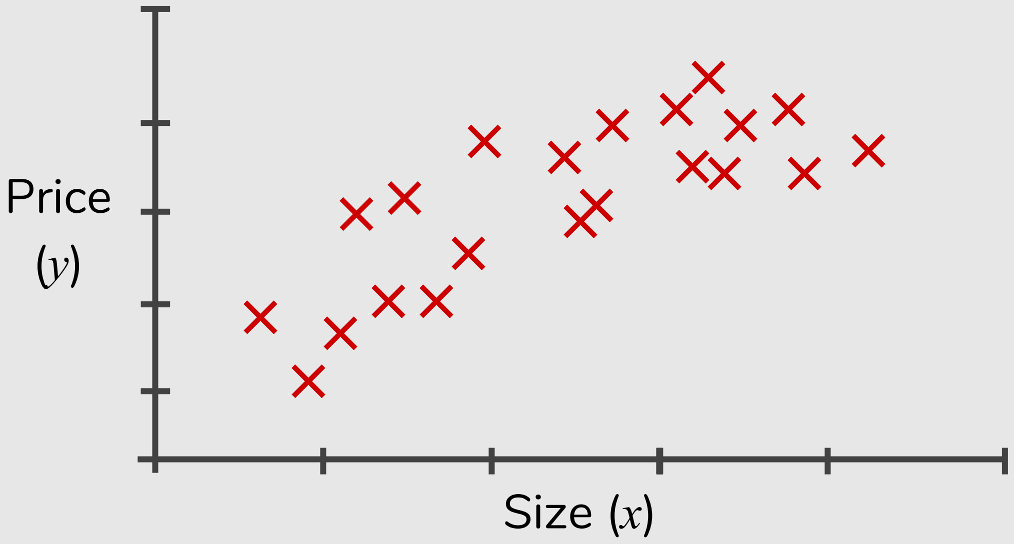
Housing prices prediction

$$h_\theta(x) = \theta_0 + \theta_1 \times \underbrace{\text{frontage}}_{x_1} + \theta_2 \times \underbrace{\text{depth}}_{x_2}$$

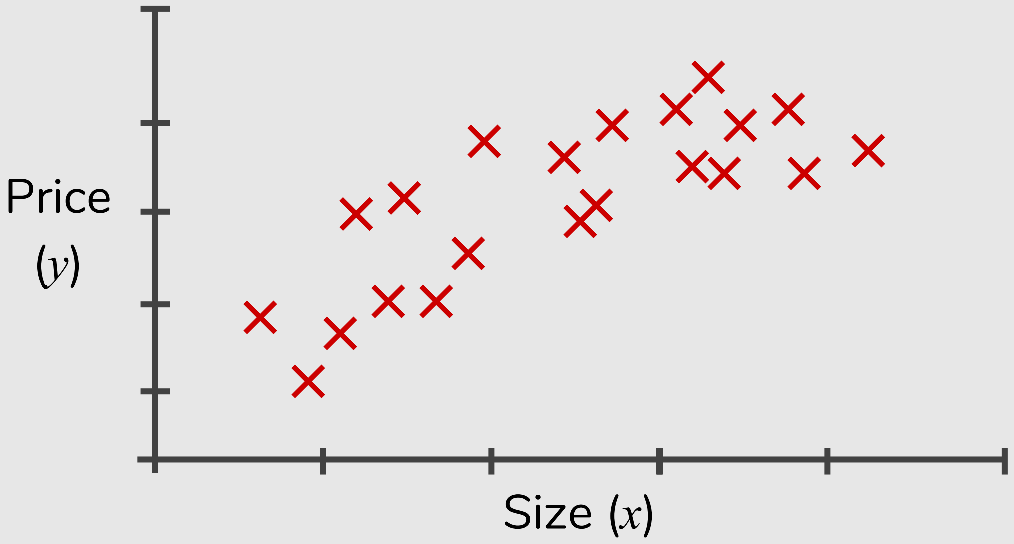
Area x = frontage $\times$ depth

$$h_\theta(x) = \theta_0 + \theta_1 x$$

Polynomial Regression

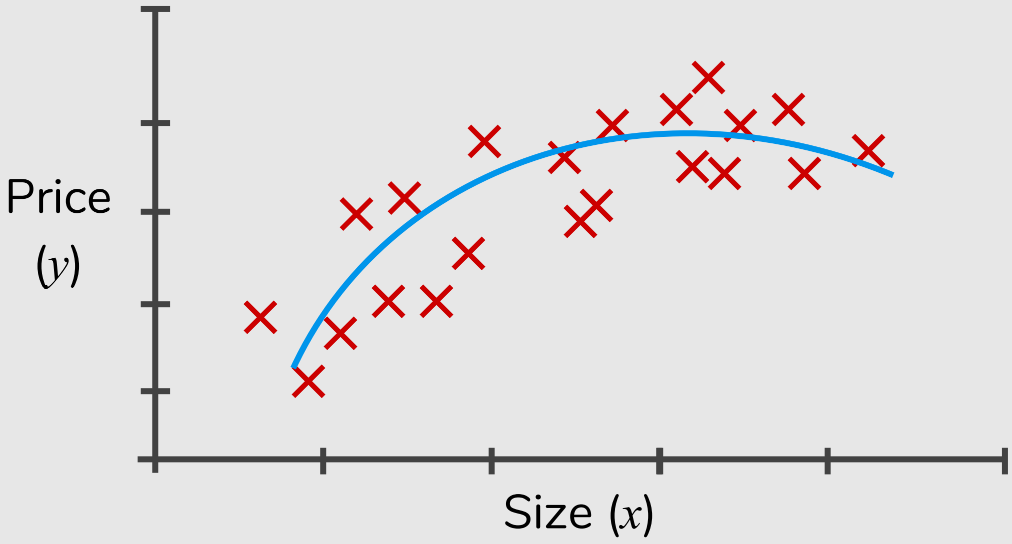


Polynomial Regression



$$\theta_0 + \theta_1 x + \theta_2 x^2$$

Polynomial Regression



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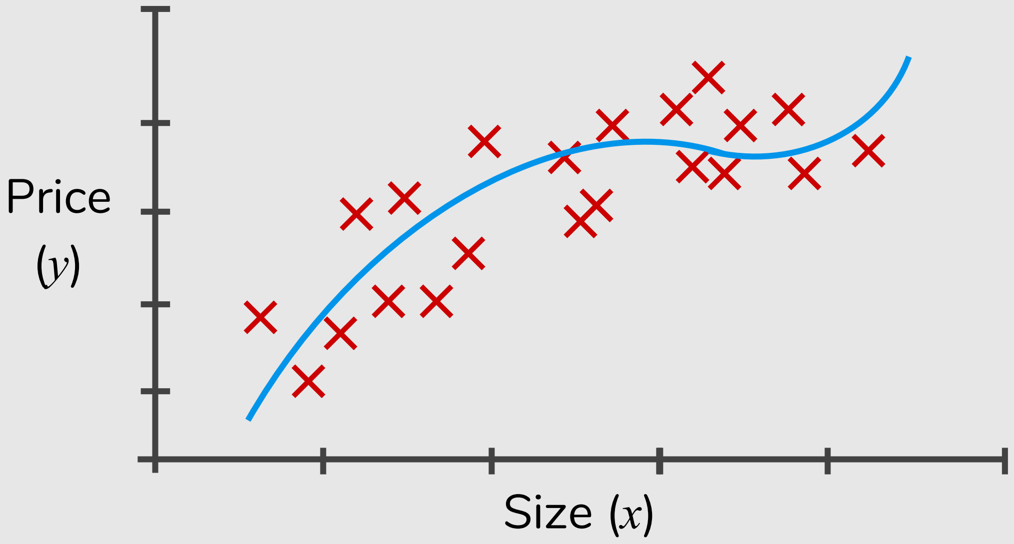

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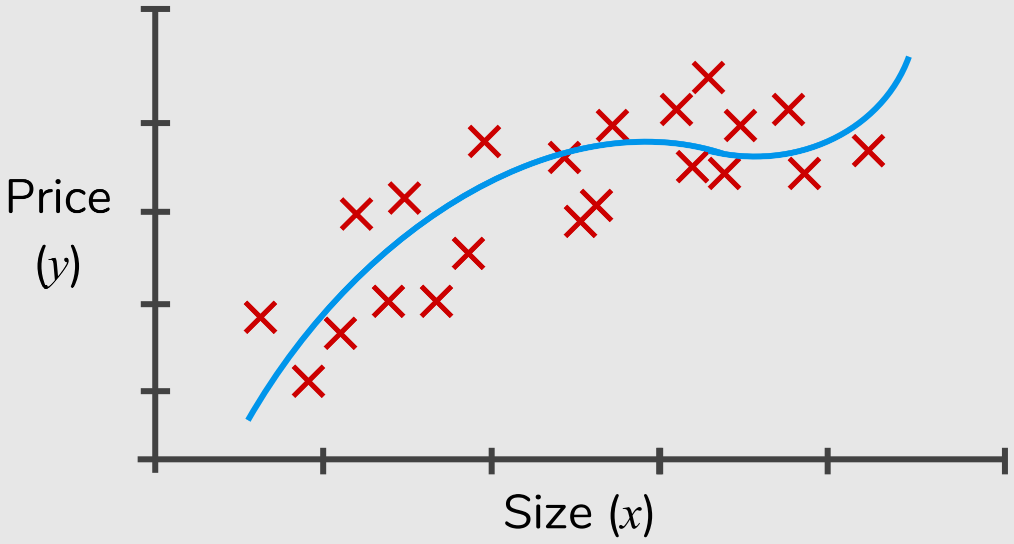


$$\theta_0 + \theta_1 x + \theta_2 x^2$$

$$\theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3$$

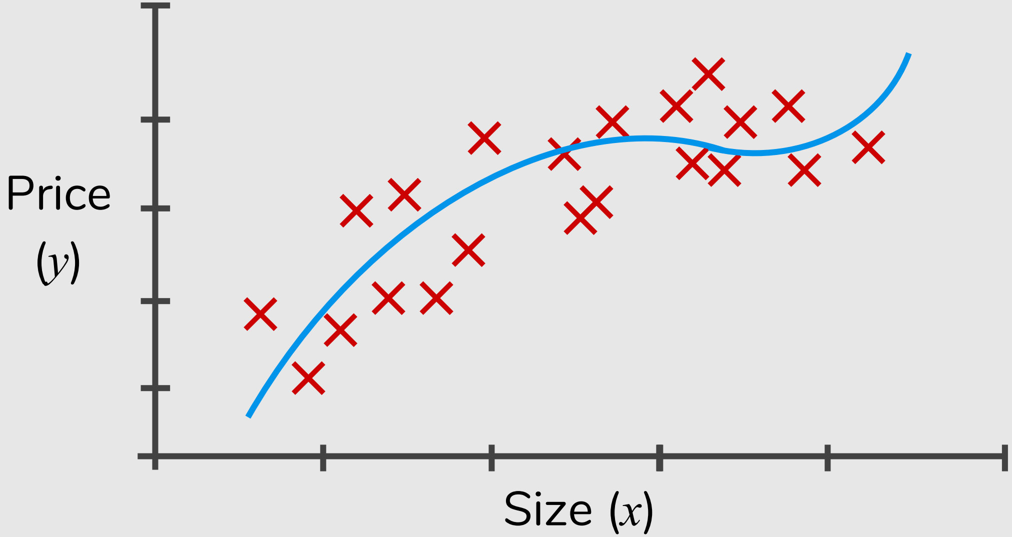
$$x_1 = (\text{size})$$

$$x_2 = (\text{size})^2$$

$$x_3 = (\text{size})^3$$

$$\begin{aligned} h_\theta(x) &= \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_3 \\ &= \theta_0 + \theta_1(\text{size}) + \theta_2(\text{size})^2 + \theta_3(\text{size})^3 \end{aligned}$$

Polynomial Regression



$$\theta_0 + \theta_1 x + \theta_2 x^2$$

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$$x_1 = (\text{size}) \quad : 1-1{,}000$$

$$x_2 = (\text{size})^2 \quad : 1-1{,}000{,}000$$

$$x_3 = (\text{size})^3 \quad : 1-10^9$$

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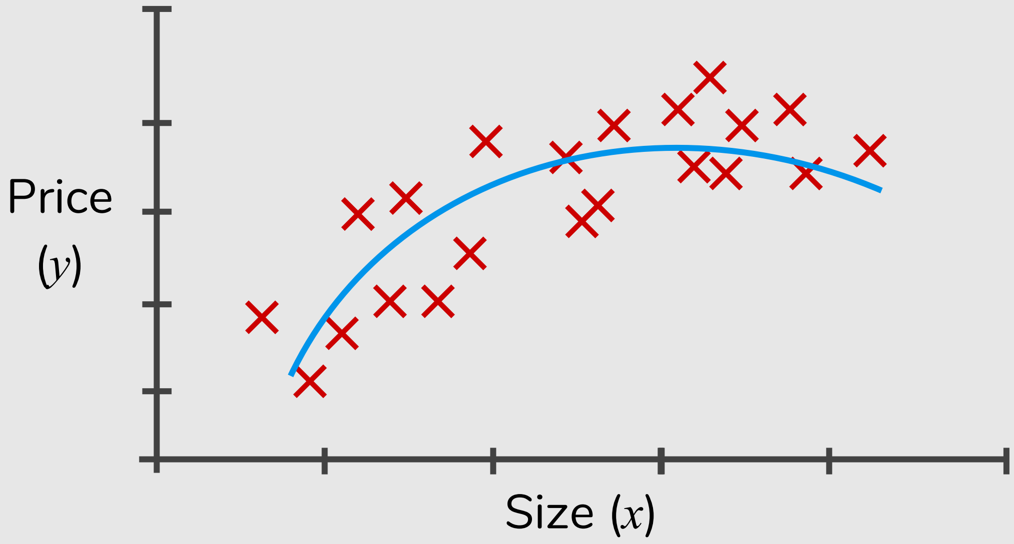
Choice of Features



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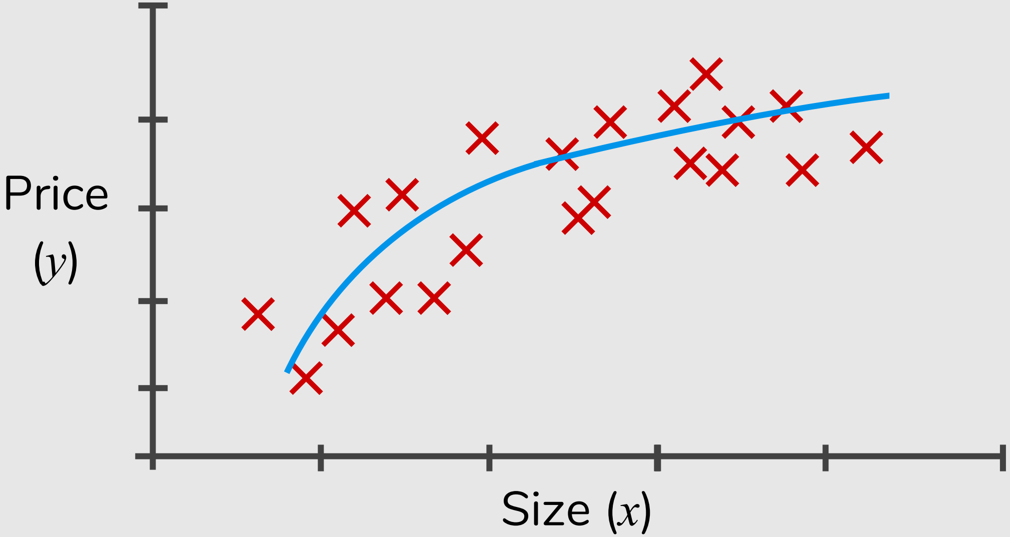
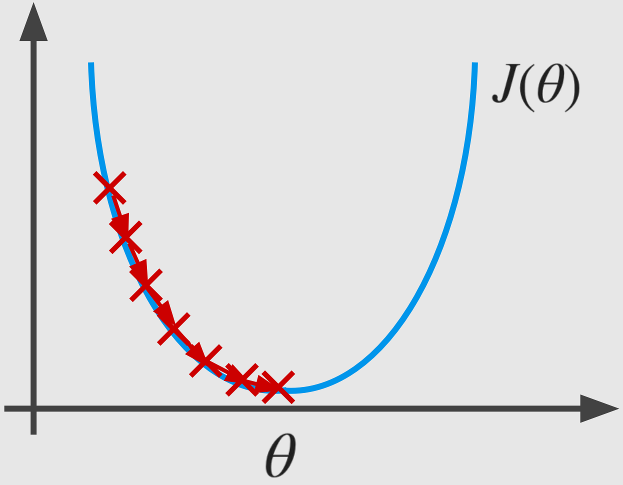


$$h_\theta(x) = \theta_0 + \theta_1(\text{ size }) + \theta_2(\text{ size })^2$$

$$h_\theta(x) = \theta_0 + \theta_1(\text{ size }) + \theta_2\sqrt{(\text{ size })}$$

Normal Equation

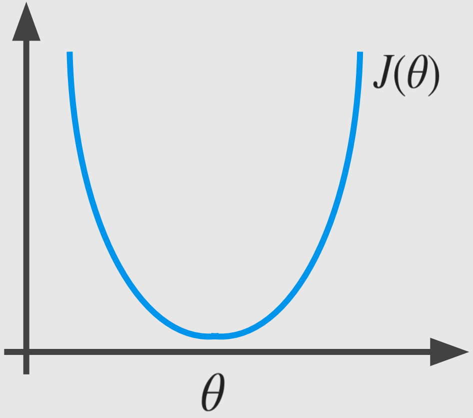
Gradient Descent



Normal equation: Method to solve θ **analytically**.

Intuition: If 1D ($\theta \in \mathbb{R}$)

$$J(\theta) = a\theta^2 + b\theta + c$$



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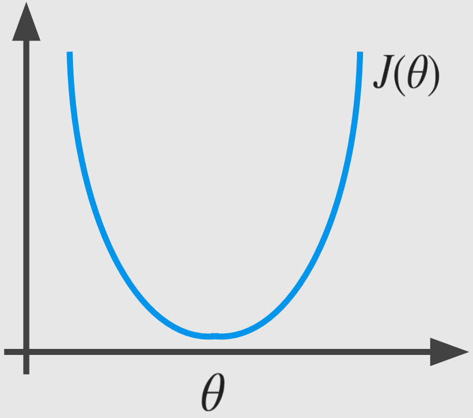
$$\frac{d}{d\theta} J(\theta) = \ldots = 0$$ Solve for θ



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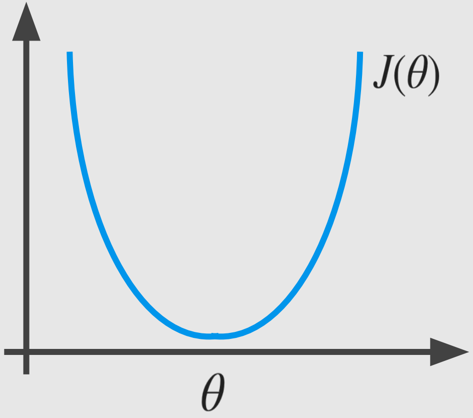

$\theta \in \mathbb{R}^{n+1}$ $$J(\theta_0, \theta_1, \ldots, \theta_n) = \frac{1}{2m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)})^2$$

$$\frac{\partial}{\partial \theta_j} J(\theta) = \ldots = 0$$ Solve for $\theta_0, \theta_1, \ldots, \theta_n$

Examples: $m = 4$.

Size (feet^2) x_1	Number of bedrooms x_2	Number of floors x_3	Age of home (years) x_4	Price ($) in 1000's y
2104	5	1	45	460
1416	3	2	40	232
1534	3	2	30	315
852	2	1	36	178

Examples: $m = 4$.

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

m examples $(x^{(1)}, y^{(1)}), \ldots, (x^{(m)}, y^{(m)})$ and n features

$$x^{(i)} = \begin{bmatrix} x_0^{(i)} \\ x_1^{(i)} \\ x_2^{(i)} \\ \vdots \\ x_n^{(i)} \end{bmatrix} \in \mathbb{R}^{n+1}$$

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E.g. $x^{(i)} = \begin{bmatrix} 1 \\ x_1^{(i)} \end{bmatrix}$

m **examples** $(x^{(1)}, y^{(1)}), \ \ldots, \ (x^{(m)}, y^{(m)})$ **and** n **features**

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E.g. $x^{(i)} = \begin{bmatrix} 1 \\ x_1^{(i)} \end{bmatrix}$ $\quad X = \begin{bmatrix} 1 & x_1^{(1)} \\ \vdots & \vdots \\ 1 & x_m^{(1)} \end{bmatrix}_{m \times 2}$

m **examples** $(x^{(1)}, y^{(1)}), \ldots, (x^{(m)}, y^{(m)})$ **and** n **features**

$$X = \begin{bmatrix} \text{——} & (x^{(1)})^{\mathrm{T}} & \text{——} \\ \text{——} & (x^{(2)})^{\mathrm{T}} & \text{——} \\ \text{——} & \vdots & \text{——} \\ \text{——} & (x^{(m)})^{\mathrm{T}} & \text{——} \end{bmatrix} \qquad y = \begin{bmatrix} y^{(1)} \\ y^{(2)} \\ \vdots \\ y^{(m)} \end{bmatrix}$$

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

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Deriving the Normal Equation using matrix calculus ...

☞ https://ayearofai.com/rohan-3-deriving-the-normal-equation-using-matrix-calculus-1a1b16f65dda

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What if $X^T X$ is noninvertible?

What if $X^T X$ is noninvertible?

The common causes might be having :

- Redundant features, where two features are very closely related (i.e. they are linearly dependent).
- Too many features (e.g. $m \leq n$). In this case, delete some features or use “regularization”.

Gradient Descent

- Need to choose α.
- Needs many iterations.

Normal Equation

- No need to choose α.
- Don't need to iterate.

m examples and n features

Gradient Descent

- Need to choose α.
- Needs many iterations.
- Works well even when n is large.

Normal Equation

- No need to choose α.
- Don't need to iterate.
- Need to compute $(X^T X)^{-1} \rightarrow O(n^3)$.
- Slow if n is very large.

m examples and n features

References

Machine Learning Books

- Hands-On Machine Learning with Scikit-Learn and TensorFlow, Chap. 2 & 4
  https://www.oreilly.com/library/view/hands-on-machine-learning/9781491962282/ch04.html
- Pattern Recognition and Machine Learning, Chap. 3

Machine Learning Courses

- https://www.coursera.org/learn/machine-learning, Week 1 & 2