DS 4400

Machine Learning and Data Mining I
Spring 2022

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Today's Outline

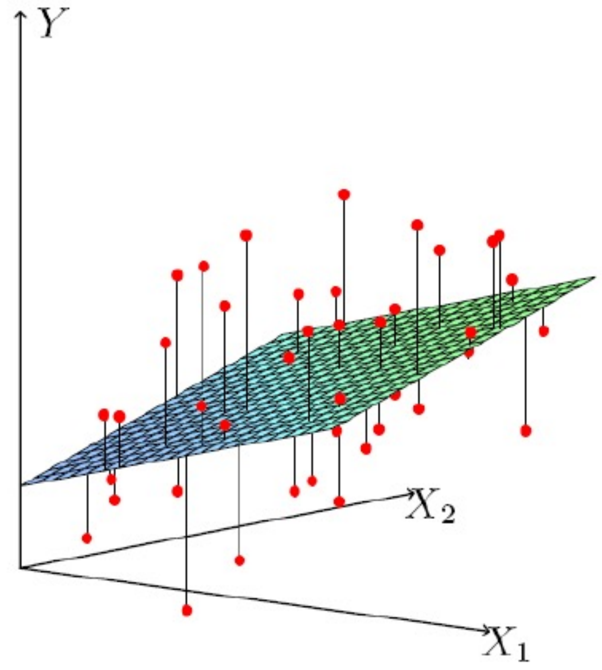
- Gradient descent
  - General optimization algorithm
  - Instantiation for linear regression
  - Issues with gradient descent
  - Comparison with closed-form solution
- Non-linear regression
  - Polynomial regression
  - Cubic, spline regression

Multiple Linear Regression

- Dataset: $x_i \in R^d, y_i \in R$
- Hypothesis $h_\theta(x) = \theta^T x$
- MSE $= \frac{1}{N}\sum (\theta^T x_i - y_i)^2$ Loss / cost

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

Closed-form optimum solution for linear regression



Recap Linear Regression

- Optimal solution to min MSE
  - Use vectorization for compact representation
- Advantages of linear regression
  - Simplicity and interpretability
  - Closed-form optimal solution (depends uniquely on training data)
- Limitations of linear regression
  - Small capacity in number of parameters (d+1)
  - Does not fit well non-linear data
- Practical issues
  - Feature standardization
  - Outliers
  - Categorical features

Practical issues: Categorical features

- Predict credit card balance
  - Age
  - Income
  - Number of cards
  - Credit limit
  - Credit rating
- Categorical variables
  - Student (Yes/No)
  - State (50 different levels)

How to generate numerical representations of these?

Indicator Variables

- One-hot encoding
- Binary (two-level) variable
  - Add new feature $x_j = 1 \text{ if student and } 0 \text{ otherwise}$
- Multi-level variable
  - State: 50 values
  - $x_{MA} = 1 \text{ if State} = \text{MA and } 0, \text{otherwise}$
  - $x_{NY} = 1 \text{ if State} = \text{NY and } 0, \text{otherwise}$
  - …
  - How many indicator variables are needed?
- Disadvantages: data becomes too sparse for large number of levels
  - Will discuss feature selection later in class

Training phase of most ML

- Input: labeled data
- Define objective / loss metric
  - MSE for regression
  - Specific loss functions for classification
- Run an optimization procedure to minimize loss (error) on training data
- Output: trained model that best fits the training data

How to optimize loss functions?

- Dataset: $x_i \in R^d, y_i \in R$
- Hypothesis $h_\theta(x) = \theta^T x$
- $J(\theta) = \frac{1}{N} \sum (\theta^T x_i - y_i)^2$ Loss / cost for regression
- General method to optimize a multi-variate function
  - Practical and efficient
  - Generally applicable to different loss functions
  - Convergence guarantees for certain loss functions (e.g., convex)

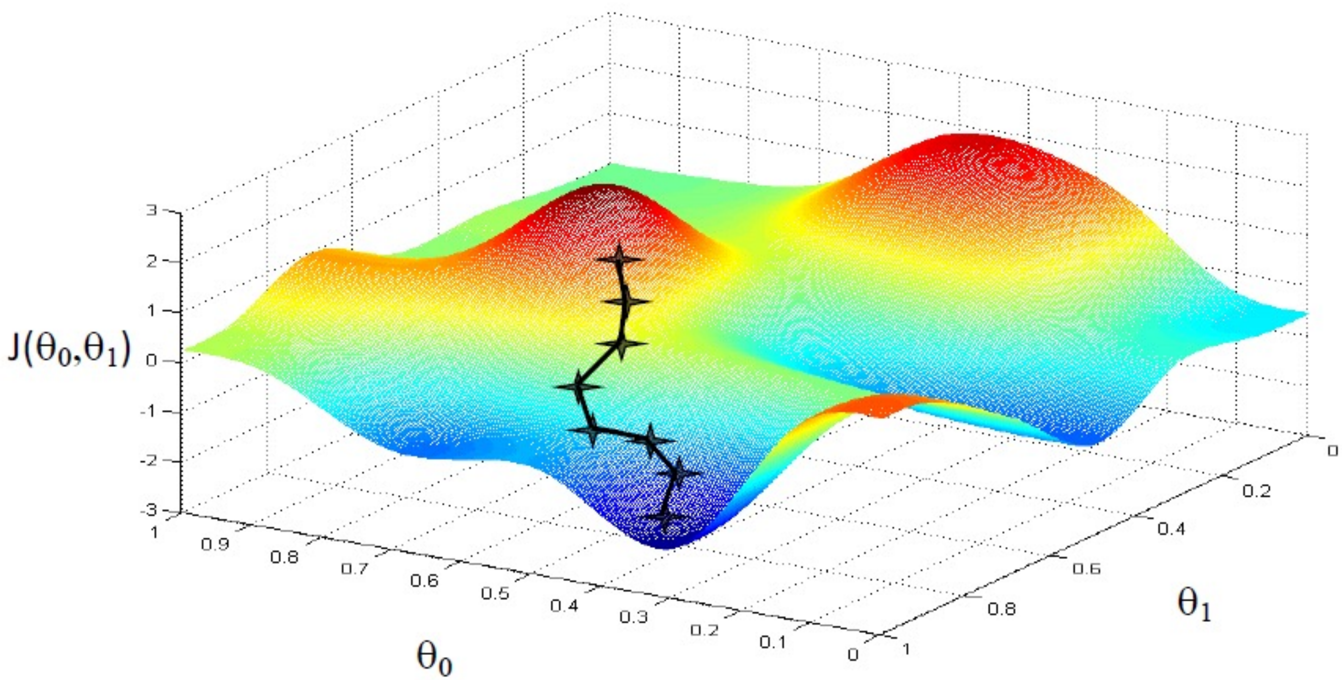
What Strategy to Use?

Follow the Slope

Follow the direction of steepest descent!

How to optimize $J(\theta)$?

- Choose initial value for θ
- Until we reach a minimum:
  - Choose a new value for $\boldsymbol{\theta}$ to reduce $J(\boldsymbol{\theta})$



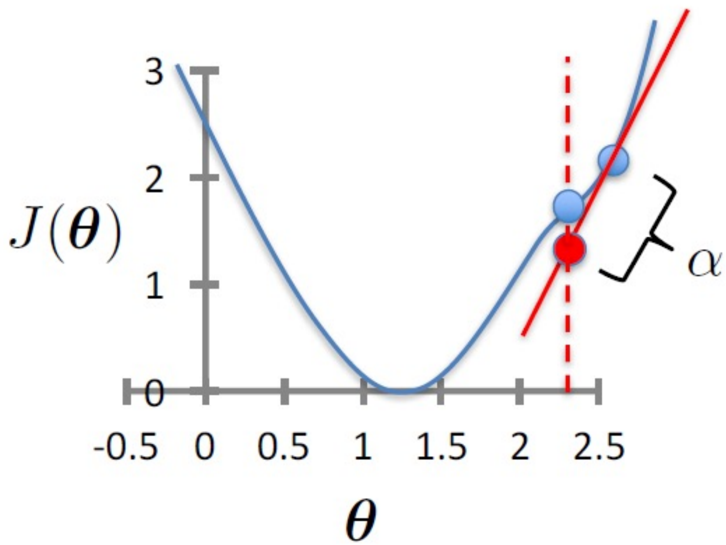
Gradient Descent

- Initialize $\boldsymbol{\theta}$
- Repeat until convergence

$$\theta_j \leftarrow \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\boldsymbol{\theta})$$

simultaneous update
for j = 0 ... d

learning rate (small)
e.g., α = 0.05



- Gradient = slope of line tangent to curve
- Function decreases faster in negative direction of gradient
- Larger learning rate => larger step

Gradient Descent

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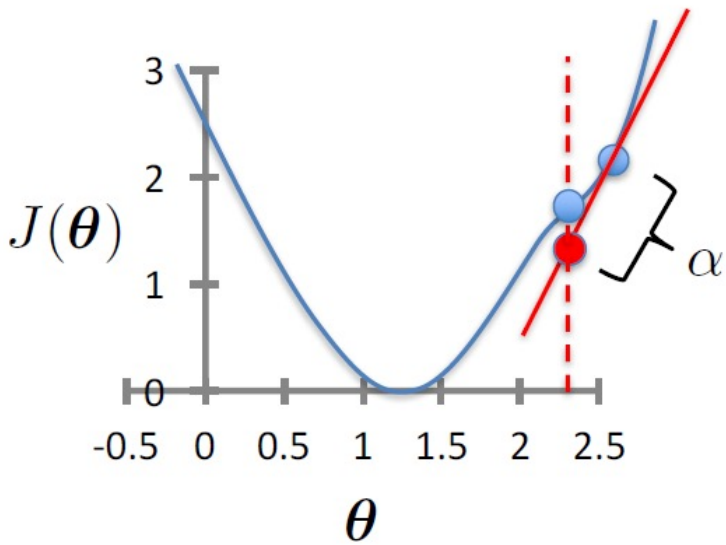
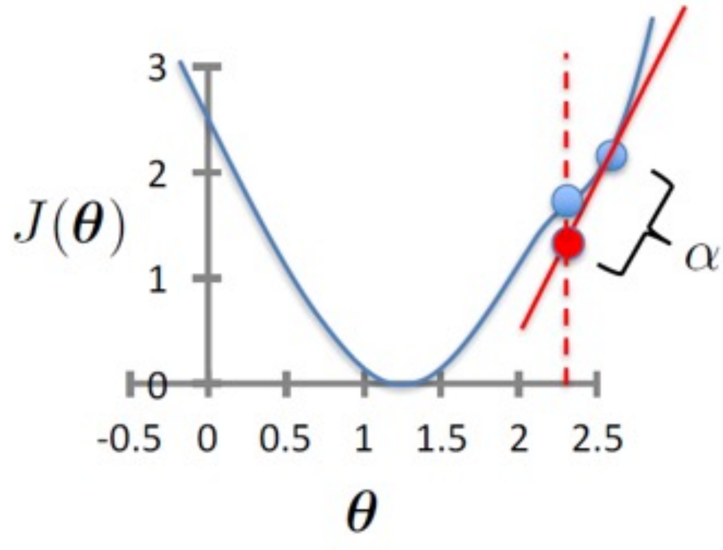
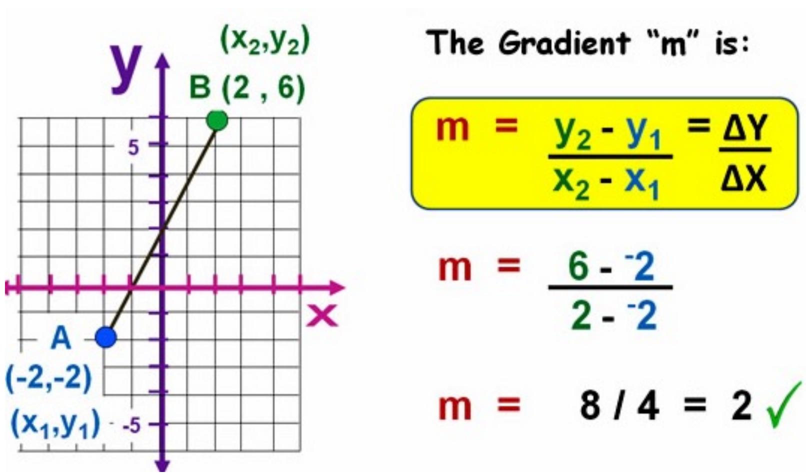


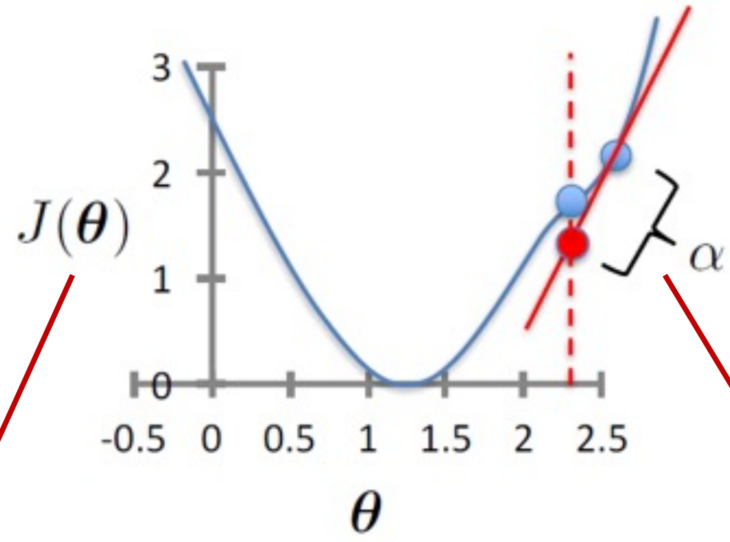
Vector update rule: $\theta \leftarrow \theta - \frac{\partial J(\theta)}{\partial \theta}$

Gradient Descent





Gradient Descent



- If θ is on the left of minimum, slope is negative
- Increase value of θ

- If θ is on the right of minimum, slope is positive
- Decrease value of θ

In both cases θ gets closer to minimum

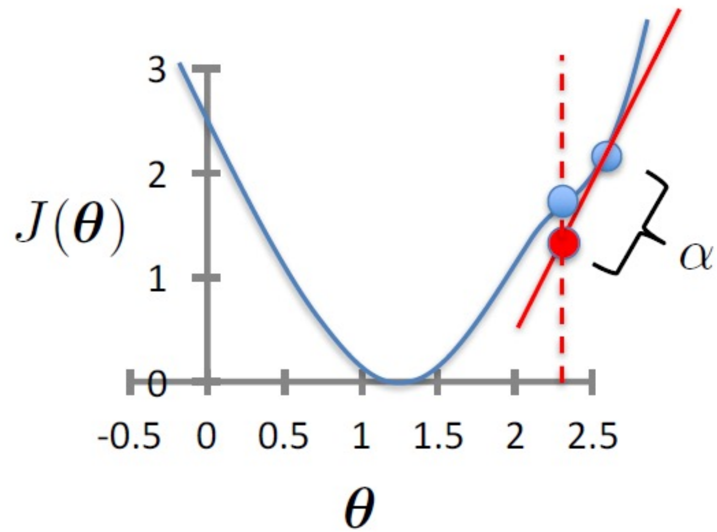
Stopping Condition

- Initialize $\boldsymbol{\theta}$
- Repeat until convergence

$$\theta_j \leftarrow \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\boldsymbol{\theta})$$

simultaneous update for j = 0 ... d

learning rate (small) e.g., α = 0.05



- When should the algorithm stop?

Stopping Condition

- Initialize $\boldsymbol{\theta}$
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simultaneous update
for j = 0 ... d

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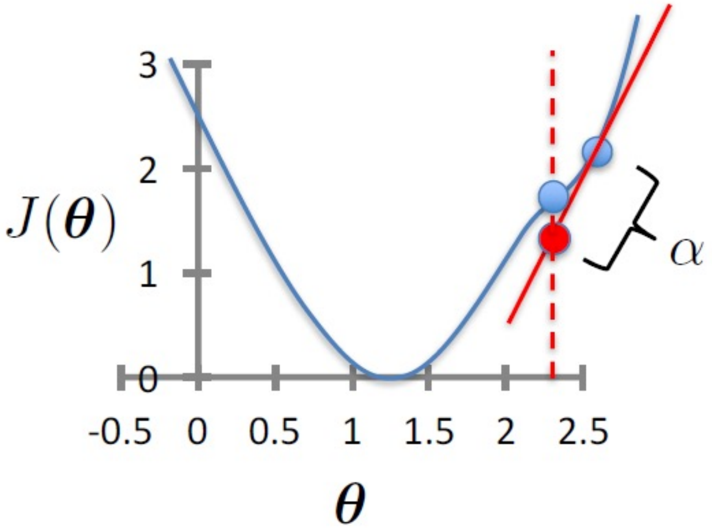
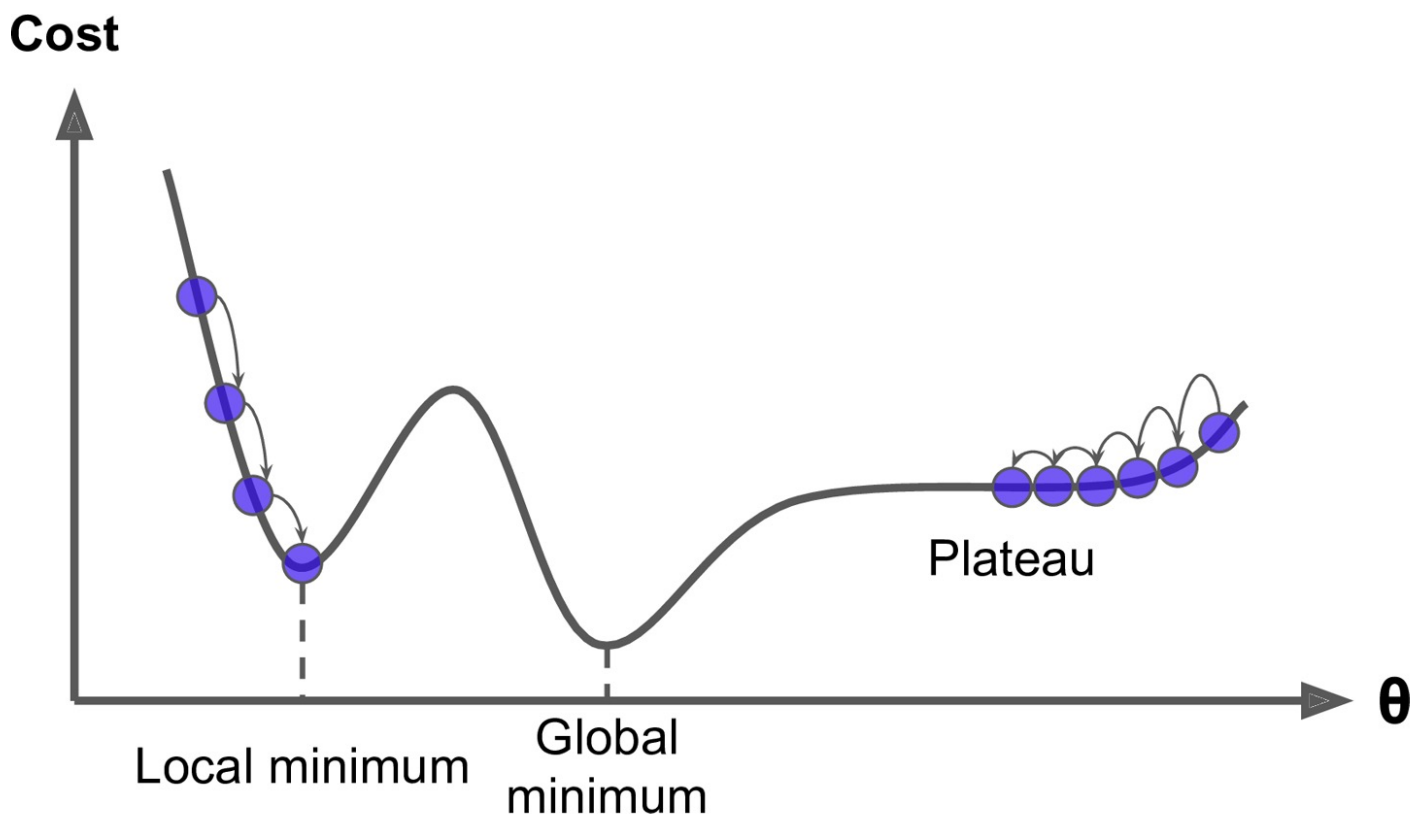


- When should the algorithm stop?
- When the update in θ is below some threshold
- Or maximum number of iterations is reached

GD Convergence Issues



Gradient Descent

- Initialize $\boldsymbol{\theta}$
- Repeat until convergence

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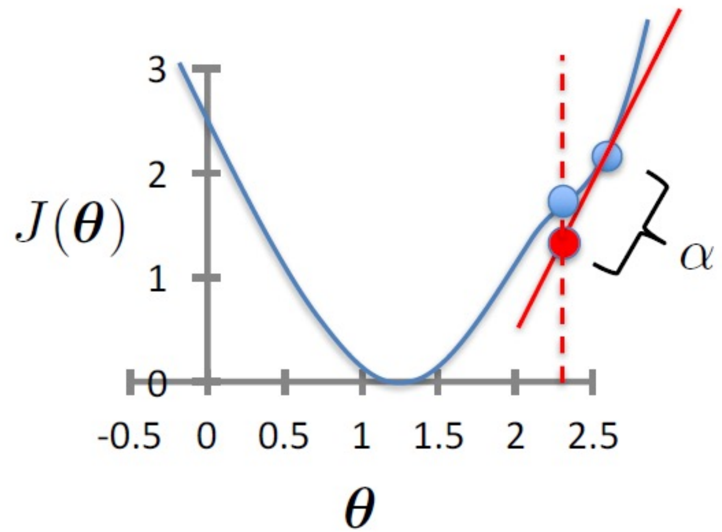
simultaneous update
for j = 0 ... d

learning rate (small)
e.g., α = 0.05



- What happens when θ reaches a local minimum?

Gradient Descent

- Initialize $\boldsymbol{\theta}$
- Repeat until convergence

$$\theta_j \leftarrow \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\boldsymbol{\theta})$$

simultaneous update
for j = 0 ... d

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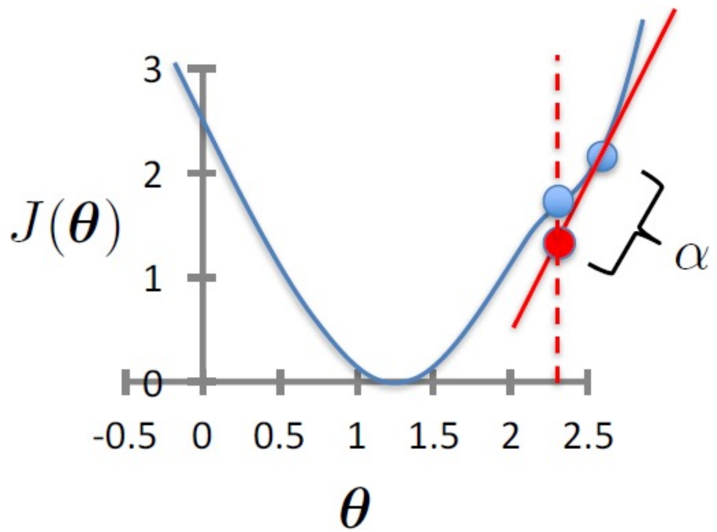
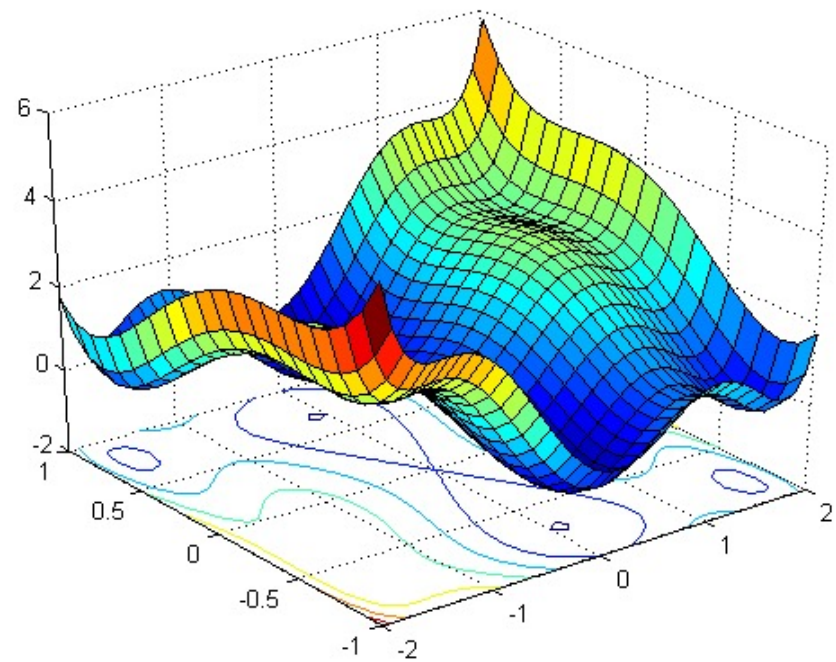


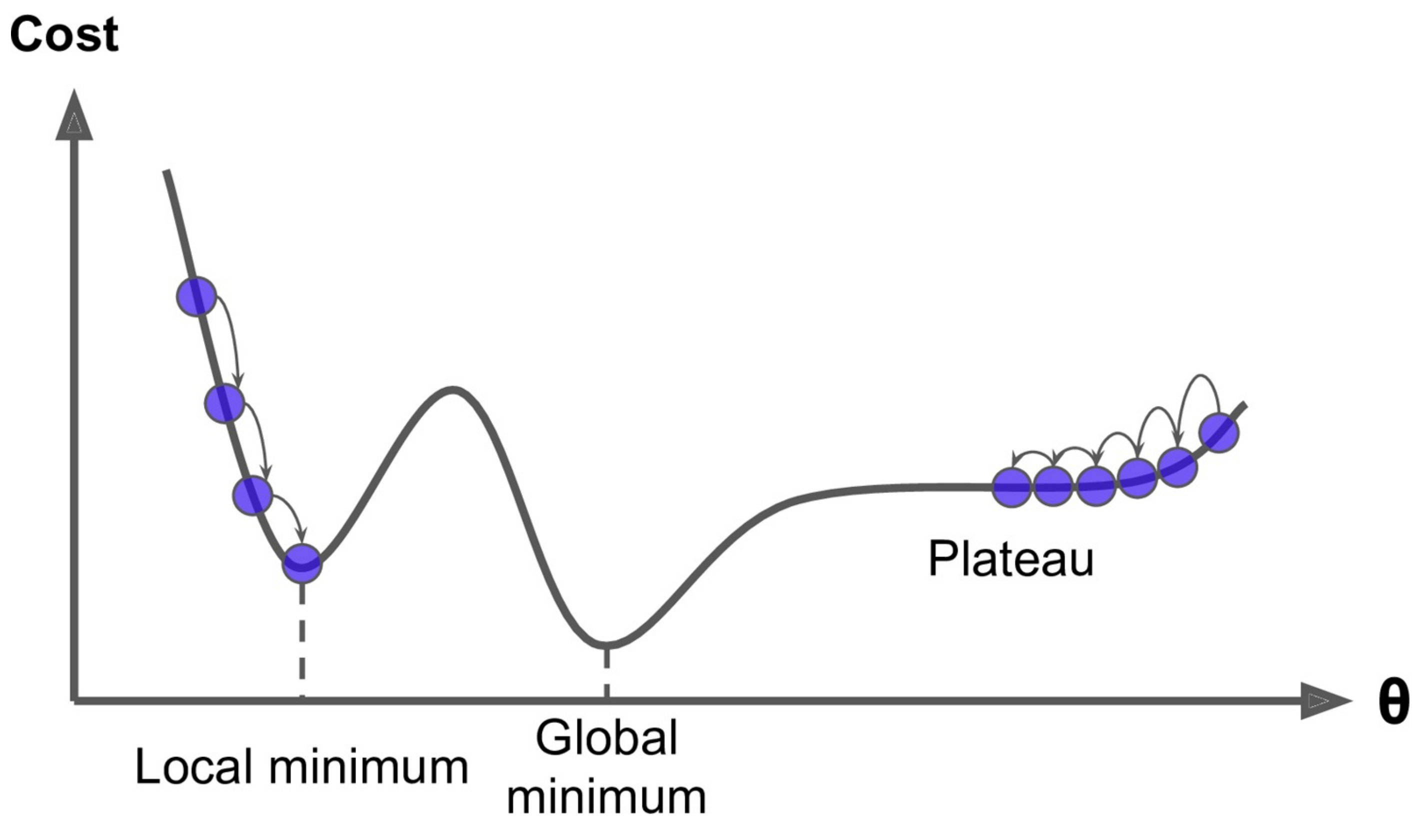
- What happens when θ reaches a local minimum?
- The slope is 0, and gradient descent converges!
- Strictly convex functions only have global minimum

Complex loss function



- Convex loss functions only have global minimum, no local minima
- Complex loss functions are more difficult to optimize as they have multiple local optima

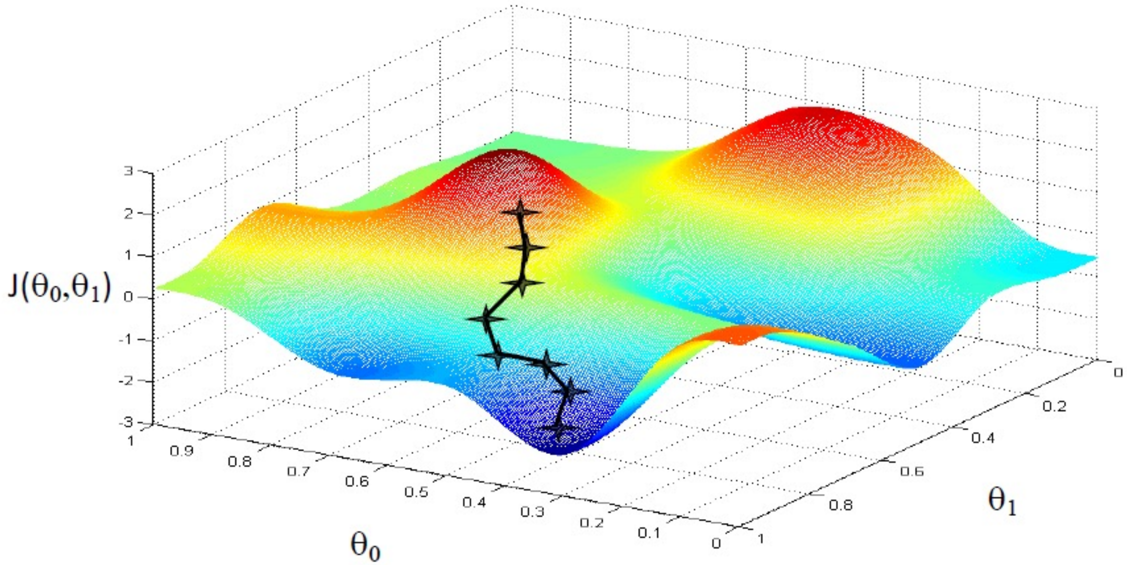
GD Convergence Issues

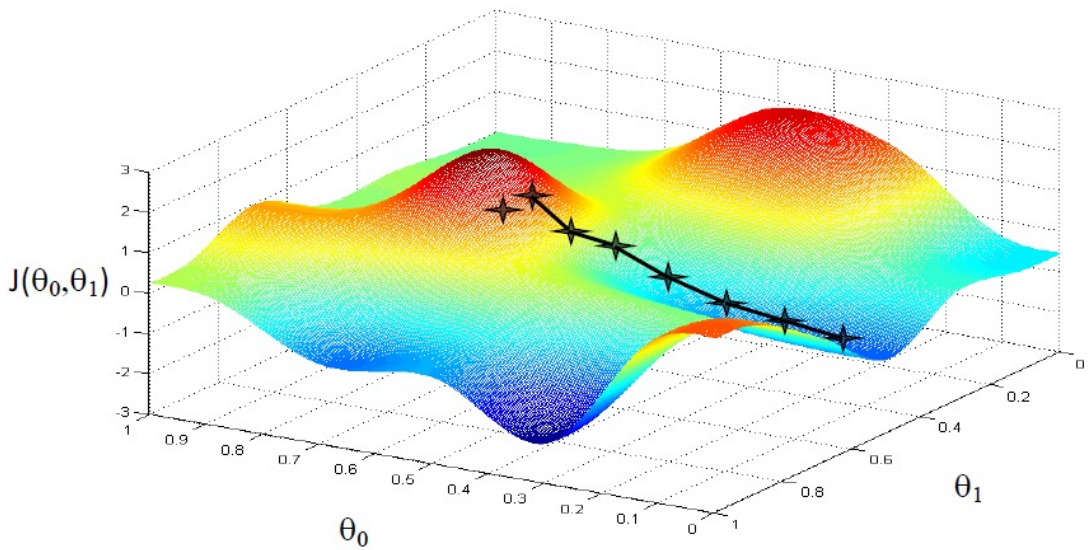


- Local minimum: Gradient descent stops
- Plateau: Almost flat region where slope is small

Solution: start from multiple random locations

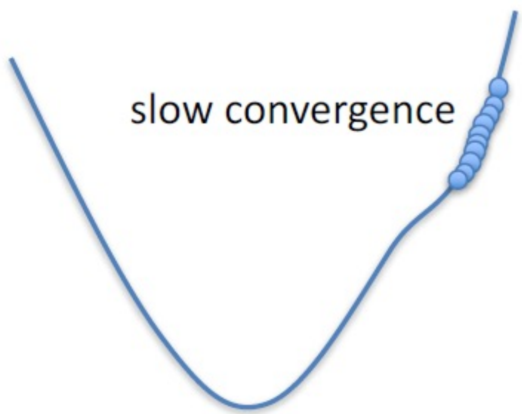
Possible Solution



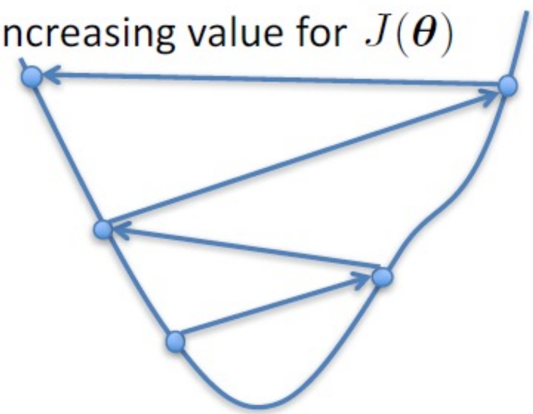


Choosing Learning Rate

α too small



α too large

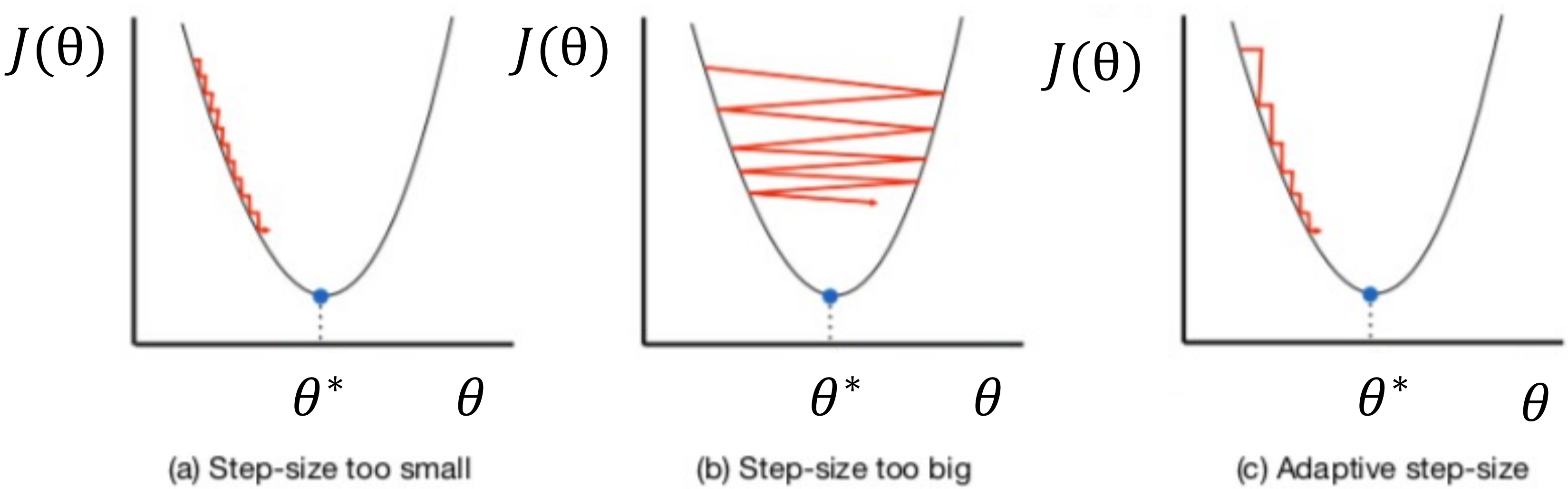


- May overshoot the minimum
- May fail to converge
- May even diverge

To see if gradient descent is working, print out $J(\boldsymbol{\theta})$ each iteration

- The value should decrease at each iteration
- If it doesn't, adjust α

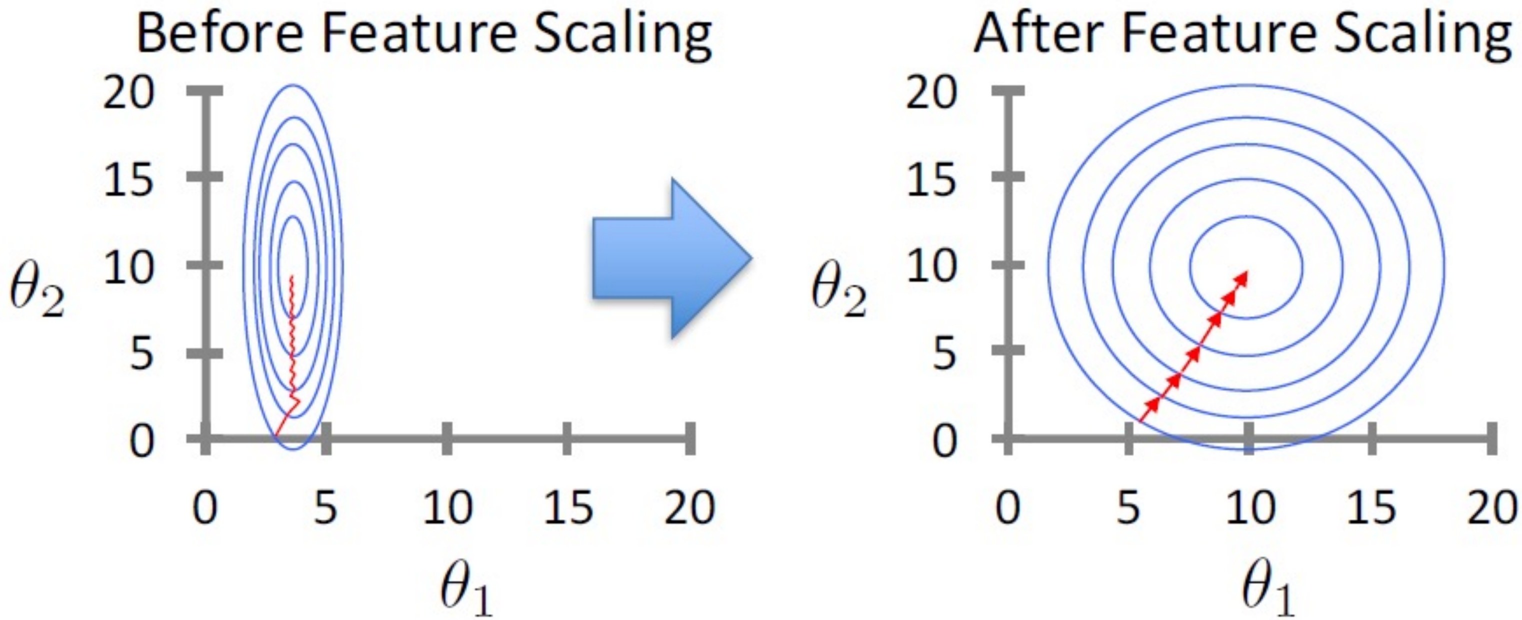
Adaptive step size



- Start with large step size and reduce over time, adaptively
- Line search method
- Measure how objective decreases

Feature Scaling

- **Idea:** Ensure that feature have similar scales



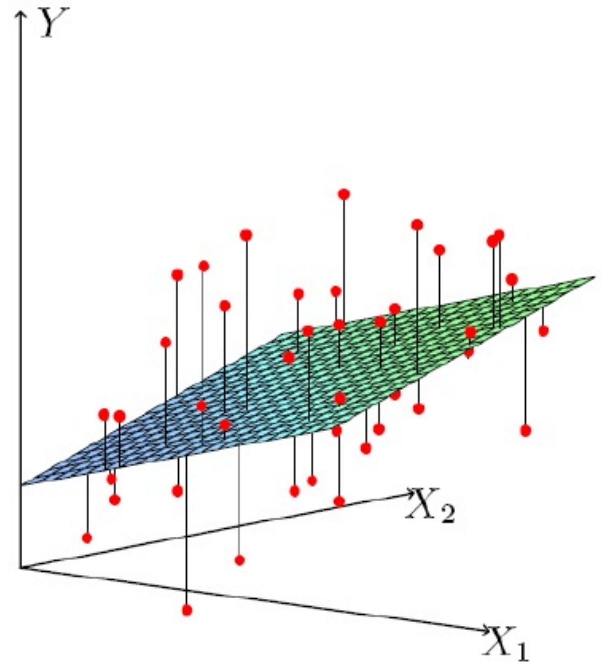
- Makes gradient descent converge *much* faster

Multiple Linear Regression

- Dataset: $x_i \in R^d, y_i \in R$
- Hypothesis $h_\theta(x) = \theta^T x$
- MSE $= \frac{1}{N} \sum (h_\theta(x_i) - y_i)^2$ Loss / cost

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

MSE is a strictly convex function and has unique minimum



GD for Multiple Linear Regression

- Initialize $\boldsymbol{\theta}$
- Repeat until convergence

$$\theta_j \leftarrow \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\boldsymbol{\theta})$$

simultaneous update
for j = 0 ... d

GD for Linear Regression

- Initialize $\boldsymbol{\theta}$
- Repeat until convergence

$||\theta_{new} - \theta_{old}|| < \epsilon$ or iterations == MAX_ITER

$$\theta \leftarrow \theta - \alpha \frac{2}{N}(X\theta - y)^T X$$

Equivalent

$$\theta_j \leftarrow \theta_j - \alpha \frac{2}{N}\sum_{i=1}^{N}(h_\theta(x_i) - y_i)x_{ij}, j = 0, \dots, d$$

- Assume convergence when $\|\boldsymbol{\theta}_{new} - \boldsymbol{\theta}_{old}\|_2 < \epsilon$

L_2 norm: $$\|\boldsymbol{v}\|_2 = \sqrt{\sum_i v_i^2} = \sqrt{v_1^2 + v_2^2 + \ldots + v_{|v|}^2}$$

Gradient Descent in Practice

- Asymptotic complexity
  - $O(NTd)$, *N* is size of training data, *d* is feature dimension, and *T* is number of iterations
- Most popular optimization algorithm in use today
- At the basis of training
  - Linear Regression
  - Logistic regression
  - SVM
  - Neural networks and Deep learning
  - Stochastic Gradient Descent variants

Gradient Descent vs Closed Form

Gradient Descent

- Initialize $\boldsymbol{\theta}$
- Repeat until convergence

$$\theta_j \leftarrow \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\boldsymbol{\theta})$$

simultaneous update for j = 0 ... d

Closed form

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

Gradient Descent	Closed Form
+ Linear increase in d and N	+ No parameter tuning
+ Generally applicable	+ Gives the global optimum
- Need to choose α and stopping conditions	- Not generally applicable
- Might get stuck in local optima	- Slow computation: $O(d^3)$

Issues with Gradient Descent

- Might get stuck in local optimum and not converge to global optimum
  - Restart from multiple initial points
- Only works with differentiable loss functions
- Small or large gradients
  - Feature scaling helps
- Tune learning rate
  - Can use line search for determining optimal learning rate

Review Gradient Descent

- Gradient descent is an efficient algorithm for optimization and training ML models
  - The most widely used algorithm in ML!
  - Faster than using closed-form solution for linear regression
  - Main issues with Gradient Descent is convergence and getting stuck in local optima (for neural networks)
- Gradient descent is guaranteed to converge to optimum for strictly convex functions if run long enough

Acknowledgements

- Slides made using resources from:
  - Andrew Ng
  - Eric Eaton
  - David Sontag
- Thanks!