CS 7775

Seminar in Computer Security: Machine Learning Security and Privacy

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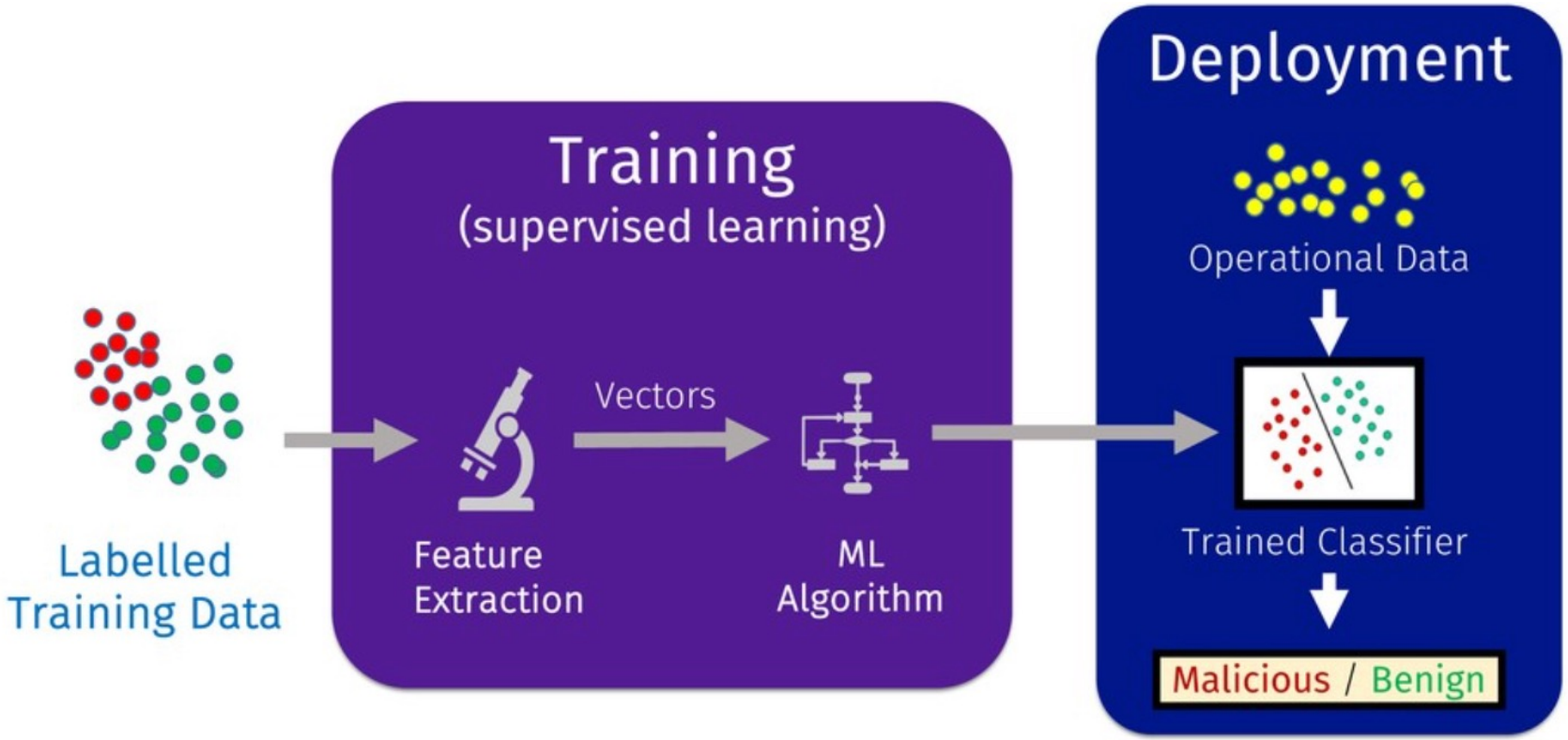
Outline: Review of ML

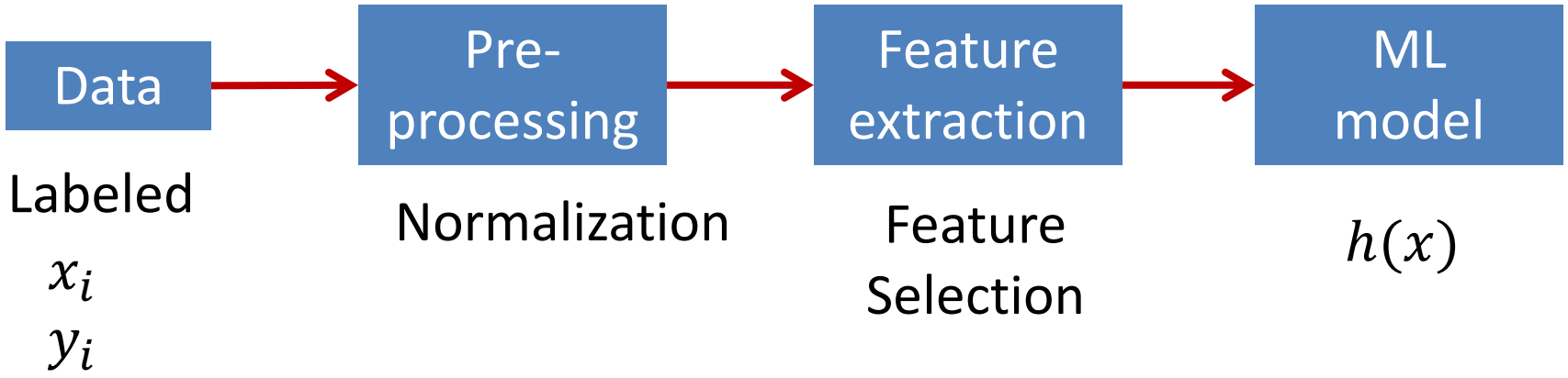
- Regression
  - Linear regression, closed form
  - Gradient descent
- Bias-variance tradeoff
  - Regularization
  - Cross validation
- Classification
  - Linear classification: logistic regression, SVM
  - Classifier metrics
  - Naïve Bayes classifier
  - Decision trees
  - Ensembles: bagging and boosting

Machine Learning Pipeline

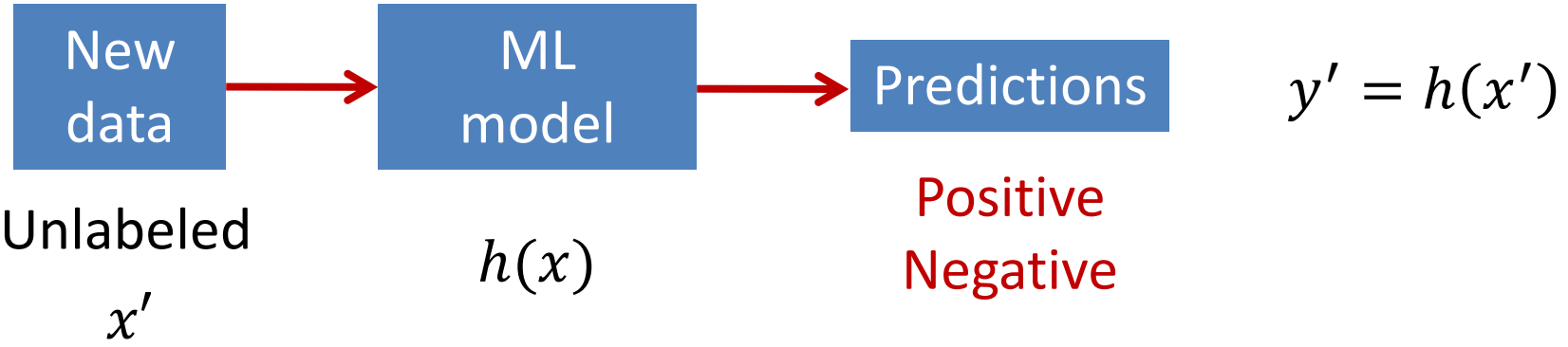


Supervised Learning: Classification

Training

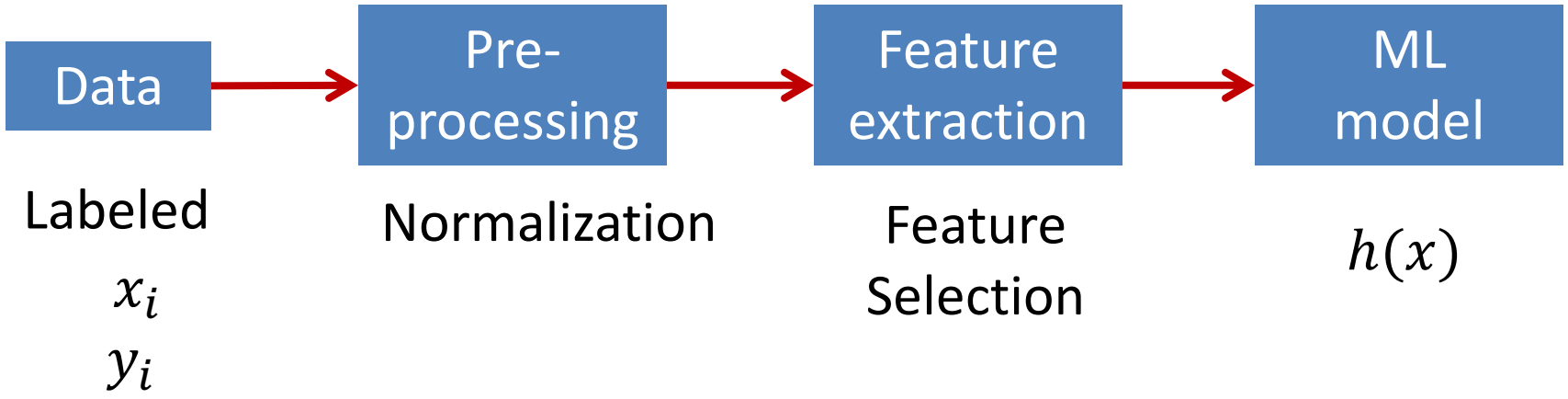


Testing

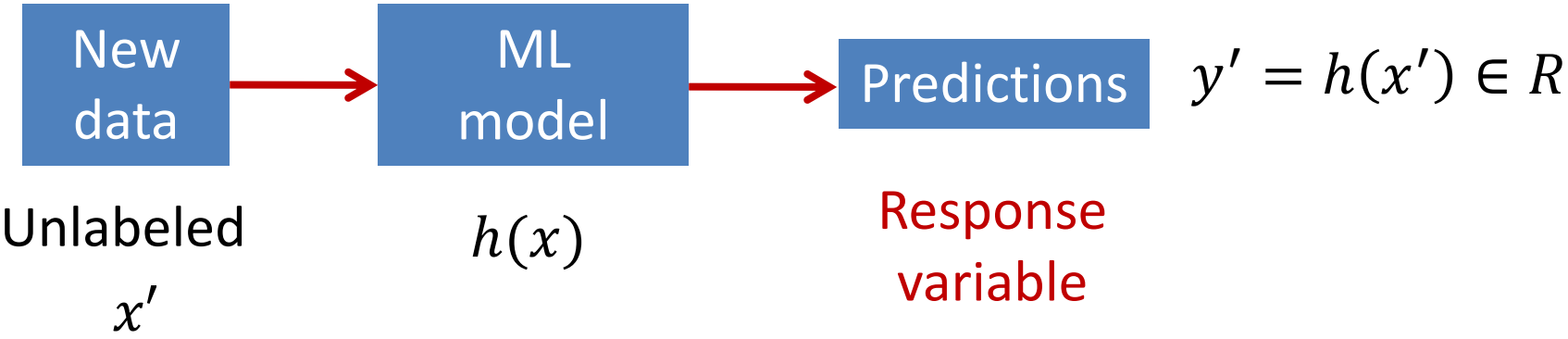


Supervised Learning: Regression

Training

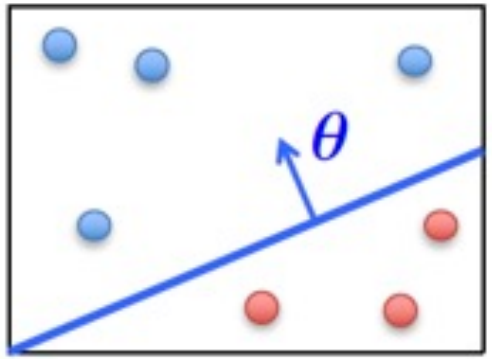


Testing



Supervised learning

- Training data
  - $x_i = [x_{i,1}, \ldots x_{i,d}]$: vector of features
  - y_i: labels
- Models (hypothesis)
  - Example: Linear model
    - $h_\theta(x) = \theta_0 + \theta_1 x$
- Loss function
  - Error function to minimize during training
- Training algorithm
  - Training: Learn model parameters θ to minimize objective
  - Output: "optimal" model according to loss function
- Testing
  - Apply learned model to new data x' and generate prediction $h(x')$



Vector Norms

Vector norms: A norm of a vector ||x|| is informally a measure of the "length" of the vector.

$$\|x\|_p = \left(\sum_{i=1}^{n} |x_i|^p \right)^{1/p}$$

- Common norms: L_1, L_2 (Euclidean)

$$\|x\|_1 = \sum_{i=1}^{n} |x_i| \qquad \|x\|_2 = \sqrt{\sum_{i=1}^{n} x_i^2}$$

- L_∞

$$\|x\|_\infty = \max_i |x_i|$$

Distance Metrics

- Euclidean Distance $\sqrt{(\sum_{i=1}^{k}(x_i - y_i)^2)}$
- Manhattan Distance $\sum_{i=1}^{k}|x_i - y_i|$
- Minkowski Distance $\left(\sum_{i=1}^{k}(|x_i - y_i|)^q\right)^{\frac{1}{q}}$

Vector Operations

- **Vector dot (inner) product:**

$$x^T y \in \mathbb{R} = \begin{bmatrix} x_1 & x_2 & \cdots & x_n \end{bmatrix} \begin{bmatrix} y_1 \\ x_2 \\ \vdots \\ y_n \end{bmatrix} = \sum_{i=1}^{n} x_i y_i.$$

Linear Regression

- Linear Model

$$h(\boldsymbol{x}) = \sum_{j=0}^{d} \theta_j x_j$$

- Let

$$\boldsymbol{\theta} = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \vdots \\ \theta_d \end{bmatrix} \qquad \boldsymbol{x}^\intercal = \begin{bmatrix} 1 & x_1 & \dots & x_d \end{bmatrix}$$

- Can write the model in vectorized form as $h(\boldsymbol{x}) = \boldsymbol{\theta}^\intercal \boldsymbol{x}$

Vectorized Form

- Consider our model for N instances:

$$h(x_i) = \sum_{j=0}^{d} \theta_j x_{ij} = \theta^T x_i$$

- Let

Model parameter

$$\boldsymbol{\theta} = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \vdots \\ \theta_d \end{bmatrix} \quad \boldsymbol{X} = \begin{bmatrix} 1 & x_{11} & \cdots & x_{1d} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_{i1} & \cdots & x_{id} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_{N1} & \cdots & x_{Nd} \end{bmatrix}$$

Training data

$\mathbb{R}^{(d+1)\times 1}$ $\mathbb{R}^{n\times(d+1)}$

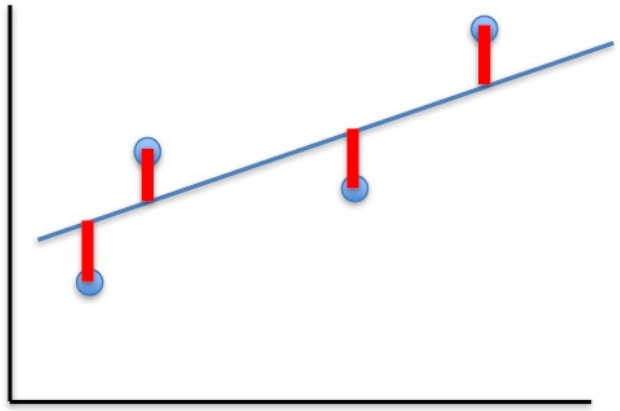
Least-Squares Linear Regression

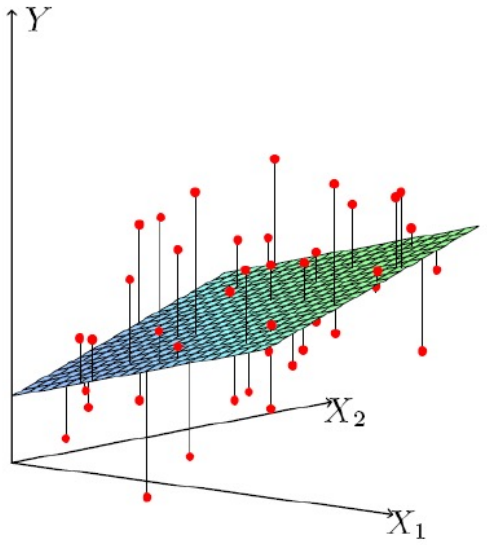
- Cost Function

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

Mean Square Error (MSE)

- Fit by solving $\min_{\theta} J(\theta)$





Optimization Methods

- Closed form solution
  - Define the exact solution as a function of X and y
  - This is available for linear regression, but not for other ML models
- Gradient descent solution
  - Iterative optimization procedure that could result in an approximate solution
  - Applicable to many ML models that optimize an objective: linear regression, logistic regression, SVM, neural networks

Matrix and vector gradients

If $y = f(x), y \in R$ scalar , $x \in R^n$ vector

$$\frac{\partial y}{\partial x} = \begin{bmatrix} \frac{\partial y}{\partial x_1} & \frac{\partial y}{\partial x_2} & \cdots & \frac{\partial y}{\partial x_n} \end{bmatrix}$$

Vector gradient (row vector)

If $y = f(x), y \in R^m, x \in R^n$

$$\frac{\partial \mathbf{y}}{\partial \mathbf{x}} = \begin{bmatrix} \frac{\partial y_1}{\partial x_1} & \frac{\partial y_1}{\partial x_2} & \cdots & \frac{\partial y_1}{\partial x_n} \\ \frac{\partial y_2}{\partial x_1} & \frac{\partial y_2}{\partial x_2} & \cdots & \frac{\partial y_2}{\partial x_n} \\ \vdots & \vdots & & \vdots \\ \frac{\partial y_m}{\partial x_1} & \frac{\partial y_m}{\partial x_2} & \cdots & \frac{\partial y_m}{\partial x_n} \end{bmatrix}$$

Jacobian matrix (Matrix gradient)

Properties

- If w, x are $(d\times1)$ vectors, $\frac{\partial w^T x}{\partial x} = w^T$
- If A: $(n\times d)$ x: $(d\times1)$, $\frac{\partial Ax}{\partial x} = A$
- If A: $(d\times d)$ x: $(d\times1)$, $\frac{\partial x^T Ax}{\partial x} = (A + A^T)x$
- If A symmetric: $\frac{\partial x^T Ax}{\partial x} = 2Ax$
- If x: $(d\times1)$, $\frac{\partial ||x||^2}{\partial x} = 2x^T$

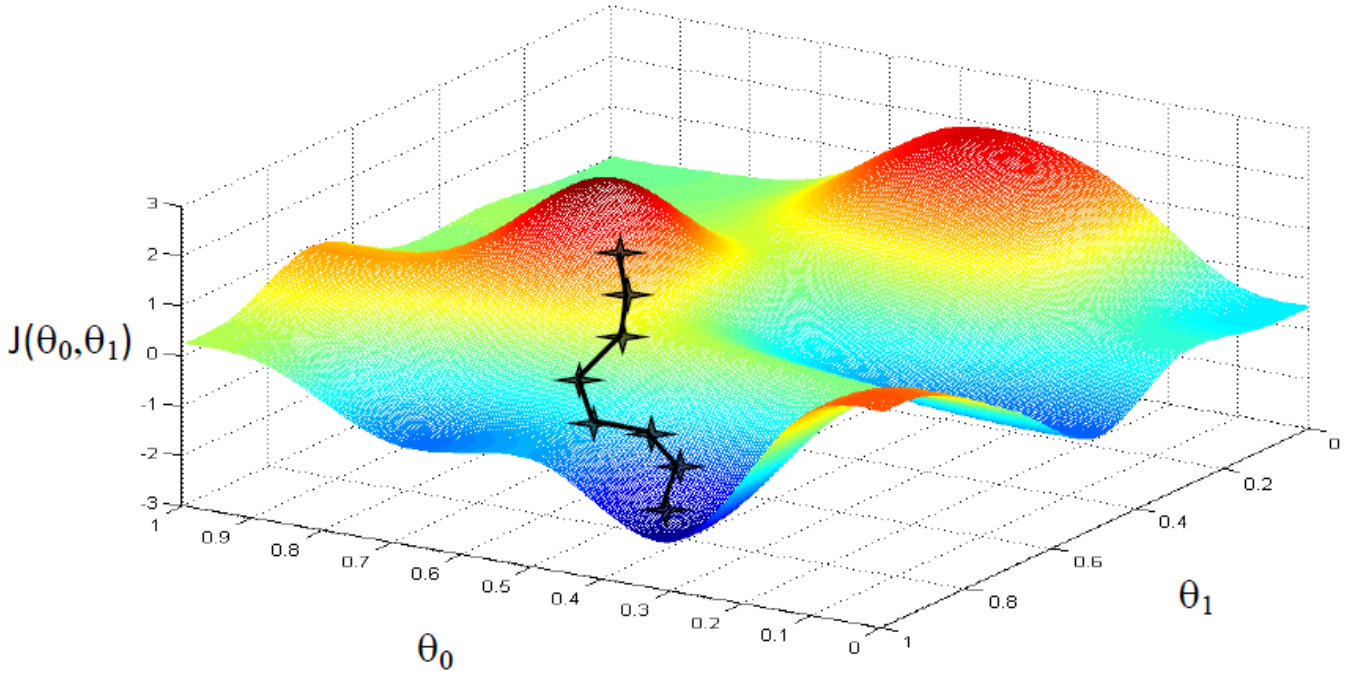
Closed-Form Solution

$$J(\theta) = \frac{1}{N} \left|\left|\mathrm{X}\theta - y\right|\right|^2$$

Gradient Descent

Goal: find $\boldsymbol{\theta}$ to min $J(\boldsymbol{\theta})$

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



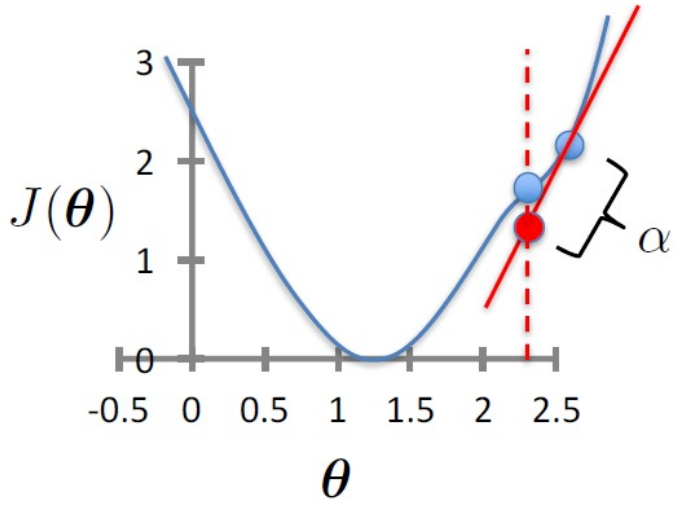
Gradient Descent

- 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

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

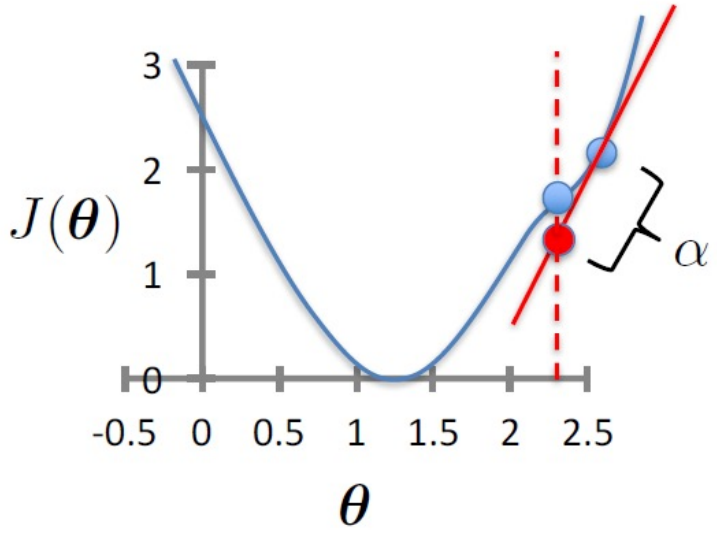
Stopping Condition

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

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

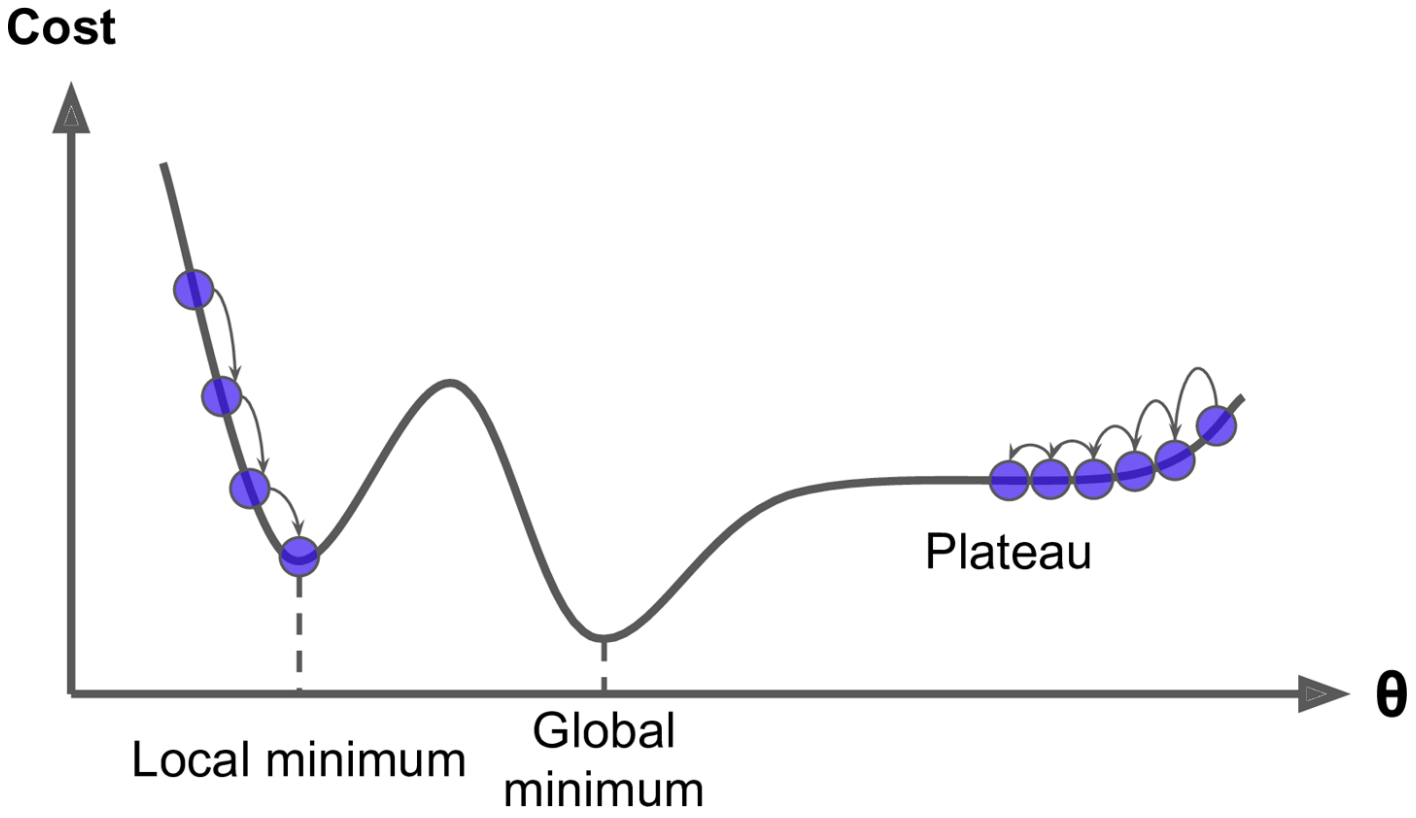
simultaneous update
for j = 0 ... d

learning rate (small)
e.g., α = 0.05



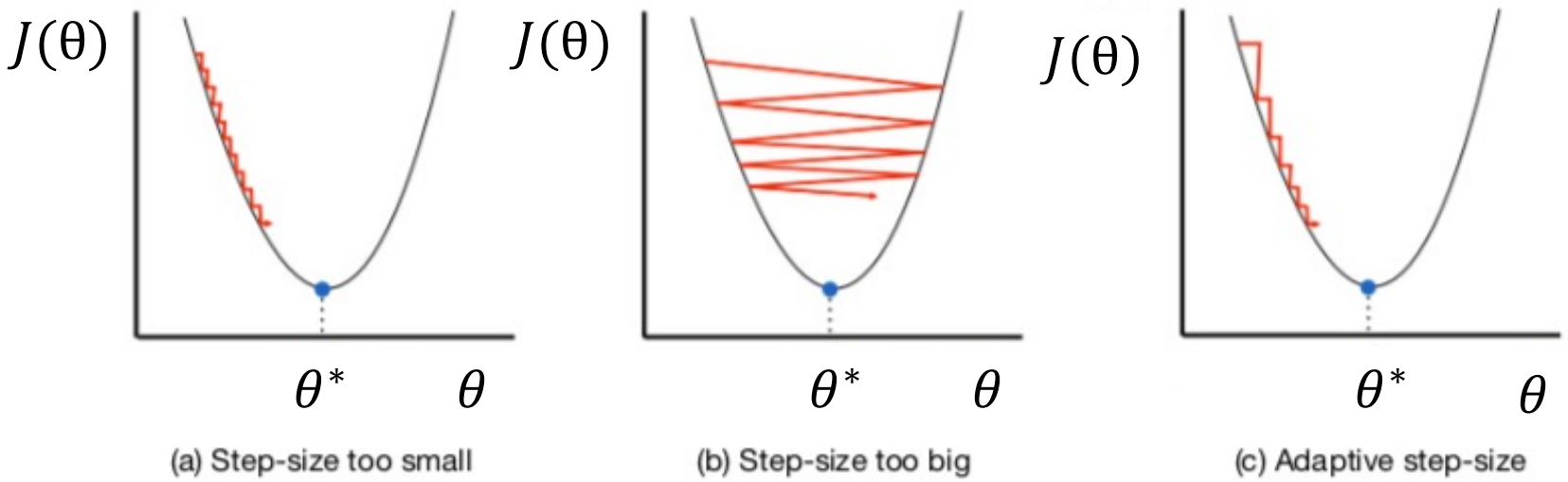
- When should the algorithm stop?

GD Convergence Issues



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

Adaptive learning rates



- Start with large step size and reduce over time, adaptively
- Measure how objective decreases
- Several optimizers use adaptive learning rates: ADAM, AdaGrad, RMSProp

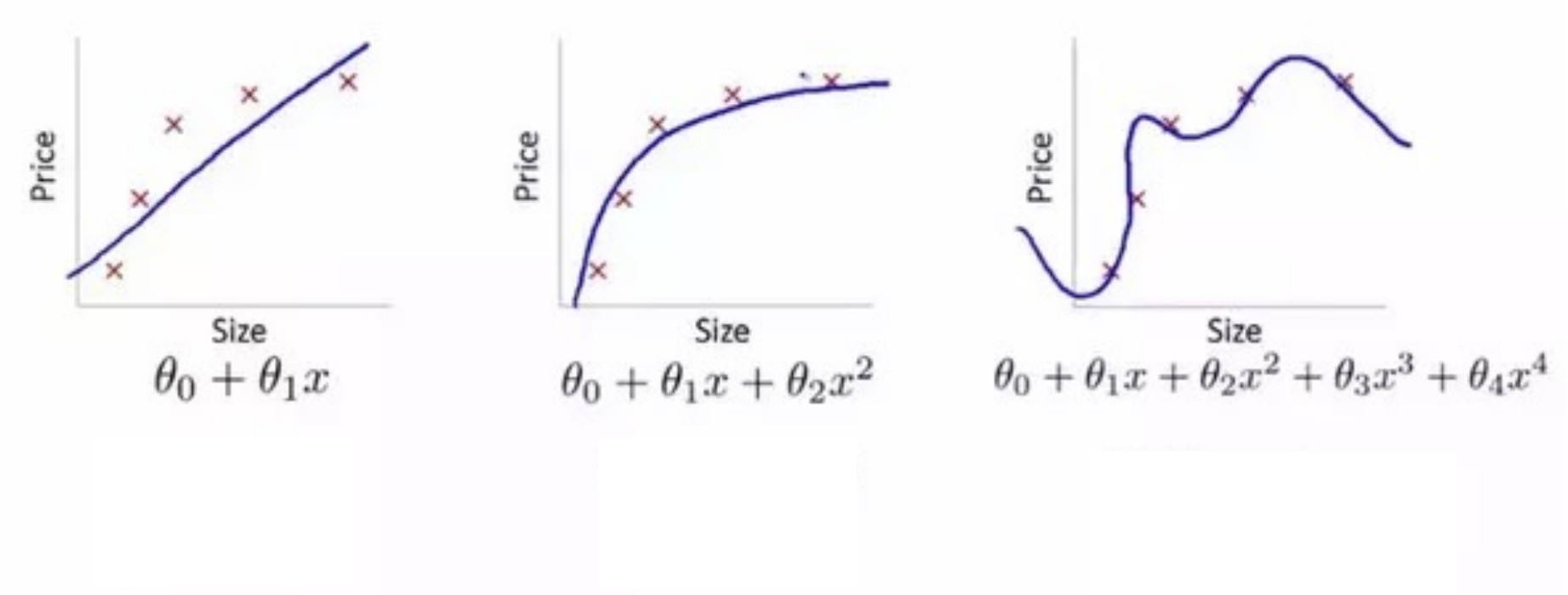
Gradient Descent for Linear Regression

Learning Challenges

- Generalization Goal
  - Classify well new testing data
  - Model **generalizes** well to new testing data
  - Minimize error (MSE or classification error) in testing
- Variance
  - Amount by which model would change if we estimated it using a different training data set
- Bias
  - Error introduced by approximating a real-life problem by a much simpler model
  - E.g., for linear models (linear regression) bias is high

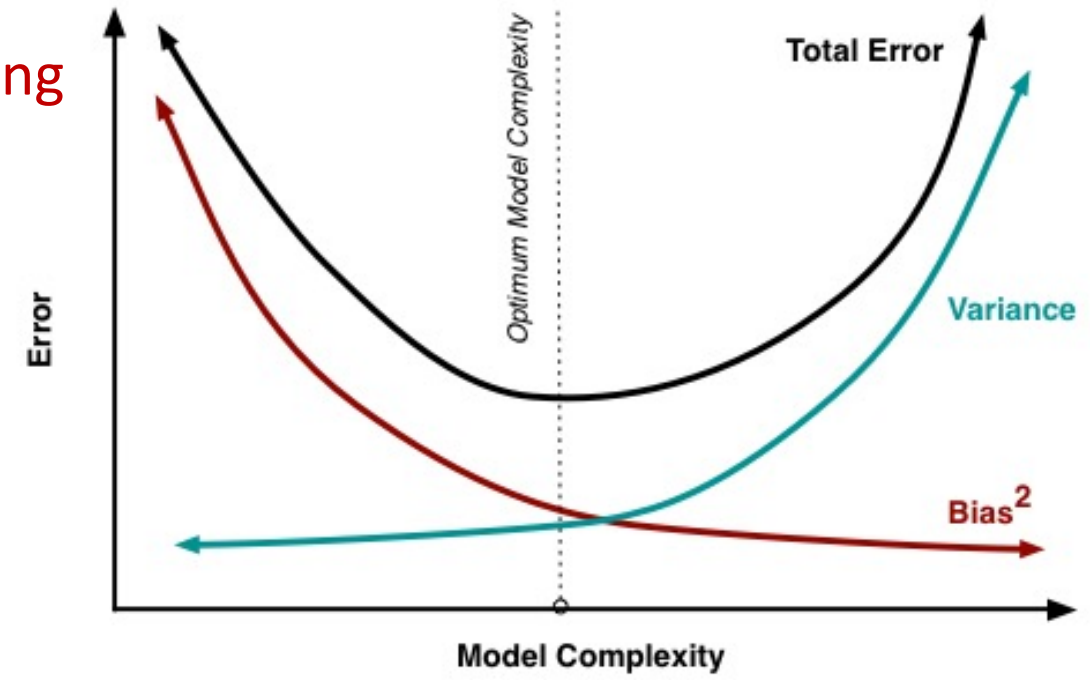
Bias-Variance tradeoff

Example: Regression



Bias-Variance Tradeoff

Under-fitting

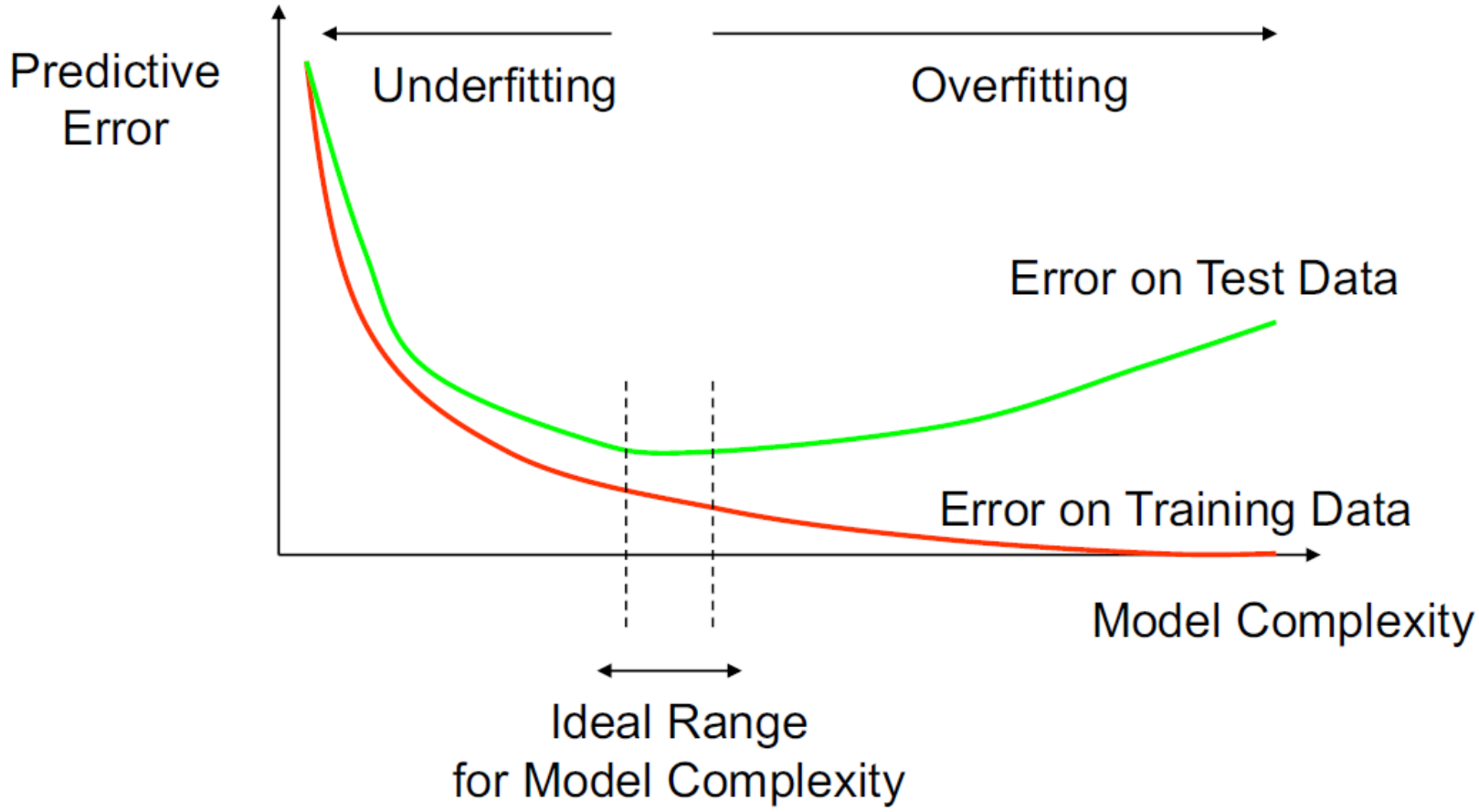


Over-fitting

- Bias = Difference between estimated and true models
- Variance = Model difference on different training sets

Test MSE is proportional to Bias + Variance

How Overfitting Affects Prediction



How can we avoid over-fitting without having access to testing data?

Regularization

- A method for automatically controlling the complexity of the learned hypothesis
- **Idea**: penalize for large values of θ_j
  - Can incorporate into the cost function
  - Works well when we have a lot of features, each that contributes a bit to predicting the label
- Can also address overfitting by eliminating features (either manually or via model selection)

Reduce model complexity

Reduce model variance

Ridge regression

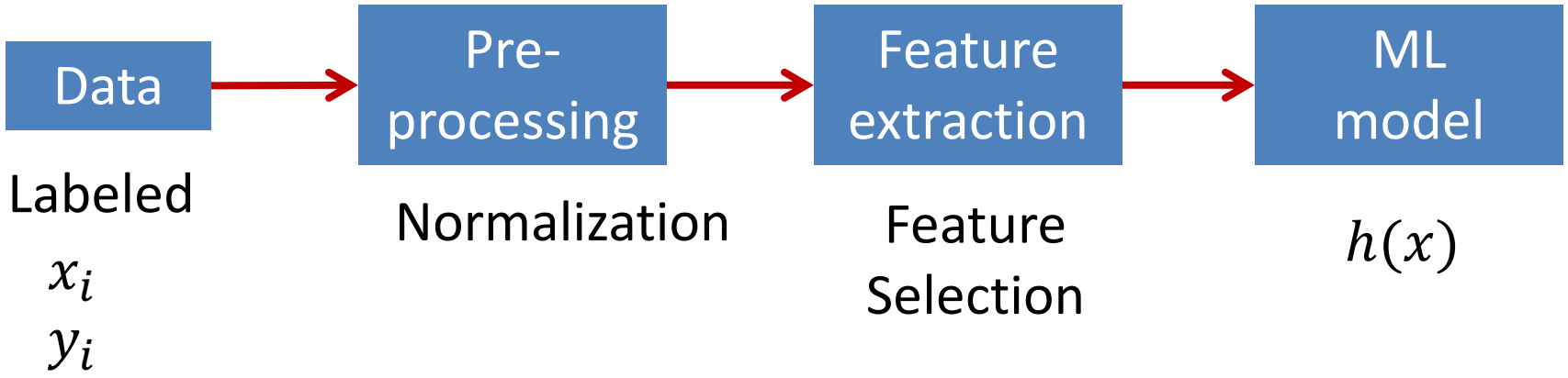
- Linear regression objective function

$$J(\theta) = \underbrace{\frac{1}{2}\sum_{i=1}^{N} \left(h_\theta(x_i) - y_i \right)^2}_{\text{model fit to data}} + \underbrace{\frac{\lambda}{2}\sum_{j=1}^{d} \theta_j^2}_{\text{regularization}}$$

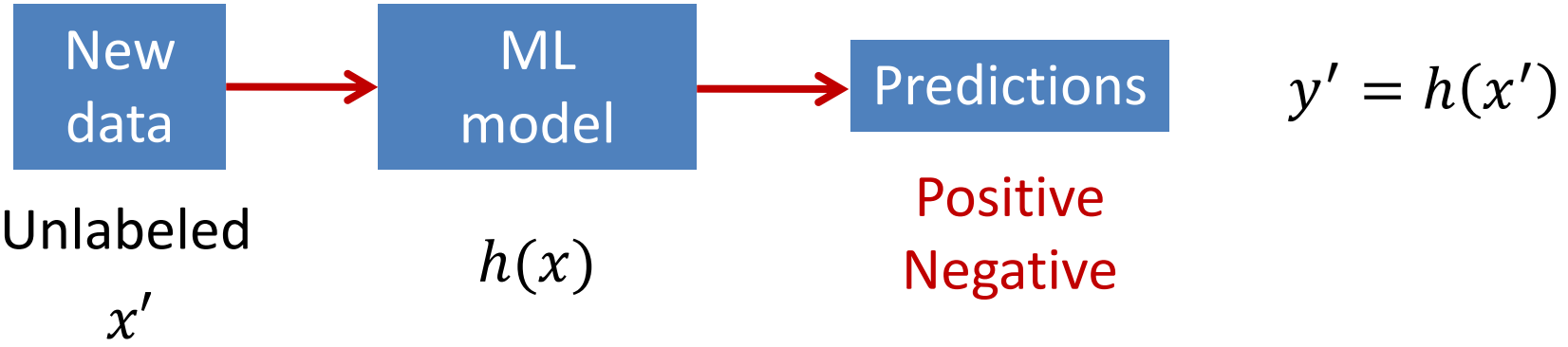
  - λ is the regularization parameter ($\lambda \geq 0$)
  - No regularization on θ_0!

Supervised Learning: Classification

Training



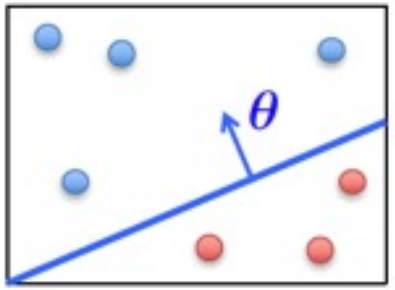
Testing



Linear Classifiers

- **Linear classifiers**: represent decision boundary by hyperplane

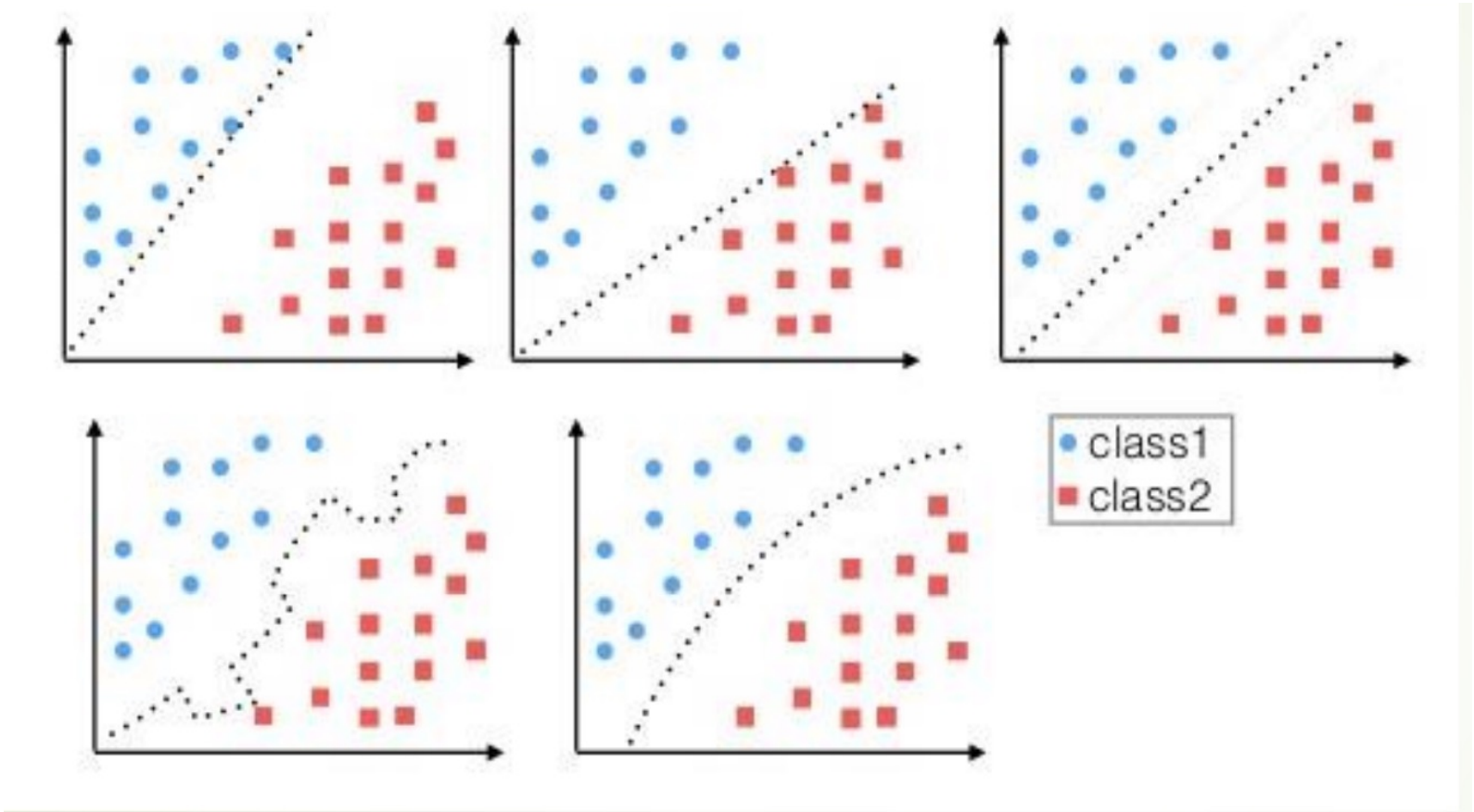
$$\boldsymbol{\theta} = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \vdots \\ \theta_d \end{bmatrix} \quad \boldsymbol{x}^\intercal = \begin{bmatrix} 1 & x_1 & \dots & x_d \end{bmatrix}$$



$h_\theta(x) = f(\theta^T x)$ linear function

- If $\theta^T x > 0$ classify "Class 1"
- If $\theta^T x < 0$ classify "Class 0"

Linear vs Non-Linear Classifiers



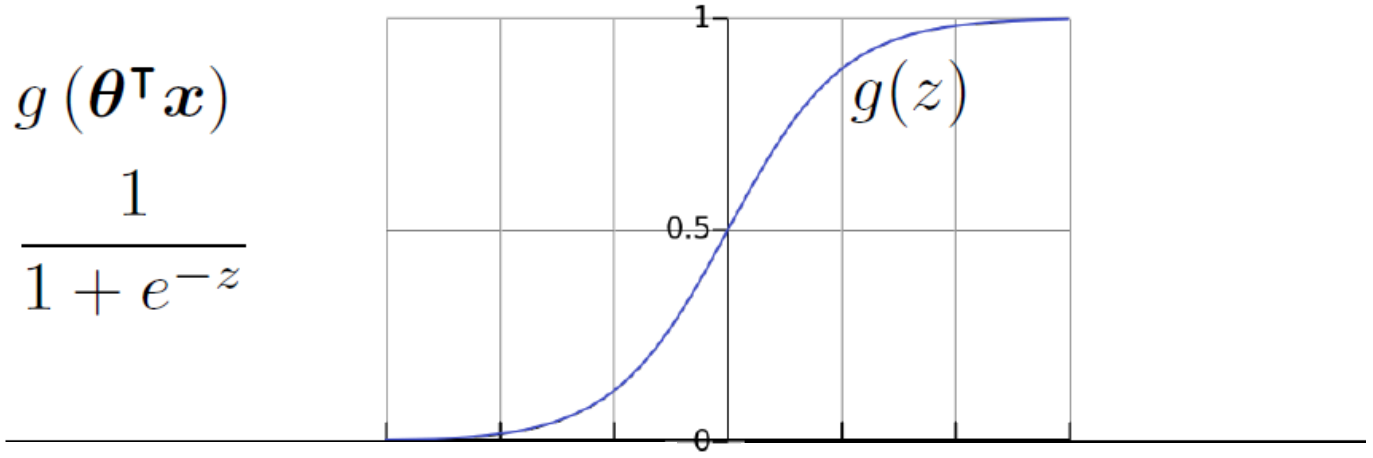
Logistic Regression

- Setup
  - Training data: $\{x_i, y_i\}$, for $i = 1, \dots, N$
  - Labels: $y_i \in \{0,1\}$
- Goals
  - Learn $h_\theta(x) = P(Y = 1|X = x)$
  - $P(Y = 1|X) + P(Y = 0|X) = 1$
- Highlights
  - Probabilistic output
  - At the basis of more complex models (e.g., neural networks)
  - Supports regularization (Ridge, Lasso)
  - Can be trained with Gradient Descent

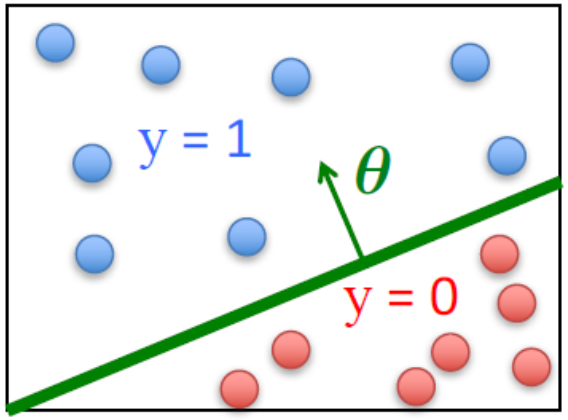
Logistic Regression

$$h_{\boldsymbol{\theta}}(\boldsymbol{x}) = g\left(\boldsymbol{\theta}^{\mathsf{T}}\boldsymbol{x}\right)$$

$$g(z) = \frac{1}{1+e^{-z}}$$



- Assume a threshold and...
  - Predict $Y = 1$ if $h_{\boldsymbol{\theta}}(\boldsymbol{x}) \geq 0.5$
  - Predict $Y = 0$ if $h_{\boldsymbol{\theta}}(\boldsymbol{x}) < 0.5$



Logistic Regression is a linear classifier!

Cross-Entropy Loss

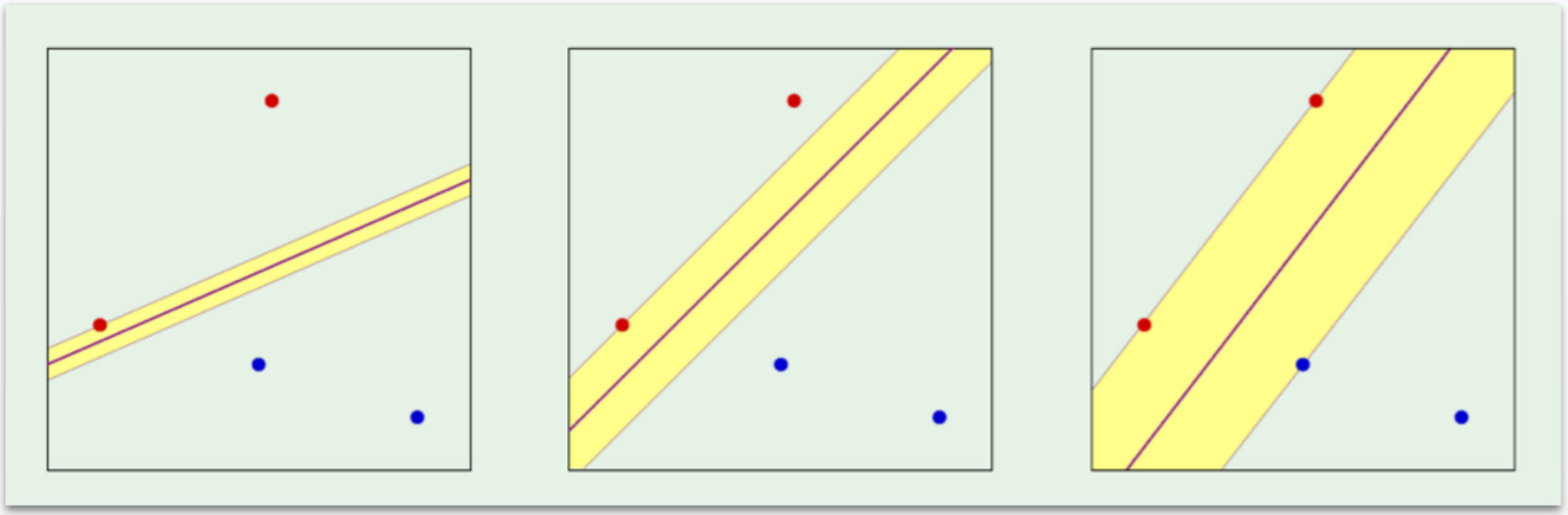
- Standard loss function for binary classification
- Derived from Maximum Likelihood Estimation (MLE)

$$\min_{\theta} J(\theta)$$

$$J(\theta) = -\sum_{i=1}^{N} [y_i \log h_\theta(x_i) + (1 - y_i) \log \left(1 - h_\theta(x_i)\right)]$$

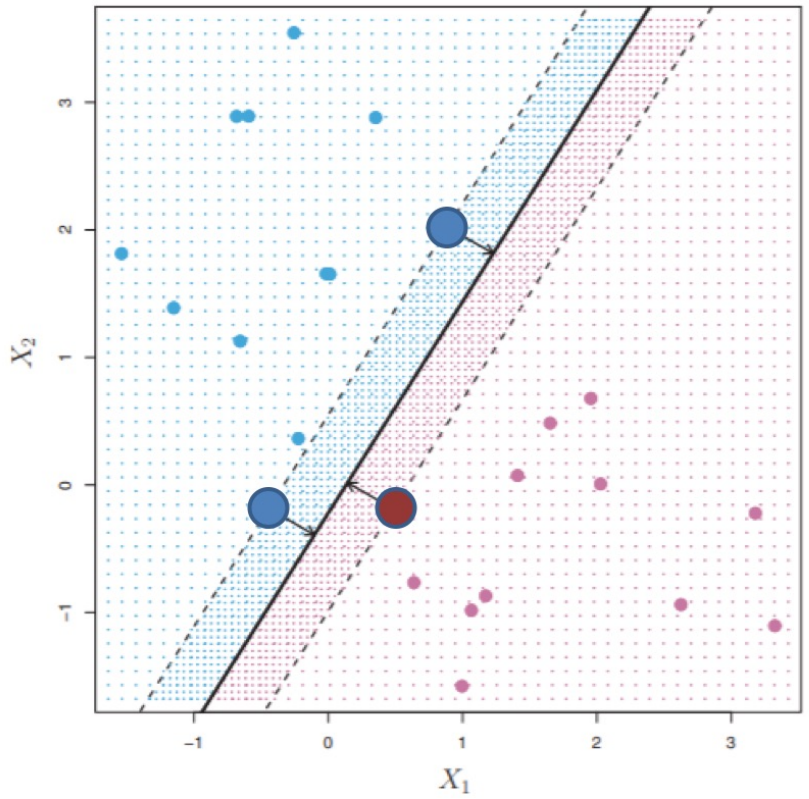
Gradient Descent for Logistic Regression

Optimal Linear Classifiers



Which of these linear classifiers is the best?

Support Vectors Classifiers



- Support vectors = points “closest” to hyperplane
- Support vector classifier: maximize the margin
- If support vectors change, classifier changes

Hinge Loss

- Linear SVM: $h_\theta(x_i) = \theta^T x_i$
- Optimization solution equivalent to:
- $J(\theta) = \sum_{i=0}^{N} \max\left(0, 1 - y_i h_\theta(x_i)\right) + \lambda \sum_{j=1}^{d} \theta_j^2$

- $J(\theta) = C \sum_{i=0}^{N} \max\left(0, 1 - y_i h_\theta(x_i)\right) + \sum_{j=1}^{d} \theta_j^2$

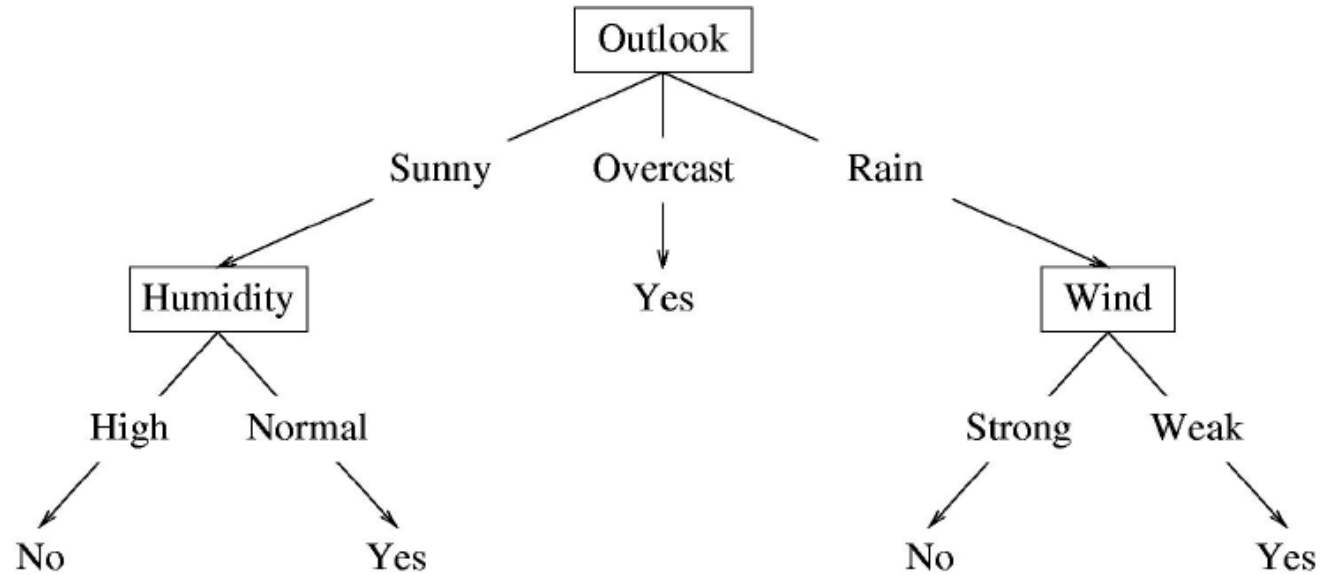
$C = \text{regularization cost}$

SVM Classifier

- Support Vector Classifier (SVC, linear SVM)
  - Train with hinge loss objective
  - Linear SVM classifier is linear combination of dot product between testing point and support vectors
  - $h(z) = \theta_0 + \sum_{i \in S} \alpha_i < z, x_i >$
- SVM classifier
  - Select a kernel function K
  - SVM classifier is linear combination of kernel between testing point and support vectors
  - $h(z) = \theta_0 + \sum_{i \in S} \alpha_i K(z, x_i)$
- Polynomial kernel of degree *p*
  - $K(x, y) = \left(1 + \sum_{i=0}^{d} x_i y_i\right)^p$
- Radial Basis Function (RBF) kernel (or Gaussian)
  - $K(x, y) = \exp\left(-\sum_{i=0}^{d} (x_i - y_i)^2 / 2\gamma^2\right)$

Decision Tree

- A possible decision tree for the data:



- Each internal node: test one attribute X_i
- Each branch from a node: selects one value for X_i
- Each leaf node: predict Y (or $p(Y \mid x \in \text{leaf})$)

Learning Decision Trees

- Start from empty decision tree
- Split on **next best attribute (feature)**
  - Use, for example, information gain to select attribute:

$$\arg\max_i IG(X_i) = \arg\max_i H(Y) - H(Y \mid X_i)$$

- Recurse

ID3 algorithm uses Information Gain
Information Gain reduces uncertainty on Y

Decision Trees Limitations

- Are prone to overfitting
  - Can train them to get training error of 0
  - Need stopping condition
  - Pruning
- They are rarely used on their own, but typically used in ensembles

Ensemble Learning

Consider a set of classifiers h_1, ..., h_L

Idea: construct a classifier $H(\mathbf{x})$ that combines the individual decisions of h_1, ..., h_L

- e.g., could have the member classifiers vote, or
- e.g., could use different members for different regions of the instance space

Successful ensembles require **diversity**

- Classifiers should make different mistakes
- Can have different types of base learners

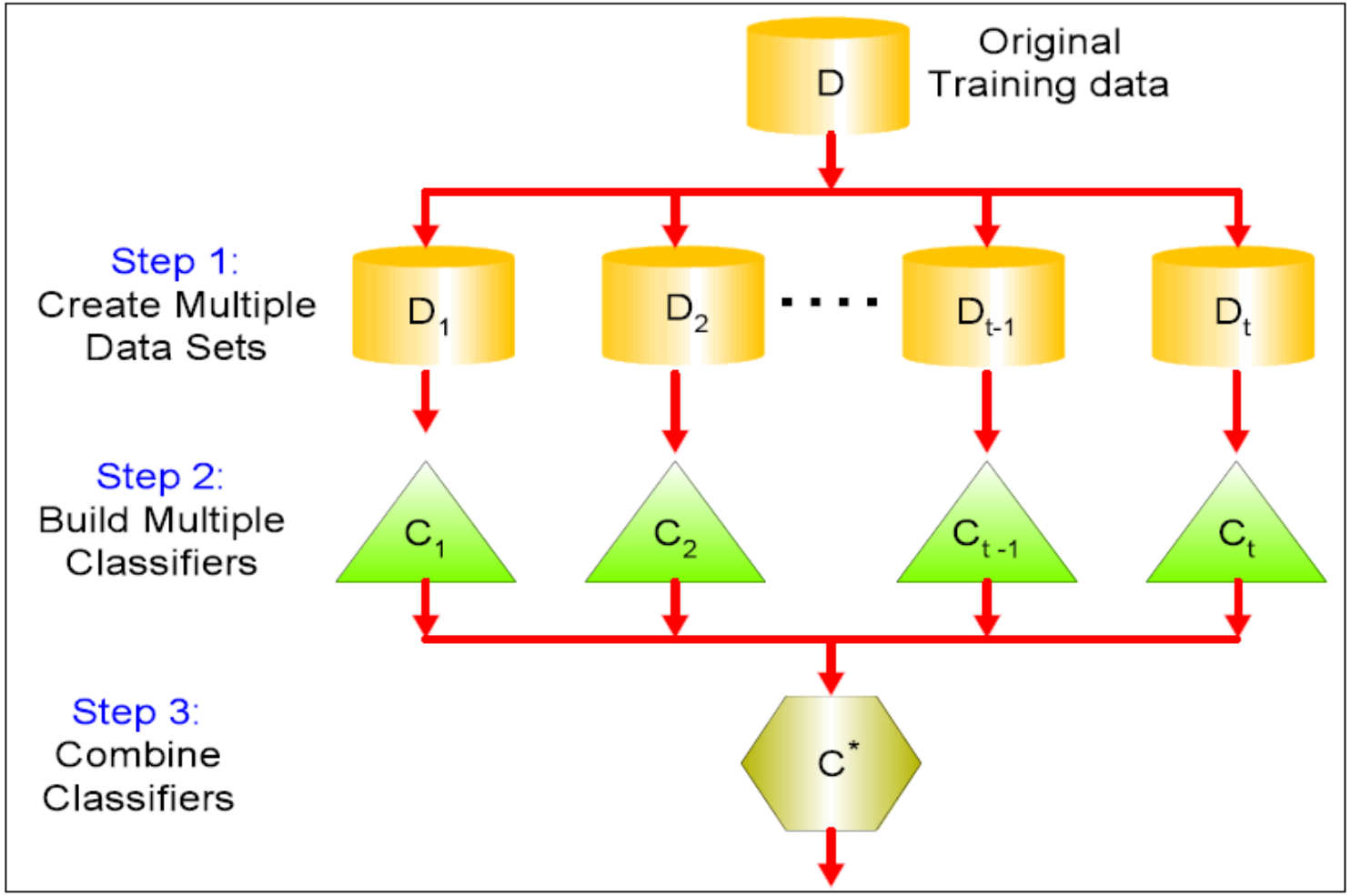
How to Achieve Diversity

- Avoid overfitting
  - Vary the training data
- Features are noisy
  - Vary the set of features

Two main ensemble learning methods

- Bagging (e.g., Random Forests)
- Boosting (e.g., AdaBoost)

Bagging

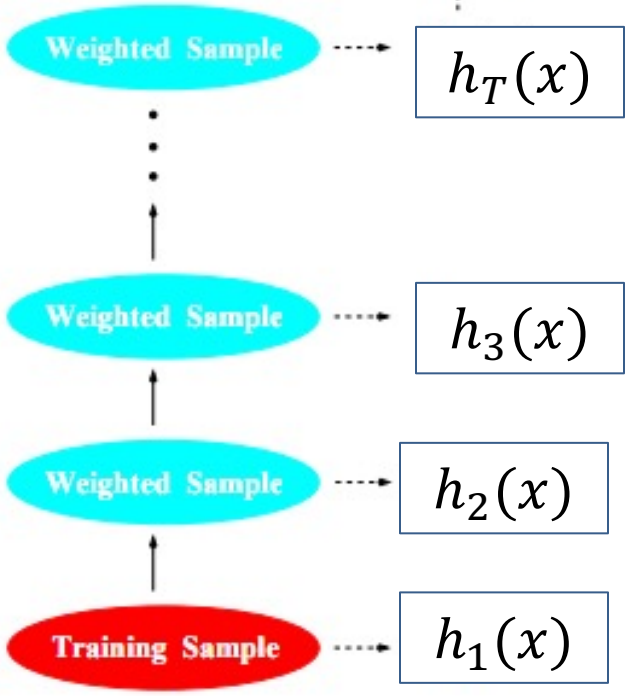


Majority Votes

Boosting

Sequential training process

$$G(x) = sign(\sum_{t=1}^{T} \beta_t h_t(x))$$



- Mis-classified examples get higher weights
- Correct examples get lower weights

Uniform weights

Better classifiers will get higher weights

FIGURE 10.1. *Schematic of AdaBoost. Classifiers are trained on weighted versions of the dataset, and then combined to produce a final prediction.*

Bagging vs Boosting

Bagging	vs.	Boosting
Resamples data points		Reweights data points (modifies their distribution)
Weight of each classifier is the same		Weight is dependent on classifier's accuracy
Only variance reduction		Both bias and variance reduced – learning rule becomes more complex with iterations

Applicable to complex models with low bias, high variance

Applicable to weak models with high bias, low variance

Summary

- Supervised learning tasks include classification and regression
- Linear regression has closed form solution for MSE loss
- Gradient Descent is a general optimization technique
  - Converges for convex objectives (MSE)
  - Applied to cross-entropy loss for logistic regression
  - Can be extended for deep learning
- Non-linear classifiers are more powerful than linear ones
  - Kernel SVMs (different kernels such as polynomial and Gaussian / RBF)
  - Decision trees (high interpretability, but prone to overfitting)
  - Ensembles (bagging and boosting) avoid overfitting and improve generalization

Acknowledgements

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  - Andrew Ng
  - Eric Eaton
  - David Sontag
- Thanks!