CY 7790

Special Topics in Security and Privacy: Machine Learning Security and Privacy
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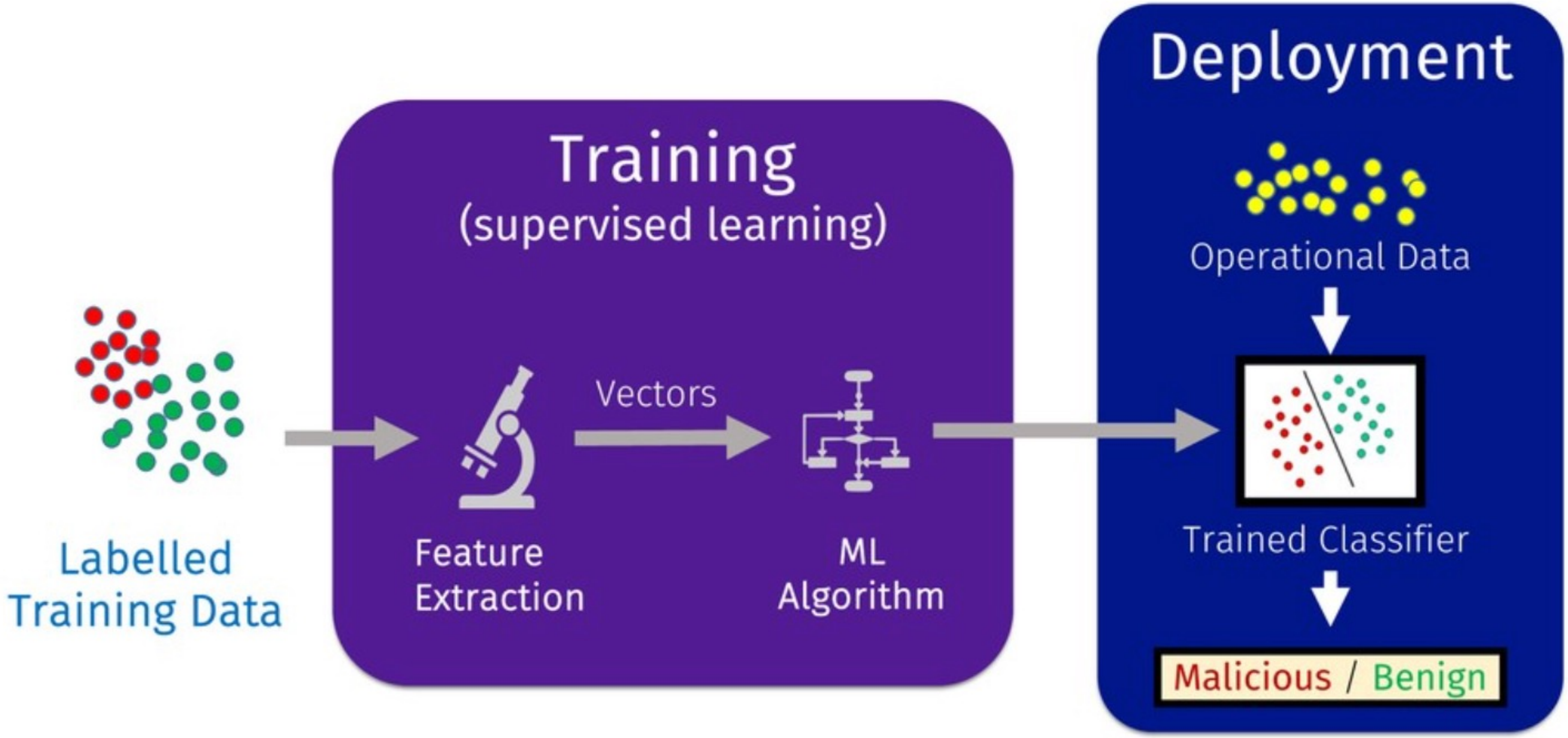
Outline: Review of ML

- 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

Data → Pre-processing → Feature extraction → ML model

Labeled

x_i. d-dim FEATURES

y_i discrete LABELS

Normalization

Feature Selection

Classification

$h(x)$

Testing

New data → ML model → Predictions

Unlabeled

x'

$h(x)$

Positive
Negative

Classification

$y' = h(x')$

Supervised Learning: Regression

Training

Data → Pre-processing → Feature extraction → ML model

Labeled

Normalization

Feature Selection

Regression

$x_i, y_i \in R$

RESPONSE VAR

$h(x)$

Testing

New data → ML model → Predictions

$y' = h(x') \in R$

Unlabeled

x'

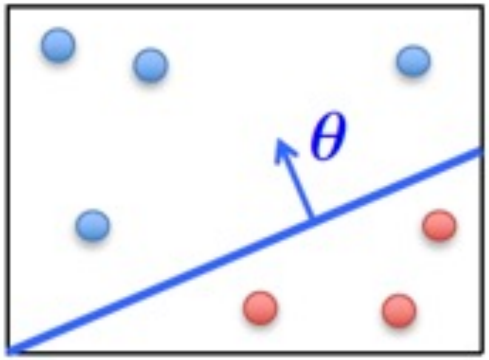
$h(x)$

Response variable

Regression

Supervised learning

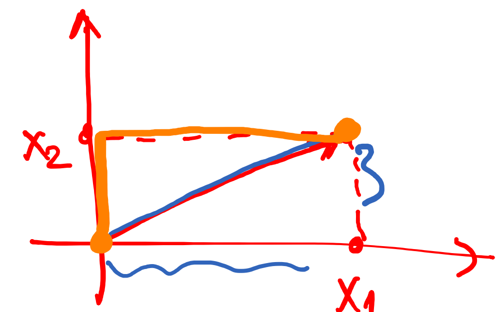
- Training data   d dim.
  - $x_i = [x_{i,1}, \ldots x_{i,d}]$: vector of features
  - y_i: labels   RES. VAR.
- Models (hypothesis)
  - Example: Linear model
    - $h_\theta(x) = \theta_0 + \theta_1 x$ θ = Model param.



- 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)

$$||x||_2 = \sqrt{x_1^2 + x_2^2} \quad L_2$$

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

$$||x||_1 = |x_1| + |x_2| \quad L_1$$

- L_∞

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

Distance Metrics

- Euclidean Distance $\sqrt{(\sum_{i=1}^{k}(x_i - y_i)^2)}$ $\|x-y\|_2$
- Manhattan Distance $\sum_{i=1}^{k}|x_i - y_i| = \|x-y\|_1$
- Minkowski Distance $\left(\sum_{i=1}^{k}(|x_i - y_i|)^q\right)^{\frac{1}{q}}$

Vector Operations

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

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

$$X+Y = [X_1+Y_1, \ldots, X_N+Y_N]$$

$$X-Y$$

Linear Regression $\simeq 1800$

- Linear Model $(x_1, \dots, x_N), (y_1, \dots, y_N)$

$\in \mathbb{R}^d$

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

$$= \theta_0 + \theta_1 x_1 + \dots + \theta_d x_d$$

- Let

Model param

$$\boldsymbol{\theta} = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \vdots \\ \theta_d \end{bmatrix} \qquad \boldsymbol{x}^\intercal = \begin{bmatrix} 1 & \underbrace{x_1 \quad \dots \quad x_d}_{d\text{-dim}} \end{bmatrix}$$

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

LEARN OPT θ

$$X = \begin{bmatrix} 1 & x_{11} & \cdots & x_{1d} \\ 1 & & & \\ \vdots & & & \\ 1 & x_{N1} & \cdots & x_{Nd} \end{bmatrix} \rightarrow i^{th} \text{ TRAINING EXAMPLE}$$

FEATURE j

size: $N \times \underline{(d+1)}$

$$\theta = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \vdots \\ \theta_d \end{bmatrix}$$

$\underline{(d+1)} \times 1$

$$X \cdot \theta = \begin{bmatrix} h_\theta(x_1) \\ \vdots \\ h_\theta(x_N) \end{bmatrix} = \hat{y}$$

PREDICTED RESPONSES

$$y = \begin{bmatrix} y_1 \\ \vdots \\ y_N \end{bmatrix}$$

TRAINING RES VAR

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

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

Training data

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

- Can write the model in vectorized form as $h_{\boldsymbol{\theta}}(\boldsymbol{x}) = \boldsymbol{X}\boldsymbol{\theta}$

Model prediction vector $\hat{y}$

Least-Squares Linear Regression

- Cost Function

  LOSS

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

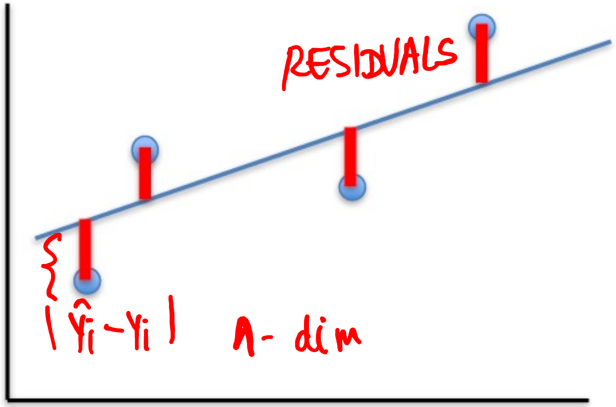
Mean Square Error (MSE)

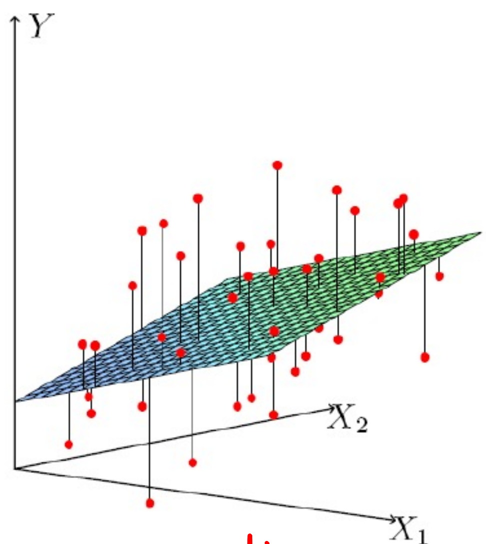
- Fit by solving $\boxed{\min_{\theta} J(\boldsymbol{\theta})}$

$$J(\theta) = \frac{1}{N}\sum_{i=1}^{N}|\hat{y}_i - y_i|^2$$

$$= \frac{1}{N}\|\hat{Y} - Y\|_2^2$$

$$= \frac{1}{N}\|X\cdot\theta - Y\|_2^2$$





2-dim

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

$$\frac{\partial y}{\partial x} = \left[\frac{\partial y}{\partial x_1} \quad \frac{\partial y}{\partial x_2} \quad \cdots \quad \frac{\partial y}{\partial x_n} \right]$$

Vector gradient (row vector)

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

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

m

n

Jacobian matrix (Matrix gradient)

Properties

- If w, x are $(d \times 1)$ vectors, $\boxed{\frac{\partial w^T x}{\partial x} = w^T}$
- If A: $(n \times d)$ x: $(d \times 1)$, $\frac{\partial Ax}{\partial x} = A$
- If A: $(d \times d)$ x: $(d \times 1)$, $\frac{\partial x^T Ax}{\partial x} = (A + A^T)x$
- If A symmetric: $\frac{\partial x^T Ax}{\partial x} = 2Ax$
- If x: $(d \times 1)$, $\boxed{\frac{\partial ||x||^2}{\partial x} = 2x^T}$

$$x = \begin{bmatrix} x_1 \\ \vdots \\ x_d \end{bmatrix}$$

$$||x||^2 = x_1^2 + \cdots + x_d^2$$

$$\frac{\partial ||x||^2}{\partial x} = \left[\frac{\partial ||x||^2}{\partial x_1}, \cdots, \frac{\partial ||x||^2}{\partial x_d} \right]$$

$$= \left[2x_1, \cdots, 2x_d \right]$$

$$= 2x^T$$

Closed-Form Solution

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

– Notice that the solution is when $\boxed{\frac{\partial}{\partial \boldsymbol{\theta}} J(\boldsymbol{\theta}) = 0}$

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

$$\frac{\partial J(\theta)}{\partial \theta} = \frac{2}{N} \cdot \underbrace{(X\theta - y)^T \cdot X} = 0$$

$(A \cdot B)^T = B^T A^T$

$$X^T (X\theta - y) = 0$$

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

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

$\rightarrow$ size $(d+1) \times 1$

$(d+1) \times (d+1)$, $(d+1) \times N$, $N \times 1$

X: $N \times (d+1)$

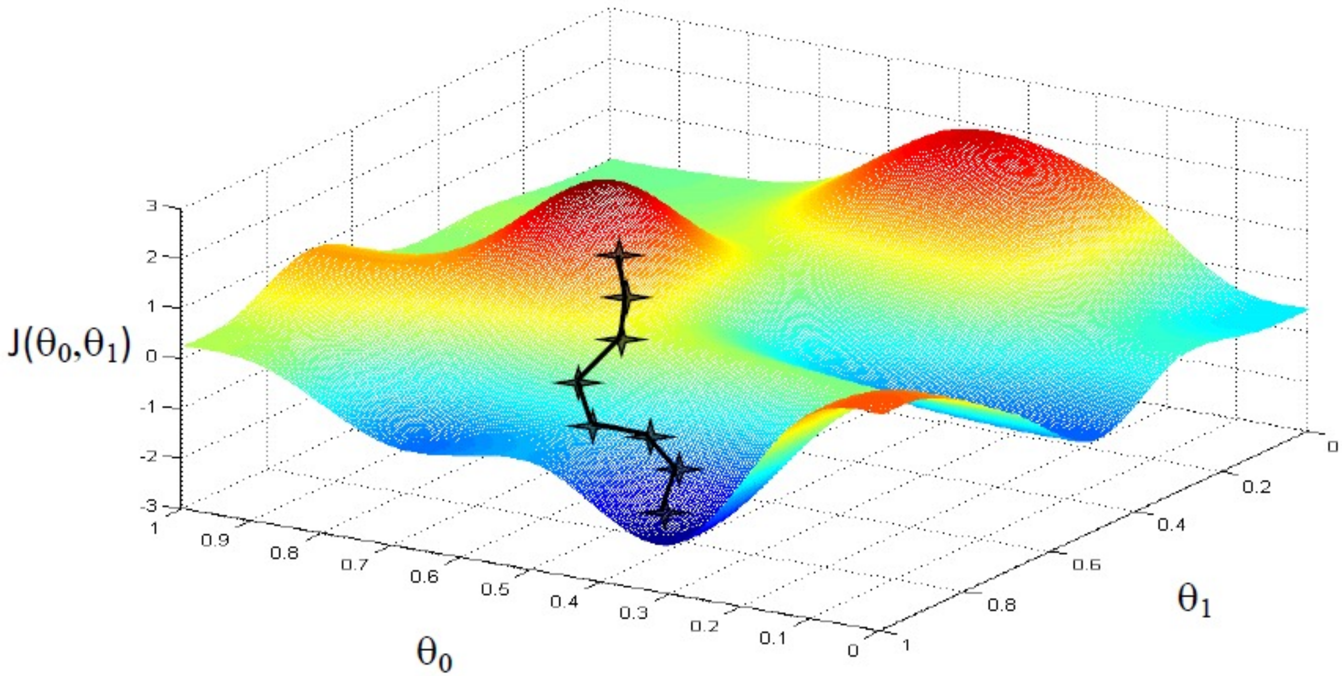
$X^T X$: $(d+1) \times (d+1)$

Gradient Descent

min $J(\theta)$

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

$$\frac{\partial J(\theta)}{\partial \theta}$$



Gradient Descent

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

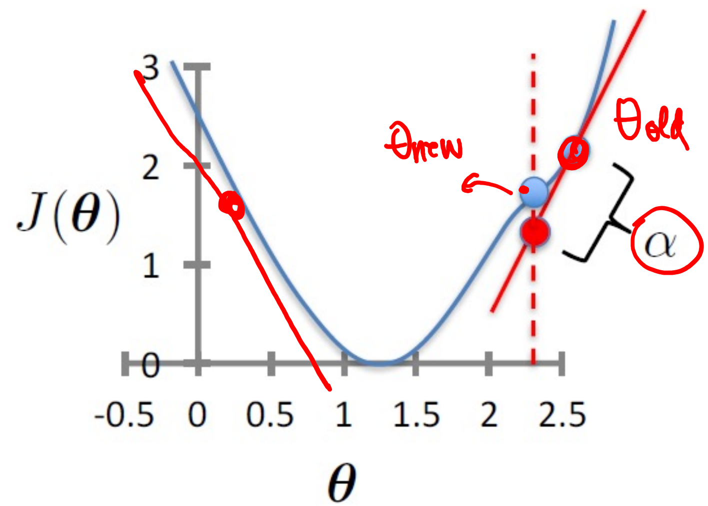
$$\theta_j \leftarrow \theta_j - \boxed{\alpha} \frac{\partial}{\partial \theta_j} J(\boldsymbol{\theta})$$

simultaneous update
for j = 0 ... d

learning rate (small)
e.g., α = 0.05

$$\theta = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \vdots \\ \theta_d \end{bmatrix}$$

$$f'(x) = \frac{f(x+\delta) - f(x)}{\delta}$$



FOR CONVEX OBJ, IT CONVERGES

- Gradient = slope of line tangent to curve
- Function decreases faster in negative direction of gradient

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

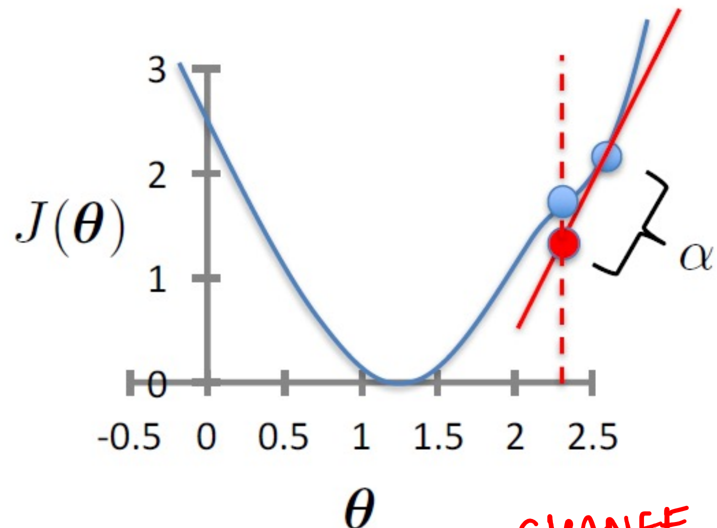
Stopping Condition

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

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

simultaneous update
for j = 0 ... d

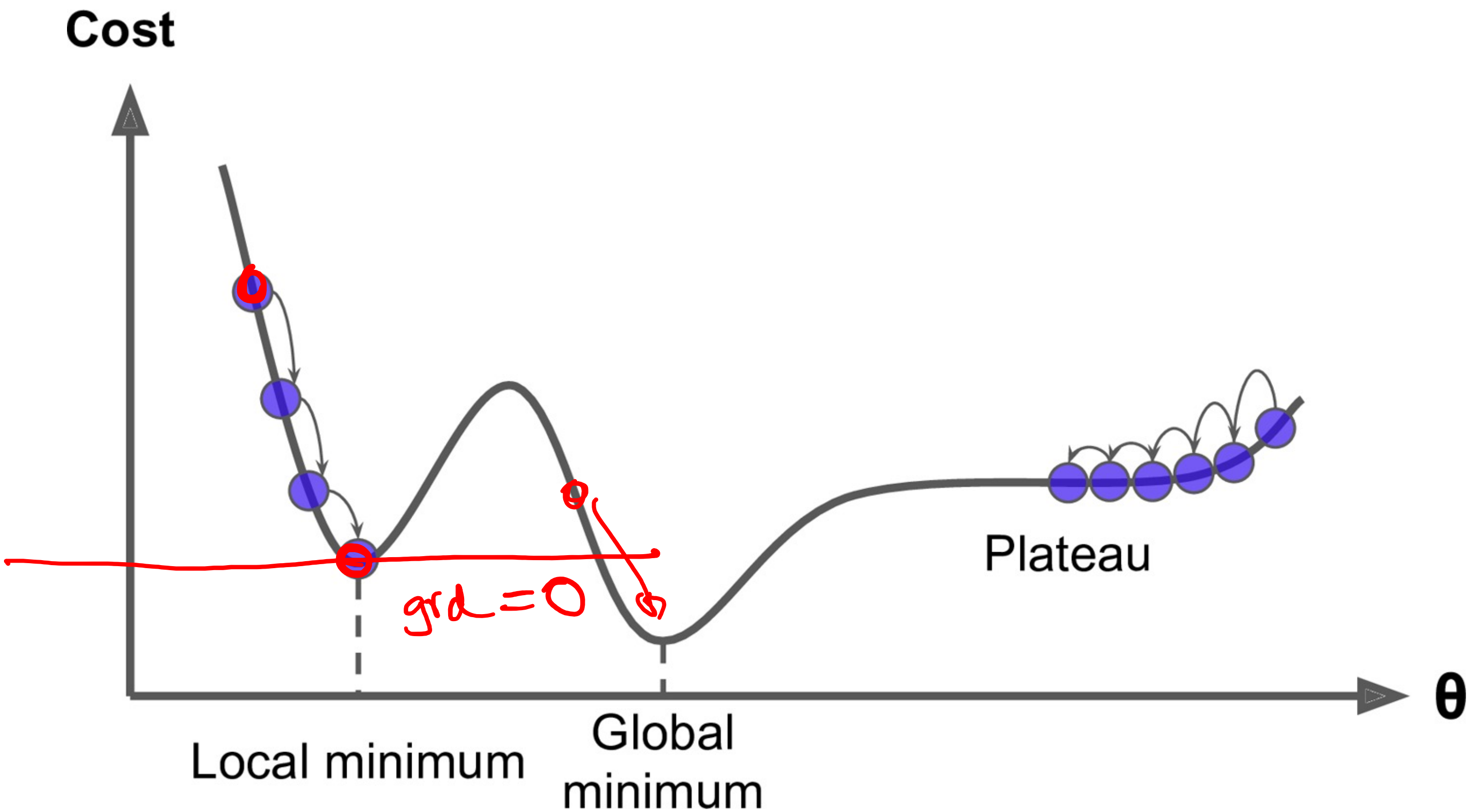
learning rate (small)
e.g., α = 0.05



- When should the algorithm stop?

CHANGE IN OBJ
FIX ITERATIONS

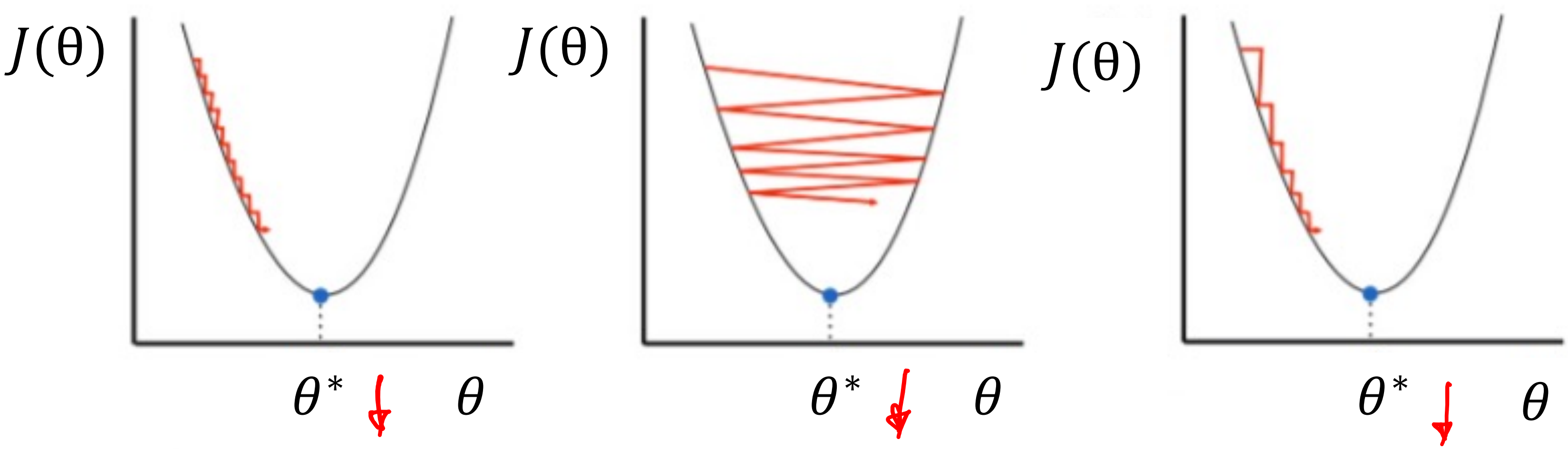
GD Convergence Issues



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

Solutions: start from multiple random locations / adaptive learning rate

Adaptive step size



(a) Step-size too small (b) Step-size too big (c) Adaptive step-size

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

Gradient Descent for Linear Regression

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

$$J(\theta) = \frac{1}{N} \|X\theta - Y\|^2 = \frac{1}{N} \sum_{i=1}^{N} \underbrace{\left[h_\theta(x_i) - y_i\right]}^2$$

$$h_\theta(x_i) = \theta^T x_i$$

$$= \theta_0 + \theta_1 \cdot x_{i1} + \dots + \theta_d x_{id}$$

$$\frac{\partial J(\theta)}{\partial \theta} = \frac{2}{N} (X\theta - Y)^T X$$

$$\rightarrow \quad \theta \leftarrow \theta - \alpha \cdot \frac{2}{N} \cdot (X\theta - Y)^T X$$

$$\rightarrow \quad \theta_j \leftarrow \theta_j - \alpha \cdot \frac{2}{N} \sum_{i=1}^{N} \left[h_\theta(x_i) - y_i\right) \cdot \boxed{\frac{\partial h_\theta(x_i)}{\partial \theta_j}}$$

$$x_{ij}$$

Learning Challenges

- 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

LINEAR

$\theta_0 + \theta_1 x$

HIGH BIAS

POL. DEG 2

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

DEG. 4

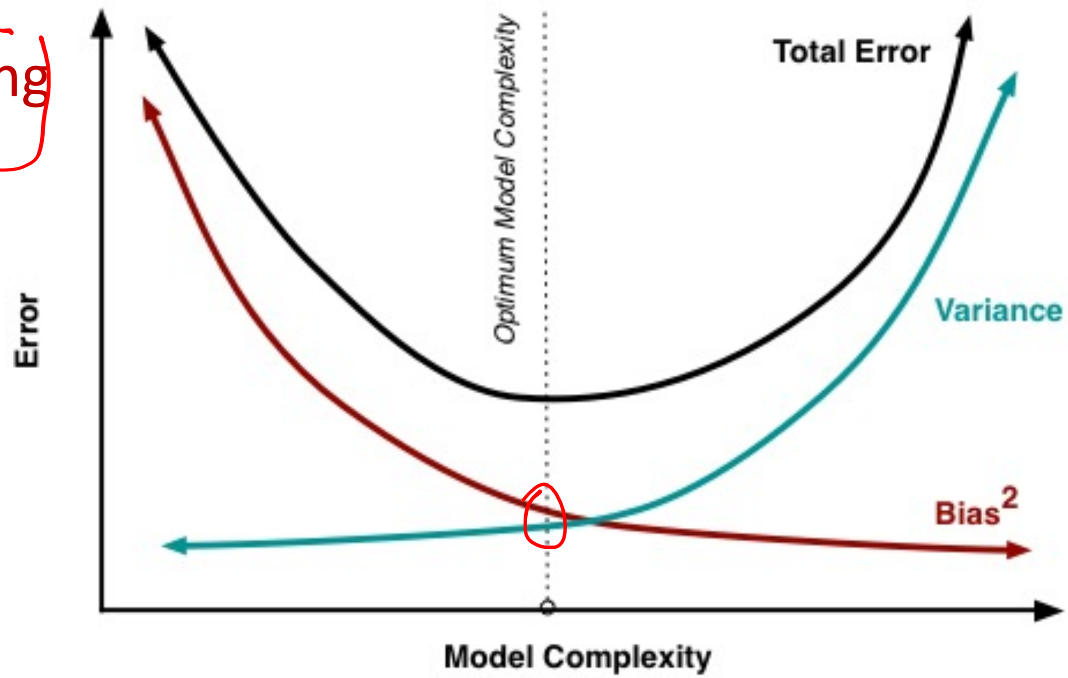
TRAIN ERROR = 0

$\theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3 + \theta_4 x^4$

HIGH VAR

Bias-Variance Tradeoff

Under-fitting

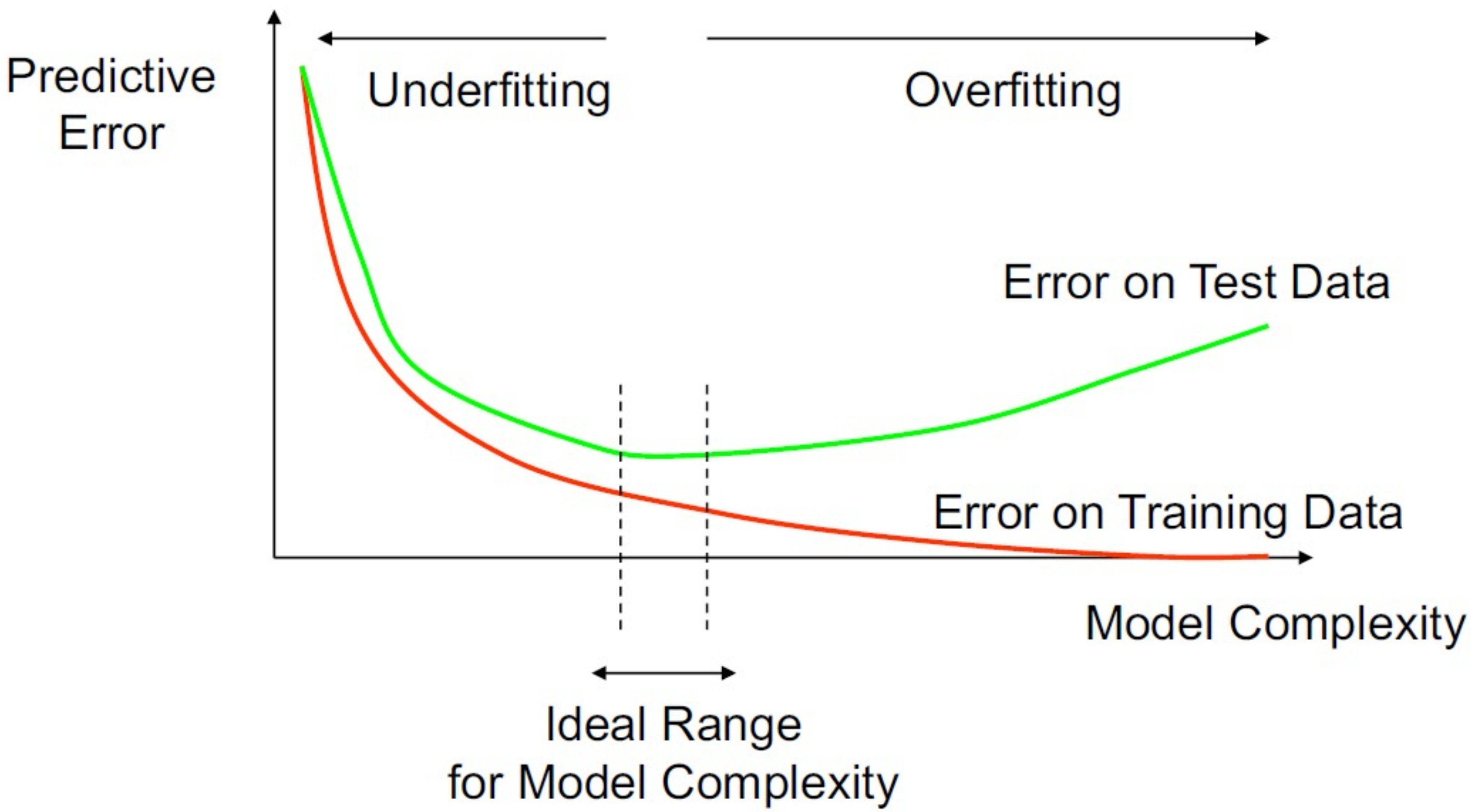


Over-fitting

- 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

$\lambda \|\theta\|^2 \quad l_2$

- Linear regression objective function

MSE

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

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

RIDGE OR L2 , $\lambda \|\theta\|_2^2$, $\lambda \uparrow \quad \theta \downarrow$

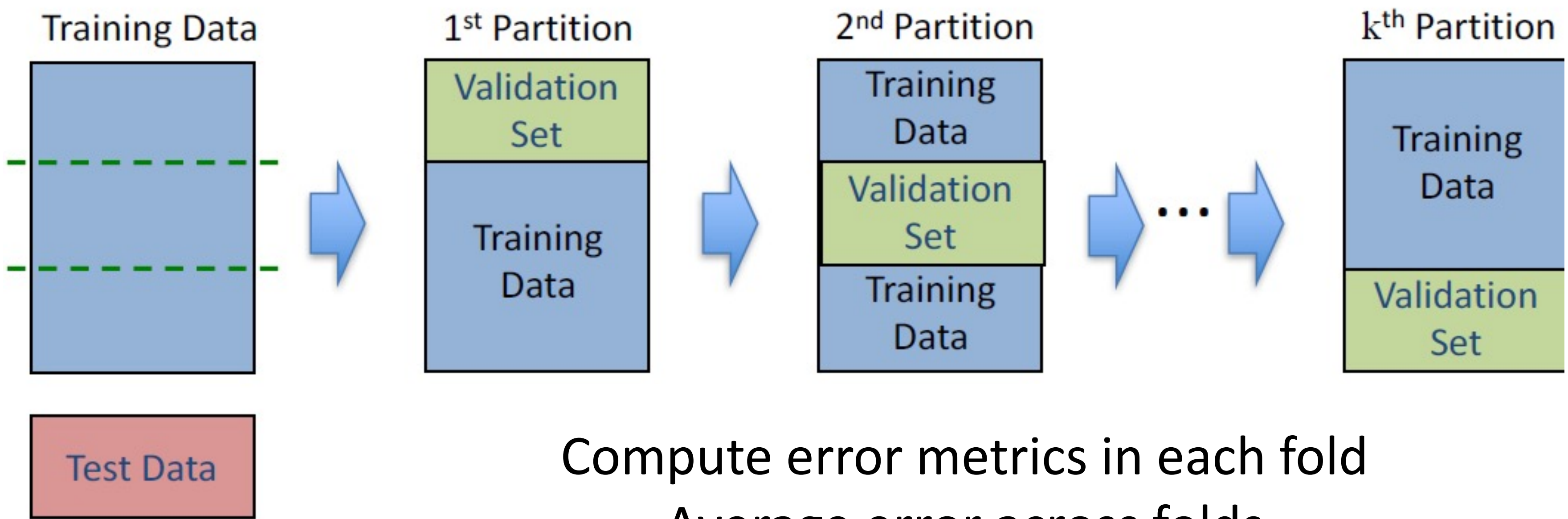
LASSO OR L1 , $\lambda |\theta|_1$

CLOSED FORM

$\theta = (X^T X + \lambda I)^{-1} X^T Y$

INVERTIBLE

k-fold Cross Validation



Compute error metrics in each fold
Average error across folds

- Split training data into k partitions (folds) of equal size
- Pick the optimal value of hyper-parameter according to error metric averaged over all folds (computed on validation set)

Supervised Learning: Classification

Training

Data → Pre-processing → Feature extraction → ML model

- Data: Labeled, x_i. d-dim, y_i discrete
- Pre-processing: Normalization
- Feature extraction: Feature Selection
- ML model: Classification, $h(x)$

Testing

New data → ML model → Predictions

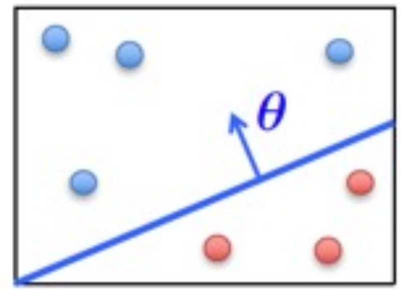
$y' = h(x')$

- New data: Unlabeled, x'
- ML model: $h(x)$
- Predictions: Positive / Negative — Classification

Linear Classifiers

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

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

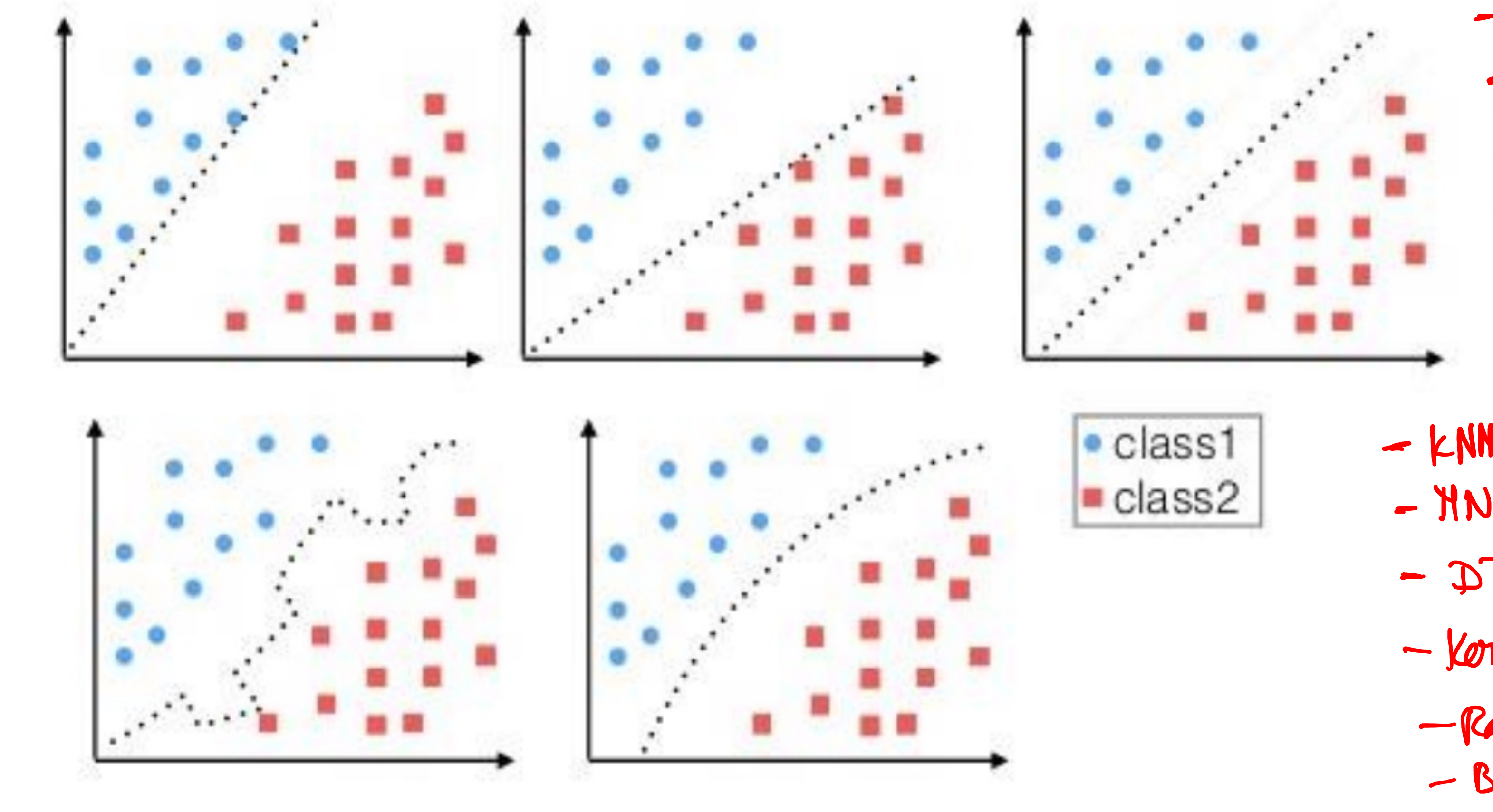


sign

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

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

Linear vs Non-Linear Classifiers



- LOG. REGRESSION
- LINEAR SVM
- PERCEPTRON
- LDA

⋮

- KNN
- NN (CNN, MLP)
- DT
- Kernel SVM
- Random forest
- Bagging

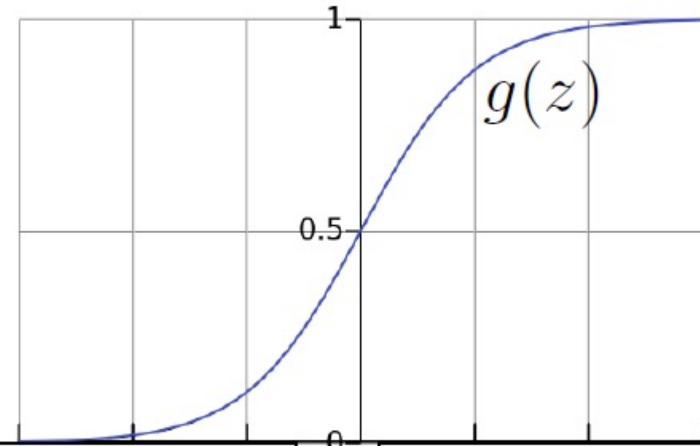
Logistic Regression

- Setup
  - Training data: $\{x_i, y_i\}$, for $i = 1, \ldots, N$
  - Labels: $y_i \in \{0,1\}$
- Goals
  - Learn $h_\theta(x) = \boxed{P(Y = 1|X = x)}$
  - $P(Y = 1|X) + P(Y = 0|X) = 1$
- 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

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

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

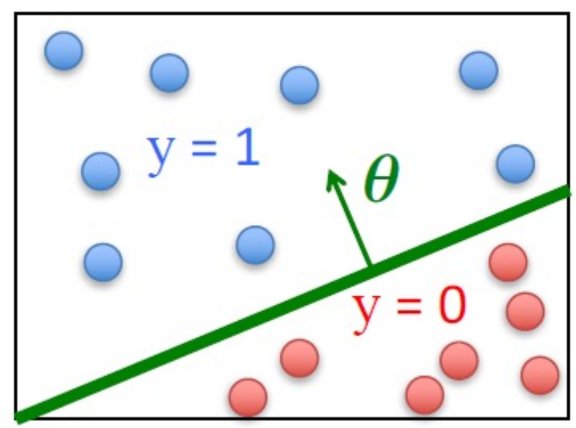


SIGMOID

$\boldsymbol{\theta}^\intercal \boldsymbol{x}$ should be large negative values for negative instances

$\boldsymbol{\theta}^\intercal \boldsymbol{x}$ should be large positive values for positive instances

- 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)

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

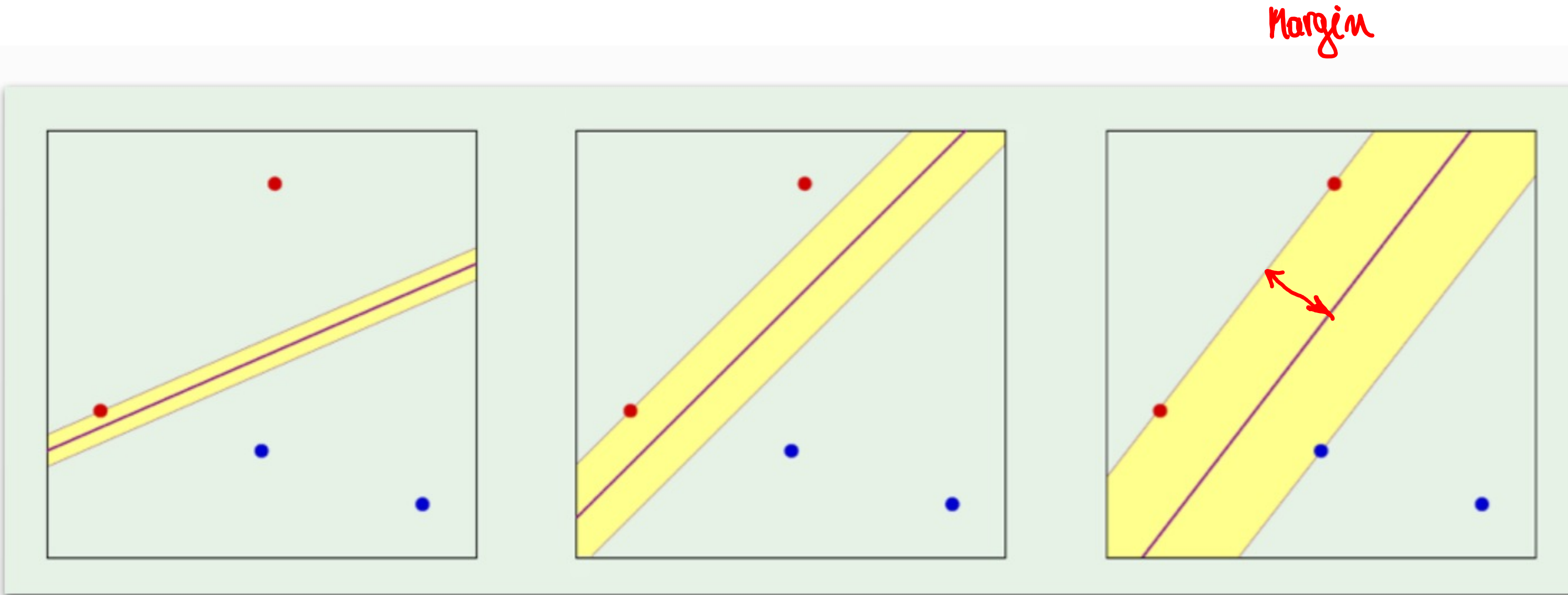
$$J(\theta) = -\sum_{i=1}^{N} [y_{\mathrm{i}} \log h_{\theta}(x_i) + (1 - y_i) \log \left(1 - h_\theta(x_i)\right)]$$

$y_i = 0$ $\qquad$ $y_i = 1$

$\log(1 - h_\theta(x_i))$ $\qquad$ $\log h_\theta(x_i)$

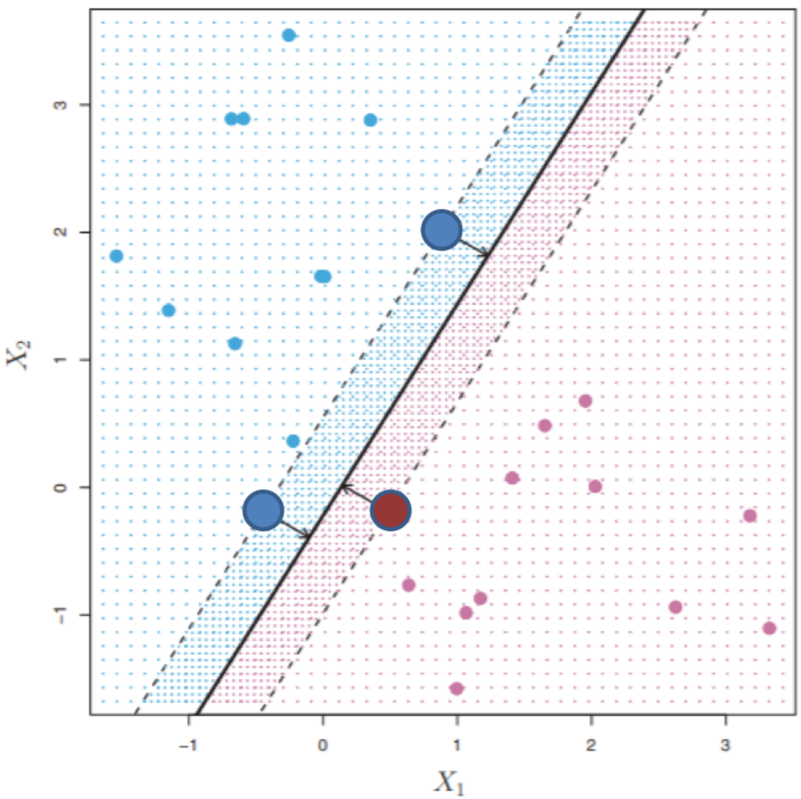
Gradient Descent for Logistic Regression

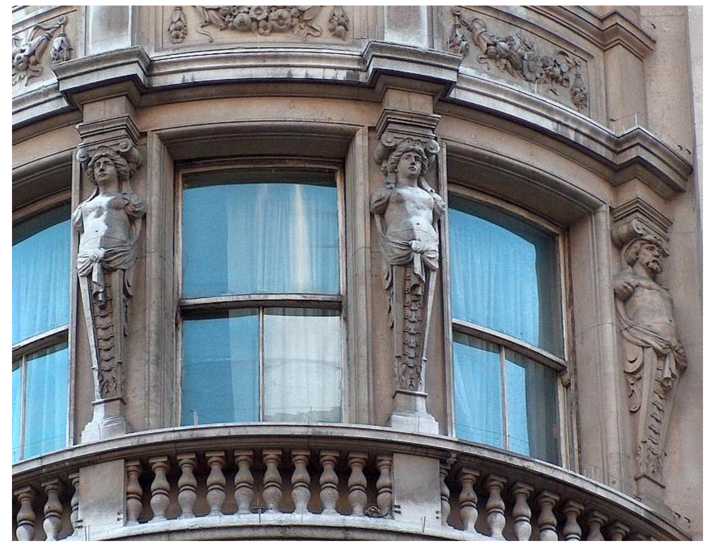
Optimal Linear Classifiers



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

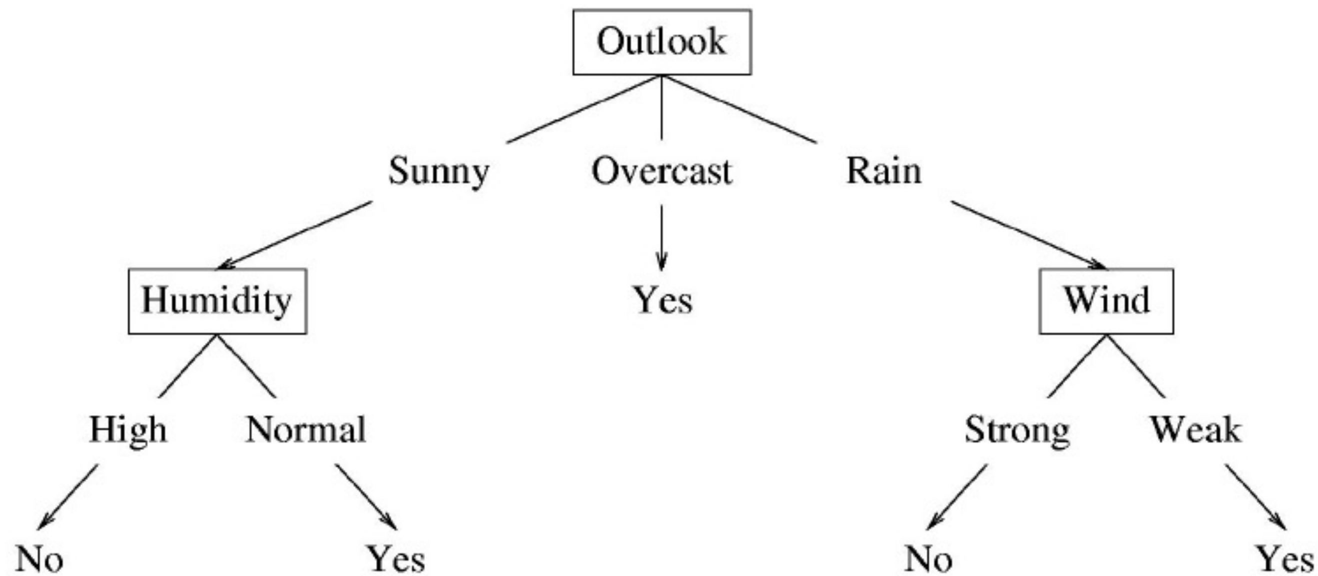
SVM Classifier

- 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
  - $h(z) = \theta_0 + \sum_{i \in S} \alpha_i < z, x_i >$ weight, support vector, S = set of support vectors
- 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)
  - $K(x, y) = \exp\left(-\sum_{i=0}^{d} (x_i - y_i)^2 / 2\gamma^2\right)$ PARAM: γ

$\frac{\|x-y\|^2}{2\gamma^2}$

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:

$$\arg\max_i IG(X_i) = \arg\max_i \underbrace{H(Y) - H(Y \mid X_i)}_{\text{GINI}}$$

- Recurse

ID3 algorithm uses Information Gain

Information Gain reduces uncertainty on Y

Ensemble Learning

Consider a set of classifiers h_1, ..., $\mathrm{h_L}$

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

- 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

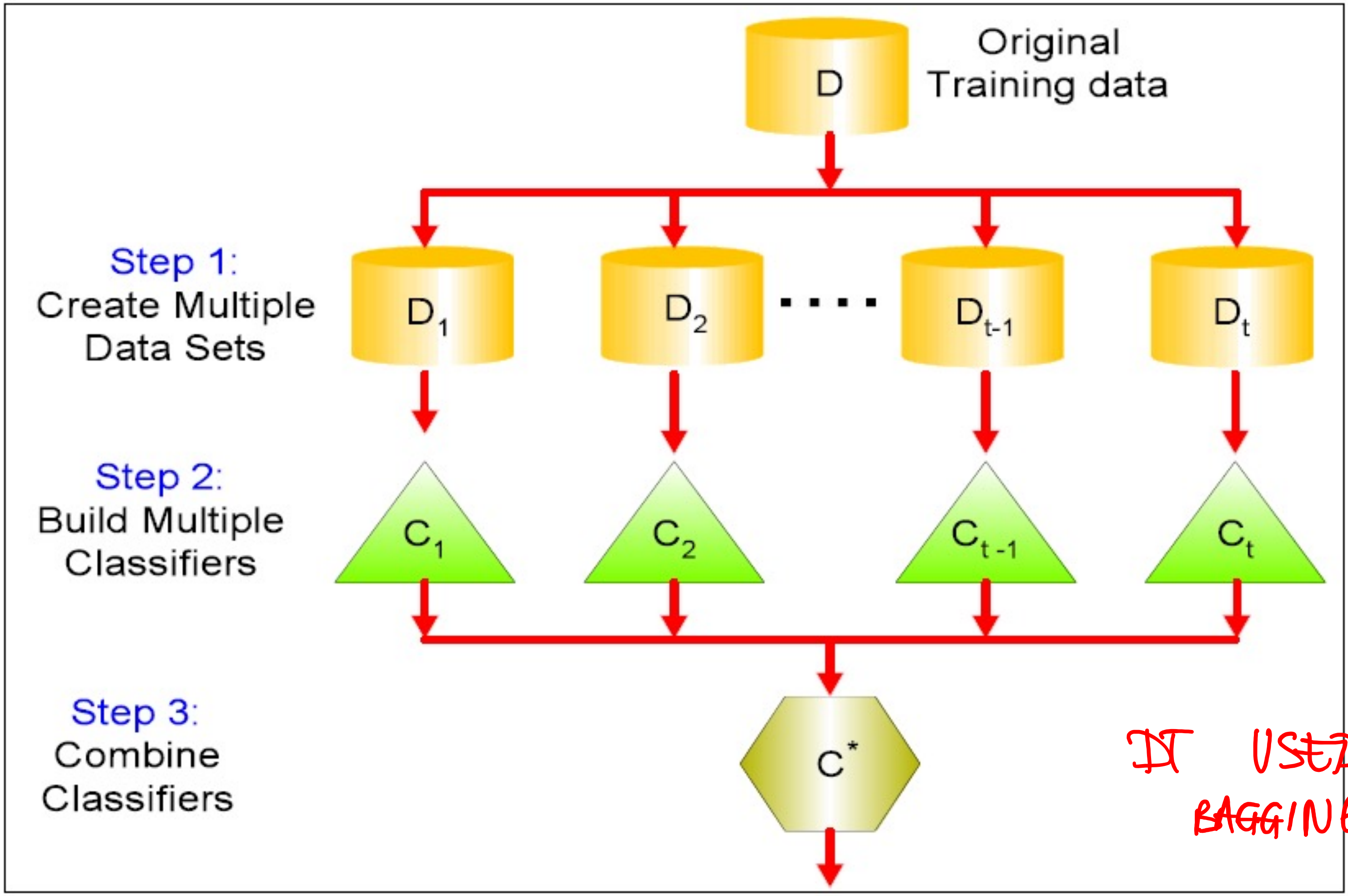
How to Achieve Diversity

- 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



RANDOM
W
REPLACEMENT

DT USED FOR
BAGGING

Majority Votes

Random Forest Algorithm

1. For $b = 1$ to B:

   (a) Draw a bootstrap sample $\mathbf{Z}^*$ of size N from the training data.

   (b) Grow a random-forest tree T_b to the bootstrapped data, by recursively repeating the following steps for each terminal node of the tree, until the minimum node size n_{min} is reached.

      i. Select m variables at random from the p variables.

      ii. Pick the best variable/split-point among the m.

      iii. Split the node into two daughter nodes.

2. Output the ensemble of trees $\{T_b\}_1^B$.

To make a prediction at a new point x:

Regression: $\hat{f}_{\text{rf}}^B(x) = \frac{1}{B}\sum_{b=1}^B T_b(x)$.

Classification: Let $\hat{C}_b(x)$ be the class prediction of the bth random-forest tree. Then $\hat{C}_{\text{rf}}^B(x) = \textit{majority vote}\ \{\hat{C}_b(x)\}_1^B$.

Summary

- 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
  - Kernel SVMs (different kernels such as polynomial and Gaussian / RBF)
  - Decision trees (high interpretability, but prone to overfitting)
  - Ensembles (bagging and boosting)