Linear Models

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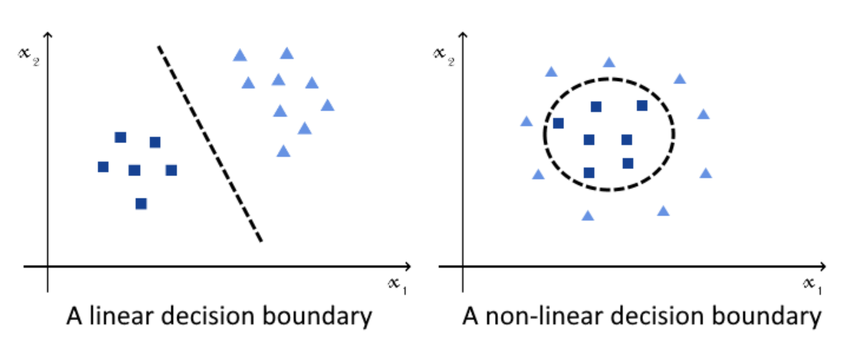
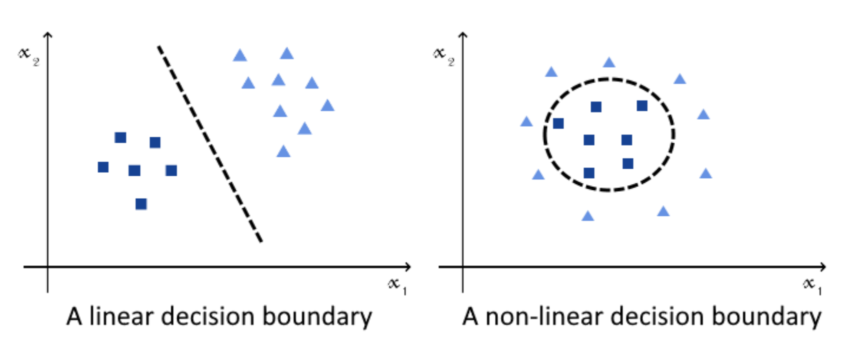
- Linear Classification
- Margins, Regularization, and Optimization
- Overfitting vs. Underfitting
- Bias-Variance Trade-off
- Linear Regression

Linear Classification

- $\theta \cdot X + \theta_0 = 0$
- X: both a vector and a point in high-dimensional space

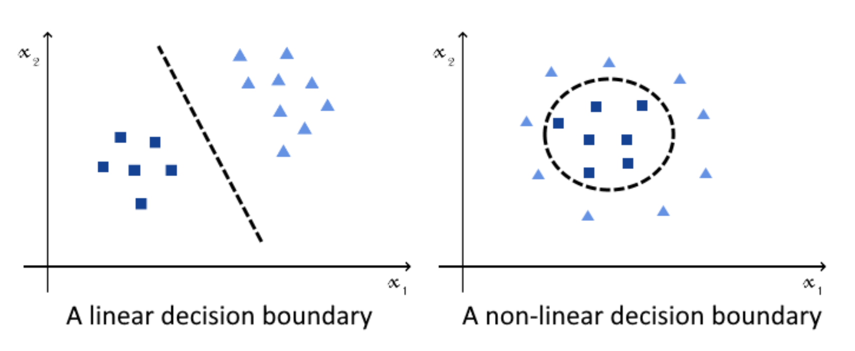


- θ: also a vector, determine the orientation of the decision boundary
  - Consider $\theta \cdot X = 0$ (a linear classifier goes through the origin), θ is perpendicular to X, thus determine the orientation



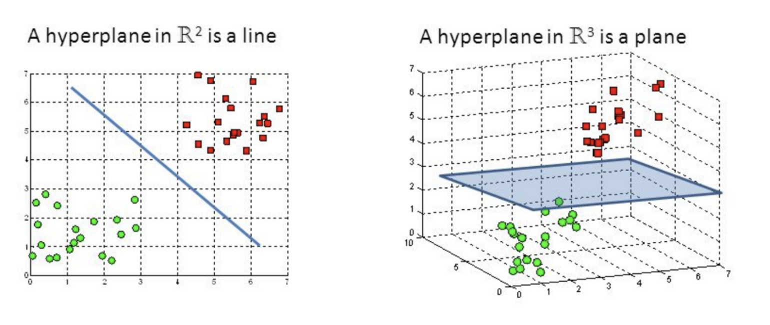
- Note that different θ can result in the same linear classifier, i.e., $c\theta \cdot X = \theta \cdot X = 0$

- $\theta \cdot X + \theta_0 = 0$
- θ_0: determine the location of the decision boundary



- Why it's called linear classifier?
- Linear operations
  - Addition
  - Multiplication with a constant
- $\theta \cdot X$: only linear operations conducted on the elements of X

- Linear classifier go beyond a “line”



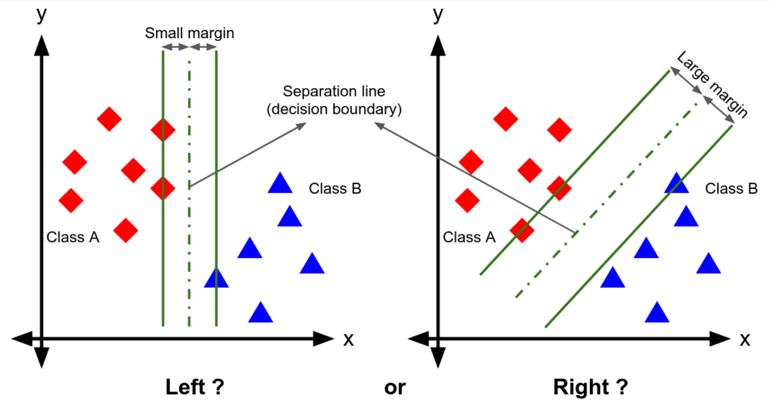
- For n training examples $S_n = \{(X^{(i)}, y^{(i)}), i = 1, \ldots, n\}$ if there exist θ and θ_0 such that $y^{(i)}(\theta \cdot X^{(i)} + \theta_0) > 0$ for all $i = 1, \ldots, n$, we call these training examples linearly separable
    - $X^{(i)}$: ith training example
    - $y^{(i)}$: ith training example's label ($+$ or $-$)
    - $\theta \cdot X^{(i)} + \theta_0$: result of the classifier ($+$ or $-$)
- $y^{(i)}$ and $\theta \cdot X^{(i)} + \theta_0$ should have the same sign if the classifier works correctly

- Occurs when classifier makes a mistake
- For linear classification, occurs when data are not linearly separable, otherwise there exist algorithms guarantee no error
- Denote h as the classifier, n as the total number of training examples, we have the classification error:

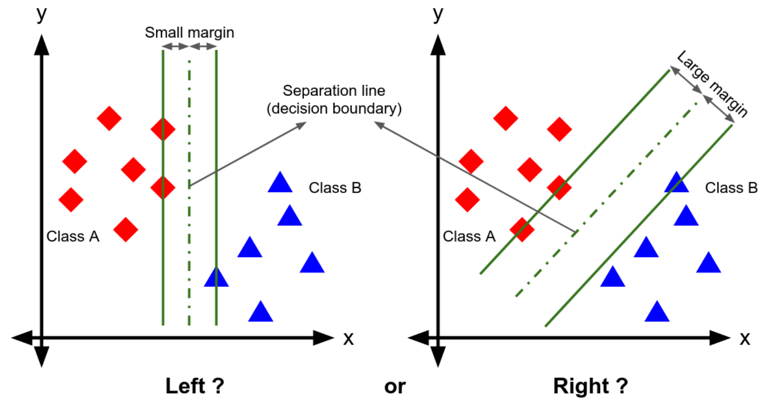
$$\epsilon_n(h) = \frac{1}{n}\sum_{i=1}^{n}[[h(X^{(i)}) \neq y^{(i)}]]$$

Margins, Regularization, and Optimization

- Large margin: more robust classifier (against noise), less accurate



- Small margin: less robust classifier, more accurate



- Hinge loss encourages large margins
- Denote ζ as the distance from the margin boundary to the decision boundary:
  - When $y^{(i)}(\theta \cdot X^{(i)} + \theta_0) > \zeta$, loss $= 0$
  - When $y^{(i)}(\theta \cdot X^{(i)} + \theta_0) \leq \zeta$, loss $= \zeta - y^{(i)}(\theta \cdot X^{(i)} + \theta_0)$

- Recall the decision boundary of linear classification

$$\theta \cdot X + \theta_0 = 0$$

- Then, the margin boundary of the decision boundary

$$\theta \cdot X + \theta_0 = \zeta$$

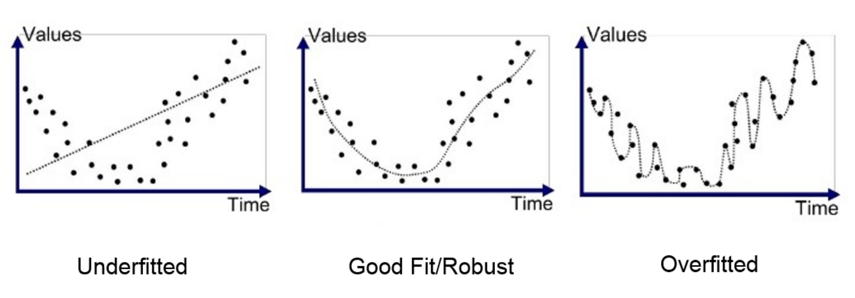
- If divide both sides by $\|\theta\|$, the decision boundary won't change but the margin boundary ($\frac{\zeta}{\|\theta\|}$) will decrease if $\|\theta\|$ increases
- In general, the goal of regularization is to obtain a more robust classifier, thus prefer large margins (small $\|\theta\|$)

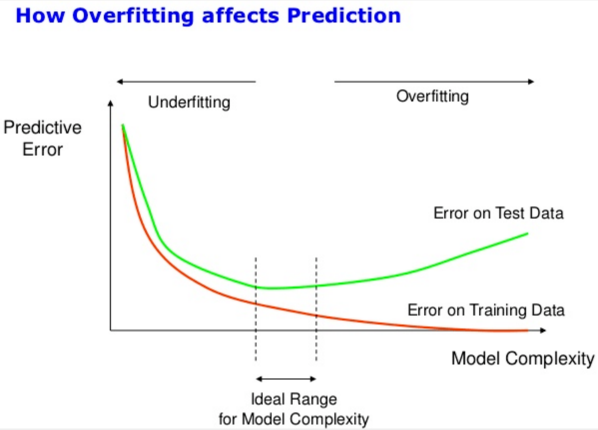
- Objective function

$$J(\theta, \theta_0) = \epsilon_n(h) + \frac{\lambda}{2}\|\theta\|^2$$

- λ: regularization parameter (a hyperparameter)

Overfitting vs. Underfitting


Values
Time
Underfitted
Values
Time
Good Fit/Robust
Values
Time
Overfitted

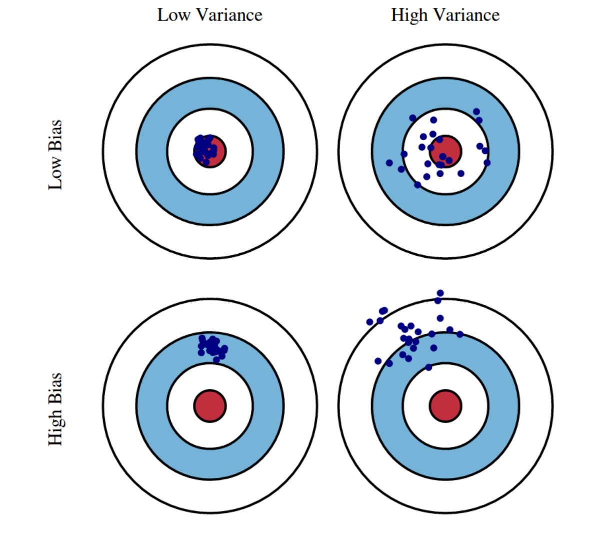


- Recall the objective function $J(\theta, \theta_0) = \epsilon_n(h) + \frac{\lambda}{2}\|\theta\|^2$
- Increase λ will encourage smaller θ (less complex model), thus prevent overfitting

Bias-Variance Trade-off

- Assume the underlying true relationship between X and y is $y = f(X) + \epsilon$
- X, y: data and label
- f: actual mapping (unknown)
- ϵ: irreducible error (unknown)
- $\hat{f}$: trained model depends on the training set (not fixed)

- $\mathbb{E}\left[\left(y - \hat{f}(x)\right)^2\right] =$
  $\left(f(x) - \mathbb{E}\left[\hat{f}(x)\right]\right)^2 + \mathbb{E}\left[\left(\hat{f}(x) - \mathbb{E}\left[\hat{f}(x)\right]\right)^2\right] + \mathbb{E}\left[\epsilon^2\right]$
- $\left(f(x) - \mathbb{E}\left[\hat{f}(x)\right]\right)^2$: bias
- $\mathbb{E}\left[\left(\hat{f}(x) - \mathbb{E}\left[\hat{f}(x)\right]\right)^2\right]$: variance
- $\mathbb{E}\left[\epsilon^2\right]$: irreducible error
- Because the left-hand side and $\mathbb{E}\left[\epsilon^2\right]$ are fixed, when bias increases variance decreases, and vice versa


Low Variance
High Variance
Low Bias
High Bias

- Overfitting: low bias and high variance
- Underfitting: high bias and low variance
- Desired model: balancing bias and variance (neither overfit nor underfit)

Linear Regression

- Denote $h(X^{(i)}) = \theta \cdot X^{(i)} + \theta_0$
- Classification
  - y takes discrete values
  - Example loss: $\frac{1}{n}\sum_{i=1}^{n}\left[\left[h(X^{(i)}) \neq y^{(i)}\right]\right]$
- Regression
  - y takes continuous values
  - Example loss: $\frac{1}{n}\sum_{i=1}^{n}\frac{\left(y^{(i)}-h\left(X^{(i)}\right)\right)^2}{2}$

- Compact representation: $\theta \cdot X + \theta_0 \to \theta' X'$ ($\theta' = [\theta, \theta_0]$, $X' = [X, 1]$)
- Step 1: initialize θ'
- Step 2: randomly select a training example (X', y)
- Step 3: update θ' via $\theta' \leftarrow \theta' + \alpha(y - \theta' \cdot X')X'$
  - α: learning rate
  - Where does this formula come from?
  - Why $+$?
- Step 4: if stopping criteria not meet, go to Step 2

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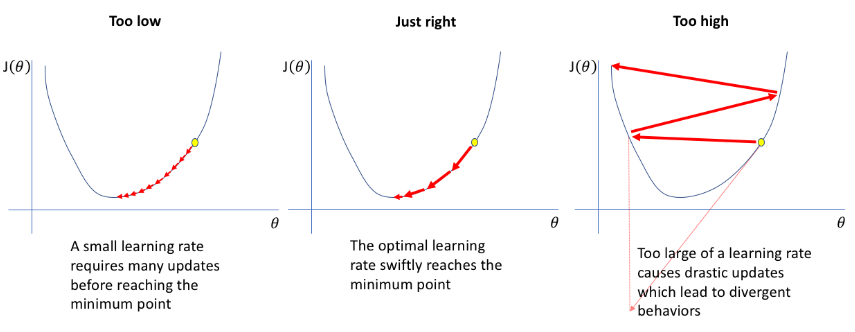
  - α: learning rate
  - Where does this formula come from? $\bigtriangledown_\theta \frac{(y-\theta' \cdot X')^2}{2}$
  - Why $+$? we need to go the opposite direction of the gradient
- Step 4: if stopping criteria not meet, go to Step 2

- Small learning rate: slow learning
- Large learning rate: overshoot (miss the optimal point)

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- Only applicable to linear problems (matrix operation is linear)
- Solution: $\theta' = \left(\frac{1}{n}\sum_{i=1}^{n} X'^{(i)}\left(X'^{(i)}\right)^T\right)^{-1}\left(\frac{1}{n}\sum_{i=1}^{n} y^{(i)} X'^{(i)}\right)$
- Pros: obtain the solution in one go
- Cons: 1) needs the matrix to be invertible, 2) matrix computation can be expensive