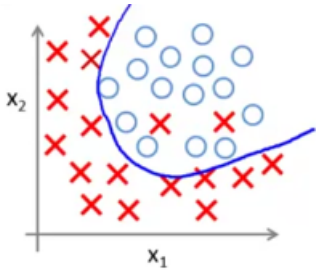
1 Logistic regression (for classification)

Categorize observations based on quantitative features.
Predict target class or probabilities of target classes.



1.1 Binary classification

- Description

  Logistic regression is a statistical method that studies the relationship between multiple variables:
  - n variables $x = \{x_1, x_2, \ldots, x_n\}$: the predictor, explanatory, independent variables,
  - one y variable: the response, outcome, dependent variable.

  Logistic regression expands the linear regression model with a *logistic function* to make it suitable for classification.
  Its dependent variable is therefore categorical instead of numerical.
  In case of a binary classification task, its dependent variable takes on one out of two possible values
  - $y \in \{0, 1\}$
  - 0 indicates the *negative* class
  - 1 indicates the *positive* class

- Model's hypothesis: output the estimated probability that $y = 1$ on input x
  - $z = \theta_0 + \theta_1 * x_1 + \theta_2 * x_2 + \ldots + \theta_n * x_n$
  - $h_\theta(x) = P(y = 1|x, \theta) = \sigma(z) = \frac{1}{1+e^{-z}} = \hat{y} \quad (0 <= h(x) <= 1)$
  - Note: $\sigma(z) \geq 0.5$ when $z \geq 0$

- Model's parameters (# $n + 1$)

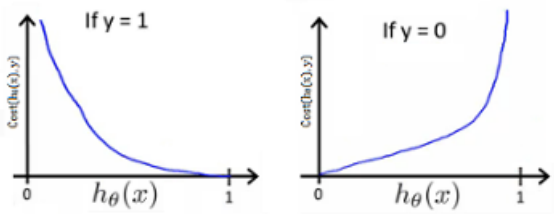
  $\theta = \{\theta_0, \theta_1, \ldots, \theta_n\}$

- Decision boundary
  - linear
  - non-linear when adding extra higher-order polynomial terms to the features

- Cost function

  $J(\theta) = \frac{1}{m} \sum_{i=1}^{m} \left(-y^{(i)} \, log \, \hat{y}^{(i)} - (1 - y^{(i)}) \, log \, (1 - \hat{y}^{(i)})\right)$

  in other words
  - $J(\theta) = \frac{1}{m} \sum_{i=1}^{m} \left(- \, log \, \hat{y}^{(i)}\right)$ when $y^{(i)} = 1$
  - $J(\theta) = \frac{1}{m} \sum_{i=1}^{m} \left(- \, log \, (1 - \hat{y}^{(i)})\right)$ when $y^{(i)} = 0$

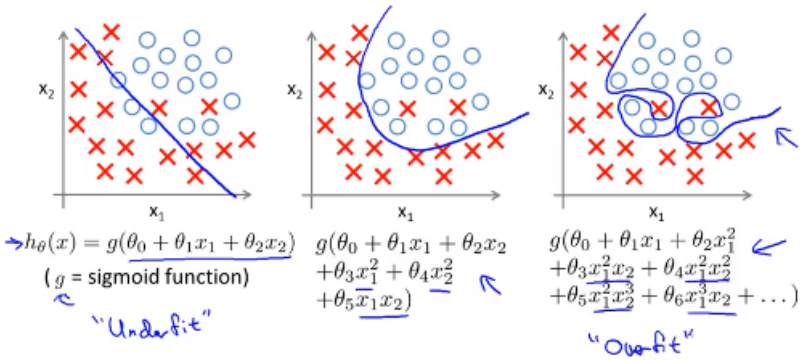
  

  intuition
  - when $y = 1$ and $\hat{y} \to 0$ then $J(\theta) \to \infty$
  - when $y = 0$ and $\hat{y} \to 1$ then $J(\theta) \to \infty$

- Goal

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

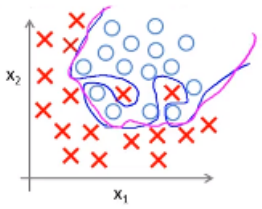
- Algorithm
  - gradient descent
    - start with some initial values for $\theta_0, \theta_1, ..., \theta_n$ (usually normal random values)
    - keep changing θs to reduce $J(\theta)$
      - $\theta_0 = \theta_0 - \alpha \frac{\partial J}{\partial \theta_0} = \theta_0 - \alpha \left(\frac{1}{m} \sum_{i=1}^{m} \left(\hat{y}^i - y^{(i)} \right) \right)$
      - $\theta_1 = \theta_1 - \alpha \frac{\partial J}{\partial \theta_1} = \theta_1 - \alpha \left(\frac{1}{m} \sum_{i=1}^{m} \left(\hat{y}^i - y^{(i)} \right) \cdot x_1^{(i)} \right)$
      - ...
      - $\theta_n = \theta_n - \alpha \frac{\partial J}{\partial \theta_n} = \theta_n - \alpha \left(\frac{1}{m} \sum_{i=1}^{m} \left(\hat{y}^i - y^{(i)} \right) \cdot x_n^{(i)} \right)$
  - hyperparameters
    - α
- Performance evaluation
  - accuracy: out of all predictions, how many of them were correct
  - precision: out of all *positive* predictions, how many of them were actually *positive* examples
  - recall: out of all positive examples, how many of them were detected as positive
  - f1-score: harmonic mean between precision and recall
- Problems
  - feature scaling is also important for logistic regression
    - feature scaling: $x' = \frac{x - min(x)}{max(x) - min(x)}$
    - feature scaling with mean normalization: $x' = \frac{x - mean(x)}{max(x) - min(x)}$
    - feature scaling with standardization: $x' = \frac{x - mean(x)}{std(x)}$
  - make sure the gradient descent is working correctly
    - plot the value of the cost function J over the number of iterations (# epochs)
    - for a sufficiently small α, $J(\theta)$ should decrease on every iteration
    - if α is too small, the gradient descent can be slow to converge
    - if α is too large, $J(\theta)$ may not decrease on every iteration; may not converge
    - try values $\alpha \in \{\dots, 0.001, 0.003, 0.01, 0.03, 0.1, 0.3, 1, \dots\}$
  - check model performance



    - in case of **underfitting**
      - try adding new features
        - e.g, use a polynomial regression

$$\theta_0 + \theta_1 * x \quad \Rightarrow \quad \theta_0 + \theta_1 * x + \theta_2 * x^2 + \theta_3 * x^3 + \dots$$

- in case of **overfitting**
  - reduce the number of features
    - manually select which features to keep
    - use a model-selection algorithm
  - use regularization
    - keep all the features, but reduce the magnitude of parameters θ;
      works well when working with a lot of features, each of which contributes a bit to predicting y
    - intuition: *shrink* model parameters in order to *smooth out* the decision boundary (generate a *simpler* hypothesis)



$$h_\theta(x) = g(\theta_0 + \theta_1 x_1 + \theta_2 x_1^2 + \theta_3 x_1^2 x_2 + \theta_4 x_1^2 x_2^2 + \theta_5 x_1^2 x_2^3 + \dots)$$

Cost function:

$$J(\theta) = -\left[\frac{1}{m}\sum_{i=1}^{m} y^{(i)} \log h_\theta(x^{(i)}) + (1 - y^{(i)}) \log (1 - h_\theta(x^{(i)}))\right] + \frac{\lambda}{2m}\sum_{j=1}^{n} \theta_j^2$$

$\theta_1, \theta_2, \dots, \theta_n$

    - cost function with the regularization term

$$J(\theta) = \frac{1}{m}\sum_{i=1}^{m}\left(-y^{(i)}\, log\, \hat{y}^{(i)} - (1 - y^{(i)})\, log\, (1 - \hat{y}^{(i)})\right) + \frac{\lambda}{2m}\sum_{j=1}^{n}\theta_j^2$$

    - parameter update in gradient descent (for $j \in \{1, 2, \dots, n\}$)

$$\theta_j = \theta_j - \alpha\frac{\partial J}{\partial \theta_j} = \theta_j - \alpha\left(\frac{1}{m}\sum_{i=1}^{m}\left(\hat{y}^i - y^{(i)}\right)\cdot x_j^{(i)} + \frac{\lambda}{m}\theta_j\right) = \theta_j\left(1 - \alpha\frac{\lambda}{m}\right) - \alpha\frac{1}{m}\sum_{i=1}^{m}\left(\hat{y}^i - y^{(i)}\right)\cdot x_j^{(i)}$$

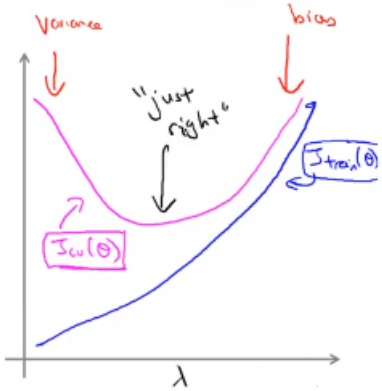
    - λ is the *regularization parameter* and needs to be tuned;
      it controls the trade-off between the goal of fitting the training data well and the goal of keeping the parameters small;
      try values $\lambda \in \{0, 0.02, 0.04, 0.08, 0.16, \dots, 10\}$
  - when using regularization, try increasing or decreasing λ

Bias/variance as a function of the regularization parameter λ

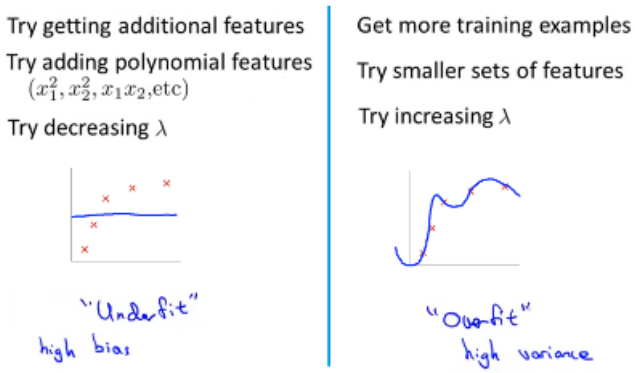
$$J(\theta) = \frac{1}{2m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})^2 + \frac{\lambda}{2m}\sum_{j=1}^{m}\theta_j^2$$

$$J_{train}(\theta) = \frac{1}{2m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})^2$$

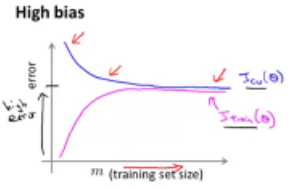
$$J_{cv}(\theta) = \frac{1}{2m_{cv}}\sum_{i=1}^{m_{cv}}(h_\theta(x_{cv}^{(i)}) - y_{cv}^{(i)})^2$$



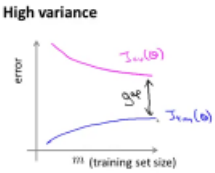
- debugging
  - choices to make when dealing with an underfit or an overtfit model



- machine learning diagnostic
  - gain guidance on how to improve the model's performance
  - draw **learning curves**: check the train and dev set error when training on various sizes of the training data set ($1 \leq i \leq m$)
    - high bias ⇒ getting more data won't help
    - high variance ⇒ getting more data might help



If a learning algorithm is suffering from high bias, getting more training data will not (by itself) help much.



If a learning algorithm is suffering from high variance, getting more training data is likely to help.

- Trading off precision and recall
  - use a different threshold for making decisions whether the class is positive or negative
  - minimize the number of false positives
    - generate a higher precision, but a lower recall
    - choose a higher threshold (e.g. $\sigma = \{0.7, \ldots, 0.9\}$)
  - minimize the number of false negatives
    - generate a higher recall, but a lower precision
    - choose a lower threshold (e.g. $\sigma = \{0.1, \ldots, 0.3\}$)
  - plot the precision-recall tradeoff curve by testing various threshold values between $[0, 1]$

1.2 Multiclass classification

- Description
  - use the one-vs-all (one-vs-rest) approach
  - turn the problem into C binary classification problems (generate C decision boundaries)
  - formally: train a logistic regression classifier $h^{(i)}(x)$ for each class i to predict the probability that $y = i$
  - on a new input x, in order to make a prediction pick the class i that maximizes the class probability $\max_i h^{(i)}(x)$