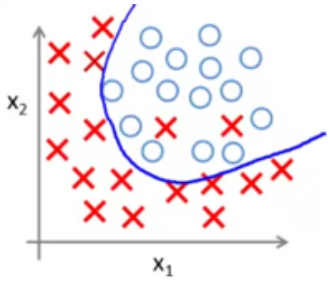
1 Logistic regression (for classification)

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
  - $z = \theta_0 + \theta_1 * x_1 + \theta_2 * x_2 + \ldots + \theta_n * x_n$
  - $h_\theta(x) = P(y = 1 \mid x, \theta) = \sigma(z) = \frac{1}{1+e^{-z}} = \hat{y} \quad (0 <= h(x) <= 1)$
  - Note: $\sigma(z) \geq 0.5$ when $z \geq 0$

- Model's parameters (# n + 1)

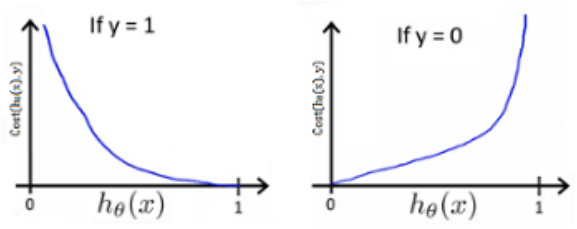
  $\theta = \{\theta_0, \theta_1, \ldots, \theta_n\}$

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

- Goal

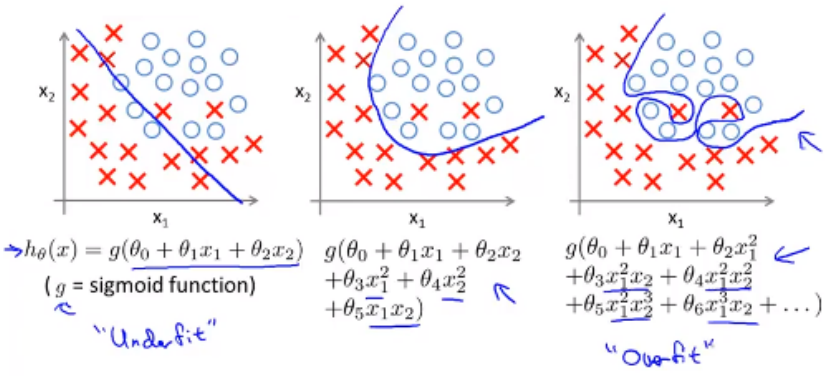
  $\min_\theta J(\theta)$

- Algorithm
  - gradient descent
    - start with some initial values for θ_0, θ_1, ..., θ_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

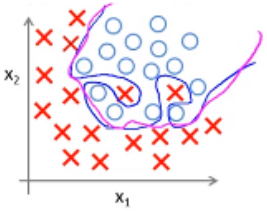
- Problems
  - feature scaling is also important for logistic regression
    - feature scaling: $x' = \frac{x - min(x)}{max(x) - min(x)}$
    - feature scaling with mean normalization: $x' = \frac{x - mean(x)}{max(x) - min(x)}$
    - feature scaling with standardization: $x' = \frac{x - mean(x)}{std(x)}$
  - 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 $\alpha \in \{\ldots, 0.001, 0.003, 0.01, 0.03, 0.1, 0.3, 1, \ldots\}$
  - check model performance



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

          $\theta_0 + \theta_1 * x \quad \Rightarrow \quad \theta_0 + \theta_1 * x + \theta_2 * x^2 + \theta_3 * x^3 + \ldots$
    - 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)



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

Cost function:

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

$\theta_1, \theta_2, \ldots, \theta_n$

        - 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 $j \in \{1, 2, \ldots, n\}$)

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

        - 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

- 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 $\max_i h^{(i)}(x)$