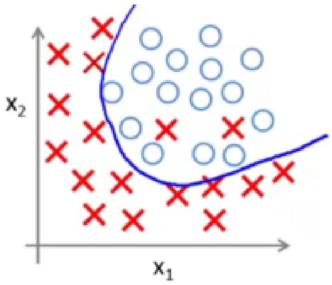
1 Logistic regression (for classification)

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

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

- 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 $y^{(i)} = 0$

- Goal

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

- 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
- Problems
  - the idea of feature scaling also aplied for logistic regression
  - make sure the gradient descent is working correctly
  - in case of **underfitting**
    - try adding new features
      - e.g, use a polynomial regression

        $$\theta_0 + \theta_1 * x \quad \Rightarrow \quad \theta_0 + \theta_1 * x + \theta_2 * x^2 + \theta_3 * x^3$$
  - 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)
      - 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
- Evaluation metrics
  - 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
- 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 $max_i h^{(i)}(x)$