CS 6170: Computational Topology, Spring 2019
Lecture 14

Topological Data Analysis for Data Scientists

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Feb 21, 2019

Announcement Project 2

- Project 2 will be posted in 2 days with due date changed to 3/21 (2-day extension from the original due date).

Machine Learning
An Intuitive Introduction

Machine Learning

Predicting things we have not seen by using what we have seen.

- Example: how photo app predicts who is in the photo
- Predict unseen data (*test data*) using seen data (*training data*)
- Two types of "prediction":
  - *Classification*: apply label to data.
  - Example: based on my previous reviews on restaurants, decides whether I will like or dislike a new restaurant.
  - *Regression*: assign a value to data.
  - Example: predict the score (from 1 to 100) for a new restaurant.
  - Classification – getting the label right.
  - Regression – predicting a value that is not far from the real value.

Shah and Pahwa (2019)

Error in Machine Learning

- Error is used to evaluate performance.
- Error is where "learning" happens.
- Error is used to train the ML algorithms.
- *Train* an algorithm: use the training data to learn some prediction scheme that can then be used on the (unseen) test data.

Shah and Pahwa (2019)

Classification Error

- Training data: points with labels, $\{(x_1, y_1), (x_2, y_2), \cdots, (x_n, y_n)\}$.
- Test data: (unlabeled) points, $\{z_1, z_2, \cdots, z_m\}$
- Classification: use training data to label test data.
- A classifier (a ML algorithm) is a function f that takes some input z_i and maps it to a label $f(z_i)$.
- *Training error*
  - $\epsilon_{train} = \frac{1}{n} \sum_{i=1}^{n} [[f(x_i) \neq y_i]]$
  - $[[S]] = 1$ if the statement S is true; $[[S]] = 0$ otherwise.
- *Test error*
  - $\epsilon_{test} = \frac{1}{m} \sum_{i=1}^{m} [[f(z_i) \neq \text{real label of } z_i)]]$

Shah and Pahwa (2019)

Other Errors

- *Regression error*: varies, i.e., mean squared error.
- Errors capture performance.
- Algorithm only knows the training data; optimize for training data does not necessarily optimize for error or test data.
- *Loss functions*: An ML algorithms defines error as *loss*.
- Different algorithms optimize for different loss functions.
- *Underfitting*: an algorithm does not use enough information of the training data.
- *Overfitting*: an algorithm overadapts to the training data.

Shah and Pahwa (2019)

Classification

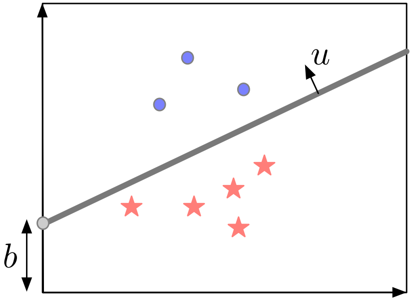
Identify to which of a set of categories a new observation belongs:

- Linear Classifiers
- Perceptron Algorithm
- Kernels
- SVM
- Neural Networks

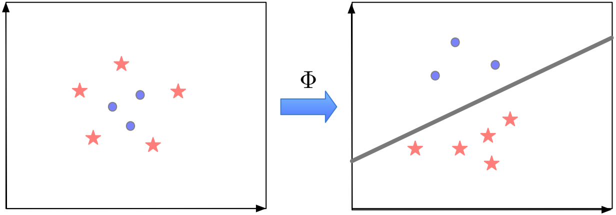
  `https://en.wikipedia.org/wiki/Statistical_classification`

Linear classifiers

- A classifier that uses a line (hypeplanes) to label the data points.
  1. Define a line by its *normal vector* (direction) u and a point on the line (e.g., offset).
  2. Points on the same side of u have $+$ labels; $-$ labels otherwise.



Limitations of linear classifiers



- What if the data is not linearly separable?
  - Solution: transform the data (via a function) into some space that is linearly separable, e.g., via kernel methods.
- What if we want more than two labels?
  - Solution: use multiple linear classifiers: $ABCD \rightarrow AB, CD \rightarrow A, B, C, D$

Shah and Pahwa (2019)

Perceptron algorithm: "error-driven learning"

- Idea: if you make a mistake, adjust the line based on the mistake
- Push the normal vector in the direction of the mistake if it was positively labeled, and away if it was negatively labeled.
- Pay attention to the notion of *inner product*.
- Additional reading: Shah and Pahwa (2019); Phillips (2019)

Inner product

- For two vectors $p = (p_1, ..., p_d)^T$,$q = (q_1, ..., q_d)^T \in \mathbb{R}^d$, the *inner product*:

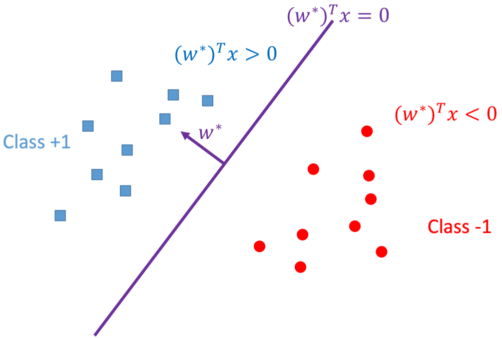
$$\langle p, q \rangle = p^T q = \sum_{i=1}^{d} p_i \cdot q_i$$

- Also: $p^T q = ||p||||q||cos\theta$, where θ is the angle between the two vectors.

Perceptron algorithm

- Learn a linear binary classifier $\mathbf{w}$
- $\mathbf{w}$ is a vector of weights (together with an intercept term b, omitted here) that is used to classify a sample vector $\mathbf{x}$ as class $+1$ or class -1 according to

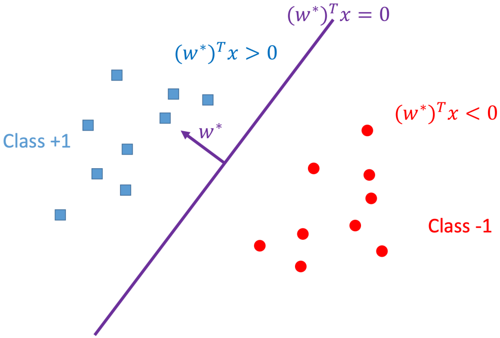
$$\hat{y} = \mathrm{sgn}(\mathbf{w}^T\mathbf{x})$$



https://en.wikipedia.org/wiki/Kernel_perceptron
https://www.cs.princeton.edu/courses/archive/spring16/cos495/slides/ML_basics_lecture3_Perceptron.pdf

Perceptron pseudocode

1. Initialize $\mathbf{w}$ to an all-zero vector.
2. For a fixed number of iterations, or until stopping criterion is met:
   - For each training example x_i with ground truth label $y_i \in \{-1, +1\}$:
     - Let $\hat{y} = \mathrm{sgn}(\mathbf{w}^T x_i)$.
     - If $\hat{y} \neq y_i$, update $\mathbf{w} \leftarrow \mathbf{w} + y_i x_i$.



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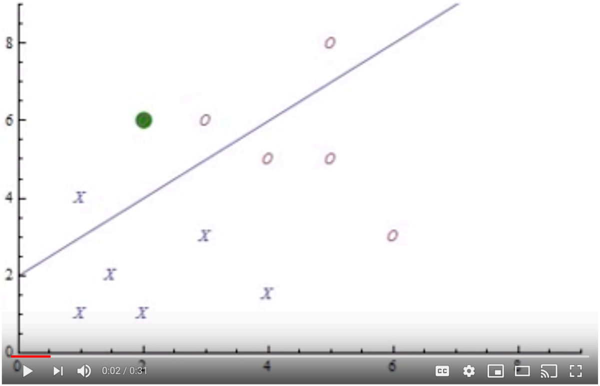
Perceptron in action



`https://www.youtube.com/watch?v=vGwemZhPlsA`

From perceptron to kernel perceptron: dual perceptron

- The weight vector $\mathbf{w}$ can be expressed as a linear combination of the n training points:

$$\mathbf{w} = \sum_i^n \alpha_i y_i \mathbf{x}_i$$

- α_i: number of times x_i was misclassified, forcing an update to $\mathbf{w}$
- A dual perceptron algorithm loops through the samples as before, making predictions, but instead of storing and updating a weight vector $\mathbf{w}$, it updates a "mistake counter" vector α:

$$\begin{aligned} \hat{y} &= \mathrm{sgn}(\mathbf{w}^T \mathbf{x}) \\ &= \mathrm{sgn}\left(\sum_i^n \alpha_i y_i \mathbf{x}_i\right)^T \mathbf{x} \\ &= \mathrm{sgn}\left(\sum_i^n \alpha_i y_i (\mathbf{x}_i \cdot \mathbf{x})\right) \end{aligned} \tag{1}$$

https://en.wikipedia.org/wiki/Kernel_perceptron

Kernel perceptron

- Kernel perceptron: replace *dot product* in the dual perceptron by an arbitrary *kernel* function, to get the effect of a feature map Φ without computing $\Phi(x)$ explicitly for any samples.
- $K(\mathbf{x}, \mathbf{x}') = \langle \Phi(\mathbf{x}), \Phi(\mathbf{x}') \rangle$.

`https://en.wikipedia.org/wiki/Kernel_method`

Kernel perceptron

- Perceptron: learns a linear classifier
- Kernel perceptron: learns a kernelized classifier
- A *kernel* is a (user-specified) similarity function over pairs of data points.
- A *kernel machine* is a classifier that stores a subset of its training examples x_i, associates with each a weight α_i, and makes decisions for new samples $\mathbf{x}$ by evaluating

$$\hat{y} = \operatorname{sgn}\left(\sum_i \alpha_i y_i K(\mathbf{x}_i, \mathbf{x})\right)$$

`https://en.wikipedia.org/wiki/Kernel_perceptron`

Kernel perceptron algorithm pseudocode

Pseudocode:

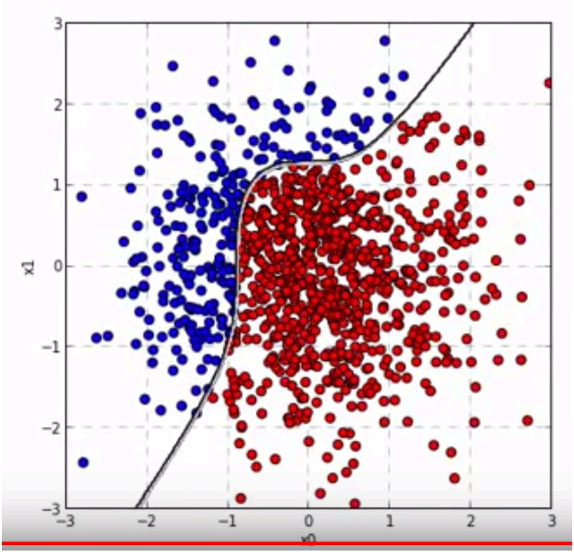
1. Initialize α to an all-zeros vector of length n
2. For a fixed number of iterations, or until stopping criterion is met:
   - For each training example $\mathbf{x}_j$ with ground truth label $y_j \in \{-1, +1\}$:
     - Let $\hat{y} = \mathrm{sgn}\left(\sum_{i=1}^{n} \alpha_i y_i K(\mathbf{x}_i, \mathbf{x}_j)\right)$.
     - If $\hat{y} \neq y_i$, update $\alpha_j \leftarrow \alpha_j + 1$.

   `https://en.wikipedia.org/wiki/Kernel_perceptron`

Commonly used kernels

- Gaussian kernel: $K(p,q) = \exp(-||p-q||^2/\sigma^2)$ with bandwidth σ
- Laplace kernel: $K(p,q) = \exp(-||p-q||/\sigma)$ with bandwidth σ
- Polynomial kernel of power r: $K(p,q) = (\langle p,q\rangle + c)^r$ with control parameter $c > 0$.

Kernel perceptron in action



`https://www.youtube.com/watch?v=mC0awsGOOcs`

Coming up next: kernels for barcodes

References I

Phillips, J. M. (2019). Mathematical foundations for data analysis. http://www.cs.utah.edu/~jeffp/M4D/M4D.html.

Shah, P. and Pahwa, R. (2019). Urban data analytics and machine learning. http://web.mit.edu/6.S097/www/about.html.