Introduction to Data Science - 1MS041

Benny Avelin

Department of Mathematics

HT 2023

Recall from last time

- We defined a stochastic process as a index family of random variables X_α where $\alpha \in I$ is the index set. The base example is a sequence of i.i.d. random variables, $X_1, \ldots, X_n$, here the index set is $\mathbb{N}$.

Recall from last time

- We defined a stochastic process as a index family of random variables X_α where $\alpha \in I$ is the index set. The base example is a sequence of i.i.d. random variables, $X_1, \ldots, X_n$, here the index set is $\mathbb{N}$.
- We defined the concept of Markov chain, which is a stochastic process which takes a finite number of states and its dependency on the past is only the previous value, i.e.

$$\mathbb{P}(X_{t+1} = x \mid X_1, \ldots, X_t) = \mathbb{P}(X_{t+1} = x \mid X_t).$$

Recall from last time

- We defined a homogeneous Markov chain, as one where the transition probabilities does not depend on the index t (or time).

  $$\mathbb{P}(X_{t+1} = y \mid X_t = x) = P_{xy}$$

  that is the probability of transitioning from state x to state y does not depend on the particular time t.

Recall from last time

- We defined a homogeneous Markov chain, as one where the transition probabilities does not depend on the index t (or time).

  $$\mathbb{P}(X_{t+1} = y \mid X_t = x) = P_{xy}$$

  that is the probability of transitioning from state x to state y does not depend on the particular time t.
- Since $X_t \in \mathbb{X}$, where $\mathbb{X}$ is called the state space and $\mathbb{X}$ is a finite set. We can define a matrix P_{xy} where $x, y \in \mathbb{X}$. We call this matrix the transition matrix.

Recall from last time

- We defined a homogeneous Markov chain, as one where the transition probabilities does not depend on the index t (or time).

$$\mathbb{P}(X_{t+1} = y \mid X_t = x) = P_{xy}$$

  that is the probability of transitioning from state x to state y does not depend on the particular time t.
- Since $X_t \in \mathbb{X}$, where $\mathbb{X}$ is called the state space and $\mathbb{X}$ is a finite set. We can define a matrix P_{xy} where $x, y \in \mathbb{X}$. We call this matrix the transition matrix.
- We can use the transition matrix to compute how distributions change when the Markov chain progresses. I.e. let us assume that at time t we have a distribution over the states p_t, then the distribution at time $t+1$ is computed as

$$p_{t+1} = p_t P \qquad p_t = p_0 P^t.$$

Today

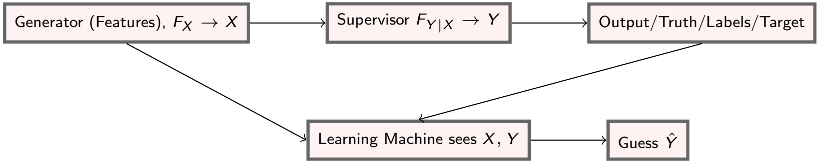
Today we will take a look at the pattern recognition problem.

- We will see the first algorithm developed for this problem the "Perceptron", which eventually became neural networks.
- We will study its limitations and how to overcome them by a concept known as kernelization.

Supervised learning

Setup

1. The generator of the data G
2. The supervisor S
3. The learning machine LM.


Generator (Features), $F_X \to X$
Supervisor $F_{Y|X} \to Y$
Output/Truth/Labels/Target
Learning Machine sees X, Y
Guess $\hat{Y}$

Pattern recognition

- Supervisors conditional distribution $F(y|x)$ is discrete, and can take k different values, $y = 0, \ldots, k-1$.

Pattern recognition

- Supervisors conditional distribution $F(y|x)$ is discrete, and can take k different values, $y = 0, \dots, k-1$.
- Model space $\mathcal{M} = \{g_\lambda(x) : g_\lambda(x) \in \{0, \dots, k-1\}\}$.

Pattern recognition

- Supervisors conditional distribution $F(y|x)$ is discrete, and can take k different values, $y = 0, \ldots, k-1$.
- Model space $\mathcal{M} = \{g_\lambda(x) : g_\lambda(x) \in \{0, \ldots, k-1\}\}$.
- g_λ a **decision function**, **decision rule**, **classifier**.

Pattern recognition

- Supervisors conditional distribution $F(y|x)$ is discrete, and can take k different values, $y = 0, \dots, k-1$.
- Model space $\mathcal{M} = \{g_\lambda(x) : g_\lambda(x) \in \{0, \dots, k-1\}\}$.
- g_λ a **decision function**, **decision rule**, **classifier**.
- $0 - 1$ loss

$$L(z, u) = \begin{cases} 0 & \text{if } y = u \\ 1 & \text{if } y \neq u \end{cases}$$

Pattern recognition

- Supervisors conditional distribution $F(y|x)$ is discrete, and can take k different values, $y = 0, \dots, k-1$.
- Model space $\mathcal{M} = \{g_\lambda(x) : g_\lambda(x) \in \{0, \dots, k-1\}\}$.
- g_λ a **decision function**, **decision rule**, **classifier**.
- $0-1$ loss

$$L(z, u) = \begin{cases} 0 & \text{if } y = u \\ 1 & \text{if } y \neq u \end{cases}$$

The pattern recognition problem

Minimize

$$R(\lambda) = \int L(y, g_\lambda(x)) dF(x, y) = \mathbb{E}[L(Y, g_\lambda(X))]$$

where $(X, Y) \sim F(x, y)$, where $g_\lambda \in \mathcal{M}$.

Example

From regression to decision function

The regression problem. The goal is to estimate the function $\mathbb{E}[Y \mid X]$, where Y are the labels and X are the features. We assume f_X is a fixed density, that we will not care about and instead assume that $f_{Y|X}$ is part of a parametrized family, i.e. $f_{Y|X} = p_{\alpha^*,X}$ for some α^*.

- $p_{\alpha^*,X} = N(\alpha_1 X + \alpha_2, \alpha_3^2)$, Linear regression
- $p_{\alpha^*,X} = \text{Bernoulli}(G(\alpha_1 X + \alpha_2))$,

$$G(x) = \frac{1}{1 + e^{-x}}$$

  Logistic regression

Definition

Let $r(x) = \mathbb{E}[Y \mid X]$, then the **Bayes classification rule** h^* is

$$h^*(x) = \begin{cases} 1 & \text{if } r(x) > 1/2 \\ 0 & \text{otherwise.} \end{cases}$$

Definition

Let $r(x) = \mathbb{E}[Y \mid X]$, then the **Bayes classification rule** h^* is

$$h^*(x) = \begin{cases} 1 & \text{if } r(x) > 1/2 \\ 0 & \text{otherwise.} \end{cases}$$

Lets say we use Logistic regression and fit the function $G(\hat{\alpha}_1 X + \hat{\alpha}_2)$, now the model is that $p_{\hat{\alpha},X} = \text{Bernoulli}(G(\hat{\alpha}_1 X + \hat{\alpha}_2))$ which is a model of the conditional density, i.e.

$$\hat{r}(x) = \mathbb{E}_{p_{\hat{\alpha},X}}[Y] = G(\hat{\alpha}_1 X + \hat{\alpha}_2)$$

Definition

Let $r(x) = \mathbb{E}[Y \mid X]$, then the **Bayes classification rule** h^* is

$$h^*(x) = \begin{cases} 1 & \text{if } r(x) > 1/2 \\ 0 & \text{otherwise.} \end{cases}$$

Lets say we use Logistic regression and fit the function $G(\hat{\alpha}_1 X + \hat{\alpha}_2)$, now the model is that $p_{\hat{\alpha},X} = \text{Bernoulli}(G(\hat{\alpha}_1 X + \hat{\alpha}_2))$ which is a model of the conditional density, i.e.

$$\hat{r}(x) = \mathbb{E}_{p_{\hat{\alpha},X}}[Y] = G(\hat{\alpha}_1 X + \hat{\alpha}_2)$$

thus we can construct

$$g_{\hat{\alpha}}(x) = \begin{cases} 1 & \text{if } \hat{r}(x) > 1/2 \\ 0 & \text{otherwise.} \end{cases}$$

Definition

Let $r(x) = \mathbb{E}[Y \mid X]$, then the **Bayes classification rule** h^* is

$$h^*(x) = \begin{cases} 1 & \text{if } r(x) > 1/2 \\ 0 & \text{otherwise.} \end{cases}$$

Lets say we use Logistic regression and fit the function $G(\hat{\alpha}_1 X + \hat{\alpha}_2)$, now the model is that $p_{\hat{\alpha},X} = \text{Bernoulli}(G(\hat{\alpha}_1 X + \hat{\alpha}_2))$ which is a model of the conditional density, i.e.

$$\hat{r}(x) = \mathbb{E}_{p_{\hat{\alpha},X}}[Y] = G(\hat{\alpha}_1 X + \hat{\alpha}_2)$$

thus we can construct

$$g_{\hat{\alpha}}(x) = \begin{cases} 1 & \text{if } \hat{r}(x) > 1/2 \\ 0 & \text{otherwise.} \end{cases}$$

Note!!

This is what scikit-learns LogisticRegression predict function does!

Pattern recognition

Pattern recognition problem from CS perspective

Suppose we have n training data points $T_n := ((X_i, Y_i))_{i=1}^n$ and are interested in a classification rule $h(X)$ that uses T_n to *predict*, i.e., assign labels to previously unseen data X.

Pattern recognition

Pattern recognition problem from CS perspective

Suppose we have n training data points $T_n := ((X_i, Y_i))_{i=1}^n$ and are interested in a classification rule $h(X)$ that uses T_n to *predict*, i.e., assign labels to previously unseen data X.

- We want our classification rule h, which is typically an algorithm, to perform well on previously unseen data by learning from the training data. This is known as *generalization*.

Definition

The space $\mathcal{X}$ where X_i belongs to is called the *instance space* or *feature space* and the space $\mathcal{Y}$ where Y_i belongs to is called the *label space*.

Definition

The space $\mathcal{X}$ where X_i belongs to is called the *instance space* or *feature space* and the space $\mathcal{Y}$ where Y_i belongs to is called the *label space*.

Typically, $\mathcal{X}$ is a subset of $\mathbb{R}^d$ and $\mathcal{Y}$ is binary label space either as $\{0, 1\}$ or $\{-1, 1\}$. For example, $\mathcal{X}$ can be $\{0, 1\}^d$ to indicate the presence or absence of something in the instance space, say a specific set of words in an email if the task is to classify emails with labels 0 and 1 for non-spam or spam.

Remark

To connect back to our previous terminology, we see that the data space $\mathbb{X} = (\mathcal{X}, \mathcal{Y})$ (we will later write $\mathbb{X} \times \mathbb{Y}$ to avoid X being used for both feature and label) is split into the featue space and the label space. The random variable we are observing is a pair (X, Y) and a collection of n samples is the training dataset.

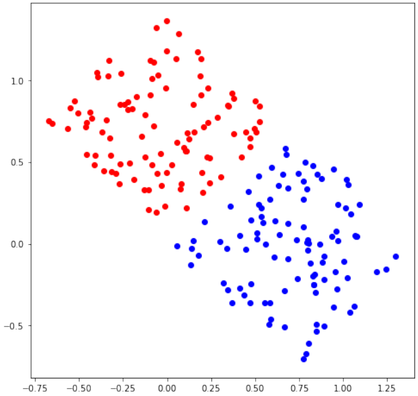
Let us say that we are trying to device a classification rule based on instance space $\mathcal{X} = \mathbb{R}^d$ and label space $\mathcal{Y} = \{-1, 1\}$.

Let us say that we are trying to device a classification rule based on instance space $\mathcal{X} = \mathbb{R}^d$ and label space $\mathcal{Y} = \{-1, 1\}$.

- Simple rules consists of finding a hyperplane that separate out the data, this is called a **linear separator**.

Let us say that we are trying to device a classification rule based on instance space $\mathcal{X} = \mathbb{R}^d$ and label space $\mathcal{Y} = \{-1, 1\}$.

- Simple rules consists of finding a hyperplane that separate out the data, this is called a **linear separator**.



How do we find such a separator?

- In two or three dimensions it is easy by just looking at the image

How do we find such a separator?

- In two or three dimensions it is easy by just looking at the image
- In higher dimension, i.e. when the number of features is high, we have to find an automated way of doing this!

The Perceptron algorithm

- The perceptron is a linear classification rule

The Perceptron algorithm

- The perceptron is a linear classification rule
- The first training algorithm was devised by Frank Rosenblatt at Cornell Aeronautical Laboratory in 1957.

The Perceptron algorithm

- The perceptron is a linear classification rule
- The first training algorithm was devised by Frank Rosenblatt at Cornell Aeronautical Laboratory in 1957.
- The goal was to build a machine that could recognize hand written letters.

Lets explain the algorithm

The dimension trick

We start by increasing the dimension, i.e. lets say we have the features $X = (x_1, \ldots, x_k)$, i.e. we have k dimensions (features), then we can create $\tilde{X} = (x_1, \ldots, x_k, 1)$ which is now in $k + 1$ dimensions. The point is that we can write

$$X \cdot w + c = 0 \iff \tilde{X} \cdot \tilde{w} = 0$$

where $\tilde{w} = (w_1, \ldots, w_k, c)$.

Lets explain the algorithm

The dimension trick

We start by increasing the dimension, i.e. lets say we have the features $X = (x_1, \ldots, x_k)$, i.e. we have k dimensions (features), then we can create $\tilde{X} = (x_1, \ldots, x_k, 1)$ which is now in $k+1$ dimensions. The point is that we can write

$$X \cdot w + c = 0 \iff \tilde{X} \cdot \tilde{w} = 0$$

where $\tilde{w} = (w_1, \ldots, w_k, c)$.

Warning

We will from now on assume that we have done **the dimension trick** but we go back to the notation X and w.

The perceptron algorithm

Let us say that we are trying to device a classification rule based on instance space $\mathcal{X} = \mathbb{R}^d$ and label space $\mathcal{Y} = \{-1, 1\}$.

The perceptron algorithm

Let us say that we are trying to device a classification rule based on instance space $\mathcal{X} = \mathbb{R}^d$ and label space $\mathcal{Y} = \{-1, 1\}$.

In the following we can take a training dataset $\{(x_1, y_1), \ldots, (x_n, y_n)\}$. For the perceptron the goal is to find

$$(w \cdot x_i) y_i > 0, \qquad i = 1, \ldots, n.$$

The perceptron algorithm

Let us say that we are trying to device a classification rule based on instance space $\mathcal{X} = \mathbb{R}^d$ and label space $\mathcal{Y} = \{-1, 1\}$.

In the following we can take a training dataset $\{(x_1, y_1), \ldots, (x_n, y_n)\}$. For the perceptron the goal is to find

$$(w \cdot x_i) y_i > 0, \qquad i = 1, \ldots, n.$$

The perceptron algorithm

1. $w = 0$
2. while there exists x_i with $x_i y_i \cdot w \leq 0$, update $w := w + x_i y_i$

Convergence is guaranteed if linearly separable

Theorem

If there exists w^* such that $w^* \cdot x_i y_i \geq 1$ for all i. Then the perceptron algorithm finds a w satisfying $w \cdot x_i y_i \geq 0$ for all i in at most $r^2 |w^*|^2$ updates, where $r = \max_i |x_i|$.

Convergence is guaranteed if linearly separable

Theorem

If there exists w^* such that $w^* \cdot x_i y_i \geq 1$ for all i. Then the perceptron algorithm finds a w satisfying $w \cdot x_i y_i \geq 0$ for all i in at most $r^2|w^*|^2$ updates, where $r = \max_i |x_i|$.

Warning

If the set is not linearly separable then the algorithm will not converge, in fact it will go all over the place.

Kernelization

The idea

If we cannot separate our data, then perhaps we can find a function ϕ which maps $\mathbb{R}^{k+1} \to \mathbb{R}^m$ where $m > k + 1$, such that our data becomes linearly separable.

Kernelization

The idea

If we cannot separate our data, then perhaps we can find a function ϕ which maps $\mathbb{R}^{k+1} \to \mathbb{R}^m$ where $m > k + 1$, such that our data becomes linearly separable.

So if we transform the $x \to \phi(x)$ for some good transformation ϕ then our perceptron will try to solve

$$w \cdot \phi(x_i) l_i > 0$$

The perceptron algorithm

1. $w = 0$
2. while there exists x_i with $x_i y_i \cdot w \leq 0$, update $w := w + x_i y_i$

The weight after n steps will have the form

$$w = \sum_{i=1}^{n} c_i \phi(x_i)$$

for numbers c_i. The perceptron algorithm becomes just addition and subtraction of certain c_i's by 1.
Furthermore

$$w \cdot \phi(x_i) = \sum_{j=1}^{n} c_j \phi(x_j) \cdot \phi(x_i) = \sum_{j=1}^{n} c_i k_{ij}$$

where $k_{ij} = \phi(x_i) \cdot \phi(x_j)$.

The kernelized perceptron algorithm

1. $c = 0$
2. While there exists an i such that $(Kc)_i y_i \leq 0$ update

$$c_i := c_i + y_i.$$

Kernel trick

Issue

If $\phi(x_i)$ is high dimensional there is a big computational cost to computing it.

What if we had a function $k(x, y)$ that could be written as

$$k(x, y) = \phi(x) \cdot \phi(y)$$

for some ϕ and k is easier to compute, then our life would be simpler. Also, what if we are given a function $k(x, y)$ and we would like to know if it is a “kernel function”.

Kernel functions

Definition

We call a function $k(x, y) : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ a kernel function if there is a mapping $\phi : \mathbb{R}^d \to \mathbb{R}^m$ (for some m) such that
$k(x, y) = \phi(x) \cdot \phi(y)$.

- $k(x, y) = (\gamma x \cdot y + r)^k$, $(k \in \mathbb{N})$ polynomial
- $k(x, y) = x \cdot y$, linear
- $k(x, y) = e^{-\gamma|x-y|}$, called Radial Basis Function
- $k(x, y) = \tanh(\gamma x \cdot y + r)$, sigmoidal