Foundation of Intelligent Systems, Part I Classification

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Last Lecture : Regression

• Mentioned the Maximum Likelihood perspective on LS-regression

$$\log \mathcal{L}(\mathbf{a}, b) = C - \frac{1}{2\sigma^2} \underbrace{\sum_{j=1}^{N} \|y_j - (\mathbf{a}^T \mathbf{x}_j + b)\|^2}_{L(\mathbf{a}, b)}$$

• Provided a geometric perspective on LS regression through projections

- Many issues with LS regression... Hence advanced regression techniques
 - \circ Ridge Regression
 - Subset selection
 - o Lasso
- we will talk about these in 3 lectures when discussing **sparsity**.

Today

- Classification, differences with regression
- Binary classification
- Linear classification algorithms
 - Logistic Regression
 - Ideally, Linear Discriminant Analysis, but no time.
 - Perceptron rule
 - Support Vector Machine
- Once this is done, we will move on to more theory in next lecture about statistical learning theory.

Classification

Starting Again With Regression

Many observations of the same data type, with label

- we still consider a database $\{\mathbf{x}_1, \cdots, \mathbf{x}_N\}$,
- each datapoint \mathbf{x}_j is represented as a vector of features $\mathbf{x}_j = \begin{bmatrix} x_{1,j} \\ x_{2,j} \\ \vdots \\ \vdots \\ x_{j} \end{bmatrix}$

- To each observation is associated a **label** y_j ...
 - If $y_i \in \mathbb{R}$, we have **regression**
 - If $y_i \in S$ where S is a finite set, **multiclass classification**.
 - \circ If S only has two elements, **binary classification**.

Examples

Multiclass Classification

• Classify images of fruits into fruit category



- $\bullet\,$ Classify images of handwritten digits into digits from 0 to 9
- Classify musical tunes, books, movies into genres
- Classify proteins into functional classes

img source

Examples

Binary Classification

- Using elementary measurements, guess if someone has or not a disease that is
 - $\circ~$ difficult to detect at an early stage
 - difficult to measure directly (fetus)
- Classify chemical compounds into toxic / nontoxic
- Classify a passenger as **suspect/not suspect**
- Classify body tumor as **begign/malign** to detect cancer
- etc.

Solve a classification problem \Leftrightarrow build a function $f : \mathbb{R}^d \to S$

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Namely, for each j, can we measure whether $f(\mathbf{x}_j) \approx y_j$?

Solve a classification problem \Leftrightarrow build a function $f : \mathbb{R}^d \to S$ for each j, can we measure whether $f(\mathbf{x}_j) \approx y_j$?

In conventional regression - linear regression

- We have used consistently $\sum_{j=1}^{N} \|\boldsymbol{f}(\mathbf{x}_j) y_j\|^2$ to select a good \boldsymbol{f} .
- \mathbb{R} is a metric space... ||37.354 JPY 36.000 JPY|| = 1354
 - $\circ\,$ sense of closeness between possible answers
- \mathbb{R} is a totally ordered set... 36.000 JPY<37.354 JPY
 - o notion of total hierarchy between possible answers

Solve a classification problem \Leftrightarrow build a function $f : \mathbb{R}^d \to S$ for each j, can we measure whether $f(\mathbf{x}_j) \approx y_j$?

In discrete labels in classification

- No distance nor order is available on ${\cal S}$
 - No order for musical genres jazz > bossa-nova ?
 - No distance between fruits

jazz > bossa-nova ? ||kiwi — banana||?

This creates challenges to quantify how $f(\mathbf{x}_j)$ is close to y_j

Digits recognition

• Use a database such as

2601927240 5420BH2947

paired with the corresponding labels,

(2, 6, 0, 1, 9, 2, 7, 1, 4, 0, 5, 4, 3, 0, 8, 4, 3, 9, 4, 7).

to build an **automated recognition system** for handwritten digits.

• useful for post office, check recognition, tax office, *etc.*.

Labels are usually unordered and without a metric

- The set of labels is $S = \{0, 1, 2, 3, 4, 5, 6, 7, 8, 9\}$
- Yet there is no distance/order in ${\mathcal S}$ for this task.
- Suppose the image given to the recognition system is



• Although |5 - 6| < |0 - 6|, the answer 5 is **not better** than 0.

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• Although $|\mathbf{5} - \mathbf{6}| < |\mathbf{0} - \mathbf{6}|$, the answer **5** is **not better** than **0**.

If all mistakes are equally wrong, then we consider the 0/1 loss:

$$l\left(f(\boldsymbol{x_j}), \boldsymbol{y_j}\right) \stackrel{\text{def}}{=} \begin{cases} 0 \text{ if } f(\boldsymbol{x_j}) = \boldsymbol{y_j}, \\ 1 \text{ if } f(\boldsymbol{x_j}) \neq \boldsymbol{y_j}. \end{cases}$$

Sometimes discrete labels are regression variables in disguise

• Suppose the task is to guess the rating of a movie

DVDs in Your Queue					Update Your Queue		
Priority	Movie Title	Star Rating	MPAA	Genre	Availability	×	7
1	Me and You and Everyone We Know	⊗ ★★★☆☆	R	Independent	Now		7
2	Melinda and Melinda	© ☆☆☆ ☆☆	PG-13	Cornedy	Now		7
3	Arrested Development: Season 2: Disc 1	◎☆☆☆☆☆	HR	Television	Nove		7
4	Arrested Developmenti Season 21 Disc 2	Series Disc	NR	Television	Now		7
5	Arrested Development: Season 2: Disc 3	Series Disc	NR	Television	Now		7
6	Lords of Dogtown	© ☆☆☆☆ ☆	UR.	Drama	Novy		7
7	The United States of Leland	0 *** **	R	Drama	Now		7
8	Donnie Darkoj Director's Cut	⊗ ☆☆☆☆ ☆	R	Independent	Now		7
9	Eternal Sunshine of the Spotless Mind	© ☆☆☆☆ ☆	R	Cornedy	Nove		7
10	Lost in Translation	© ☆☆☆☆ ☆	R	Drama	Now		7
11	Girl with a Pearl Earring	0 *** **	PG-13	Drama	Now		2
12	Stage Beauty	⊗☆☆☆ ☆☆	R	Romance	Novy		2
13	Elephant	♦★★☆☆☆	R	Drama	Now		7
14	The Red Violin	0 ***	R	Drama	Nove		7
15	Grash	0****	R	Drama	Novy		7

- User inputs are in $\mathcal{S} = \{1, 2, 3, 4, 5\}$
- In this case **standard regression techniques** may be applied because,
 - $\circ\,$ the natural metric $\|5-3\|$ is meaningful
 - \circ the final user does not mind getting fractional predictions (e.g. 3.85)

Binary Classification

 $\operatorname{card} \mathcal{S} = 2.$

Usually
$$S = \{0, 1\}$$
 or $S = \{-1, 1\}$ or $S = \{-, +\}$ or $S = \{Y, N\}$

Data

- **Data**: vectors $\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \cdots, \mathbf{x}_N$.
- To infer a "yes/no" rule, we need the **correct answer** for each vector.
- We consider thus a set of **pairs of (vector,bit)**

"training set"
$$= \left\{ \left(\mathbf{x}_i = \begin{bmatrix} x_1^i \\ x_2^i \\ \vdots \\ x_d^i \end{bmatrix} \in \mathbb{R}^d, \ \mathbf{y}_i \in \{0, 1\} \right)_{i=1..N} \right\}$$

- For illustration purposes only we will consider vectors in the plane, d = 2.
- Points are easier to represent in 2 dimensions than in 20.000...
- The ideas for $d \gg 3$ are **exactly the same**.



What is a classification rule?



Classification rule = a partition of \mathbb{R}^d into two sets



This partition is recovered as the level set of a function on \mathbb{R}^d



Namely, $\{\mathbf{x} \in \mathbb{R}^d | \mathbf{f}(\mathbf{x}) > 0\}$ and $\{\mathbf{x} \in \mathbb{R}^d | \mathbf{f}(\mathbf{x}) \le 0\}$



What kind of function? any. For instance, a curved line



Even more **simple**: using **straight lines** and halfspaces.

Linear Classifiers

- Straight lines (hyperplanes when d > 2) are the simplest type of classifiers.
- A hyperplane $H_{\mathbf{c},b}$ is a set in \mathbb{R}^d defined by
 - \circ a normal vector $\mathbf{c} \in \mathbb{R}^d$
 - \circ a constant $b \in \mathbb{R}$. as

$$H_{\mathbf{c},b} = \{ \mathbf{x} \in \mathbb{R}^d \, | \, \mathbf{c}^T \mathbf{x} \, = \, b \}$$

• Letting b vary we can "slide" the hyperplane across \mathbb{R}^d



Linear Classifiers

• Exactly like lines in the plane, hypersurfaces divide \mathbb{R}^d into two halfspaces,

$$\left\{ \mathbf{x} \in \mathbb{R}^d \, | \, \mathbf{c}^T \mathbf{x} < b \right\} \cup \left\{ \mathbf{x} \in \mathbb{R}^d \, | \, \mathbf{c}^T \mathbf{x} \ge b \right\} = \mathbb{R}^d$$

• Linear classifiers attribute the "yes" and "no" answers given arbitrary c and b.



• Assuming we only look at halfspaces for the decision surface... ...how to choose the "best" (c*, b*) given a training sample?

Linear Classifiers

• This specific question,

"training set"
$$\left\{ \left(\mathbf{x}_i \in \mathbb{R}^d, \ \mathbf{y}_i \in \{0, 1\} \right)_{i=1..N} \right\} \stackrel{????}{\Longrightarrow}$$
 "best" $\mathbf{c}^{\star}, \ b^{\star}$

has different answers. Depends on the meaning of "best" ?:

- Linear Discriminant Analysis (or Fisher's Linear Discriminant);
- Logistic regression maximum likelihood estimation;
- **Perceptron**, a one-layer neural network;
- Support Vector Machine, the result of a convex program
- *etc*.



Given two sets of points...



It is sometimes possible to separate them perfectly



Each choice might look equivalently good on the training set, but it will have obvious impact on new points









Specially close to the border of the classifier





For each different technique, different results, different performance.
A few linear classifiers: (1) Linear Discriminant Analysis

Reminder: Gaussian Multivariate Density

Gaussian Multivariate Density

A multivariate (= for vectors) generalization of the Gaussian density for $x \in \mathbb{R}$

$$p(x) = \frac{1}{\sqrt{2\pi\sigma}} e^{-\frac{1}{2}x^2}$$

A very common density to characterize random vectors.

Reminder: Gaussian Multivariate Density

Gaussian Multivariate Density

 $\mathbf{x} \in \mathbb{R}^d \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma}), \boldsymbol{\Sigma}$ positive definite

$$\label{eq:Density} \begin{tabular}{l} \begin{tabu$$

Reminder: Gaussian Multivariate Density



Linear Discriminant Analysis in a Nutshell

- Assume points from two classes, $0 \ {\rm and} \ 1$ are generated by two Gaussian densities
- Estimate ML covariance Σ_0, Σ_1 and mean μ_0 and μ_1 for **each** class



$$\mu_{0} = \frac{1}{N_{0}} \sum_{i | y_{i} = 0} \mathbf{x}_{i}, \quad \mathbf{\Sigma}_{0} = \frac{1}{N_{0} - 1} \sum_{i | y_{i} = 0} (\mathbf{x}_{i} - \mu_{0}) (\mathbf{x}_{i} - \mu_{0})^{T}$$
$$\mu_{1} = \frac{1}{N_{1}} \sum_{i | y_{i} = 1} \mathbf{x}_{i}, \quad \mathbf{\Sigma}_{1} = \frac{1}{N_{1} - 1} \sum_{i | y_{i} = 1} (\mathbf{x}_{i} - \mu_{1}) (\mathbf{x}_{i} - \mu_{1})^{T}$$

https://onlinecourses.science.psu.edu/stat557/book/export/html/45

Linear Discriminant Analysis

• Define the **two** resulting densities, i = 0 or 1,

$$p_i(\mathbf{x}) = \frac{1}{(2\pi)^{d/2} |\Sigma_i|} e^{(\mathbf{x} - \mu_i)^T \Sigma_i^{-1} (\mathbf{x} - \mu_i)}$$

- Decide that **x** belongs to 1 if $p_1(\mathbf{x}) > p_0(\mathbf{x})$ and 0 otherwise.
- In practice (after some computations), this means that:
 - $\circ x$ belongs to class 1 if

$$(x - \mu_0)^T \Sigma_0^{-1} (x - \mu_0) + \ln |\Sigma_0| - (x - \mu_1)^T \Sigma_1^{-1} (x - \mu_1) - \ln |\Sigma_1| > T$$

• 0 otherwise

Linear Discriminant Analysis

• If one assumes that $\Sigma_0 = \Sigma_1 = \Sigma$, the decision becomes a simple dot-product:

 $w^T x > T$

where

$$w = \Sigma^{-1}(\mu_1 - \mu_0).$$

• Using the assumption that 0 and 1 have been generated with the same covariance, we get a **linear boundary**.

A few linear classifiers: (2) Logistic Regression

Regression does not work

• Consider the toy classification example:

• Points \mathbf{x}_j are taken randomly between -10 and 50.

 $\circ~$ The label

$$y_j = \begin{cases} 0 \text{ if } \mathbf{x}_j < \pi, \\ 1 \text{ if } \mathbf{x}_j > \pi. \end{cases}$$

• What happens if we feed this directly to regression?... matlab demo



How can we adapt regression? logistic map

• Logistic map :

$$g(z) = \frac{e^z}{e^z + 1} = \frac{1}{e^{-z} + 1}$$



 \circ for any z, $0 \le g(z) \le 1$

How can we adapt regression? logistic map

Basic Idea

• Rather than find the best \mathbf{c} and b such that

$$f(\mathbf{x}_j) = \mathbf{c}^T \mathbf{x}_j + b \quad \approx \quad y_j \in \{0, 1\}$$

• logistic regression considers instead the best ${f c}$ and b such that

$$g \circ f(\mathbf{x}_j) = \frac{1}{e^{-(\mathbf{c}^T \mathbf{x}_j + b)} + 1} \approx y_j \in \{0, 1\}.$$

- if for a new point **x**,
 - $g \circ f(\mathbf{x}) > 1/2$, guess that the class is 1 ◦ $g \circ f(\mathbf{x}) < 1/2$, guess that the class is 0

Probabilistic Interpretation of Logistic Regression

- Suppose there is a probability density $\mathbf{p}(X, Y)$ on couples $(\mathbf{x}, y) \in \mathbb{R}^d \times \{0, 1\}$.
- Suppose for now that we **know** *p*.

• The ratio

$$r(\mathbf{x}) = \frac{p(Y=1|X=\mathbf{x})}{p(Y=0|X=\mathbf{x})}$$

is called the odds-ratio of a given point **x**.

• Obviously,

• if $r(\mathbf{x}) > 1$, then it is more likely that y = 1 than y = 0. • if $r(\mathbf{x}) < 1$, then one is tempted to guess that y = 0 than y = 1.

Probabilistic Interpretation of Logistic Regression

• In other words...

$$\log \frac{p(Y=1|X=\mathbf{x})}{p(Y=0|X=\mathbf{x})}, \quad \begin{cases} > 0 \text{ then } y=1 \text{ is the likely answer} \\ < 0 \text{ then } y=0 \text{ is the likely answer} \end{cases}$$

• Logistic regression assumes that the log-odds ratio follows a linear relationship

$$\log \frac{p(Y=1|X=\mathbf{x})}{p(Y=0|X=\mathbf{x})} \approx \mathbf{c}^T \mathbf{x} + b$$

• This implies that the decision surface is **linear**.

Note that Logistic Regression assumes a model only for the log-odds ratio, not for the whole probability p

Probabilistic Interpretation of Logistic Regression

• Since
$$p(Y = 0 | X = \mathbf{x}) = 1 - p(Y = 1 | X = \mathbf{x})$$
, we hence have

$$\log \frac{p(Y=1|X=\mathbf{x})}{1-p(Y=1|X=\mathbf{x})} = \mathbf{c}^T \mathbf{x} + b$$

• which in turn implies

$$p(Y = 1 | X = \mathbf{x}) = \frac{1}{e^{-(\mathbf{c}^T \mathbf{x} + b)} + 1} = g(\mathbf{c}^T \mathbf{x} + b).$$

Predictor variables contribute **linearly** to the increase/decrease of the probability that y = 1.

Estimation of c and *b* **through Maximum Likelihood**

- Flip coin, setting p(y = 1) = p and p(y = 0) = 1 p for binary random variable y,
 - $\circ\,$ Likelihood of a draw y knowing that probability is p,

$$p^y(1-p)^{1-y}$$

• In the context of logistic regression, p depends on \mathbf{c}, b and \mathbf{x}_j for each point,

$$\mathcal{L}(\mathbf{c},b) = \prod_{j=1}^{N} g(\mathbf{c}^T \mathbf{x}_j + b)^{y_j} (1 - g(\mathbf{c}^T \mathbf{x}_j + b))^{1-y_j}$$

Estimation of ${\bf c}$ and b through Maximum Likelihood

• Using again the log transformation,

$$\log \mathcal{L}(\mathbf{c}, b) = \sum_{j=1}^{N} y_j \log g(\mathbf{c}^T \mathbf{x}_j + b) + (1 - y_j) \log g(1 - (\mathbf{c}^T \mathbf{x}_j + b)).$$

• Maximizing this log-likelihood is equivalent to

$$\max_{\mathbf{c},b} \log \mathcal{L}(\mathbf{c},b) \Leftrightarrow \max_{\mathbf{c},b} \sum_{j=1}^{N} y_j(\mathbf{c}^T \mathbf{x}_j + b) - \log(1 + e^{\mathbf{c}^T \mathbf{x}_j + b}).$$

- No closed form solution for this unfortunately... need efficient optimization.
- For datasets of reasonable size, Newton method for instance.

Estimation of \mathbf{c} and b through Maximum Likelihood



...with



Compare...

A few linear classifiers: (3) Perceptron Rule

Estimation of c and b through iterative updates

- Iterative algorithm that considers each data point successively.
- Here we consider $S = \{-1, 1\}$
- Start from any arbitrary estimate $\omega = \begin{bmatrix} b \\ c \end{bmatrix}$.
- Loop over j until ω does not change for a while...
 - Consider a point $\begin{bmatrix} 1 \\ \mathbf{x}_j \end{bmatrix}$ and his label y_j . • Do $u_j = \operatorname{sign}(\omega^T \begin{bmatrix} 1 \\ \mathbf{x}_j \end{bmatrix})$ and y_j match? • it not, set $\omega \leftarrow \omega + \rho(y_j - u_j) \begin{bmatrix} 1 \\ \mathbf{x}_j \end{bmatrix}$.
- Not much more to add, better see in practice.



A few linear classifiers: (4) Support Vector Machine











Largest Margin Linear Classifier ?



Support Vectors with Large Margin



In equations



 We assume (for the moment) that the data are linearly separable, i.e., that there exists (w, b) ∈ ℝ^d × ℝ such that:

$$\begin{cases} \mathbf{w}^T \mathbf{x}_i + b > 0 & \text{if } \mathbf{y}_i = 1 ,\\ \mathbf{w}^T \mathbf{x}_i + b < 0 & \text{if } \mathbf{y}_i = -1 . \end{cases}$$

- Next, we give a formula to compute the margin as a function of \mathbf{w} .
- Obviously, for any $t \in \mathbb{R}$,

$$H_{\mathbf{w},b} = H_{t\mathbf{w},tb}$$

- Thus w and b are defined up to a multiplicative constant.
- We need to take care of this in the definition of the margin

How to find the largest separating hyperplane?

For the linear classifier $f(\mathbf{x}) = \mathbf{w}^T \mathbf{x} + b$,

consider the **interstice** defined by the hyperplanes:

•
$$f(\mathbf{x}) = \mathbf{w}^T \mathbf{x} + b = \mathbf{+1}$$

• $f(\mathbf{x}) = \mathbf{w}^T \mathbf{x} + b = -\mathbf{1}$



• Consider \mathbf{x}_1 and \mathbf{x}_2 such that $\mathbf{x}_2 - \mathbf{x}_1$ is parallel to \mathbf{w} .

The margin is $2/||\mathbf{w}||$

• Margin = $2/||\mathbf{w}||$: the points \mathbf{x}_1 and \mathbf{x}_2 satisfy:

$$\begin{cases} \mathbf{w}^T \mathbf{x}_1 + b = 0, \\ \mathbf{w}^T \mathbf{x}_2 + b = 1. \end{cases}$$

• By subtracting we get $\mathbf{w}^T(\mathbf{x}_2 - \mathbf{x}_1) = 1$, and therefore:

$$\gamma \stackrel{\text{def}}{=} 2||\mathbf{x}_2 - \mathbf{x}_1|| = \frac{2}{||\mathbf{w}||}.$$

where γ is by definition the margin.

All training points should be on the appropriate side

• For positive examples $(y_i = 1)$ this means:

 $\mathbf{w}^T \mathbf{x}_i + b \ge 1$

• For negative examples $(y_i = -1)$ this means:

$$\mathbf{w}^T \mathbf{x}_i + b \le -1$$

• in both cases:

$$\forall i = 1, \dots, n, \qquad \mathbf{y}_i \left(\mathbf{w}^T \mathbf{x}_i + b \right) \ge 1$$

Finding the optimal hyperplane



• Find (**w**, *b*) which minimize:

 $\|\mathbf{w}\|^2$

under the constraints:

$$\forall i = 1, \dots, n, \quad \mathbf{y}_i \left(\mathbf{w}^T \mathbf{x}_i + b \right) - 1 \ge 0.$$

This is a classical quadratic program on \mathbb{R}^{d+1} linear constraints - quadratic objective

Another interpretation: Convex Hulls ?



go back to 2 sets of points that are linearly separable

Another interpretation: Convex Hulls



Linearly separable = convex hulls do not intersect

Another interpretation: Convex Hulls



Find two closest points, one in each convex hull

Another interpretation: Convex Hulls



The SVM = bisection of that segment
Another interpretation: Convex Hulls



support vectors = extreme points of the faces on which the two points lie

The non-linearly separable case for SVM's

(when convex hulls intersect)









Soft-margin SVM ?

- Find a trade-off between large margin and few errors.
- Mathematically:

$$\min_{f} \left\{ \frac{1}{\mathsf{margin}(f)} + C \times \mathsf{errors}(f) \right\}$$

• C is a parameter



Soft-margin SVM formulation ?

• The margin of a labeled point (\mathbf{x}, \mathbf{y}) is

 $margin(\mathbf{x}, \mathbf{y}) = \mathbf{y} \left(\mathbf{w}^T \mathbf{x} + b \right)$

- The error is
 - \circ 0 if margin(**x**, **y**) > 1, \circ 1 − margin(**x**, **y**) otherwise.
- The soft margin SVM solves:

$$\min_{\mathbf{w},b} \{ \|\mathbf{w}\|^2 + C \sum_{i=1}^n \max\{0, 1 - \mathbf{y}_i \left(\mathbf{w}^T \mathbf{x}_i + b\right) \}$$

- $c(u, y) = \max\{0, 1 yu\}$ is known as the hinge loss.
- $c(\mathbf{w}^T \mathbf{x}_i + b, \mathbf{y}_i)$ associates a mistake cost to the decision \mathbf{w}, b for example \mathbf{x}_i .