Classification with generative models I

DSE 210

Machine learning versus Algorithms

In both fields, the goal is to develop

procedures that exhibit a desired input-output behavior.

- **Algorithms**: the input-output mapping can be precisely defined.
  Input: Graph G.
  Output: MST of G.
- **Machine learning**: the mapping cannot easily be made precise.
  Input: Picture of an animal.
  Output: Name of the animal.

Instead, we simply provide examples of (input,output) pairs and ask the machine to *learn* a suitable mapping itself.

Inputs and outputs

Basic terminology:

- The input space, $\mathcal{X}$.
  E.g. 32×32 RGB images of animals.
- The output space, $\mathcal{Y}$.
  E.g. Names of 100 animals.

x:

y: "bear"

After seeing a bunch of examples (x, y), pick a mapping

$$f : \mathcal{X} \to \mathcal{Y}$$

that accurately replicates the input-output pattern of the examples.

Learning problems are often categorized according to the type of *output space*: (1) discrete, (2) continuous, (3) probability values, or (4) more general structures.

Discrete output space: classification

Binary classification:

- Spam detection
  $\mathcal{X} = \{\text{email messages}\}$
  $\mathcal{Y} = \{\text{spam}, \text{not spam}\}$
- Credit card fraud detection
  $\mathcal{X} = \{\text{descriptions of credit card transactions}\}$
  $\mathcal{Y} = \{\text{fraudulent}, \text{legitimate}\}$

Multiclass classification:

- Animal recognition
  $\mathcal{X} = \{\text{animal pictures}\}$
  $\mathcal{Y} = \{\text{dog}, \text{cat}, \text{giraffe}, \ldots\}$
- News article classification
  $\mathcal{X} = \{\text{news articles}\}$
  $\mathcal{Y} = \{\text{politics}, \text{business}, \text{sports}, \ldots\}$

Continuous output space: regression

- A parent's concerns
  How cold will it be tomorrow morning?
  $\mathcal{Y} = [-273, \infty)$
- For the asthmatic
  Predict tomorrow's air quality (max over the whole day)
  $\mathcal{Y} = [0, \infty)$ (< 100: okay, > 200: dangerous)
- Insurance company calculations
  In how many years will this person die?
  $\mathcal{Y} = [0, 200]$

What are suitable predictor variables ($\mathcal{X}$) in each case?

Conditional probability functions

Here $\mathcal{Y} = [0, 1]$ represents probabilities.

- Dating service
  What is the probability these two people will go on a date if introduced to each other?
  If we modeled this as a classification problem, the binary answer would basically always be "no". The goal is to find matches that are slightly less unlikely than others.
- Credit card transactions
  What is the probability that this transaction is fraudulent?
  The probability is important, because – in combination with the amount of the transaction – it determines the overall risk and thus the right course of action.

Structured output spaces

The output space consists of structured objects, like sequences or trees.

Dating service

Input: description of a person
Output: rank-ordered list of all possible matches

$\mathcal{Y}$ = space of all permutations

Example:
$x = Tom$
$y = (Nancy, Mary, Chloe, \ldots)$

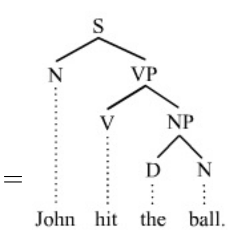
Language processing

Input: English sentence
Output: parse tree showing grammatical structure

$\mathcal{Y}$ = space of all trees

Example:
$x =$ "John hit the ball"

$y =$



A basic classifier: nearest neighbor

Given a labeled training set $(x^{(1)}, y^{(1)}), \ldots, (x^{(n)}, y^{(n)})$.

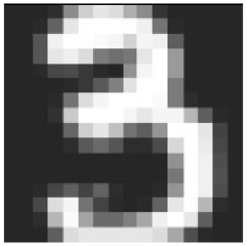
Example: the MNIST data set of handwritten digits.

To classify a new instance x:

- Find its nearest neighbor amongst the $x^{(i)}$
- Return $y^{(i)}$

The data space

We need to choose a distance function.



Each image is 28×28 grayscale.
One option: Treat images as 784-dimensional vectors, and use Euclidean (ℓ_2) distance:

$$\|x - x'\| = \sqrt{\sum_{i=1}^{784} (x_i - x_i')^2}.$$

Summary:

- Data space $\mathcal{X} = \mathbb{R}^{784}$ with ℓ_2 distance
- Label space $\mathcal{Y} = \{0, 1, \ldots, 9\}$

Performance on MNIST

Training set of 60,000 points.

- What is the error rate on training points? **Zero.**
  In general, **training error** is an overly optimistic predictor of future performance.
- A better gauge: separate test set of 10,000 points.
  Test error = fraction of test points incorrectly classified.
- What test error would we expect for a random classifier? **90%.**
- Test error of nearest neighbor: **3.09%.**

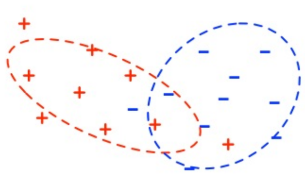
Examples of errors:

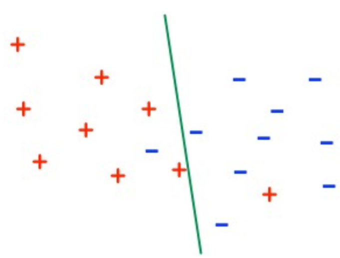
Properties of NN: (1) Can model arbitrarily complex functions
(2) Unbounded in size

Classification with parametrized models

Classifiers with a fixed number of parameters can represent a limited set of functions. Learning a model is about picking a good approximation.

Typically the x's are points in p-dimensional Euclidean space, $\mathbb{R}^p$.





Two ways to classify:

- **Generative**: model the individual classes.
- **Discriminative**: model the decision boundary between the classes.

Quick review of conditional probability

Formula for conditional probability: for any events A, B,

$$\Pr(A|B) = \frac{\Pr(A \cap B)}{\Pr(B)}.$$

Applied twice, this yields Bayes' rule:

$$\Pr(H|E) = \frac{\Pr(E|H)}{\Pr(E)} \Pr(H).$$

Summation rule: Suppose events $A_1, \ldots, A_k$ are disjoint events, one of which must occur. Then for any other event E,

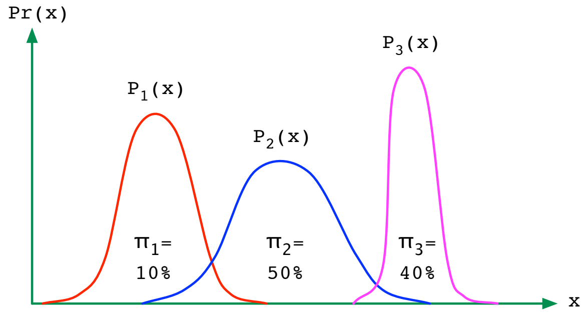
$$\begin{aligned}\Pr(E) &= \Pr(E, A_1) + \Pr(E, A_2) + \cdots + \Pr(E, A_k) \\ &= \Pr(E|A_1)\Pr(A_1) + \Pr(E|A_2)\Pr(A_2) + \cdots + \Pr(E|A_k)\Pr(A_k)\end{aligned}$$

Generative models

Generating a point (x, y) in two steps:

1. First choose y
2. Then choose x given y

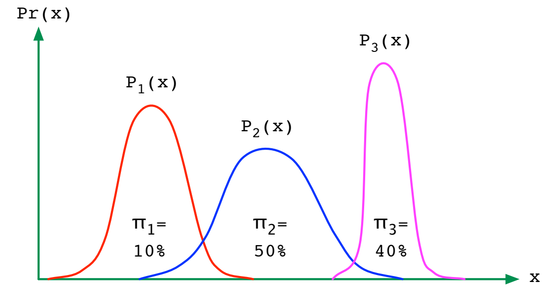
Example:
$\mathcal{X} = \mathbb{R}$
$\mathcal{Y} = \{1, 2, 3\}$



The overall density is a mixture of the individual densities,

$$\Pr(x) = \pi_1 P_1(x) + \cdots + \pi_k P_k(x).$$

The Bayes-optimal prediction



Labels $\mathcal{Y} = \{1, 2, \ldots, k\}$, density $\Pr(x) = \pi_1 P_1(x) + \cdots + \pi_k P_k(x)$.

For any $x \in \mathcal{X}$ and any label j,

$$\Pr(y = j|x) = \frac{\Pr(y = j)\Pr(x|y = j)}{\Pr(x)} = \frac{\pi_j P_j(x)}{\sum_{i=1}^{k} \pi_i P_i(x)}$$

Bayes-optimal (minimum-error) prediction: $h^*(x) = \arg\max_j \pi_j P_j(x)$.

Estimating the π_j is easy. Estimating the P_j is hard.

Estimating class-conditional distributions

Estimating an arbitrary distribution in $\mathbb{R}^p$:

- Can be done, e.g. with kernel density estimation.
- But number of samples needed is exponential in p.

Instead: approximate each P_j with a simple, parametric distribution.

Some options:

- Product distributions.
  Assume coordinates are independent: naive Bayes.
- Multivariate Gaussians.
  Linear and quadratic discriminant analysis.
- More general graphical models.

Naive Bayes

Labels $\mathcal{Y} = \{1, 2, \ldots, k\}$, density $\Pr(x) = \pi_1 P_1(x) + \cdots + \pi_k P_k(x)$.

Binarized MNIST:

- $k = 10$ classes
- $\mathcal{X} = \{0, 1\}^{784}$

Assume that **within each class**, the individual pixel values are independent:

$$P_j(x) = P_{j1}(x_1) \cdot P_{j2}(x_2) \cdots P_{j,784}(x_{784}).$$

Each P_{ji} is a coin flip: trivial to estimate!

Smoothed estimate of coin bias

Pick a class j and a pixel i. We need to estimate

$$p_{ji} = \Pr(x_i = 1 | y = j).$$

Out of a training set of size n,

$$\begin{aligned} n_j &= \# \text{ of instances of class } j \\ n_{ji} &= \# \text{ of instances of class } j \text{ with } x_i = 1 \end{aligned}$$

Then the maximum-likelihood estimate of p_{ji} is

$$\widehat{p}_{ji} = n_{ji}/n_j.$$

This causes problems if $n_{ji} = 0$. Instead, use "Laplace smoothing":

$$\widehat{p}_{ji} = \frac{n_{ji}+1}{n_j+2}.$$

Form of the classifier

Data space $\mathcal{X} = \{0,1\}^p$, label space $\mathcal{Y} = \{1,\ldots,k\}$. Estimate:

- $\{\pi_j : 1 \leq j \leq k\}$
- $\{p_{ji} : 1 \leq j \leq k, 1 \leq i \leq p\}$

Then classify point x as

$$\arg\max_j \quad \pi_j \prod_{i=1}^{p} p_{ji}^{x_i} (1-p_{ji})^{1-x_i}.$$

To avoid underflow: take the log:

$$\arg\max_j \quad \underbrace{\log \pi_j + \sum_{i=1}^{p} (x_i \log p_{ji} + (1-x_i)\log(1-p_{ji}))}_{\text{of the form } w \cdot x + b}$$

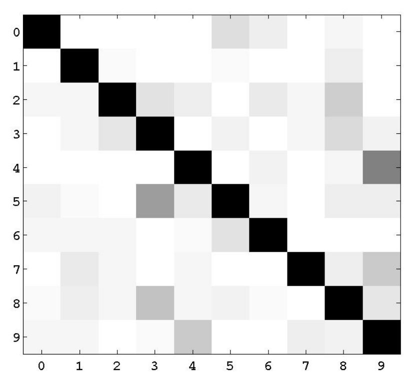
A linear classifier!

Example: MNIST

Result of training: mean vectors for each class.

Test error rate: 15.54%.

Visualization of the "confusion matrix" $\longrightarrow$



Other types of data

How would you handle data:

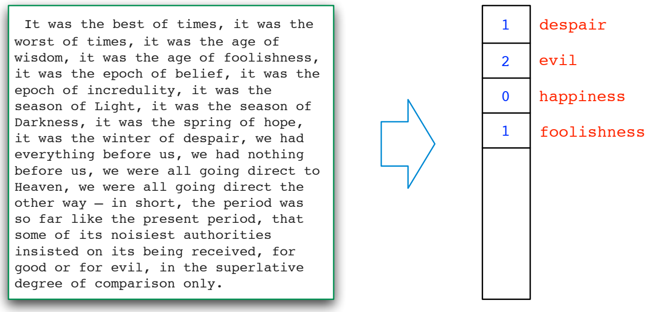
- Whose features take on more than two discrete values (such as ten possible colors)?
- Whose features are real-valued?
- Whose features are positive integers?
- Whose features are mixed: some real, some Boolean, etc?

How would you handle "missing data": situations in which data points occasionally (or regularly) have missing entries?

- At train time: **???**
- At test time: **???**

Handling text data

Bag-of-words: vectorial representation of text documents.



- Fix V = some vocabulary.
- Treat each document as a vector of length $|V|$:

$$x = (x_1, x_2, \ldots, x_{|V|}),$$

where x_i = # of times the ith word appears in the document.

A standard distribution over such document-vectors x: the **multinomial**.

Multinomial naive Bayes

Multinomial distribution over a vocabulary V:

$$p = (p_1, \ldots, p_{|V|}), \quad \text{such that } p_i \geq 0 \text{ and } \sum_i p_i = 1$$

Document $x = (x_1, \ldots, x_{|V|})$ has probability $\propto p_1^{x_1} p_2^{x_2} \cdots p_{|V|}^{x_{|V|}}$.

For naive Bayes: one multinomial distribution per class.

- Class probabilities $\pi_1, \ldots, \pi_k$
- Multinomials $p^{(1)} = (p_{11}, \ldots, p_{1|V|}), \ldots, p^{(k)} = (p_{k1}, \ldots, p_{k|V|})$

Classify document x as

$$\arg\max_j \quad \pi_j \prod_{i=1}^{|V|} p_{ji}^{x_i}.$$

(As always, take log to avoid underflow: linear classifier.)

Improving performance of multinomial naive Bayes

A variety of heuristics that are standard in text retrieval, such as:

1. Compensating for burstiness.
   Problem: Once a word has appeared in a document, it has a much higher chance of appearing again.

   Solution: Instead of the number of occurrences f of a word, use $\log(1+f)$.

2. Downweighting common words.
   Problem: Common words can have a unduly large influence on classification.

   Solution: Weight each word w by **inverse document frequency**:

$$\log \frac{\#\text{ docs}}{\#(\text{docs containing } w)}$$