# Nearest neighbor classification

CSE 250B

## Nearest neighbor classification

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 $28 \times 28$ grayscale.
One option: Treat images as 784-dimensional vectors, and use Euclidean ($\ell_2$) distance:

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

Summary:

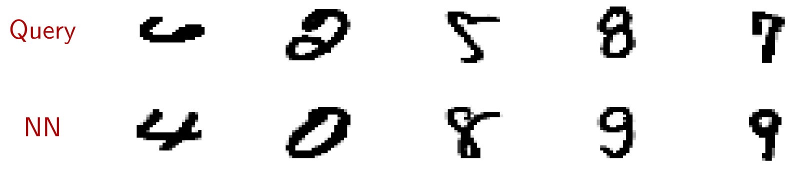
- Data space $\mathcal{X} = \mathbb{R}^{784}$ with $\ell_2$ distance
- Label space $\mathcal{Y} = \{0, 1, \ldots, 9\}$

## 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:



Ideas for improvement: (1) $k$-NN (2) better distance function.

## $K$-nearest neighbor classification

Classify a point using the labels of its $k$ nearest neighbors among the training points.

MNIST:

| $k$ | 1 | 3 | 5 | 7 | 9 | 11 |
|---|---|---|---|---|---|---|
| Test error (%) | 3.09 | 2.94 | 3.13 | 3.10 | 3.43 | 3.34 |

How to choose $k$ in general?
Let $S \in \mathcal{Z}^n$ be the training set, where $\mathcal{Z} = \mathcal{X} \times \mathcal{Y}$ is the space of *labeled* points. Let $\Gamma_k(S, x)$ be the prediction made on $x$ using its $k$-NN in $S$.

1. Hold-out set. Choose a subset $V \subset S$ as a *validation set*.

$$\arg\min_k \sum_{(x,y)\in V} \mathbf{1}(\Gamma_k(S \setminus V, x) \neq y)$$

2. Leave-one-out cross-validation.

$$\arg\min_k \sum_{(x,y)\in S} \mathbf{1}(\Gamma_k(S \setminus \{(x,y)\}, x) \neq y)$$

## Better distance functions

Let $x$ be an image. Consider an image $x'$ that is just like $x$, but is either:

- shifted one pixel to the right, or
- rotated slightly.

Then $\|x - x'\|$ could easily be quite large.

It makes sense to choose distance measures that are invariant under:

- Small translations and rotations. e.g. *tangent distance*.
- A broader family of natural deformations. e.g. *shape context*.

Test error rates:

| $\ell_2$ | tangent distance | shape context |
|---|---|---|
| 3.09 | 1.10 | 0.63 |

Are there families of distance functions that are often useful?

## $\ell_p$ norms

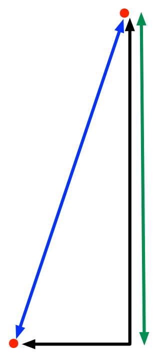
How can we measure the length of a vector in $\mathbb{R}^m$?
Usual choice is the *Euclidean norm*:

$$\|x\|_2 = \sqrt{\sum_{i=1}^m x_i^2}.$$

Generalization: For $p \geq 1$, the $\ell_p$ norm is

$$\|x\|_p = \left(\sum_{i=1}^m |x_i|^p\right)^{1/p}$$

- $p = 2$: Euclidean norm
- $\ell_1$ norm: $\|x\|_1 = \sum_{i=1}^m |x_i|$
- $\ell_\infty$ norm: $\|x\|_\infty = \max_i |x_i|$



## Quick quiz

Suppose data lie in $\mathbb{R}^p$.

1. What is the $\ell_2$ norm of the all-ones vector?
2. Suppose $\|x\|_1 = 1$.
   In what range must $\|x\|_2$ lie?

## Metric spaces

A more general notion is a *metric space*.

Let $\mathcal{X}$ be the space in which data lie. A distance function $d : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is a *metric* if it satisfies these properties:

- $d(x, y) \geq 0$ (nonnegativity)
- $d(x, y) = 0$ if and only if $x = y$
- $d(x, y) = d(y, x)$ (symmetry)
- $d(x, z) \leq d(x, y) + d(y, z)$ (triangle inequality)

For instance:

- $\mathcal{X} = \mathbb{R}^m$ and $d(x, y) = \|x - y\|_p$
- $\mathcal{X} = \{\text{strings over some alphabet}\}$ and $d =$ edit distance.

Later in the course: methods for *learning* suitable distance measures.

## Outline

- Nearest neighbor classification
- Statistical analysis
- Algorithmic analysis
- Some questions to ponder

## The statistical learning framework

**Why does training data help us develop a model that will work well on future data? Because they come from the same source: the same underlying distribution.**

**Model of reality: there is an (unknown) underlying distribution, call it $P$, from which pairs $(X, Y)$ are generated.**

- Training points $(x, y)$ come from this distribution.
- Future test points will also come from this distribution.

We want a classifier

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

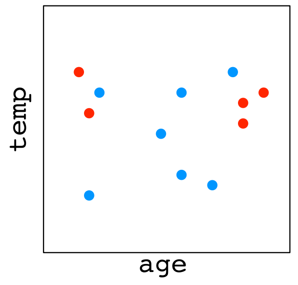
which will do well on future data, i.e., do well on distribution $P$.

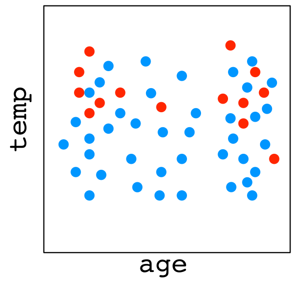
But we don't know $P$, so we treat the training data as a proxy for it.

## The underlying distribution: example

A new strain of flu is highly contagious and seems to particularly affect children and the elderly. We want to predict whether patients waiting in an emergency room have this flu, based only on age and temperature.

- $\mathcal{X} = \mathbb{R}^2$ (age, temperature)
- $\mathcal{Y} = \{0, 1\}$ (1 = flu)





As we get more and more samples, we get a better idea of the underlying distribution over $\mathcal{X} \times \mathcal{Y}$.

## Three ways to sample

Three ways to draw a sample from a distribution $P$ over pairs $(x, y)$:

1. Draw the pair $(x, y)$ in one go.
2. First draw $y$ according to its *marginal distribution*.
   Then draw $x$ according to its *conditional distribution* given $y$.
3. First draw $x$ according to its marginal distribution.
   Then draw $y$ according to its conditional distribution given $x$.

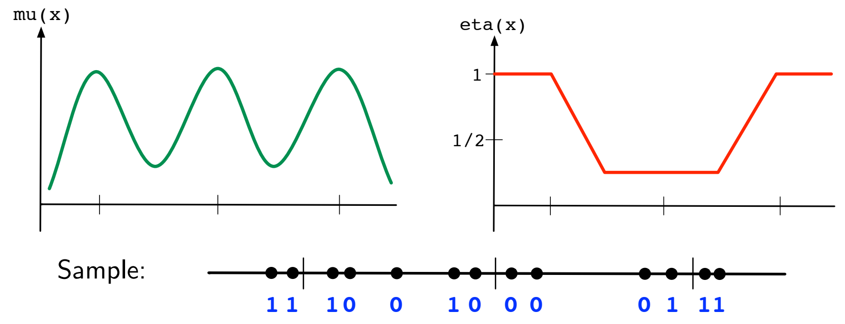
## The underlying distribution

Reality $\equiv$ the underlying distribution on pairs $(X, Y)$
Can factor this distribution into two parts:

- The distribution of $X$. Call this $\mu$.
- The distribution over labels $Y$ given $X$. In the binary case ($\mathcal{Y} = \{0, 1\}$) this can be specified as $\eta(x) = \Pr(Y = 1|X = x)$.

For instance, distribution of patients in a community:

$x$ = age
$y = 1$ if visited doctor in the last year



## Quick quiz

Suppose there are two possible labels, $Y \in \{0, 1\}$, that each occur 50% of the time. Data points $X$ lie in $\mathbb{R}$ and have the following distribution:

- When $Y = 0$, points $X$ are distributed uniformly in $[-2, 1]$.
- When $Y = 1$, points $X$ are distributed uniformly in $[-1, 2]$.

What is the marginal distribution $\mu$ of $X$?

What is the conditional probability distribution $\eta(x) = \Pr(Y = 1|X = x)$?

## Statistical learning framework, cont'd

Let's look at the binary case, $\mathcal{Y} = \{0, 1\}$.

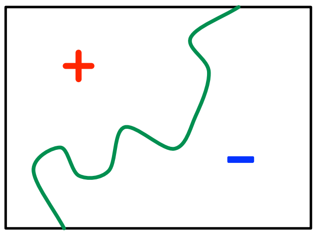
- There is an (unknown) underlying probability distribution on $\mathcal{X}$ from which *all* points are generated. Call this distribution $\mu$.
- The label of any point $x$ can, in general, be *stochastic*. It is a coin flip with bias $\eta(x) = \Pr(Y = 1|X = x)$.
- A classifier is a rule $h : \mathcal{X} \to \{0, 1\}$. Its misclassification rate, or *risk*, is $R(h) = \Pr(h(X) \neq Y)$.

The Bayes-optimal classifier

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

has minimum risk,

$$R^* = R(h^*) = \mathbb{E}_X \min(\eta(X), 1 - \eta(X)).$$



## Quick quiz, cont'd

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What is the Bayes risk $R^*$?

What is the risk of a classifier that always predicts 0?

## Statistical theory of nearest neighbor

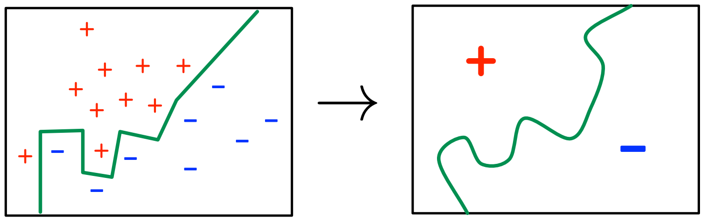
Let $h_n$ be a classifier based on $n$ training points from the underlying distribution.

- Its risk is $R(h_n) = \Pr(h_n(X) \neq Y)$.
- We say it is **consistent** if, as $n$ grows to infinity, $R(h_n) \to R^*$ .

Consistency of NN (Fix and Hodges, 1951; Cover and Hart, 1967):

- Suppose $\eta(x) = \Pr(Y = 1 | X = x)$ is continuous in $x$.
- Set $k$ to a growing function of $n$, with (1) $k \to \infty$ and (2) $k/n \to 0$, as $n \to \infty$.

Then $k$-NN is consistent.



## Statistical theory of 1-NN

1-NN is not consistent.

E.g. $\mathcal{X} = \mathbb{R}$ and $\eta(x) \equiv 1/4$. Every label is a coin flip with bias 1/4.

- Bayes optimal classifier: always predict 0. Risk $R^* = 1/4$.
- 1-NN risk: what is the probability that two coins of bias 1/4 disagree?

$$R(h_n) = 2 \cdot \frac{1}{4} \cdot \frac{3}{4} = \frac{3}{8} > \frac{1}{4}.$$

But (Cover-Hart 1967) it is always within a factor two of optimal:

$$R(h_n) \to 2R^*(1 - R^*).$$

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## Fast NN search

Naive search is $O(n)$ for training set of size $n$: very slow.

Two popular approaches to fast nearest neighbor search, for data set $S \subset \mathcal{X}$ and query $q$.

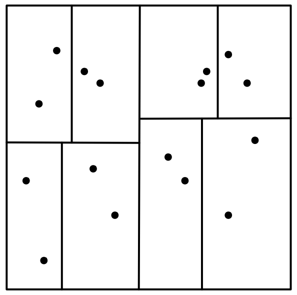
1. Locality sensitive hashing
   Collection of special hash functions $h_1, \ldots, h_m : \mathcal{X} \to \mathbb{Z}$.
   Search for nearest neighbor in
   $$\bigcup_{i=1}^{m} \{x \in S : h_i(x) = h_i(q)\}$$
   This set is smaller than $S$, and is likely to contain the nearest neighbor of $q$.
2. Tree-based search
   Build tree structure on $S$, and use it to discard subsets of $S$ that are far from a query $q$.
   Common options: $k$-d tree, PCA tree, cover tree.

## $K$-d trees for NN search

A hierarchical, rectilinear spatial partition.

For data set $S \subset \mathbb{R}^p$:

- Pick a coordinate $1 \leq i \leq p$.
- Compute $v = \text{median}(\{x_i : x \in S\})$.
- Split $S$ into two halves:
$$S_L = \{x \in S : x_i < v\}$$
$$S_R = \{x \in S : x_i \geq v\}$$
- Recurse on $S_L, S_R$



Two types of search, given a query $q \in \mathbb{R}^p$:

- *Defeatist search*: Route $q$ to a leaf cell and return the NN in that cell. This might not be the true NN.
- *Comprehensive search*: Grow the search region to other cells that cannot be ruled out using the triangle inequality.

## The curse of dimension

Situation: $n$ data points in $\mathbb{R}^p$.

1. Storage is $O(np)$
2. Time to compute distance is $O(p)$ for $\ell_p$ norms
3. Geometry
   It is possible to have $2^{O(p)}$ points that are roughly equidistant from each other.

Current methods for fast exact NN search have time complexity proportional to $2^p$ and $\log n$.

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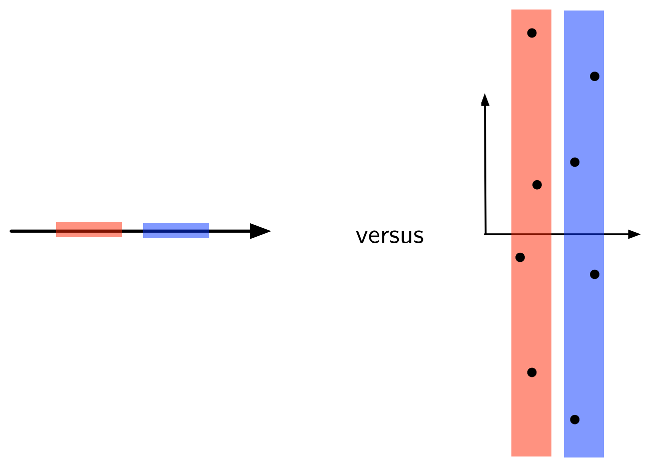
## Beyond classification

How might nearest neighbor be used for the following tasks?

- Regression
- Conditional probability estimation
- Classification with confidence intervals

## Sensitivity to noise

Adding a single sufficiently noisy feature can wreak havoc with nearest neighbor classifiers.



How to do feature selection/reweighting for nearest neighbor?