Nearest neighbor classifiers

COMS 4771
1. Nearest neighbor rule
1. Classify images of handwritten digits by the actual digits they represent.

2. Classification problem: $\mathcal{Y} = \{0, 1, 2, 3, 4, 5, 6, 7, 8, 9\}$ (a discrete set).
Nearest neighbor (NN) classifier

**Given:** labeled examples $D := \{(x_i, y_i)\}_{i=1}^n$

**Predictor:** $\hat{f}_D : \mathcal{X} \to \mathcal{Y}$

On input $x$,

1. Find the point $x_i$ among $\{x_i\}_{i=1}^n$ that is “closest” to $x$ (the nearest neighbor).
2. Return $y_i$. 

\[
\begin{array}{c}
4 \\
\xrightarrow{\hat{f}_D} \\
\text{“4”}
\end{array}
\]
How to measure distance?

A default choice for distance between points in $\mathbb{R}^d$ is the *Euclidean distance* (also called $\ell_2$ distance):

$$
\|u - v\|_2 := \sqrt{\sum_{i=1}^{d} (u_i - v_i)^2}
$$

(where $u = (u_1, u_2, \ldots, u_d)$ and $v = (v_1, v_2, \ldots, v_d)$).

Grayscale $28 \times 28$ pixel images.

Treat as vectors (of 784 real-valued features) that live in $\mathbb{R}^{784}$. 

2. Evaluation
Example: OCR for digits with NN classifier

- Classify images of handwritten digits by the digits they depict.
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\[ \mathcal{X} = \mathbb{R}^{784}, \mathcal{Y} = \{0, 1, \ldots, 9\}. \]
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\[ 0 \ 1 \ 2 \ 3 \ 4 \ 5 \ 6 \ 7 \ 8 \ 9 \]

- \( \mathcal{X} = \mathbb{R}^{784}, \ \mathcal{Y} = \{0, 1, \ldots, 9\} \).

- **Given**: labeled examples \( D := \{(x_i, y_i)\}_{i=1}^n \subset \mathcal{X} \times \mathcal{Y} \).
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- Construct NN classifier \( \hat{f}_D \) using \( D \).
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- Construct NN classifier \( \hat{f}_D \) using \( D \).

- **Question:** Is this classifier any good?
Error rate of classifier $f$ on a set of labeled examples $D$:

$$\text{err}(f; D) := \frac{\# \text{ of } (x, y) \in D \text{ such that } f(x) \neq y}{|D|}$$

(i.e., the fraction of $D$ on which $f$ disagrees with paired label).
Error rate

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(i.e., the fraction of $D$ on which $f$ disagrees with paired label).

- **Question**: What is $\text{err}(\hat{f}_D; D)$?
A better way to evaluate the classifier

- Split the labeled examples \( \{(x_i, y_i)\}_{i=1}^{n} \) into two sets (randomly).
  - Training data \( S \).
  - Test data \( T \).
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- Split the labeled examples \( \{(x_i, y_i)\}_{i=1}^{n} \) into two sets (randomly).
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- Only use training data \( S \) to construct NN classifier \( \hat{f}_S \).
A better way to evaluate the classifier

- Split the labeled examples $\{(x_i, y_i)\}_{i=1}^n$ into two sets (randomly).
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  - Training error rate of $\hat{f}_S$: $\text{err}(\hat{f}_S; S) = 0\%$.
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- Split the labeled examples \( \{(x_i, y_i)\}_{i=1}^{n} \) into two sets (randomly).
  - *Training data* \( S \).
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- Use *test data* \( T \) to evaluate accuracy of \( \hat{f}_S \).
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Is this good?
3. Upgrading the nearest neighbor rule
Diagnostics

Some mistakes made by the NN classifier (test point in $T$, nearest neighbor in $S$):

28
35
54
Diagnostics

- Some mistakes made by the NN classifier (test point in $T$, nearest neighbor in $S$):

  2 8 5 5 5 4

- First mistake (correct label is “2”) could’ve been avoided by looking at the *three* nearest neighbors (whose labels are “8”, “2”, and “2”).

  2 8 2 2
  test point  three nearest neighbors
\textit{k}-nearest neighbors classifier

\textbf{Given:} labeled examples \( D := \{(x_i, y_i)\}_{i=1}^{n} \)

\textbf{Predictor:} \( \hat{f}_{D,k} : \mathcal{X} \rightarrow \mathcal{Y} \):

On input \( x \),

1. Find the \( k \) points \( x_{i_1}, x_{i_2}, \ldots, x_{i_k} \) among \( \{x_i\}_{i=1}^{n} \) “closest” to \( x \) (the \( k \) nearest neighbors).
2. Return the plurality of \( y_{i_1}, y_{i_2}, \ldots, y_{i_k} \).

(Break ties in both steps arbitrarily.)
Effect of $k$

- Smaller $k$: smaller training error rate.
- Larger $k$: higher training error rate, but predictions are more “stable” due to voting.

<table>
<thead>
<tr>
<th>OCR digits classification</th>
<th>$k$</th>
<th>1</th>
<th>3</th>
<th>5</th>
<th>7</th>
<th>9</th>
</tr>
</thead>
<tbody>
<tr>
<td>Test error rate</td>
<td></td>
<td>0.0309</td>
<td>0.0295</td>
<td>0.0312</td>
<td>0.0306</td>
<td>0.0341</td>
</tr>
</tbody>
</table>
Choosing $k$

The hold-out set approach

1. Pick a subset $V \subset S$ (hold-out set, a.k.a. validation set).
2. For each $k \in \{1, 3, 5, \ldots \}$:
   - Construct $k$-NN classifier $\hat{f}_{S \setminus V, k}$ using $S \setminus V$.
   - Compute error rate of $\hat{f}_{S \setminus V, k}$ on $V$ ("hold-out error rate").
3. Pick the $k$ that gives the smallest hold-out error rate.
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(There are many other approaches.)
4. Other issues with nearest neighbor prediction
Better distance functions

- **Strings**: edit distance

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- **Audio waveforms**: dynamic time warping

- Etc.
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<tr>
<td>Distance</td>
</tr>
<tr>
<td>Test error rate</td>
</tr>
</tbody>
</table>
**Caution**: nearest neighbor classifier can be broken by bad/noisy features!
Naïve method for computing NN predictions: $O(n)$ distance computations.
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Better: organize training data in a data structure to improve look-up time.
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- Space: $O(nd)$ for $n$ points in $\mathbb{R}^d$.
- Query time: $O(2^d \log n)$ time in worst-case.
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E.g., how to quickly find a point among the top-1% closest points?
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- Popular technique: Locality sensitive hashing
Questions

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- Why is test error rate a better way to evaluate the classifier?
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- Why is test error rate a better way to evaluate the classifier?

We will answer these questions in the context of a statistical model.

(Next lecture!)
Key takeaways

1. $k$-NN learning procedure; role of $k$, distance functions, features.
2. Training and test error rates.