k-nearest neighbors (kNN)

## The problem we'll solve today

Given an image of a handwritten digit, say which digit it is


$$
\Longrightarrow \quad 3
$$

Some more examples:


## MNIST dataset



- Training set of 60,000 images and their labels
- Test set of 10,000 images and their labels


## Nearest neighbor classification

- Training images $x^{(1)}, x^{(2)}, x^{(3)}, \ldots, x^{(60000)}$
- Labels $y^{(1)}, y^{(2)}, y^{(3)}, \ldots, y^{(60000)}$ are numbers from $0-9$

$$
\begin{aligned}
& 1410119154857268032264141 \\
& 8663597202992997225100467 \\
& 0130841115910106154061036 \\
& 3110641110304752620099799 \\
& 6689120 \text { \#世 } 4085541314279554 \\
& 6010182501871129910899709 \\
& 8401097075973319720155190 \\
& 5610755182551828143580909 \\
& \text { 6317875416554603546035460 } \\
& 5518255108503047520439401
\end{aligned}
$$

## Nearest neighbor classification

- Training images $x^{(1)}, x^{(2)}, x^{(3)}, \ldots, x^{(60000)}$
- Labels $y^{(1)}, y^{(2)}, y^{(3)}, \ldots, y^{(60000)}$ are numbers from $0-9$ 1410119154857268032264141 8663597202992997225100467 0130841115910106154061036 3110641110304752620099799 6689120 \#世 4085541314279554 6010187501871129910899709 8401097075973319720155190 5510755182551828143580909 4317875416554605546035460 5518255108503047520439401

How to classify a new image $x$ ?

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


## Data as vectors

How to measure the distance between images?


Stretch each image into a vector with 784 coordinates

$$
\begin{aligned}
& x^{(1)}=(0,0,0, \ldots, 0.6,1,1,1,0,0,1,1,0.8, \ldots, 0,0,0) \\
& y^{(1)}=6
\end{aligned}
$$

## The distance function

Euclidean distance in two dimensions is

## Euclidean distance in higher dimension

Two images $a$ and $b$ :

$$
\begin{aligned}
a & =\left(a_{1}, a_{2}, a_{3}, \ldots, a_{784}\right) \\
b & =\left(b_{1}, b_{2}, b_{3}, \ldots, b_{784}\right)
\end{aligned}
$$

The Euclidean distance between $a$ and $b$ is

$$
\begin{aligned}
\|a-b\|_{2} & =\sqrt{\left(a_{1}-b_{1}\right)^{2}+\left(a_{2}-b_{2}\right)^{2}+\ldots+\left(a_{784}-b_{784}\right)^{2}} \\
& =\sqrt{\sum_{i=1}^{784}\left(a_{i}-b_{i}\right)^{2}}
\end{aligned}
$$

## Nearest neighbor classification

Training images $x^{(1)}, x^{(2)}, x^{(3)}, \ldots, x^{(60000)}$ Labels $y^{(1)}, y^{(2)}, y^{(3)}, \ldots, y^{(60000)}$

$$
\begin{aligned}
& \text { 1410119154857268032264141 } \\
& 8663597202992997225100467 \\
& 0130841115910106154061036 \\
& 3110641110304752620099799 \\
& 6689120 \text { \#世 } 7885571314279554 \\
& 6010187501871129990899709 \\
& 8401097075973319720155190 \\
& 5610755182551828143580909 \\
& 6317875416554605546035460 \\
& 5518255108503047520439401
\end{aligned}
$$

## Nearest neighbor classification

Training images $x^{(1)}, x^{(2)}, x^{(3)}, \ldots, x^{(60000)}$ Labels $y^{(1)}, y^{(2)}, y^{(3)}, \ldots, y^{(60000)}$

```
1410119154857268032264141
8663597202992997225100467
01308411115910106154061036
3110641110304752620099799
6689120%H47085541314279554
6010187501871129940899709
8401097075973319720155190
561075518255182-8143580909
6317875416554605S46035460
5518255108503047520439401
```

To classify a new image $x$

- Find its nearest neighbor in Euclidean distance, say $x^{(i)}$
- Return $y^{(i)}$


## Accuracy of Nearest Neightbor on MNIST

$$
\begin{aligned}
& 1410119154857268032264141 \\
& 8663597202992997225100467 \\
& 0130841115910106154061036 \\
& 3110641110304752620099799 \\
& 668912074085541314279554 \\
& 6060187801871129950899709 \\
& 8401097075973319720155190 \\
& 5510755182551828143580909 \\
& 631787571654645546035460 \\
& 5518255108503047520439401
\end{aligned}
$$

Predictions on all points in the Training set
Question: What is the accuracy?

## Accuracy of Nearest Neightbor on MNIST

```
1410119154857268032264141
8663597202992997225100467
01308411115910106154061036
3110641110304752620099799
6689120%4%7085541314279554
6010187501871129990899709
8401097075973319720155190
5510755182551828143580909
4317875416554605S46035460
5518255108503047520439401
```

Predictions on all points in the Test set
Question: What is the accuracy?

## Examples of errors

Test set of 10,000 points

- 309 are misclassified

Examples of errors:

Test image


2


8
7
Nearest neighbor


0


9
9
Ideas for improvement: $k$-NN

## $k$-nearest neighbor classification

To classify a new point:

- Find the $k$ nearest neighbors in the training set
- Return the most common label amongst them

MNIST:

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

need to find $k$ before final eval on the test set

## Validation



Train on Training set with $k=1 \Longrightarrow$ Evaluate on the Validation set Train on Training set with $k=3 \Longrightarrow$ Evaluate on the Validation set Train on Training set with $k=5 \Longrightarrow$ Evaluate on the Validation set

## Cross-validation

| Training Data |  |  |  | Validation | Holdout |
| :---: | :---: | :---: | :---: | :---: | :---: |
| Training Data |  |  | Validation |  | Holdout |
| Training Data |  | Validation |  |  | Holdout |
| Training Data | Validation |  |  |  | Holdout |
| Validation | Training Data |  |  |  | Holdout |
| 10\% | 20\% 30\% | 40\% | \% 60\% | 70\% | 90\% |

## Other distance function

$$
a=\left(a_{1}, a_{2}, \ldots, a_{m}\right) \quad b=\left(b_{1}, b_{2}, \ldots, b_{m}\right)
$$

- Cosine similarity

$$
d_{\mathrm{cos}}(a, b)=\frac{a \cdot b}{\|a\|_{2}\|b\|_{2}}=\frac{a}{\|a\|_{2}} \cdot \frac{b}{\|b\|_{2}}
$$

measures the angle between vector $a$ and $b$.

$$
-1 \leq d_{\cos }(a, b) \leq 1 .
$$

## Examples

$$
a=(1,2,2) \quad b=(3,4,0)
$$

## Distance between time series


use dynamic time warping

## $k$-NN regression

$$
y \text { is continuous } \quad x=\text { test data }
$$

$\left(x_{1}, y_{1}\right),\left(x_{2}, y_{2}\right), \ldots,\left(x_{k}, y_{k}\right)$ are $k$-nearest neighbors of $x$.

## Prediction:

$$
\hat{y}=\frac{1}{k} \sum_{i=1}^{k} y_{i}
$$

## Example

