K-nearest Neighbor
Announcements:

1. HW1 will be out today / early tomorrow and Due Sep 12

2. P1 will be out later this week

3. First paper reading quiz will be out later this week (for 5780)
Recap on ML basics

T/F: A hypothesis that achieves zero training error is always good

T/F: zero-one loss is a good loss function for regression

T/F: We can use validation dataset to check if our model overfits
Objective

Understand KNN — our first ML algorithm that can do both regression and classification
Outline for Today

1. The K-NN Algorithm

2. Why/When does K-NN work

3. Curse of dimensionality (i.e., when it can fail)
The K-NN Algorithm

**Input:** classification training dataset \( \{x_i, y_i\}_{i=1}^n \), and parameter \( K \in \mathbb{N}^+ \), and a distance metric \( d(x, x') \) (e.g., \( \|x - x'\|_2 \) euclidean distance)

**K-NN Algorithm:**

\[
x - x' = \sqrt{(x - x') \cdot (x - x')}
\]
The K-NN Algorithm

**Input**: classification training dataset \( \{ x_i, y_i \}_{i=1}^{n} \), and parameter \( K \in \mathbb{N}^+ \), and a distance metric \( d(x, x') \) (e.g., \( \| x - x' \|_2 \) euclidean distance)

**K-NN Algorithm:**

Store all training data
The K-NN Algorithm

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For any test point \( x \):
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**K-NN Algorithm:**

Store all training data

For any test point \( x \):

- Find its top \( K \) nearest neighbors (under metric \( d \))
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**K-NN Algorithm:**

1. Store all training data
2. For any test point \( x \):
   - Find its top \( K \) nearest neighbors (under metric \( d \))
   - Return the most common label among these \( K \) neighbors
The K-NN Algorithm

**Input:** classification training dataset \( \{x_i, y_i\}_{i=1}^n \), and parameter \( K \in \mathbb{N}^+ \), and a distance metric \( d(x, x') \) (e.g., \( \|x - x'\|_2 \) euclidean distance)

**K-NN Algorithm:**

Store all training data

For any test point \( x \):

- Find its top \( K \) nearest neighbors (under metric \( d \))
- Return the most common label among these \( K \) neighbors
  (If for regression, return the average value of the \( K \) neighbors)
The K-NN Algorithm

Example: 3-NN for binary classification using Euclidean distance
The choice of metric

1. We assume our metric $d$ captures similarities between examples:

Examples that are close to each other under distance $d$ share similar labels
The choice of metric

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   Examples that are close to each other under distance \( d \) share similar labels

Another example: Manhattan distance (\( \ell_1 \))

\[
d(x, x') = \sum_{j=1}^{d} | x[j] - x'[j] |
\]
The choice of $K$

1. What if we set $K$ very large?

\[ K = n \]
The choice of $K$

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Top $K$-neighbors will include examples that are very far away…
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Top $K$-neighbors will include examples that are very far away…

2. What if we set $K$ very small ($K=1$)?
The choice of \( K \)

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Top \( K \)-neighbors will include examples that are very far away…

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label has noise (easily overfit to the noise)
The choice of $K$

1. What if we set $K$ very large?

Top $K$-neighbors will include examples that are very far away…

2. What if we set $K$ very small (K=1)?

label has noise (easily overfit to the noise)

(What about the training error when $K = 1$?)
Outline for Today

1. The K-NN Algorithm

2. Why/When does K-NN work

3. Curse of dimensionality (i.e., why it can fail in high-dimension data)
Bayes Optimal Predictor

Assume our data is collected in an i.i.d fashion, i.e., \((x, y) \sim P\) (say \(y \in \{-1, 1\}\))
Bayes Optimal Predictor

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Assume we know \(P(y \mid x)\) for now

Q: what label you would predict?
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Assume we know \(P(y|x)\) for now

Q: what label you would predict?

A: we will simply predict the most-likely label,

\[
h_{opt}(x) = \arg \max_{y \in \{-1, 1\}} P(y|x)
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Bayes optimal predictor: 
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h_{opt}(x) = \arg \max_{y \in \{-1, 1\}} P(y | x)
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Example:

\[
\begin{align*}
P(1 | x) &= 0.8 \\
P(-1 | x) &= 0.2
\end{align*}
\]
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\[y_b := h_{opt}(x) = 1\]
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Q: What’s the probability of \(h_{opt}\) making a mistake on \(x\)?

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Bayes optimal predictor: \[ h_{opt}(x) = \arg \max_{y \in \{-1, 1\}} P(y \mid x) \]

Example:

\[
\begin{aligned}
P(1 \mid x) &= 0.8 \\
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\end{aligned}
\]

Q: What’s the probability of \(h_{opt}\) making a mistake on \(x\)?

\[ \epsilon_{opt} = 1 - P(y_b \mid x) = 0.2 \]
Guarantee of KNN when $K = 1$ and $n \to \infty$

Assume $x \in [-1,1]^2$, $P(x)$ has support everywhere $P(x) > 0, \forall x \in [-1,1]^2$
Guarantee of KNN when $K = 1$ and $n \to \infty$

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Assume $x \in [-1,1]^2$, $P(x)$ has support everywhere $P(x) > 0$, $\forall x \in [-1,1]^2$

What does it look when $n \to \infty$?

Given test $x$, as $n \to \infty$, its nearest neighbor $x_{NN}$ is super close, i.e., $d(x, x_{NN}) \to 0$!
Guarantee of KNN when $K = 1$ and $n \to \infty$

Theorem: as $n \to \infty$, 1-NN prediction error is no more than twice of the error of the Bayes optimal classifier

Proof:
Guarantee of KNN when $K = 1$ and $n \to \infty$

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Proof:
1. Fix a test example $x$, denote its NN as $x_{NN}$. When $n \to \infty$, we have $x_{NN} \to x$
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2. WLOG assume for $x$, the Bayes optimal predicts $y_b = h_{opt}(x) = 1$
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3. Calculate the 1-NN’s prediction error:
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   **Case 1** when \( y_{NN} = 1 \) (it happens w/ prob \( P(1 \mid x_{NN}) = P(1 \mid x) \)): 

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   **Case 1** when $y_{NN} = 1$ (it happens w/ prob $P(1 \mid x_{NN}) = P(1 \mid x)$):
   
   The probability of making a mistake: $\epsilon = P(y \neq 1 \mid x) = P(y = -1 \mid x)$. 

Guarantee of KNN when $K = 1$ and $n \to \infty$

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   $\epsilon = 1 - P(y_b \mid x)$
Guarantee of KNN when $K = 1$ and $n \rightarrow \infty$

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Guarantee of KNN when $K = 1$ and $n \to \infty$

Theorem: as $n \to \infty$, 1-NN prediction error is no more than twice of the error of the Bayes optimal classifier.

Case 1 when $y_{NN} = 1$ (it happens w/ prob $P(1 | x_{NN}) = P(1 | x)$):

The probability of making a mistake: $\epsilon = 1 - P(y_b | x)$

Case 2 when $y_{NN} = -1$ (it happens w/ prob $P(-1 | x_{NN}) = P(-1 | x)$):

The probability of making a mistake: $\epsilon = P(y \neq -1 | x) = P(y = 1 | x) = P(y_b | x)$

Final prediction error at $x$:

$$P(1 | x)(1 - P(y_b | x)) + P(-1 | x)P(y_b | x) \leq (1 - P(y_b | x)) + (1 - P(y_b | x))P(y_b | x) = 2\epsilon_{opt}$$
What happens if $K$ is large?
(e.g., $K = 1e6$, $n \to \infty$)

\[
\frac{K}{\eta} \to 0
\]
What happens if $K$ is large?
(e.g., $K = 1e6, n \to \infty$)

A: Given any $x$, the K-NN should return the $y_b$ — the solution of the Bayes optimal
Outline for Today

1. The K-NN Algorithm

2. Why/When does K-NN work

3. Curse of dimensionality (i.e., why it can fail in high-dimension data)
Finite sample error rate of 1-NN in high-dimension setting

(Informal result and no proof)
Finite sample error rate of $1$-NN in high-dimension setting

(Informal result and no proof)

Fix $n \in \mathbb{N}^+$, assume $x \in [0,1]^d$, assume $P(y \mid x)$ is Lipschitz continuous with respect to $x$, i.e., $|P(y \mid x) - P(y \mid x')| \leq d(x, x')$
Finite sample error rate of 1-NN in high-dimension setting

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Then, we have:
Finite sample error rate of 1-NN in high-dimension setting

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Fix $n \in \mathbb{N}^+$, assume $x \in [0,1]^d$, assume $P(y|x)$ is Lipschitz continuous with respect to $x$, i.e., $|P(y|x) - P(y|x')| \leq d(x,x')$

Then, we have:

$$\mathbb{E}_{x,y \sim P} \left[ 1(y \neq 1\text{NN}(x)) \right] \leq 2\mathbb{E}_{x,y \sim P} \left[ 1(y \neq h_{opt}(x)) \right] + O \left( \left( \frac{1}{n} \right)^{1/d} \right)$$
Finite sample error rate of 1-NN in high-dimension setting

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The bound is meaningless when $d \to \infty$, while $n$ is some finite number!
Finite sample error rate of 1-NN in high-dimension setting

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Fix \( n \in \mathbb{N}^+ \), assume \( x \in [0,1]^d \), assume \( P(y \mid x) \) is Lipschitz continuous with respect to \( x \), i.e., \(|P(y \mid x) - P(y \mid x')| \leq d(x,x')\)

Then, we have:

\[
\mathbb{E}_{x,y \sim P} \left[ 1(y \neq \text{1-NN}(x)) \right] \leq 2\mathbb{E}_{x,y \sim P} \left[ 1(y \neq h_{\text{opt}}(x)) \right] + O \left( \left( \frac{1}{n} \right)^{1/d} \right)
\]

Curse of dimensionality!

The bound is meaningless when \( d \to \infty \), while \( n \) is some finite number!
Curse of Dimensionality Explanation

Key problem: in high dimensional space, points that are drawn from a distribution tends to be far away from each other!
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Example: let us consider uniform distribution over a cube $[0,1]^d$
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Example: let us consider uniform distribution over a cube \([0,1]^d\)

Q: sample \(x\) uniformly, what is the probability that \(x\) is inside the small cube?
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Example: let us consider uniform distribution over a cube $[0,1]^d$

Q: sample $x$ uniformly, what is the probability that $x$ is inside the small cube?

A: $\frac{\text{Volume(small cube)}}{\text{volume}([0,1]^d)}$
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Example: let us consider uniform distribution over a cube $[0,1]^d$

Q: sample $x$ uniformly, what is the probability that $x$ is inside the small cube?

A: $\frac{\text{Volume(small cube)}}{\text{volume}([0,1]^d)} = l^d$
Curse of Dimensionality Explanation

Example: let us consider uniform distribution over a cube $[0,1]^d$

Now assume we sampled $n$ points uniform randomly, and we observed $K$ points fall inside the small cube.
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So empirically, the probability of sampling a point inside the small cube is roughly $K/n$
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Example: let us consider uniform distribution over a cube $[0,1]^d$

Now assume we sampled $n$ points uniform randomly, and we observed $K$ points fall inside the small cube.

So empirically, the probability of sampling a point inside the small cube is roughly $K/n$.

Thus, we have $l^d \approx \frac{K}{n}$.
Curse of Dimensionality Explanation

Example: let us consider uniform distribution over a cube $[0,1]^d$

We have $l^d \approx \frac{K}{n}$
Curse of Dimensionality Explanation

Example: let us consider uniform distribution over a cube $[0,1]^d$

We have $l^d \approx \frac{K}{n}$

Q: how large we should set $l$, s.t., we will have $K$ examples (out of $n$) fall inside the small cube?

$$l = \left( \frac{k}{n} \right)^{\frac{1}{d}}$$
Curse of Dimensionality Explanation

Example: let us consider uniform distribution over a cube $[0,1]^d$

We have $l^d \approx \frac{K}{n}$

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$$l \approx (K/n)^{1/d} \rightarrow 1, \text{ as } d \rightarrow \infty$$
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We have \(l^d \approx \frac{K}{n}\)

Q: how large we should set \(l\), s.t., we will have \(K\) examples (out of \(n\)) fall inside the small cube?

\[l \approx (K/n)^{1/d} \rightarrow 1, \text{ as } d \rightarrow \infty\]

Bad news: when \(d \rightarrow \infty\), the \(K\) nearest neighbors will be all over the place! (Cannot trust them, as they are not nearby points anymore!)
The distance between two sampled points increases as $d$ grows.
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In $[0, 1]^d$, we uniformly sample two points $x, x'$, calculate
\[ d(x, x') = \|x - x'\|_2 \]
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In $[0, 1]^d$, we uniformly sample two points $x, x'$, calculate

$$d(x, x') = \|x - x'\|_2$$

Let's plot the distribution of such distance:
The distance between two sampled points increases as $d$ grows.

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\[
d(x, x') = \|x - x'\|_2
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Let’s plot the distribution of such distance:

Distance increases as \( d \to \infty \)
The distance between two sampled points increases as $d$ grows.

In $[0, 1]^d$, we uniformly sample two points $x, x'$, calculate $d(x, x') = \|x - x'\|_2$.

Let's plot the distribution of such distance:

Q: can you compute $\mathbb{E}_{x, x'} \|x - x'\|_2^2$?
Well, can we just increase $n$ to avoid this?

Example: let us consider uniform distribution over a cube $[0,1]^d$

We have $l^d \approx \frac{K}{n}$
Well, can we just increase $n$ to avoid this?

Example: let us consider uniform distribution over a cube $[0,1]^d$

We have

$$l^d \approx \frac{K}{n}$$

Q: to make sure that we have one sample inside a small cube, how large $n$ needs to be?

$$n = \frac{K}{l^d} \quad k = 1$$

$$= \frac{1}{l^d}$$
Well, can we just increase \( n \) to avoid this?

Example: let us consider uniform distribution over a cube \([0,1]^d\)

We have \( l^d \approx \frac{K}{n} \)

Q: to make sure that we have one sample inside a small cube, how large \( n \) needs to be?

Set \( \ell = 0.1, K = 1 \), then \( n = 1 / (0.1)^d = 10^d \)
Well, can we just increase $n$ to avoid this?

Example: let us consider uniform distribution over a cube $[0,1]^d$

We have $l^d \approx \frac{K}{n}$

Q: to make sure that we have one sample inside a small cube, how large $n$ needs to be?

Set $\ell = 0.1$, $K = 1$, then $n = 1/(0.1)^d = 10^d$

Bad news: when $d \geq 100$, # of samples needs to be larger than total # of atoms in the universe!
Luckily, real world data often has low-dimensional structure!

Data lives in 2-d manifold
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Example: face images

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Example: face images

Data lives in 2-d manifold

Original image: $\mathbb{R}^{64^2}$

Next week: we will see that these faces approximately live in 100-d space!
Summary for Today

1. K-NN: the simplest ML algorithm (very good baseline, should always try!)
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2. Works well when data is low-dimensional (e.g., can compare against the Bayes optimal)
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1. K-NN: the simplest ML algorithm (very good baseline, should always try!)

   2. Works well when data is low-dimensional (e.g., can compare against the Bayes optimal)

3. Suffer when data is high-dimensional, due to the fact that in high-dimension space, data tends to spread far away from each other