# **Upcoming Deadlines**

- HW 2 due Monday (3/3) at 8pm
- Midterm 1 will be on Wednesday (3/5)
- Still working out project details

# Recap

- Linear regression for regression
  - Model family, loss function
  - Bias-variance tradeoff, regularization
  - Optimization, gradient descent
- Logistic regression for classification
  - Maximum likelihood framework
  - Different evaluation metrics
- Neural networks
  - Backpropagation
  - Optimization tricks

# Lecture 9: kNNs

CIS 4190/5190 Spring 2025

## Parametric vs. Non-Parametric Learning

- The algorithms we have seen so far are **parametric** 
  - Assume the model family has the form  $\{f_{\beta} \mid \beta \in \mathbb{R}^d\}$
- Not all model families have this form!
- Non-parametric models
  - Very high capacity model families that can fit "arbitrary" functions

# k-Nearest Neighbors (kNN)

- **Classification:** Given a new input *x*:
  - Step 1: Find k nearest neighbors  $\{i_1, \dots, i_k\}$  in the training dataset

$$i_1, \dots, i_k = k \operatorname{ArgMin}_{i \in \{1, \dots, n\}} \operatorname{dist}(x, x_i)$$

• Step 2: Return the majority label (i.e., label that occurs most frequently):

$$y = Majority \{y_{i_1}, \dots, y_{k_k}\}$$



| Based on data from | https:/ | //www.listendata.com | /2017/12 | /k-nearest-nei | ghbor-step-b | y-step-tutorial.html |
|--------------------|---------|----------------------|----------|----------------|--------------|----------------------|
|                    |         |                      |          |                | · ·          |                      |

| Height (cm) | Weight (kg) | Large (vs Medium)<br>t-shirt? |
|-------------|-------------|-------------------------------|
| 158         | 58          | F                             |
| 158         | 59          | F                             |
| 158         | 63          | F                             |
| 160         | 59          | F                             |
| 160         | 60          | F                             |
| 163         | 60          | F                             |
| 163         | 61          | F                             |
| 160         | 64          | Т                             |
| 163         | 64          | Т                             |
| 165         | 61          | Т                             |
| 165         | 62          | Т                             |
| 165         | 65          | т                             |
| 168         | 62          | Т                             |
| 168         | 63          | Т                             |
| 168         | 66          | Т                             |
| 170         | 63          | Т                             |
| 170         | 64          | Т                             |
| 170         | 68          | Т                             |

Inputs <u>x</u>i



| Based on data from | https:/ | /www.listendata.com | /2017 | /12/ | k-nearest-nei | ghbor- | -step-by | /-step | -tutorial | .html |
|--------------------|---------|---------------------|-------|------|---------------|--------|----------|--------|-----------|-------|
|                    |         |                     |       |      | ,             |        |          |        |           |       |

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| 163         | 60          | F                             |
| 163         | 61          | F                             |
| 160         | 64          | т                             |
| 163         | 64          | т                             |
| 165         | 61          | т                             |
| 165         | 62          | т                             |
| 165         | 65          | т                             |
| 168         | 62          | т                             |
| 168         | 63          | т                             |
| 168         | 66          | Т                             |
| 170         | 63          | Т                             |
| 170         | 64          | Т                             |
| 170         | 68          | Т                             |

Inputs <u>x</u>i



| Based on data from | https://www.listendata.com | /2017/12/k-nearest-nei | ghbor-step-by-step-tutorial.htm |
|--------------------|----------------------------|------------------------|---------------------------------|
|                    |                            |                        |                                 |

| Height (cm) | Weight (kg) | Large (vs Medium)<br>t-shirt? |
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| 158         | 63          | F                             |
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| 160         | 60          | F                             |
| 163         | 60          | F                             |
| 163         | 61          | F                             |
| 160         | 64          | т                             |
| 163         | 64          | т                             |
| 165         | 61          | т                             |
| 165         | 62          | т                             |
| 165         | 65          | Т                             |
| 168         | 62          | т                             |
| 168         | 63          | Т                             |
| 168         | 66          | т                             |
| 170         | 63          | т                             |
| 170         | 64          | т                             |
| 170         | 68          | Т                             |

Inputs <u>x</u>i



Based on data from https://www.listendata.com/2017/12/k-nearest-neighbor-step-by-step-tutorial.html

| Height (cm) | Weight (kg) | Large (vs Medium)<br>t-shirt? |
|-------------|-------------|-------------------------------|
| 158         | 58          | F                             |
| 158         | 59          | F                             |
| 158         | 63          | F                             |
| 160         | 59          | F                             |
| 160         | 60          | F                             |
| 163         | 60          | F                             |
| 163         | 61          | F                             |
| 160         | 64          | Т                             |
| 163         | 64          | Т                             |
| 165         | 61          | Т                             |
| 165         | 62          | Т                             |
| 165         | 65          | Т                             |
| 168         | 62          | Т                             |
| 168         | 63          | Т                             |
| 168         | 66          | Т                             |
| 170         | 63          | Т                             |
| 170         | 64          | Т                             |
| 170         | 68          | Т                             |

Inputs <u>x</u>i

# k-Nearest Neighbors (kNN)

- **Regression:** Given a new input *x*:
  - Step 1: Find k nearest neighbors  $\{i_1, \dots, i_k\}$  in the training dataset

$$i_1, \dots, i_k = k \operatorname{ArgMin}_{i \in \{1, \dots, n\}} \operatorname{dist}(x, x_i)$$

• Step 2: Return the average label (i.e., label that occurs most frequently):

$$y = \text{Average}\left\{y_{i_1}, \dots, y_{k_k}\right\}$$

• We can use this approach to get probabilities for classification

# k-Nearest Neighbors (kNN)

#### General framework

- **Design decision 1:** What notion of "distance" to use? (e.g., L<sub>2</sub> distance)
- **Design decision 2:** How to aggregate labels? (e.g., majority or average)

### **Choice of Distance Function**

•  $L_1$  distance: dist $(x, x') = ||x - x'||_1 = \sum_{j=1}^d |x_j - x'_j|$ 

• 
$$L_2$$
 distance: dist $(x, x') = ||x - x'||_2 = \left(\sum_{j=1}^d (x_j - x'_j)^2\right)^{\frac{1}{2}}$ 

• 
$$L_{\infty}$$
 distance: dist $(x, x') = ||x - x'||_{\infty} = \max_{j \in \{1, ..., d\}} |x_j - x'_j|$ 

• 
$$L_p$$
 distance: dist $(x, x') = ||x - x'||_p = \left(\sum_{j=1}^d |x_j - x'_j|^p\right)^{\frac{1}{p}}$ 

## **Choice of Distance Function**



# **Distances for Strings**

- Hamming distance: Number of characters that are different
  - **Example:** <u>ABCDE</u> vs. <u>AGDDF</u>  $\rightarrow$  Hamming distance = 3
  - Assumes strings have the same length
- Edit distance: Number of insert/delete/replace operations needed to transform one string into the other
  - **Example:** <u>ROBOT</u> vs. BOT  $\rightarrow$  Edit distance = 2
  - Can be computed using dynamic programming

# **Distances for Strings**

- Jaccard distance between sets  $1 \frac{|A \cap B|}{|A \cup B|}$ 
  - Apply to set of *n*-grams (i.e., *n*-character substrings)
  - Example: ROBOT vs. BOT yields

 $A = \{R, RO, ROB, OBO, BOT, OT, T\}$  $B = \{B, BO, BOT, OT, T\}$ 

• 
$$\rightarrow$$
 Jaccard distance =  $1 - \frac{3}{9} = \frac{2}{3}$ 

# Loss Minimization Framework

- What is the model family?
  - What are the "parameters"?

# Loss Minimization Framework

#### • What is the model family?

- What are the "parameters"? The training dataset Z!
- The model family is the set of kNN functions induced by Z
- In general, "non-parametric" means the number of "parameters" scales with the number of training examples *n*

#### • What is the loss function?

- kNN does not directly minimize a loss function
- But, evaluate using standard losses (e.g., accuracy or MSE)

## **Feature Standardization**

- We saw that feature standardization is not necessary for vanilla linear regression but is necessary for regularized linear regression
- It is very important for kNN!



https://stats.stackexchange.com/questions/287425/why-do-you-need-to-scale-data-in-knn

# Curse of Dimensionality

- Example: Predict acceleration of an object being pushed by a robot
- Features:
  - $x_1 = mass$
  - $x_2 = Force$
  - $x_3 = \text{color of object}$
  - $x_4$  = what the operator ate for breakfast that morning
- When more irrelevant variables, distance function becomes dominated by irrelevant dimensions in x
  - Amount of data needed by kNN scales exponentially in dimension

# Curse of Dimensionality

- Adding more dimensions makes a lot of things counterintuitive
- **Example:** The percentage of the volume of a d-dimensional sphere with radius r, that lies beyond  $\ell_2$  distance 0.99r from the center is:
  - 3% if d = 3
  - 63% if d = 100
  - 99.99% if d = 1000
  - Intuition: Volume inside radius scales as roughly 0.99<sup>d</sup>
- For kNN, nearest neighbors become very far apart, and of similar distance, making it an **unreliable predictor**

# Scalability

**Scaling:** Naively, must compute n distances between pairs of d-dimensional vectors to compute kNN

# Scalability

#### Indexing

- Use kd-trees and other multidimensional indices to capture the training data
- Each lookup is O(log *n*) but on disk

#### Parallelism

- Use multiple cores, and compare against in-memory data or kd trees
- E.g., PANDA, LBL

#### Approximation

- Compare against a sample, not all of the training data
- See, e.g., https://www.kaggle.com/code/pawanbhandarkar/knn-vsapproximate-knn-what-s-the-difference/notebook

# kNNs

#### • Strengths

- Very simple algorithm
- Nonparametric, can learn complex decision boundaries

#### Weaknesses

- Requires an enormous (exponential) amount of data in high dimensions
- Evaluating the model at test time scales with size of training data
- Modern usage: Look up nearest examples according to "learned" features (in the context of deep learning)

# Lecture 8: Decision Trees

CIS 4190/5190 Fall 2023

- Much more practical nonparametric learning algorithm
  - Idea: Can fit complex decision boundaries, but learns simpler ones first
- Interpretable models: Humans can look at the decision tree and understand what it is doing

## **Example:** Diabetes Prediction

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Over the years, I've collected data from lots of patients, recording their physical information, their demographic information, habits, and done their lab work to diagnose diabetes. I'm wondering now: from all this data, could I model the risk of other people with similar characteristics having diabetes given all this other information about them? And would your applied ML class be able to help? I've attached the data here for you to take a look.

Eventually, we'll want to explain our findings to patients, and point out any behavioral changes that would mitigate their risk for diabetes. Even if the risk factors we find are non-modifiable, insurance companies would be interested in understanding and estimating this risk. Either way, it'd be great to have something that we can understand and interpret well!

## **Example:** Diabetes Prediction

| SEQN              | RIDAGEYR | BMXWAIST | вмхнт | LBXTC | BMXLEG | вмхwт | вмхвмі | RIDRETH1              | BPQ020 | ALQ120Q | DMDEDUC2                   | RIAGENDR | INDFMPIR | LBXGH    | DIABETIC |
|-------------------|----------|----------|-------|-------|--------|-------|--------|-----------------------|--------|---------|----------------------------|----------|----------|----------|----------|
| 73557             | 69.0     | 100.0    | 171.3 | 167.0 | 39.2   | 78.3  | 26.7   | Non-Hispanic Black    | yes    | 1.0     | high school graduate / GED | male     | 0.84     | 13.9     | yes      |
| 73558             | 54.0     | 107.6    | 176.8 | 170.0 | 40.0   | 89.5  | 28.6   | Non-Hispanic White    | yes    | 7.0     | high school graduate / GED | male     | 1.78     | 9.1      | yes      |
| 73559             | 72.0     | 109.2    | 175.3 | 126.0 | 40.0   | 88.9  | 28.9   | Non-Hispanic White    | yes    | 0.0     | some college or AA degree  | male     | 4.51     | 8.9      | yes      |
| 73562             | 56.0     | 123.1    | 158.7 | 226.0 | 34.2   | 105.0 | 41.7   | Mexican American      | yes    | 5.0     | some college or AA degree  | male     | 4.79     | 5.5      | no       |
| 73564             | 61.0     | 110.8    | 161.8 | 168.0 | 37.1   | 93.4  | 35.7   | Non-Hispanic White    | yes    | 2.0     | college graduate or above  | female   | 5.0      | 5.5      | no       |
| 73566             | 56.0     | 85.5     | 152.8 | 278.0 | 32.4   | 61.8  | 26.5   | Non-Hispanic White    | no     | 1.0     | high school graduate / GED | female   | 0.48     | 5.4      | no       |
| 73567             | 65.0     | 93.7     | 172.4 | 173.0 | 40.0   | 65.3  | 22.0   | Non-Hispanic White    | no     | 4.0     | 9th-11th grade             | male     | 1.2      | 5.2      | no       |
| 73568             | 26.0     | 73.7     | 152.5 | 168.0 | 34.4   | 47.1  | 20.3   | Non-Hispanic White    | no     | 2.0     | college graduate or above  | female   | 5.0      | 5.2      | no       |
| 73571             | 76.0     | 122.1    | 172.5 | 167.0 | 35.5   | 102.4 | 34.4   | Non-Hispanic White    | yes    | 2.0     | college graduate or above  | male     | 5.0      | 6.9      | yes      |
| 73577             | 32.0     | 100.0    | 166.2 | 182.0 | 36.5   | 79.7  | 28.9   | Mexican American      | no     | 20.0    | Less than 9th grade        | male     | 0.29     | 5.3      | no       |
| 73581             | 50.0     | 99.3     | 185.0 | 202.0 | 42.8   | 80.9  | 23.6   | Other or Multi-Racial | no     | 0.0     | college graduate or above  | male     | 5.0      | 5.0      | no       |
| 73585             | 28.0     | 90.3     | 175.1 | 198.0 | 40.5   | 92.2  | 30.1   | Other or Multi-Racial | no     | 4.0     | some college or AA degree  | male     | 2.26     | 5.0      | no       |
| 73589             | 35.0     | 94.6     | 172.9 | 192.0 | 39.1   | 78.3  | 26.2   | Non-Hispanic White    | no     | 2.0     | high school graduate / GED | male     | 1.74     | 5.5      | no       |
| 73595             | 58.0     | 114.8    | 175.3 | 165.0 | 40.1   | 96.0  | 31.2   | Other Hispanic        | no     | 1.0     | some college or AA degree  | male     | 3.09     | 7.7      | no       |
| 73596             | 57.0     | 117.8    | 164.7 | 151.0 | 35.3   | 104.0 | 38.3   | Other or Multi-Racial | yes    | 1.0     | college graduate or above  | female   | 5.0      | 5.9      | no       |
| 73600             | 37.0     | 122.9    | 185.1 | 189.0 | 48.1   | 126.2 | 36.8   | Non-Hispanic Black    | yes    | 2.0     | high school graduate / GED | male     | 0.63     | 6.2      | yes      |
| 73604             | 69.0     | 96.6     | 156.9 | 203.0 | 37.0   | 59.5  | 24.2   | Non-Hispanic White    | no     | 1.0     | some college or AA degree  | female   | 2.44     | 5.4      | no       |
| 73607             | 75.0     | 130.5    | 169.6 | 161.0 | 36.5   | 111.9 | 38.9   | Non-Hispanic White    | yes    | 0.0     | high school graduate / GED | male     | 1.08     | 5.0      | no       |
| 73610             | 43.0     | 102.6    | 176.8 | 200.0 | 38.8   | 90.2  | 28.9   | Non-Hispanic White    | no     | 5.0     | college graduate or above  | male     | 2.03     | 4.9      | no       |
| 73613             | 60.0     | 113.6    | 163.8 | 203.0 | 41.6   | 104.9 | 39.1   | Non-Hispanic Black    | yes    | 2.0     | 9th-11th grade             | female   | 5.0      | 6.1      | no       |
| 73614             | 55.0     | 90.9     | 167.9 | 256.0 | 43.5   | 60.9  | 21.6   | Non-Hispanic White    | no     | 0.0     | high school graduate / GED | female   | 1.29     | 5.0      | no       |
| 73615             | 65.0     | 100.3    | 145.9 | 166.0 | 30.0   | 55.4  | 26.0   | Other Hispanic        | yes    | 1.0     | Less than 9th grade        | female   | 1.22     | 6.3      | yes      |
| 12-22-22-22-22-22 |          |          |       |       |        |       |        |                       |        |         |                            |          |          | 0.0 0.00 |          |



## Aside: Data Dictionaries

- Datasets are often accompanied by a **data dictionary** 
  - Describes each column in the dataset
  - Important to understand dataset before doing any machine learning!
  - E.g., which columns have missing values
- The dictionary for our data: <u>https://wwwn.cdc.gov/nchs/nhanes/Default.aspx</u>

- A kind of flowchart based on tests
  - Commonly used in medicine
- "Explainable", easy to mentally evaluate





Decision tree example from: Martignon and Monti. (2010). Conditions for risk assessment as a topic for probabilistic education. Proceedings of the Eighth International Conference on Teaching Statistics (ICOTS8).

- Binary tree
- Each internal node has a Boolean condition that is a function of  $\boldsymbol{x}$ 
  - Typically reference a single feature  $x_i$
  - **Real-valued feature:** Condition  $1(x_j \ge t)$  (where  $t \in \mathbb{R}$ )
  - Categorical feature: Condition  $1(x_j = t)$  (where  $t \in \{1, ..., k_j\}$  is a category)
- Each leaf node is a label
  - Can be either regression or classification
  - Can also be a probability distribution

# Intuition: Dataset Splitting



# Visualizing the Model Family

• Axis-aligned decision boundaries

















# **Decision Boundary and Depth**

• Complexity increases with depth



# **Decision Boundary and Depth**

Complexity increases with depth



- Similar to kNN, traditional decision tree learning algorithms do not fit in the loss minimization framework
  - Computing the optimal decision tree is NP complete
  - Recent work has tried to devise more efficient algorithms
- Instead, they are heuristically constructed in a top-down fashion











• Let  $Z[C] = \{ (x, y) \in Z \mid C(x, y) \}$  be the subset of Z where C holds

Ζ

**def** LearnTree(Z):

**if** all labels in Z are the same and equal y: **return** LeafNode(y)  $(j,t) \leftarrow \text{BestSplit}(Z)$   $T_{\text{left}} \leftarrow \text{LearnTree}(Z[x_j \ge t])$   $T_{\text{right}} \leftarrow \text{LearnTree}(Z[x_j < t])$ **return** InternalNode $(j, t, T_{\text{left}}, T_{\text{right}})$ 

• Let  $Z[C] = \{ (x, y) \in Z \mid C(x, y) \}$  be the subset of Z where C holds

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