DSC 140A

Probabilistic Modeling & Machine Learning

Lecture 01 | Part 1

What is Machine Learning??

What is Machine Learning?

- Computers can do things very quickly.

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- Computers can do things very quickly.
- But must be given really specific instructions.

What is Machine Learning?

- Computers can do things very quickly.
- But must be given really specific instructions.
- **Problem**: Not all tasks are easy to dictate.

Example

How old is this person?

The Trick: Use Data

age = 28

age = 42

age = 63

age = 24

age = 37

age = 39

age = ?

age = 35

What is Machine Learning?

- Before: Computer is **told** how to do a task.
- Instead: **learn** how to do a task using data.

What is Machine Learning?

- Before: Computer is **told** how to do a task.
- Instead: **learn** how to do a task using data.
- We still have to **tell** the computer how to learn.

A **machine learning algorithm** is a set of precise instructions telling the computer how to learn from data.

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Spoiler: the algorithms are usually pretty simple. It's the **data** that does the real work.

Machine Learning Tasks

- Prediction
- Clustering
- Representation Learning
- Reinforcement Learning
- Anomaly Detection
- ...

Machine Learning Tasks

- **Prediction**
- Clustering
- Representation Learning
- Reinforcement Learning
- Anomaly Detection
- ...

But first...

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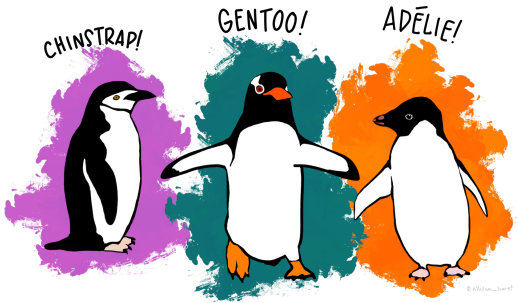
Probabilistic Modeling & Machine Learning

Lecture 01 | Part 2

A Simple Prediction Algorithm

Penguin Prediction



[1]

- **Task:** given a new penguin, predict its species.

[1] Artwork by @allison_horst

First Step: Featurization

- We represent each penguin as a collection of measurements (a **feature vector**).
- Most often, features are numerical.
- Why?
  1. Computers process numbers (not penguins).
  2. Allows us to use mathematical machinery.

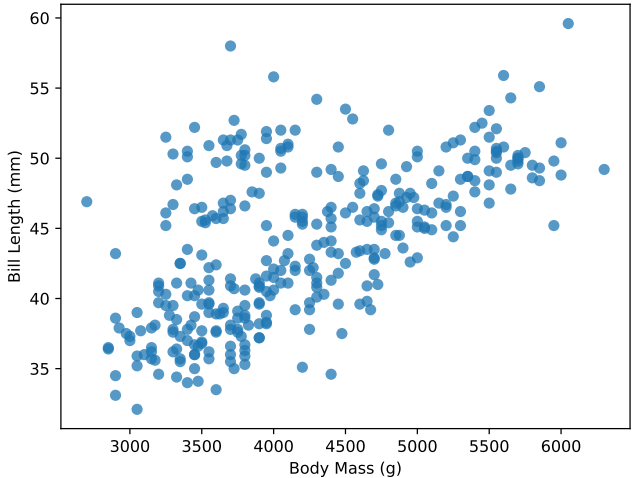
First Step: Featurization

- Chosen features should contain enough info to distinguish between species.

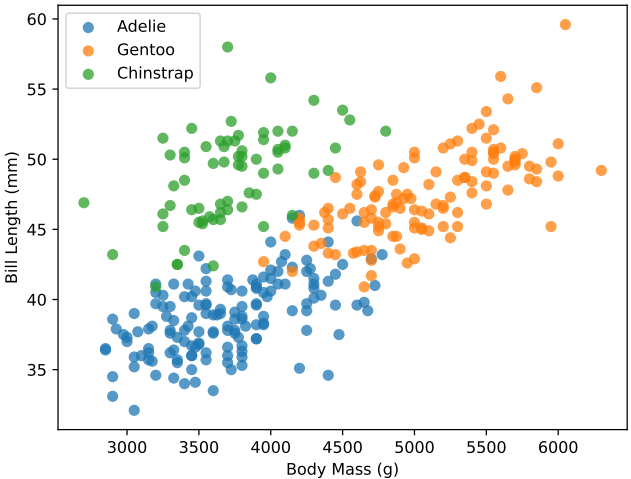
- We will represent each penguin by two numbers:
  1. Body Mass (in grams)
  2. Bill Length (in millimeters)

- Allows us to **embed** penguins as **point cloud** in $\mathbb{R}^2$.

Penguin Embedding

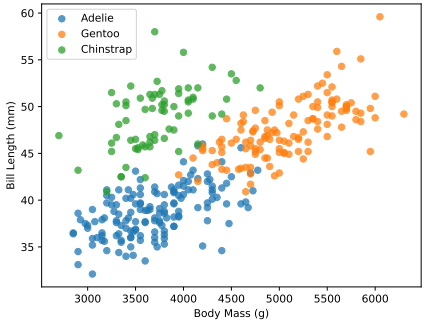


Penguin Embedding



Exercise

We see a new penguin with body mass of 5300 g and bill length of 46 mm. What is its species, most likely?



A Simple Intuition

- New penguin's embedding is close to Gentoo penguins $\implies$ it is mostly likely also Gentoo.
- **Our Assumption**: *locality*. Similar inputs have similar outputs.

A Simple Prediction Algorithm

- **Data:** a set of penguins (as feature vectors) and their species.
- **Given:** a new penguin whose species is unknown.
- **Predict:**
  1. Find the *nearest* penguin whose species is known.
  2. Use that penguin's species as our prediction.

Nearest Neighbor Classification

- **Data:** a set $\mathcal{D}$ of n feature vectors with labels: $\{(\vec{x}^{(i)}, y_i)\} = \{(\vec{x}^{(1)}, y_1), \ldots, (\vec{x}^{(n)}, y_n)\}$

- **Given:** a new point, $\vec{z}$ with unknown label.

- **Predict:**
  1. Find the closest point to $\vec{z}$ in $\mathcal{D}$:

$$i^* = \arg\min_{i \in \{1,\ldots,n\}} \|\vec{x}^{(i)} - \vec{z}\|$$

  2. Use y_{i^*} as the predicted label.

A Note About Distances

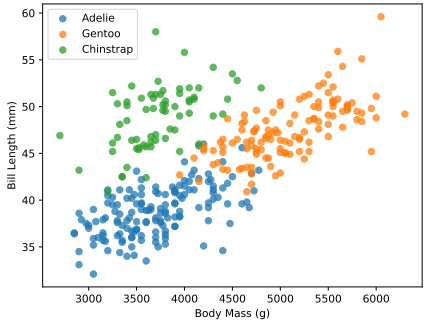
- We found the nearest neighbor with **Euclidean distance**:

$$\begin{aligned}\|\vec{p} - \vec{q}\| &= \sqrt{(p_1 - q_1)^2 + \ldots + (p_d - q_d)^2} \\ &= \sqrt{\sum_{k=1}^{d} (p_k - q_k)^2} \\ &= \sqrt{(\vec{p} - \vec{q}) \cdot (\vec{p} - \vec{q})}\end{aligned}$$

- Note that this is just one choice – there are other valid distances. E.g., cosine distance.

Exercise

We see a new penguin with body mass of 4800 g and bill length of 53 mm. What is its species, most likely?



Scale Matters!

- Not just a visual trick – Euclidean distance treats all directions the same.

- **Example.** Suppose $P = (5000g, 45mm)$. Both of these penguins are the same distance away:

$$Q_1 = (5050g, 45mm) \qquad Q_2 = (5000g, 95mm)$$

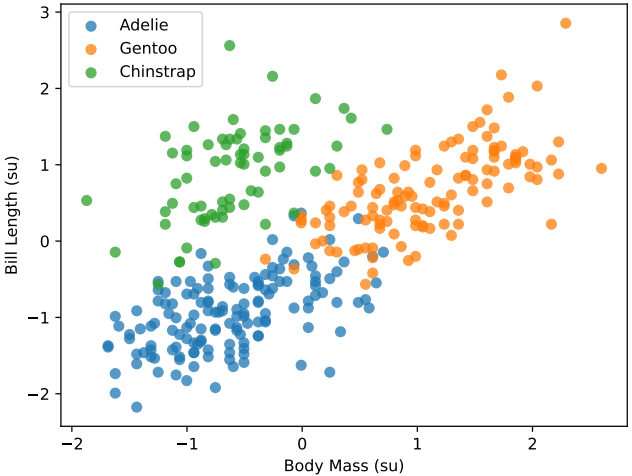
A Common Fix

- It is sometimes useful to **scale** each feature independently.
- E.g., through **standardization**:

$$(\text{new body mass}) = \frac{(\text{old body mass}) - (\text{mean body mass})}{(\text{std. body mass})}$$

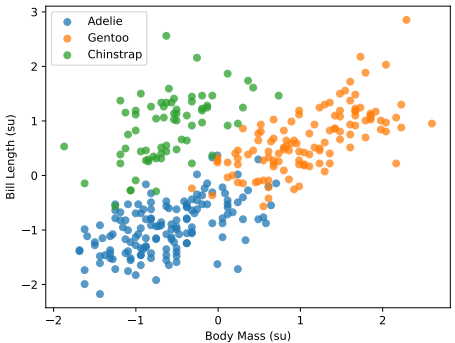
- Not always the right approach, though!

Standardized Penguins



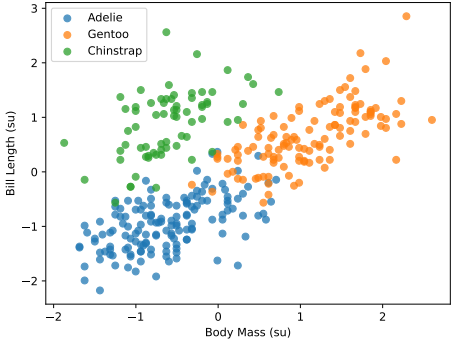
The Decision Boundary

- We can visualize the prediction for every possible input.
- **Decision boundary**: where the prediction changes.

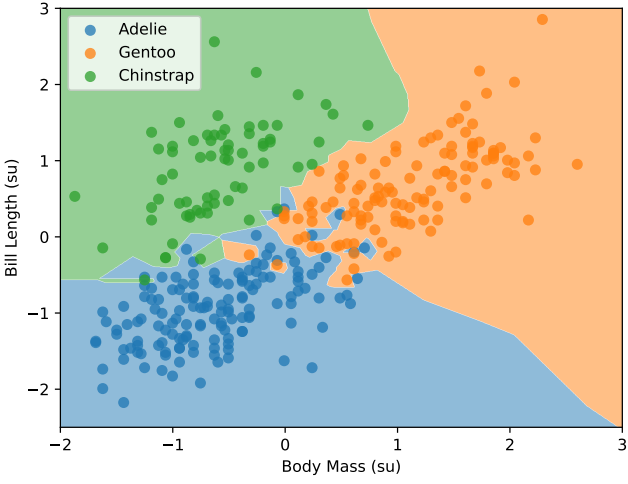


Exercise

What will the decision boundary look like for our NN penguin classifier?



The Decision Boundary

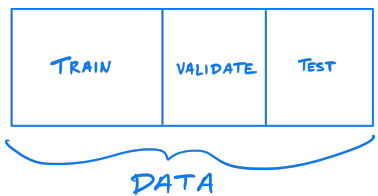


k-Nearest Neighbors

- Before: *single* closest neighbor determined prediction.
- Idea: have *k* closest neighbors “vote”.
- Can be useful to reduce noise.

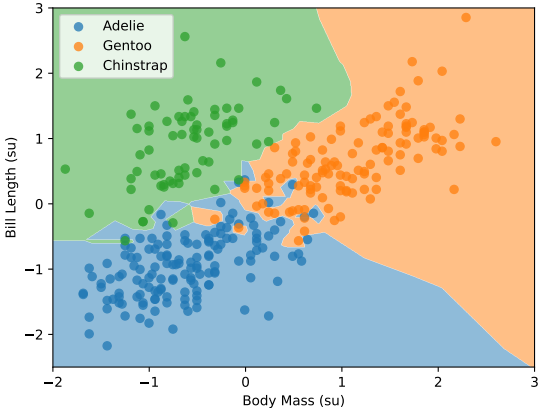
Choosing k

- The number of neighbors, k, is a **hyperparameter** of the algorithm.
- We typically choose k to be odd to break ties.
- One approach: choose k with a **validation set**.



k and the Decision Boundary

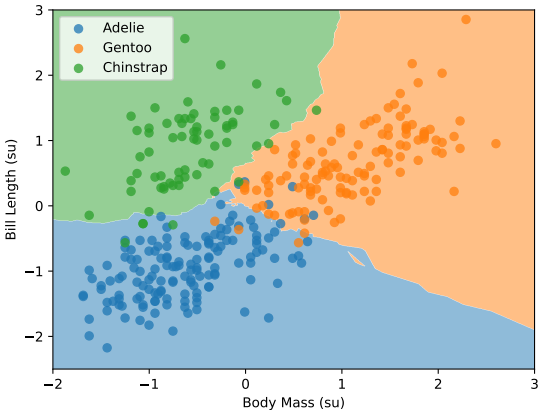
- How might the decision boundary change as we increase k?



$k = 1$

k and the Decision Boundary

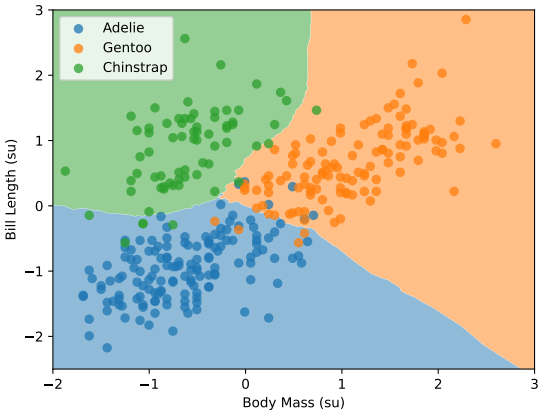
- How might the decision boundary change as we increase k?



k = 10

k and the Decision Boundary

- How might the decision boundary change as we increase k?



k = 20

k and "Complexity"

- *k* controls the "complexity" of the decision boundary.
- Recall **overfitting**: when predictor learns patterns that do not appear outside of the training data.
- *k* can be used to control overfitting.

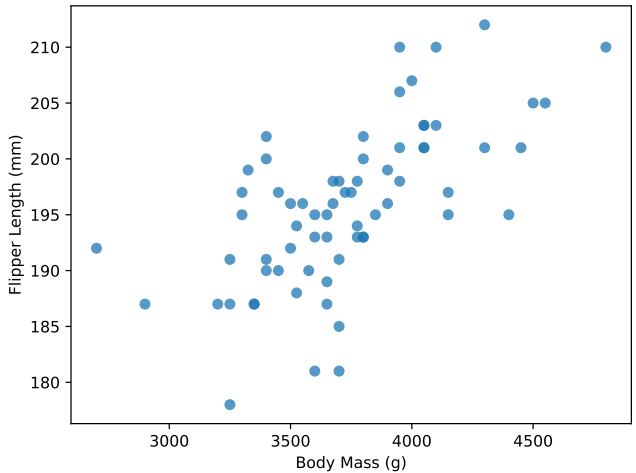
Exercise

What the prediction be if we set $k = n$?

Nearest Neighbor Regression

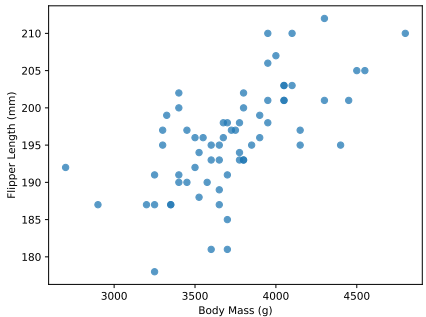
- The nearest neighbor rule can be used for **regression**, too.

A Simple Prediction Algorithm



Exercise

We see a new penguin with body mass of 4000 g. What is a likely flipper length for this penguin?



A Simple Prediction Algorithm

- **Data:** a set of penguins (as feature vectors) and their flipper lengths.
- **Given:** a new penguin whose flipper length is unknown.
- **Predict:**
  1. Find the *nearest* penguin whose species is known.
  2. Use that penguin's flipper length as our prediction.

Nearest Neighbor Regression

- **Data:** a set $\mathcal{D}$ of n feature vectors with targets: $\{(\vec{x}^{(i)}, y_i)\} = \{(\vec{x}^{(1)}, y_1), \ldots, (\vec{x}^{(n)}, y_n)\}$

- **Given:** a new point, $\vec{z}$ with unknown target.

- **Predict:**
  1. Find the closest point to $\vec{z}$ in $\mathcal{D}$:

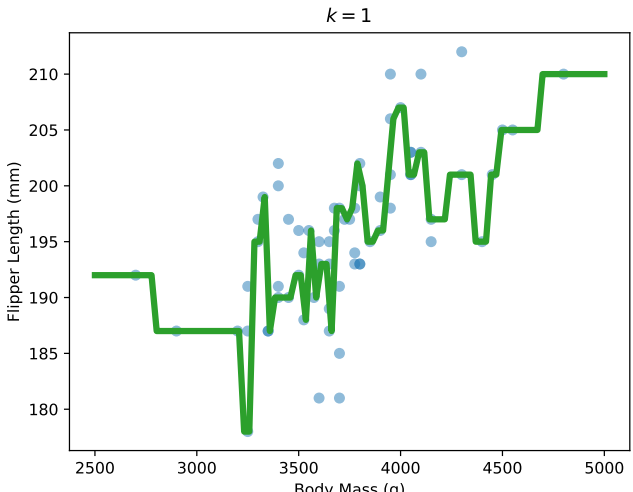
$$i^* = \arg\min_{i \in \{1,\ldots,n\}} \|\vec{x}^{(i)} - \vec{z}\|$$

  2. Use y_{i^*} as the predicted target.

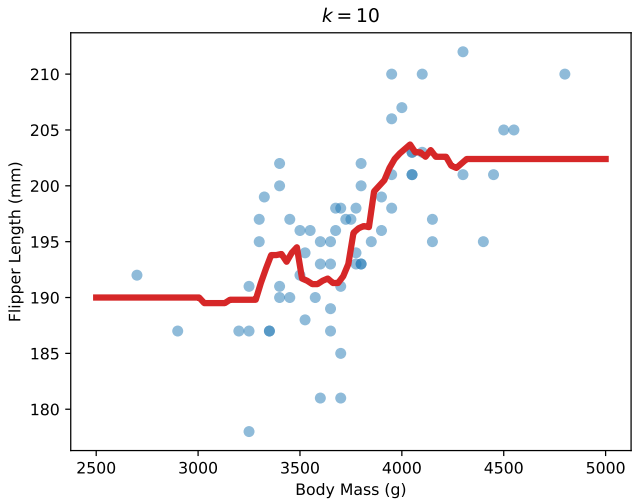
*k*NN Regression

- As with classification, can generalize to *k* nearest neighbors.
- Natural prediction: the **mean** of the targets of the *k* closest neighbors.

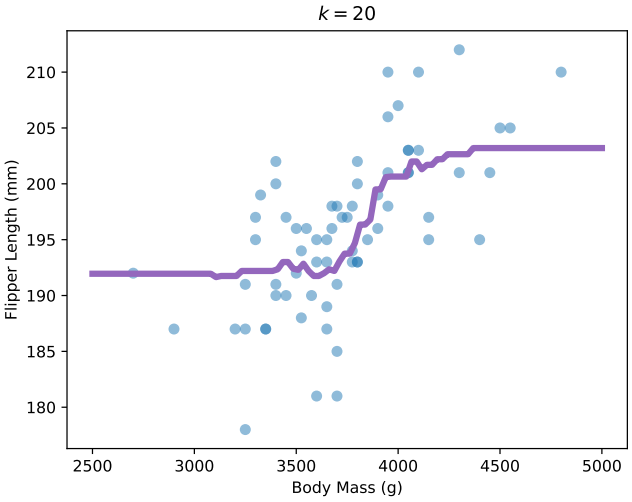
kNN Penguin Regression



kNN Penguin Regression



kNN Penguin Regression



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Probabilistic Modeling & Machine Learning

Lecture 01 | Part 3

Demo: Classifying Handwritten Digits

The Problem

- **Given** an image of a handwritten digit.
- **Classify** the image as a one, two, three, etc.

The Machine Learning Approach

- Gather a **training set** of images with **labels**.
- Let the computer **learn** the underlying patterns.
- We'll use a freely available data set, **MNIST**:

MNIST

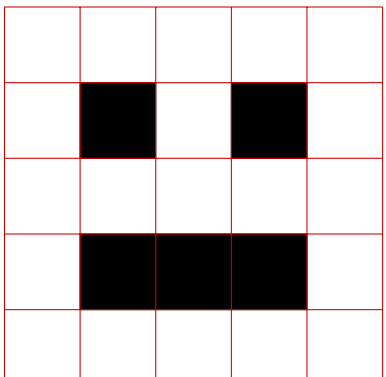
- 60,000 training images and associated labels.
- Each image is 28 × 28 pixels.
- Each pixel is 8 bit grayscale (0 - 255)

kNN on MNIST

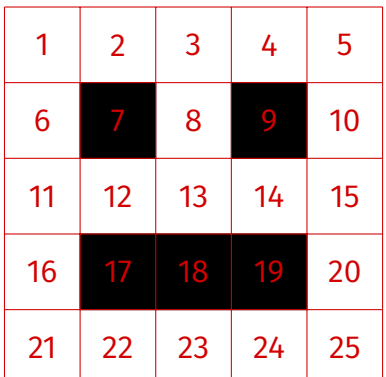
- We'll use kNN to do **character recognition**.
  - $\mathcal{X}$ = set of 28 × 28, 8-bit grayscale images
  - $\mathcal{Y} = \{0, 1, 2, 3, 4, 5, 6, 7, 8, 9\}$.

- How do we represent an image as a feature vector?

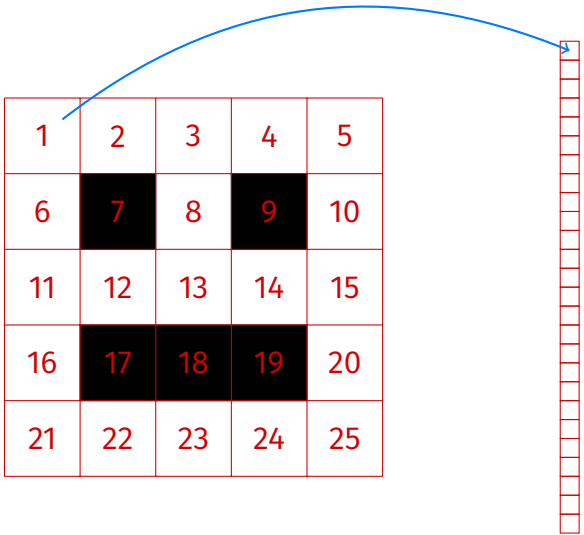
Images as Feature Vectors



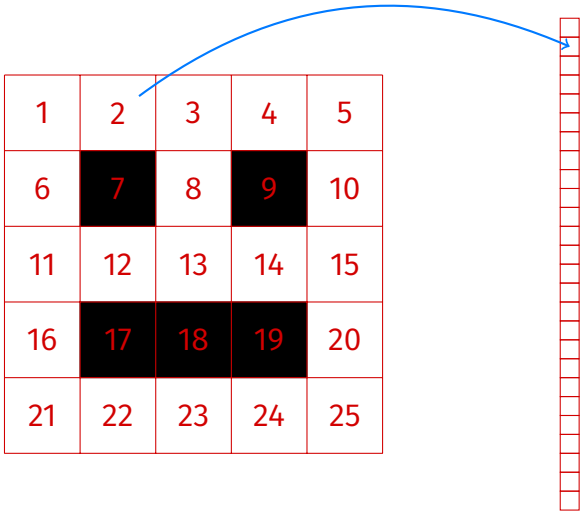
Images as Feature Vectors



Images as Feature Vectors



Images as Feature Vectors



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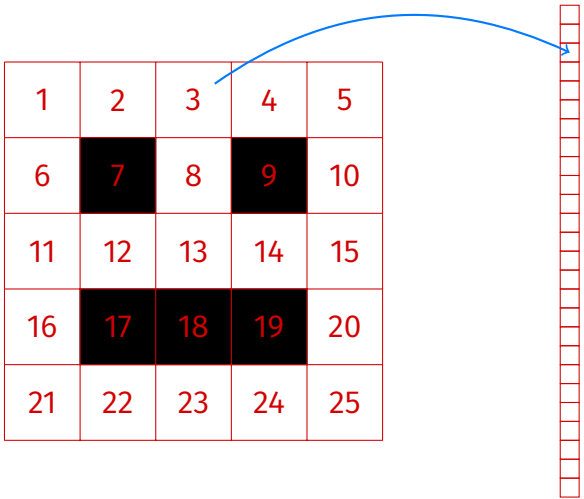

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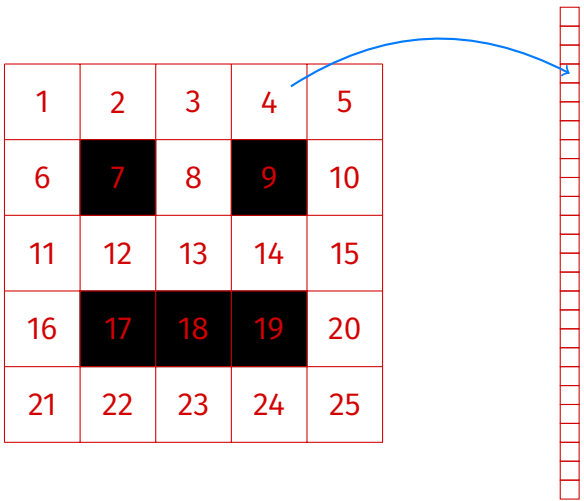

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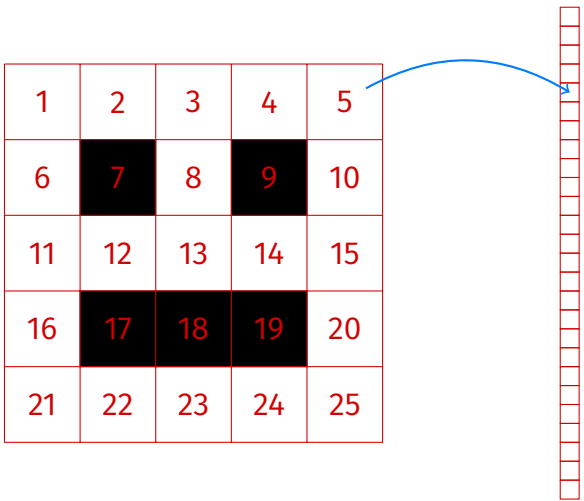

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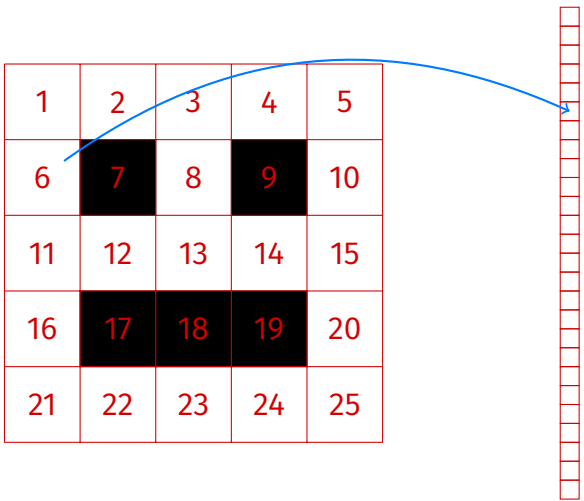

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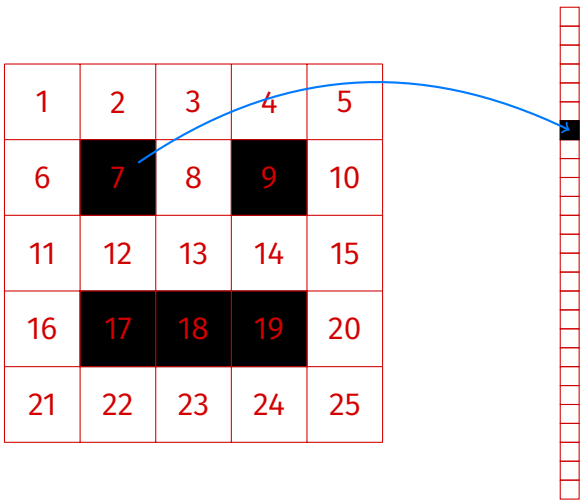

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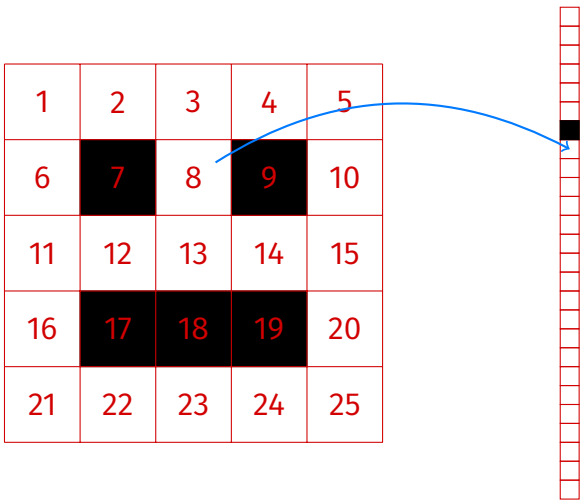

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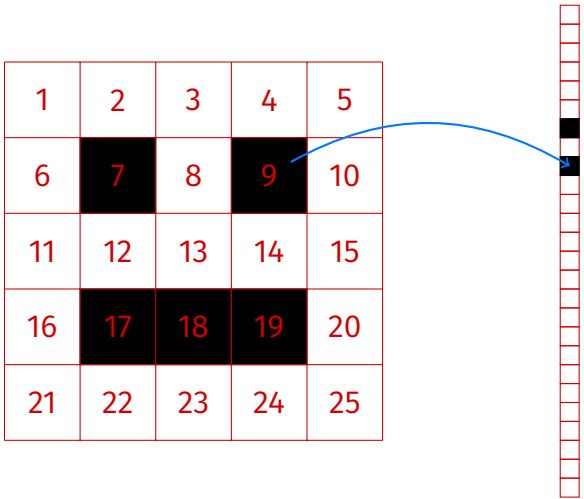

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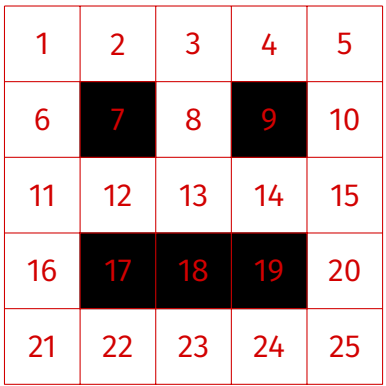


Euclidean Distance Between Images

- We “unroll” a 28×28 image into a vector in $\mathbb{R}^{784}$.
- Euclidean distance between two images $\vec{p}^{(1)}$, $\vec{p}^{(2)}$ in $\mathbb{R}^{784}$:

$$\begin{aligned}\|\vec{p}^{(1)} - \vec{p}^{(2)}\| &= \sqrt{\left(p_1^{(1)} - p_1^{(2)}\right)^2 + \left(p_2^{(1)} - p_2^{(2)}\right)^2 + \ldots + \left(p_{784}^{(1)} - p_{784}^{(2)}\right)^2} \\ &= \sqrt{\sum_{i=1}^{784} \left(p_i^{(1)} - p_i^{(2)}\right)^2}\end{aligned}$$

How well does it work?

- Does this make accurate predictions?
- Use 1-NN to classify each image in **training set**.
- **Question**: What will be the accuracy?

$$\text{error} = \frac{\#\ \textbf{incorrect}\ \text{predictions}}{60{,}000}$$

How well does it work?

- The error will be 0!
- Accuracy on training set is **misleading**, overly-optimistic.
- MNIST also includes a **test set** of 10,000 images and labels. Let's test on this set.

The Test Error

- Test set contains 1,000 images from each digit.
- Suppose our classifier always guesses 7.
  Question: what will be the test error?

The Test Error

- Test set contains 1,000 images from each digit.
- Suppose our classifier always guesses 7.
  Question: what will be the test error?
- **Answer**: 90%.

The Test Error

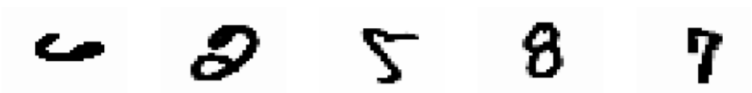
- Test set contains 1,000 images from each digit.
- Suppose our classifier guesses at random.
  Question: what is the expected test error?

The Test Error

- Test set contains 1,000 images from each digit.
- Suppose our classifier guesses at random.
  Question: what is the expected test error?
- **Answer**: 90%.

The Test Error

- The test error of nearest neighbor is only 3.09%.
- Examples of errors:

Input: 

NN: 

Does k-NN do better?

k	1	3	5	7	9	11
Test Error (%):	3.09	2.94	3.13	3.10	3.43	3.34

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Probabilistic Modeling & Machine Learning

Lecture 01 | Part 4

The End?

The End?

- We have developed a simple prediction algorithm: k-nearest neighbors.
- Often works well!
- Have we “solved” machine learning?

No

- Nearest neighbor predictors have significant limitations in two areas:

1. Computational efficiency

2. Predictive performance

Computational Efficiency

- Three main areas to consider when evaluating efficiency:
  1. Time taken to **train** the model.
  2. Memory taken to **store** the trained model.
  3. Time taken to **predict**.

Time Taken in Training

- “Training” a NN predictor is trivial.
  - The training data is simply stored.
- **Takes very little time.**

Memory Taken by Trained Model

- In NN predictors, the model *is* the training data.
- We store the **entire training data**.
- Potentially **very costly**.

Time Taken in Prediction

- To predict, we search the **entire training set** for the nearest neighbor(s): $\Theta(nd)$ time.
- Also potentially **very costly**.

Analogy: Studying

- Approach #1: do many practice problem to learn core principles, recognize patterns.
- I.e., learn “compressed” knowledge.
- During the exam, answer unseen questions by reasoning.

Analogy: Studying

- Approach #2: memorize answers to practice problems.
- During the exam, answer each question by finding most similar practice question.

Analogy: Studying

- Approach #2 is most similar to nearest neighbor.
- Can we find methods that work like approach #1?

Note

- There are methods for improving the efficiency of NN predictors.
  - Approximate NN search, k – d trees, thinning the data, etc.
- However, they break down in high dimensions (many features).

Predictive Performance

- NN predictors can work quite well.
- Still, often outperformed by other methods, especially when many features are used.

The Main Problem

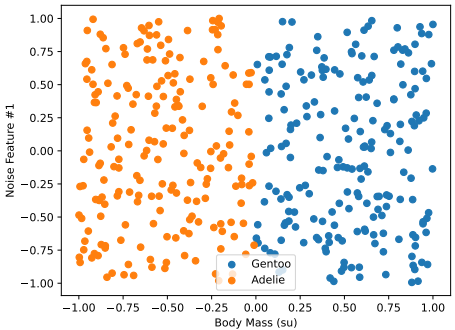
- Nearest neighbor approaches **do not learn** which features are **useful** and which **are not**.

Example

- Suppose all Adelie penguins weigh less than all Gentoo penguins.
- I.e., we can **predict perfectly** based on body mass alone.

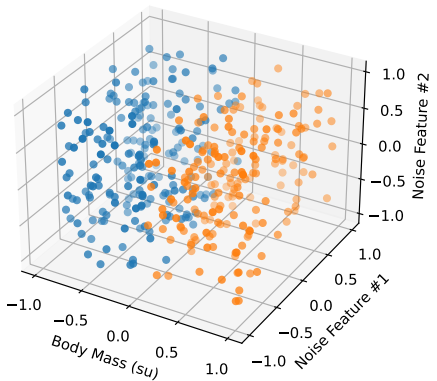
Example: One Noisy Feature

- Suppose we add a feature that is total noise.
- Still enough information to perfectly classify.
- 1-NN: 98% test accuracy.



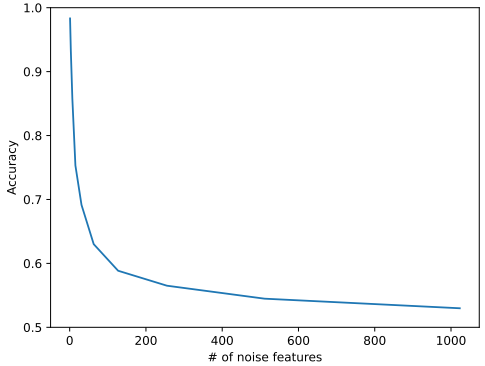
Example: Two Noisy Features

- Suppose we add a second feature that is total noise.
- *Still* enough information to perfectly classify.
- 1-NN: 95% test accuracy (**-3%**).



Example: Noisy Features

- No matter how many noisy features we add, there is enough information to classify perfectly.
- But 1-NN performance **degrades** with # of (noisy) features:



Explanation

- Euclidean distance treats all features the same.
  - Even those that are pure noise.
- NN does not **learn** which features are useful.[2]
- Distance becomes less meaningful as *noisy* features are added.

[2] For extensions of kNN which learn a distance metric from data, see: (Weinberger and Saul, 2009; Goldberger et al., 2005; Shalev-Shwartz et al., 2004)

Summary

- *k*NN prediction is simple and can work well.
- It may be computationally intensive.
- It does not:
  - “learn” in the sense of “compressing knowledge”.
  - learn which features are useful.

Next time...

- A different approach that attempts to learn a “weight” for each feature.