DSC 140A

Probabilistic Modeling & Machine Learning

Lecture 01 | Part 1

Welcome

machine learning $\overset{?}{=}$ magic

(demo)[1]

[1] Source code: `https://gist.github.com/eldridgejm/b8cdac34bf77a4c3add9a9bf2d7362c8`

machine learning $\overset{?}{=}$ magic

machine learning = math + data

But first...

- The syllabus: dsc140a.com
- Labs + Homeworks + Exams + “Super Homework”
- This class has some policies you may/may not be familiar with:
  - slip days
  - lab redemption
  - one homework dropped
  - exam redemption

This Class

- This course focuses on machine learning **theory**.
  - 80% theory, 20% practice

- Other classes (DSC 80, DSC 148) focus on machine learning **practice**.

Math Background

- The most important prereqs for this class are:
  - DSC 40A (mathematical foundations of ML)
  - DSC 80 (ML practice + pandas)
  - MATH 20C (multivariable calculus)
  - MATH 18 (linear algebra)
  - MATH 183 (probability/statistics)

- We’ll review some of the math, but you might want to fill in some gaps on your own.

If you’re a DSC major/minor...

- There are several ways to satisfy the DSC major’s ML requirement
  - CSE 150A, CSE 151A, DSC 140A, DSC 140B
- **Recommendation:** take DSC 140A and DSC 140B
- Avoid “mixing and matching”
  - e.g., avoid DSC 140A + CSE 151A

If you’re not a DSC major/minor...

- Welcome!
- This class assumes that you’ve seen some machine learning before.
  - least squares regression, gradient descent, empirical risk minimization
- If not, DSC 40A might be a good place to start.
- You’ll also want to be comfortable with Python.

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Probabilistic Modeling & Machine Learning

Lecture 01 | Part 2

Prediction

Prediction

- **Prediction** is the most common task in machine learning.
    - **Given** some input information...
    - **Predict** some related output.

Examples

- **Given** a data scientist’s age, college GPA, and state of residence, **predict** their salary.
- **Given** a penguin’s bill length and body mass, **predict** its species.
- **Given** a digital image, **predict** the gesture being made.

Features and Labels

- Each piece of input information is called a **feature**.
- The output we're trying to predict is called the **label** (or **target**).
- **Example:**
  - Features: age, college GPA, state of residence
  - Label: salary

Regression

- When the label is a continuous number, we call it a **regression** problem.
- **Examples:** predicting salary

Classification

- When the label is one of a finite number of choices, we call it a **classification** problem.
- **Examples:** predicting species, predicting gestures

Binary vs. Multiclass Classification

- In **binary classification**, there are only two possible labels.

- In **multiclass classification**, there are more than two possible labels.

- For simplicity, we'll focus on binary classification.

Features

- Features are most often numerical.
- Why?
    1. Computers process numbers (not penguins).
    2. Allows us to use mathematical machinery.

Feature Vectors

- We often package features into a **feature vector**.
- **Example:**

$$\vec{x} = (\text{bill length}, \text{body mass})^T$$

- The **dimensionality** of a feature vector is the number of features it contains.

Choosing Features

- Features should contain information relevant to predicting the label.

- There should be a relationship between them.
  - It might be quite complex!

- Choosing good features is crucial.
  - "Garbage in, garbage out."

Learning from Data

$\vec{x}_2$

- To teach the computer, we provide it with many **training examples**.
- Each example consists of an input feature vector $\vec{x}$ and the correct output label y.
- The set of examples is called the **training set**:

$$\mathcal{X} = \{(\vec{x}^{(1)}, y_1), (\vec{x}^{(2)}, y_2), \ldots, (\vec{x}^{(n)}, y_n)\}$$

Learning from Data

- Hope: given enough examples, the computer will detect a pattern between the features and labels.
- This process is called **learning**.
- The more complex the relationship, the more examples we'll need.

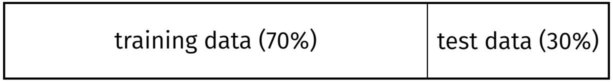
Train Error

- To see how well the computer has learned, we can compute the **train error**.
    - Make predictions on the training set.
    - E.g., for classification, the fraction of training examples misclassified.

- But this is not always a good indicator of how well the computer will do on **new** examples.

Test Error

- Instead, we reserve some examples for a **test set**.
- Randomly choose, say, 30% of the examples to be in the test set.



- Randomizing is important!

Test Error

- Train **only** on the training set.
- Make predictions on the test set.
- The error on the test set is the **test error**.
- The test error is a better indicator of how well the computer will do on new examples.

Generalization

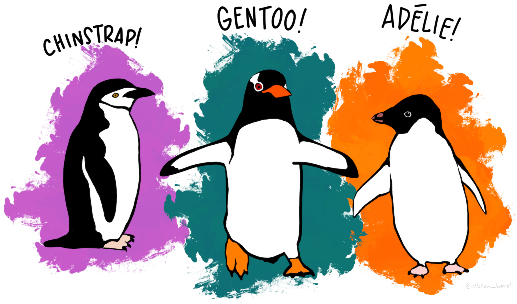
- The ability of the model to perform well on new, unseen examples is called **generalization**.
- In prediction, it's what we're after.
- Training error can be useful, but we care mostly about test error.

Overfitting and Underfitting

- **Overfitting:** model does not generalize.
  - Train error is much lower than test error.

- **Underfitting:** model is not learning the pattern.
  - Both train and test error are high.
  - Need more features, more complex model, etc.

Example: Penguin Prediction



[2]

- **Task:** given bill length and body mass, predict species.

[2] Artwork by @allison_horst

Training Set

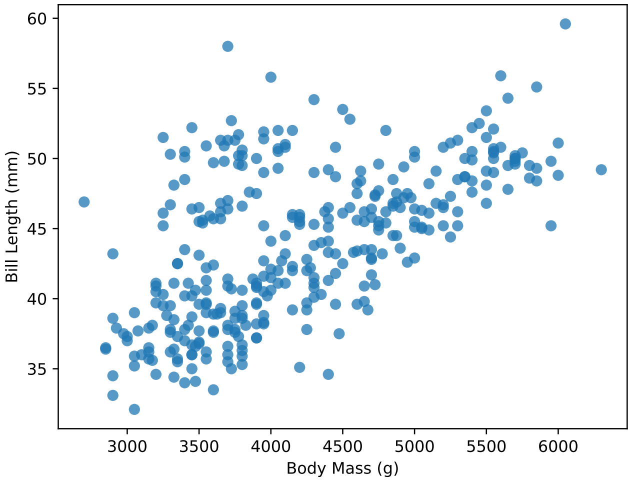
- We collect a training set of 344 penguins. For each penguin, we record:
  - The features: bill length, body mass
  - The label: species

- Each penguin becomes a feature vector in $\mathbb{R}^2$.

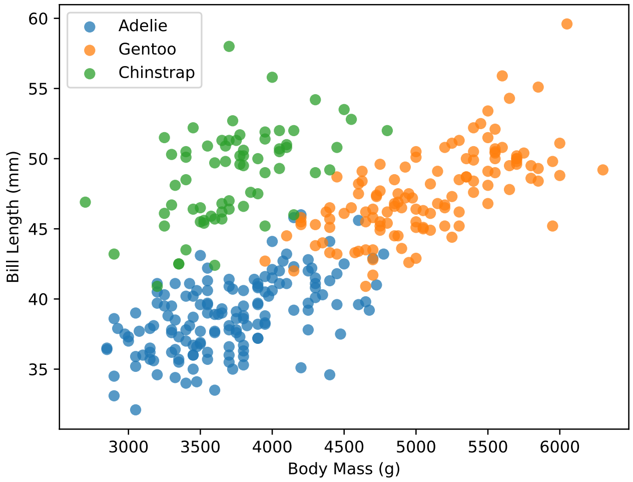
$$\vec{x}^{(i)} = (\text{body mass of penguin } i, \text{bill length of penguin } i)^T$$

- We can **embed** penguins as **point cloud** in $\mathbb{R}^2$.

Penguin Embedding

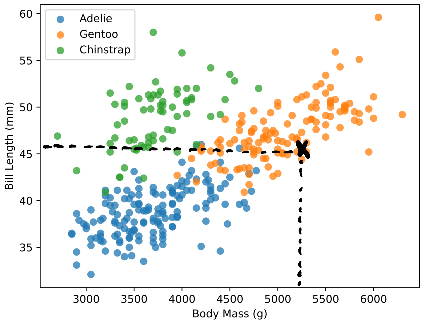


Penguin Embedding



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*. Nearby (similar) feature vectors have similar labels.

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Probabilistic Modeling & Machine Learning

Lecture 01 | Part 3

Nearest Neighbors Predictors

Nearest Neighbors Predictors

- **Idea:** to predict the label of a new example:
  1. find the most similar example in the training set
  2. predict the same label
- This is called a **nearest neighbor predictor**.
- Useful for both regression and classification.

Nearest Neighbor Classifier

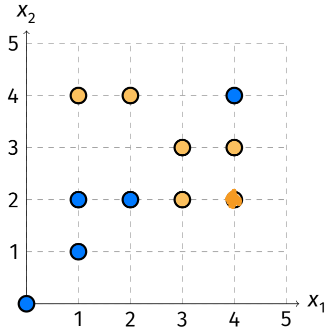
- **Data:** a training set $\mathcal{X}$ of n feature vectors with labels: $\{(\vec{x}^{(i)}, y_i)\} = \{(\vec{x}^{(1)}, y_1), \ldots, (\vec{x}^{(n)}, y_n)\}$
- **Given:** a new point, $\vec{z}$ with unknown label.
- **Predict:**
  1. Find the closest point to $\vec{z}$ in $\mathcal{X}$:

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

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

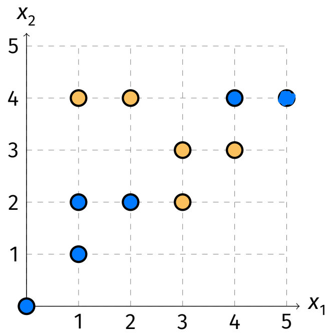
Exercise

What is the predicted label for the new point?



Exercise

What about for this new point?



A Note About Distances

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

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

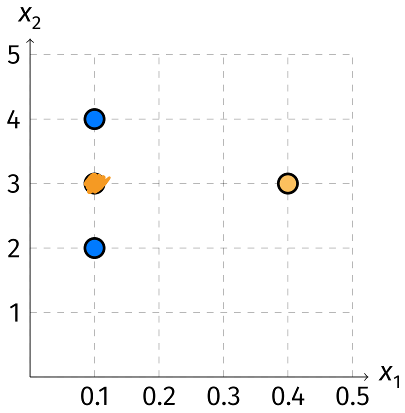
- Note that this is just one choice – there are other valid distances. E.g., cosine distance.

A Note About Distances

- The Euclidean distance treats all features equally.
- In other words, all features contribute equally to the prediction.

Exercise

What is the predicted label for the new point?



Answer

- Predicted label: **yellow**.
- The features are measured on different scales.
- The blue points *look* closer, but the yellow point is closer in Euclidean distance.
- Not just a visual illusion; sometimes, features on different scales can cause problems.

Example

- Person A is 6 ft tall, 180 lbs.
- Person B is 7 ft tall, 185 lbs.
- A new person is 7 ft tall, 180 lbs. Intuitively speaking, are they more similar to A or B?

Standardizing Features

- When features are measured on different scales, it can help to **standardize**.
- **Idea:** shift and scale to make each feature have mean 0 and standard deviation 1.

0 , 0

Standardizing Features

- Suppose we have two features, x_1 and x_2, and let:
  - μ_1, μ_2 be the means of each feature in the training set,
  - σ_1, σ_2 be the standard deviations.

, 1

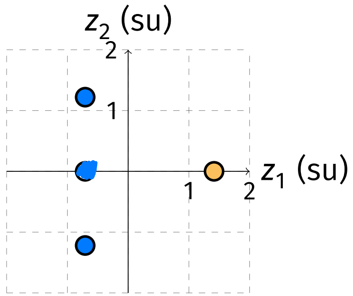
- When standardizing:

$$(x_1, x_2)^T \qquad \text{becomes} \qquad (z_1, z_2)^T = \left(\frac{x_1 - \mu_1}{\sigma_1}, \frac{x_2 - \mu_2}{\sigma_2}\right)^T$$

- Do this for all training data, **and** new test examples.

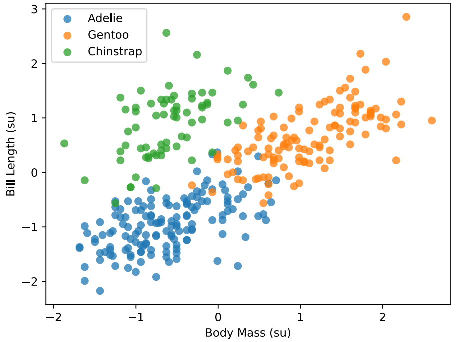
Example

When plotted in standard units, the data now looks like this:



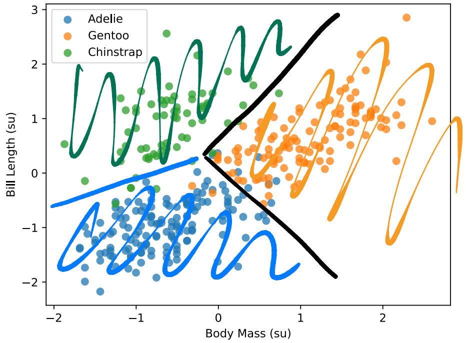
The Decision Boundary

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

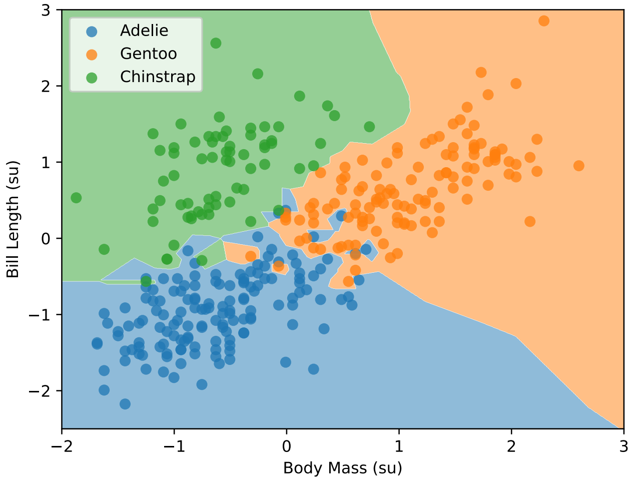


Exercise

What will the decision boundary look like for our NN penguin classifier, roughly-speaking?



The Decision Boundary



Exercise

Suppose there are no duplicates in the training data.

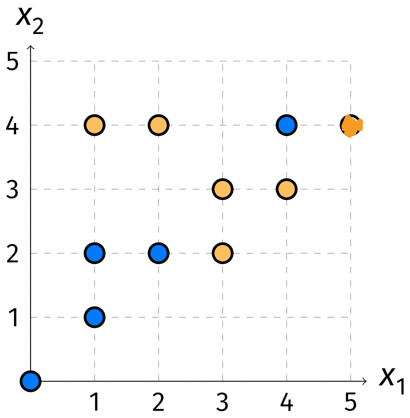
True or False: the nearest neighbor classifier will have 100% training accuracy.

Answer

- **True**.
- If no duplicates, each training example is its own nearest neighbor.
- So for each training example, we predict the correct label.
- Takeaway: training accuracy can be **misleading**.

Problem

- What if the nearest neighbor is an **outlier**?



k-Nearest Neighbors

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

k-Nearest Neighbors Classifier

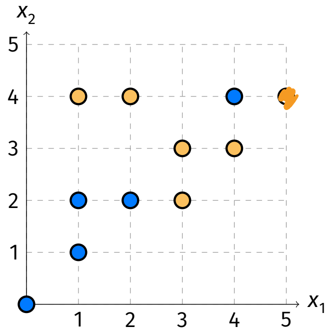
- **Data:** a training set $\mathcal{X}$ of n feature vectors with labels: $\{(\vec{x}^{(i)}, y_i)\} = \{(\vec{x}^{(1)}, y_1), \ldots, (\vec{x}^{(n)}, y_n)\}$

- **Given:** a new point, $\vec{z}$ with unknown label, a choice for the parameter k.

- **Predict:**
    1. Find the k closest points to $\vec{z}$ in $\mathcal{X}$:
    2. Use the most common label among those k points as the predicted label.

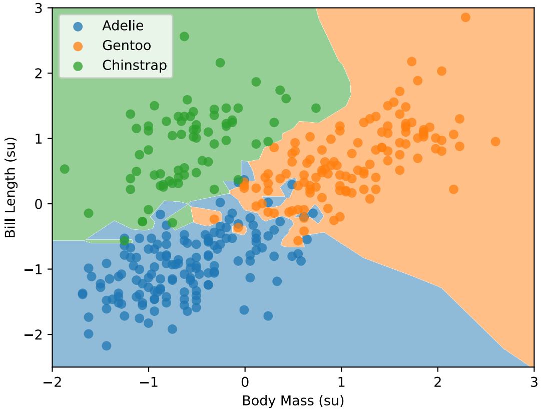
Exercise

What is the predicted label for the new point using *k*NN with $k = 3$?



k and the Decision Boundary

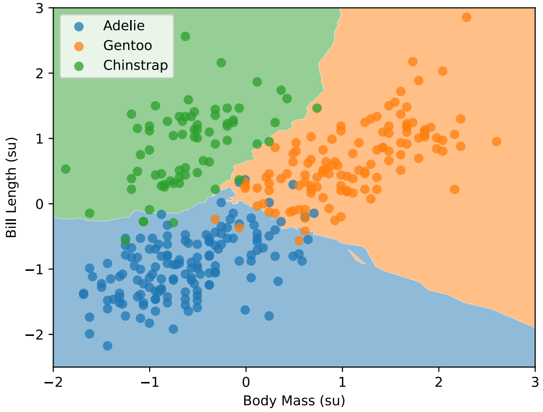
- How might the decision boundary change as we increase *k*?



$k = 1$

k and the Decision Boundary

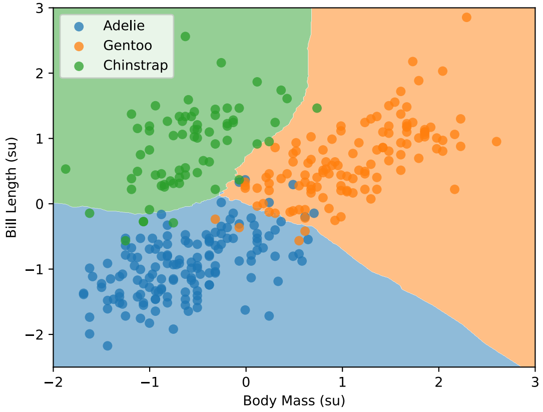
- How might the decision boundary change as we increase *k*?



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.
- The larger *k*, the simpler the boundary.
- Choosing *k* appropriately controls overfitting/underfitting.

$$\underset{\textbf{overfitting}}{\overset{k \text{ too small}}{}} \longleftrightarrow \underset{\textbf{underfitting}}{\overset{k \text{ too large}}{}}$$

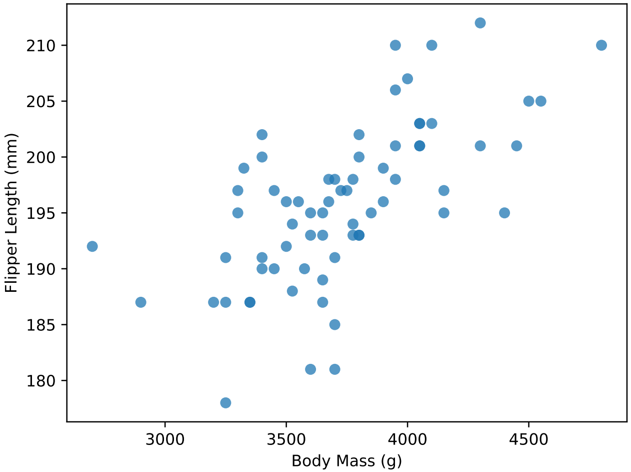
Exercise

What will the prediction be if we set $k = n$, where n is the number of training examples?

Nearest Neighbor Regression

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

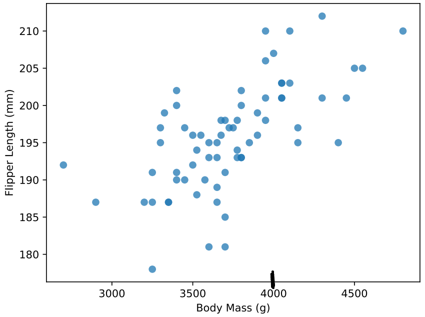
Motivation



Flipper Length (mm)
210
205
200
195
190
185
180
3000
3500
4000
4500
Body Mass (g)

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 flipper length is known.
    2. Use that penguin's flipper length as our prediction.

Nearest Neighbor Regression

- **Data:** a set $\mathcal{X}$ 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 $\mathcal{X}$:
  $$i^* = \arg\min_{i \in \{1,\ldots,n\}} \|\vec{x}^{(i)} - \vec{z}\|$$
  2. Use y_{i^*} as the predicted target.

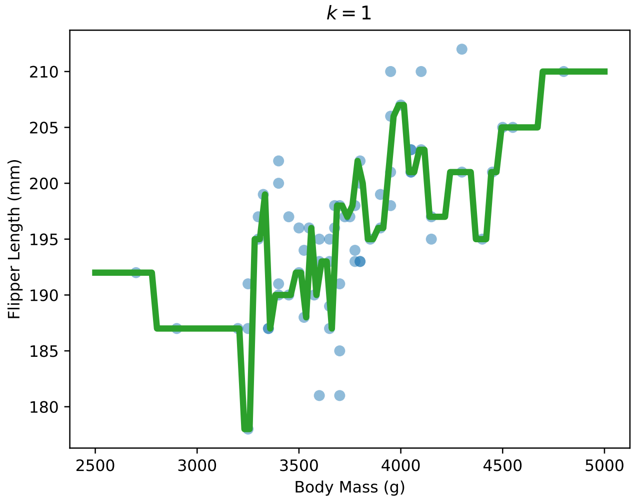
*k*NN Regression

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

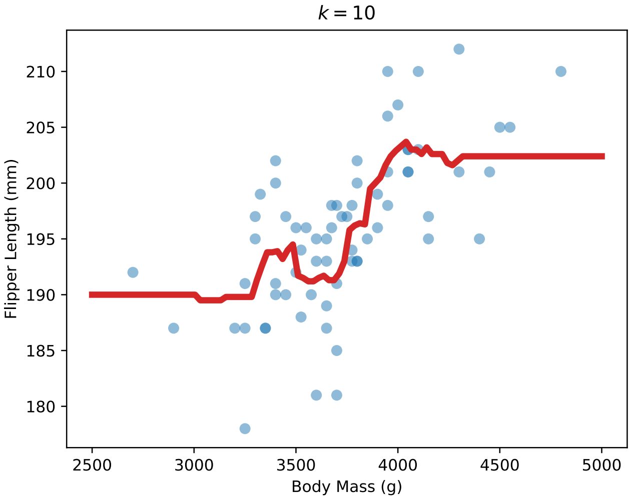
k-Nearest Neighbors Regression

- **Data:** a set $\mathcal{X}$ 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 k closest points to $\vec{z}$ in $\mathcal{X}$
  2. Use the average of their labels as the predicted target

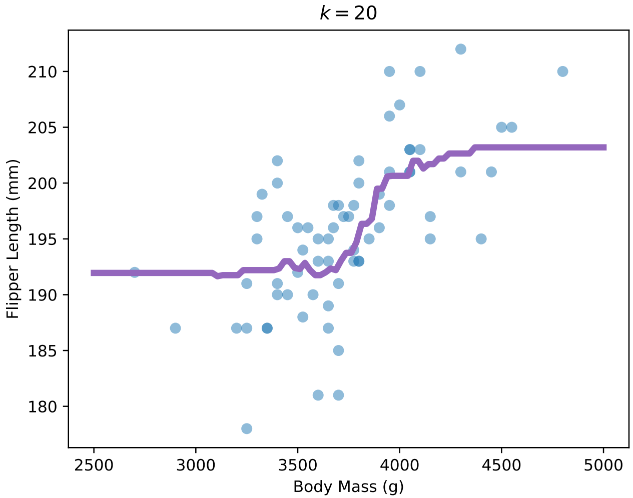
Example: *kNN* Penguin Regression



Example: kNN Penguin Regression



Example: kNN Penguin Regression



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Probabilistic Modeling & Machine Learning

Lecture 01 | Part 4

Gesture Recognition Demo, Revisited

Gesture Recognition

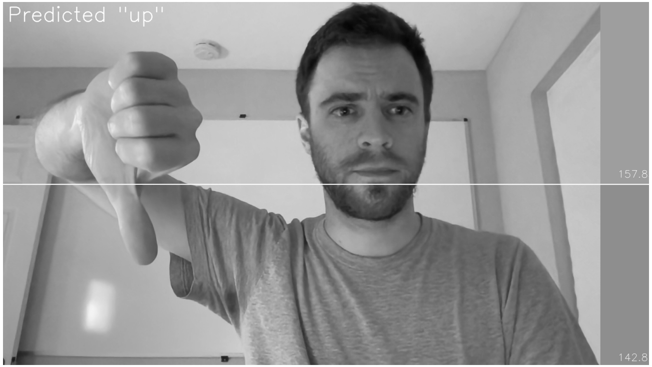
- The gesture recognition demo we saw earlier is a kNN classifier.

Features

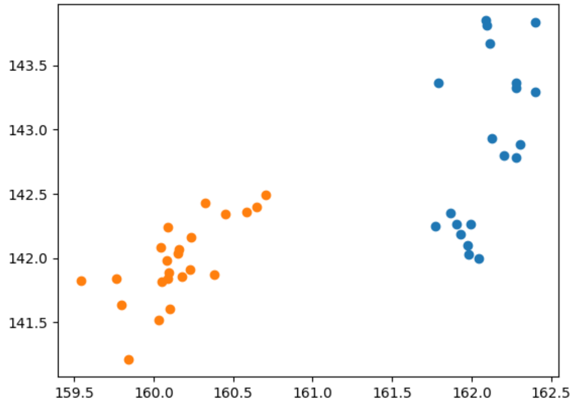
- Each video frame is made into a d-dimensional feature vector.
    1. Converted to grayscale.
    2. Divided into d horizontal strips.
    3. Feature i is the average brightness of strip i.

Example: $d = 2$

Example: d = 2



Example: d = 2



Observation

- The feature vectors for the same gesture are close together.
- The data has “organized” itself.

Prediction

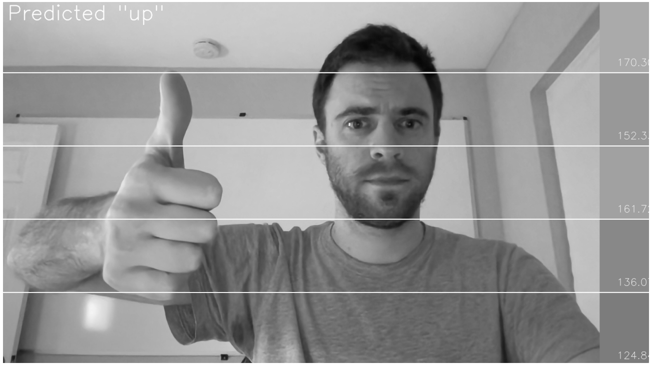
- Given a new frame, convert it to a feature vector and find the *k* closest training frames.

Beyond $d = 2$

- We can use more features.
    - We can still apply kNN in high dimensions.
    - (But we can’t visualize the feature vectors with a scatter plot)

- The original demo used $d = 5$ features.

$d = 5$



Takeaway

- Even seemingly-intelligent behavior can be achieved with simple algorithms + data.

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Probabilistic Modeling & Machine Learning

Lecture 01 | Part 5

From Theory to Practice

Tip #0: Implementation

- `sklearn` has a kNN implementation.
- `sklearn.neighbors.KNeighborsClassifier` for classification.
- But this a theory class; we'll implement it ourselves.

Tip #0: Implementation

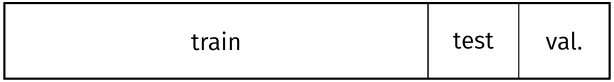
- *k*NN can be implemented in a few lines of code with `numpy`.

- useful functions:
  - `np.linalg.norm`: computes distances,
  - `np.argmin`: finds index of the minimum value
  - `np.argpartition`: finds indices of *k* smallest values
  - `np.bincount`: counts occurrences of each value

```python
import numpy as np

def knn_predict(X_train, y_train, x, k=1):
    # compute distances between test and training examples
    distances = np.linalg.norm(X_train - x, axis=1)

    # find the indices of the k smallest distances
    nearest = np.argpartition(distances, k, axis=0)[:k]

    # get the labels of the k nearest neighbors
    nearest_labels = y_train[nearest]

    # return the most common label
    return np.bincount(nearest_labels).argmax()
```

Tip #1: Choosing *k*

- To choose *k*, further divide your data into training, test, and **validation** sets.



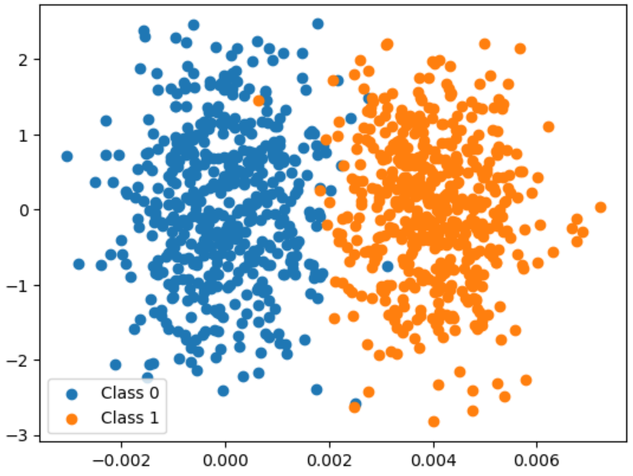
Tip #1: Choosing k

- Pick a few different values of k, train model on each, and compute error on the validation set.
- Keep the k that gives the lowest error; this is your choice.
- Compute test error using this k.

Tip #1: Choosing *k*

- When you're done and ready to use the model "in production":
    1. combine all of your data into one large training set,
    2. use the *k* you chose in validation,
    3. train the final model.

Tip #2: Standardizing Features



```
»> knn = sklearn.neighbors.KNeighborsClassifier(n_neighbors=1)
»> knn.fit(X_train, y_train)
»> knn.score(X_test, y_test)
0.672
```

```
»> mu, sigma = X_train.mean(axis=0), X_train.std(axis=0)
»> Z_train = (X_train - mu) / sigma
»> Z_test = (X_test - mu) / sigma
»> knn.fit(Z_train, y_train)
»> knn.score(Z_test, y_test)
0.972
```

Trivia: Speeding it Up

- Making a prediction requires computing the distance to *every* training example.
- There are ways of speeding this up:
  - Approximate nearest neighbors,
  - *k*-d trees, ball trees, etc.
  - Subsampling the data.

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Probabilistic Modeling & Machine Learning

Lecture 01 | Part 6

The End?

The End?

- We have developed a simple prediction algorithm: k-nearest neighbors.
- Can used for both **classification** and **regression.**
- Often works well!
- Have we “solved” machine learning?

No

- Nearest neighbor predictors have significant limitations in two areas:

1. Computational efficiency
   - I.e., they are slow, or require a lot of memory.
2. Predictive performance
   - I.e., they aren’t always as accurate as other methods.

Something Unsatisfying

- Do nearest neighbor models **learn** anything?
- They seem to just “memorize” the training data.

The Main Problem

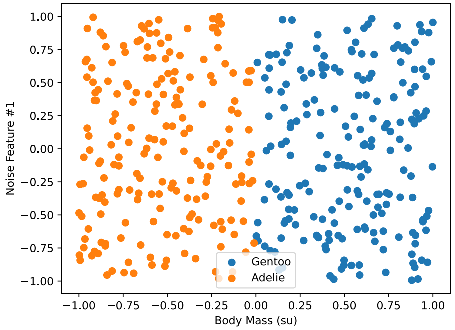
- Nearest neighbor approaches **do not learn** which features are **useful** and which **are not**.

Example

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

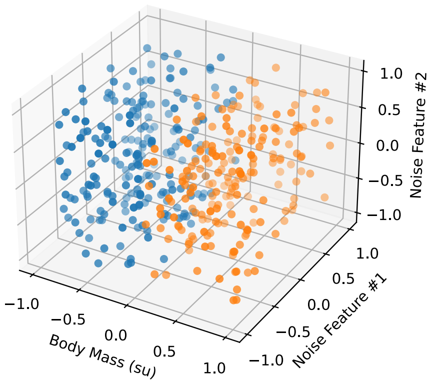
Example: One Noisy Feature

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



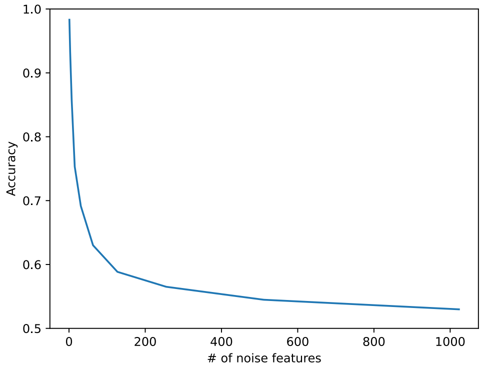
Example: Two Noisy Features

- Suppose we add another 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.[3]
- Distance becomes less meaningful as *noisy* features are added.

[3]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

- kNN 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.