CPSC 340: Machine Learning and Data Mining

Non-Parametric Models

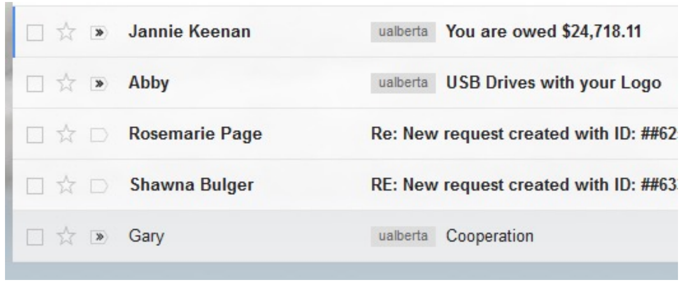
Term2, 2021

Admin

- Add/drop deadline is today.
- Audit: Anyone who wants to audit the course should email their registration form to cpsc340-admin@cs.ubc.ca.

Last Time: E-mail Spam Filtering

- Want a build a system that filters spam e-mails:



Jannie Keenan	ualberta	You are owed $24,718.11
Abby	ualberta	USB Drives with your Logo
Rosemarie Page		Re: New request created with ID: ##62
Shawna Bulger		RE: New request created with ID: ##63
Gary	ualberta	Cooperation

- We formulated as supervised learning:
  - ($y_i = 1$) if e-mail ‘i’ is spam, ($y_i = 0$) if e-mail is not spam.
  - ($x_{ij} = 1$) if word/phrase ‘j’ is in e-mail ‘i’, ($x_{ij} = 0$) if it is not.

$	Hi	CPSC	340	Vicodin	Offer	…
1	1	0	0	1	0	…
0	0	0	0	1	1	…
0	1	1	1	0	0	…
…	…	…	…	…	…	…

Spam?
1
1
0
…

Last Time: Naïve Bayes

- We considered spam filtering methods based on naïve Bayes:

$$p(y_i = \text{"spam"} \mid x_i) = \frac{p(x_i \mid y_i = \text{"spam"})\, p(y_i = \text{"spam"})}{p(x_i)}$$

- Makes conditional independence assumption to make learning practical:

$$p\underbrace{(\text{hello}=1, \text{vicodin}=0, 340=1 \mid \text{spam})}_{\text{HARD}} \approx p\underbrace{(\text{hello}=1 \mid \text{spam})}_{\text{easy}}\, p\underbrace{(\text{vicodin}=0 \mid \text{spam})}_{\text{easy}}\, p\underbrace{(340=1 \mid \text{spam})}_{\text{easy}}$$

- Predict "spam" if $p(y_i = \text{"spam"} \mid x_i) > p(y_i = \text{"not spam"} \mid x_i)$.
  - We don't need $p(x_i)$ to test this.

Naïve Bayes

- Naïve Bayes formally:

$$p(y_i \mid x_i) = \frac{p(x_i \mid y_i)\,p(y_i)}{p(x_i)} \qquad \text{(first use Bayes rule)}$$

$$\propto p(x_i \mid y_i)\,p(y_i) \qquad \text{("}\underbrace{\text{denominator doesn't matter}}_{\text{same for all } y_i \text{ values}}\text{")}$$

$$\approx \prod_{j=1}^{d} \Big[\underbrace{p(x_{ij} \mid y_i) \Big] p(y_i)}_{\text{Only needs } \underline{\text{easy}} \text{ probabilities.}} \qquad \text{(conditional independence assumption)}$$

- Post-lecture slides: how to train/test by hand on a simple example.

Laplace Smoothing

- Our estimate of p('lactase' = 1| 'spam') is:

$$\frac{\text{\# spam messages with lactase}}{\text{\# spam messages}}$$

  - But there is a problem if you have no spam messages with lactase:
    - p('lactase' | 'spam') = 0, so spam messages with lactase automatically get through.
  - Common fix is Laplace smoothing:
    - Add 1 to numerator,
      and 2 to denominator (for binary features).
      - Acts like a "fake" spam example that has lactase,
        and a "fake" spam example that doesn't.

$$\frac{(\text{\# spam messages with lactase}) + 1}{(\text{\# spam messages}) + 2}$$

Laplace Smoothing

- Laplace smoothing: $\dfrac{(\#\text{spam messages with lactase}) + 1}{(\#\text{spam messages}) + 2}$
  - Typically you do this for all features.
    - Helps against overfitting by biasing towards the uniform distribution.
- A common variation is to use a real number β rather than 1.
  - Add 'βk' to denominator if feature has 'k' possible values (so it sums to 1).

$$p(x_{ij} = c \mid y_i = \text{class}) \approx \frac{(\text{number of examples in class with } x_{ij} = c) + \beta}{(\text{number of examples in class}) + \beta K}$$

bonus!

This is a "maximum a posteriori" (MAP) estimate of the probabiliy. We'll discuss MAP and how to derive this formula later.

Decision Theory

- Are we equally concerned about "spam" vs. "not spam"?
- True positives, false positives, false negatives, true negatives:

Predict / True	True 'spam'	True 'not spam'
Predict 'spam'	True Positive	False Positive
Predict 'not spam'	False Negative	True Negative

- The costs mistakes might be different:
  - Letting a spam message through (false negative) is not a big deal.
  - Filtering a not spam (false positive) message will make users mad.

Decision Theory

- We can give a cost to each scenario, such as:

Predict / True	True ‘spam’	True ‘not spam’
Predict ‘spam’	0	100
Predict ‘not spam’	10	0

- Instead of most probable label, take $\hat{y}_i$ minimizing expected cost:

$$\underbrace{\mathbb{E}}_{\text{expectation of model with respect to } \tilde{y}_i}\left[\underbrace{\text{cost}(\hat{y}_i, \tilde{y}_i)}_{\text{cost of predicting } \hat{y}_i \text{ if it's really } \tilde{y}_i}\right]$$

- Even if “spam” has a higher probability, predicting “spam” might have a higher expected cost.

Decision Theory Example

Predict / True	True ‘spam’	True ‘not spam’
Predict ‘spam’	0	100
Predict ‘not spam’	10	0

- Consider a test example we have p($\tilde{y}_i$ = “spam” | $\tilde{x}_i$) = 0.6, then:

$$\mathbb{E}[\text{cost}(\hat{y}_i = \text{"spam"}, \tilde{y}_i)] = p(\tilde{y}_i = \text{"spam"} \mid \tilde{x}_i)\,\text{cost}(\hat{y}_i = \text{"spam"}, \tilde{y}_i = \text{"spam"})$$

$$+ \, p(\tilde{y}_i = \text{"not spam"} \mid \tilde{x}_i)\,\text{cost}(\hat{y}_i = \text{"spam"}, \tilde{y}_i = \text{"not spam"})$$

$$= (0.6)(0) + (0.4)(100) = 40$$

$$\mathbb{E}[\text{cost}(\hat{y}_i = \text{"not spam"}, \tilde{y}_i)] = (0.6)(10) + (0.4)(0) = 6$$

- Even though “spam” is more likely, we should predict “not spam”.

bonus!

Decision Theory Discussion

- In other applications, the costs could be different.
  - In cancer screening, some false positives are ok, but don't want to have false negatives.

- Decision theory and "darts":
  - http://www.datagenetics.com/blog/january12012/index.html

- Decision theory and video poker:
  - http://datagenetics.com/blog/july32019/index.html

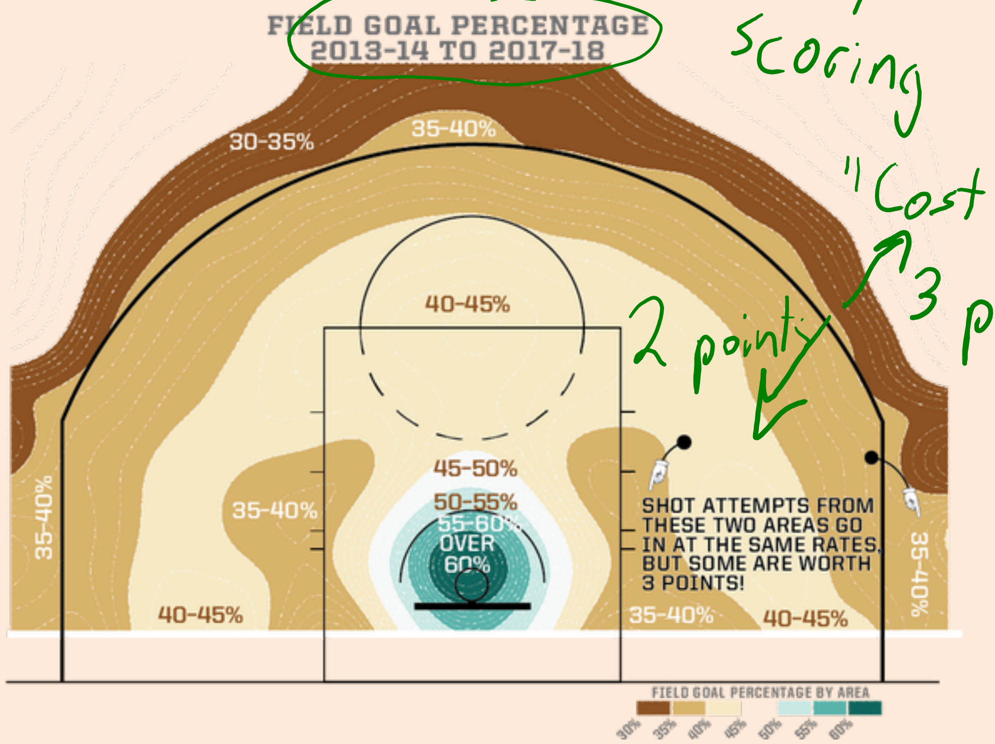
- Decision theory can help with "unbalanced" class labels:
  - If 99% of e-mails are spam, you get 99% accuracy by always predicting "spam".
  - Decision theory approach avoids this.
  - See also precision/recall curves and ROC curves in the bonus material.

bonus!

Decision Theory and Basketball

- "How Mapping Shots In The NBA Changed It Forever"

Probability of scoring


FIELD GOAL PERCENTAGE
2013-14 TO 2017-18

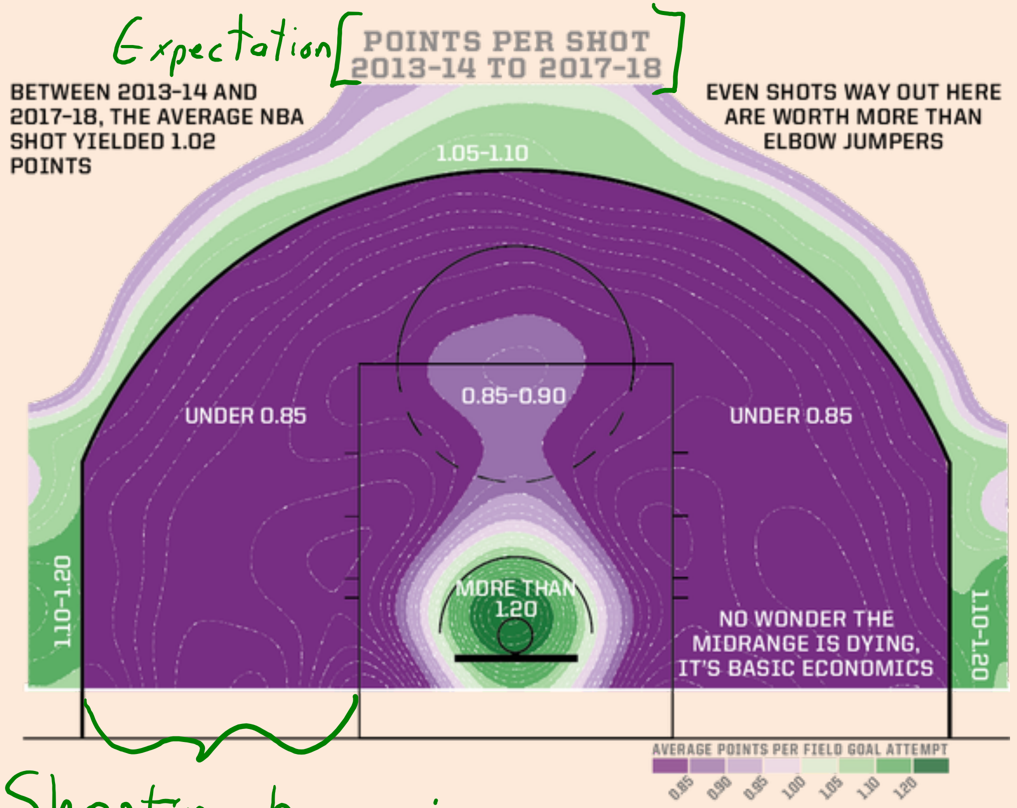
SHOT ATTEMPTS FROM THESE TWO AREAS GO IN AT THE SAME RATES, BUT SOME ARE WORTH 3 POINTS!

"Cost"

2 points

3 points

Expectation


POINTS PER SHOT
2013-14 TO 2017-18

BETWEEN 2013-14 AND 2017-18, THE AVERAGE NBA SHOT YIELDED 1.02 POINTS

EVEN SHOTS WAY OUT HERE ARE WORTH MORE THAN ELBOW JUMPERS

NO WONDER THE MIDRANGE IS DYING, IT'S BASIC ECONOMICS

Shooting here is a bad decision

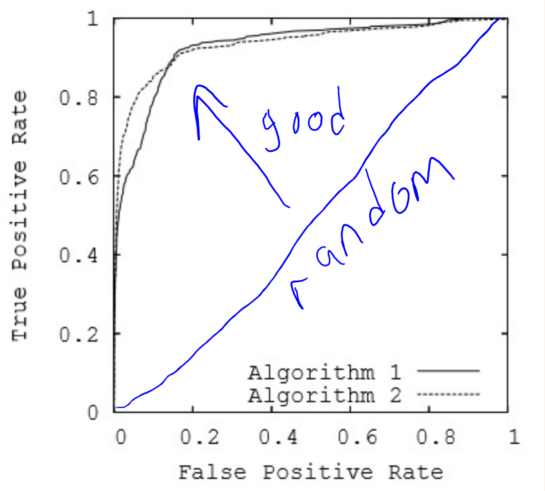
https://fivethirtyeight.com/features/how-mapping-shots-in-the-nba-changed-it-forever/

bonus!

Unbalanced Class Labels

- A related is that of “unbalanced” class labels.
  - If 99% of the e-mails are spam,
    you can get 99% accuracy by always predicting spam.

- There are a variety of other performance measures available:
  - Weighted classification error.
  - Jaccard similarity.
  - Precision and recall.
  - False positive and false negative rate.
  - ROC curves.

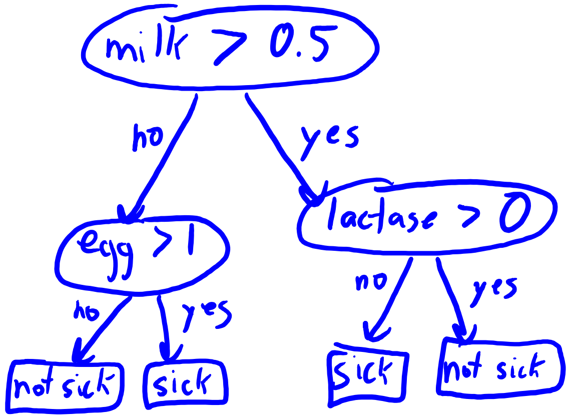


- See the post-lecture bonus slides for additional details.

(pause)

Decision Trees vs. Naïve Bayes

- Decision trees:



1. Sequence of rules based on 1 feature.
2. Training: 1 pass over data per depth.
3. Greedy splitting as approximation.
4. Testing: just look at features in rules.
5. New data: might need to change tree.
6. Accuracy: good if simple rules based on individual features work (“symptoms”).

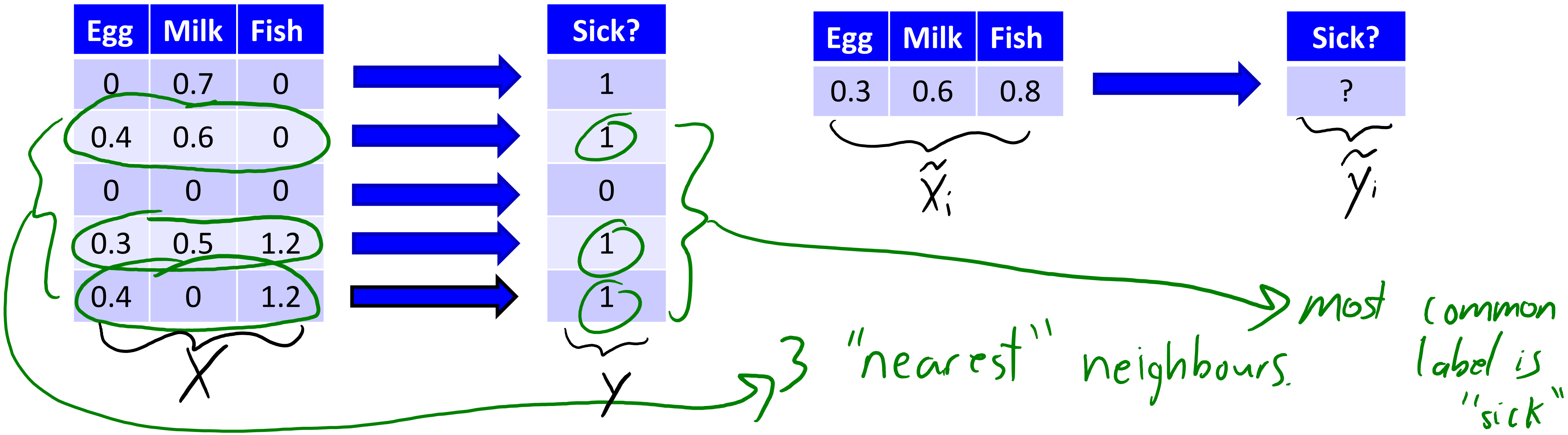
- Naïve Bayes:

$$p(\text{sick} \mid \text{milk}, \text{egg}, \text{lactase})$$
$$\approx p(\text{milk} \mid \text{sick})\, p(\text{egg} \mid \text{sick})\, p(\text{lactase} \mid \text{sick})\, p(\text{sick})$$

1. Simultaneously combine all features.
2. Training: 1 pass over data to count.
3. Conditional independence assumption.
4. Testing: look at all features.
5. New data: just update counts.
6. Accuracy: good if features almost independent given label (bag of words).

k-Nearest Neighbours (kNN)

- An old/simple classifier: k-nearest neighbours (kNN).
- To classify an example $\tilde{x}_i$:
  1. Find the ‘k’ training examples x_i that are “nearest” to $\tilde{x}_i$.
  2. Classify using the most common label of “nearest” training examples.



Egg	Milk	Fish
0	0.7	0
0.4	0.6	0
0	0	0
0.3	0.5	1.2
0.4	0	1.2

Sick?
1
1
0
1
1

X $\quad y$

Egg	Milk	Fish
0.3	0.6	0.8

Sick?
?

$\tilde{X}_i$ $\quad \tilde{y}_i$

3 "nearest" neighbours.

most common label is "sick"

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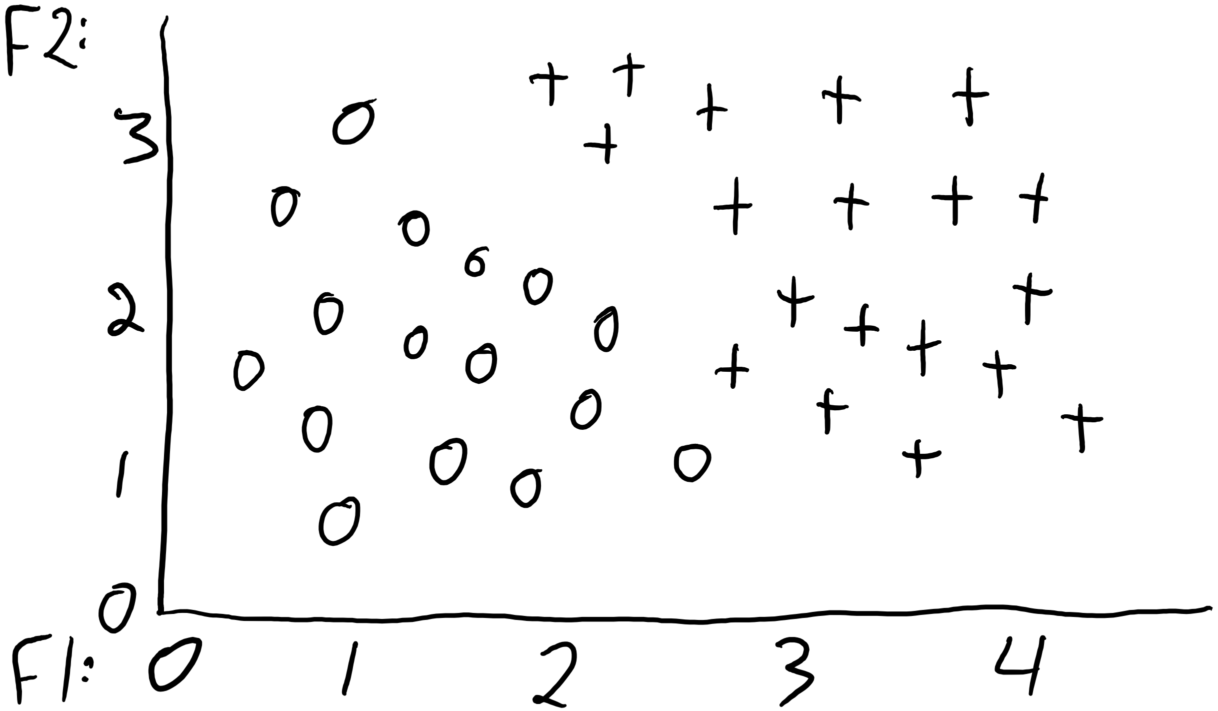
F1	F2	Label
1	3	O
2	3	+
3	2	+
2.5	1	O
3.5	1	+
…	…	…



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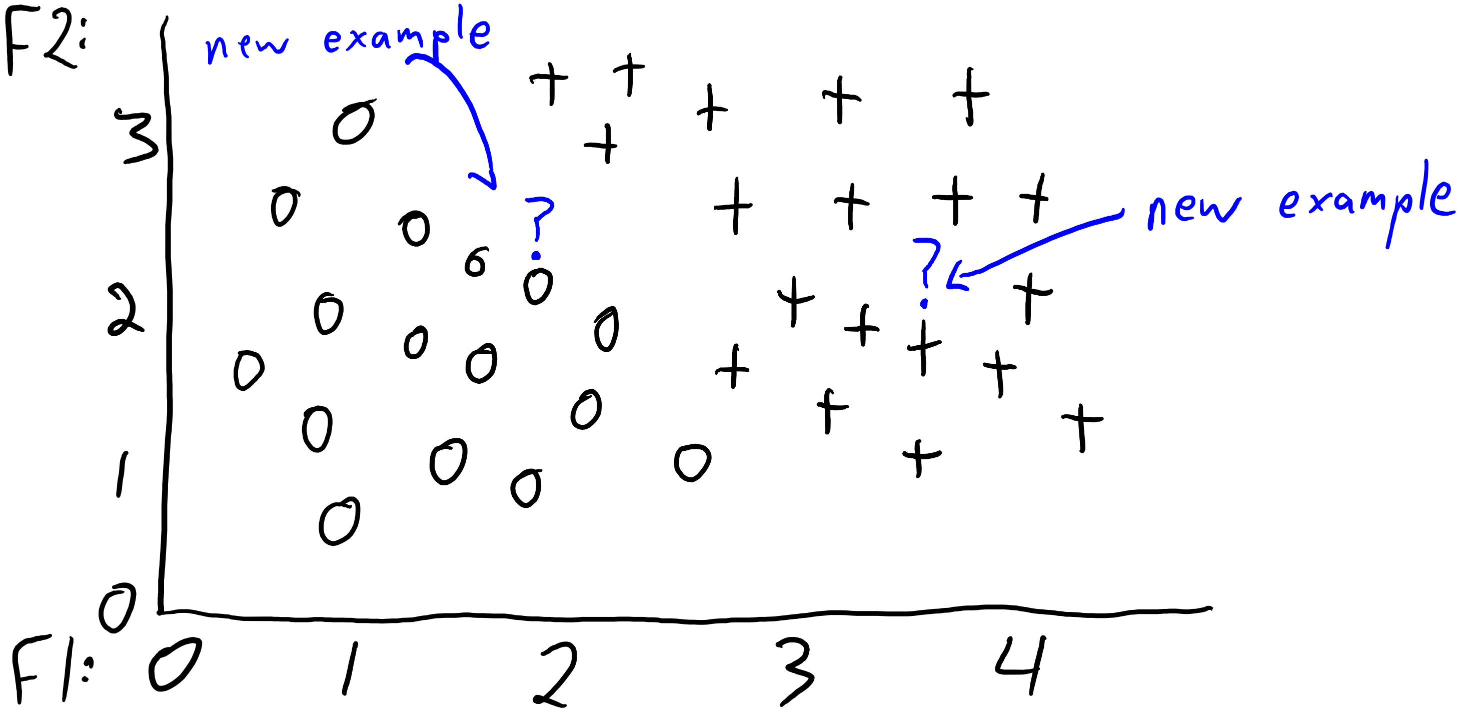
F1	F2		Label
1	3	→	O
2	3	→	+
3	2	→	+
2.5	1	→	O
3.5	1	→	+
…	…		…



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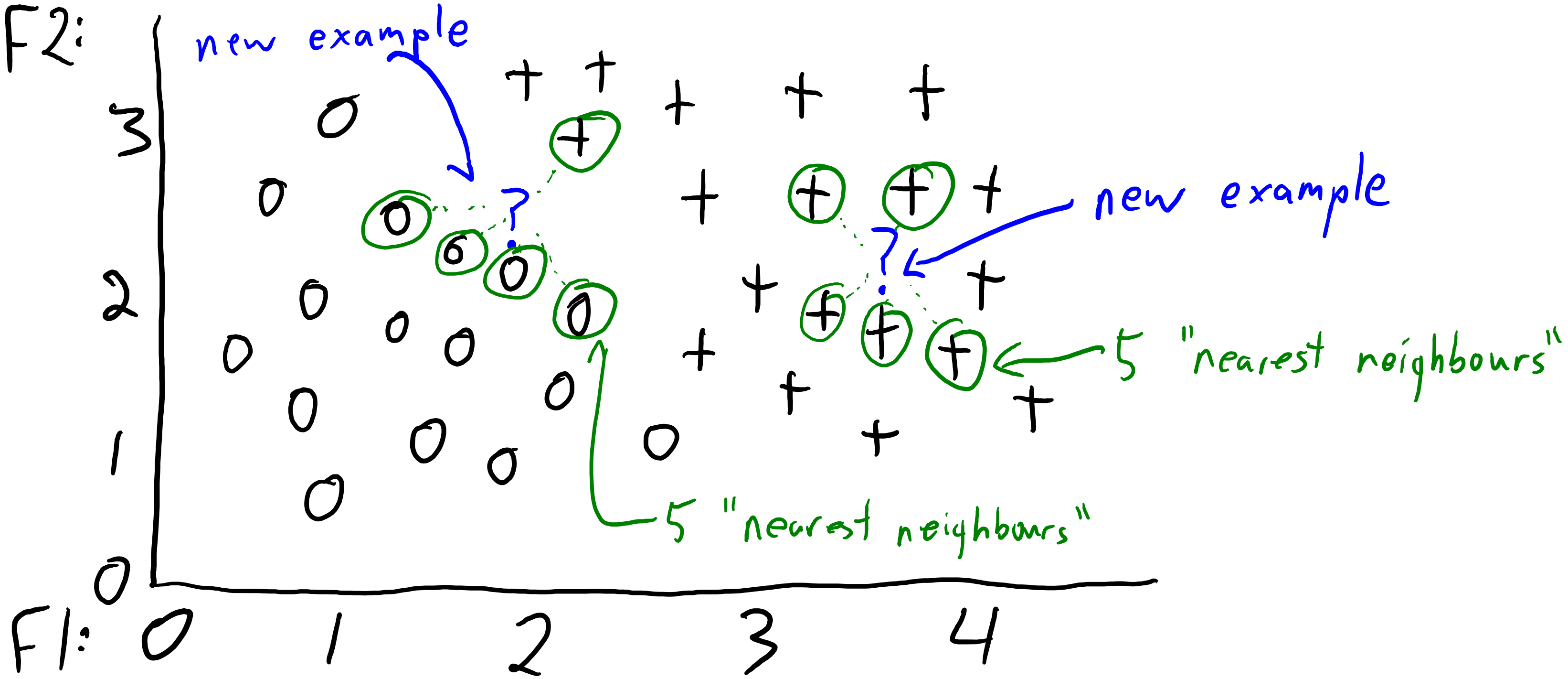
F1	F2	Label
1	3	O
2	3	+
3	2	+
2.5	1	O
3.5	1	+
…	…	…



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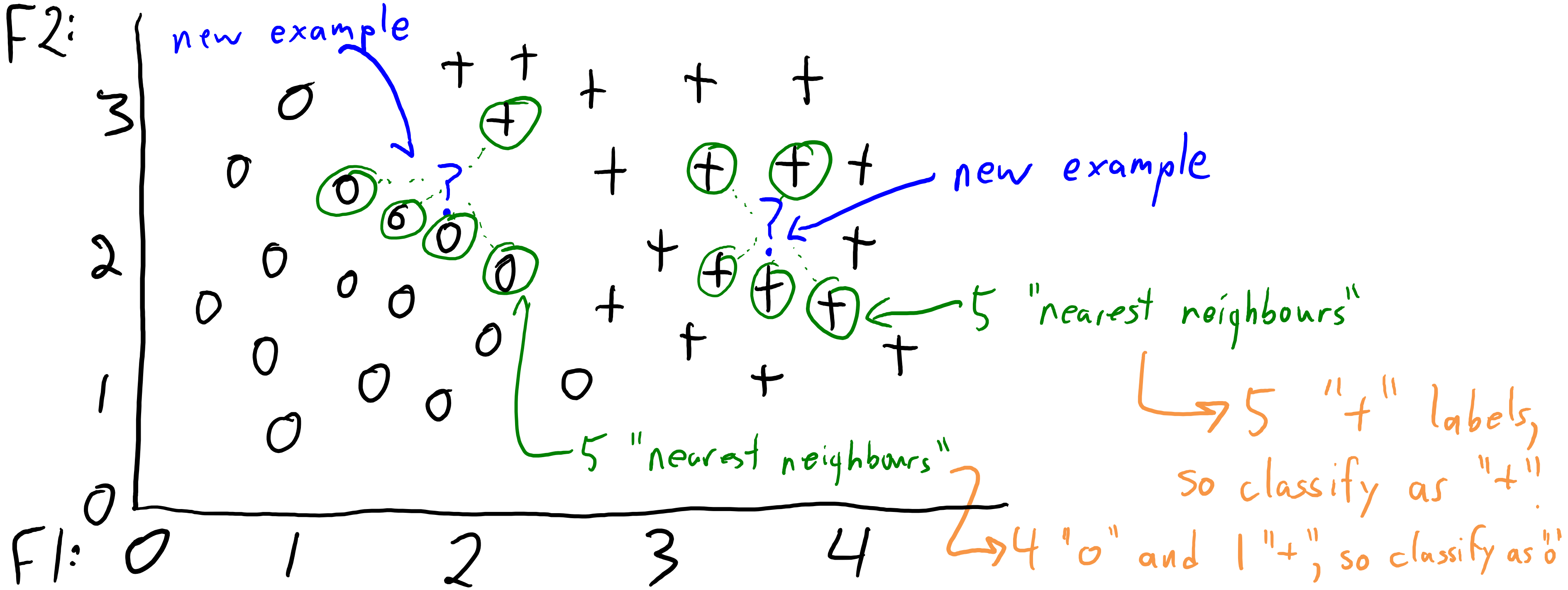
  1. Find the ‘k’ training examples x_i that are “nearest” to $\tilde{x}_i$.
  2. Classify using the most common label of “nearest” training examples.

F1	F2		Label
1	3	➡	O
2	3	➡	+
3	2	➡	+
2.5	1	➡	O
3.5	1	➡	+
…	…		…



k-Nearest Neighbours (kNN)

- Assumption:
  - Examples with similar features are likely to have similar labels.

- Seems strong, but all good classifiers basically rely on this assumption.
  - If not true there may be nothing to learn and you are in “no free lunch” territory.
  - Methods just differ in how you define “similarity”.

- Most common distance function is Euclidean distance:

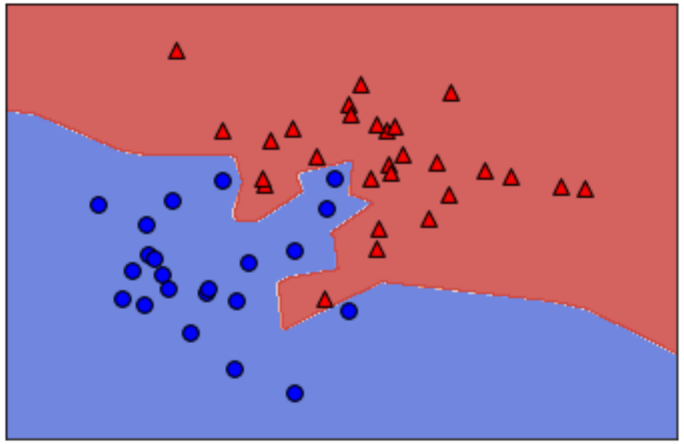
$$\|x_i - \tilde{x}_{\tilde{i}}\| = \sqrt{\sum_{j=1}^{d} (x_{ij} - \tilde{x}_{\tilde{i}j})^2}$$

  - x_i is features of training example ‘i’, and $\tilde{x}_{\tilde{\imath}}$ is features of test example ‘$\tilde{\imath}$’.
  - Costs O(d) to calculate for a pair of examples.

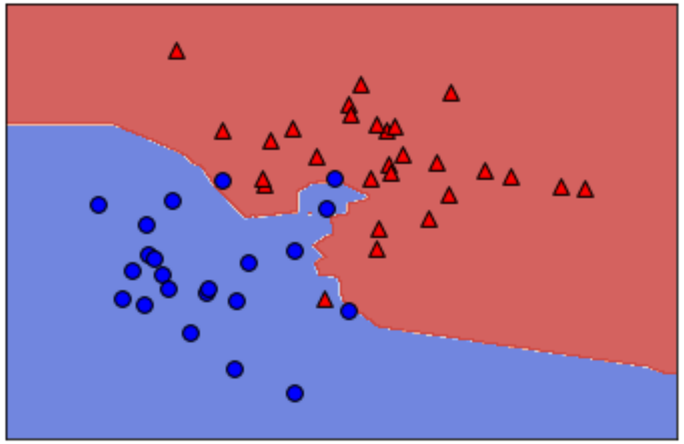
Effect of ‘k’ in kNN.

- With large ‘k’ (hyper-parameter), kNN model will be very simple.
  - With k=n, you just predict the mode of the labels.
  - Model gets more simple as ‘k’ increases.

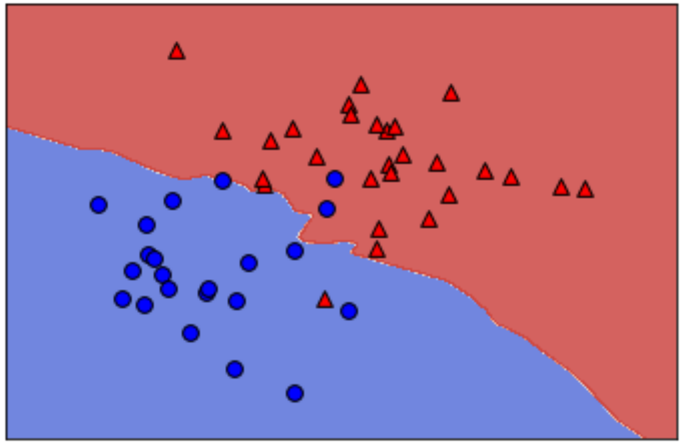
k=1



k=3



k=10



- Effect of ‘k’ on fundamental trade-off:
  - As ‘k’ grows, training error increases and approximation error decreases.

kNN Implementation

- There is no training phase in kNN (“lazy” learning).
  - You just store the training data.
  - Costs O(1) if you use a pointer.

- But predictions are expensive: O(nd) to classify 1 test example.
  - Need to do O(d) distance calculation for all ‘n’ training examples.
  - So prediction time grows with number of training examples.
    - Tons of work on reducing this cost (we’ll discuss this later).

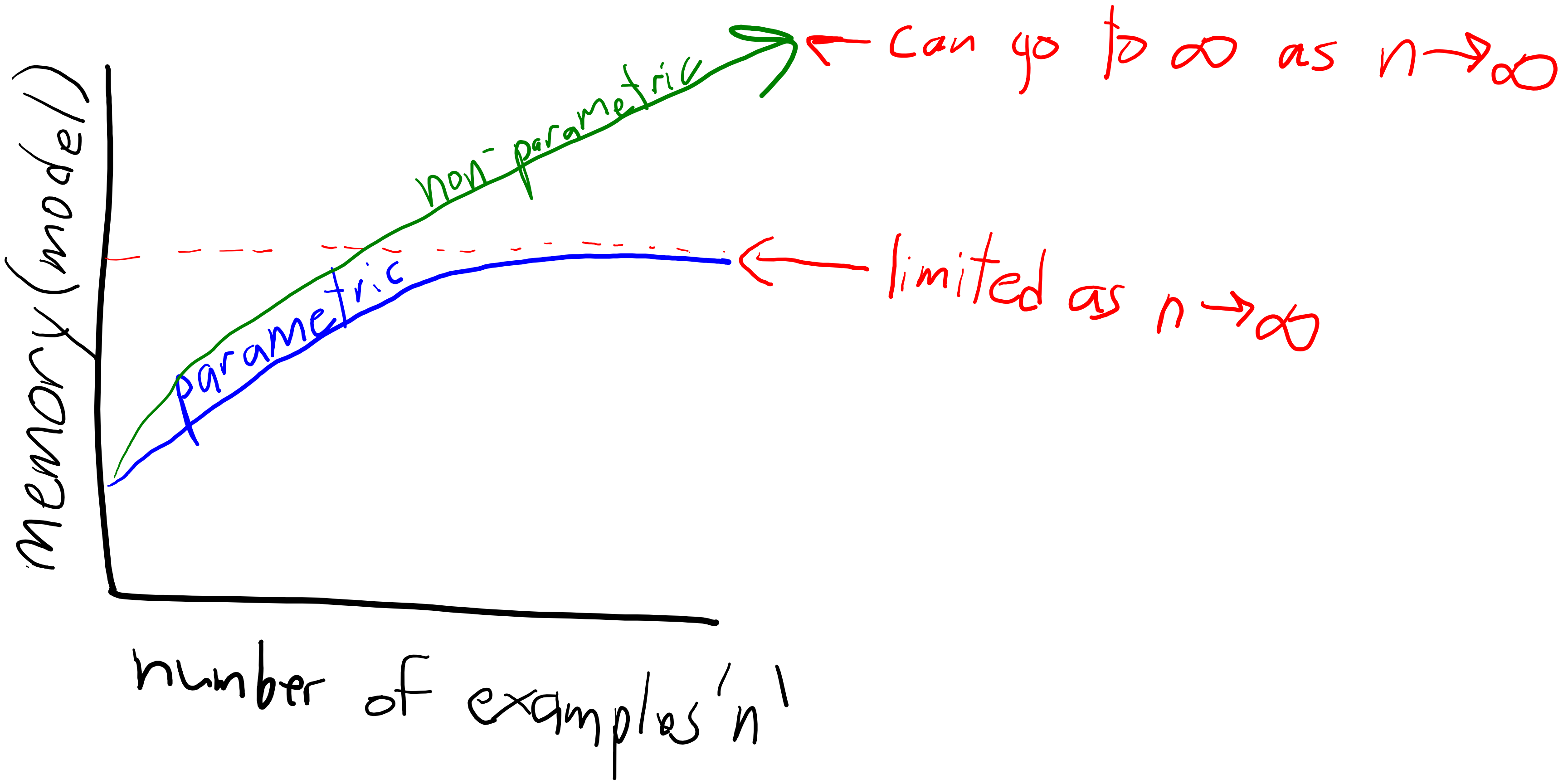
- But storage is expensive: needs O(nd) memory to store ‘X’ and ‘y’.
  - So memory grows with number of training examples.
  - When storage depends on ‘n’, we call it a non-parametric model.

Parametric vs. Non-Parametric

- Parametric models:
  - Have fixed number of parameters: trained “model” size is O(1) in terms ‘n’.
    - E.g., naïve Bayes just stores counts.
    - E.g., fixed-depth decision tree just stores rules for that depth.
  - You can estimate the fixed parameters more accurately with more data.
  - But eventually more data doesn’t help: model is too simple.
- Non-parametric models:
  - Number of parameters grows with ‘n’: size of “model” depends on ‘n’.
  - Model gets more complicated as you get more data.
    - E.g., kNN stores all the training data, so size of “model” is O(nd).
    - E.g., decision tree whose depth *grows with the number of examples*.

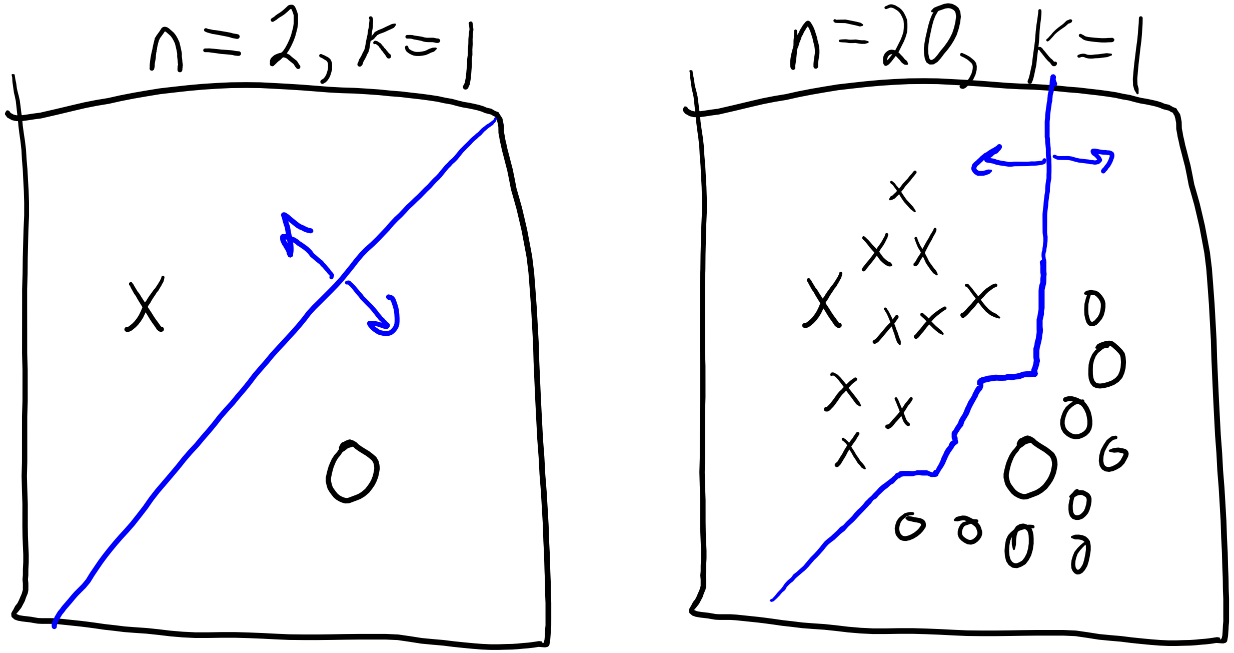
Parametric vs. Non-Parametric Models

- Parametric models have bounded memory.
- Non-parametric models can have unbounded memory.



Effect of ‘n’ in kNN.

- With a small ‘n’, kNN model will be very simple.



- Model gets more complicated as ‘n’ increases.
  - Requires more memory, but detects subtle differences between examples.

bonus!

Consistency of kNN (n → ∞)

- KNN has appealing consistency properties:
  - As ‘n’ goes to ∞, KNN test error is at most twice the best possible error.
    - For fixed ‘k’ and binary labels (under mild assumptions).

- Stone’s Theorem: kNN is “universally consistent”.
  - If k/n goes to zero and ‘k’ goes to ∞, converges to the best possible error.
    - For example, k = log(n).
    - First algorithm shown to have this property.

- Does Stone’s Theorem violate the no free lunch theorem?
  - No: it requires a continuity assumption on the labels.
  - Consistency says nothing about finite ‘n’ (see "Dont Trust Asymptotics”).
    - The “speed” at which universal consistency happens is exponential in the dimension ‘d’.

Curse of Dimensionality

- "Curse of dimensionality": problems with high-dimensional spaces.
  - Volume of space grows exponentially with dimension.
    - Circle has area O(r^2), sphere has area O(r^3), 4d hyper-sphere has area O(r^4),…
  - Need exponentially more points to 'fill' a high-dimensional volume.
    - "Nearest" neighbours might be really far even with large 'n'.

- KNN is also problematic if features have very different scales.
  - Comparing a feature measured in grams vs one measure in kilograms.
    - Measurement in grams can have much more influence (values 1000 times larger).

- Nevertheless, KNN is really easy to use and often hard to beat!

bonus!

Consistency of Non-Parametric Models

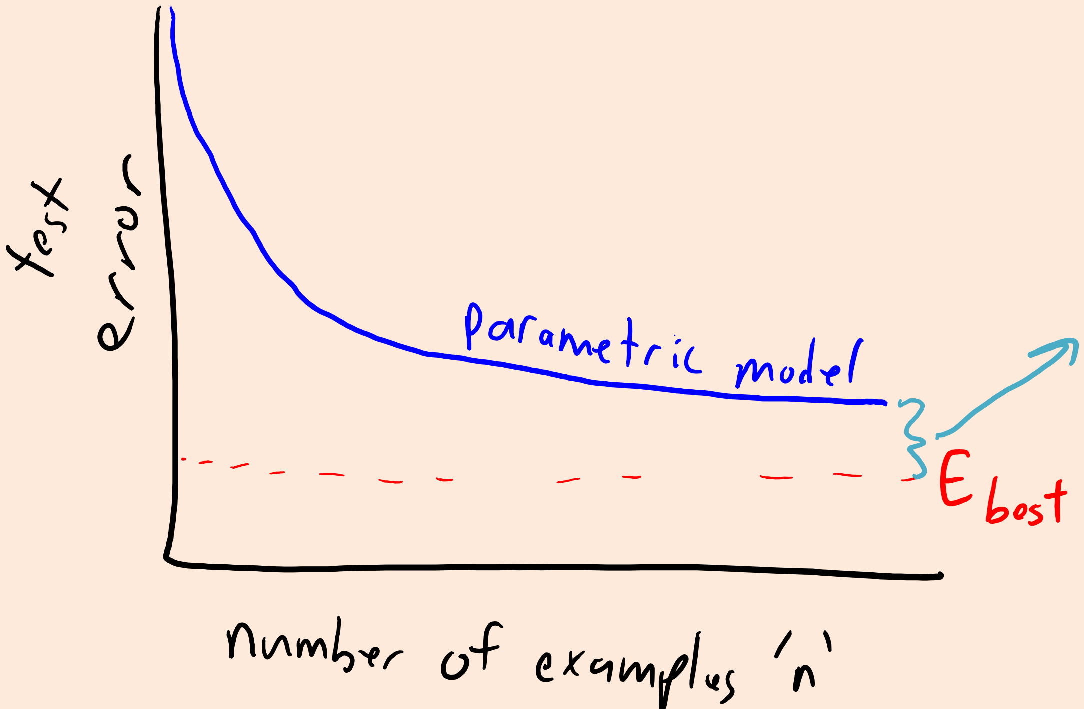
- Universal consistency can be shown for many models in 340:
  - “Linear” models with “polynomial” or “RBFs” as features (later).
  - “Neural network” and “deep learning” models (also covered later).

- But it’s always the non-parametric versions that are consistent:
  - Where size of model is a function of ‘n’.
  - Examples:
    - KNN needs to store all ‘n’ training examples.
    - Degree of the polynomial must grow with ‘n’ (not true for fixed polynomial).
    - Number of “hidden units” must grow with ‘n’ (not true for fixed neural network).

bonus!

Parametric vs. Non-Parametric Models

- With parametric models, there is an accuracy limit.
  - Even with infinite ‘n’, may not be able to achieve optimal error (E_{best}).

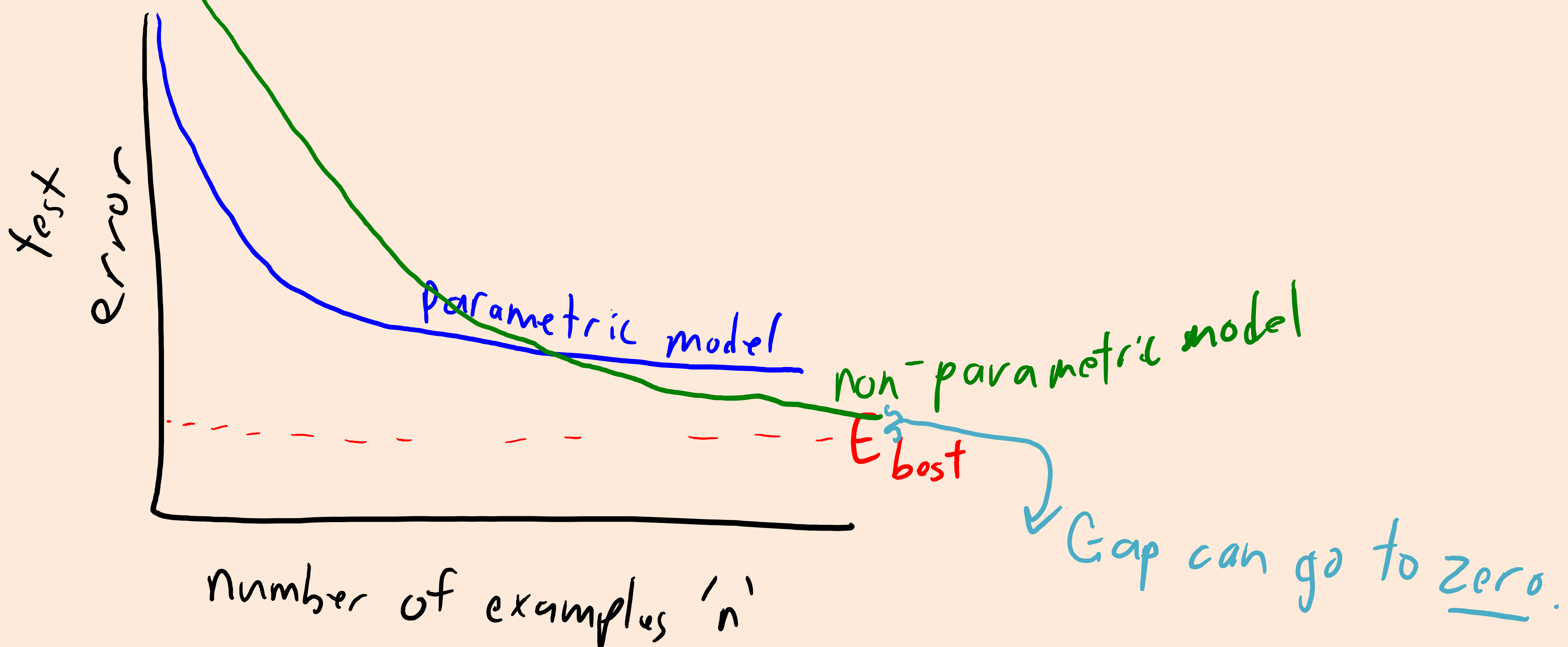


Gap may never go to zero.

bonus!

Parametric vs. Non-Parametric Models

- With parametric models, there is an accuracy limit.
  - Even with infinite ‘n’, may not be able to achieve optimal error (E_{best}).
- Many non-parametric models (like kNN) converge to optimal error.
  - Though may also converge to needing infinite memory.



Summary

- Decision theory allows us to consider costs of predictions.
- K-Nearest Neighbours: use most common label of nearest examples.
  - Often works surprisingly well.
  - Suffers from high prediction and memory cost.
  - Canonical example of a "non-parametric" model.
  - Can suffer from the "curse of dimensionality".
- Non-parametric models grow with number of training examples.
  - Can have appealing "consistency" properties (test error goes down to smallest possible error the model can make, as n goes to infinity).

- Next Time:
  - Fighting the fundamental trade-off.

Naïve Bayes Training Phase

- Training a naïve Bayes model:

$$X = \begin{bmatrix} 0 & 1 \\ 1 & 1 \\ 0 & 0 \\ 1 & 1 \\ 1 & 1 \\ 0 & 0 \\ 1 & 0 \\ 1 & 0 \\ 1 & 1 \\ 1 & 0 \end{bmatrix}, \quad y = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

Naïve Bayes Training Phase

- Training a naïve Bayes model:

1. Set n_c to the number of times $(y_i = c)$.

$n_1 = 6$

$$X = \begin{bmatrix} 0 & 1 \\ 1 & 1 \\ 0 & 0 \\ 1 & 1 \\ 1 & 1 \\ 0 & 0 \\ 1 & 0 \\ 1 & 0 \\ 1 & 1 \\ 1 & 0 \end{bmatrix}, \quad y = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

$n_0 = 4$

Naïve Bayes Training Phase

- Training a naïve Bayes model:

1. Set n_c to the number of times $(y_i = c)$.
2. Estimate $p(y_i = c)$ as $\frac{n_c}{n}$.

$p(y_i = 1) = \frac{6}{10} \leftarrow n_1 = 6$

$$X = \begin{bmatrix} 0 & 1 \\ 1 & 1 \\ 0 & 0 \\ 1 & 1 \\ 1 & 1 \\ 0 & 0 \\ 1 & 0 \\ 1 & 0 \\ 1 & 1 \\ 1 & 0 \end{bmatrix}, \quad y = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

$p(y_i = 0) = \frac{4}{10} \leftarrow n_0 = 4$

Naïve Bayes Training Phase

- Training a naïve Bayes model:

1. Set n_c to the number of times $(y_i = c)$.
2. Estimate $p(y_i = c)$ as $\frac{n_c}{n}$.
3. Set n_{cjk} as the number of times $(y_i = c, x_{ij} = k)$

$$p(y_i = 1) = \frac{6}{10} \leftarrow n_1 = 6$$

$$X = \begin{bmatrix} 0 & 1 \\ 1 & 1 \\ 0 & 0 \\ 1 & 1 \\ 1 & 1 \\ 0 & 0 \\ 1 & 0 \\ 1 & 0 \\ 1 & 1 \\ 1 & 0 \end{bmatrix}, \quad y = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

$$n_{121} = 4$$

$$p(y_i = 0) = \frac{4}{10} \leftarrow n_0 = 4$$

Naïve Bayes Training Phase

- Training a naïve Bayes model:

1. Set n_c to the number of times $(y_i = c)$.
2. Estimate $p(y_i = c)$ as $\frac{n_c}{n}$.
3. Set n_{cjk} as the number of times $(y_i = c, x_{ij} = k)$
4. Estimate $p(x_{ij} = k, y_i = c)$ as $\frac{n_{cjk}}{n}$

$$X = \begin{bmatrix} 0 & 1 \\ 1 & 1 \\ 0 & 0 \\ 1 & 1 \\ 1 & 1 \\ 0 & 0 \\ 1 & 0 \\ 1 & 0 \\ 1 & 1 \\ 1 & 0 \end{bmatrix}, \quad y = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

$p(y_i = 1) = \frac{6}{10} \leftarrow n_1 = 6$

$n_{121} = 4$

$p(x_{i2} = 1, y_i = 1) = \frac{4}{10}$

$p(y_i = 0) = \frac{4}{10} \leftarrow n_0 = 4$

Naïve Bayes Training Phase

- Training a naïve Bayes model:

1. Set n_c to the number of times $(y_i = c)$.
2. Estimate $p(y_i = c)$ as $\frac{n_c}{n}$.
3. Set n_{cjk} as the number of times $(y_i = c, x_{ij} = k)$
4. Estimate $p(x_{ij} = k, y_i = c)$ as $\frac{n_{cjk}}{n}$
5. Use that $p(x_{ij} = k \mid y_i = c) = \frac{p(x_{ij} = k, y_i = c)}{p(y_i = c)}$

$$= \frac{n_{cjk}/n}{n_c/n} = \frac{n_{cjk}}{n_c}$$

$$X = \begin{bmatrix} 0 & 1 \\ 1 & 1 \\ 0 & 0 \\ 1 & 1 \\ 1 & 1 \\ 0 & 0 \\ 1 & 0 \\ 1 & 0 \\ 1 & 1 \\ 1 & 0 \end{bmatrix}, \quad y = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

$p(y_i = 1) = \frac{6}{10} \leftarrow n_1 = 6$

$n_{121} = 4$

$p(x_{i2} = 1, y_i = 1) = \frac{4}{10}$

$p(y_i = 0) = \frac{4}{10} \leftarrow n_0 = 4$

$p(x_{i2} = 1 \mid y_i = 1) = \frac{4}{6} = \frac{2}{3}$

Naïve Bayes Prediction Phase

- Prediction in a naïve Bayes model:

Given a test example $\tilde{x}_i$ we set prediction $\hat{y}_i$ to the 'c' maximizing $p(\tilde{x}_i \mid \tilde{y}_i = c)$

Under the naive Bayes assumption we can maximize:

$$p(\tilde{y}_i = c \mid \tilde{x}_i) \propto \prod_{j=1}^{d} \left[p(\tilde{x}_{ij} \mid \tilde{y}_i = c) \right] p(\tilde{y}_i = c)$$

Naïve Bayes Prediction Phase

- Prediction in a naïve Bayes model:

Consider $\tilde{x}_i = [1\ 1]$ in this data set →

$$X = \begin{bmatrix} 0 & 1 \\ 1 & 1 \\ 0 & 0 \\ 1 & 1 \\ 1 & 1 \\ 0 & 0 \\ 1 & 0 \\ 1 & 0 \\ 1 & 1 \\ 1 & 0 \end{bmatrix}, \quad y = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

Naïve Bayes Prediction Phase

- Prediction in a naïve Bayes model:

Consider $\tilde{x}_i = [1 \ 1]$ in this data set ⟶

$$p(\tilde{y}_i = 0 \mid \tilde{x}_i) \propto p(\tilde{x}_{i1} = 1 \mid \tilde{y}_i = 0)\, p(\tilde{x}_{i2} = 1 \mid \tilde{y}_i = 0)\, p(\tilde{y}_i = 0)$$

$$= (1) \quad (0.25) \quad (0.4) = 0.1$$

$$X = \begin{bmatrix} 0 & 1 \\ 1 & 1 \\ 0 & 0 \\ 1 & 1 \\ 1 & 1 \\ 0 & 0 \\ 1 & 0 \\ 1 & 0 \\ 1 & 1 \\ 1 & 0 \end{bmatrix}, \quad y = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

Naïve Bayes Prediction Phase

- Prediction in a naïve Bayes model:

Consider $\tilde{x}_i = [1 \;\; 1]$ in this data set →

$$p(\tilde{y}_i = 0 \mid \tilde{x}_i) \propto p(\tilde{x}_{i1} = 1 \mid \tilde{y}_i = 0)\, p(\tilde{x}_{i2} = 1 \mid \tilde{y}_i = 0)\, p(\tilde{y}_i = 0)$$

$$= (1) \quad (0.25) \quad (0.4) = 0.1$$

$$p(\tilde{y}_i = 1 \mid \tilde{x}_i) \propto p(\tilde{x}_{i1} = 1 \mid \tilde{y}_i = 1)\, p(\tilde{x}_{i2} = 1 \mid \tilde{y}_i = 1)\, p(\tilde{y}_i = 1)$$

$$= (0.5) \quad (0.666\ldots) \quad (0.6) = 0.2$$

$$X = \begin{bmatrix} 0 & 1 \\ 1 & 1 \\ 0 & 0 \\ 1 & 1 \\ 1 & 1 \\ 0 & 0 \\ 1 & 0 \\ 1 & 0 \\ 1 & 1 \\ 1 & 0 \end{bmatrix}, \quad y = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

Naïve Bayes Prediction Phase

- Prediction in a naïve Bayes model:

Consider $\tilde{x}_i = [1 \ 1]$ in this data set →

$$p(\tilde{y}_i = 0 \mid \tilde{x}_i) \propto p(\tilde{x}_{i1} = 1 \mid \tilde{y}_i = 0)\, p(\tilde{x}_{i2} = 1 \mid \tilde{y}_i = 0)\, p(\tilde{y}_i = 0)$$
$$= (1) \quad (0.25) \quad (0.4) = 0.1$$

$$p(\tilde{y}_i = 1 \mid \tilde{x}_i) \propto p(\tilde{x}_{i1} = 1 \mid \tilde{y}_i = 1)\, p(\tilde{x}_{i2} = 1 \mid \tilde{y}_i = 1)\, p(\tilde{y}_i = 1)$$
$$= (0.5) \quad (0.666\ldots) \quad (0.6) = 0.2$$

$$X = \begin{bmatrix} 0 & 1 \\ 1 & 1 \\ 0 & 0 \\ 1 & 1 \\ 1 & 1 \\ 0 & 0 \\ 1 & 0 \\ 1 & 0 \\ 1 & 1 \\ 1 & 0 \end{bmatrix}, \quad y = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

Since $p(\tilde{y}_i = 1 \mid \tilde{x}_i)$ is bigger than $p(\tilde{y}_i = 0 \mid \tilde{x}_i)$, naive Bayes predicts $\hat{y}_i = 1$.

(Don't sum to 1 because we're ignoring $p(\tilde{x}_i)$)

bonus!

“Proportional to” for Probabilities

- When we say “p(y) ∝ exp(-y^2)” for a function ‘p’, we mean:

$p(y) = \beta \exp(-y^2)$ for some constant ‘β’.

- However, if ‘p’ is a probability then it must sum to 1.
  - If $y \in \{1,2,3,4\}$ then $p(1)+p(2)+p(3)+p(4)=1$

- Using this fact, we can find β:

$$\beta \exp(-1^2) + \beta \exp(-2^2) + \beta \exp(-3^2) + \beta \exp(-4^2) = 1$$

$$\Leftrightarrow \beta [\exp(-1^2) + \exp(-2^2) + \exp(-3^2) + \exp(-4^2) = 1$$

$$\Leftrightarrow \beta = \frac{1}{\exp(-1^2) + \exp(-2^2) + \exp(-3^2) + \exp(-4^2)}$$

Probability of Paying Back a Loan and Ethics

bonus!

- Article discussing predicting "whether someone will pay back a loan":
  - https://www.thecut.com/2017/05/what-the-words-you-use-in-a-loan-application-reveal.html
- Words that increase probability of paying back the most:
  - *debt-free, lower interest rate, after-tax, minimum payment, graduate.*
- Words that decrease probability of paying back the most:
  - *God, promise, will pay, thank you, hospital.*
- Article also discusses an important issue: are all these features ethical?
  - Should you deny a loan because of religion or a family member in the hospital?
  - ICBC is limited in the features it is allowed to use for prediction.

bonus!

Avoiding Underflow

- During the prediction, the probability can underflow:

$$p(y_i = c \mid x_i) \propto \prod_{j=1}^{d} \Big[\underbrace{p(x_{ij} \mid y_i = c)}_{}\Big] \underbrace{p(y_i = c)}_{}$$

All these are < 1 so the product gets <u>very small</u>.

- Standard fix is to (equivalently) maximize the logarithm of the probability:

Rember that $\log(ab) = \log(a) + \log(b)$ so $\log(\prod a_i) = \sum_i \log(a_i)$

Since log is <u>monotonic</u> the 'c' maximizing $p(y_i = c \mid x_i)$ also maximizes $\log p(y_i = c \mid x_i)$,

so maximize $\log\left(\prod_{j=1}^{d}\left[p(x_{ij} \mid y_i = c)\right] p(y_i = c)\right) = \sum_{j=1}^{d} \log(p(x_{ij} \mid y_i = c)) + \log(p(y_i = c))$

bonus!

Less-Naïve Bayes

- Given features {x1,x2,x3,…,xd}, naïve Bayes approximates p(y|x) as:

$$p(y \mid x_1, x_2, \dots, x_d) \propto p(y)\, p(x_1, x_2, \dots, x_d \mid y)$$

product rule applied repeatedly

$$= p(y)\, p(x_1 \mid y)\, p(x_2 \mid x_1, y)\, p(x_3 \mid x_2, x_1, y) \cdots p(x_d \mid x_1, x_2, \dots, x_{d-1}, y)$$

$$\approx p(y)\, p(x_1 \mid y)\, p(x_2 \mid y)\, p(x_3 \mid y) \cdots p(x_d \mid y) \quad \text{(naive Bayes assumption)}$$

- The assumption is very strong, and there are “less naïve” versions:
  - Assume independence of all variables except up to ‘k’ largest ‘j’ where j < i.
    - E.g., naïve Bayes has k=0 and with k=2 we would have:

$$\approx p(y)\, p(x_1 \mid y)\, p(x_2 \mid x_1, y)\, p(x_3 \mid x_2, x_1, y)\, p(x_4 \mid x_3, x_2, y) \cdots p(x_d \mid x_{d-2}, x_{d-1}, y)$$

    - Fewer independence assumptions so more flexible, but hard to estimate for large ‘k’.
  - Another practical variation is “tree-augmented” naïve Bayes.

bonus!

Computing $p(x_i)$ under naïve Bayes

- Generative models don’t need $p(x_i)$ to make decisions.
- However, it’s easy to calculate under the naïve Bayes assumption:

$$p(x_i) = \sum_{c=1}^{K} p(x_i, y=c) \qquad \text{(marginalization rule)}$$

$$= \sum_{c=1}^{K} p(x_i \mid y=c)\, p(y=c) \qquad \text{(product rule)}$$

$$= \sum_{c=1}^{K} \underbrace{\left[\prod_{j=1}^{d} p(x_{ij} \mid y=c)\right] p(y=c)}_{\text{These are the quantities we compute during training.}} \qquad \text{(naive Bayes assumption)}$$

bonus!

Gaussian Discriminant Analysis

- Classifiers based on Bayes rule are called generative classifier:
  - They often work well when you have tons of features.
  - But they need to know $p(x_i \mid y_i)$, probability of features given the class.
    - How to “generate” features, based on the class label.

- To fit generative models, usually make BIG assumptions:
  - Naïve Bayes (NB) for discrete x_i:
    - Assume that each variables in x_i is independent of the others in x_i given y_i.
  - Gaussian discriminant analysis (GDA) for continuous x_i.
    - Assume that $p(x_i \mid y_i)$ follows a multivariate normal distribution.
    - If all classes have same covariance, it’s called “linear discriminant analysis”.

bonus!

Other Performance Measures

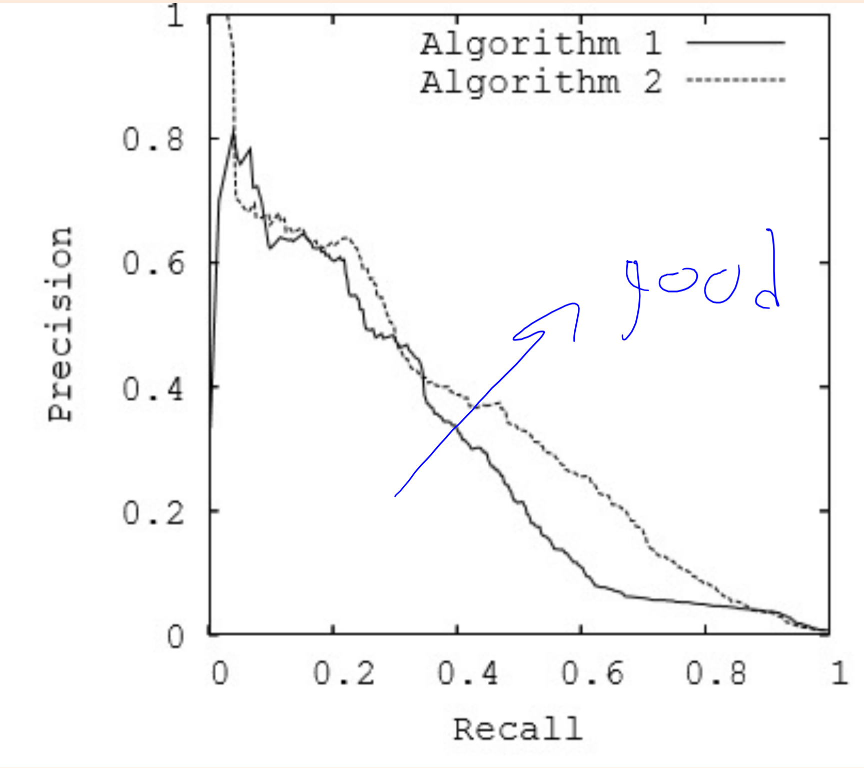
- Classification error might be wrong measure:
  - Use weighted classification error if have different costs.
  - Might want to use things like Jaccard measure: TP/(TP + FP + FN).

- Often, we report precision and recall (want both to be high):
  - Precision: "if I classify as spam, what is the probability it actually is spam?"
    - Precision = TP/(TP + FP).
    - High precision means the filtered messages are likely to really be spam.
  - Recall: "if a message is spam, what is probability it is classified as spam?"
    - Recall = TP/(TP + FN)
    - High recall means that most spam messages are filtered.

bonus!

Precision-Recall Curve

- Consider the rule $p(y_i = \text{'spam'} \mid x_i) > t$, for threshold 't'.
- Precision-recall (PR) curve plots precision vs. recall as 't' varies.

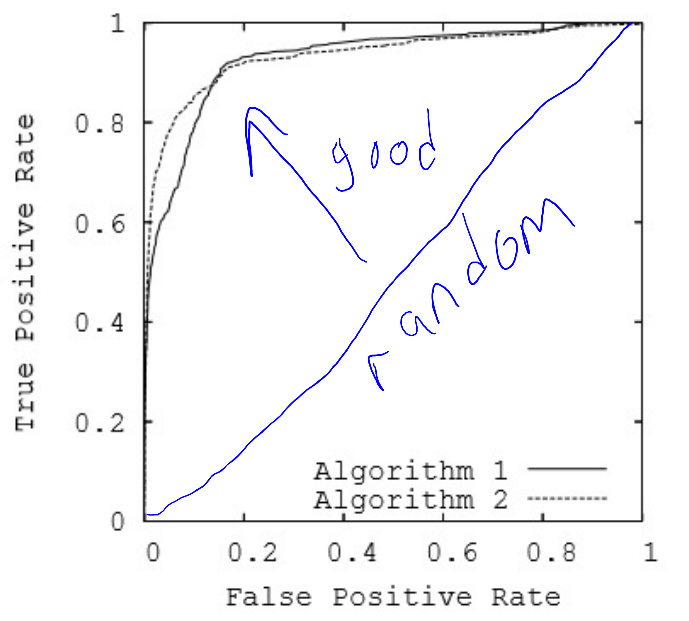


http://pages.cs.wisc.edu/~jdavis/davisgoadrichcamera2.pdf

bonus!

ROC Curve

- Receiver operating characteristic (ROC) curve:
  - Plot true positive rate (recall) vs. false positive rate (FP/FP+TN).
    (negative examples classified as positive)



  - Diagonal is random, perfect classifier would be in upper left.
  - Sometimes papers report area under curve (AUC).
    - Reflects performance for different possible thresholds on the probability.

http://pages.cs.wisc.edu/~jdavis/davisgoadrichcamera2.pdf

bonus!

More on Unbalanced Classes

- With unbalanced classes, there are many alternatives to accuracy as a measure of performance:
  - Two common ones are the Jaccard coefficient and the F-score.

- Some machine learning models don't work well with unbalanced data. Some common heuristics to improve performance are:
  - Under-sample the majority class (only take 5% of the spam messages).
    - https://www.jair.org/media/953/live-953-2037-jair.pdf
  - Re-weight the examples in the accuracy measure (multiply training error of getting non-spam messages wrong by 10).
  - Some notes on this issue are here.

bonus!

More on Weirdness of High Dimensions

- In high dimensions:
  - Distances become less meaningful:
    - All vectors may have similar distances.
  - Emergence of “hubs” (even with random data):
    - Some datapoints are neighbours to many more points than average.
  - Visualizing high dimensions and sphere-packing

bonus!

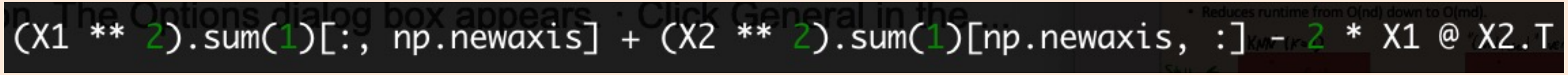
Vectorized Distance Calculation

- To classify 't' test examples based on kNN, cost is O(ndt).
  - Need to compare 'n' training examples to 't' test examples, and computing a distance between two examples costs O(d).

- You can do this using matrix multiplication:
  - Let D be a matrix such that D_{ij} contains:

$$||x_i - x_j||^2 = ||x_i||^2 - 2x_i^T x_j + ||x_j||^2$$

    where 'i' is a training example and 'j' is a test example.
  - In numpy: (like sklearn.metrics.pairwise.euclidean_distances)



```
(X1 ** 2).sum(1)[:, np.newaxis] + (X2 ** 2).sum(1)[np.newaxis, :] - 2 * X1 @ X2.T
```

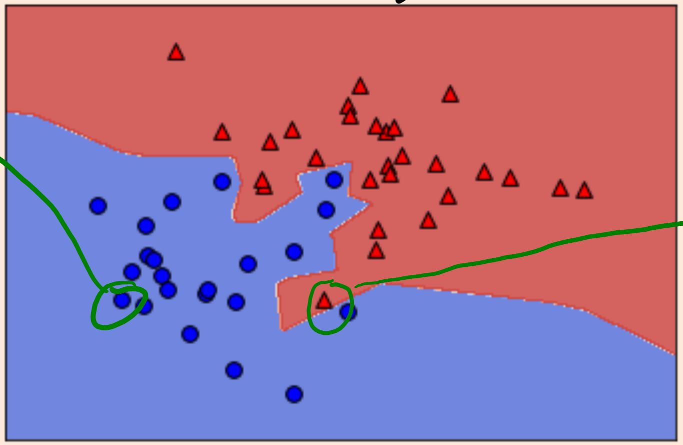
  - Can be better than optimized C loops (scipy.spatial.distance.cdist)

bonus!

Condensed Nearest Neighbours

- Disadvantage of kNN is slow prediction time (depending on ‘n’).
- Condensed nearest neighbours:
  - Identify a set of ‘m’ “prototype” training examples.
  - Make predictions by using these “prototypes” as the training data.
- Reduces runtime from O(nd) down to O(md).

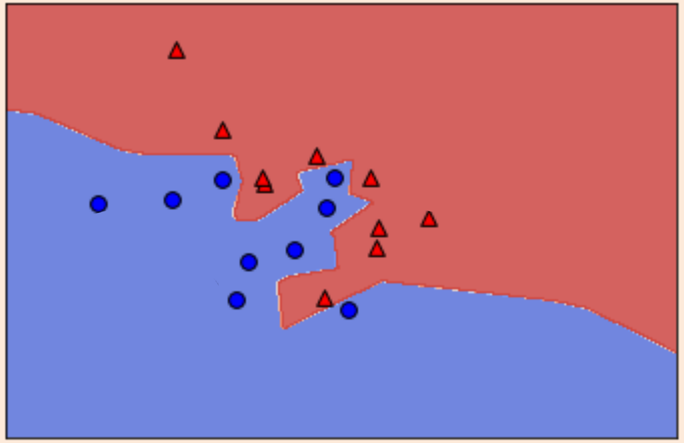
KNN (K=1)



Still blue if you remove this point

Decision would change if you remove this one.

"Condensed" version



same predictions, fewer examples

bonus!

Condensed Nearest Neighbours

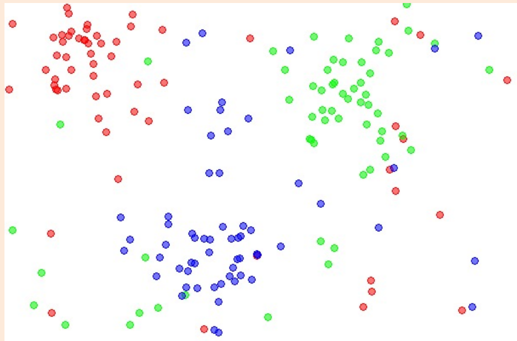
- Classic condensed nearest neighbours:
  - Start with no examples among prototypes.
  - Loop through the non-prototype examples ‘i’ in some order:
    - Classify x_i based on the current prototypes.
    - If prediction is not the true y_i, add it to the prototypes.
  - Repeat the above loop until all examples are classified correctly.
- Some variants first remove points from the original data, if a full-data KNN classifier classifies them incorrectly (“outliers’).

bonus!

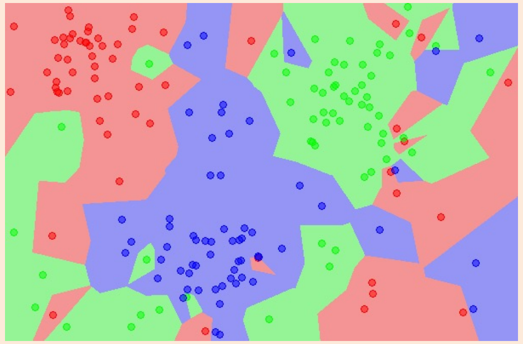
Condensed Nearest Neighbours

- Classic condensed nearest neighbours:

Data:



1NN



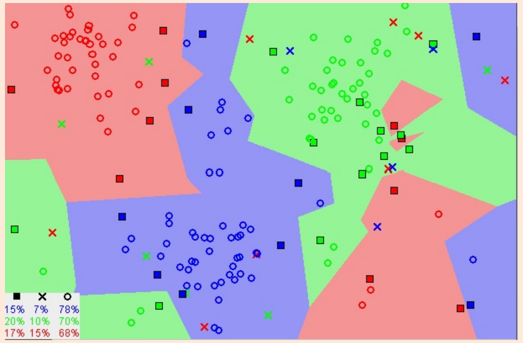
CNN:

□: prototype

O: removed

X: outlier

(using 3NN)



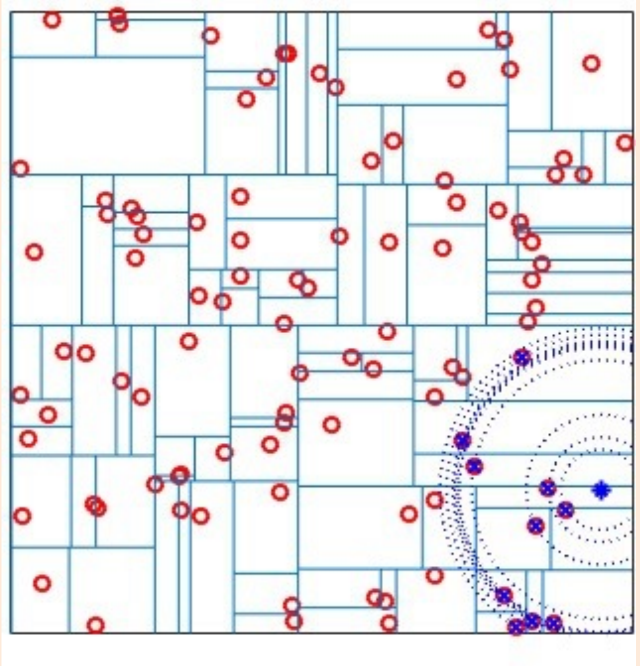
- Recent work shows that finding optimal compression is NP-hard.
  - An approximation algorithm algorithm was published in 2018:
    - "Near optimal sample compression for nearest neighbors"

https://en.wikipedia.org/wiki/K-nearest_neighbors_algorithm

bonus!

Approximate Nearest Neighbours

- Store data in a special data structure, e.g. k-d tree
  - Partition points into regions, only check nearby regions
  - Only helps for exact checks if n is at least about 2^d
  - But making several trees on different projections can give good approximations (that might miss true NNs)



from vlfeat docs

- Locality-sensitive hashing
  - Like traditional hashing but we *try to get collisions* for nearby points
  - Simple method (SimHash): choose random hyperplanes, track which side of each the result is on

https://en.wikipedia.org/wiki/K-nearest_neighbors_algorithm

bonus!

Refined Fundamental Trade-Off

- Let E_{best} be the irreducible error (lowest possible error for *any* model).
  - For example, irreducible error for predicting coin flips is 0.5.
- Some learning theory results use E_{best} to further decompose E_{test}:

$$E_{test} = \underbrace{(E_{test} - E_{train})}_{E_{approx}} + \underbrace{(E_{train} - E_{best})}_{E_{model}} + \underbrace{E_{best}}_{\text{"noise"}}$$

- E_{approx} measures *how sensitive we are to training data*.
- E_{model} measures *if our model is complicated enough to fit data*.
- E_{best} measures how low can **any** model make test error.
  - E_{best} does not depend on what model you choose.

bonus!

Consistency and Universal Consistency

- A model is consistent for a particular learning problem if:
  - E_{test} converges to E_{best} as ‘n’ goes to infinity, for that particular problem.

- A model is universally consistent for a class of learning problems if:
  - E_{test} converges to E_{best} as ‘n’ goes to infinity, for all problems in the class.

- Class of learning problems will usually be “all problems satisfying”:
  - A continuity assumption on the labels y^i as a function of x^i.
    - E.g., if x^i is close to x^j then they are likely to receive the same label.
  - A boundedness assumption of the set of x^i.

bonus!

Consistency of KNN (Discrete/Deterministic Case)

- Let’s show universal consistency of KNN in a simplified setting.
  - The x^i and y^i are binary, and y^i being a deterministic function of x^i.
    - Deterministic y^i implies that E_{best} is 0.

- Consider KNN with k=1:
  - After we observe an x_i, KNN makes right test prediction for that vector.
  - As ‘n’ goes to ∞, each feature vectors with non-zero probability is observed.
  - We have E_{test} = 0 once we’ve seen all feature vectors with non-zero probability.

- Notes:
  - “No free lunch” isn’t relevant as ‘n’ goes to ∞: we eventually see everything.
    - But there are 2^d possible feature vectors, so might need a huge number of training examples.
  - It’s more complicated if labels aren’t deterministic and features are continuous.

bonus!

Consistency of Non-Parametric Models

- Universal consistency can be been shown for many models we'll cover:
  - Linear models with polynomial basis.
  - Linear models with Gaussian RBFs.
  - Neural networks with one hidden layer and standard activations.
    - Sigmoid, tanh, ReLU, etc.

- But it's always the non-parametric versions that are consistent:
  - Where size of model is a function of 'n'.
  - Examples:
    - KNN needs to store all 'n' training examples.
    - Degree of polynomial must grow with 'n' (not true for fixed polynomial).
    - Number of hidden units must grow with 'n' (not true for fixed neural network).