CPSC 340:
Machine Learning and Data Mining

Non-Parametric Models

Fall 2020

Admin

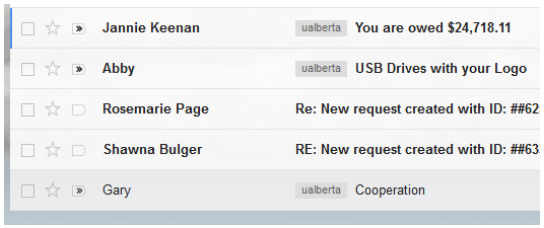
- Course webpage:
  - https://www.cs.ubc.ca/~fwood/CS340/

- Assignment 2 is out.
  - Due Wednesday the 30th. It's long so start early.

- Submission guidelines *will be enforced* starting with Assignment 2
  - Answers in green text
  - Match questions to pages in Gradescope
  - Mark all pages corresponding to each question in Gradescope

Last Time: E-mail Spam Filtering

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



- 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	…	Spam?
1	1	0	0	1	0	…	1
0	0	0	0	1	1	…	1
0	1	1	1	0	0	…	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:

$$p(\text{hello}=1, \text{viagra}=0, \text{340}=1 \mid \text{spam}) \approx p(\text{hello}=1 \mid \text{spam})\, p(\text{viagra}=0 \mid \text{spam})\, p(\text{340}=1 \mid \text{spam})$$

HARD

easy easy 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:

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

$$\propto p(x_i \mid y_i)\,p(y_i) \quad \text{("denominator doesn't matter")}$$

same for all y_i values

$$\approx \prod_{j=1}^{d} \left[p(x_{ij} \mid y_i) \right] p(y_i) \quad \text{(conditional independence assumption)}$$

Only needs easy probabilities.

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

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

This is a "maximum a posteriori" (MAP) estimate of the probability. 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:

$$\mathbb{E}[\text{cost}(\hat{y}_i, \tilde{y}_i)]$$

expectation of model with respect to $\tilde{y}_i$

cost of predicting $\hat{y}_i$ if it's really $\tilde{y}_i$

- Even if "spam" has a higher probability, predicting "spam" might have a expected higher 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 $p(\tilde{y}_i = \text{"spam"} \mid \tilde{x}_i) = 0.6$, then:

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

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

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

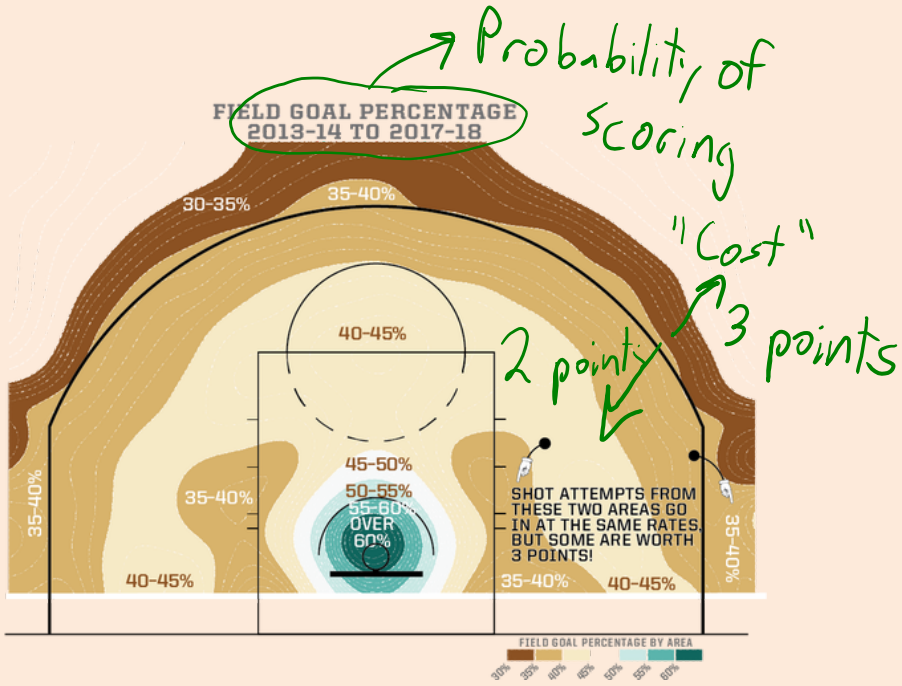
- Even though "spam" is more likely, we should predict "not spam".

Decision Theory Discussion

- In other applications, the costs could be different.
  - In cancer screening, maybe 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 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.

Decision Theory and Basketball

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

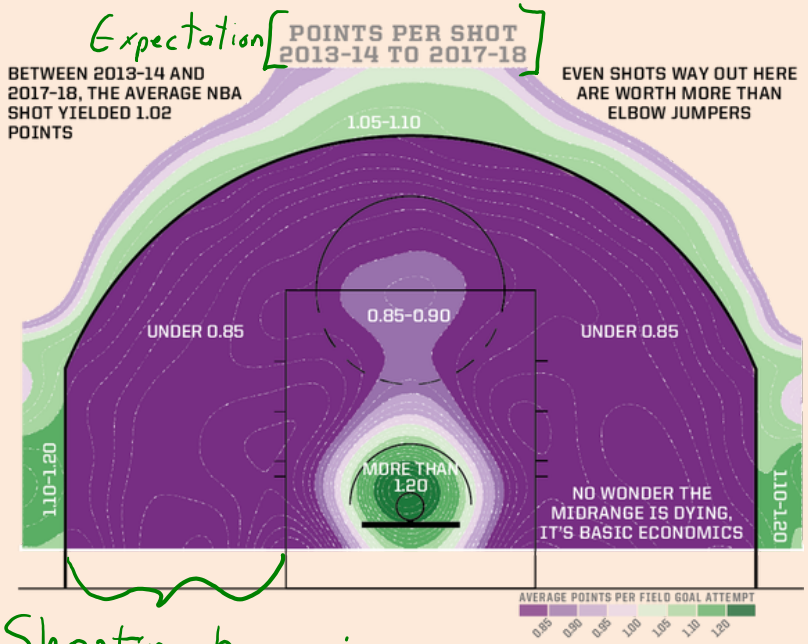


Probability of scoring

"Cost"

2 points

3 points



Expectation

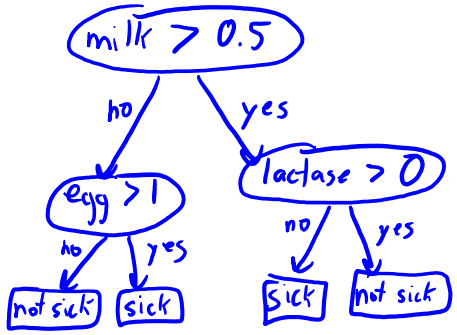
Shooting here is a bad decision

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

(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").

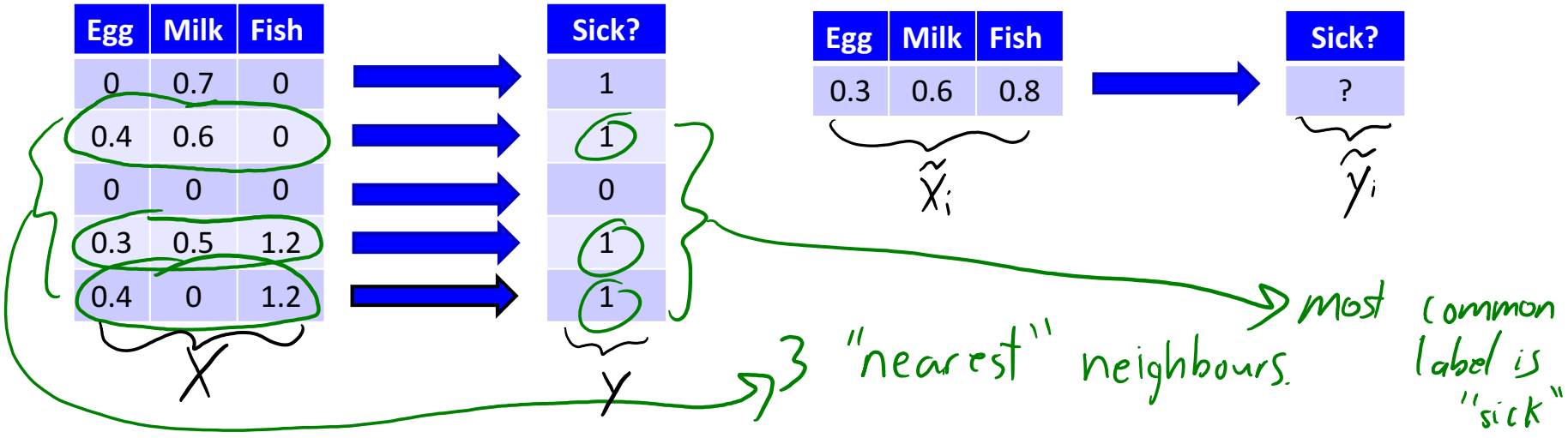
- Naïve Bayes:

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

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.



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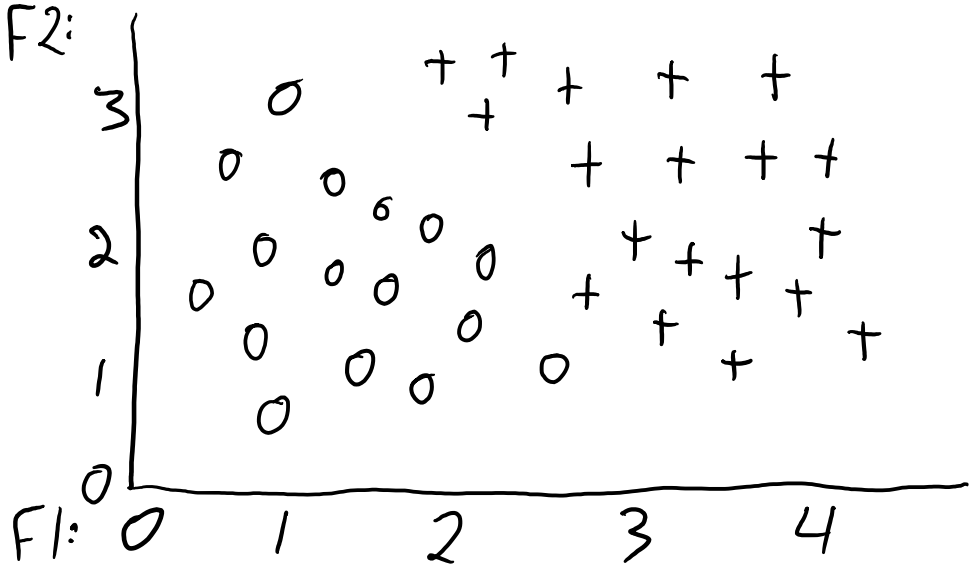
F1	F2	Label
1	3	O
2	3	+
3	2	+
2.5	1	O
3.5	1	+
…	…	…



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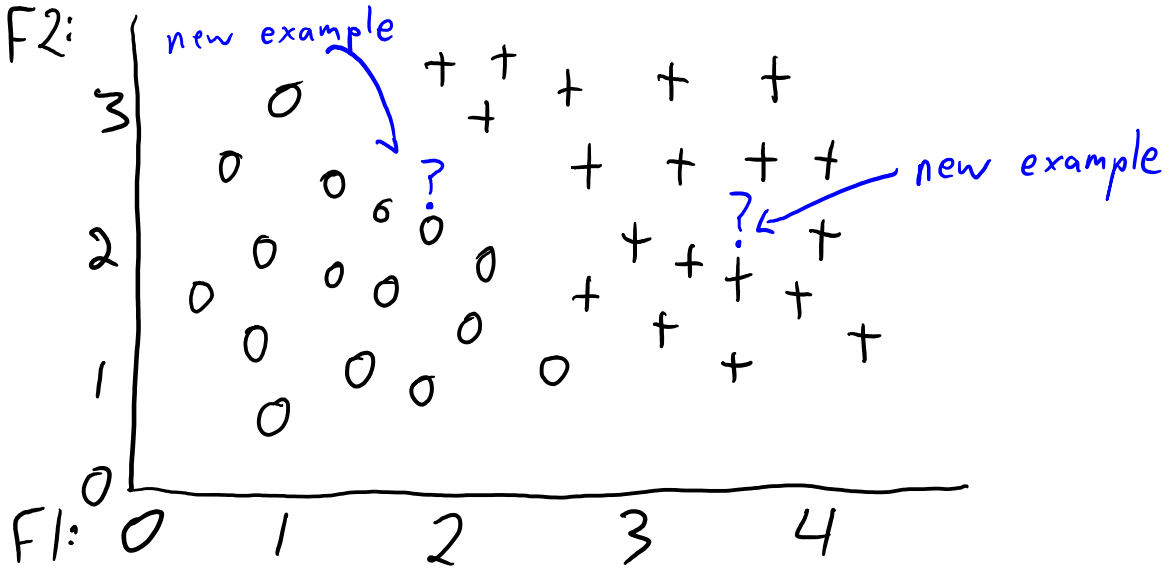

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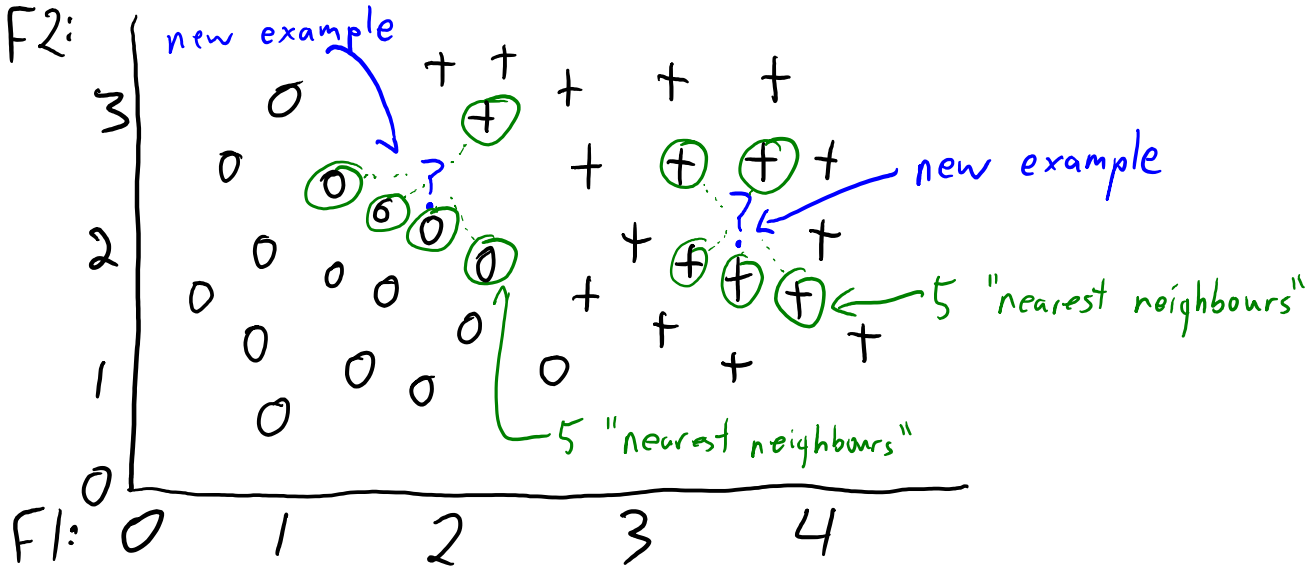

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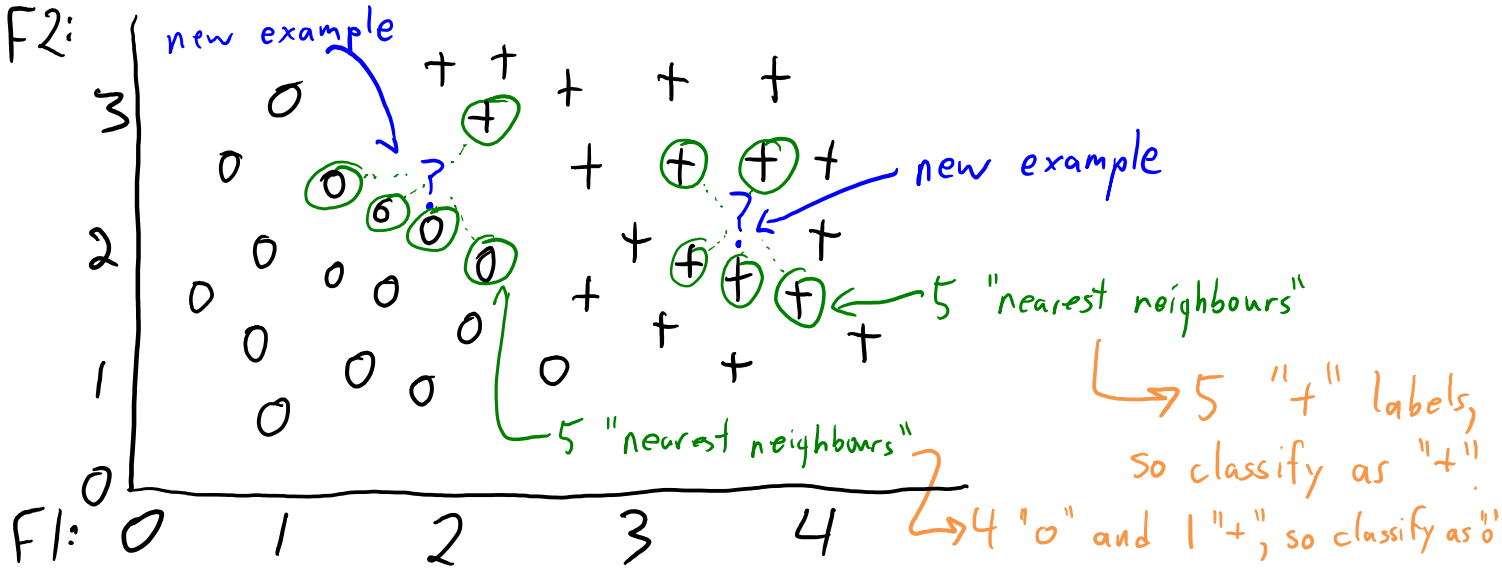


K-Nearest Neighbours (KNN)

- 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".

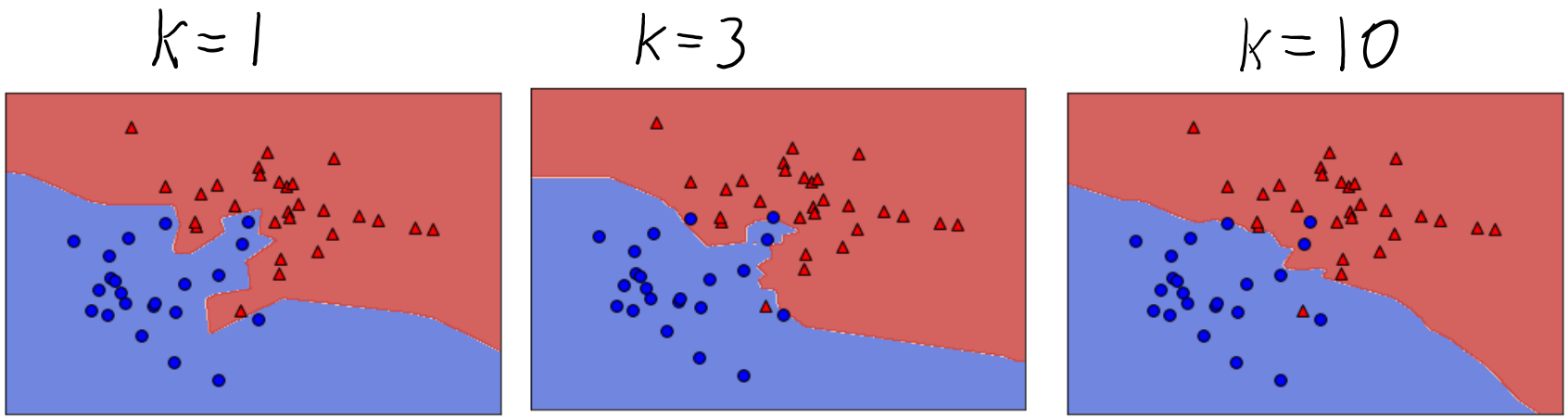
- Most common distance function is Euclidean distance:

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

  - x_i is features of training example 'i', and $\tilde{x}_{\tilde{i}}$ is features of test example '$\tilde{i}$'.
  - 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 complicated as ‘k’ decreases.



- Effect of ‘k’ on fundamental trade-off:
  - As ‘k’ grows, training error increase 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).

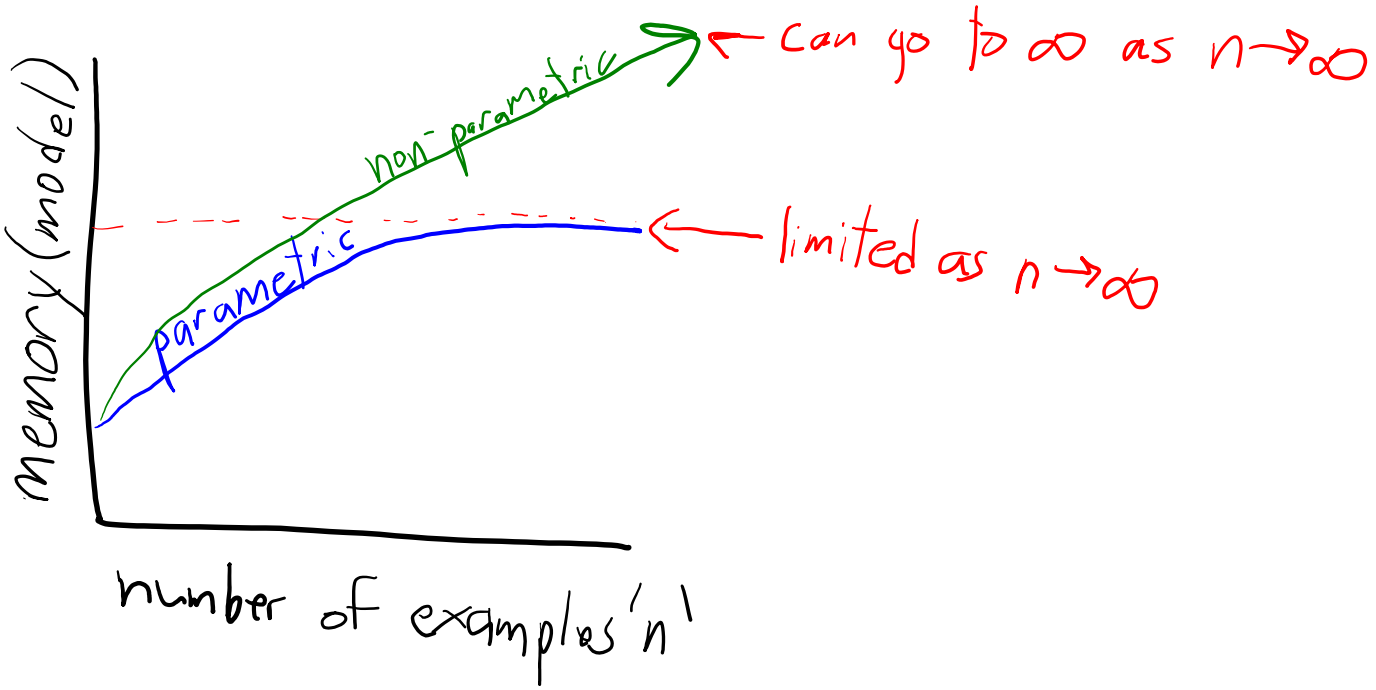
- But storage is expensive: needs O(nd) memory to store 'X' and 'y'.
  - So memory grows with number of training examples.
  - When storage depends on 'n', we call it a non-parametric model.

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*.

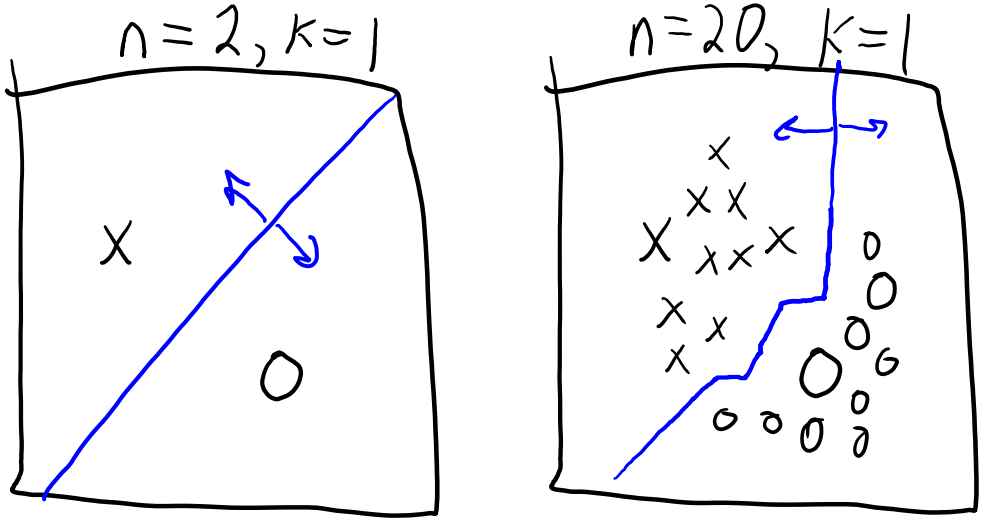
Parametric vs. Non-Parametric Models

- 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.



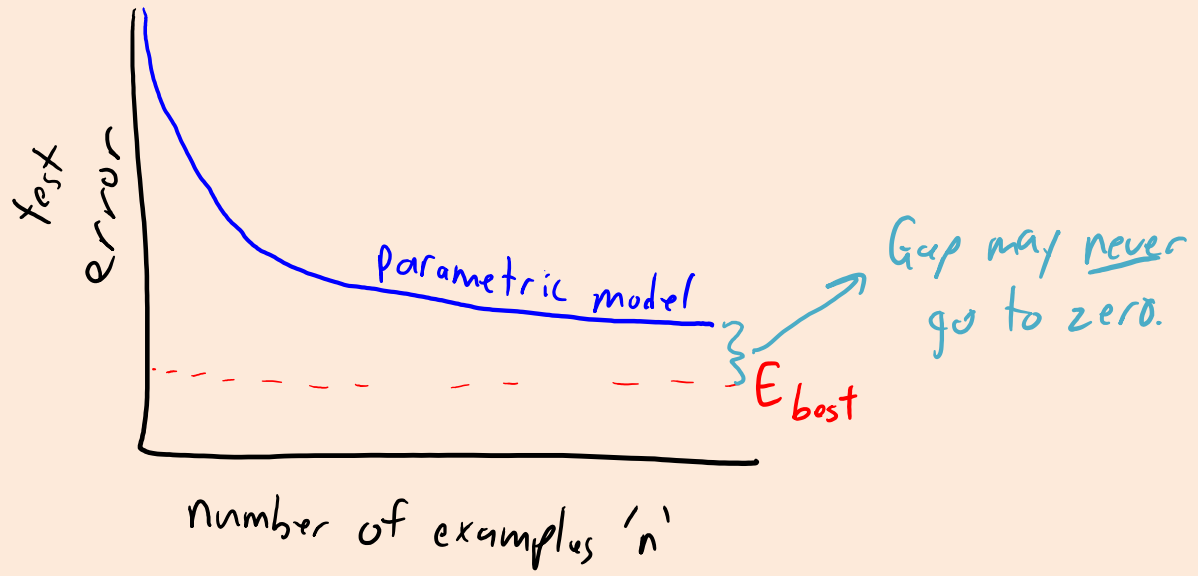
- Model gets more complicated as ‘n’ increases.
  - Requires more memory, but detects subtle differences between examples.

Consistency of KNN (‘n’ going to ‘∞’)

- KNN has appealing consistency properties:
  - As ‘n’ goes to ∞, KNN test error is less than twice 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”).

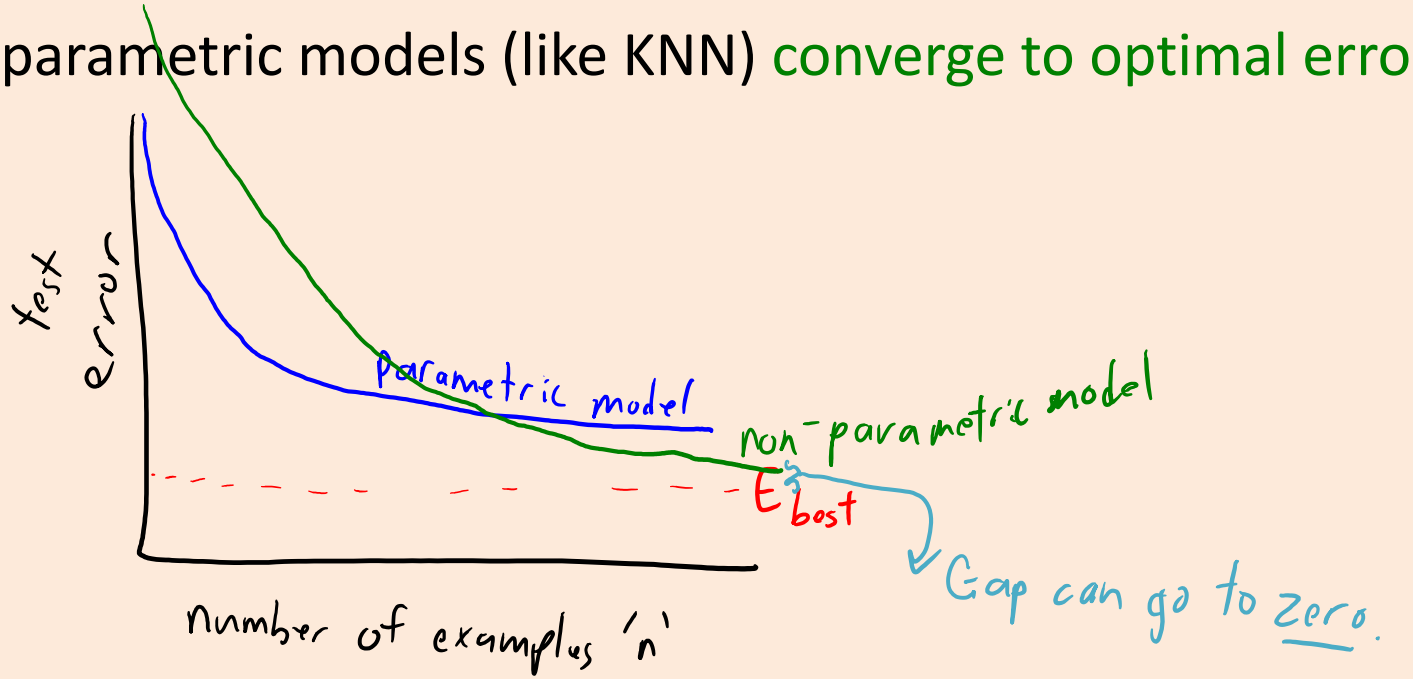
Parametric vs. Non-Parametric Models

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



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.



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.

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

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.

- Next Time:
  - Fighting the fundamental trade-off and Microsoft Kinect.

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 $(y_i = c)$.

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$n_1 = 6$

$n_0 = 4$

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 $\frac{n_c}{n}$.

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

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

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

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 $(y_i = c, x_{ij} = k)$

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

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

$n_{121} = 4$

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

Naïve Bayes Training Phase

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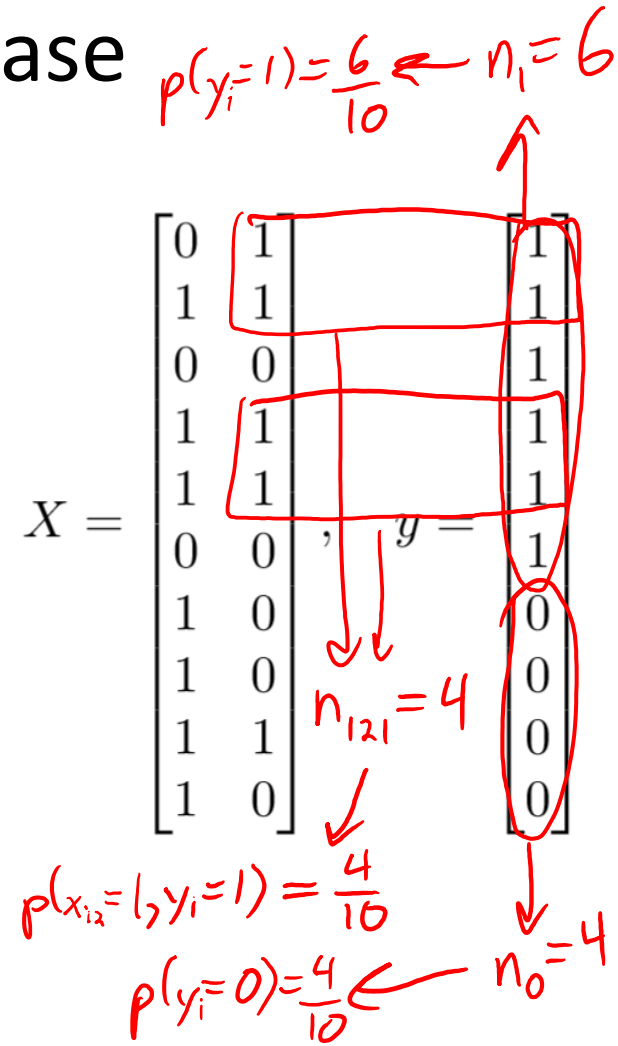
3. Set n_{cjk} as the number of times $(y_i = c, x_{ij} = k)$
4. Estimate $p(x_{ij} = k, y_i = c)$ as $\frac{n_{cjk}}{n}$

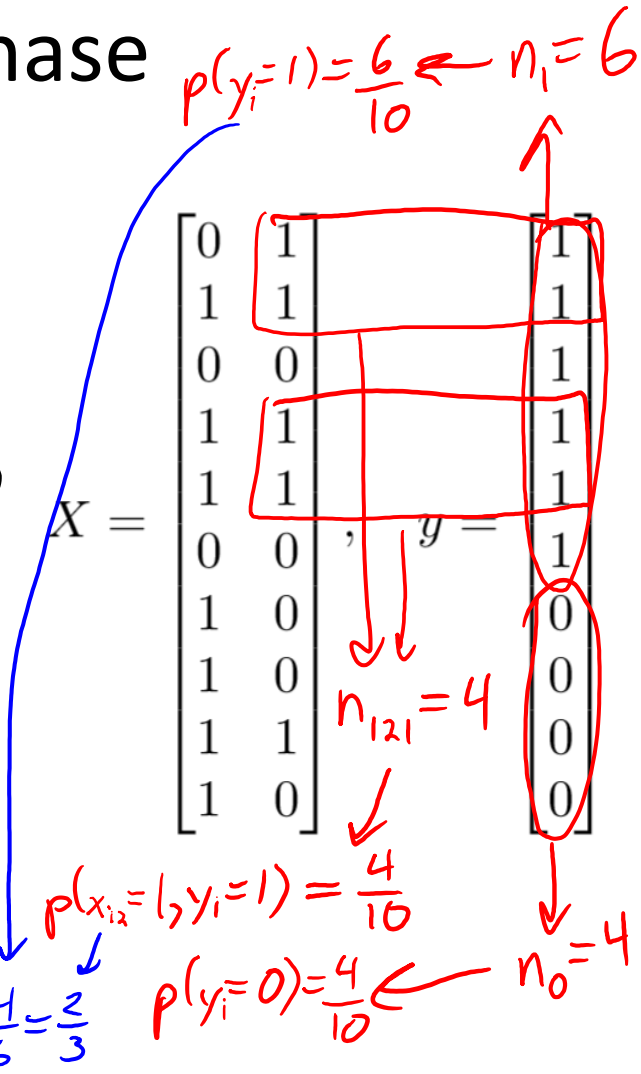


Naïve Bayes Training Phase

- 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 $p(x_{ij} = k \mid y_i = c) = \frac{p(x_{ij} = k, y_i = c)}{p(y_i = c)}$

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



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 $\longrightarrow$

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

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

Naïve Bayes Prediction Phase

- Prediction in a naïve Bayes model:

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

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

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

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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 $p(\tilde{x}_i)$)

"Proportional to" for Probabilities

- When we say "p(y) ∝ exp(-y^2)" for a function 'p', we mean:

$$p(y) = \beta \exp(-y^2) \quad \text{for some constant } \beta.$$

- 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

- 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.

Avoiding Underflow

- During the prediction, the probability can underflow:

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

All these are < 1 so the product gets very small!

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

Rember that $\log(ab) = \log(a) + \log(b)$ so $\log\left(\prod_i a_i\right) = \sum_i \log(a_i)$

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

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

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.

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:

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

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

$$= \sum_{c=1}^{K} \left[\prod_{j=1}^{d} p(x_{ij} \mid y=c) \right] p(y=c) \qquad \text{(naive Bayes assumption)}$$

These are the quantities we compute during training.

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".

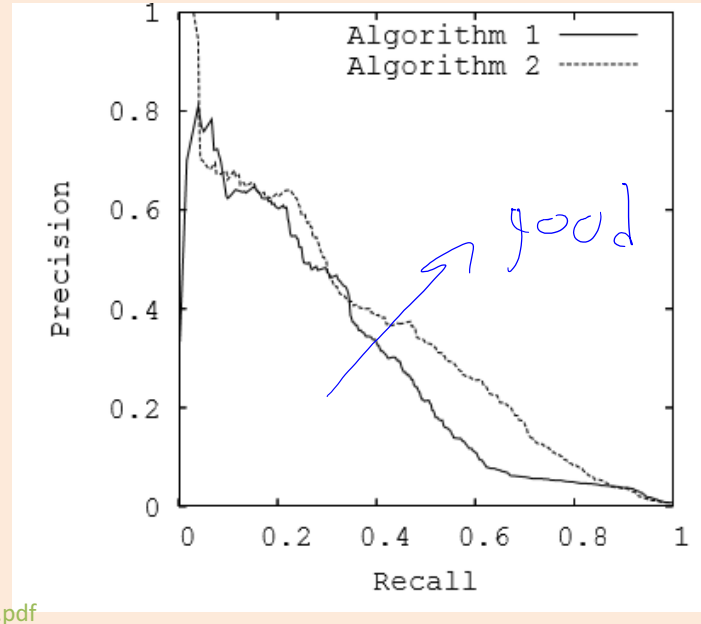
Other Performance Measures

- 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.

Precision-Recall Curve

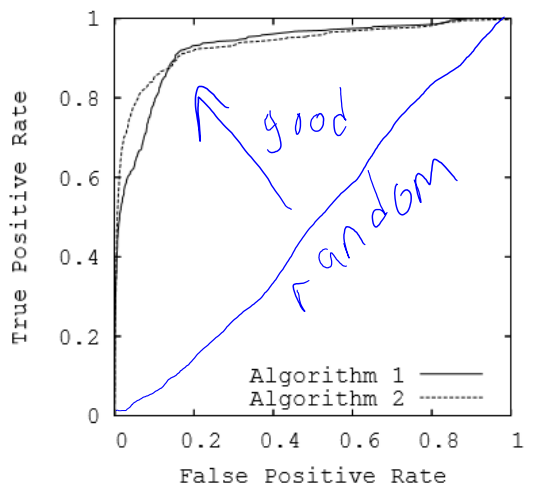
- Consider the rule $p(y_i = \text{'spam'} \mid x_i) > t$, for threshold 't'.
- Precision-recall (PR) curve plots precision vs. recall as 't' varies.



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

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

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.

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

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 slightly faster using fast matrix multiplication:
  - Let D be a matrix such that D_{ij} contains:

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

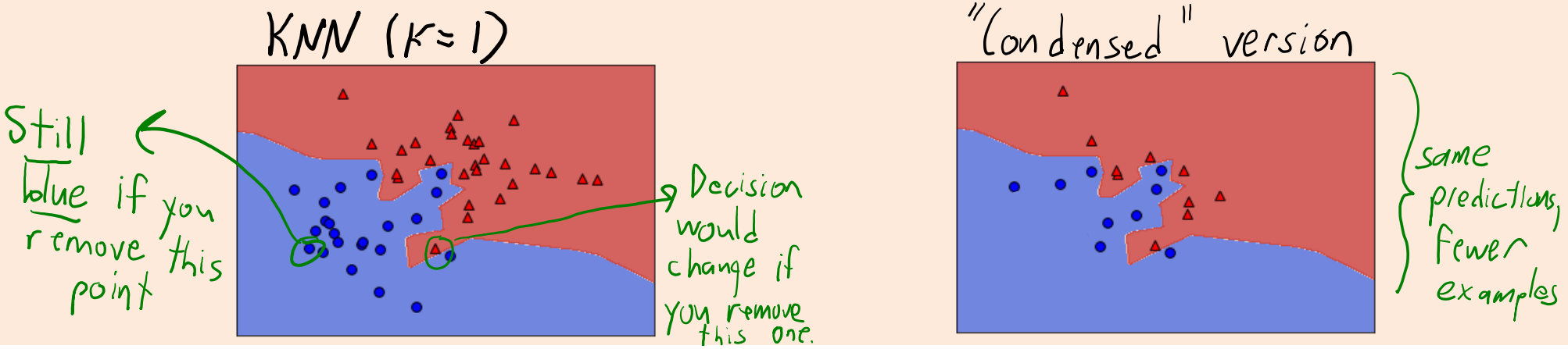
    where 'i' is a training example and 'j' is a test example.
  - We can compute D in Julia using:

```
X1.^2*ones(d,t) .+ ones(n,d)*(X2').^2 .- 2X1*X2'
```

  - And you get an extra boost because Julia uses multiple cores.

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).



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’).

Condensed Nearest Neighbours

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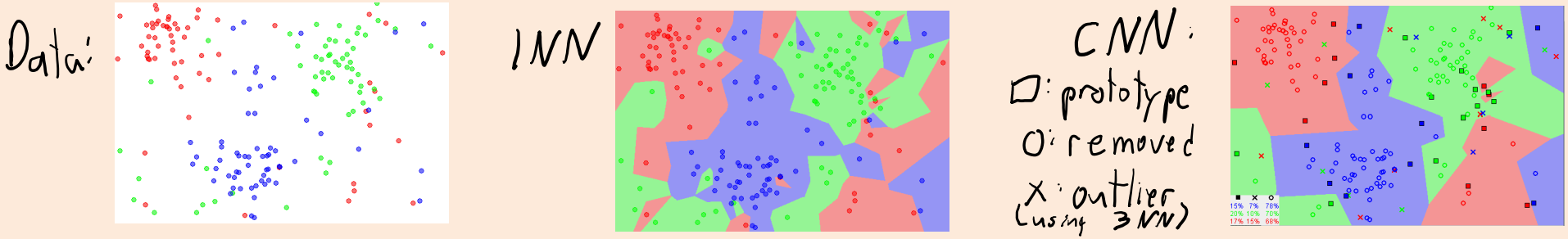

- Recent work shows that finding optimal compression is NP-hard.
  - An approximation algorithm algorithm was published in 2018:
    - "Near optimal sample compression for nearest neighbors"

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