CPSC 340: Machine Learning and Data Mining

Non-Parametric Models

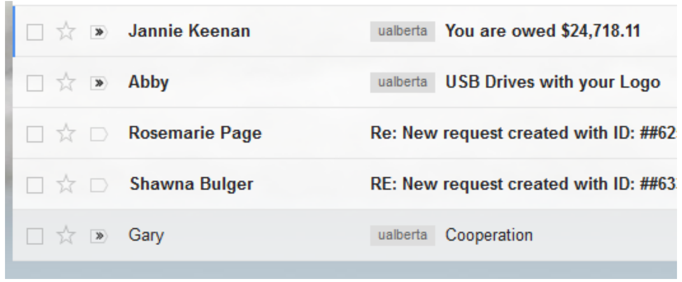
Fall 2016

Admin

- Assignment 0:
  - 1 late day to hand it in tonight, 2 late days for Wednesday.
- Assignment 1 is out:
  - Due Friday of next week. It’s long so start early.

- Add/drop deadline is tomorrow.

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:

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

- 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.

Laplace Smoothing

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

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

  – Problem if you have no spam messages with lactase:
    - p('lactase' | 'spam') = 0, and message automatically gets through filter.

  – Common fix is Laplace smoothing estimate:
    - Add 1 to numerator, and add 1 for each possible label to denominator.

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

    - A common variation is to use a different number β rather than 1.

Decision Theory

- Are we equally concerned about “spam” vs. “not spam”?
- True positives, false positives, false negatives, false 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 yhat minimizing expectated cost:

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

- Even if "spam" has a higher probability, predicting "spam" might have a higher cost.

Decision Theory Example

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

- If for a test example we have p($\tilde{y}_i$ = “spam” | $\tilde{y}_i$) = 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

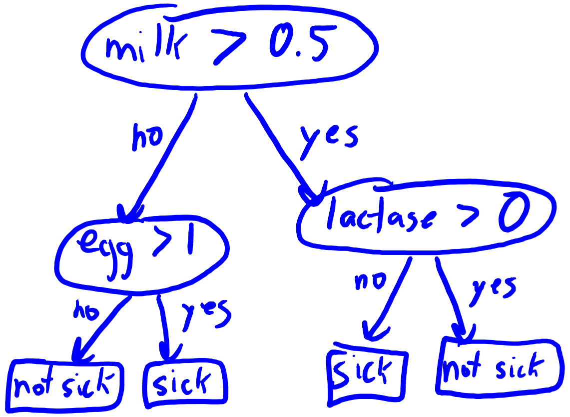
- In other applications, the costs could be different.
  - In cancer screening, maybe false positives are ok,
    but don't want to miss false negatives.

- 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 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 (text).

Parametric vs. Non-Parametric

- Decision trees and naïve Bayes are often not very accurate.
  - Greedy rules or conditional independence might be bad assumptions.
  - They are also parametric models.

Parametric vs. Non-Parametric

- Parametric models:
  - Have a fixed number of parameters: size of "model" is O(1) in terms 'n'.
    - E.g., fixed-depth decision tree just stores rules.
    - E.g., naïve Bayes just stores counts.
  - 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., decision tree whose depth *grows with the number of examples*.

K-Nearest Neighbours (KNN)

- Classical non-parametric classifier is k-nearest neighbours (KNN).
- To classify an object $\tilde{x}_i$:
  1. Find the ‘k’ training examples x_i that are “nearest” to $\tilde{x}_i$.
  2. Classify using the most common label of “nearest” 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

X

Sick?
1
1
0
1
1

y

Egg	Milk	Fish
0.3	0.6	0.8

$\tilde{X}_i$

Sick?
?

$\tilde{y}_i$

3 "nearest" neighbours

most common label is "sick"

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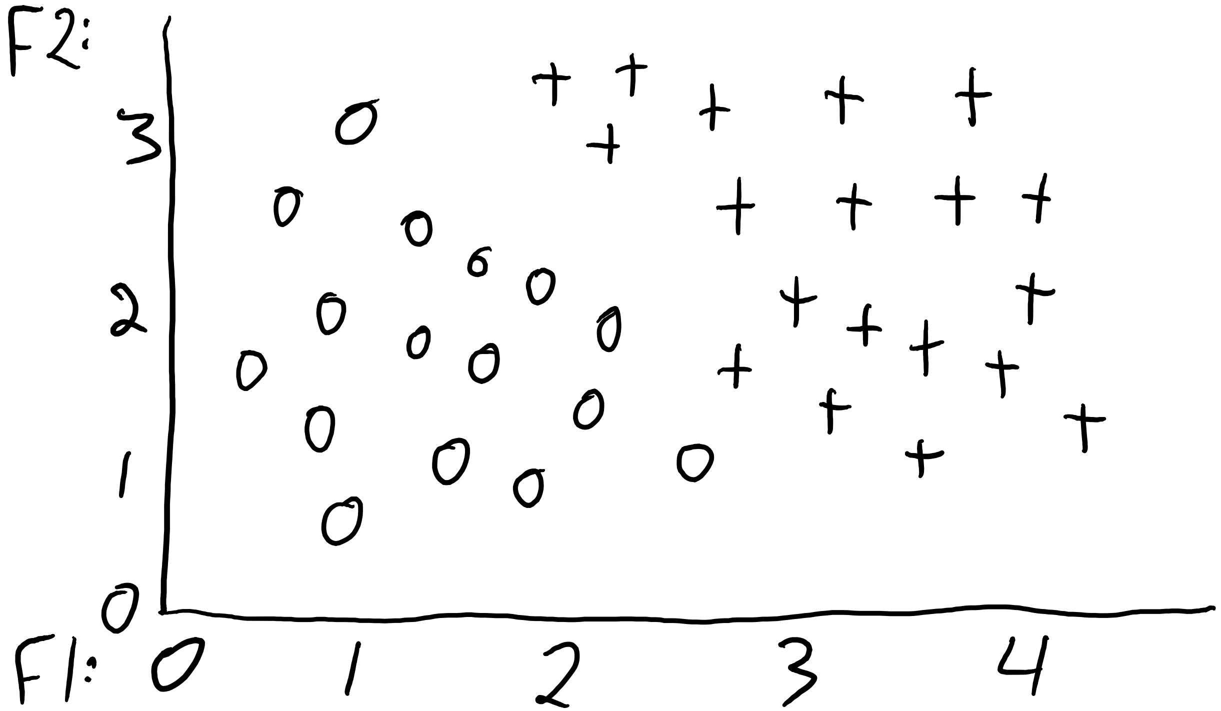
F1	F2		Label
1	3	→	O
2	3	→	+
3	2	→	+
2.5	1	→	O
3.5	1	→	+
…	…		…



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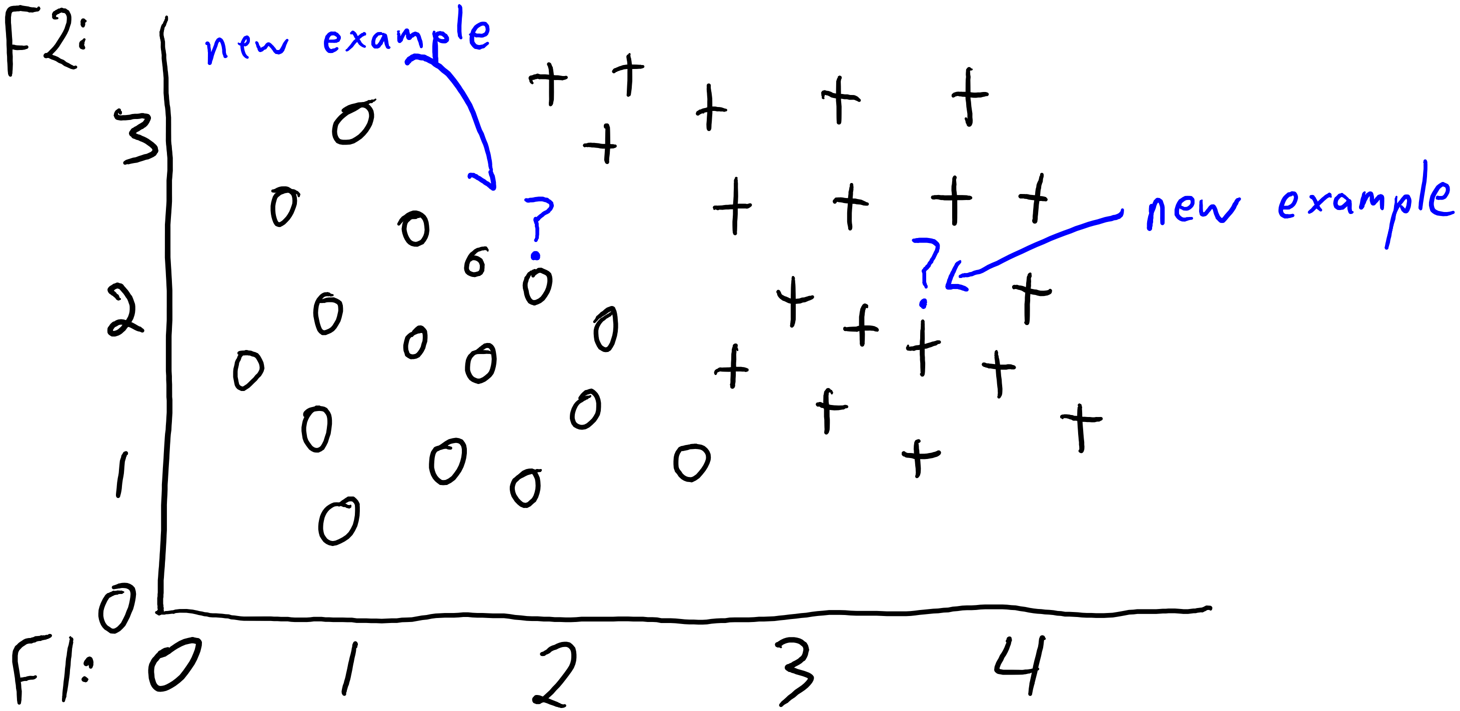

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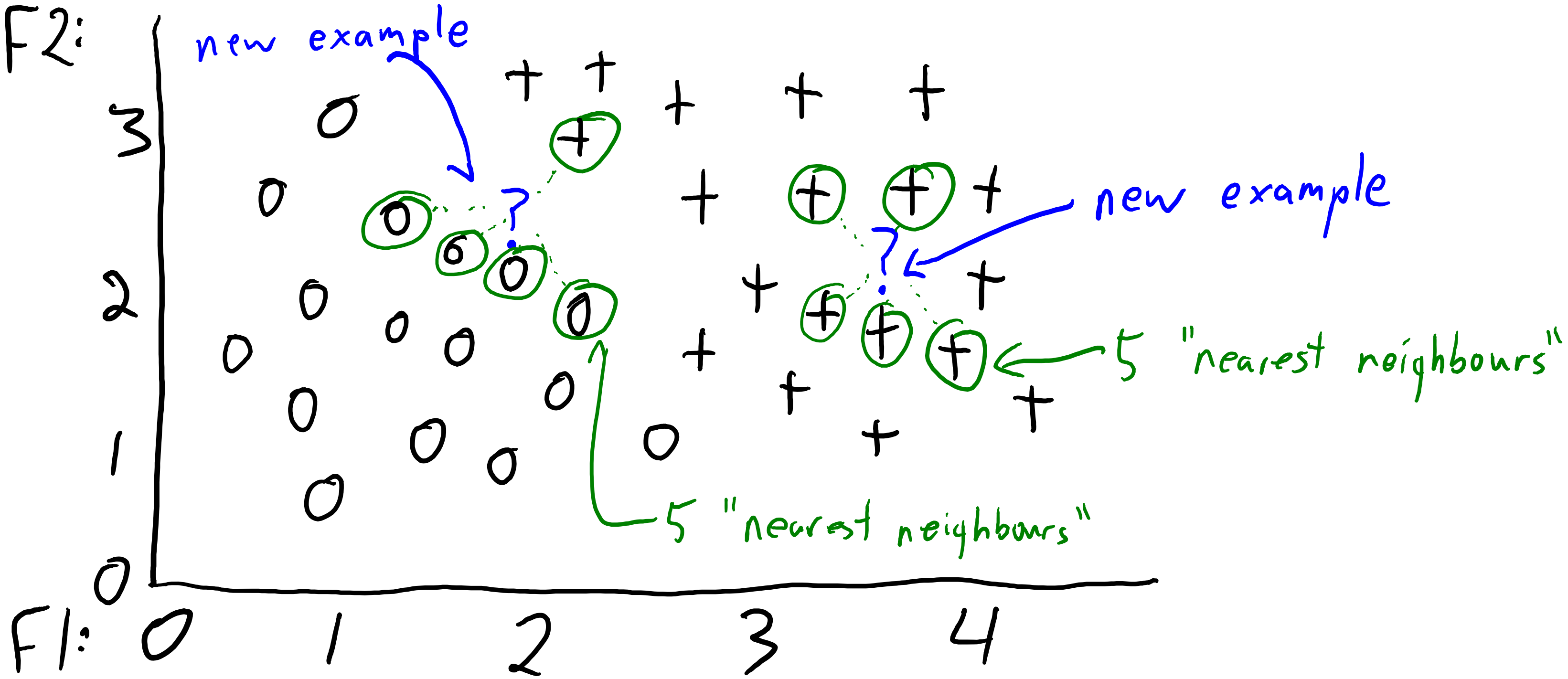
3.5	1
…	…

Label
O
+
+
O
+
…



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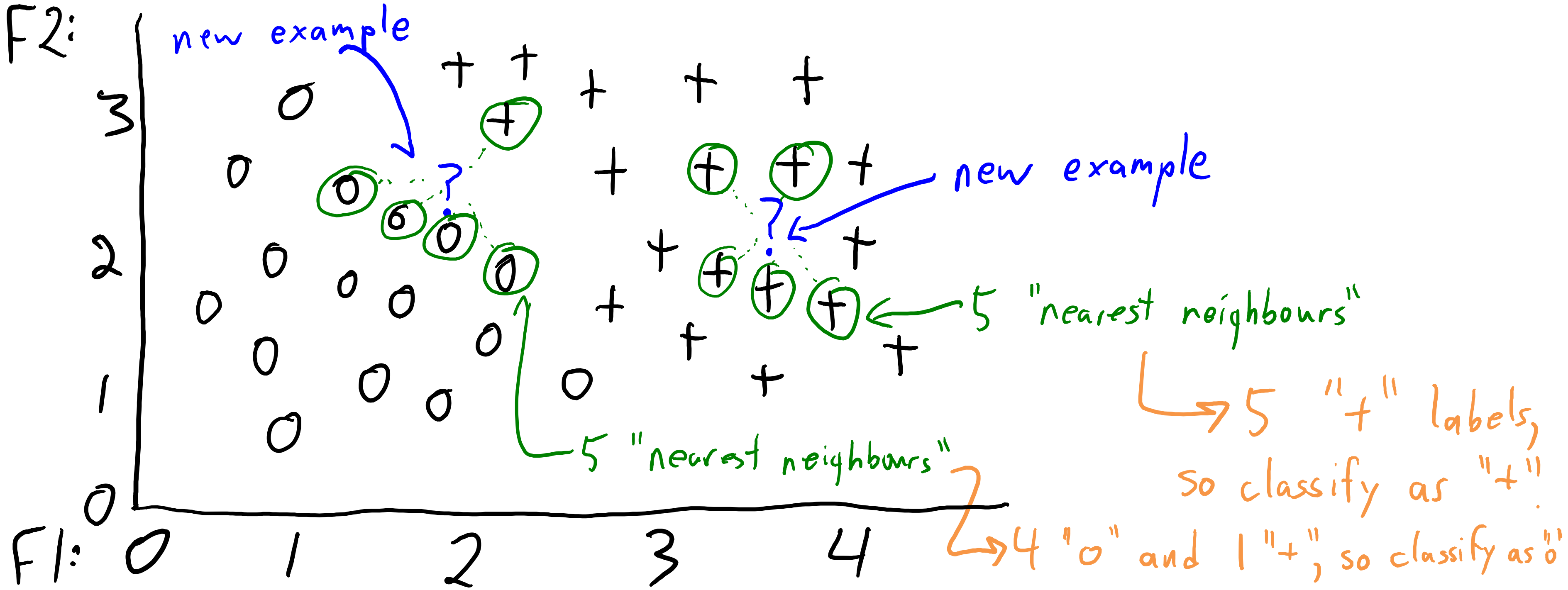
…	…	…



K-Nearest Neighbours (KNN)

- 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 '$\tilde{\imath}$'.
- Assumption:
  – Objects with similar features likely have similar labels.

- With a small 'n', KNN model will be very simple.
- Model gets more complicated as 'n' increases.
  – Starts to detect subtle differences between examples.

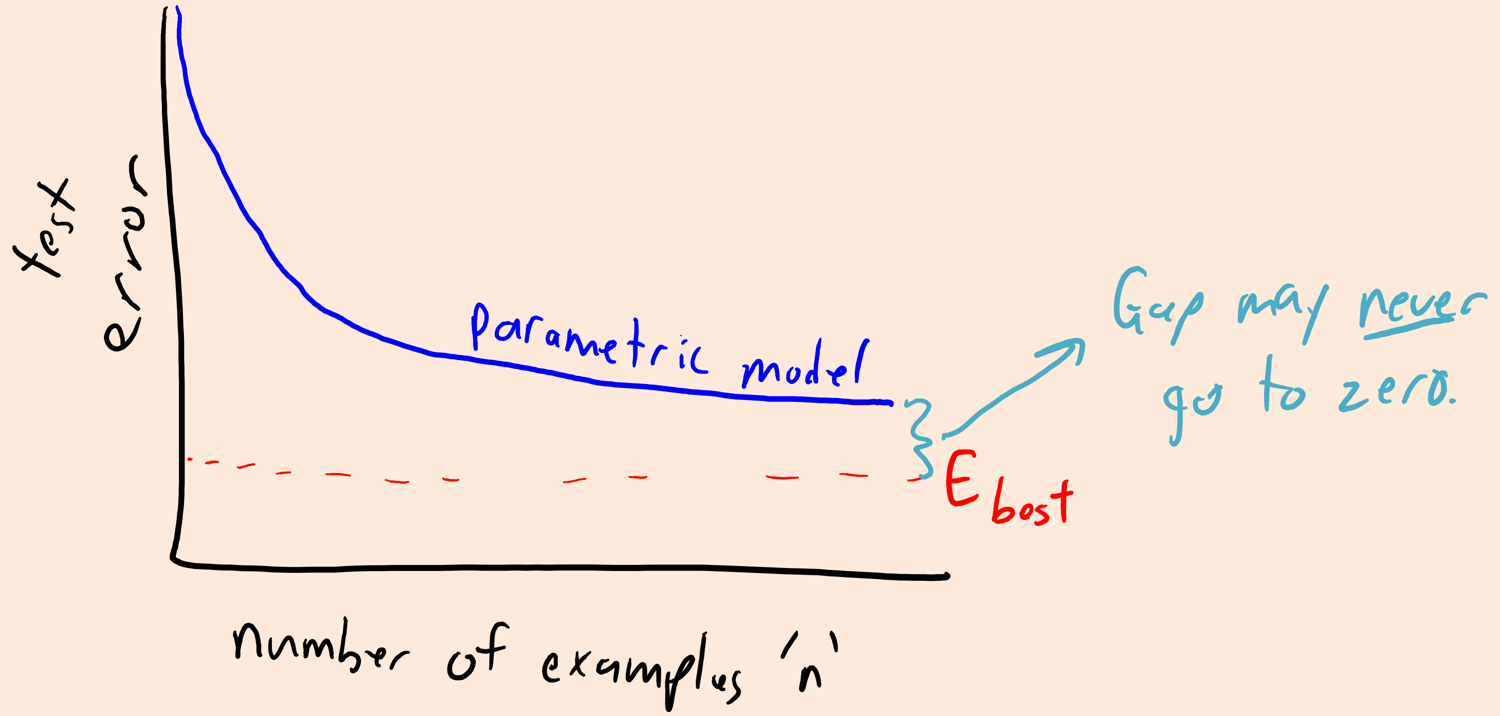
Consistency of KNN

- 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.
    - 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



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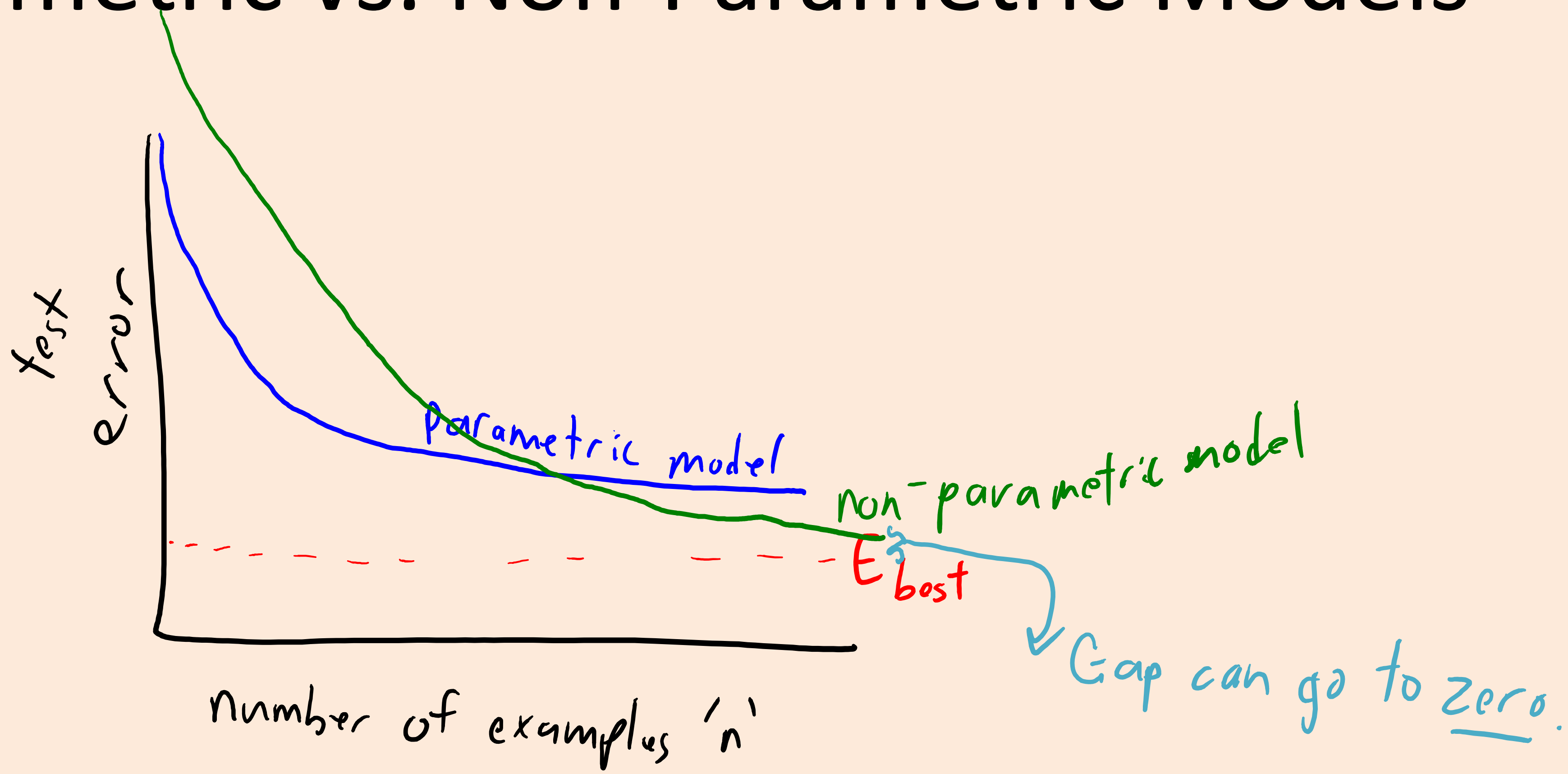


Curse of Dimensionality

- "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.

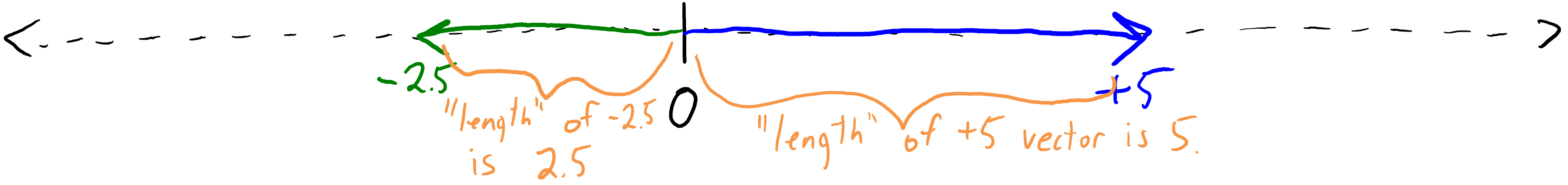
- Nevertheless, KNN is really easy to use and often hard to beat!

KNN Implementation

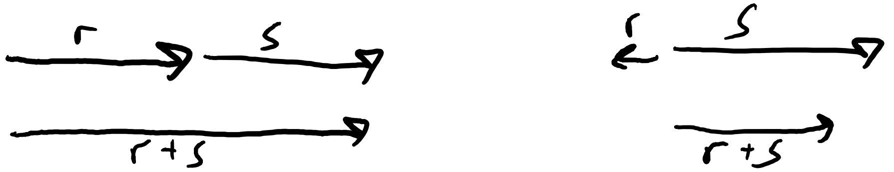
- There is no training phase in KNN ("lazy" learning).
  - You just store the training data.
  - Non-parametric because the size of the model is O(nd).
- But predictions are expensive: O(nd) to classify 1 test object.
  - Tons of work on reducing this cost (we'll discuss this later).
- There are also alternatives to Euclidean distance…

Norms in 1-Dimension

- We can view absolute value, $|r|$, as 'size' or 'length' of a number 'r':



- It satisfies three intuitive properties of 'length':
  1. Only '0' has a 'length' of zero.
  2. Multiplying 'r' by constant 'α' multiplies length by $|\alpha|$: $|\alpha r| = |\alpha||r|$.
     - "If be will twice as long if you multiply by 2".
  3. Length of 'r+s' is not more than length of 'r' plus length of 's':
     - "You can't get there faster by a detour".
     - "Triangle inequality": $|r + s| <= |r| + |s|$.

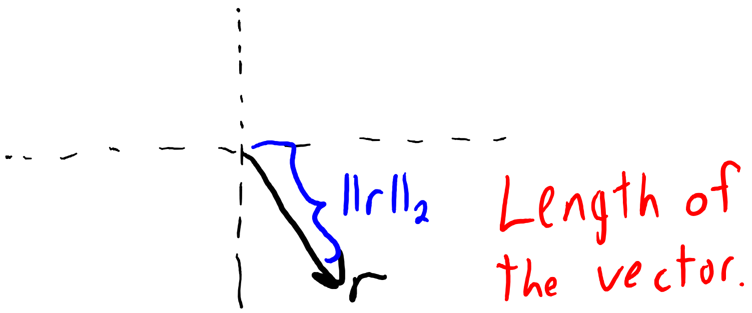


Norms in 2-Dimensions

- In 1-dimension, only scaled absolute values satisfy the 3 properties.
- In 2-dimensions, there is no unique function satisfying them.
- We call any function satisfying them a norm:
  - Measures of “size” or “length” in 2-dimensions.
- Three most common examples:

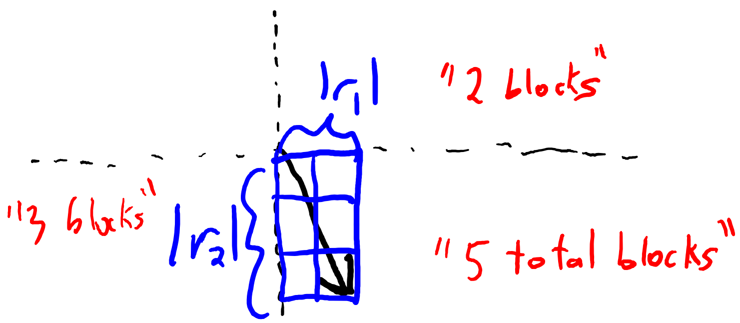
L_2 or "Euclidean" norm.

$\|r\|_2 = \sqrt{r_1^2 + r_2^2}$



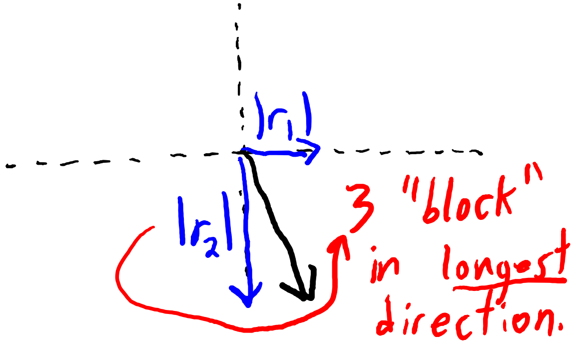
L_1 or "Manhattan" norm:

$\|r\|_1 = |r_1| + |r_2|$



L_∞ or "max" norm:

$\|r\|_\infty = \max\{|r_1|, |r_2|\}$



Norms as Measures of Distance

- By taking norm of difference, we get a "distance" between vectors:

$$\|r - s\|_2 = \sqrt{(r_1 - s_1)^2 + (r_2 - s_2)^2}$$

$= \|r - s\|$ "Euclidean distance"

$$\|r - s\|_1 = |r_1 - s_1| + |r_2 - s_2|$$

"Number of blocks you need to walk to get from r to s."

$$\|r - s\|_\infty = \max\{|r_1 - s_1|, |r_2 - s_2|\}$$

"Most number of blocks in any direction you would have to walk."

[Infinite Series Video]

Norms in d-Dimensions

- We can generalize these common norms to d-dimensional vectors:

L_2: $\|r\|_2 = \sqrt{\sum_{j=1}^{d} r_j^2}$

L_1: $\|r\|_1 = \sum_{j=1}^{d} |r_j|$

L_∞: $\max_j \{|r_j|\}$

E.g., in 3-dimensions:

$\|r\|_2 = \sqrt{r_1^2 + r_2^2 + r_3^2}$

in 4-dimensions:

$\|r\|_2 = \sqrt{r_1^2 + r_2^2 + r_3^2 + r_4^2}$

Notation: $\|r\|_2^2 = (\|r\|_2)^2$

$= \left(\sqrt{\sum_{j=1}^{d} r_j^2}\right)^2$

$= \sum_{j=1}^{d} r_j^2$

$= r^T r$

Different ways to write the same thing

- These norms place different "weights" on large values:
  - L_1: all values are equal.
  - L_2: bigger values are more important (because of squaring).
  - L_∞: only biggest value is important.

KNN Distance Functions

- Most common KNN distance functions: norm($x_i - x_j$).
  - L1-, L2-, and Linf-norm.
  - Weighted norms (if some features are more important): $\sum_{j=1}^{d} v_j |x_j|$
    "weight" of feature 'j'
  - "Mahalanobis" distance (takes into account correlations).

- But we can consider other distance/similarity functions:
  - Hamming distance.
  - Jaccard similarity (if x_i are sets).
  - Edit distance (if x_i are strings).
  - Metric learning (*learn* the best distance function).

Summary

- Decision theory allows us to consider costs of predictions.
- Non-parametric models grow with number of training examples.
- K-Nearest Neighbours: simple non-parametric classifier.
  - Appealing “consistency” properties.
  - Suffers from high prediction cost and curse of dimensionality.

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

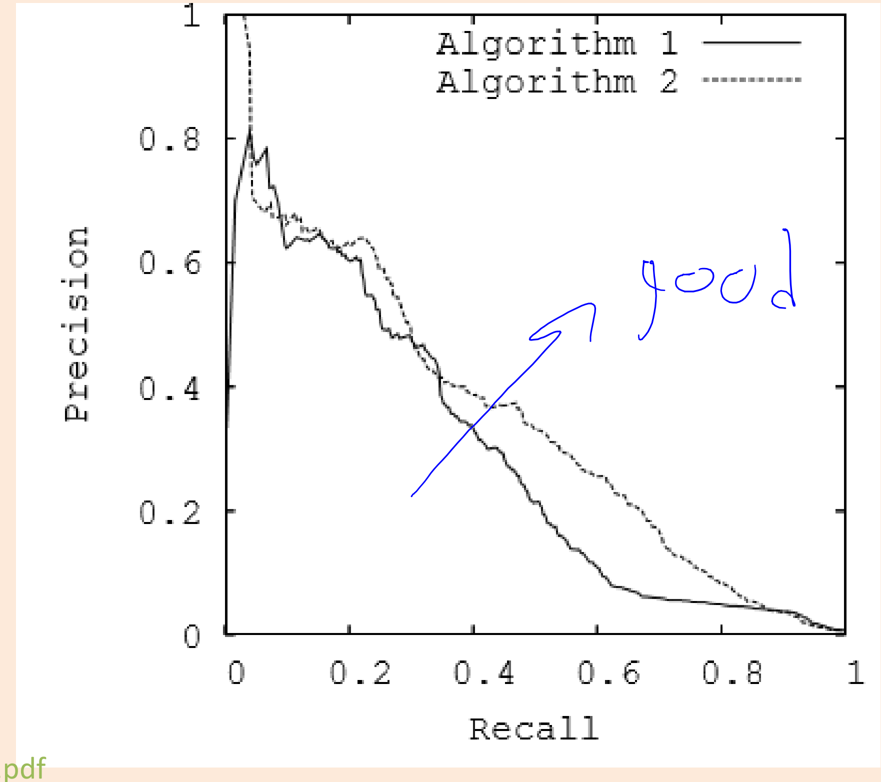
Other Performance Measures

- 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.

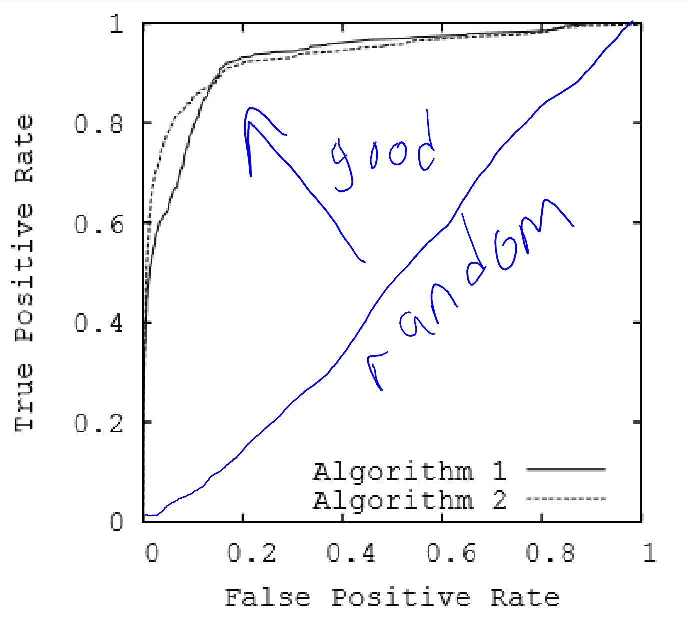


http://pages.cs.wisc.edu/~jdavis/davisgoadrichcamera2.pdf

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.

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:

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

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

```
D = X.^2*ones(d,t) + ones(n,d)*(Xtest').^2 - 2*X*Xtest';
```

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

Squared/Euclidean-Norm Notation

We're using the following conventions:

The subscript after the norm is used to denote the p-norm, as in these examples:

$$\|x\|_2 = \sqrt{\sum_{j=1}^{d} w_j^2}.$$
$$\|x\|_1 = \sum_{j=1}^{d} |w_j|.$$

If the subscript is omitted, we mean the 2-norm:

$$\|x\| = \|x\|_2.$$

If we want to talk about the *squared* value of the norm we use a superscript of "2":

$$\|x\|_2^2 = \sum_{j=1}^{d} w_j^2.$$
$$\|x\|_1^2 = \left(\sum_{j=1}^{d} |w_j|\right)^2.$$

If we omit the subscript and have a superscript of "2", we're taking about the squared L2-norm:

$$\|x\|^2 = \sum_{j=1}^{d} w_j^2.$$

Lp-norms

- The L_1-, L_2-, and L_∞-norms are special cases of Lp-norms:

$$\|x\|_p = \left(\sum_{j=1}^{d} x_j^p\right)^{1/p}$$

- This gives a norm for any (real-valued) $p \geq 1$.
  - The L_∞-norm is limit as 'p' goes to ∞.

- For $p < 1$, not a norm because triangle inequality not satisfied.