CSE/STAT 416

Precision/Recall
k-Nearest Neighbors

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Reflection

Go to 9:50

Spend 10 minutes writing a reflection on a piece of paper

What did you learn ~~this~~ last week?

How does it relate to what we learned earlier in the quarter?

Hold on to papers til end

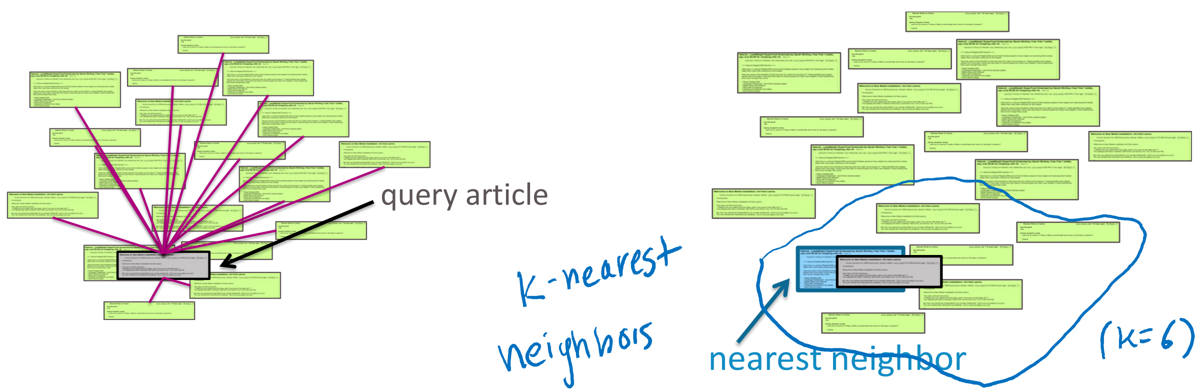
Roadmap

1. Housing Prices - Regression
   - Regression Model
   - Assessing Performance
   - Ridge Regression
   - LASSO
2. Sentiment Analysis – Classification
   - Classification Overview
   - Logistic Regression
   - Decision Trees
   - Ensemble Methods
3. Document Retrieval – Clustering and Similarity
   - Precision / Recall
   - k-Nearest Neighbor
   - Kernel Methods
   - Locality Sensitive Hashing
   - Clustering
   - Hierarchical Clustering

Document Retrieval

- Consider you had some time to read a book and wanted to find other books similar to that one.
- If we wanted to write an system to recommend books
  - How do we measure similarity?
  - How do we search over books?
  - How do we measure accuracy?

Big Idea: Define an **embedding** and a **similarity metric** for the books, and find the **"nearest neighbor"** to some query book.



Detecting Spam

Imagine I made a “Dummy Classifier” for detecting spam

- The classifier ignores the input, and always predicts spam.
- This actually results in 90% accuracy! Why?
  - Most emails are spam…

This is called the **majority class classifier.**

A classifier as simple as the majority class classifier can have a high accuracy if there is a **class imbalance**.

- A class imbalance is when one class appears much more frequently than another in the dataset

This might suggest that accuracy isn’t enough to tell us if a model is a good model.

Assessing Accuracy

Always digging in and ask critical questions of your accuracy.

- Is there a **class imbalance**?
- How does it compare to a baseline approach?
  - Random guessing
  - Majority class
  - ...
- Most important: **What does my application need?**
  - What's good enough for user experience?
  - What is the impact of a mistake we make?

Confusion Matrix

For binary classification, there are only two types of mistakes

- $\hat{y} = +1, \;\; y = -1$
- $\hat{y} = -1, \;\; y = +1$

Generally we make a **confusion matrix** to understand mistakes.

		Predicted Label	
		+	−
True Label	+	True Positive (TP)	False Negative (FN)
	−	False Positive (FP)	True Negative (TN)

Confusion Matrix Example

		Predicted Label	
		+	−
True Label	+	True Positive (TP)	False Negative (FN)
	−	False Positive (FP)	True Negative (TN)

Binary Classification Measures

Notation

- $C_{TP} = \#\mathrm{TP}, \quad \mathrm{C_{FP}} = \#\mathrm{FP}, \quad \mathrm{C_{TN}} = \#\mathrm{TN}, \quad \mathrm{C_{FN}} = \#\mathrm{FN}$
- $N = C_{TP} + C_{FP} + C_{TN} + C_{FN}$
- $N_P = C_{TP} + \cancel{C_{FP}}, \quad N_N = C_{FP} + C_{TN}$

C_{FN}

Error Rate

$$\frac{C_{FP} + C_{FN}}{N}$$

Accuracy Rate

$$\frac{C_{TP} + C_{TN}}{N}$$

False Positive rate (FPR)

$$\frac{C_{FP}}{N_N}$$

False Negative Rate (FNR)

$$\frac{C_{FN}}{N_P}$$

True Positive Rate or Recall

$$\frac{T_P}{N_P}$$

Precision

$$\frac{T_P}{C_{TP} + C_{FP}}$$

F1-Score

$$2\,\frac{Precision \cdot Recall}{Precison + Recall}$$

[See more!]

Assessing Accuracy

Often with binary classification, we treat the positive label as being the more important of the two. We then often then focus on these metrics:

Precision: Of the ones I predicted positive, how many of them were actually positive?

Recall: Of all the things that are truly positive, how many of them did I correctly predict as positive?

Precision

What fraction of the examples I predicted positive were correct?

Sentences predicted to be positive:

$\hat{y}_i = +1$

- Easily best sushi in Seattle. ✓
- The seaweed salad was just OK, vegetable salad was just ordinary. ✗
- I like the interior decoration and the blackboard menu on the wall. ✓
- The service is somewhat hectic. ✗
- The sushi was amazing, and the rice is just outstanding. ✓
- All the sushi was delicious. ✓

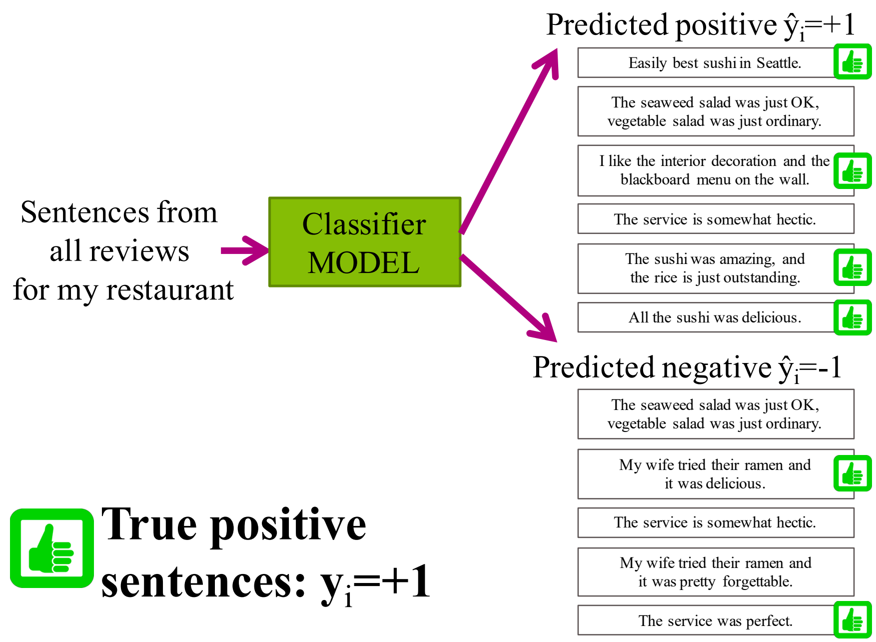
Only 4 out of 6 sentences predicted to be **positive** are actually **positive**

$$precision = \frac{C_{TP}}{C_{TP} + C_{FP}} = \frac{4}{4+2} = \frac{2}{3}$$

num pred. positive

Recall

Of the truly positive examples, how many were predicted positive?



$$recall = \frac{C_{TP}}{N_P} = \frac{C_{TP}}{C_{TP} + C_{FN}} = \frac{4}{4+2} = 2/3$$

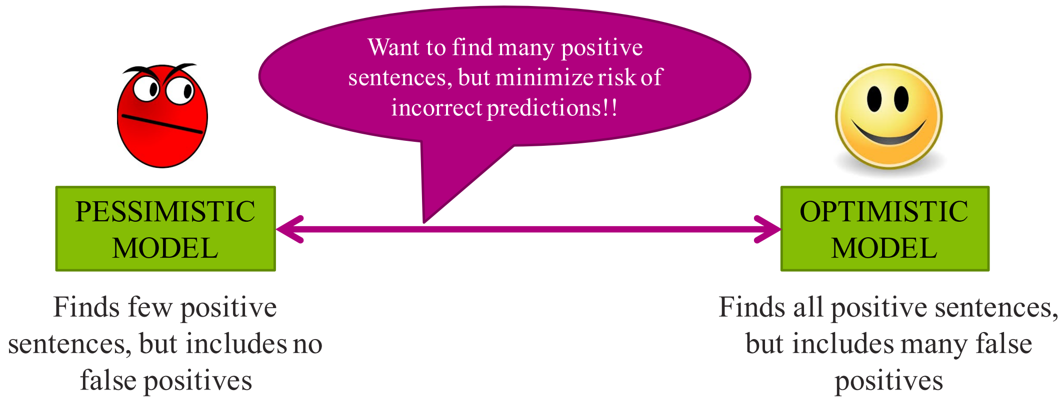
Precision & Recall

An optimistic model will predict almost everything as positive

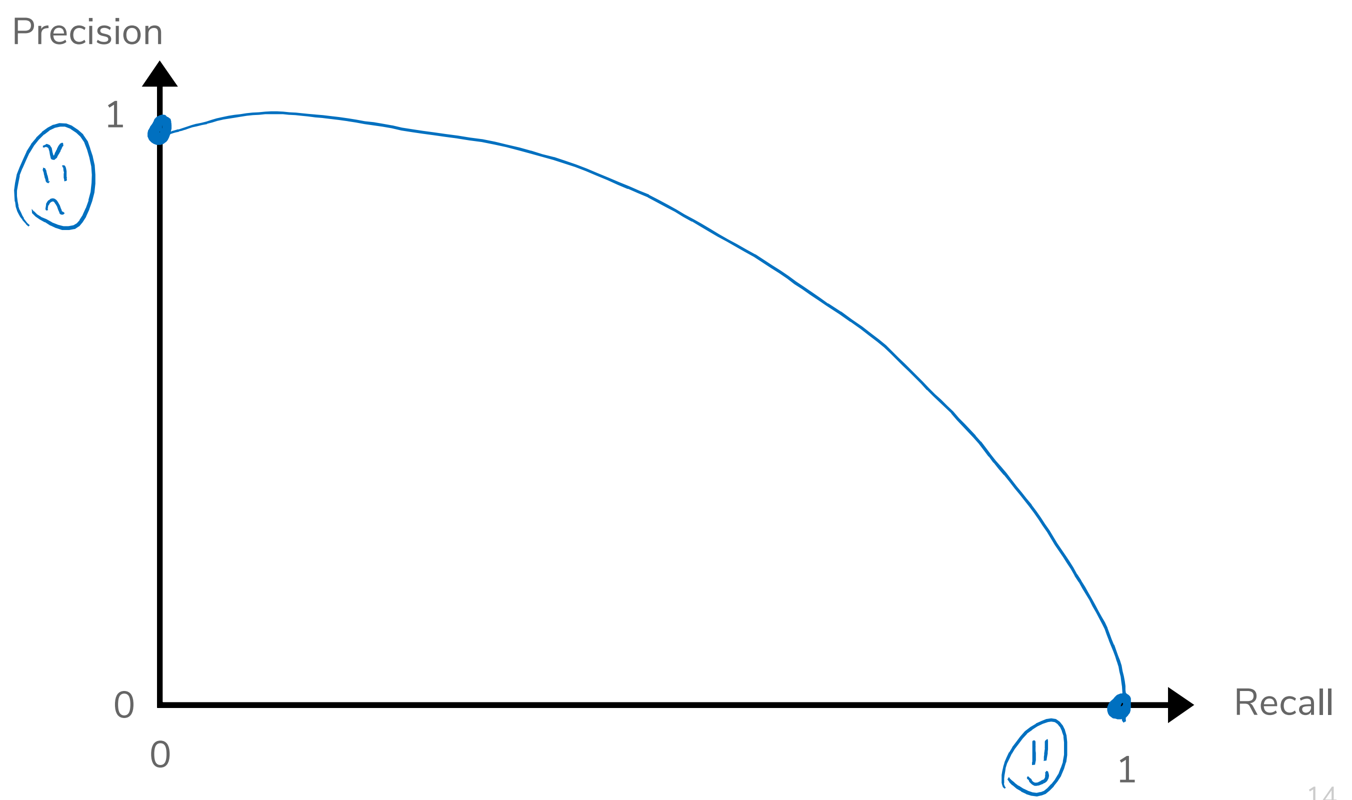
- High recall, low precision

A pessimistic model will predict almost everything as negative

- High precision, low recall



Precision-Recall Curve



Controlling Precision/Recall

Depending on your application, precision or recall might be more important

- Ideally you will have high values for both, but generally increasing recall will decrease precision and vice versa.

For logistic regression, we can control for how optimistic the model is by changing the threshold for positive classification

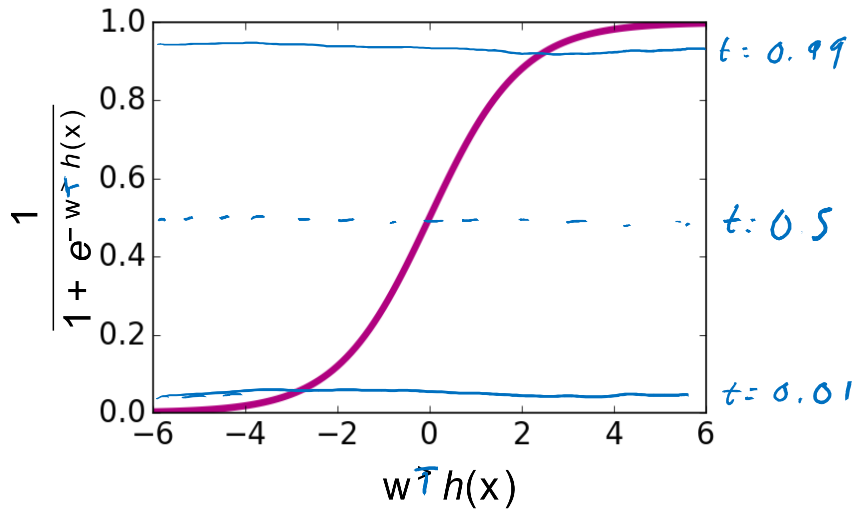
Before

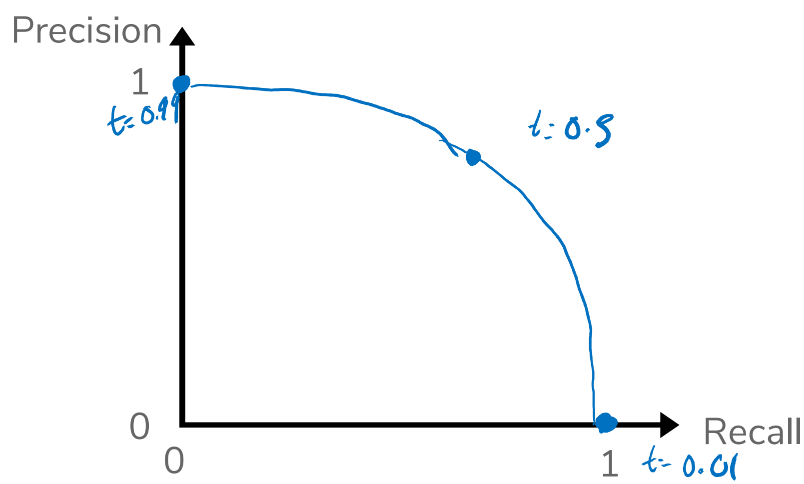
$\hat{y}_i = +1$ if $\hat{P}(y = +1|x_i) > 0.5$ else $\hat{y}_i = -1$

Now

$\hat{y}_i = +1$ if $\hat{P}(y = +1|x_i) > t$ else $\hat{y}_i = -1$

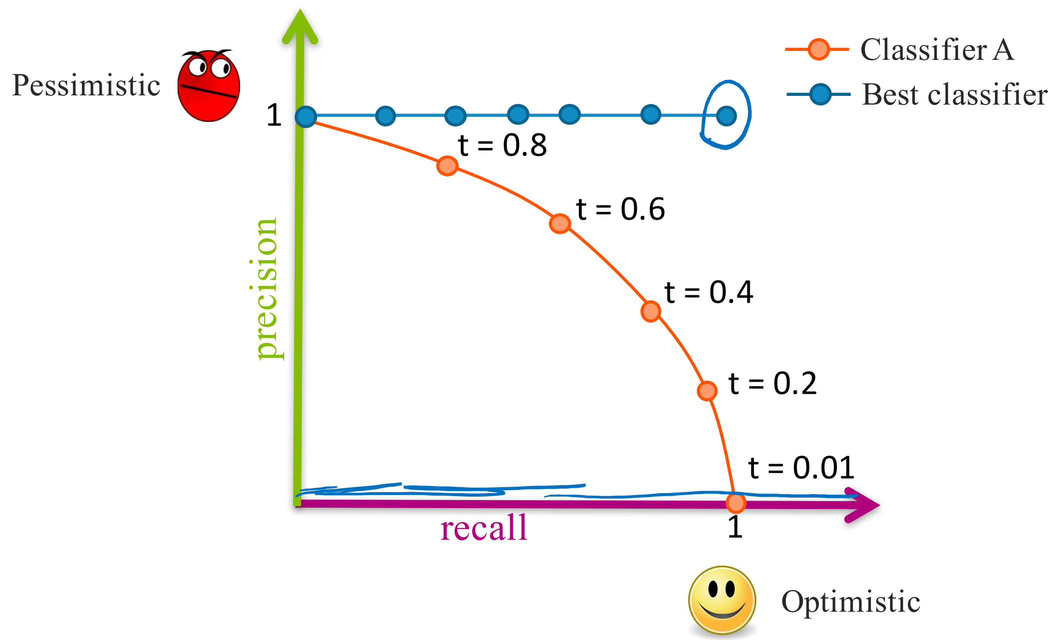
Precision-Recall Tradeoff





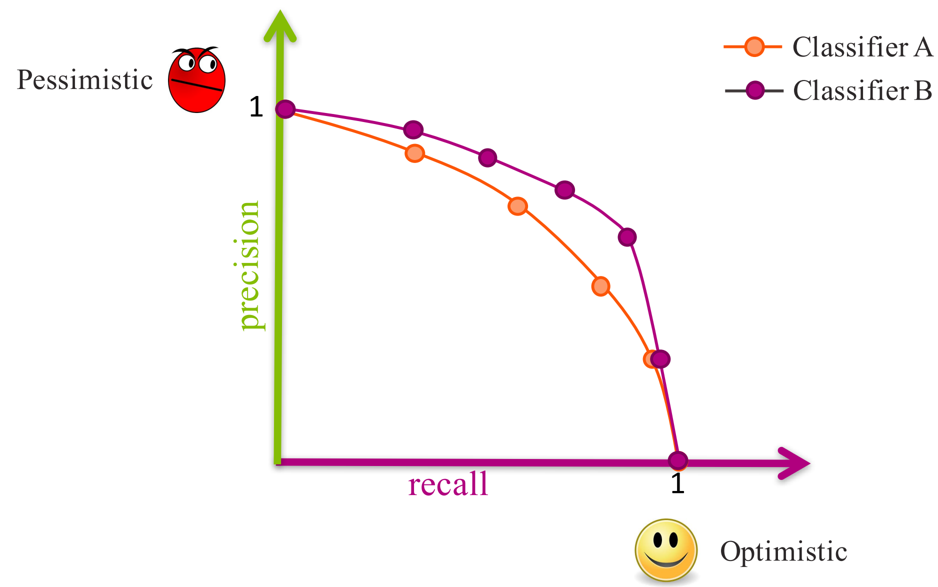
Precision-Recall Curve

Can try every threshold to get a curve like below



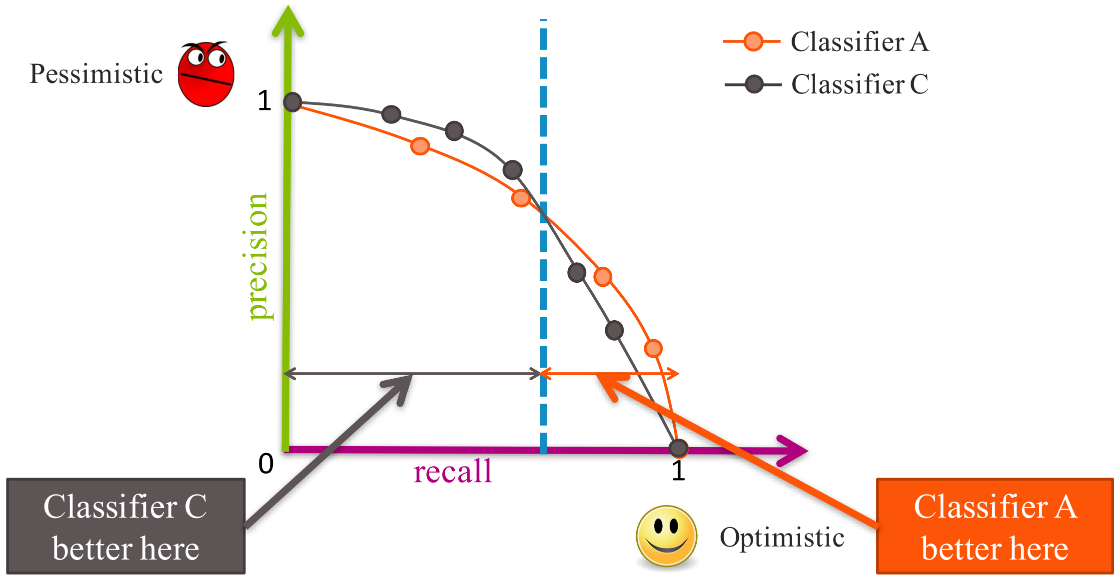
Precision-Recall Curve

Sometimes, Classifier B is strictly better than Classifier A



Precision-Recall Curve

Most times, the classifiers are incomparable



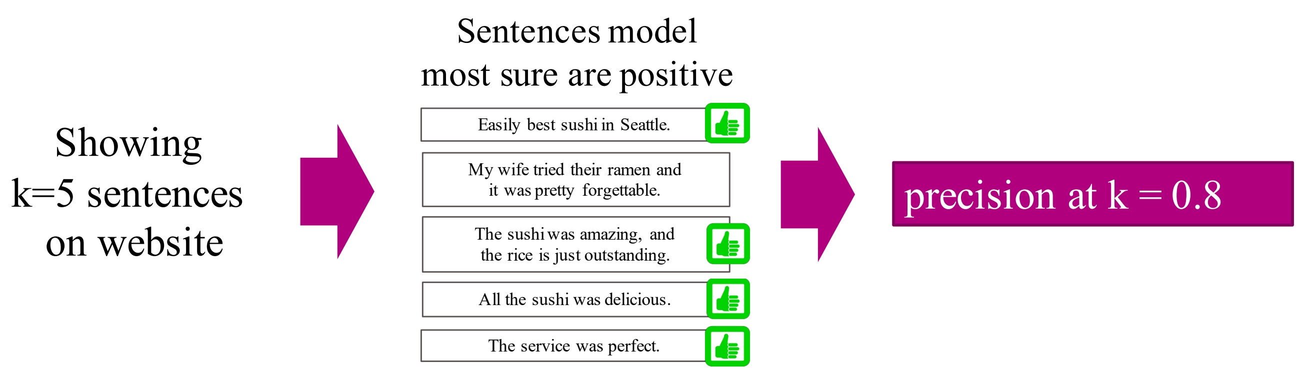
Compare Classifiers

Often come up with a single number to describe it

- F1-score, AUC, etc.
- Remember, what your application needs is most important

Also common to use **precision at k**

- If you show the top **k** most likely positive examples, how many of them are true positives



Poll Everywhere

Think

1 min

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A model with high bias will have high precision and low recall.

- True
- False

Poll Everywhere

Pair

2 min

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A model with high bias will have high precision and low recall.

- True
- False

2:00

Brain Break

10:53

Nearest Neighbors

1-Nearest Neighbor

Input

- x_q: Query example (e.g. my book)
- $x_1, \ldots, x_n$: Corpus of documents (e.g. Amazon books)

Output

- The document in corpus that is most similar to x_q

$$x^{NN} = \underset{x_i \in [x_1, \ldots, x_n]}{\arg\min}\ distance(x_q, x_i)$$

It's very critical to properly define how we represent each document x_i and the similarity metric $distance$! Different definitions will lead to very different results.

1-Nearest Neighbor

Runtime: $\mathcal{O}(n)$

How long does it take to find the 1-NN? About n operations

Input: x_q

$x^{NN} = \emptyset$

$nn\_dist = \infty$

$for\ x_i \in [x_1, \dots, x_n]$:

    $dist = distance(x_q, x_i)$

    $if\ dist < nn\_dist$:

        $x^{NN} = x_i$

        $nn\_dist = dist$

Output: x^{NN}

k-Nearest Neighbors

Input

- x_q: Query example (e.g. my book)
- $x_1, \ldots, x_n$: Corpus of documents (e.g. Amazon books)

Output

- List of k documents most similar to x_q

Formally

$$X^{k\text{-}NN} = \{x^{NN_1}, x^{NN_2}, \ldots, x^{NN_k}\}$$

For all x_i <u>not</u> in $X^{k\text{-}NN}$

$$dist(x_i, x_q) \geq \max_{j \in [1,\ldots,k]} dist(x^{NN_j}, x_q)$$

k-Nearest Neighbors

Same idea as 1-NN algorithm, but maintain list of k-NN

Input: x_q

$X^{k-NN} = [x_1, \dots, x_k]$

$nn\_dists = [dist(x_1, x_q), dist(x_2, x_q), \dots, dist(x_k, x_q)]$

$for\ x_i \in [x_{k+1}, \dots, x_n]$:

$\quad dist = distance(x_q, x_i)$

$\quad if\ dist < \max(nn\_dists)$:

$\quad\quad remove\ largest\ dist\ from\ X^{k-NN}\ and\ nn\_dists$

$\quad\quad add\ x_i\ to\ X^{k-NN} and\ distance(x_q, x_i)\ to\ nn\_dists$

Output: X^{k-NN}

k-Nearest Neighbors

Can be used in many circumstances!

Retrieval

$$\text{Return } X^{k-NN}$$

Regression

$$\hat{y}_i = \frac{1}{k}\sum_{j=1}^{k} x^{NN_j}$$

Classification

$$\hat{y}_i = majority\_class(X^{k-NN})$$

Important Points

While the formalization of these algorithms are fairly tedious, the intuition is fairly simple. Find the 1 or k nearest neighbors to a given document and return those as the answer.

embedding / representation

This intuition relies on answering two important questions

- How do we represent the documents x_i?
- How do we measure the distance $distance(x_q, x_i)$?

distance metric

Document Representation

[# "I", # "love", # "dogs", # "cats"]

Like our previous ML algorithms, we will want to make a vector out of the document to represent it as a point in space.

Simplest representation is the **bag-of-words** representation.

- Each document will become a ~~W~~ D dimension vector where ~~W~~ D is the number of words in the entire corpus of documents
- The value of $x_i[j]$ will be the number of times word j appears in document i.
- This ignores order of words in the document, just the counts.

"I like dogs dogs" [1, 1, 2, 0]

"I like cats" [1, 1, 0, 1]

Bag of Words

Pros

- Very simple to describe
- Very simple to compute

Cons

- Common words like “the” and “a” dominate counts of uncommon words
- Often it’s the uncommon words that uniquely define a doc.

TF-IDF

docs w/ Obama = 4

$\log\left(\frac{1000000}{1+4}\right) \gg 0$

docs in corpus = 1,000,000

docs w/ "the" = 1,000,000

$\log\left(\frac{1000000}{1+1000000}\right) \approx 0$

Goal: Emphasize important words

- Appear frequently in the document (common locally)

Term frequency = | 22 | word counts |

"the"

- Appears rarely in the corpus (rare globally)

Inverse doc freq. = | 0 | $\log \frac{\text{\# docs}}{1 + \text{\# docs using word}}$ |

"the"

| 0 | tf * idf |

"the"

Do a pair-wise multiplication to compute the TF-IDF for each word

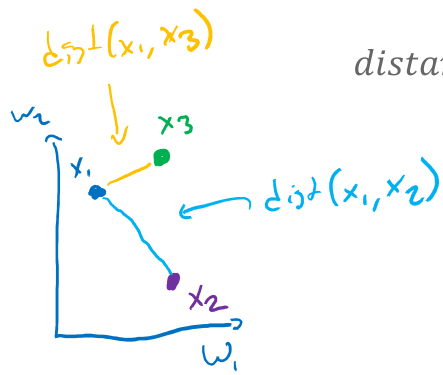
- Words that appear in every document will have a small IDF making the TF-IDF small!

Distance

Now we will define what similarity/distance means

Want to define how "close" two vectors are. A smaller value for distance means they are closer, a large value for distance means they are farther away.

The simplest way to define distance between vectors is the **Euclidean distance**

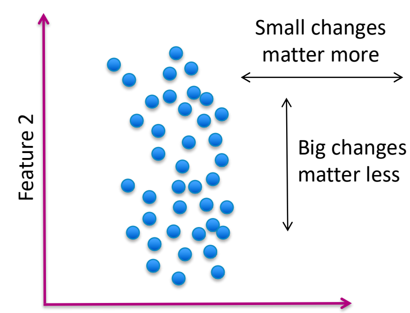


$$distance(x_i, x_q) = \left\| x_i - x_q \right\|_2$$

$$= \sqrt{\sum_{j=1}^{D} \left(x_i[j] - x_q[j]\right)^2}$$

Weighted Distances

Some features vary more than others or are measured in different units. We can weight different dimensions differently to make the distance metric more reasonable.



Specify weights as a function of feature spread

For feature j: $$\frac{1}{\max_i(x_i[j])-\min_i(x_i[j])} = a_j$$

Weighted Educlidean distance

$$distance(x_i, x_q) = \sqrt{\sum_{j=1}^{D} a_j^2 \left(x_i[j] - x_q[j]\right)^2}$$

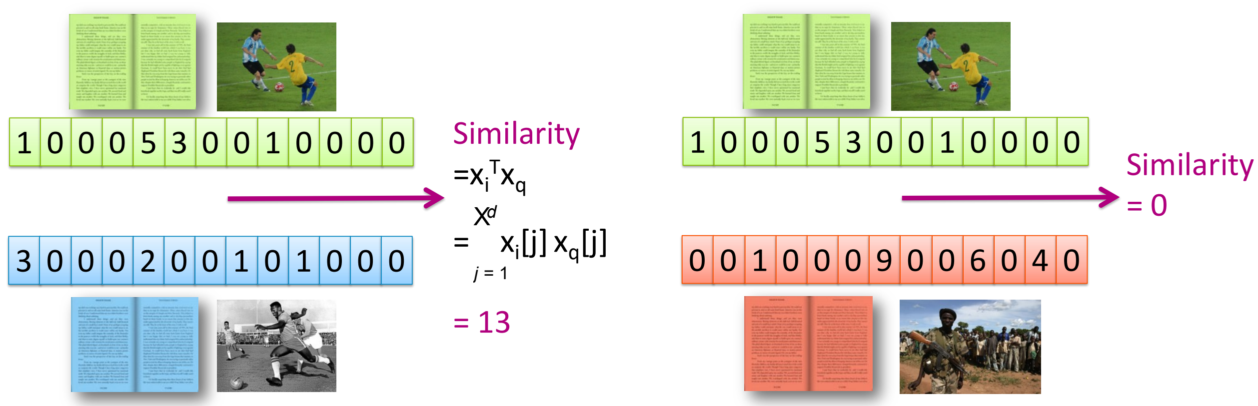
Similarity

Another natural similarity measure would use

$$x_i^T x_q = \sum_{j=1}^{D} x_i[j] x_q[j]$$

Notice this is a measure of similarity, not distance

- This means a bigger number is better



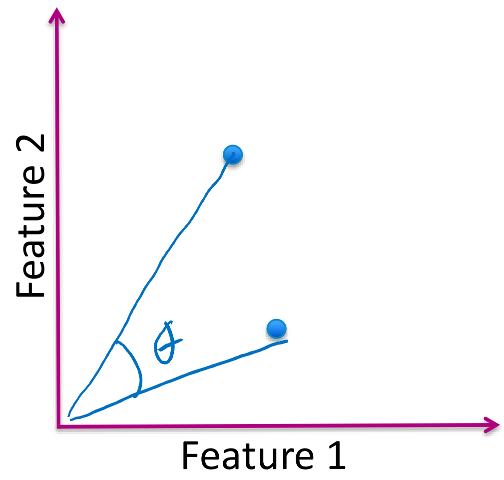
Cosine Similarity

Should we normalize the vectors before finding the similarity?

$$similarity = \frac{x_i^T x_q}{\left\|x_i\right\|_2 \left\|x_q\right\|_2} = \cos(\theta)$$

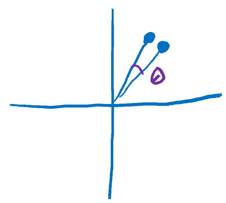
Note:

- Not a true distance metric
- Efficient for sparse vectors!

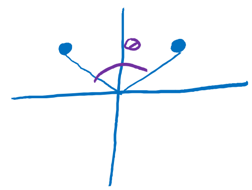


Cosine Similarity

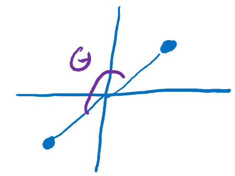
$\cos(\theta) \approx 1$



$\cos(\theta) \approx 0$



$\cos(\theta) \approx -1$



In general

$$-1 \leq cosine\ similarity \leq 1$$

For positive features (like TF-IDF)

$$0 \leq cosine\ similarity \leq 1$$

Define

$$distance = 1 - similarity$$

To Normalize or Not To Normalize?

Not normalized

similarity $= x_i^T x_q$

1	0	0	0	5	3	0	0	1	0	0	0	0

Similarity = 13

3	1	0	0	2	0	0	1	0	1	0	0	0

2	0	0	0	10	6	0	0	2	0	0	0	0

Similarity = 52

6	2	0	0	4	0	0	2	0	2	0	0	0

To Normalize or Not To Normalize?

Normalized

$$\text{cosine similarity} = \frac{x_i^T x_q}{\|x_i\|_2 \|x_q\|_2}$$

1/6	0	0	0	5/6	3/6	0	0	1/6	0	0	0	0
3/4	1/4	0	0	1/2	0	0	1/4	0	1/4	0	0	0

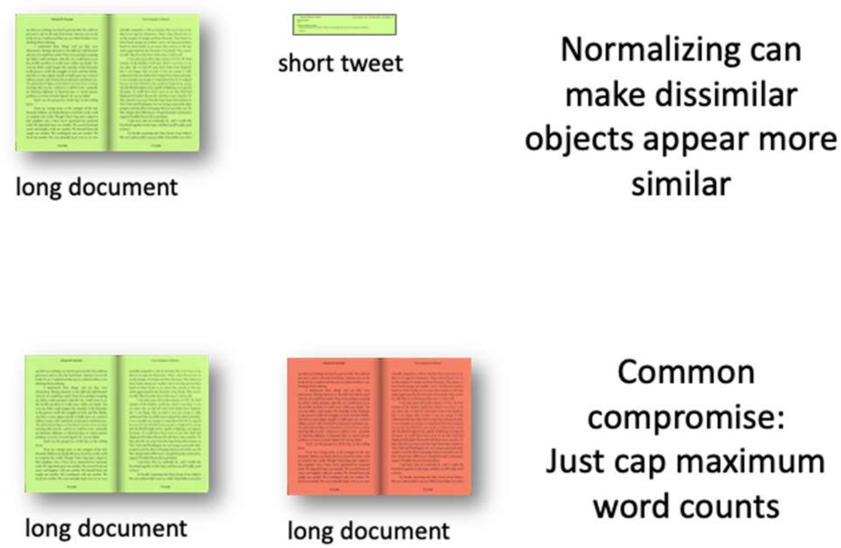
Similarity = 13/24

1/6	0	0	0	5/6	3/6	0	0	1/6	0	0	0	0
3/4	1/4	0	0	1/2	0	0	1/4	0	1/4	0	0	0

Similarity = 13/24

To Normalize or Not To Normalize?

Normalization is not desired when comparing documents of different sizes since it ignores length.



In practice, can use multiple distance metrics and combine them using some defined weights

Poll Everywhere

Pair

3 min

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Not a real Poll Everywhere question, just time to work!

For the given documents, what are their Euclidean Distance and Cosine Similarity?

Assume we are using a bag of words representation

Document 1: “I really like dogs”

Document 2: “dogs are really really awesome”

see next slide

Steps:

- Write out bag of words vectors
- Compute Euclidean distance
- Compute cosine distance

Poll Everywhere

Think

3 min

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Document 1: “I really like dogs”

Document 2: “dogs are really really awesome”

Bag of Words: [# "I", # "really", # "like", # "dogs", # "are", # "awesome"]

$x_1 = [1, 1, 1, 1, 0, 0]$, $x_2 = [0, 2, 0, 1, 1, 1]$

Euclidean Distance $(\|x_i - x_q\|_2)$

$$distance(x_1, x_2) = \sqrt{(1-0)^2 + (1-2)^2 + (1-0)^2 + (1-1)^2 + (0-1)^2 + (0-1)^2} = \sqrt{5}$$

Cosine Distance $\left(1 - \frac{x_i^T x_q}{\|x_i\|_2 \|x_q\|_2}\right)$

$$distance(x_1, x_2) = 1 - \frac{1\cdot0 + 1\cdot2 + 1\cdot0 + 1\cdot1 + 0\cdot1 + 0\cdot1}{\sqrt{1^2+1^2+1^2+1^2+0^2+0^2}\sqrt{0^2+2^2+0^2+1^2+1^2+1^2}}$$

$$= 1 - \frac{3}{\sqrt{4}\sqrt{7}}$$

$$\approx 0.433$$

Recap

Theme: Use nearest neighbors to recommend documents.

Ideas:

- Precision and Recall Curves
- Implement a nearest neighbor algorithm
- Compare and contrast different document representations
  - Emphasize important words with TF-IDF
- Compare and contrast different measurements of similarity
  - Euclidean and weighted Euclidean
  - Cosine similarity and inner-product similarity