Machine Learning

Topic 4: Measuring Distance

Why measure distance?

- Clustering requires distance measures.
- Local methods require a measure of "locality"
- Search engines require a measure of similarity

What is a "metric"?

- A function of two values with these four qualities.

$$d(x,y)=0 \quad \text{iff} \quad x=y \qquad \text{(reflexivity)}$$

$$d(x,y)\geq 0 \qquad \text{(non-negative)}$$

$$d(x,y)=d(y,x) \qquad \text{(symmetry)}$$

$$d(x,y)+d(y,z)\geq d(x,z) \qquad \text{(triangle inequality)}$$

What is a norm ||v|| ?

- Loosely, it is a function that applies a positive value to all vectors (except the 0 vector) in a vector space.
- 3 properties:

For all a $\in$ F and u,v $\in$ V, a function $p: V \to F$

$p(av) = |a|\, p(v)$ (positive scalability)

$p(u) = 0$ iff u is the zero vector

$p(u) + p(v) \geq p(u+v)$ (triangle inequality)

2 definitions (AKA why this is confusing)

- A vector norm

  A function that assigns a strictly positive value to all vectors in a vector space….except the 0 vector, which has a 0 assigned to it. (see previous slide)

- A normal vector

  A vector is called a **normal** to another object if they are perpendicular to each other. So, a **normal vector** is perpendicular to (the tangent plane of) a surface at some point *P*.

Metric == Norm??

- Every norm determines a metric.

  Given a normed vector space, we can make a metric by saying

$$d(x,y) \equiv \left\| x - y \right\|$$

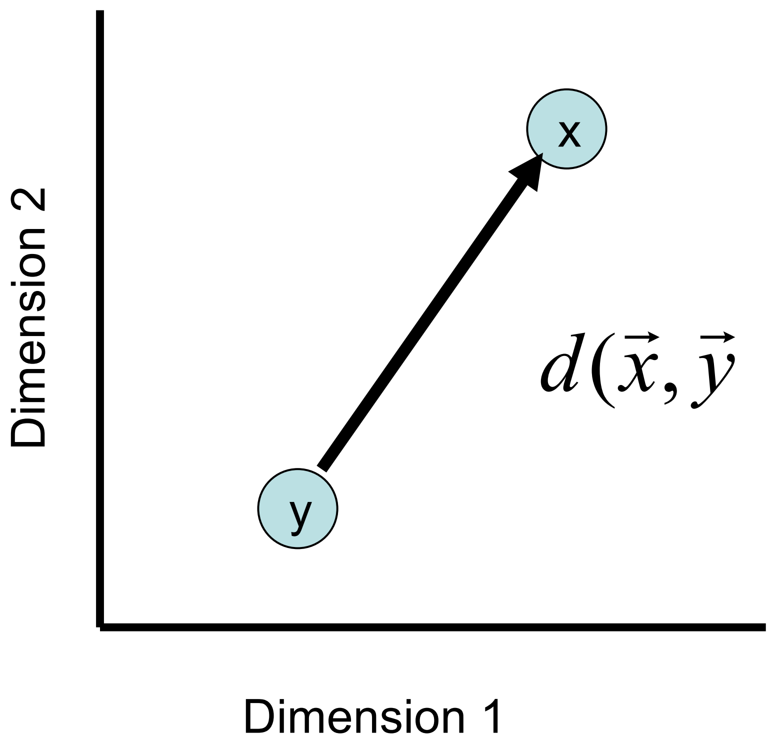
- Some metrics determine a norm.

  <u>If</u> the metric is on a vector space, you can define a norm by saying…

$$\left\| x \right\| \equiv d(x,0)$$

Euclidean Distance

- What people intuitively think of as "distance"
- Is it a metric?
- Is it a norm?



$$d(\vec{x},\vec{y}\ )=\sqrt{(x_1-y_1)^2+(x_2-y_2)^2}$$

Generalized Euclidean Distance

n = the number of dimensions

$$d(\vec{x}, \vec{y}) = \left[\sum_{i=1}^{n} | x_i - y_i |^2 \right]^{1/2}$$

$$\text{where } \vec{x} =< x_1, x_2, \ldots, x_n >,$$

$$\vec{\mathrm{y}} =< y_1, y_2, \ldots, y_n \}$$

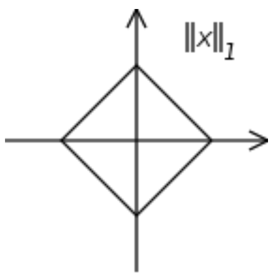
$$\text{and} \quad \forall i (x_i, y_i \in \Re)$$

L^p norms

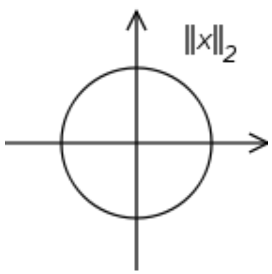
- L^p norms are all special cases of this:

$$d(\vec{x},\vec{y}) = \left[\sum_{i=1}^{n} | x_i - y_i |^p \right]^{1/p}$$

p changes the norm



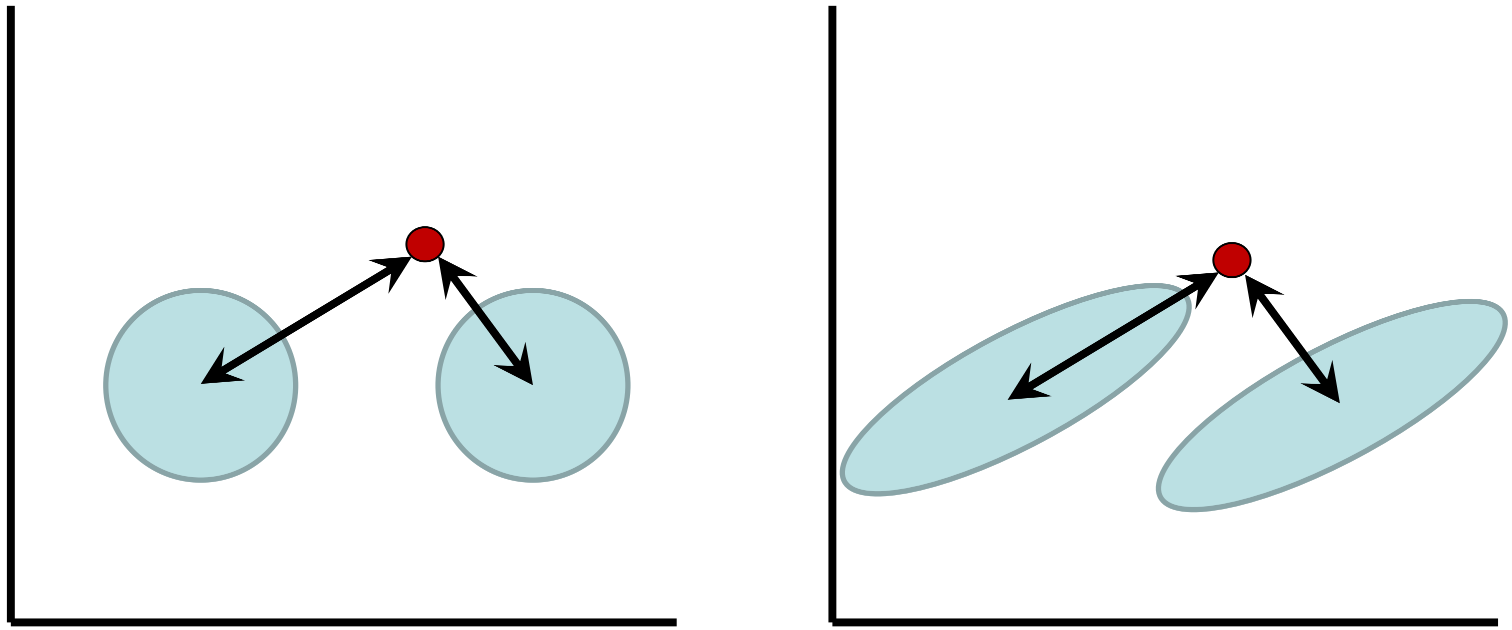
$$\|\mathrm{x}\|_1 = \mathrm{L}^1 \text{ norm} = \text{Manhattan Distance}: p = 1$$



$$\|\mathrm{x}\|_2 = \mathrm{L}^2 \text{ norm} = \text{Euclidean Distance}: p = 2$$

$$\text{Hamming Distance}: p = 1 \text{ and } x_i, y_i \in \{0,1\}$$

Weighting Dimensions



- Put point in the cluster with the closest center of gravity
- Which cluster <u>should</u> the red point go in?
- How do I measure distance in a way that gives the "right" answer for both situations?

Weighted Norms

- You can compensate by weighting your dimensions….

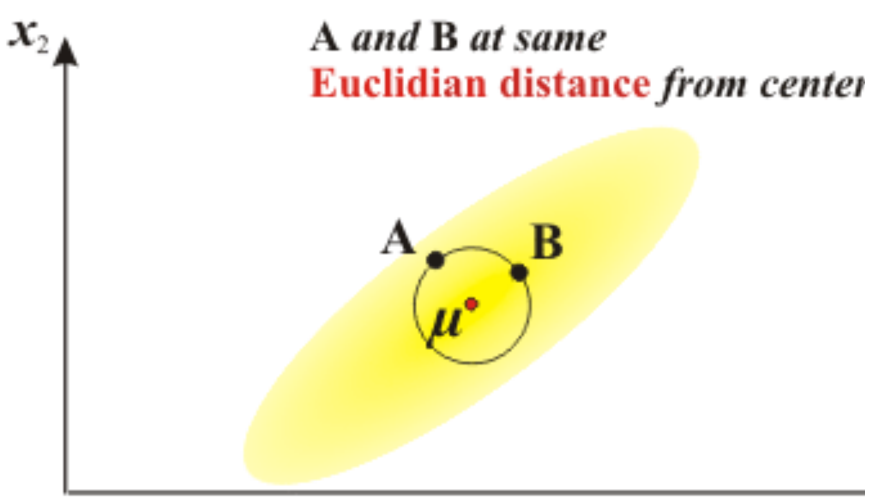
$$d(\vec{x}, \vec{y}) = \left[\sum_{i=1}^{n} w_i \, | x_i - y_i |^p \right]^{1/p}$$

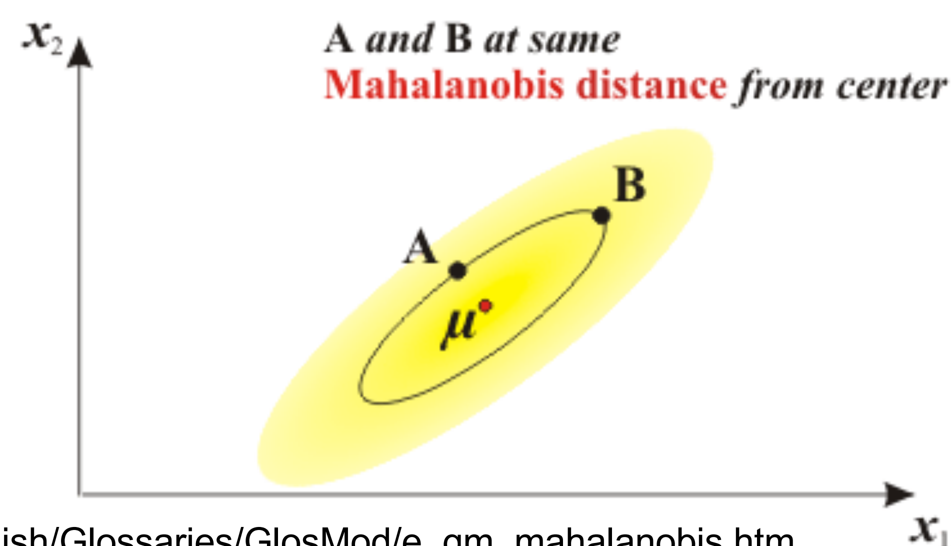
This lets you turn your circle of equal-distance into an elipse with axes parallel to the dimensions of the vectors.

Mahalanobis distance

The region of constant Mahalanobis distance around the mean of a distribution forms an ellipsoid.

The axes of this ellipsiod don't have to be parallel to the dimensions describing the vector





Images from: http://www.aiaccess.net/English/Glossaries/GlosMod/e_gm_mahalanobis.htm

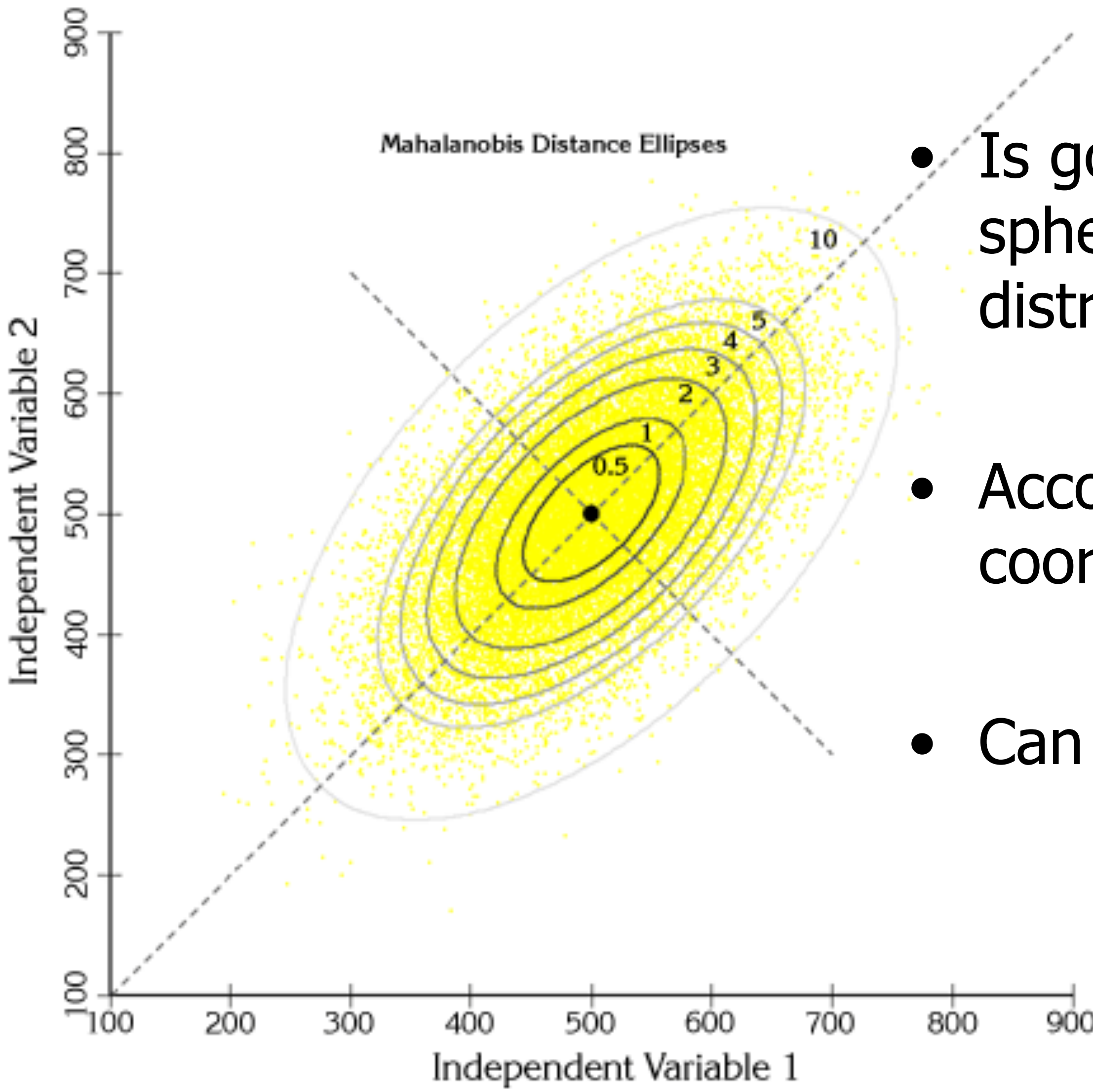
Calculating Mahalanobis

$$d(\vec{x},\vec{y}) = \sqrt{(\vec{x}-\vec{y})^T S^{-1} (\vec{x}-\vec{y})}$$

- This matrix S^{-1} is called the "covariance" matrix and is calculated from the data distribution
- Let's look at the demo here:

http://www.aiaccess.net/English/Glossaries/GlosMod/e_gm_mahalanobis.htm#Animation%20Mahalanobis

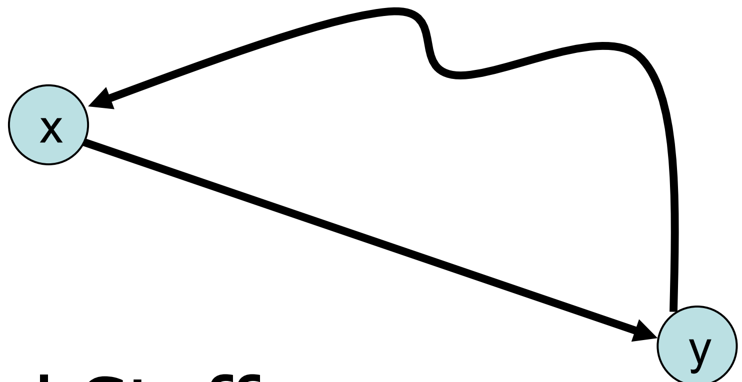
Take-away on Mahalanobis



- Is good for non-spherically symmetric distributions.
- Accounts for scaling of coordinate axes
- Can reduce to Euclidean

Metric, or not?

- Driving distance with 1-way streets



- Categorical Stuff :
  - Is distance (Jazz to Blues to Rock) no less than distance (Jazz to Rock)?

Categorical Variables

- Consider feature vectors for genre & vocals:
  - Genre: {Blues, Jazz, Rock, Zydeco}
  - Vocals: {vocals,no vocals}

s1 = {rock, vocals}

s2 = {jazz, no vocals}

s3 = { rock, no vocals}

- Which two songs are more similar?

One Solution:Hamming distance

Blues	Jazz	Rock	Zydeco	Vocals
0	0	1	0	1
0	1	0	0	0
0	0	1	0	0

s1 = {rock, vocals}
s2 = {jazz, no_vocals}
s3 = { rock, no_vocals}

Hamming Distance = number of bits different between binary vectors

Hamming Distance

$$d(\vec{x},\vec{y}) = \sum_{i=1}^{n} | x_i - y_i |$$

$$\text{where } \vec{x} =< x_1, x_2, \ldots, x_n >,$$

$$\vec{\mathrm{y}} =< y_1, y_2, \ldots, y_n \}$$

$$\text{and } \quad \forall i(x_i, y_i \in \{0,1\})$$

Defining your own distance (an example)

How often does artist *x* quote artist *y*?

Quote Frequency

	Beethoven	Beatles	Kanye
Beethoven	7	0	0
Beatles	4	5	0
Kanye	?	1	2

Let's build a distance measure!

Defining your own distance (an example)

	Beethoven	Beatles	Kanye
Beethoven	7	0	0
Beatles	4	5	0
Kanye	?	1	2

$$\text{Quote frequency } Q_f(x, y) = \text{value in table}$$

$$\text{Distance } d(x, y) = 1 - \frac{Q_f(x, y)}{\sum_{z \in Artists} Q_f(x, z)}$$

Missing data

- What if, for some category, on some examples, there is no value given?

- Approaches:
  - Discard all examples missing the category
  - Fill in the blanks with the mean value
  - Only use a category in the distance measure if both examples give a value

(one way of) handling missing attributes

$$w_i = \begin{cases} 0, & \text{if both } x_i \text{ and } y_i \text{ are defined} \\ 1, & \text{else} \end{cases}$$

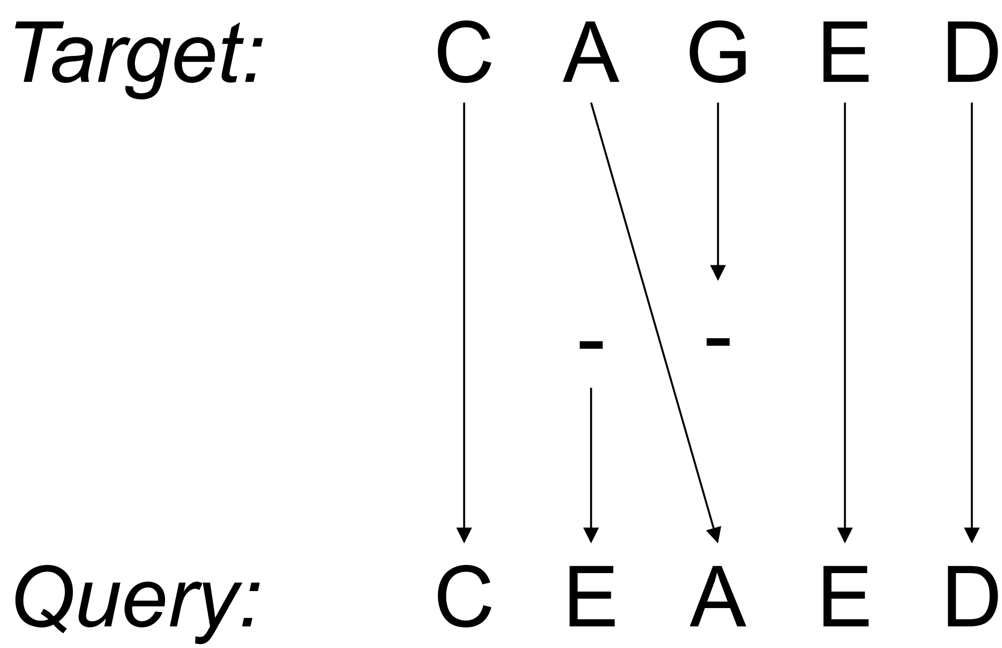
$$d(\vec{x}, \vec{y}) = \frac{n}{n - \sum_{i=1}^{n} w_i} \left[\sum_{i=1}^{n} \phi(x_i, y_i) \right]$$

A scaling factor that adds weight to the distance, as there are fewer attributes used

A distance measure that works on individual attributes

Edit Distance

- Query = string from finite alphabet
- Target = string from finite alphabet
- Cost of Edits = Distance



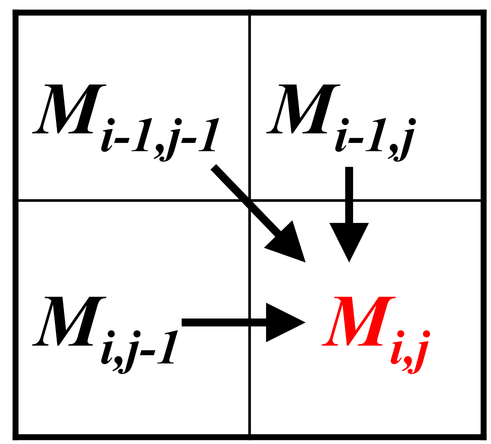
Levenshtein edit distance

$$M_{0,0} = 0$$

3 possible operations

$$M_{i,j} = \min \begin{cases} M_{i-1,j} + 1 & \textbf{Insertion} \\ M_{i,j-1} + 1 & \textbf{Deletion} \\ M_{i-1,j-1} + \mu(s_i, q_j) & \textbf{Substitution} \end{cases}$$

$$\mu(s_i, q_j) = \begin{cases} 0 & \text{if } s_i = q_j \\ 1 & \text{otherwise} \end{cases}$$



Pseudocode of Levenshtein (after Wagner and Fischer)

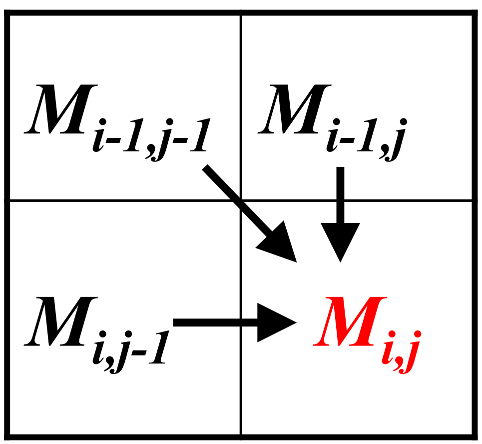
```
return int LevenshteinDistance(char s[1..m], char t[1..n], deletionCost,  insertionCost,
substitutionCost)

// A standard approach is to set deletionCost = insertionCost = substitutionCost = 1

  declare int M[0..m, 0..n]    // M has (m+1) by (n+1) values
  for i from 0 to m
              M[i, 0] := i*deletionCost  // distance of any 1st string to an empty 2nd string
  for j from 0 to n
              M[0, j] := j*insertionCost // distance of any 2nd string to an empty 1st string

  for j from 1 to n
     for i from 1 to m
        if s[i] = t[j] then
           M[i, j] := M[i-1, j-1]   // no operation cost, because they match
        else
           M[i, j] := minimum(M[i-1, j] + deletionCost,
                              M[i, j-1] + insertionCost,
                              M[i-1, j-1] + substitutionCost)
  return M[m,n]
```

Working through an example

$$M_{i,j} = \min \begin{cases} M_{i-1,j} + 1 \\ M_{i,j-1} + 1 \\ M_{i-1,j-1} + \mu(s_i, q_j) \end{cases}$$

$$\mu(s_i, q_j) = \begin{cases} 0 & \text{if } s_i = q_j \\ 1 & \text{otherwise} \end{cases}$$

$$M_{0,0} = 0$$



		F	R	O	G
	0	**1**,-,-	2,-,-	3,-,-	4,-,-
D	-,-,1	2,**1**,2	**2,2**,3	3,3,4	4,4,5
O	-,-,2	3,2,2	3,2,3	3,**2**,4	**3**,4,5
G	-,-,3	4,3,3	4,3,3	4,3,3	4,**2**,4

Edit distance is 2 edits

Working through an example

- The final edit cost is the lowest value calculated for the lower right-hand corner of the matrix.
- Tracing a path from the lower right to the beginning shows 2 minimal-cost alignments, each with 1 substitution and one deletion:

```
FROG    FROG
D-OG    -DOG
```

		F	R	O	G
	0	**1**,-,-	2,-,-	3,-,-	4,-,-
D	-,-,1	2,**1**,2	**2,2**,3	3,3,4	4,4,5
O	-,-,2	3,2,2	3,2,3	3,**2**,4	**3**,4,5
G	-,-,3	4,3,3	4,3,3	4,3,3	4,**2**,4

del F

sub D for F

sub D for R

del R

O = O

G= G

Edit distance is 2 edits

(Somewhat more) General Edit Distance

$$M_{i,j} = \min \begin{cases} M_{i-1,j} + \mu(-, q_j) & \textbf{Insert} \\ M_{i,j-1} + \mu(s_i, -) & \textbf{Delete} \\ M_{i-1,j-1} + \mu(s_i, q_j) & \textbf{Match} \end{cases}$$

$\mu(s_i, q_j) =$ whatever you want.

The distance between s_i and q_j on a keyboard?

The probability of substituting s_i for q_j?

Final notes on edit distance

- Used in many applications
  - Gene sequence matching (google: BLAST)
  - Spell checking
  - Music melody matching
- There are many variants of the algorithms
- The parameter weights strongly affect performance
- You need to pick the algorithm and parameters that make sense for your problem.

One more distance measure

- Kullback–Leibler (KL) divergence
  - a non-symmetric measure of the difference between two probability distributions
  - not a metric, since it is not symmetric
  - Here's the definition of KL divergence for discrete probability distributions P and Q

$$D_{KL}(P \| Q) = \sum_i \ln\left(\frac{P(i)}{Q(i)}\right) P(i)$$

KL Divergence as Cross Entropy

$$D_{KL}(P \,\|\, Q) = \sum_i \ln\left(\frac{P(i)}{Q(i)}\right) P(i)$$

$$= \sum_i \left(\ln(P(i)) - \ln(Q(i))\right) P(i)$$

$$= \sum_i P(i) \ln P(i) - \sum_i P(i) \ln Q(i)$$

Some take-away thoughts

- Many machine learning methods are helped by having a distance measure
- Some methods require metrics
- Not all measures are metrics
- Some common distance measures:

  "P-norms": Euclidean, Manhattan

  "Edit distance": Levenshtein

  KL Divergence

  Mahalanobis