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Statistical and Machine Learning

Inter-point Distances

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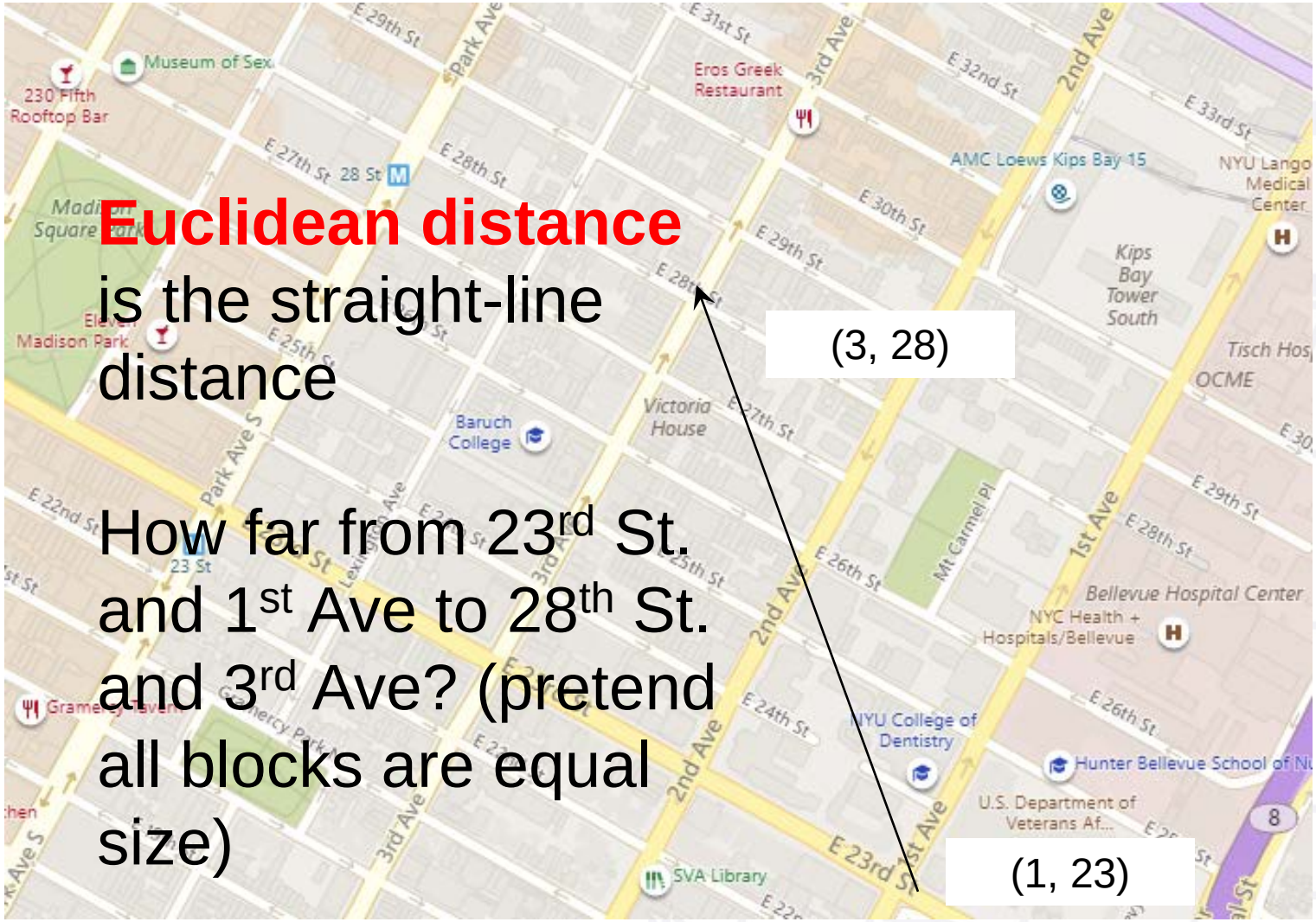
Inter-point Distances

- Many statistics techniques (like clustering, to come) rely on a measure of **distance** (or ***dissimilarity***) between two points, between a point and a cluster, and between two clusters
- **Concerns: How do we…**
  1. Evaluate the contribution of a variable to the clustering (selection, weighting)?
  2. Account for correlation (or duplication) among variables?
  3. How do we incorporate categorical variables?

Euclidean Distance



Euclidean distance is the straight-line distance

How far from 23rd St. and 1st Ave to 28th St. and 3rd Ave? (pretend all blocks are equal size)

Source: Bing Maps

Euclidean Distance

Answer:

$\sqrt{[(1 - 3)^2 + (23 - 28)^2]}$

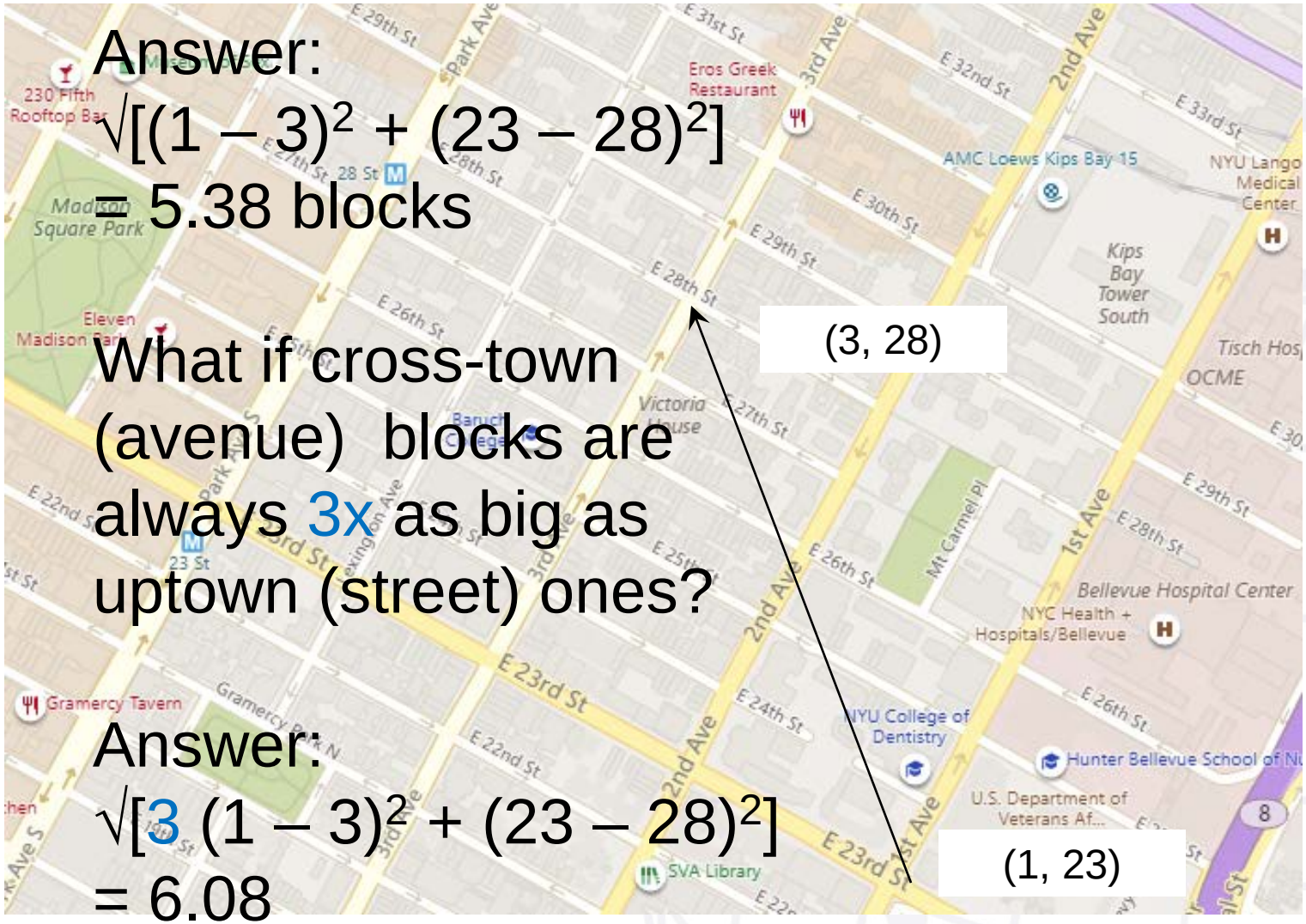
= 5.38 blocks

What if cross-town (avenue) blocks are always 3x as big as uptown (street) ones?

Answer:

$\sqrt{[3\ (1 - 3)^2 + (23 - 28)^2]}$

= 6.08



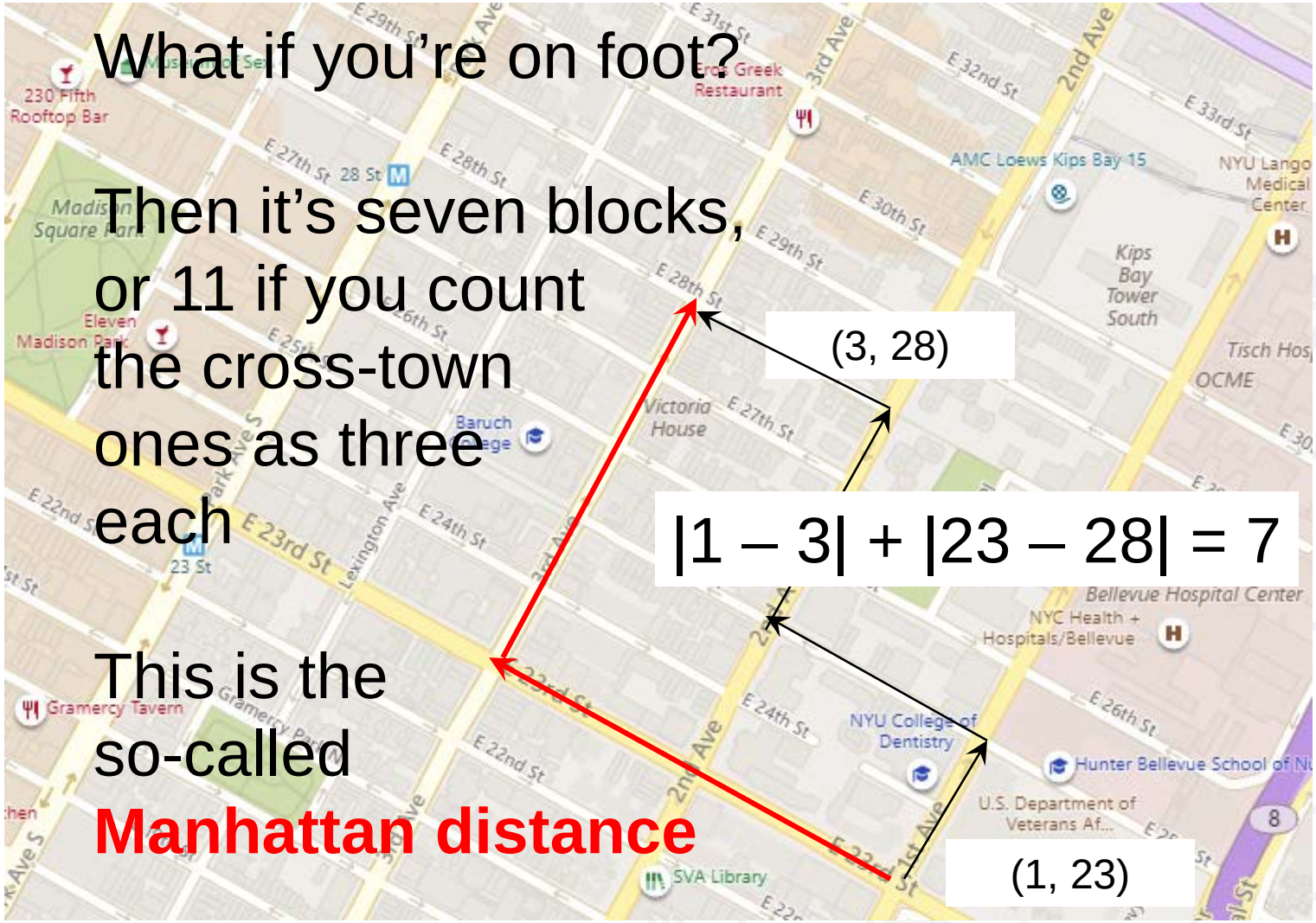
Source: Bing Maps

Manhattan Distance

What if you're on foot?

Then it's seven blocks, or 11 if you count the cross-town ones as three each

This is the so-called **Manhattan distance**



Source: Bing Maps

Distances

- Most techniques measure distance between two observations x_1, x_2 with:

$$d(x_1, x_2) = \sqrt{\sum_j \left(x_{1j} - x_{2j}\right)^2} \text{ (Euclidean) or}$$

$$d(x_1, x_2) = \sqrt{\sum_j w_j \left(x_{1j} - x_{2j}\right)^2} \text{ (wtd. Euc.)}$$

  - Weights w_j are 1, or sd (x_j), or range (x_j)
    - But are these good choices? Scale is not the same as "importance"
  - Correlation among X's usually ignored
  - Still needs modification for categorical data

Distances

- The weighted **Manhattan** distance is one alternative:

$$d(x_1, x_2) = \sum_j w_j \, |x_{1j} - x_{2j}|$$

More generally we could use the **Minkowski** distance for some value p:

$$d(x_1, x_2) = [\sum_j w_j \, |x_{1j} - x_{2j}|^p]^{(1/p)}$$

  - Again, choice of weights w_j are 1, or sd (x_j), or range (x_j)
  - Correlation among X's usually ignored
  - Still needs modification for categorical data

Mahalanobis Distance

- Suppose your data vectors x1, x2 come from a distribution with cov. matrix $\boldsymbol{\Sigma}$
- Then a "natural" way to account for correlation among observations is to weight by the inverse of that matrix:

$$d(x_1, x_2) = \sqrt{(\boldsymbol{x_1} - \boldsymbol{x_2})^{\mathrm{T}} \boldsymbol{\Sigma^{-1}} (\boldsymbol{x_1} - \boldsymbol{x_2})}$$

- This **Mahalanobis** distance generalizes the Euclidean…but the $\boldsymbol{\Sigma}$ matrix, $n \times n$, is unknown and hard to estimate

Distance Measure

- R's `daisy() {cluster}` computes inter-point distances (replaces `dist()`)
- Scale, choice of metric **can** matter
- If all variables numeric, choose "euclidean" or "manhattan"
- We can scale columns differently, but correlation among columns ignored
- Otherwise daisy uses **Gower** distance

Gower Distance

- If some columns are not numeric, the "dissimilarity" between numeric X_{ik} and X_{jk} scaled to $|X_{ik} - X_{jk}|$ / range (X_k)
  - (What happens when one entry in X_k has an outlier – like Age = 999?)
- For binary variables the usual dissimilarity is 0 if $X_{ij} = X_{ik}$, 1 if not
  - What if 1's are very rare (e.g. speaks Esperanto, attended Sorbonne)?
  - Asymmetric binary

Gower Distance

- Our observations are vectors $\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_n$
- The dist $d_{ij,k}$ between $\mathbf{x}_i$ and $\boldsymbol{x}_j$ on var. k is:
  - For categorical k, 0 if $x_{ik} = x_{jk}$, otherwise 1
  - For numeric k, $|x_{ik} - x_{jk}|$ / (range of column k)
- The overall distance d_{ij} is a weighted sum of these: $d_{ij} = \frac{\sum_{i=1}^{p} \partial_{ij,k}\, d_{ij,k}}{\sum_{i=1}^{p} \partial_{ij,k}}$
- Weights $\partial_{ij,k}$ are 1 except when one $\boldsymbol{x}$ is missing, or both 0 and $\boldsymbol{x}$ asymm.binary
- Case weights are also possible

Thoughts on Gower

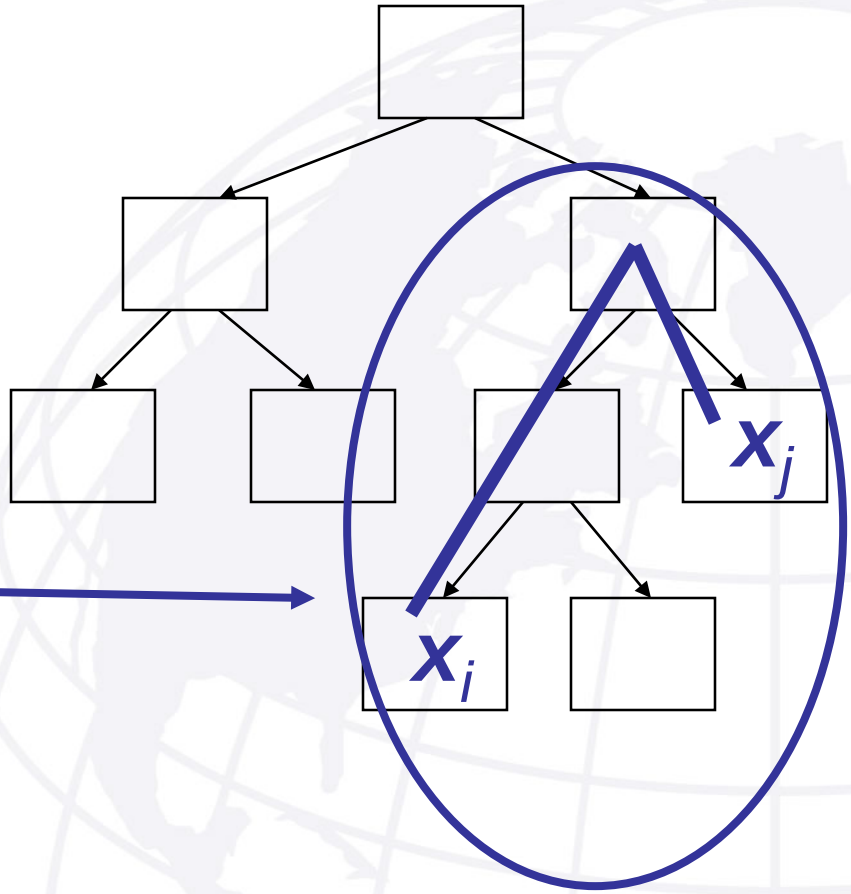
- Natural adjustment for missing values
  - Euclidean dist: inflate by √[ncol(X)/#non-NA]
- All these choices can matter!
- `daisy()` computes all the pairwise distances up front
- There are $n(n-1)/2$ of these, which causes trouble in really big data
- Things are different in high dimensions – our intuition is not very good here
- Dimensionality reduction is always good!

treeDist

- "Two observations are alike if they tend to fall in the same leaves of trees"
  - But trees require a response variable
- The treeDist distance computes *p* trees, with each column in turn as response
- Trees are pruned – some may be discarded
- The distance between points *i* and *j* on tree *t* is $d_1^t(i,j) = 0$ if *i* and *j* land in the same leaf, otherwise 1
- d_2 is like d_1 but with tree "quality" weights

Enhancements

- **Local** quality
- If two obs. are in different leaves, compute the change in deviance associated with the smallest sub-tree containing both



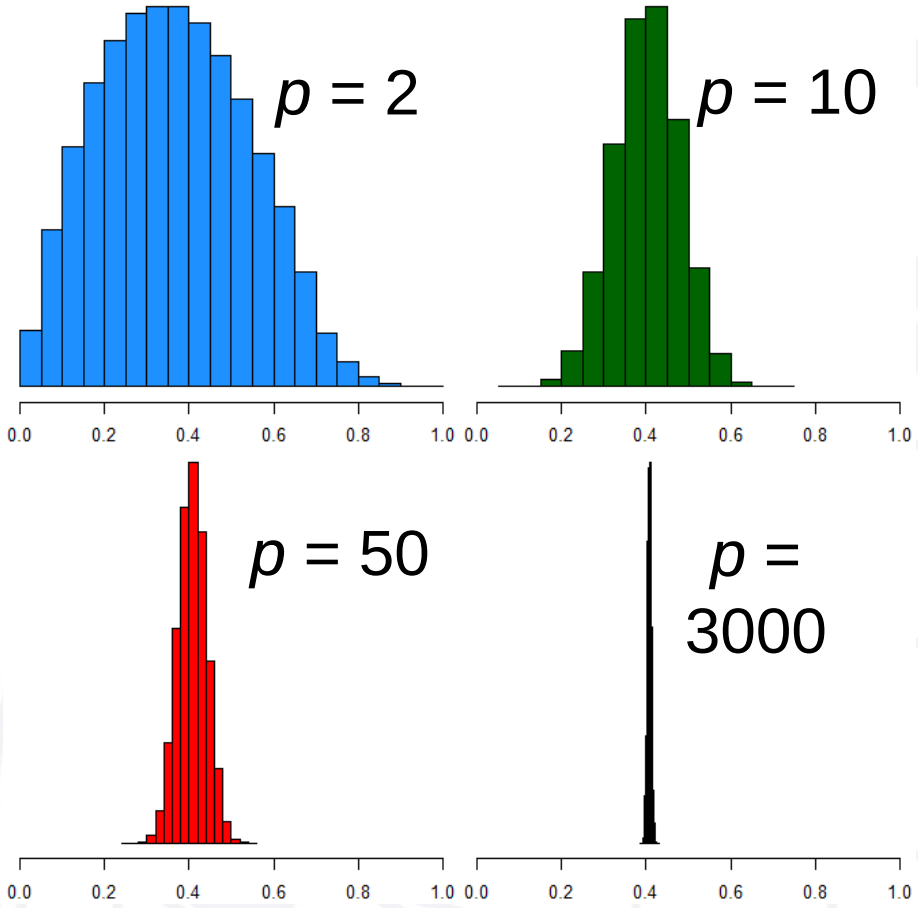
- Scale the (i, j) distance "accordingly" → d_3
- d_4: this "local" measure, weighted by tree quality
- The treeDist is unlike other measures in that it's learned from the data

Distances in Big Data Sets

- Instead of computing all $\binom{n}{2}$ pairwise distances, we can compute the set of pairwise **leaf distances** for each tree, which is much smaller
- We can also generate a new **numeric** data matrix whose inter-point distances "mirror" the inter-leaf ones
  - This data can be clustered or visualized in lower-d space via, e.g., multi-dim scaling
  - B. and W., *R Journal* 7/2, Dec. 2015
  - treeClust library at CRAN respository

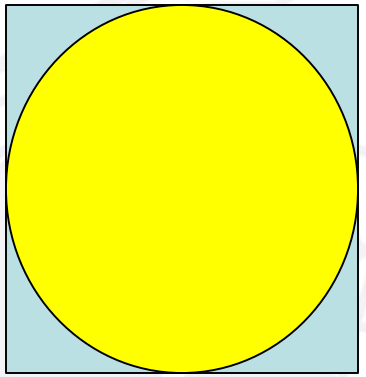
Digression: High-Dimensional Data

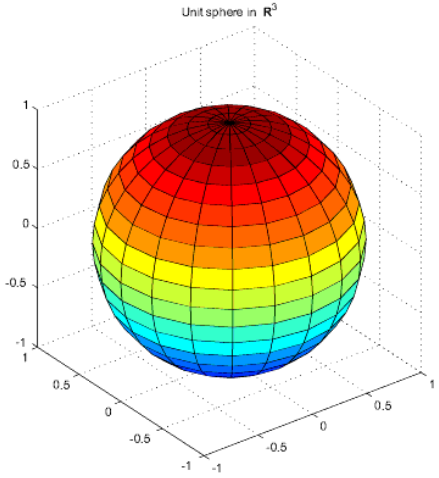
- High-dimensional data is just *different*
- Here are the pairwise distances among 1,000 points in *p* dimensions where each component is indep. U(–.5, +.5), scaled to (0, 1)
- In high dimensions, everything is "equally far away"
- Hopefully our data lies in a lower-dimensional subspace



Digression Part 2

- What proportion of the unit square is occupied by the unit circle?
- A: $\pi(1)^2 / 2^2 = \pi/4 = 0.79$
- What proportion of the unit cube is occupied by the unit sphere? A: $(4/3)\ \pi(1)^3 / 2^3 = \pi/6 = 0.52$





- How about in 30 dimensions? A: ≈ Zero!

Source: Matlab via http://www.ic.unicamp.br

Shameless Plug

- Remember random forests?
- "Proximity" measured by number of times two observations fell in the same leaf
  - But every tree has the same response variable
- The `treeClust()` dissimilarity of Buttrey and Whitaker (2015) creates (0 or) one tree from each response variable
  - Some trees are pruned to the root, dropped
  - Inherits tree missing value, outlier etc. handling
- Often performs well

Dimensionality Reduction

- **How** can we reduce dimensionality while preserving as much info as possible?
  - Principal Components, based on variance
  - "Projection Pursuit" is the name of techniques that use other criteria of "interestingness," like "as non-Gaussian as possible"
  - Sammon mapping: preserve the *ranking* of inter-point distances as much as possible
  - t-SNE seems pretty successful
- **Why**?
  - For plotting, visualization

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Similar Items part 2 (Mostly a Digression)

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Finding Similar Items

- Goal: locate neighbors in scalable way
  - i.e. without computing $n(n-1)/2$ distances
  - Tasks
    - Find exact duplicates
    - Find nearest neighbor – or the k nearest
    - Find all, or at least one, neighbors within distance r
    - Find distribution of distances to k^{th} nearest
    - Find average number of points within r…

- Lescovec, Rajmaran, & Ullman, “Mining Massive Datasets,” On-line Textbook (2014)

Applications

- Numeric vectors:
  - Clustering
  - Multidimensional Scaling (more to follow)
    - These often require numeric variables – like most of the examples we've looked at
    - Need to handle mixed variables (e.g. Gower)
- Text documents
  - Plagiarism, mirror pages, same source articles
- Sets
  - Recommender systems

Distances

- Numeric vectors
  - **Euclidean** and **Manhattan** distances…
  - We know how to incorporate categoricals, asymmetric binaries…
  - …though scaling/weighting still needs to be considered…
  - …as does correlation – perhaps a simple sum of column distances is insufficient
  - `dist()` and `daisy()` in R

Distances (cont'd)

- Numeric vectors (cont'd)
  - **Cosine** similarity
    - $c(\mathbf{x}_1, \mathbf{x}_2) = \mathbf{x}_1^T\mathbf{x}_2 / [\ ||\mathbf{x}_1||\ ||\mathbf{x}_2||]$
    - Often we take distance as 1 – similarity
  - Proportional to the "dot product" between the two vectors, but insensitive to scale
  - Recall $\mathbf{x}_1^T\mathbf{x}_2 = ||\mathbf{x}_1||\ ||\mathbf{x}_2||\ \cos(\theta)$, so the similarity is the cosine of the angle between the two vectors
  - $\cos(\theta) = 0 \Rightarrow \mathbf{x}_1, \mathbf{x}_2$ are parallel; $\cos(\theta) = 1 \Rightarrow \mathbf{x}_1, \mathbf{x}_2$ are perpendicular
  - E.g. in text mining, to compare two docs

Cosine Similarity Example

- Example: documents counts by word

	Doc 1	Doc 2	Doc 3
Gambia	15	0	0
baseball	0	23	12
Senegal	8	0	0
cotton	5	2	0
Oakland	0	0	9
peanuts	11	2	7
exports	0	0	1
shortstop	0	8	6
market	3	2	3

- $c(d_1, d_2) = 0.07$; $c(d_1, d_3) = 0.23$; $c(d_2, d_3) = 0.78$

Distances (cont'd)

- Numeric (usually binary) vectors
  - **Hamming** distance: the number of components on which the two differ
- E.g. $h(\texttt{001011}, \texttt{010011}) = 2$
- Extended to character sequences, possibly of different lengths:
  - **Levenshtein** (or "edit") distance: the number of one-character inserts, deletions, or changes necessary to turn one string into another
- E.g. L("button", "builtin") = 3

Distances (cont'd)

- Sets:
  - **Jaccard** distance, $d(A, B) = 1 - |A \cap B| / |A \cup B|$
  - The part on the right of the minus sign is "the fraction of all the items in both sets that appear in the intersection" – that is, set similarity
  - $d(A, B)$ measures how dissimilar two sets are
- Probability Distributions:
  - The distance from a dist'n p(x) to q(x) is often measured by the **Kullback-Leibler divergence**

$$\int_x p(x) \log \frac{p(x)}{q(x)} dx$$

Multidimensional Scaling

- Multidimensional scaling (MDS) is the general term for "compressing" a set of high-dimensional inter-point distances into a lower dimension (usually, 2 or 3)
- Find the low-d configuration whose inter-point distances are as similar as possible to the originals
  - So not the same as PCA, where we try to find new coordinates to capture the variance
  - Minimze **stress** between old and new

MDS, cont'd

- If the original distances are d_{ij}, and the lower-d ones are d^*_{ij}, then we might take

$$\text{Stress} = \sqrt{\frac{\sum\left(d^*_{ij} - d_{ij}\right)^2}{\sum d^2_{ij}}} \text{ or } \left(\frac{\sum\left|d^*_{ij} - d_{ij}\right|^p}{\sum d^p_{ij}}\right)$$

- MDS solutions will normally be insensitive to shift, rotation and reflection
- As with PCA we might need to **scale** data
- **Classical** MDA: minimize stress
  - There's a closed form solution for this

MDS, cont'd

- In **Metric MDS**, we minimize the stress based on a non-linear transformation of the distances

$$\text{Stress} = \left(\frac{\sum \left| d_{ij}^{*} - d_{ij} \right|^{p}}{\sum d_{ij}^{p}} \right)$$

with, e.g., $d_{ij}^{*} = a + b \log (d_{ij})$

- Some applications in, e.g. psychology
- Lots of alternate formulations of d_{ij}^{*} available

Non-Metric MDS

- In **Non-metric** MDS we try to respect the **ordering** of distances rather than their numeric values
- In "stochastic neighbor embedding" (SNE) we model the probabilities that observation *i* would pick *j* as a neighbor, and try to match those in the lower-d space…
  - Cost function from Kullback-Leibler
- …Leading to the widely used modification called **t-SNE**

MDS in R

- R has `cmdscale()` for classical MDS built in
- Metric MDS comes from packages, among them `smacof`
- Non-metric MDS from (among others) `ismMDS` and `sammon` in MASS library
- t-SNE from `Rtsne`
  - Best with smaller sample sizes
  - Remove duplicates

MDS Example

- **Splice data**
  - Primate spice-junction gene sequences
  - Each observation has a class EI, IE or n
  - Each observation has 60 A, C, T, G values
    - Except, inevitably, data prep required
  - Goal: Compute inter-point distances (excluding classes), map in 2 or 3 dimensions...
  - …with colors given by “real” class to try to see if the classes look different

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Statistical and Machine Learning

Hashing (A Digression)

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Scalability

- We need algorithms to operate without computing all $n(n-1)/2$ distances
- For some applications it will be enough to identify a small number of candidate pairs, distances for which can then be computed explicitly

Hash

- A **hash** is a function (or verb, or noun) that describes converting the contents of an item (vector, document, video, set…) to one of a much smaller number of possibilities (e.g. an integer, a 32-byte string)
- The “hash table” is a related storage and look-up scheme
- Example: Dewey Decimal System

Hashing

- Goals of hashing:

1. Hash value should be easy to compute
2. The same source should produce the same hash value, but sources different by even a little should produce different values (*)
3. The hash should be **one-way**; that is, given a hash value, you should not be able to construct a string that also produces that hash value

Hashing

- The set of items with a particular hash value is called a **bucket**
  - So we hope each bucket has 0 or 1 items
  - A “collision” is when two different items end up in the same bucket
  - If we can’t have a unique hash output from each item, we at least want a uniform distribution of items over buckets

Hashing for Duplicates

- Imagine searching for duplicate documents
- Each doc has an ID and some contents
- 1.) Hash every document's contents; build list of (bucket, ID)
- 2.) If no bucket has two members, there are no duplicates
  - And we never had to compare two docs!
- 3.) Otherwise, examine all buckets with > 1 members for collisions/duplicates

Hashing for Data Integrity

- R packages carry MD5 signatures
- If your downloaded package produces the same signature as the one reported, you can be pretty sure you got the exact set of bits they sent
  - Or a collision of really tiny probability
  - If your MD5 value differs, your download is wrong, but you have no idea how

Bash example

- echo "The quick brown fox" | md5sum
- echo "The quick brown f0x" | md5sum
- Other algorithms (sha1sum, sha256sum) available
- For data integrity, these are all fine
- For crypto-strength, use SHA-2 or SHA-3 algorithms; md5 and sha1 have been “broken”

Digression: Public-Key Encryption

- A good hash is one-way: non-invertible
- A code or cipher needs to be reversible to recover the message
  - The “key” might be symmetric – same key encrypts and decrypts – in which case it must be protected
  - Asymmetric keys let recipient make the encoding key public while keeping the decoding key private: **public key encryption**
  - Asymmetric encryption is slow (by a factor of 1,000 compared to conventional?)

Digression: PGP

- Pretty Good Privacy (PGP) uses a random, symmetric **session key**
  - Session key must be kept secret, so…
- The message is encrypted with the session key; the session key is then encrypted with the receiver's public key
  - A hash of the message might be encrypted with the sender's private key, as well, and sent along as authentication

Digression: PGP (cont'd)

- Recipient decodes session key with receiver's private key, then decodes message using the session key
  - If she decodes the hash with the sender's public key she can compare the sender's hash with one she computes herself
  - If they match, there's a **digital signature** that can't be repudiated

Hashing for Crypto

- The CS and Crypto communities love hashing
  - They hate collisions
  - Tiny changes in the message need to produce big changes in the hash (*)
  - It should be difficult to generate a message with a particular hash – since collisions are rare, you would be “inverting” the hash and maybe recovering the original message

Locality Sensitive Hashing

- **LSH** takes a different approach
- Items that are “close together” should land in the same bucket with high probability
  - We welcome collisions, and want small changes in input to have small changes, or no change, in hash value
  - Anti-spam example: replacing “Rolex” with “R0lex” should have no effect w/high prob.

Families of Hash Functions

- Consider a family of functions, each function $f_i()$ producing a different hash
  - Ex: for Hamming distance, f_1 might be "value of bit *i* "
- We can **AND** or **OR** these functions together to try to control error rates
  - For Hamming, pick 40 of these, say
  - False positives: items that hash together but aren't alike (here, match at only 40 points)

LSH

- LSH measures have been implemented for Euclidean, Hamming, Jaccard and other distances
- Ex.: fingerprint matching[1] (Hamming)
- Imagine each fingerprint represented in a 1000-pixel image
- Each pixel may have a “minutia”

1 Lescovec, Rajmaran, & Ullman, “Mining Massive Datasets,” On-line Textbook (2014)

Fingerprints

- Problems:
  - 1.) Is this print in our database? (“one-many”)
  - 2.) Do any pairs in our database come from the same individual? (“many-many”)
- Assume that overall Pr (minutia) = **.20**
- Pr ($m_{ij \cdot k}$) = Prob. of a minutia at pixel *ij* of image *k*)
- Assume that, given two different images of the same finger, Pr ($m_{ij \cdot 2} \mid m_{ij \cdot 1}$) = .80
- For different fingers, Pr ($m_{ij \cdot 2} \mid m_{ij \cdot 1}$) = **.20**

Hash functions

- Pick three points at random
- Define the function $f()$:
  = 1 if all three have minutia, else = 0
- For two random fingerprints A and B,
  $\Pr(f(A) = 1, f(B) = 1) = .2^3.2^3 = .000064$
- For two images from the same finger,
  $\Pr(f(A) = 1, f(B) = 1) = .2^3.8^3 = .004096$
- What if we use lots of f () functions?
  – AND reduces false positives, OR reduces false negatives – usual trade-off

Combining $f()$s

- Create 1024 separate $f()$ functions, each referring to three random pixels
- What's the prob. that two fingerprints from the same finger match on **at least one** [this is OR] of the $f()$ functions?
  - A: $1 - (1 - .004096)^{1024} = .985$
- What's that prob. for two random prints?
  - A: $1 - (1 - .000064)^{1024} = .063$
- 1.4% false neg, 6.3% false pos

LSH

- The hash is easy to compute, even for a large database of prints, and the “at least one” part is easy to evaluate
- We can do even better than this in the fingerprints example (using AND)
- LSH works best when the overall level of similarity is not too high; different hashing approaches have been proposed for the case of lots of similarity

Ensembles

- This acts much the same way as bagging and other ensemble methods on classification and regression
- Combining lots of simple models (hash functions) can be more effective than creating one complex one
- Readily parallelizable; database can be distributed