Euclidean vs. City block geometry

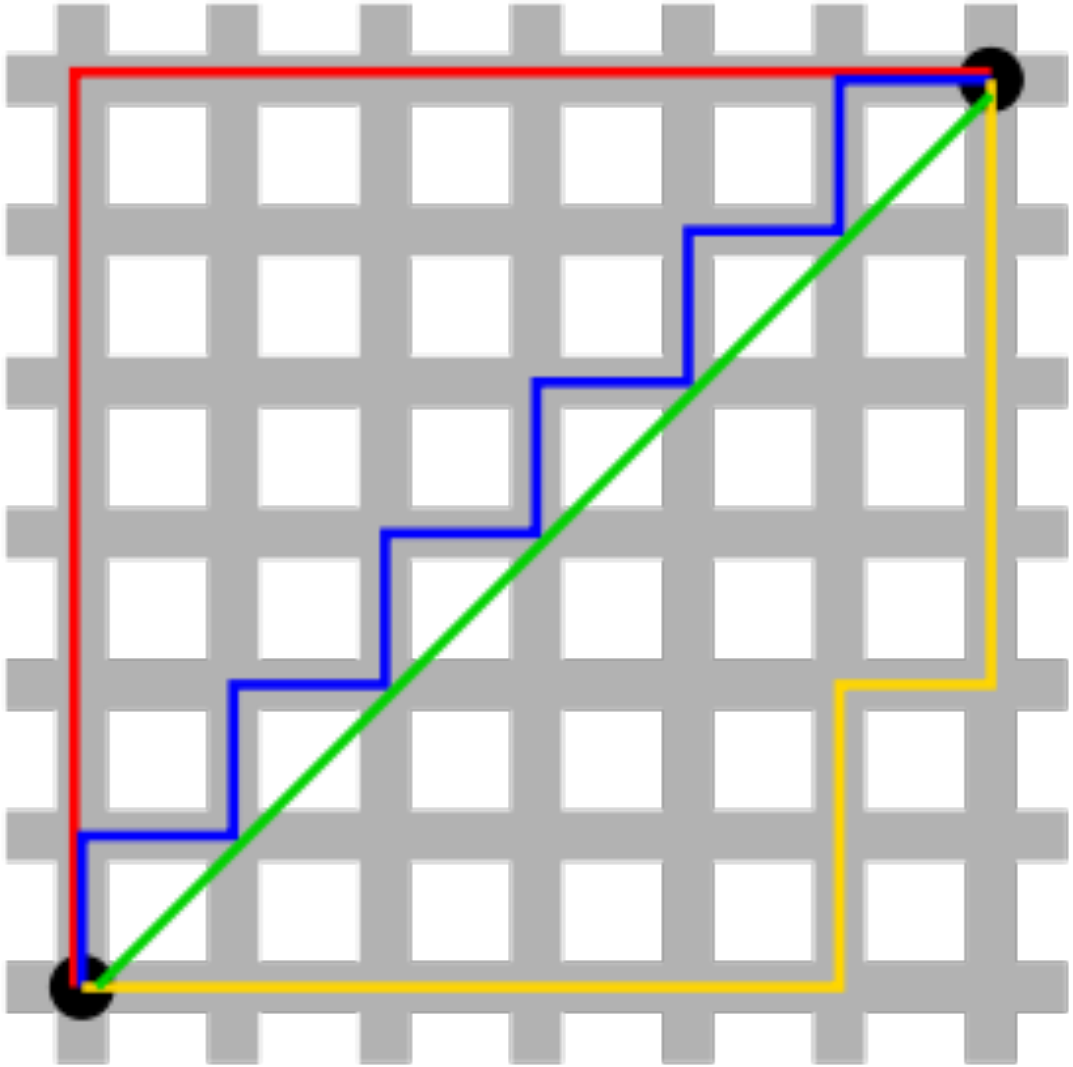


Figure taken from Wikipedia

Mahalanobis Distance

- Multi-dimensional generalization of the idea of measuring how many standard deviations away P is from the mean of D.
- Accounts for correlations

$$\text{mahalanobis}(p,q) = (p-q)\sum^{-1}(p-q)^T$$

Σ is the covariance matrix of the input data *X*

$$\Sigma_{j,k} = \frac{1}{n-1}\sum_{i=1}^{n}(X_{ij} - \overline{X}_j)(X_{ik} - \overline{X}_k)$$

Common Properties of a Similarity

- Similarities, also have some well known properties.
  - s(p, q) = 1 (or maximum similarity) only if p = q.
  - s(p, q) = s(q, p) for all p and q. (Symmetry)

Similarity Between Binary Vectors

- Common situation is that objects, *p* and *q*, have only binary attributes
- Compute similarities using the following quantities

  M_{01} = the number of attributes where p was 0 and q was 1

  M_{10} = the number of attributes where p was 1 and q was 0

  M_{00} = the number of attributes where p was 0 and q was 0

  M_{11} = the number of attributes where p was 1 and q was 1

- Simple Matching and Jaccard Coefficients

  SMC = number of matches / number of attributes

  $= (M_{11} + M_{00}) / (M_{01} + M_{10} + M_{11} + M_{00})$

  J = number of 11 matches / number of not-both-zero attribute values

  $= (M_{11}) / (M_{01} + M_{10} + M_{11})$

- Exercise: Construct an example with Jaccard similarity of 0 and SMC > 0.5

SMC versus Jaccard: Example

p = 1 0 0 0 0 0 0 0 0 0

q = 0 0 0 0 0 0 1 0 0 1

M_{01} = 2 (the number of attributes where p was 0 and q was 1)

M_{10} = 1 (the number of attributes where p was 1 and q was 0)

M_{00} = 7 (the number of attributes where p was 0 and q was 0)

M_{11} = 0 (the number of attributes where p was 1 and q was 1)

$SMC = (M_{11} + M_{00})/(M_{01} + M_{10} + M_{11} + M_{00}) = (0+7) / (2+1+0+7) = 0.7$

$J = (M_{11}) / (M_{01} + M_{10} + M_{11}) = 0 / (2 + 1 + 0) = 0$

Cosine Similarity

- If d_1 and d_2 are two document vectors, then

$$\cos(d_1, d_2) = (d_1 \bullet d_2) / \|d_1\| \|d_2\| ,$$

where • indicates vector dot product and $\|d\|$ is the length of vector d.

- Example:

d_1 = **3 2 0 5 0 0 0 2 0 0**

d_2 = **1 0 0 0 0 0 0 1 0 2**

$d_1 \bullet d_2 = 3*1 + 2*0 + 0*0 + 5*0 + 0*0 + 0*0 + 0*0 + 2*1 + 0*0 + 0*2 = 5$

$\|d_1\| = (3*3+2*2+0*0+5*5+0*0+0*0+0*0+2*2+0*0+0*0)^{0.5} = (42)^{0.5} = 6.481$

$\|d_2\| = (1*1+0*0+0*0+0*0+0*0+0*0+0*0+1*1+0*0+2*2)^{0.5} = (6)^{0.5} = 2.245$

$$\cos(d_1, d_2) = .3150$$

Correlation

Correlation measures the linear relationship between objects

$$corr(x, y) = \frac{\text{Covariance}(x, y)}{\text{standard\_dev(x)*standard\_dev(y)}}$$

$$= \frac{S_{xy}}{S_x S_y}$$

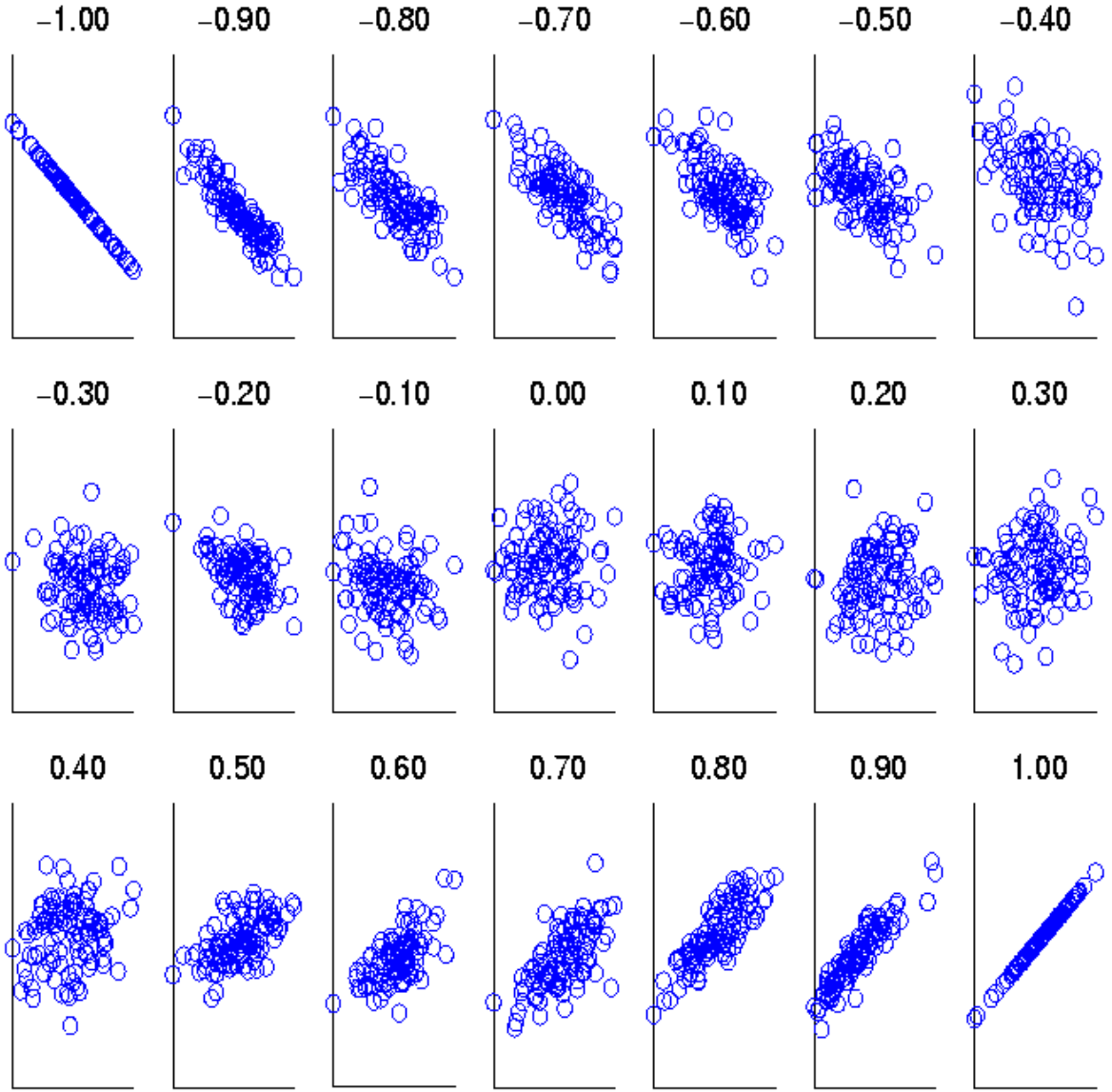
Correlation (cont.)

$$\text{covariance}(x,y) = \frac{1}{n-1}\sum_{k=1}^{n}(x_k - \bar{x})(y_k - \bar{y})$$

$$\text{standard\_dev}(x) = S_x = \sqrt{\frac{1}{n-1}\sum_{k=1}^{n}(x_k - \bar{x})^2}$$

$$\text{standard\_dev}(y) = S_y = \sqrt{\frac{1}{n-1}\sum_{k=1}^{n}(y_k - \bar{y})^2}$$

Visually Evaluating Correlation



General Approach for Combining Similarities

- Sometimes attributes are of many different types, but an overall similarity is needed.

1. For the k^{th} attribute, compute a similarity, s_k, in the range $[0, 1]$.
2. Define an indicator variable, δ_k, for the k_{th} attribute as follows:

$$\delta_k = \begin{cases} 0 & \text{if the } k^{th} \text{ attribute is a binary asymmetric attribute and both objects have a value of 0, or if one of the objects has a missing values for the } k^{th} \text{ attribute} \\ 1 & \text{otherwise} \end{cases}$$

3. Compute the overall similarity between the two objects using the following formula:

$$similarity(p, q) = \frac{\sum_{k=1}^{n} \delta_k s_k}{\sum_{k=1}^{n} \delta_k}$$

Using Weights to Combine Similarities

- May not want to treat all attributes the same.
  - Use weights w_k which are between 0 and 1 and sum to 1.

$$similarity(p,q) = \frac{\sum_{k=1}^{n} w_k \delta_k s_k}{\sum_{k=1}^{n} \delta_k}$$

$$distance(p,q) = \left(\sum_{k=1}^{n} w_k |p_k - q_k|^r \right)^{1/r}$$

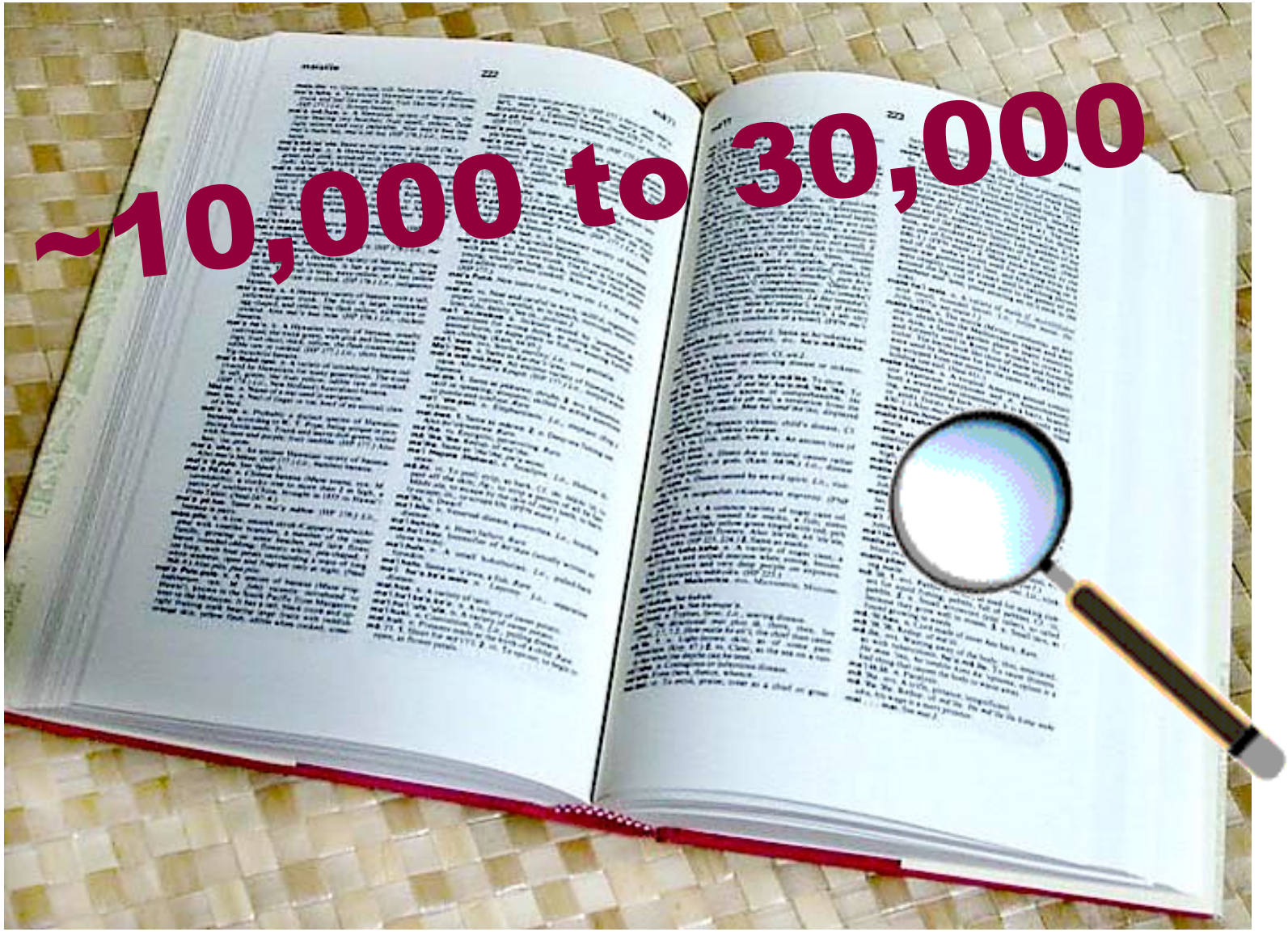
Which similarity function to use ?

- Depends on the application.
  - Analyze the attributes.
  - See their properties, min, max, etc
  - See their dependency on other attributes
  - Do you need similarity or distance ?
  - Do you need a metric ?
  - Try several functions.
  - Combine/merge.
- Active area of research!

Curse of Dimensionality

- Many problems of interest have objects with a large number of dimensions.
- An example…

What's the size of the dictionary?



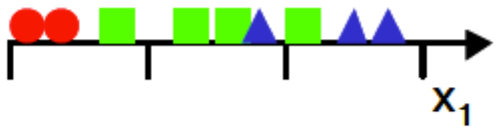
Curse of Dimensionality

- When dimensionality increases, data becomes increasingly sparse in the space that it occupies

- Also distances between objects gets skewed
  - More dimensions that contribute to the notion of distance or proximity which makes it uniform. This leads to trouble in clustering and classification settings.

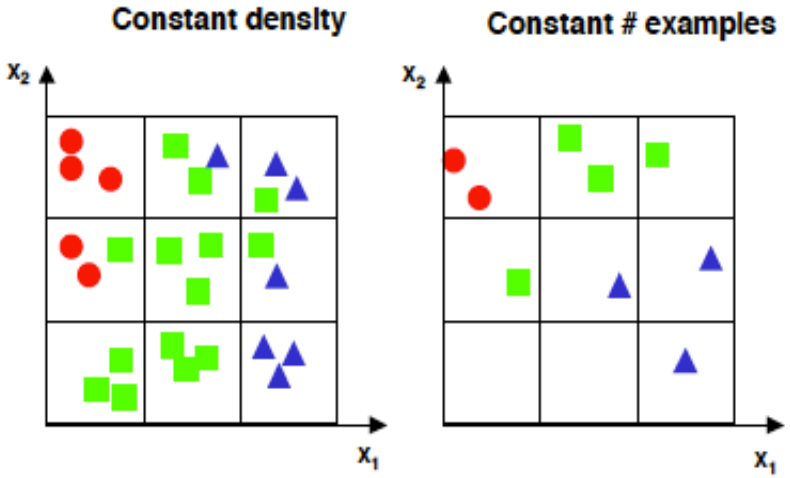
Driving the point home…

- **Consider a 3-class pattern recognition problem**
  - A simple approach would be to
    - Divide the feature space into uniform bins
    - Compute the ratio of examples for each class at each bin and,
    - For a new example, find its bin and choose the predominant class in that bin
  - In our toy problem we decide to start with one single feature and divide the real line into 3 segments

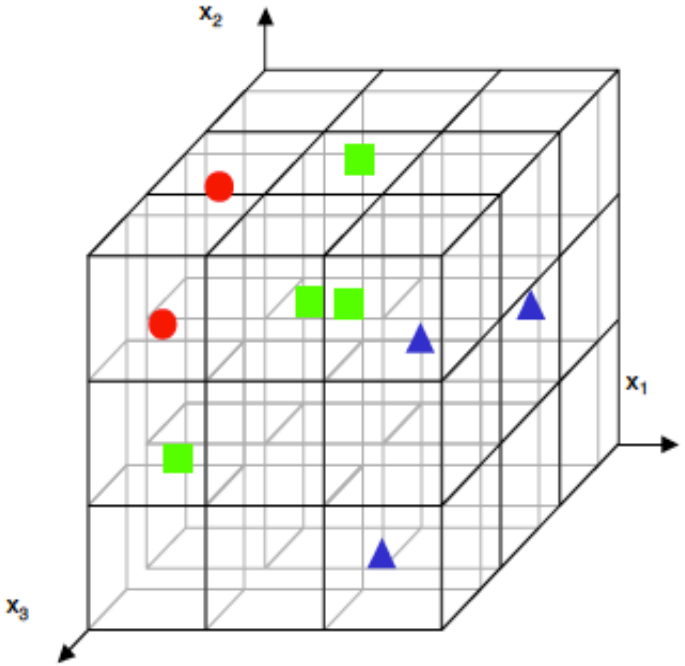


  - After we have done this, we notice that there exists too much overlap for the classes, so we decide to incorporate a second feature to try and improve the classification rate

- **We decide to preserve the granularity of each axis, which raises the number of bins from 3 (in 1D) to 3^2=9 (in 2D)**
  - At this point we are faced with a decision: do we maintain the density of examples per bin or do we keep the number of examples we used for the one-dimensional case?
    - Choosing to maintain the density increases the number of examples from 9 (in 1D) to 27 (in 2D)
    - Choosing to maintain the number of examples results in a 2D scatter plot that is very sparse

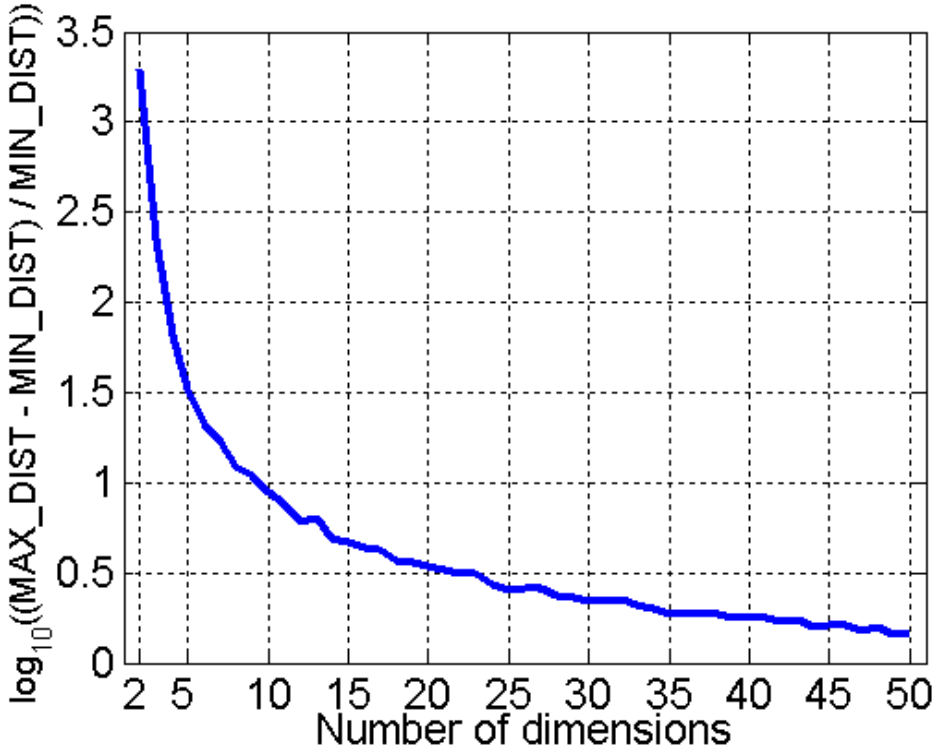


- **Moving to three features makes the problem worse:**
  - The number of bins grows to 3^3=27
  - For the same density of examples the number of needed examples becomes 81
  - For the same number of examples, well, the 3D scatter plot is almost empty



Curse of Dimensionality

- Definitions of density and distance between points, which is critical for clustering and outlier detection, become less meaningful



- **Randomly generate 500 points**
- **Compute difference between max and min distance between any pair of points**

Dimensionality Reduction

- Purpose:
  - Avoid curse of dimensionality
  - Reduce amount of time and memory required by data mining algorithms
  - Allow data to be more easily visualized
  - May help to eliminate irrelevant features or reduce noise
- Techniques
  - Principle Component Analysis
  - Singular Value Decomposition
  - Others: supervised and non-linear techniques

Nearest Neighbor Classification…

- Scaling issues
  - Attributes may have to be scaled to prevent distance measures from being dominated by one of the attributes
  - Example:
    - height of a person may vary from 1.5m to 1.8m
    - weight of a person may vary from 90lb to 300lb
    - income of a person may vary from $10K to $1M