

# Python for Computational Linguistics

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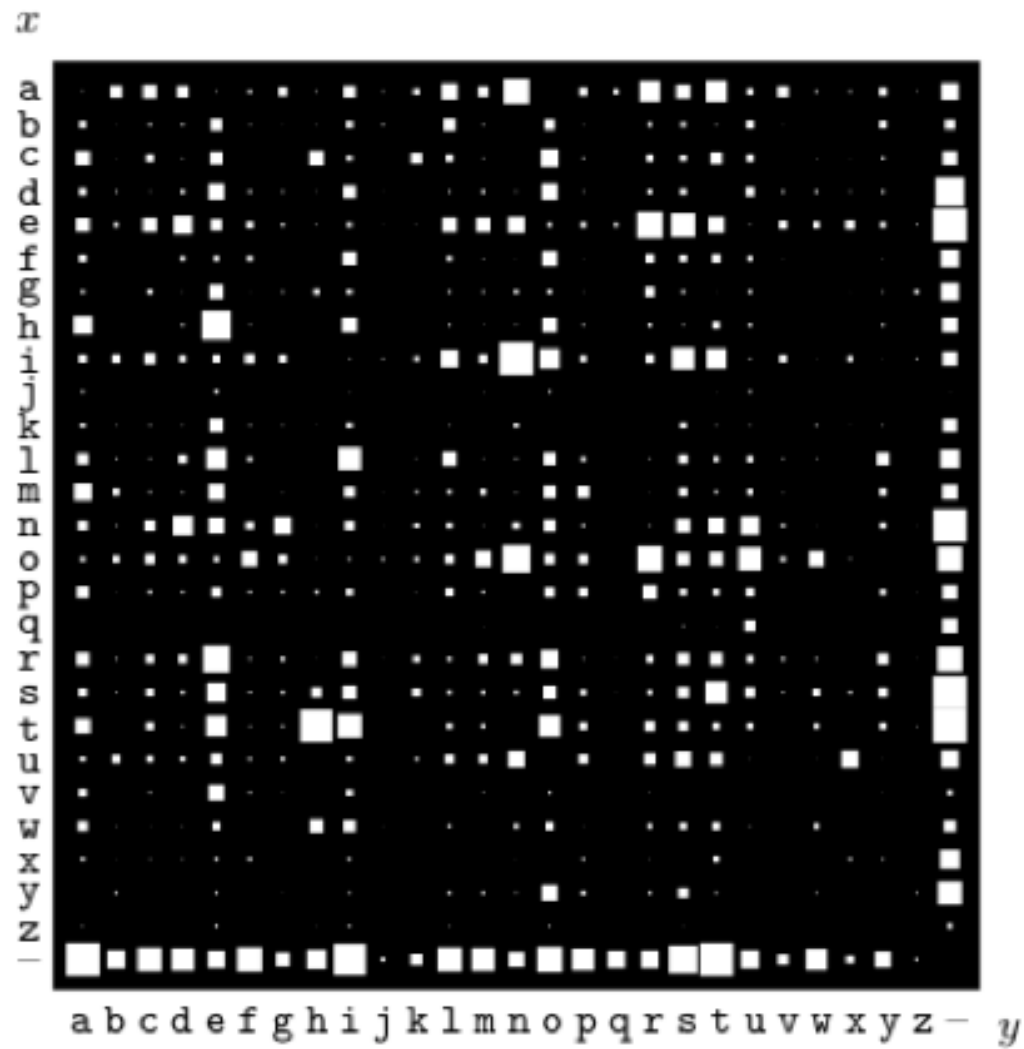
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# Frequency Profiles

- *Uni-gram* frequencies: freq.py, . . .
- *Bi-gram* frequencies:
- General  $n$ -gram models
- Examples: from [[MacKay\(2003\)](#)]

| $i$ | $a_i$ | $p_i$  |   |
|-----|-------|--------|---|
| 1   | a     | 0.0575 | a |
| 2   | b     | 0.0128 | b |
| 3   | c     | 0.0263 | c |
| 4   | d     | 0.0285 | d |
| 5   | e     | 0.0913 | e |
| 6   | f     | 0.0173 | f |
| 7   | g     | 0.0133 | g |
| 8   | h     | 0.0313 | h |
| 9   | i     | 0.0599 | i |
| 10  | j     | 0.0006 | j |
| 11  | k     | 0.0084 | k |
| 12  | l     | 0.0335 | l |
| 13  | m     | 0.0235 | m |
| 14  | n     | 0.0596 | n |
| 15  | o     | 0.0689 | o |
| 16  | p     | 0.0192 | p |
| 17  | q     | 0.0008 | q |
| 18  | r     | 0.0508 | r |
| 19  | s     | 0.0567 | s |
| 20  | t     | 0.0706 | t |
| 21  | u     | 0.0334 | u |
| 22  | v     | 0.0069 | v |
| 23  | w     | 0.0119 | w |
| 24  | x     | 0.0073 | x |
| 25  | y     | 0.0164 | y |
| 26  | z     | 0.0007 | z |
| 27  | -     | 0.1928 | - |





# Frequency Profiles

- What can we do with  $n$ -gram frequency profiles?
  - Compression, modeling expectations, study of quantitative language properties, ...
- What value for  $n$  is best for what purpose?

# Language Identification

- *N*-gram models for Language Identification
- Files: `lid.py`, `lidtrainer.py`, `*.dat`
- Calculations:
  - Mean of frequencies
  - Deviation

# Numerical Statistics

- Measures of central tendencies of data
  - Mean
  - Median
  - Mode
- Measures of variation/variability
  - Spread in data

# Numerical Statistics

- Arithmetic Mean
  - Data set:

| File           | Count words |
|----------------|-------------|
| Flo031201.txt  | 10346       |
| Flo031202a.txt | 5031        |
| Flo031202b.txt | 11876       |
| Flo031203.txt  | 12175       |
| Flo031204.txt  | 10943       |



# Numerical Statistics

- Arithmetic Mean

$$\text{arithmetic mean} = \frac{\text{sum of measures}}{\text{number of measures}}$$

– example:

$$\frac{10346 + 5031 + 11876 + 12175 + 10943}{5} = 10074.2$$

# Numerical Statistics

- Median
  - Middle value of ordered measure values

| File                 | Count words  |
|----------------------|--------------|
| Flo031202a.txt       | 5031         |
| Flo031201.txt        | 10346        |
| <b>Flo031204.txt</b> | <b>10943</b> |
| Flo031202b.txt       | 11876        |
| Flo031203.txt        | 12175        |

# Numerical Statistics

- Median
  - Decrease relevance of outliers:

| File           | Count words |
|----------------|-------------|
| Flo031202a.txt | 5031        |
| Flo031201.txt  | 10346       |
| Flo031204.txt  | 10943       |
| Flo031202b.txt | 11876       |
| Flo031203.txt  | 12175       |

# Numerical Statistics

- Median
  - with even number of elements:

| File           | Count words |
|----------------|-------------|
| Flo031202a.txt | 5031        |
| Flo031201.txt  | 10346       |
| Flo031204.txt  | 10943       |
| Flo031202b.txt | 11876       |

- Arithmetic mean of the two middle values:

$$\frac{10346 + 10943}{2} = 10644.5$$

# Numerical Statistics

- Mean: 10074.2
- Median: 10943
- Mean is reduced on the basis of the outlier:
  - Flo031202a.txt          5031
- Median may be a better indicator of central tendency if outliers/extreme values are present.

# Numerical Statistics

- Mode
  - The measure value that occurs most often:

| File           | Count words |
|----------------|-------------|
| Flo031202a.txt | 5031        |
| Flo031201.txt  | 10943       |
| Flo031204.txt  | 10943       |
| Flo031202b.txt | 6329        |
| Flo031203.txt  | 12175       |

- Mode = 10943

# Numerical Statistics

- Approximation of
  - Mode
    - $mean - 3 (mean - median)$
  - Median
    - $(2 mean + mode) / 3$
  - Mean
    - $(3 median - mode) / 2$

# Numerical Statistics

- Notation

- Mean (x bar):  $\bar{x}$

- Mean of a population:  $\mu$

- Sum of values:  $\Sigma$



# Numerical Statistics

- Notation example:
  - Arithmetic mean:

$$\bar{x} = \frac{\sum x}{n} = \frac{x_1 + x_2 + \dots + x_n}{n}$$

# Numerical Statistics

- Arithmetic mean for grouped data:

| Files | Count words |
|-------|-------------|
| 35%   | 0-4999      |
| 30%   | 5000-9999   |
| 25%   | 10000-14999 |
| 10%   | 15000-19999 |

- With 100 sample documents what is the arithmetic mean?

# Numerical Statistics

- Arithmetic mean for grouped data:

$$\bar{x} = \frac{\sum fx}{n}$$

- $f$  = frequency
- $x$  = midpoint

# Numerical Statistics

- Arithmetic mean for grouped data:

| Files | Midpoint | $fx$   | Count words |
|-------|----------|--------|-------------|
| 35    | 2500     | 87500  | 0-4999      |
| 30    | 7500     | 225000 | 5000-9999   |
| 25    | 12500    | 312500 | 10000-14999 |
| 10    | 17500    | 175000 | 15000-19999 |

$$\bar{x} = \frac{\sum fx}{n} = \frac{87500 + 225000 + 312500 + 175000}{100} = \frac{800000}{100} = 8000$$

# Numerical Statistics

- Median for grouped data:

$$median = L + \frac{w}{f_{med}} \left( .5n - \sum f_b \right)$$

- $L$  = lower class limit that contains the interval
- $n$  = total number of measurements
- $w$  = class width
- $f_{med}$  = frequency of the class containing the median
- $\bullet f_b$  = sum of the frequencies for all classes before the median class

# Numerical Statistics

- Median for grouped data:

| Files | Count words |
|-------|-------------|
| 35    | 0-4999      |
| 30    | 5000-9999   |
| 25    | 10000-14999 |
| 10    | 15000-19999 |

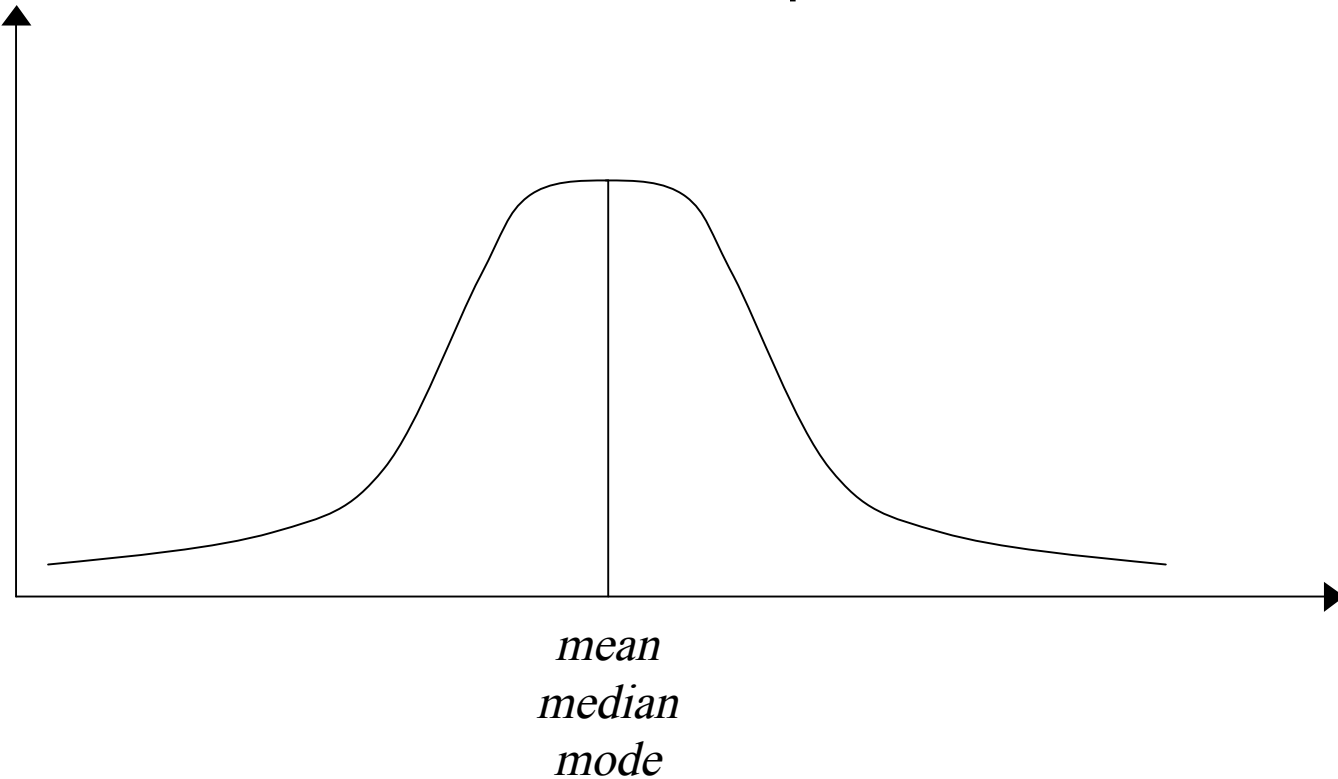
$$median = 5000 + \frac{4999}{30}(50 - 35) = 7499.5$$

# Numerical Statistics

- Distribution
  - Symmetric distribution
  - Skewed curves
    - negatively skewed curves
    - positively skewed curves

# Numerical Statistics

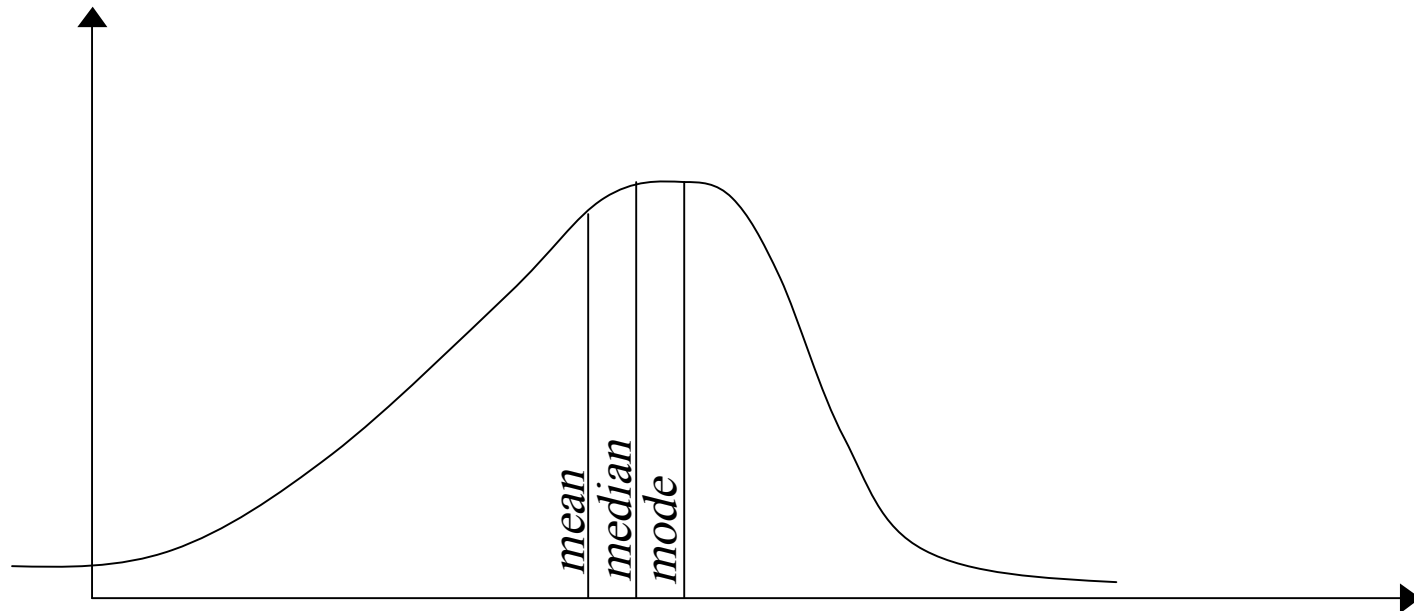
- Symmetric distribution
  - Mean, median and mode are equal.





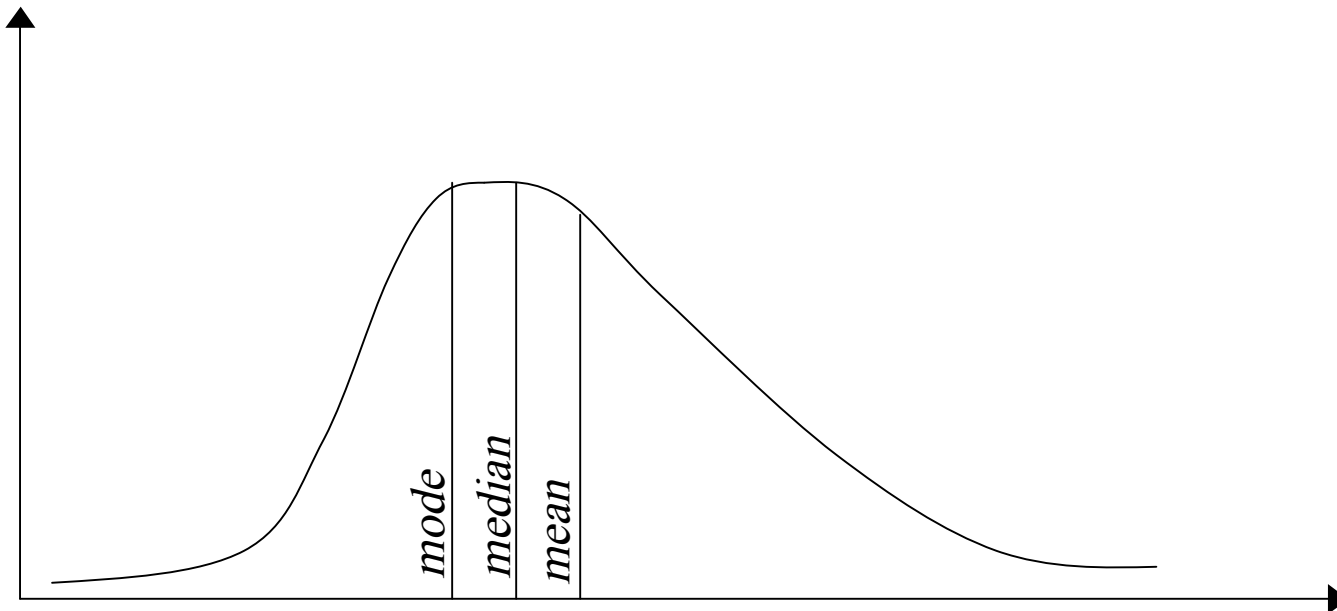
# Numerical Statistics

- Skewed curves
  - Negatively skewed distribution:  $\text{mean} < \text{median} < \text{mode}$



# Numerical Statistics

- Skewed curves
  - Positively skewed distribution:  $\text{mode} < \text{median} < \text{mean}$



# Numerical Statistics

- Variability

| Experiment 1 | Experiment 2 |
|--------------|--------------|
| 195          | 10           |
| 210          | 0            |
| 199          | 400          |
| 200          | 20           |
| 205          | 380          |
| 190          | 200          |
| 200          | 390          |
| 201          | 200          |

# Numerical Statistics

- Variability
  - For both experiments:
    - mean: 200
    - mode: 200
    - median: 200
  - Experiment 2 has greater variation.
- Measure of variation:
  - Range
  - Deviation
  - Variance

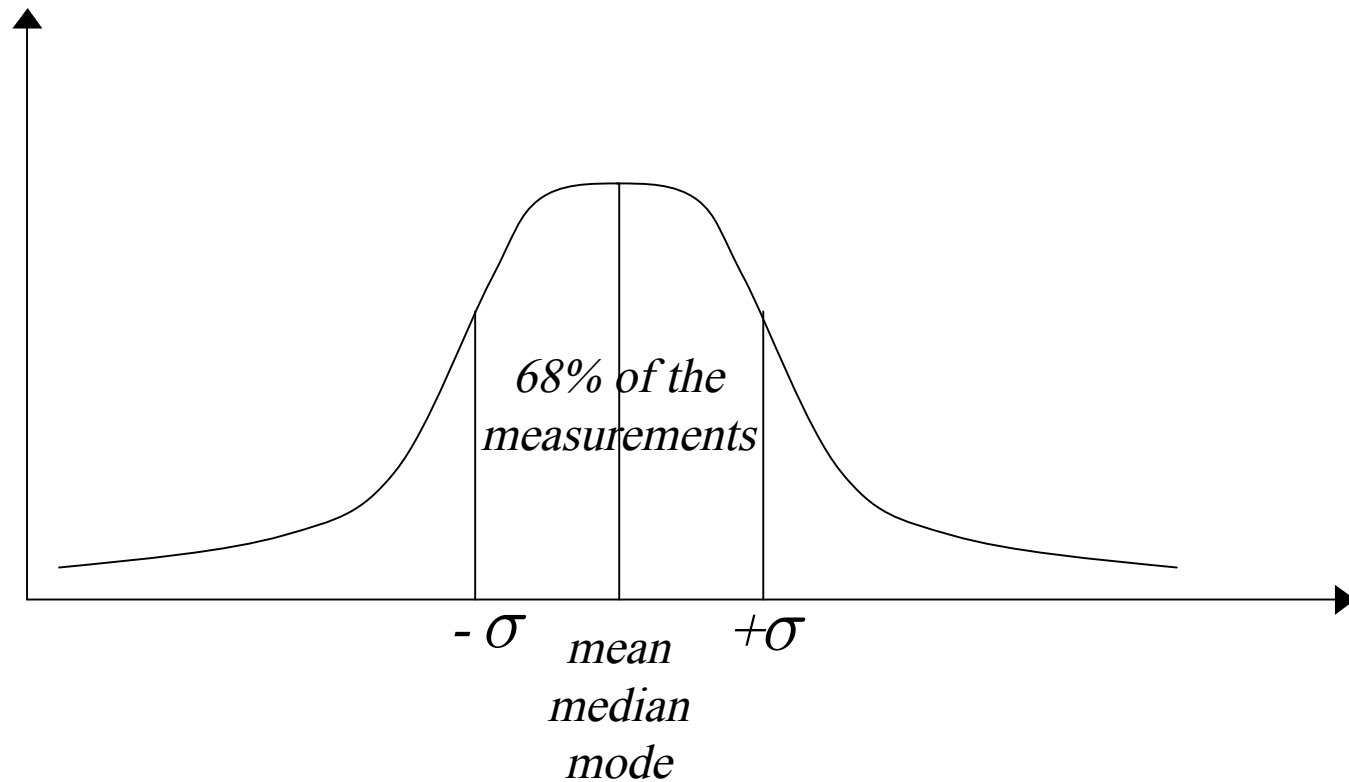
# Numerical Statistics

- Range
  - Difference between largest and smallest value:
    - Experiment 1:  $210 - 190 = 20$
    - Experiment 2:  $400 - 0 = 400$
- Deviation
  - Distance of the measurements away from the mean:
    - Experiment 1: less
    - Experiment 2: more

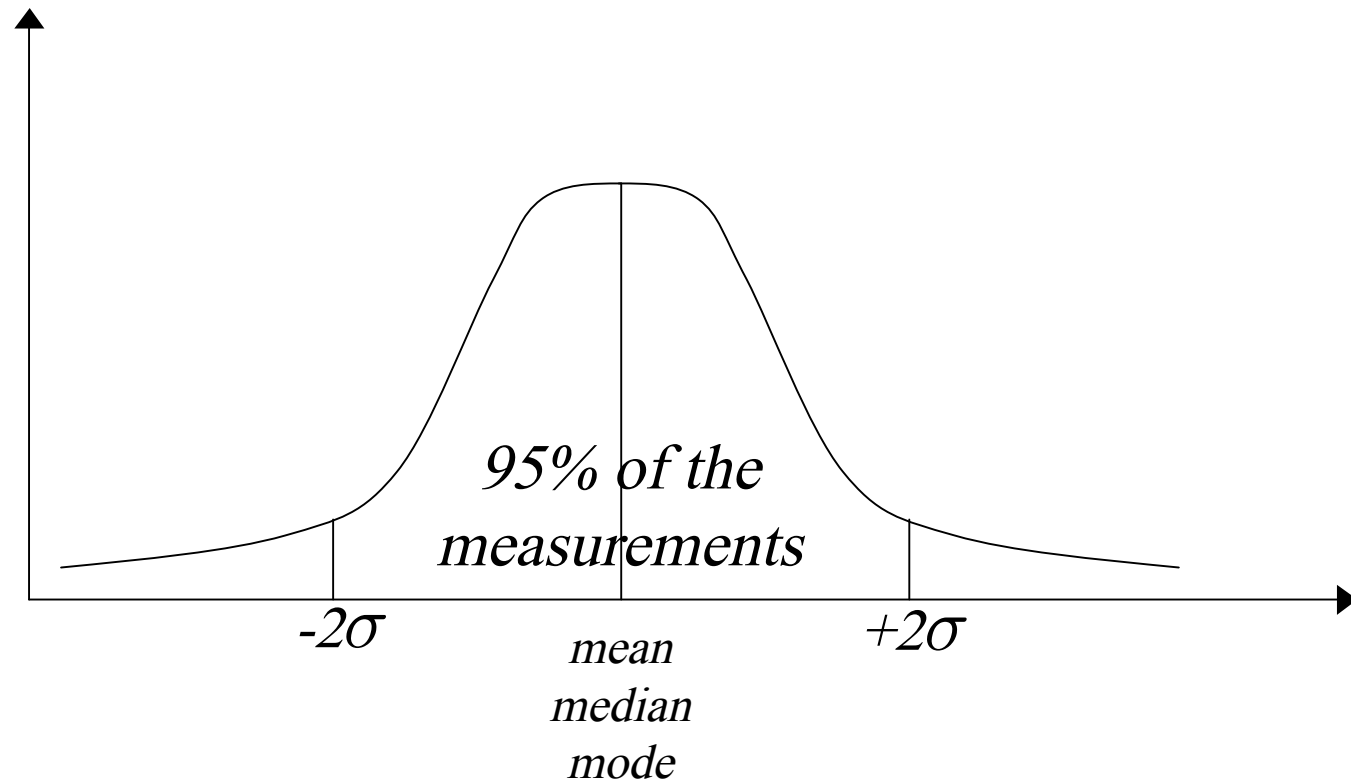
# Numerical Statistics

- Notation
  - $s^2$  = variance of a sample
  - $\sigma^2$  = variance of a population
  - $s$  = standard deviation of a sample
  - $\sigma$  = standard deviation of a population

# Numerical Statistics

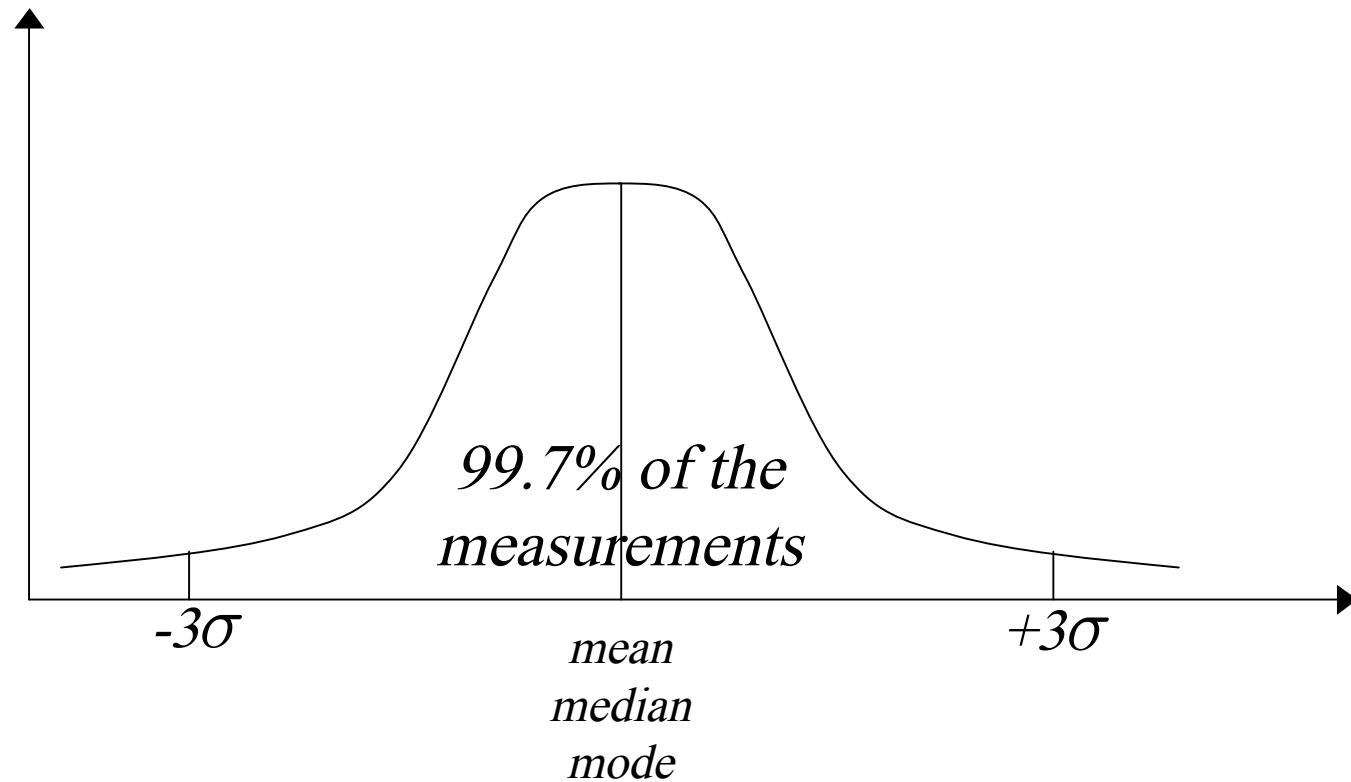


# Numerical Statistics





# Numerical Statistics



# Language Identification

- General  $n$ -gram class
- Files: `ngram.py`
- Task:
  - Develop a simple  $n$ -gram script on the basis of the  $n$ -gram class for uni-gram, bi-gram, and tri-gram models
  - Read in the data from the Brown corpus: a.  $n$ -gram model of the tokens and b.  $n$ -gram model of the types

# Collocations

- Words in context
  - distribution
  - fixed expressions
  - collocations
    - statistical properties
    - function words

# Tests for collocations

- Statistics
- Significance tests

# Significance

- Notations:
  - Type I error rate of .05
  - Alpha level of .05 or  $\alpha = .05$
  - Finding is significant at the .05 level
  - Confidence level is 95%
  - 95% certainty that a result is not due to chance
  - A 1 in 20 chance of obtaining the result

# Testing

- Statistics as testing of scientific hypotheses
- Strategies:
  - Formulating a Research Hypothesis or Alternative Hypothesis ( $H_a$ )
    - Statement of the expectation to be tested

# Testing

- Strategies:
  - Derivation of a statement that is the opposite of the research hypothesis: Null Hypothesis ( $H_0$ )
  - Testing the null hypothesis

# Testing

- Statistics as testing of scientific hypotheses
- Strategies:
  - If the null hypothesis can be rejected, this is evidence in favor of the research hypothesis.



# Testing

- Strategies:
- Usually:
  - No prove for research hypothesis, just support for it.

# Testing

- Research Hypothesis:
  - At IU linguistics students perform differently in statistics than computer science students.
    - $H_a: \mu_1 \neq \mu_2$
    - $H_a: \mu_1 - \mu_2 \neq 0$

# Testing

- Null Hypothesis:
  - At IU linguistics students perform the same in statistics as computer science students.
    - $H_0: \mu_1 = \mu_2$
    - $H_0: \mu_1 - \mu_2 = 0$

# Testing

- More specific: Research Hypothesis:
  - At IU linguistics students perform better in statistics than computer science students.
    - $H_a: \mu_1 > \mu_2$
    - $H_a: \mu_1 - \mu_2 > 0$

# Testing

- More specific: Null Hypothesis
  - At IU linguistics students perform worse in statistics, or equal to computer science students.
    - $H_0: \mu_1 \leq \mu_2$
    - $H_0: \mu_1 - \mu_2 \leq 0$

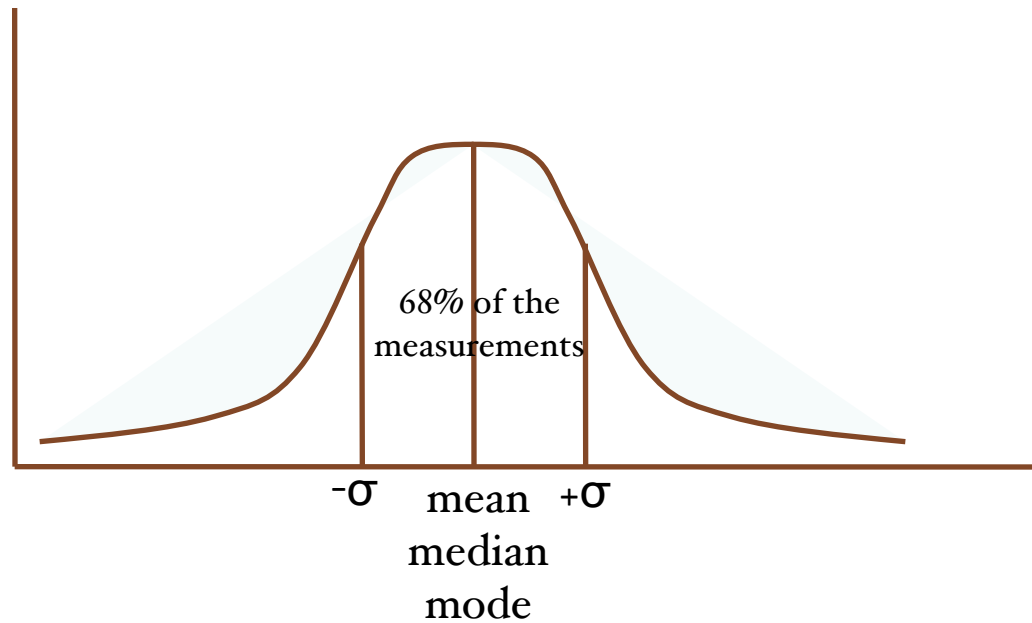
# Testing

- Given the distribution of a known area
  - e.g. normal distribution
- estimate the probability of obtaining a certain value as a result of chance.
- If the probability is low, the likelihood for a mere coincidence is low, i.e. a certain theory is correct.

# Testing

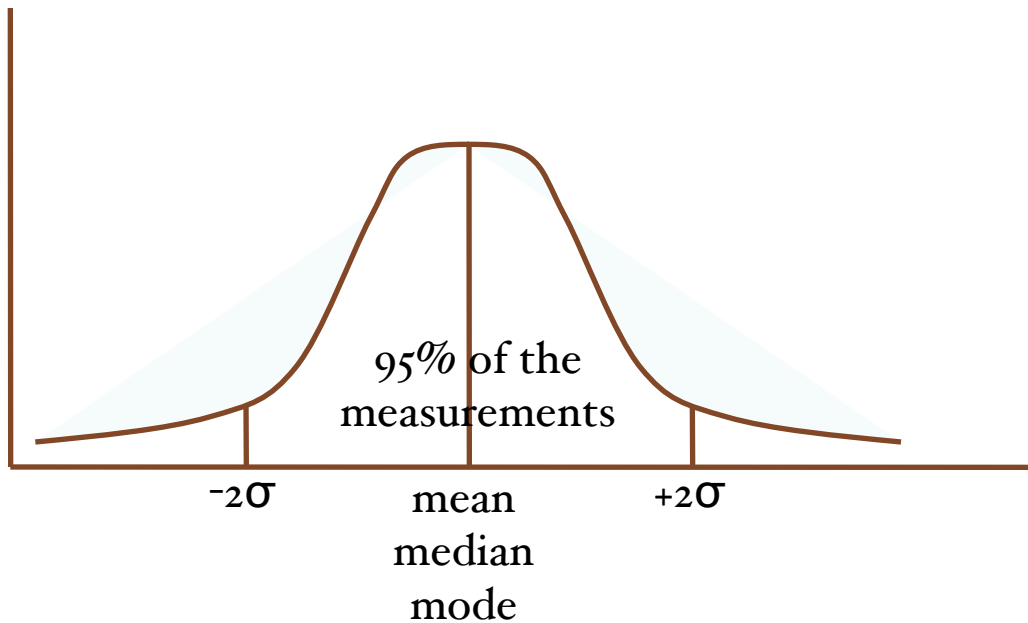
- Two possible outcomes of test:
  - Rejection of null hypothesis
  - Acceptance of null hypothesis

# Numerical Statistics

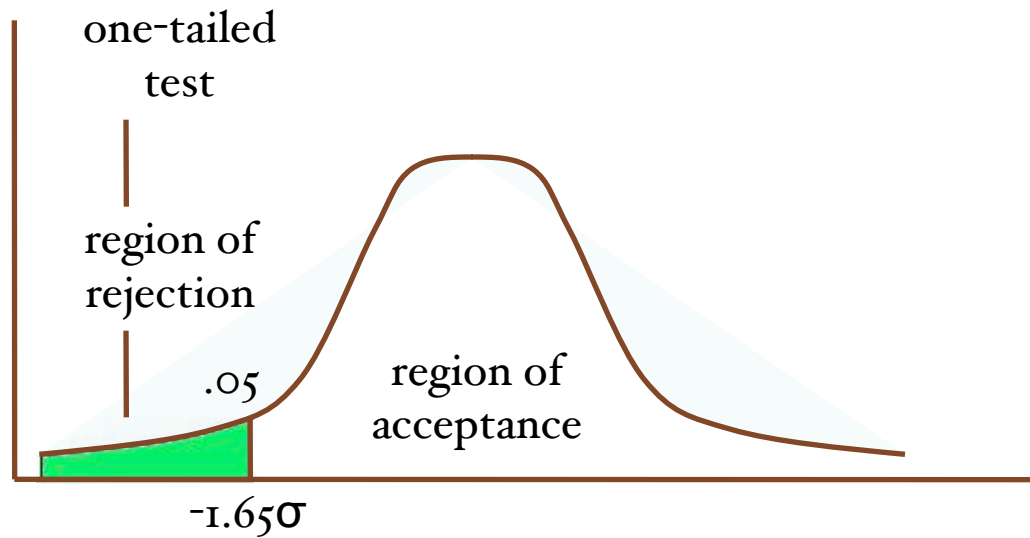




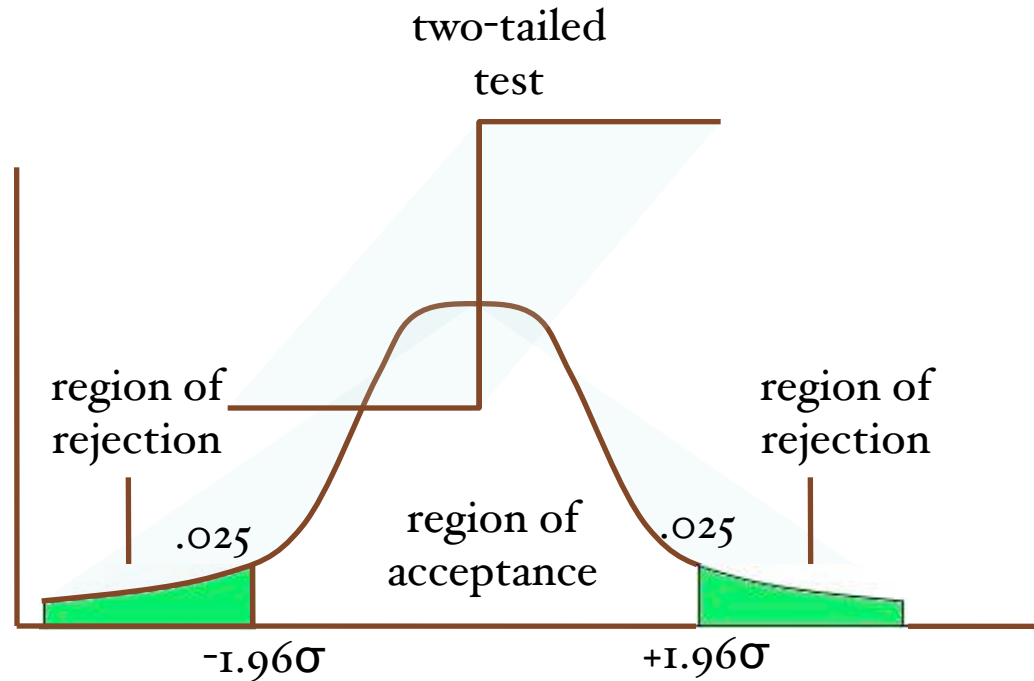
# Numerical Statistics



# Numerical Statistics



# Numerical Statistics



# Significance Table

| <i>P</i> | <b>0.99</b> | <b>0.95</b> | 0.10  | 0.05  | 0.01  | 0.005 | 0.001 |
|----------|-------------|-------------|-------|-------|-------|-------|-------|
| d.f. 1   | 0.00016     | 0.0039      | 2.71  | 3.84  | 6.63  | 7.88  | 10.83 |
| 2        | 0.020       | 0.10        | 4.60  | 5.99  | 9.21  | 10.60 | 13.82 |
| 3        | 0.115       | 0.35        | 6.25  | 7.81  | 11.34 | 12.84 | 16.27 |
| 4        | 0.297       | 0.71        | 7.78  | 9.49  | 13.28 | 14.86 | 18.47 |
| 100      | 70.06       | 77.93       | 118.5 | 124.3 | 135.8 | 140.2 | 149.4 |

# Testing

- Probability as significance level
- Example: Collocations
  - Null Hypothesis: independence of two words
  - $P(w_1w_2) = P(w_1) P(w_2)$

# chi-square ( $\chi^2$ ) test

- Preferred activities over a population sample of 125 people:

|               | <b>bowling</b> | <b>dancing</b> | <b>computer</b> | <b>total</b> |
|---------------|----------------|----------------|-----------------|--------------|
| <b>male</b>   | 30             | 29             | 16              | 75           |
| <b>female</b> | 12             | 33             | 5               | 50           |
| <b>total</b>  | 42             | 62             | 21              | 125          |

# chi-square ( $\chi^2$ ) test

- Is the choice of activities related to the gender?
- If the two variables are independent, we can use these probabilities to predict how many people should be in each cell.
- If the actual number is different from the expectation for independence, the two variables must be related.

# chi-square ( $\chi^2$ ) test

- Research Hypothesis:
  - The variables are dependent.
- Null Hypothesis:
  - The variables are independent.



# chi-square ( $\chi^2$ ) test

- Overall probability of a person in the sample being:
  - male:  $75/125 = .6$
  - female:  $50/125 = .4$

# chi-square ( $\chi^2$ ) test

- Overall probability of each preference:
  - bowling:  $42/125 = .336$
  - dancing:  $62/125 = .496$
  - computer games:  $21/125 = .168$

# chi-square ( $\chi^2$ ) test

- Independent events: multiplication rule
- The probability of two events occurring is the product of their two probabilities.

# chi-square ( $\chi^2$ ) test

- Probability of a person in the sample being male and preferring bowling:
  - P(male & bowling):  $.6 \times .336 = .202$
  - Expectation:  $.202 \times 125 = 25.2$

# chi-square ( $\chi^2$ ) test

- Multiplication of row total with column total and division by total number in sample:
- $(75 \times 42) / 125 = 25.2$

|        | bowling   | dancing   | computer  | total |
|--------|-----------|-----------|-----------|-------|
| male   | 30 (25.2) | 29 (37.2) | 16 (12.6) | 75    |
| female | 12 (16.8) | 33 (24.8) | 5 (8.4)   | 50    |
| total  | 42        | 62        | 21        | 125   |

# chi-square ( $\chi^2$ ) test

- Formula: 
$$\chi^2 = \sum \frac{(\textit{observed} - \textit{expected})^2}{\textit{expected}}$$

$$\chi^2 = \frac{(30 - 25.2)^2}{25.2} + \frac{(29 - 37.2)^2}{37.2} + \frac{(16 - 12.6)^2}{12.6} + \frac{(12 - 16.8)^2}{16.8} + \frac{(33 - 24.8)^2}{24.8} + \frac{(5 - 8.4)^2}{8.4} = 9.097$$

# chi-square ( $\chi^2$ ) test

- The larger  $\chi^2$ , the more likely the variables are related.
- Square effect of cells with large differences.

# chi-square ( $\chi^2$ ) test

- Probability distribution of  $\chi^2$ :
  - Critical values in table
  - Degree-of-freedom:
    - $df = (\text{number-of-rows} - 1) \times (\text{number-of-columns} - 1)$
    - Example:  $(2 - 1) \times (3 - 1) = 2$
    - Example: 9.097 ( $< .025$ ;  $> .01$ )



# chi-square ( $\chi^2$ ) test

- Example: 9.097 ( $< .025$ ;  $> .01$ )
  - Significance (at levels: .05, .01)!
  - Rejection of Null Hypotheses (independence of variables)

# chi-square ( $\chi^2$ ) test

- Collocations
  - new, companies

|              | w1=new | w1-new   | total    |
|--------------|--------|----------|----------|
| w2=companies | 8      | 4667     | 4675     |
| w2-companies | 15820  | 14287181 | 14303001 |
| total        | 15828  | 14291848 | 14307676 |

# Statistics

- Maximum Likelihood Estimate
  - Frequency oriented
  - No inclusion of prior belief: here e. g. assuming a normal distribution, i. e.
  - No inclusion of a prior probability distribution

# Statistics

- Example: Coin tossing
  - Observation:  $8 \times \textit{head} \ \& \ 2 \times \textit{tail}$
  - Prior probability distribution:  $5 \times \textit{head} \ \& \ 5 \times \textit{tail}$
  - Probability mass:  $\frac{1}{2}$
  - How does observation:  $X = \textit{tail}$  change our expectation?

# Statistics

- Example: Coin tossing
  - Bayesian answer: update prior belief (= prior probability distribution) in face of evidence and generate posterior probability estimate

# Bayesian Statistics

- Example:
  - Data is added incrementally/sequentially
  - Given an a-priori probability distribution
    - \* Update our beliefs with every new datum
    - \* Calculate Maximum A Posteriori (MAP) distribution
  - MAP probability becomes the new prior probability for the next datum

# Information Theory

- Surprise effect:
  - Coin tossing and observing the results
  - What is our prior believe or expectation about an outcome?
  - How surprised are we to see a certain outcome?
- Data compression:
  - Knowing about the distributional properties of some data
  - What is the best compression we can get by mapping it to bit-representations?
  - Is there a formal way to calculate the optimal representation for data transmission?

# Information Theory

- Entropy:
  - Entropy as uncertainty
    - \* Tossing a coin = not knowing what the outcome will be.
    - \* Probability distribution:
      - Fair coin
      - Biased coin, unlimited probability distributions



# Information Theory

- Entropy:
  - Entropy as uncertainty
    - \* Is there a way to calculate the uncertainty and formulate a function on the basis of a probability distribution?
    - \* Let us design such a function:
      - $H[X]$  is the measure for  $X$ , with  $X$  a probability distribution
      - $H$  takes  $X$ , with  $X = \{P(1), P(2), \dots, P(N)\}$  as an argument
      - and returns a real number, the value of uncertainty

# Information Theory

- Designing a function for Entropy:
  1. Maximum uncertainty in uniform distribution: every possible outcome is equally likely
    - This is the maximum  $H$  can return
  2.  $H$  is a continuous function over the probabilities
    - changing the probabilities slightly leads to slight changes of  $H$

# Information Theory

- Grouping Probabilities:

- $X = \{P(1) = .5, P(2) = .2, P(3) = (.3)\}$ :

- is equivalent to:

- \*  $X = \{P(1) = .5, P(Y) = .5\}$

- \*  $Y = \{P(2) = .4, P(3) = .6\}$

3. Uncertainty  $H$  cannot depend on the grouping of events for a random variable.

# Information Theory

- Entropy: Formal reformulation of (1–3)
  - $H(p)$  is a real valued function of  $P(1), P(2), \dots, P(N)$ , with  $N$  the number of values for the random variable or length of *domain*, then
    1.  $H(P(1), P(2), \dots, P(N))$  reaches a maximum if the distribution is uniform:  $P(i) = 1/N, N = \text{len}(i), \forall i$ .
    2.  $H(P(1), P(2), \dots, P(N))$  is a continuous function of all  $P(i)$ 's.

# Information Theory

- Entropy: Formal reformulation of (1–3)
  3. Independence of subsets of probability groups: for  $N$  probabilities grouped into  $k$  subsets,  $w_k$ :

$$w_1 = \sum_{i=1}^{n_1} p_i; w_2 = \sum_{i=n_1+1}^{n_2} p_i; \dots$$

# Information Theory

- Entropy: Formal reformulation of (1–3)

3. Independence of subsets of probability groups: assumption

$$H[p] = H[w] + \sum_{j=1}^k w_j H[\{p_i/w_j\}_j]$$

–  $\{p_i/w_j\}$  is: sum extends over  $p_i$ 's that make up a particular  $w_j$

# Information Theory

- Entropy: Summary

- Given the three requirements it follows that:

$$H[X] = k \sum_{x \in X} Pr(x) \log Pr(x)$$

- with  $k$  and arbitrary constant [8, 40, 44]. For  $k = -1$  and  $\log_2$  the units are bit.

# Information Theory

- Average Shannon Entropy: measured in bits

$$H[X] = -1 \sum_{x \in X} Pr(x) \lg Pr(x)$$

$$H[X] = \sum_{x \in X} Pr(x) \lg \frac{1}{Pr(x)}$$



# Information Theory

- Average Shannon Entropy of one outcome: measured in bits

$$h[x] = Pr(x) \lg \frac{1}{Pr(x)}$$

# Joint Entropy

- For a pair of random variables:  $X, Y \sim p(x, y)$

$$H(X, Y) = - \sum_{x \in X} \sum_{y \in Y} p(x, y) \lg p(x, y)$$

- $X = \{A = .4, B = .6\}$
- $Y = \{C = .2, D = .8\}$

# Joint Entropy

- $X \wedge Y = \{AC = .4 \times .2, AD = .4 \times .8, BC = .6 \times .2, BD = .6 \times .8\}$
- $X \wedge Y = \{AC = .08, AD = .32, BC = .12, BD = .48\}$
- $Z = \{AC = .08, AD = .32, BC = .12, BD = .48\}$

# Mutual Information

- Reduction of uncertainty of one random variable due to knowing about another.
- Amount of information one random variable contains about another.
- Symmetric, Non-negative
- $MI = 0$ , if two random variables are independent
- MI is high, if two random variables are dependent, depending on their entropy.

# Mutual Information

- MI over random variables!

→ Pointwise Mutual Information

- Pointwise MI over selected values of random variables!

$$I(X; Y) = P(XY) \lg \frac{P(XY)}{P(X)P(Y)}$$

- How many bits can we spare by storing two elements, rather than each single element alone?

## Relative Entropy – KL Divergence

- Average number of bits that are wasted by encoding events from random variable  $X$  with a code based on random variable  $Y$ . How close are two pmf's?

$$D(y||x) = p(y) \lg \frac{p(y)}{p(y|x)}$$

$$D(y||x) = p(y) \lg \frac{p(y)}{\frac{p(xy)}{p(x)}} = p(y) \lg \frac{p(y)p(x)}{p(xy)}$$

- How many bits more would we use by storing  $\langle xy \rangle$ , rather than each single element alone?

# Vector Space

- Representing elements in a vector space:
  - $x = [2.0, 4.9, 12.4, \dots]$
  - Matrix:
    - \* row = elements
    - \* column = features
  - Representation in an n-dimensional space
  - Linear Algebra for analysis of vector similarity
  - Vector similarity for clustering, grouping, association

# Vector Space

$$\mathcal{X} = \begin{bmatrix} \mathbf{X}_{1,1} & \mathbf{X}_{1,2} & \cdots & \mathbf{X}_{1,d} \\ \mathbf{X}_{2,1} & \mathbf{X}_{2,2} & \cdots & \mathbf{X}_{2,d} \\ \vdots & & & \\ \mathbf{X}_{k,1} & \mathbf{X}_{k,2} & \cdots & \mathbf{X}_{k,d} \end{bmatrix}$$

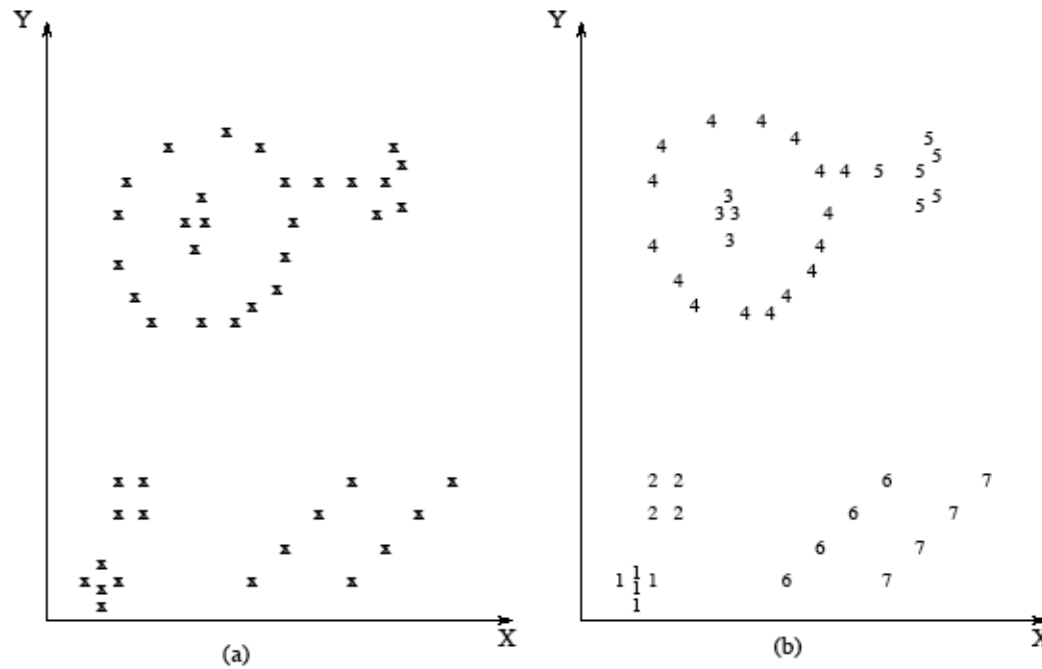


# Vector Space

- What is mapped on the vector space?
  - Number of individual words in a document: each row one document, each column a word
  - Number of individual words in the context of one word (left and right)
  - Features of words, documents, etc.

# Vector Space

- Each vector is a point in  $n$ -dimensional space: Example for  $n$



# Optimization Clustering

- Given a clustering criterion
  - How to find a partition into  $n$  groups that optimizes the criterion?
- Find all possible partitions and calculate their value of the given criterion.
- Choose the partition with the optimal value.

# Optimization Clustering

- Complexity:
  - Number of possible partitions given  $n$  objects into  $g$  groups (Liu, 1968):

$$N(n, g) = \frac{1}{g!} \sum_{m=1}^g (-1)^{g-m} \binom{g}{m} m^n \quad (1)$$

# Optimization Clustering

- Complexity example:

$$N(50, 4) = 5.3 \times 10^{28} \quad (2)$$

$$N(100, 5) = 6.6 \times 10^{67} \quad (3)$$

# Optimization Clustering

- Complexity solution
  - Programming strategies
    - \* Dynamic programming
    - \* Branch and bound algorithms
- Hill-climbing algorithms
  - Iterative search for optimum value of clustering criteria via rearrangement of existing partitions

# Optimization Clustering

- K-means generates
  - $k$  number of disjoint clusters (non-hierarchical)
  - globular clusters (spherical, elliptical, convex)
- properties:
  - numerical
  - unsupervised (limited!)
  - iterative

# Optimization Clustering

- K-means
  - $k$  clusters
  - At least one element per cluster
  - No overlapping clusters
  - Non-hierarchical
  - Every member of a cluster is closer to its cluster than to any other cluster
  - Procedure



# Optimization Clustering

- K-means
  - Initial partitioning of data set into  $k$  clusters
  - For each data point: calculate distance to each cluster
  - If one data point is closer to another cluster, relocate it
  - Repeat until no further relocations possible

# Optimization Clustering

- K-means advantages
  - For large number of variables it is faster than hierarchical algorithms (for small  $k$ 's)
  - Tighter clusters than hierarchical clustering, if cluster are globular
- K-means disadvantages
  - Initial set of  $k$  clusters can affect the result
  - Does not work well with non-globular clusters

# Optimization Clustering

- K-means example

| Individual | Variable 1 | Variable 2 |
|------------|------------|------------|
| 1          | 1.0        | 1.0        |
| 2          | 1.5        | 2.0        |
| 3          | 3.0        | 4.0        |
| 4          | 5.0        | 7.0        |
| 5          | 3.5        | 5.0        |
| 6          | 4.5        | 5.0        |
| 7          | 3.5        | 4.5        |

# Optimization Clustering

- Initial 2 clusters on the basis of the most distant individuals:

|         | Individual | Mean Vector |
|---------|------------|-------------|
| Group 1 | 1          | (1.0, 1.0)  |
| Group 2 | 4          | (5.0, 7.0)  |

# Optimization Clustering

- Initial clustering of all remaining individuals:
  - For every other individual:
    - \* Calculate Euclidean distance to the centroid of every cluster
    - \* Assign individual to cluster
    - \* Recalculate centroid for every cluster

# Optimization Clustering

- Mean vector or centroid (with coordinates  $x_1$  to  $x_n$ ) with equal weight coordinates:

$$\bar{x} = \frac{\sum_{i=1}^n x_i}{n} \quad (4)$$

# Optimization Clustering

- Mean vector or centroid example for  $x = \{(3, 5), (7, 9)\}$ , i. e.  $n = |x| = 2$ :

$$\begin{aligned}\bar{x} &= \frac{\sum_{i=1}^2 x_i}{2} = \frac{(3, 5) + (7, 9)}{2} = \\ &= \frac{(3 + 7, 5 + 9)}{2} = \left(\frac{10}{2}, \frac{14}{2}\right) = (5, 7)\end{aligned}$$

# Optimization Clustering

- Initial clustering of all remaining individuals:

|        | Group 1    |             | Group 2    |             |
|--------|------------|-------------|------------|-------------|
|        | Individual | Mean Vector | Individual | Mean Vector |
| Step 1 | 1          | (1.0, 1.0)  | 4          | (5.0, 7.0)  |
| Step 2 | 1, 2       | (1.3, 1.5)  | 4          | (5.0, 7.0)  |
| Step 3 | 1, 2, 3    | (1.8, 2.3)  | 4          | (5.0, 7.0)  |
| Step 4 | 1, 2, 3    | (1.8, 2.3)  | 4, 5       | (4.3, 6.0)  |
| Step 5 | 1, 2, 3    | (1.8, 2.3)  | 4, 5, 6    | (4.3, 5.7)  |
| Step 6 | 1, 2, 3    | (1.8, 2.3)  | 4, 5, 6, 7 | (4.1, 5.4)  |



# Optimization Clustering

- Initial partitions and clustering criterion:

|         | Individual | Mean Vector | Sum of SQR error |
|---------|------------|-------------|------------------|
| Group 1 | 1, 2, 3    | (1.8, 2.3)  | 6.84             |
| Group 2 | 4, 5, 6, 7 | (4.1, 5.4)  | 5.38             |
| total   |            |             | 12.22            |

# Optimization Clustering

- Error = for every point distance to centroid
  - Criterion: the smaller the sum of square errors, the better the cluster
- Two dimensional Euclidean distance:

$$\sqrt{(x_1 - x_2)^2 + (y_1 - y_2)^2} \quad (5)$$

# Optimization Clustering

- Error = for every point distance to centroid
- $N$ -dimensional Euclidean distance, with  $p_i$  and  $q_i$  the coordinates for  $p$  and  $q$  in dimension  $i$ :

$$\sqrt{\sum_{i=1}^N (p_i - q_i)^2} \quad (6)$$

# Optimization Clustering

- Optimization Iteration:
  - Compare each individual's distance to its own mean with distance to the opposite group mean.
  - If distance to the mean in opposite group is smaller, relocate the individual.
  - Calculate the sum of square errors, if smaller than before, this is an improvement.

# Optimization Clustering

- Distance to means:

| Individual | distance to mean 1 | distance to mean 2 |
|------------|--------------------|--------------------|
| 1          | 1.5                | 5.4                |
| 2          | 0.4                | 4.3                |
| 3          | 2.1                | 1.8                |
| 4          | 5.7                | 1.8                |
| 5          | 3.2                | 0.7                |
| 6          | 3.8                | 0.8                |
| 7          | 2.8                | 1.1                |

# Optimization Clustering

- Subsequent partitions and new clustering criterion:

|         | Individual    | Mean Vector | Sum of SQR error |
|---------|---------------|-------------|------------------|
| Group 1 | 1, 2          | (1.3, 1.5)  | 0.63             |
| Group 2 | 3, 4, 5, 6, 7 | (3.9, 5.1)  | 7.9              |
| total   |               |             | 8.53             |

- Decrease of clustering criterion (from 12.22 to 8.53).

# Optimization Clustering

- Remember:
  - *k-means* or *k-nearest neighbors* is a fast and efficient algorithm.
  - You have to know how many clusters you are looking for.
  - Specific cluster shapes will not be discovered.

# Optimization Clustering

- Expectation Maximization
  - Assume different Gaussian distribution for each cluster
  - Calculate the Expectation of belonging to each Gaussian for each data point
  - Assign each data point to the Gaussian with the highest expectation
  - Recalculate Gaussians given the new data points
  - Repeat until no significant improvement of expectation

$$f(X) = \frac{1}{\sqrt{2\pi} \textit{deviation}} e^{-\frac{(\textit{value}-\textit{mean})^2}{2 \textit{deviation}^2}} \quad (1)$$



## Keep in mind...

Schlage die Trommel und fürchte dich nicht,  
Und küsse die Marketenderin!  
Das ist die ganze Wissenschaft,  
Das ist der Bücher tiefster Sinn.  
(Heinrich Heine, *Doktrin*)

Thanks for your attendance and hope to see you again!

## References

[MacKay(2003)] David J. C. MacKay. *Information theory, inference, and learning algorithms*. Cambridge University Press, Cambridge, UK; New York, 2003.