CS685: Data Mining
Data Reduction

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Data Reduction

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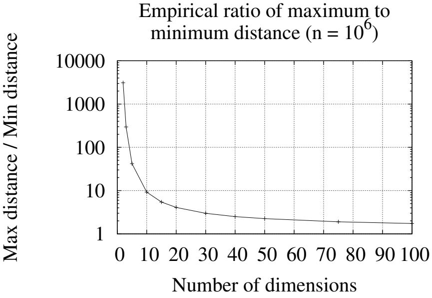
- Important ways of data reduction
  - Dimensionality reduction
  - Numerosity reduction
  - Data discretization
  - Data modeling
  - Feature selection

Dimensionality Reduction

- Dimensionality reduction reduces the number of dimensions
- New dimensions are generally different from original ones
- Curse of dimensionality
  - Data becomes too sparse as dimensions increase
  - Data is mostly at the boundaries
  - Classification: Not enough data to create good models or methods
  - Clustering: Density becomes irrelevant and distance between points becomes similar



Singular Value Decomposition (SVD)

- Singular value decomposition is factorization of a matrix

$$A = U \Sigma V^T$$

- If A is of size $m \times n$, then U is $m \times m$, V is $n \times n$ and Σ is $m \times n$
- Columns of U are *eigenvectors* of AA^T
    - Left singular vectors
    - $UU^T = I_m$ (orthonormal)
- Columns of V are *eigenvectors* of $A^T A$
    - Right singular vectors
    - $V^T V = I_n$ (orthonormal)
- σ_{ii} are the singular values
    - Σ is *diagonal*
    - Singular values are *positive square roots* of *eigenvalues* of AA^T or $A^T A$
- $\sigma_{11} \geq \sigma_{22} \geq \cdots \geq \sigma_{nn}$ (assuming n singular values)

Transformation using SVD

- Transformed data

$$T = AV = U\Sigma$$

- V is called SVD transform matrix
- Essentially, T is just a rotation of A
- Dimensionality of T is n
- n different basis vectors than the original space
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- V shows how each *object* can be represented as a linear combination of other objects
- U shows how each *dimension* can be represented as a linear combination of other dimensions
- Lengths of vectors are preserved

$$||\vec{a_i}||_2 = ||\vec{t_i}||_2$$

SVD of Real Symmetric Matrix

- A is real symmetric of size $n \times n$
- $A = A^T$
- $U = V$ since $A^T A = AA^T = A^2$

$$A = Q \Sigma Q^T$$

- Q is of size $n \times n$ and contains eigenvectors of A^2
- This is called spectral decomposition of A
- Σ contains n singular values
- Eigenvectors of A = eigenvectors of A^2
- Eigenvalues of A = square root of eigenvalues of A^2
- Eigenvalues of A = singular values of A

Example

$$
A \begin{bmatrix} 2 & 4 & 1 \\ 1 & 3 & 0 \\ 5 & 2 & 1 \\ 0 & 0 & 7 \\ 3 & 3 & 3 \end{bmatrix} = U \begin{bmatrix} -0.41 & 0.29 & 0.49 & -0.41 & -0.56 \\ -0.23 & 0.27 & 0.48 & 0.77 & 0.18 \\ -0.48 & 0.36 & -0.71 & 0.23 & -0.25 \\ -0.47 & -0.83 & 0.02 & 0.18 & -0.19 \\ -0.55 & 0.05 & 0.01 & -0.37 & 0.73 \end{bmatrix}
$$

$$
\times \Sigma \begin{bmatrix} 9.30 & 0 & 0 \\ 0 & 6.47 & 0 \\ 0 & 0 & 2.91 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \times V^T \begin{bmatrix} -0.55 & 0.44 & -0.70 \\ -0.53 & 0.45 & 0.70 \\ -0.63 & -0.77 & 0.01 \end{bmatrix}^T
$$

Transformed Data

$$
\begin{aligned}
T = AV = U\Sigma &= \begin{bmatrix} 2 & 4 & 1 \\ 1 & 3 & 0 \\ 5 & 2 & 1 \\ 0 & 0 & 7 \\ 3 & 3 & 3 \end{bmatrix} \times \begin{bmatrix} -0.55 & 0.44 & -0.70 \\ -0.53 & 0.45 & 0.70 \\ -0.63 & -0.77 & 0.01 \end{bmatrix} \\
&= \begin{bmatrix} -3.89 & 1.93 & 1.44 \\ -2.16 & 1.80 & 1.42 \\ -4.47 & 2.36 & -2.08 \\ -4.45 & -5.39 & 0.08 \\ -5.18 & 0.38 & 0.05 \end{bmatrix} \\
\text{Lengths} &= [4.58, 3.16, 5.47, 7.00, 5.19]
\end{aligned}
$$

Compact Form

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- If A is of size $m \times n$, then U is $m \times n$, V is $n \times n$ and Σ is $n \times n$
- Works because there at most n non-zero singular values in Σ

Dimensionality Reduction using SVD

$$A = U \Sigma V^T = \sum_{i=1}^{n} (u_i \sigma_{ii} v_i^T)$$

- Use only k dimensions
- Retain first k columns for U and V and first k values for Σ
- First k columns of V give the basis vectors in reduced space

$$A_k \approx \sum_{i=1}^{k} (u_i \sigma_{ii} v_i^T) = U_{1 \ldots k} \Sigma_{1 \ldots k} V_{1 \ldots k}^T$$

$$T_k \approx A V_{1 \ldots k}$$

Reduced Dimensionality

$$A \approx A_k = U_k \begin{bmatrix} -0.41 & 0.29 \\ -0.23 & 0.27 \\ -0.48 & 0.36 \\ -0.47 & -0.83 \\ -0.55 & 0.05 \end{bmatrix} \times \Sigma \begin{bmatrix} 9.30 & 0 \\ 0 & 6.47 \end{bmatrix} \times V^T \begin{bmatrix} -0.55 & 0.44 \\ -0.53 & 0.45 \\ -0.63 & -0.77 \end{bmatrix}^T$$

$$= \begin{bmatrix} 3.01 & 2.97 & 0.98 \\ 2.00 & 1.98 & -0.01 \\ 3.52 & 3.48 & 1.02 \\ 0.05 & -0.05 & 6.99 \\ 3.03 & 2.96 & 2.99 \end{bmatrix}$$

$$T \approx T_k = AV_k = U_k \Sigma_k = \begin{bmatrix} -3.89 & 1.93 \\ -2.16 & 1.80 \\ -4.47 & 2.36 \\ -4.45 & -5.39 \\ -5.18 & 0.38 \end{bmatrix}$$

$$\text{Reduced Lengths} = [4.34, 2.82, 5.06, 6.99, 5.19]$$

$$\text{Length Ratios} = [0.95, 0.89, 0.92, 1.00, 1.00]$$

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- Consider any rank-k approximation A_k of A
- SVD produces A_k^* that minimizes the Frobenius norm of the difference
  - Best in terms of sum squared error

$$A_k^* = \arg \min_{A_k : rank = k} ||A - A_k||_F$$

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- Generally, p is between 80 % to 95 %
- In the above example, $k = 1$ (resp. $k = 2$) retains 63 % (resp. 94 %) of the energy
- Running time: $O(m.n.r)$ for A of size $m \times n$ and rank r

Principal Component Analysis (PCA)

- Way of identifying patterns in data
  - How input basis vectors are correlated for the given data
- A transformation from a set of (possibly) correlated axes to another set of uncorrelated axes
- Orthogonal linear transformation (i.e., rotation)
- New axes are principal components
- First principal component produces projections that are best in the squared error sense
- Optimal least squares solution

Algorithm

- Mean center the data (optional)
- Compute the *covariance matrix* of the dimensions
- Find eigenvectors of covariance matrix
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- Compute the *covariance matrix* of the dimensions
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- Assume data matrix is B of size $m \times n$
- For each dimension, compute mean μ_i
- Mean center B by subtracting μ_i from each column i to get A
- Compute covariance matrix C of size $n \times n$
  - If mean centered, $C = A^T A$
- Find eigenvectors and corresponding eigenvalues (V, E) of C
- Sort eigenvalues such that $e_1 \geq e_2 \geq \cdots \geq e_n$
- Project step-by-step onto the principal components $\vec{v_1}, \vec{v_2}, \ldots,$ etc.

Example

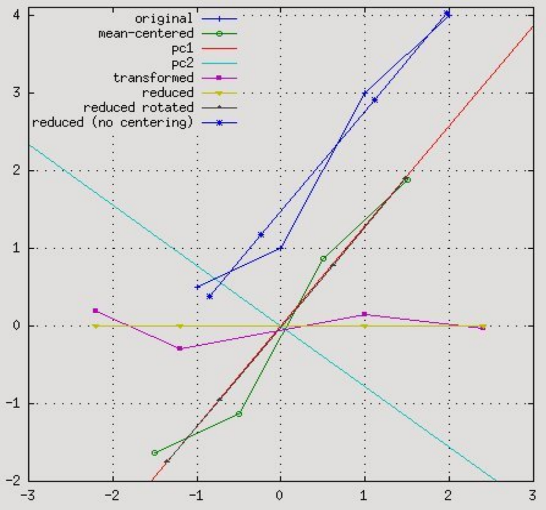
$$B = \begin{bmatrix} 2 & 4 \\ 1 & 3 \\ 0 & 1 \\ -1 & 0.5 \end{bmatrix}; \ \mu(B) = \begin{bmatrix} 0.500 & 2.125 \end{bmatrix}$$

$$\therefore A = \begin{bmatrix} 1.5 & 1.875 \\ 0.5 & 0.875 \\ -0.5 & -1.125 \\ -1.5 & -1.625 \end{bmatrix} \text{ and, } C = A^T A = \begin{bmatrix} 5.000 & 6.250 \\ 6.250 & 8.187 \end{bmatrix}$$

$$\text{Eigenvectors } V = \begin{bmatrix} 0.613 & -0.789 \\ 0.789 & 0.613 \end{bmatrix}; \ \text{eigenvalues } E = \begin{bmatrix} 13.043 \\ 0.143 \end{bmatrix}$$

$$\text{Transformed data } T = AV = \begin{bmatrix} 2.400 & -0.034 \\ 0.997 & 0.142 \\ -1.195 & -0.295 \\ -2.203 & 0.187 \end{bmatrix}$$

Visual Example



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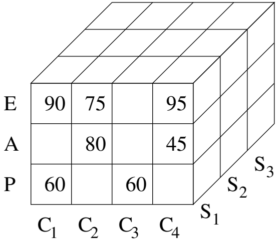
- Reduction in number of data objects
- Compression
- Modeling
- Discretization

Aggregation

- Considers a set of data objects having some similar attribute(s)
- Aggregates some other attribute(s) into single value(s)
- Example: sum, average
- Benefits of aggregation
  - Aggregate value has less variability
  - Absorbs individual errors
  - Reduces noise

Data Cube



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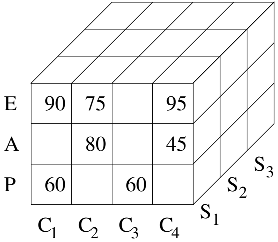

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- Each cell or face or lower dimensional surface represents a certain *projection* operation
- Aggregation can also happen along different resolutions in each dimension

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- Progressive sampling or adaptive sampling
  - Start with a small sample size
  - Keep on increasing till it is acceptable

Histograms

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- MaxDiff histograms
  - Values are first sorted
  - To get b bins, the largest $b-1$ differences are made bin boundaries

Data Summarization

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  - Mean: may be weighted
  - Median: "middle" value
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- Graphical measures help in data visualization

Data Visualization

- Histogram:

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- Histogram: frequency versus grouped values
- Bar chart:

Data Visualization

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- Bar chart: histograms where bins are categorical
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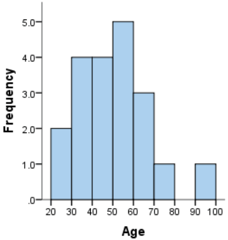
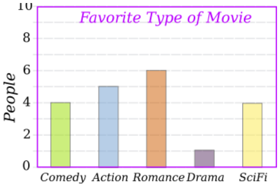
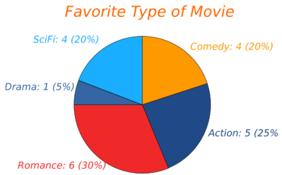
- Bar chart: histograms where bins are categorical
- Pie chart: relative frequencies shown as secalert in a circle







Data Plots

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- Quantile plot: quantiles against value
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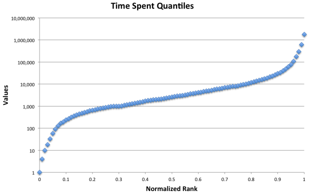

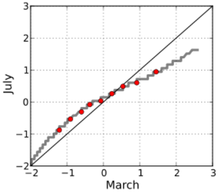

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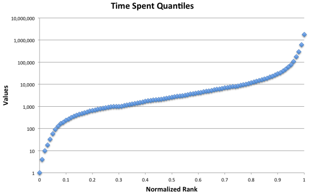

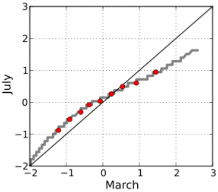

- Scatter plot:

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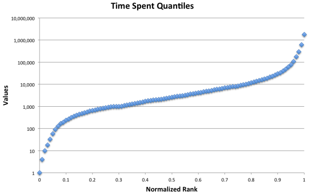
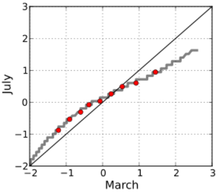
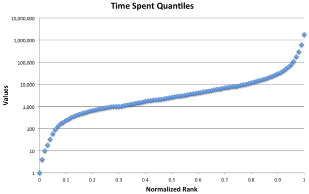
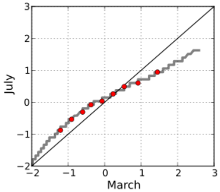




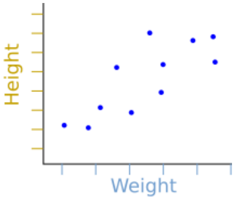
- Scatter plot: values of one variable against another
- Scatter plot matrix:

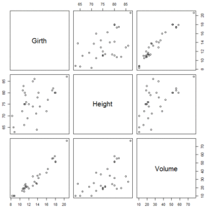
- Quantile plot: quantiles against value
- Quantile-quantile plot (q-q plot): quantiles against quantiles





- Scatter plot: values of one variable against another
- Scatter plot matrix: n^2 scatter plots for n variables





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- Can predict missing values
- The general form of regression model is

$$Y = f(X) + \varepsilon$$

- The function f can be chosen using domain knowledge
- For *linear regression*, f is linear
- ε encodes the *error* (includes *noise*) terms associated with each observation

Linear Regression

- The function f is chosen to be linear
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- *Feature weighting:* Variant of feature selection
  - SVM does it naturally

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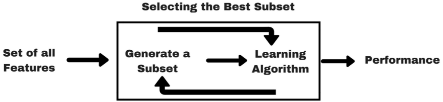

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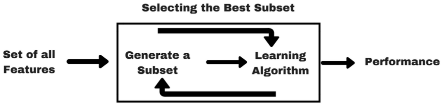
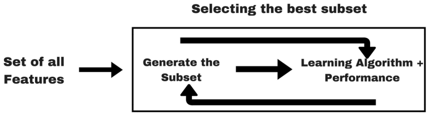


- Embedded
  - Algorithm has built-in feature selection strategy
  - Example: decision trees, LASSO regression



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