

# CS685: DATA MINING DATA REDUCTION

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# Data Reduction

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  - Simpler model
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  - Faster algorithms
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  - Avoids *overfitting*
- Important ways of data reduction
  - Dimensionality reduction
  - Numerosity reduction
  - Data discretization
  - Data modeling
  - Feature selection

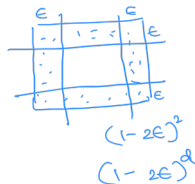
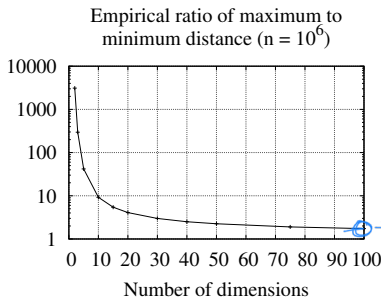
# Dimensionality Reduction

- 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

⊙ new set

All clusters are equally close

Max distance / Min distance



⊙ Everything is at the border

# 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  $\Sigma$  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)
- $\sigma_{ii}$  are the **singular** values
  - $\Sigma$  is *diagonal*
  - Singular values are *positive square roots of eigenvalues* of  $AA^T$  or  $A^T A$
- $\sigma_{11} \geq \sigma_{22} \geq \dots \geq \sigma_{nn}$  (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



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- $U$  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  $A^T A = A A^T = A^2$

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

- $Q$  is of size  $n \times n$  and contains eigenvectors of  $A^2$
- This is called **spectral decomposition** of  $A$
- $\Sigma$  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  $\Sigma$  is  $n \times n$
- Works because there at most  $n$  non-zero singular values in  $\Sigma$

# 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  $\Sigma$
- First  $k$  columns of  $V$  give the basis vectors in reduced space

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

$$T_k \approx AV_{1\dots k}$$

# Reduced Dimensionality

$$\begin{aligned} A \approx A_k &= U_k \begin{bmatrix} -0.41 & 0.29 \\ -0.23 & 0.27 \\ -0.48 & 0.36 \\ -0.47 & -0.83 \\ -0.55 & 0.05 \end{bmatrix} \times \Sigma \begin{bmatrix} 9.30 & 0 \\ 0 & 6.47 \end{bmatrix} \times V^T \begin{bmatrix} -0.55 & 0.44 \\ -0.53 & 0.45 \\ -0.63 & -0.77 \end{bmatrix}^T \\ &= \begin{bmatrix} 3.01 & 2.97 & 0.98 \\ 2.00 & 1.98 & -0.01 \\ 3.52 & 3.48 & 1.02 \\ 0.05 & -0.05 & 6.99 \\ 3.03 & 2.96 & 2.99 \end{bmatrix} \\ T \approx T_k &= AV_k = U_k \Sigma_k = \begin{bmatrix} -3.89 & 1.93 \\ -2.16 & 1.80 \\ -4.47 & 2.36 \\ -4.45 & -5.39 \\ -5.18 & 0.38 \end{bmatrix} \end{aligned}$$

Reduced Lengths = [4.34, 2.82, 5.06, 6.99, 5.19]

Length Ratios = [0.95, 0.89, 0.92, 1.00, 1.00]

# Best Approximation

- **Frobenius norm** of a matrix  $C$  of size  $n \times m$  is

$$\|C\|_F = \sqrt{\sum_{i=1}^n \sum_{j=1}^m C_{ij}^2}$$



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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

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

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- 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)
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- Assume data matrix is  $B$  of size  $m \times n$
- For each dimension, compute mean  $\mu_i$
- Mean center  $B$  by subtracting  $\mu_i$  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  $e_1 \geq e_2 \geq \dots \geq e_n$
- Project step-by-step onto the principal components  $\vec{v}_1, \vec{v}_2, \dots$ , etc.

## Example

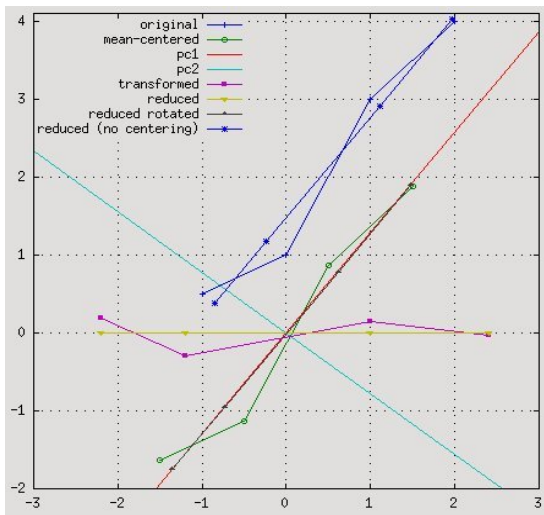
$$B = \begin{bmatrix} 2 & 4 \\ 1 & 3 \\ 0 & 1 \\ -1 & 0.5 \end{bmatrix}; \mu(B) = \begin{bmatrix} 0.500 & 2.125 \end{bmatrix}$$

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

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

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

# Visual Example



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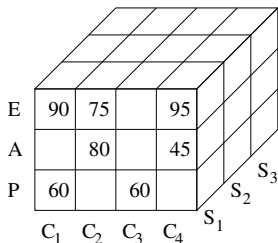
# Numerosity Reduction

- Numerosity reduction reduces the *volume* of data
  - Reduction in number of data objects
  - Compression
  - Modeling  $\Rightarrow$  Model derives the data points
  - Discretization
- Dimensionality reduction also reduces volume.*
- But here no. of data objects is being reduced*

# Aggregation

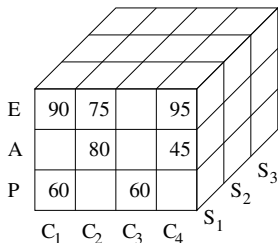
- Considers a set of data objects having some similar attribute(s)
- **Aggregates** some other attribute(s) into single value(s)
- Example: sum, average
- Benefits of aggregation
  - Aggregate value has less variability
  - Absorbs individual errors
  - Reduces noise

# Data Cube



- For multi-dimensional datasets, aggregation can happen along different dimensions
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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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- Mostly useful for one-dimensional data
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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

- **Central tendency** measures
  - Mean: may be weighted
  - Median: “middle” value
  - Mode: dataset may be *unimodal* or *multimodal*
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- **Holistic** measures
  - Cannot be computed by partitioning the dataset
  - Example: median
- Graphical measures help in **data visualization**

- Histogram:

# Data Visualization

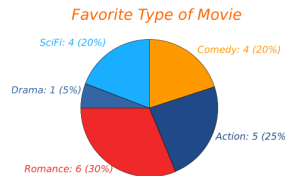
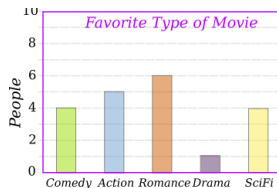
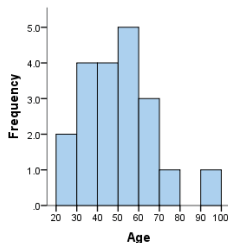
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- **Bar chart:** histograms where bins are categorical
- **Pie chart:** relative frequencies shown as sectors in a circle



# Data Plots

- Quantile plot:

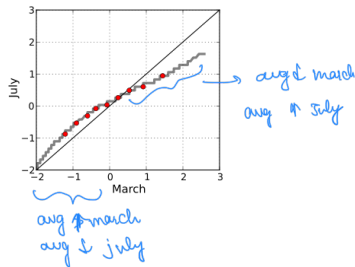
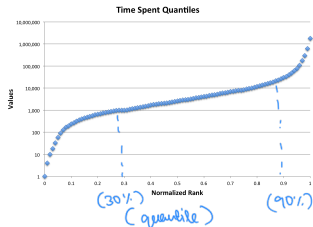


# Data Plots

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

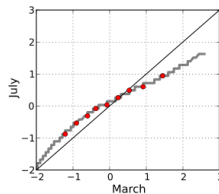
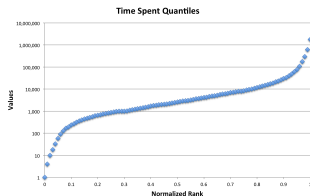
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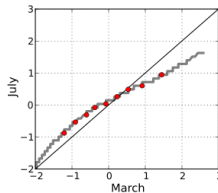
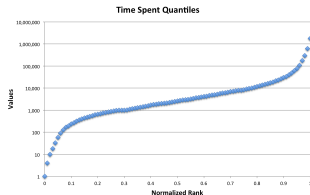
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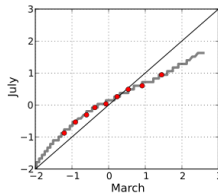
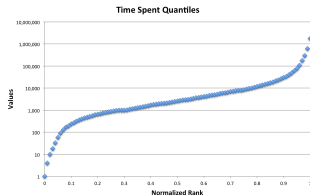
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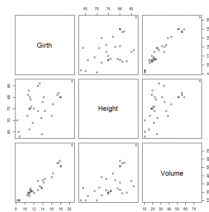
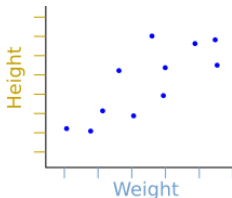
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- Produces a model of  $Y$
- Can predict missing values
- The general form of regression model is

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

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

# Linear Regression

- The function  $f$  is chosen to be linear
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- $W$  can be solved through *least squares* method

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- *Feature weighting*: Variant of feature selection
  - SVM does it naturally

feature1: 80%      feature2: 5%  
(drop)

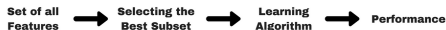
- \* Unlike dim-reduction  $\Rightarrow$  we get completely new values in (new features)

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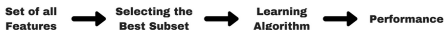


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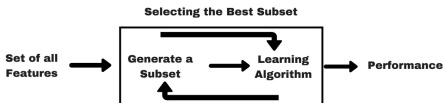
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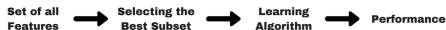


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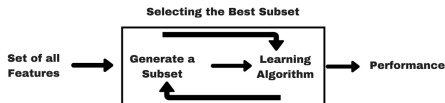
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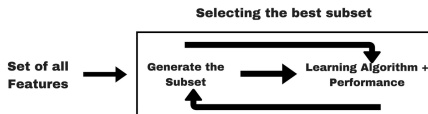
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- **Embedded**

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





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*↳ each object has a class and we know it*
- Update the score of feature  $i$  as  $x_1 = \begin{matrix} f_1 & f_2 & f_3 \\ [1, & 2, & 3] \end{matrix} \quad x_2 = \begin{matrix} f_1 & f_2 & f_3 \\ [4, & 6, & 7] \end{matrix}$

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- All features with score less than threshold  $\tau$  are removed

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