

# Structured Low Rank Approximation

## Lecture I: Introduction

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presented at

XXII School of Computational Mathematics  
Numerical Linear Algebra and Its Applications  
September 13, 2004

# Syllabus

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- Objectives:
  - ◇ To provide some preliminaries.
  - ◇ To treat some mathematics.
  - ◇ To point out some applications.
  - ◇ To describe some algorithms.
- Topics:
  - ◆ Lecture I: Introduction
  - ◇ Lecture II: General Approach
  - ◇ Lecture III: Distance Geometry and Protein Structure
  - ◇ Lecture IV: Singular Value Reassignment with Low Rank Matrices
  - ◇ Lecture V: Nonnegative Matrix Factorization
- Assignments:
  - ◇ Be able to relate the various subjects.
  - ◇ Answer the various open problems.
  - ◇ Get excited and enjoy the lectures.

**Lecture I:**  
**Introduction**

# Outline

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- Problem Description
- The Meaning of Rank Reduction
  - ◇ Karhunen-Loève Expansion
  - ◇ Low Rank Modeling
  - ◇ Random sampling
  - ◇ TSVD
- Applications
  - ◇ Data Mining
  - ◇ Factor Retrieval
- The Involvement of Structure
  - ◇ Types of Structures
  - ◇ Difficulties

# Structure Preserving Rank Reduction Problem

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- Given
  - ◇ A target matrix  $A \in \mathbb{R}^{n \times n}$ ,
  - ◇ An integer  $k$ ,  $1 \leq k < \text{rank}(A)$ ,
  - ◇ A class of matrices  $\Omega$  with a specified structure,
  - ◇ a fixed matrix norm  $\|\cdot\|$ ;

Find

- ◇ A matrix  $\hat{B} \in \Omega$  of rank  $k$ , such that

$$\|A - \hat{B}\| = \min_{B \in \Omega, \text{rank}(B)=k} \|A - B\|. \quad (1)$$

# Some Known Facts

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- It seems that we know a lot about low rank approximations.
  - ◇ Truncated singular value decomposition.
  - ◇ Noise removal.
  - ◇  $\vdots$
- Exactly what do we know about low rank approximations?
  - ◇ Why is low rank doing what we think it is doing?

# Karhunen-Loève Expansion

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- Let  $\mathcal{X} \in \mathbb{R}^n$  denote a random column vector.
  - ◊  $C := \mathcal{E}[(\mathcal{X} - \mathcal{E}[\mathcal{X}])(\mathcal{X} - \mathcal{E}[\mathcal{X}])^\top] \in \mathbb{R}^{n \times n}$  is defined as the *covariance matrix* of  $\mathcal{X}$ .
  - ◊ Being symmetric and positive semi-definite,  $C$  has a spectral decomposition

$$\text{cov}(\mathcal{X}) = \sum_{j=1}^n \lambda_j \mathbf{u}_j \mathbf{u}_j^\top.$$

- ◊  $\mathbf{u}_1, \dots, \mathbf{u}_p$  are deterministic and form an orthonormal basis for  $\mathbb{R}^n$ .
- The random column vector  $\mathcal{X}$  can be expressed as

$$\mathcal{X} = \sum_{j=1}^n (\mathbf{u}_j^\top \mathcal{X}) \mathbf{u}_j.$$

- Each coefficient  $\alpha_j := \mathbf{u}_j^\top \mathcal{X}$  itself is a random variable.
- Properties of  $\boldsymbol{\alpha}$ :

$$\begin{aligned} \mathcal{E}[\boldsymbol{\alpha}] &= U^\top \mathcal{E}[\mathcal{X}], \\ \text{cov}(\boldsymbol{\alpha}) &= \text{diag}\{\lambda_1, \dots, \lambda_n\}. \end{aligned}$$

# Low Rank Modeling

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- Since the basis vectors  $\mathbf{u}_j, j = 1, \dots, n$ , are deterministic,
  - ◇ Stochastic properties of  $\mathcal{X}$  are caused only by stochastic properties of coefficients  $\boldsymbol{\alpha}$ .
  - ◇ The randomness of  $\mathcal{X}$  is due to the randomness of  $\boldsymbol{\alpha}$ .
- Random variables  $\alpha_j, j = 1, \dots, n$ , are mutually stochastically independent.
  - ◇ Variance measures the unpredictability or scattering of a random variable.
  - ◇ The larger the eigenvalue  $\lambda_j$  is, the larger the variance of  $\alpha_j$  is and, hence, the more randomness it contributes.

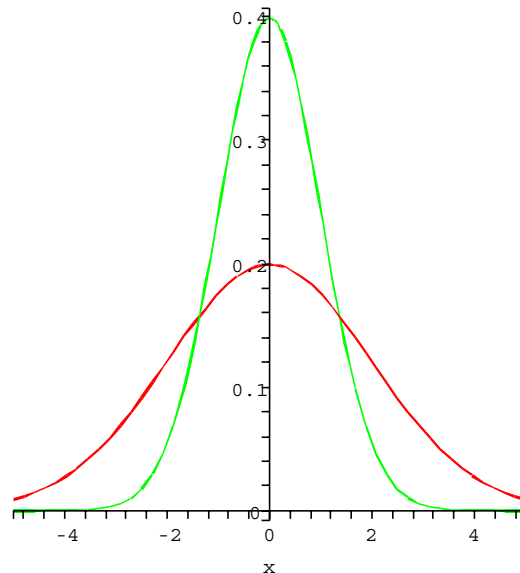


Figure 1: Normal distributions with different variances ( $\sigma = 1, 2$ ).



# Feature Selection

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- The effectiveness of basis vectors:
  - ◇ Those coefficients with larger variances and the corresponding directions are the more important components in representing the stochastic nature of  $\mathcal{X}$ .
  - ◇ Rank the importance of corresponding eigenvectors  $\mathbf{u}_j$  as *essential* components for the variable  $\mathcal{X}$  according to the magnitude of  $\lambda_j$ .
- If truncation is necessary, those eigenvectors corresponding to smaller variances should be thrown away first.
  - ◇ A Maple demonstration.

# Minimum-Variance Approximation

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- Assume  $\lambda_1 \geq \dots \geq \lambda_r \geq \dots \geq \lambda_n$ . The low rank model

$$\hat{\mathcal{X}} := \sum_{j=1}^r (\mathbf{u}_j^\top \mathcal{X}) \mathbf{u}_j \tag{2}$$

is an approximate reconstruction of  $\mathcal{X}$ .

- Consider the error

$$\mathbf{e} := \mathcal{X} - \hat{\mathcal{X}} = \sum_{j=r+1}^n \alpha_j \mathbf{u}_j.$$

- Assume  $\mathcal{E}[\mathcal{X}] = 0$ . Among *all* unbiased variables restricted to *any*  $r$ -dimensional subspaces in  $R^n$ , the random variable  $\hat{\mathcal{X}}$  defined in (2) is the **best linear minimum-variance estimate** of  $\mathcal{X}$  in the sense that

$$\mathcal{E}[\|\mathcal{X} - \hat{\mathcal{X}}\|^2] = \sum_{j=r+1}^n \lambda_j$$

is minimized.

# An Application of Low Rank Modeling

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- Consider the transmission of a data vector  $\mathcal{X}$  over a noisy communication channel.

- ◊  $\mathcal{X}$  resides in the data space.

- ◊ The reduced-rank approximation  $\hat{\mathcal{X}}$ , represented by

$$\hat{\boldsymbol{\alpha}} = [\alpha_1, \dots, \alpha_r]^\top,$$

resides in the feature space.

- Assume the signal is corrupted by an additive white noise of zero mean  $\mathbf{v}$ , that is,

- ◊ The noise vector  $\mathbf{v}$  is uncorrelated to the data vector  $\mathcal{X}$ ,

$$\mathcal{E}[\mathcal{X}\mathbf{v}^\top] = 0.$$

- ◊ Elements of the noise vector  $\mathbf{v}$  are identical independently distributed random variables,

$$\mathcal{E}[\mathbf{v}\mathbf{v}^\top] = \sigma^2 I.$$

# Direct Transmission

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- In the direct transmission, the received signal is given by

$$\mathcal{Y} = \mathcal{X} + \mathbf{v}.$$

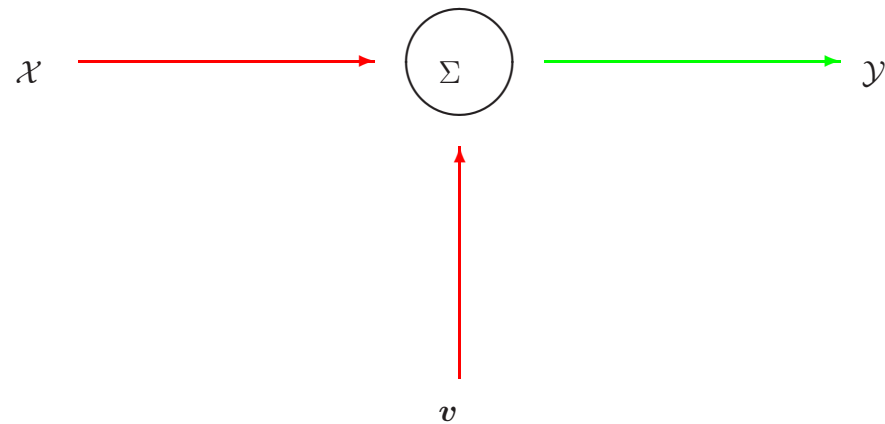


Figure 2: Direct data transmission.

- The mean-square transmission error is

$$\begin{aligned}\epsilon_{direct} &= \mathcal{E}[\|\mathcal{Y} - \mathcal{X}\|^2] = \mathcal{E}[\|\mathbf{v}\|^2] \\ &= \sum_{j=1}^n \mathcal{E}[v_j^2] \quad (\text{by independence}) \\ &= n\sigma^2.\end{aligned}$$

# Indirect Transmission

- In the indirect transmission, the signal  $\mathcal{X}$  is first applied to a transmit filter bank made of  $U_1^\top = [\mathbf{u}_1, \dots, \mathbf{u}_r]^\top$ . The resulting  $\hat{\boldsymbol{\alpha}} = U_1^\top \mathcal{X}$  is sent through the noisy channel and the received signal is given by

$$\boldsymbol{\beta} = \hat{\boldsymbol{\alpha}} + \hat{\mathbf{v}},$$

which is then applied to the receive filter bank  $U_1$  to obtain

$$\mathcal{Z} = U_1 \boldsymbol{\beta} = U_1 \hat{\boldsymbol{\alpha}} + U_1 \hat{\mathbf{v}}.$$

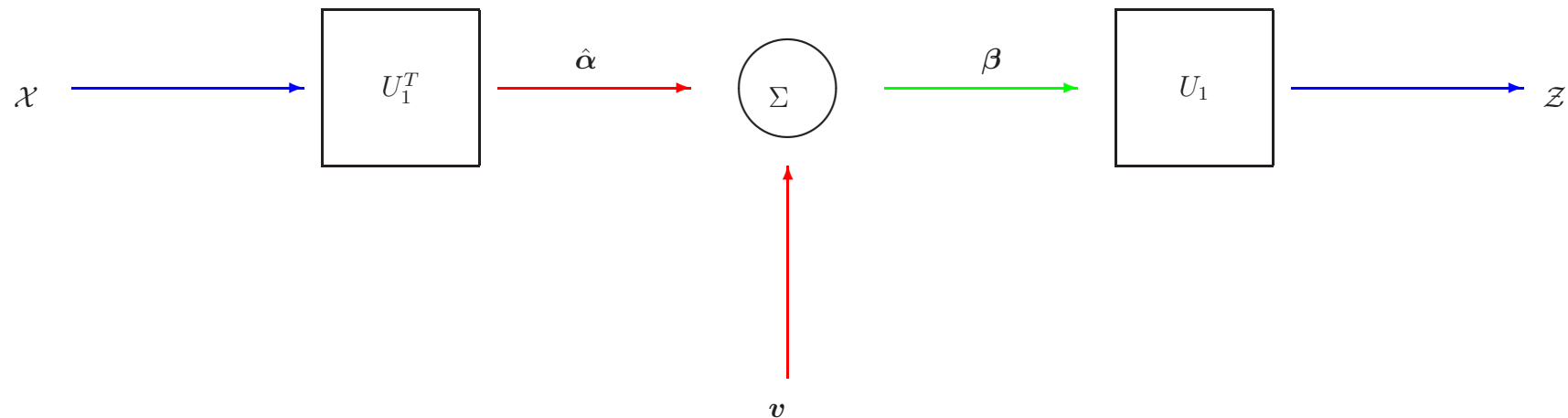


Figure 3: Indirect data transmission.

- The mean-square transmission error of the entire process is given by

$$\epsilon_{indirect} = \mathcal{E}[\|\mathcal{Z} - \mathcal{X}\|^2] = \mathcal{E}[\|(U_1 U_1^\top - I)\mathcal{X} + U_1 \hat{\mathbf{v}}\|^2] = \sum_{j=r+1}^n \lambda_j + r\sigma^2.$$

# Bias-Variance Tradeoff

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- Note that  $\epsilon_{indirect} < \epsilon_{direct}$  if and only if

$$\sum_{j=r+1}^n \lambda_j < (n-r)\sigma^2.$$

- ◊ If the tail-end eigenvalues of the correlation matrix  $C$  are sufficient small, then truncation is better than no-truncation.
- Truncation introduces a bias.
- The reduced yet biased low rank model is less susceptible to noise.

# Random Sampling in Sample Space

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- The distribution of a random variable is often simulated by a collection of  $\ell$  random samples.
  - ◇ Samples are recorded in a  $n \times \ell$  matrix  $X$ .
  - ◇ Each column of  $X$  represents one random sample of the underlying random (column vector) variable  $\mathcal{X} \in \mathbb{R}^n$ .
- Law of large numbers: When  $\ell$  is large enough, many of the stochastic properties of  $\mathcal{X}$  can be recouped from  $X$ .
  - ◇ Sample mean  $\boldsymbol{\mu} = X \frac{1}{\ell}$  converges stochastically to  $\mathcal{E}(\mathcal{X})$ .
  - ◇ Sample covariance  $R = \frac{1}{\ell}(X - \boldsymbol{\mu}\mathbf{1}^\top)(X - \boldsymbol{\mu}\mathbf{1}^\top)^\top$  converges stochastically to  $\text{cov}(\mathcal{X})$ .

# Low Rank Representation of Sample Data

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- How to retrieve a sample data matrix from  $X$  to represent the minimum-variance approximation  $\hat{\mathcal{X}}$  of  $\mathcal{X}$ ?

◇ Spectral decomposition of sample covariance:

$$R = \sum_{i=1}^n \lambda_i \mathbf{u}_i \mathbf{u}_i^\top. \quad (3)$$

- Comparison:

◇ Best *low dimension* minimum-variance estimate of the *continuous* random variable  $\mathcal{X}$ .

$$\hat{\mathcal{X}} := \sum_{j=1}^r (\mathbf{u}_j^\top \mathcal{X}) \mathbf{u}_j.$$

◇ Best *low rank* minimum-variance estimate of the *discrete* random sample of  $X$ ?

$$\hat{X} := \sum_{j=1}^r \mathbf{u}_j (\mathbf{u}_j^\top X). \quad (4)$$



# TSVD

- The singular value decomposition of  $X$ :

$$X = U\Sigma V^\top = \sum_{i=1}^n \sigma_i \mathbf{u}_i \mathbf{v}_i^\top \quad (5)$$

- ◊ Share the same eigenvectors of  $R$  as its left singular vectors, i.e.,  $U = [\mathbf{u}_1, \dots, \mathbf{u}_n]$ .
- ◊ Singular values  $\sigma_i = \sqrt{\ell\lambda_i}$  are ranked in the same ordering as eigenvalues  $\lambda_i$ ,  $i = 1, \dots, n$ .
- ◊ The notion of the truncated singular value decomposition of  $X$  is simply the partial sum

$$\hat{X} = \sum_{i=1}^r \mathbf{u}_i (\sigma_i \mathbf{v}_i^\top).$$

- The TSVD of a give data matrix  $X$  representing random samples of an unknown random variable  $\mathcal{X}$  has a statistical meaning.
  - ◊ The truncated rank- $r$  SVD  $\hat{X}$  represents random samples of the best minimum-variance linear estimate  $\hat{\mathcal{X}}$  to  $\mathcal{X}$  among all possible  $r$ -dimensional subspaces.

# Data Mining

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- Data mining is about extracting **interesting information** from raw data.
- What constitutes “information”?
  - ◇ Patterns of appearance.
  - ◇ Association rules between sets of items.
  - ◇ Clustering of the data points.
  - ◇ Concepts or categories.
  - ◇ Principal components or factors.
  - ◇ ...
- What should be counted as “interesting”?
  - ◇ Confidence and support.
  - ◇ Information content.
  - ◇ Unexpectedness.
  - ◇ Actionability — The ability to suggest concrete and profitable decision-making.
  - ◇ ...
- For different information retrievals, different techniques should be used.
  - ◇ Factors — Rank reduction or lower dimension approximation.
  - ◇ Clusters — Centroids or  $k$ -means.
  - ◇ ...

# From Complexity to Simplicity

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- Data analysis:
  - ◇ An indispensable task in almost every discipline of science.
  - ◇ Search for relationships between a set of externally caused and internal variables.
  - ◇ Especially important in this era of information and digital technologies when massive amounts of data are generated at almost all levels of applications.
- Data observed from complex phenomena:
  - ◇ Often represent the **integrated result** of several interrelated variables acting together.
  - ◇ These variables sometimes are **less precisely defined**.
- What to distinguish which variable is related to which and how the variables are related.

# Two Classical Approaches

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- Factor analysis:
  - ◇ A class of procedures that can help identify and test what *constructs*, or *factors*, might be used to explain the interrelationships among the variables.
  - ◇ Each construct itself is a complex image, idea, or theory formed from a number of simpler elements.
- Cluster analysis:
  - ◇ A procedure used to organize information about cases so that relatively *homogenous groups*, or *clusters*, can be formed.
    - ▷ Group members should be highly internally homogenous (members are “similar” to one another in their characteristics) and highly externally heterogenous (members are not “like” members of other clusters).
    - ▷ Need a measurement of similarity or dissimilarity.
    - ▷ Need a decision on how many clusters to keep.
- Either analysis is meant to bring forth the effect of **reducing the size** of the data table.

# Basic Model

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- Making observation, data gathering and processing:
  - ◇ Assume  $\ell$  **entities** and  $n$  **variable**.
  - ◇ Record raw scores that entity  $j$  received from all variables.
  - ◇ **Normalize** raw scores to have mean 0 and standard deviation 1 (standardized score).
  - ◇ Let  $Y = [y_{ij}] \in \mathbb{R}^{n \times \ell}$  denote the matrix of observed data.
    - ▷  $y_{ij} =$  *standard score* of entity  $j$  on variable  $i$ .
- **Correlation matrix** of all  $n$  variables:

$$R := \frac{1}{\ell} Y Y^T. \tag{6}$$

# Linear Relationship (Only an Assumption)

- Assume that  $y_{ij}$  is a linearly weighted score of entity  $j$  on several factors.

$$Y = AF. \tag{7}$$

- $A = [a_{ik}] \in \mathbb{R}^{n \times m}$  is the factor loading matrix.

◇  $a_{ik}$  = the loading of variable  $i$  on factor  $k$ , or the **influence** of factor  $k$  on variable  $i$ .

- $F = [f_{kj}] \in \mathbb{R}^{m \times \ell}$  is the factor scoring matrix.

◇  $f_{kj}$  = the score of factor  $k$  on entity  $j$ , or the **response** of entity  $j$  to factor  $k$ .

$$\begin{bmatrix}
 & & y_{1j} & & & \\
 & & \vdots & & & \\
 \dots & \dots & \boxed{y_{ij}} & \dots & \dots & \\
 & & \vdots & & & \\
 & & y_{nj} & & & \\
 \end{bmatrix}
 =
 \underbrace{\begin{bmatrix}
 & & a_{i1} & \dots & a_{ik} & \dots & a_{im} & \\
 \end{bmatrix}}_{\text{influence of factors}}
 \begin{bmatrix}
 & & f_{1j} & & & \\
 & & \vdots & & & \\
 \dots & \dots & f_{kj} & \dots & \dots & \\
 & & \vdots & & & \\
 & & f_{mj} & & & \\
 \end{bmatrix}
 \left. \vphantom{\begin{bmatrix} f_{1j} \\ \vdots \\ f_{kj} \\ \vdots \\ f_{mj} \end{bmatrix}} \right\} \text{response to factors}$$

# Four Examples

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- Factor retrieval
- Latent semantic indexing
- Cluster analysis
- Receptor model

## Example 1: What Factors Affect Students' Academic Performance?

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- $Y$  represents the transcripts of  $\ell$  college students (the entities) at the end of freshman year. Each column denote one student's grades on  $n$  fixed subjects (the variables), e.g., Calculus, English, Chemistry, and so on.
- A college freshman's academic performance depends on a number of factors including, for instance, family social status, finance, high school GPA, cultural background, and so on.
- Upon entering the college, each student could be asked to fill out a questionnaire inquiring these factors of his/her background. In turn, individual responses to those factors are translated into scores and placed in the corresponding column of the scoring matrix  $F$ .
- What is not clear to the educators/administrators is [how to choose the factors to compose the questionnaire](#) or [how each of the chosen factors would be weighted](#) (the loadings) to reflect the effect on each particular subject.
- In practice, we usually do not have a priori knowledge about the number and character of underlying factors in  $A$ . Sometimes we do not even know the factor scores in  $F$ .
- Only the data matrix  $Y$  is observable.
- Explaining the complex phenomena observed in  $Y$  with the help of a minimal number of factors extracted from the data matrix is the primary and most important goal of factor analysis.



# Factor Analysis and Matrix Decomposition

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- Two additional assumptions:
  - ◇ All sets of factors being considered are uncorrelated with each other.
  - ◇ Similar to  $Y$ , the scores in  $F$  for each factor are normalized.

$$\frac{1}{\ell} F F^T = I_m. \tag{8}$$

- The correlation matrix  $R$  can be expressed directly in terms of the loading matrix  $A$ , i.e.,

$$R = A A^T. \tag{9}$$

- ◇ Factor extraction now becomes a problem of decomposing the correlation matrix  $R$  into the product  $A A^T$ .
- ◇ Would like to use as few factors as possible.

# Interpretation of the Loading Matrix $A$

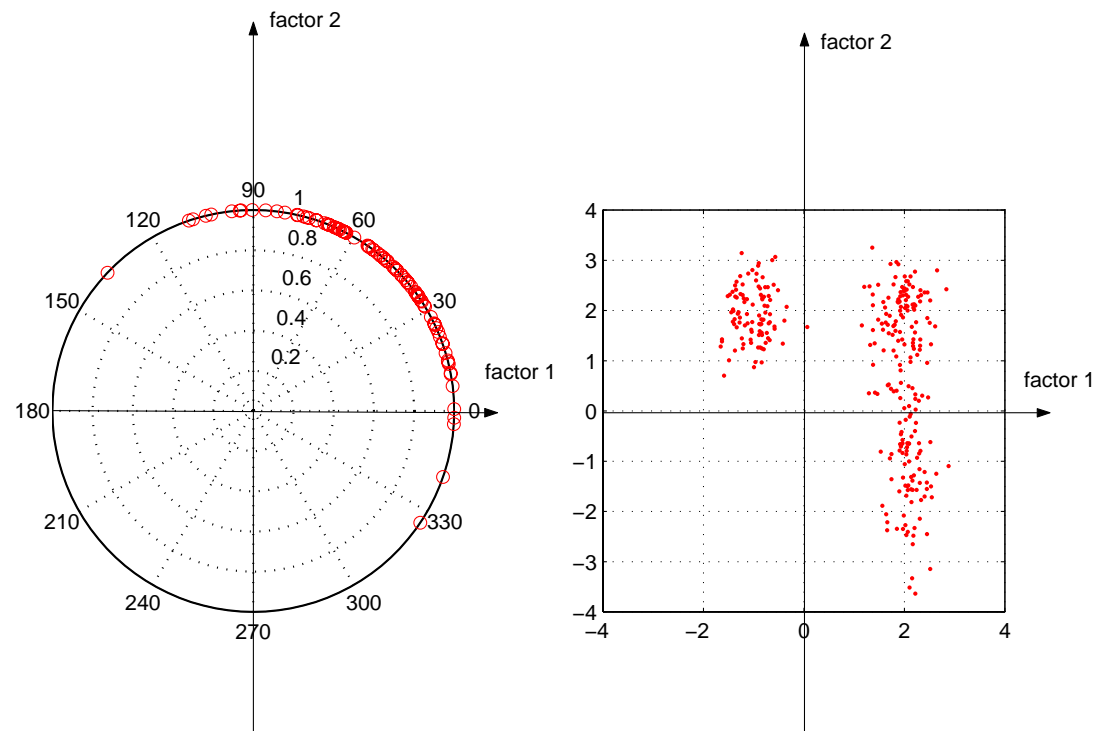
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- $a_{i*}$  = how the data variable  $i$  is weighted across/influenced by the list of current factors.
  - ◊  $\|a_{i*}\|_2^2$  = the *communality* of variable  $i$ .
    - ▷ If  $\|a_{i*}\|_2$  is small, variable  $i$  is of little consequence to the current factors.
- $a_{*k}$  = correlations of the data variables with that particular  $k$ th factor.
  - ◊  $\|a_{*k}\|$  = the *significance* of factor  $k$ .
    - ▷ Variables with high factor loadings are more “like” the factor in some sense.
    - ▷ Variables with zero or near-zero loadings are treated as being unlike the factor.

$$\begin{bmatrix}
 & & & y_{1j} & & & \\
 & & & \vdots & & & \\
 y_{i1} & \cdots & \cdots & y_{ij} & \cdots & \cdots & y_{il} \\
 & & & \vdots & & & \\
 & & & y_{nj} & & & 
 \end{bmatrix} = \underbrace{\begin{bmatrix}
 & & & a_{1k} & & & \\
 & & & \vdots & & & \\
 a_{i1} & \cdots & a_{ik} & \cdots & a_{im} & & \\
 & & & \vdots & & & \\
 & & & a_{nk} & & & 
 \end{bmatrix}}_{\text{factors}} \begin{bmatrix}
 & & & f_{1j} & & & \\
 & & & \vdots & & & \\
 f_{k1} & \cdots & \cdots & f_{kj} & \cdots & \cdots & f_{kl} \\
 & & & \vdots & & & \\
 & & & f_{mj} & & & 
 \end{bmatrix}$$

# Tasks to Do in Factor Analysis

- Want to rewrite the loadings of variables over some *newly selected* factors.
  - ◊ Fewer factors.
  - ◊ Manifest more clearly the correlation between variables and factors.
- Represent the loading of each variable (each row of  $A$ ) as a single point in the factor space  $\mathbb{R}^m$ .
  - ◊ What does it mean if these points cluster around a certain direction?
  - ◊ How to find the clustering direction?



# What Is Going On?

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- Suppose the newly selected factors are expressed in terms of columns of the orthogonal matrix

$$V := [\mathbf{v}_1, \dots, \mathbf{v}_m] \in \mathbb{R}^{m \times m}. \quad (10)$$

- ◇ Determine some appropriate new basis for  $V$ .
  - ◇ The rewriting of factor loadings with respect to  $V$  is mathematically equivalent to a change of basis, i.e.,  $A$  is now written as  $B := AV$ .
  - ◇ Because  $Y = AF = (AV)(V^T F) = BG$ ,
    - ▷  $B = AV$  denotes new factor loadings.
    - ▷  $G = V^T F$  denotes new factor scores.
  - ◇ The correlation matrix  $R = AA^T = BB^T \in \mathbb{R}^{n \times n}$  is independent of factors selected.
    - ▷ Would like that the significance of factors concentrates on “fewer” columns of  $B$ .
    - ▷ Lower rank approximation of  $A$ .
- In the process of defining new factors it is often desirable to retrieve information ...
  - ◇ Directly from the correlation matrix  $R$  rather than from any particular loading matrix  $A$ , if  $A$  is not readily available; or
  - ◇ Approximate  $A$ , if  $A$  is too large or too expensive.

## Example 2: Latent Semantic Indexing

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- Indexing matrix  $H = [h_{ik}] \in \mathbb{R}^{n \times m}$ :
  - ◇ Each document is represented by one row in  $H$ .
  - ◇  $h_{ik}$  = the *weight* of one particular *term*  $k$  in document  $i$ .
    - ▷ Each term could be just one single word or a string of phrases.
    - ▷ The weight  $h_{ik}$  could simply be the number of occurrence of term  $k$  in document  $i$ .
    - ▷ More elaborate weighting schemes are available and yield better performance.

$$h_{ik} = t_{ik} g_k n_i,$$

$$\begin{array}{c} \text{terms} \\ \downarrow \\ \begin{array}{c} h_{1k} \\ \vdots \\ h_{ik} \\ \vdots \\ h_{nk} \end{array} \end{array} \quad \begin{array}{c} \left[ \begin{array}{cccc} h_{i1} & \dots & h_{ik} & \dots & h_{im} \end{array} \right] \end{array}$$

documents  $\rightarrow$

- Watch out the constraint: **Each row should be normalized to unit length.**

# Search Similarities

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- Queries  $\mathbf{q}_j = [q_{1j}, \dots, q_{mj}]^T \in \mathbb{R}^m$ :
  - ◊  $q_{kj}$  = the weight of term  $k$  in the query  $j$ .
- Would like to find documents relevant to given queries.
  - ◊ To measure how the query  $\mathbf{q}_j$  matches the documents,
    - ▷ Calculate the dots product
  - ▷ Rank the relevance of documents to  $\mathbf{q}_j$  according to the *scores* in  $\mathbf{s}_j$ .

$$\mathbf{s}_j = H\mathbf{q}_j. \tag{11}$$

# Comparison of LSI with Linear Model

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- Analogies:

indexing matrix $H$	$\longleftrightarrow$	loading matrix $A$
document $i$	$\longleftrightarrow$	variable $i$
one query $\mathbf{q}_j$	$\longleftrightarrow$	one column in scoring matrix $F$
term $k$	$\longleftrightarrow$	factor $k$
weight $h_{ik}$	$\longleftrightarrow$	loading of factor $k$ on variable $i$
weights $q_{kj}$ of term $k$ in query $\mathbf{q}_j$	$\longleftrightarrow$	response $f_{kj}$ of entity $j$ on factor $k$
scores $s_{ij}$ in of document $i$ in query $\mathbf{q}_j$	$\longleftrightarrow$	scores $y_{ij}$ of variable $i$ in entity $j$

- Differences:

- ◇ In LSI, terms/factors are predetermined.
  - ▷ How are the terms/factors predetermined?
  - ▷ What is the notion of “orthogonal words”?
  - ▷ What is the notion of “term/factor reduction”?
- ◇ LSI is not trying to compute factors based on the scores in  $\mathbf{s}_j$ ,  $j = 1, \dots, \ell$ .
  - ▷ Though, this information may be used as [a learning process](#) for selecting terms/factors.
- ◇ LSI emphasizes effective vector-matrix multiplication (11).
  - ▷ Want to represent the indexing matrix and the queries in a more *compact form* so as to facilitate the computation of the scores.

## Example 3: Electronic Model Design

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- Consider the switch manufacturing in the telecommunication industry.
  - ◊ A cabinet consists of  $m$  slots.
  - ◊ Each slot may be filled with a selection from  $r$  types of boards.

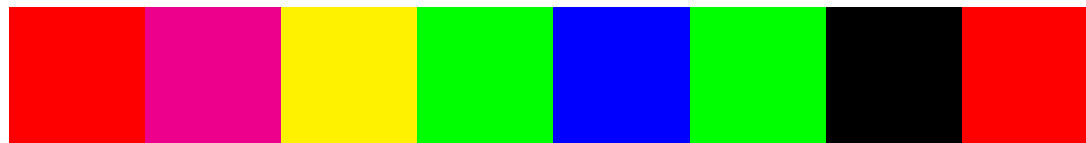


Figure 5: An electronic cabinet with 8 slots to be filled with 6 boards.

- History of past  $n$  customer orders have been recorded into a matrix  $A \in \mathbb{R}^{n \times m}$ .
- Would like to preassemble  $q$  semi-finished cabinet models.
- Determine the model configurations and the corresponding customer-to-model assignment of semi-finished cabinets based on  $A$  so as to minimize the total number of insertions required to manufacture the entire order.



## Example 4: Receptor Model

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- An observational technique within the air pollution research community.
- Make use of the ambient data and source profile data to apportion sources or source categories.
- Fundamental principle:
  - ◇ Mass conservation can be assumed.
  - ◇ Mass balance analysis can identify and apportion sources of airborne particulate matter in the atmosphere.

# Ideas

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- Obtain a large number of chemical constituents such as elemental concentrations in a number of samples.
- Mass balance equation describes the relationships between  $p$  sources which contribute  $m$  chemical species to  $n$  samples.

$$y_{ij} = \sum_{k=1}^p a_{ik} f_{kj}, \quad (12)$$

- ◇  $y_{ij}$  = the elemental concentration of the  $i$ th chemical measured in the  $j$ th sample.
- ◇  $a_{ik}$  = the gravimetric concentration of the  $i$ th chemical in the  $k$ th source.
- ◇  $f_{kj}$  = the airborne mass concentration that the  $k$ th source has contributed to the  $j$ th sample.
- Application:
  - ◇ Typically, only values of  $y_{ij}$  are observable.
  - ◇ Neither the sources are known nor the compositions of the local particulate emissions are measured.
  - ◇ A critical question is to estimate the number  $p$ , the compositions  $a_{ik}$ , and the contributions  $f_{kj}$  of the sources.
- The source compositions  $a_{ik}$  and the source contributions  $f_{kj}$  must all be nonnegative. The identification and apportionment, therefore, becomes a **nonnegative matrix factorization problem of  $Y$** .

# Types of Structures

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- Structural constraints:
  - ◇ Toeplitz or circulant matrices.
  - ◇ Covariance matrices.
  - ◇ Euclidean distance matrices.
  - ◇ Data on the unit sphere.
  - ◇ Nonnegative matrix factorizations.
- Applications:
  - ◇ Signal and image processing with Toeplitz structure.
  - ◇ Model reduction problem in speech encoding and filter design with Hankel structure.
  - ◇ Protein folding problem with Euclidean distance structure.
  - ◇ Data mining with normalized information.
  - ◇ Principal component analysis with nonnegative structure.
- Each of the above topics is a major research effort.

# Difficulties

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- No easy way to characterize, either algebraically or analytically, a given class of structured lower rank matrices.
- Lack of explicit description of the feasible set  $\implies$  Difficult to apply classical optimization techniques.
- Little discussion on whether lower rank matrices with specified structure actually exist.