CPSC 340: Machine Learning and Data Mining

Sparse Matrix Factorization

Summer 2021

Admin

- Assignment 5 is due 11:55pm today
- Assignment 6 will be released today

- Final exam is Wednesday, June 23
  - 24-hour take-home exam (NOT timed!)
  - Prep materials will go up Wednesday, June 16

Assignment 7

- Assignment 7 will be released next Friday-ish
  - Optional, but "due" Wednesday, June 30
  - Outside final exam coverage
  - Covers things previously not covered in assignments
    - E.g. automatic differentiation and backpropagation

- Graded on completeness not correctness
  - If you submit A7, I will
    replace your lowest assignment grade with A7 grade

- Office hours will be upon request for A7

In This Lecture

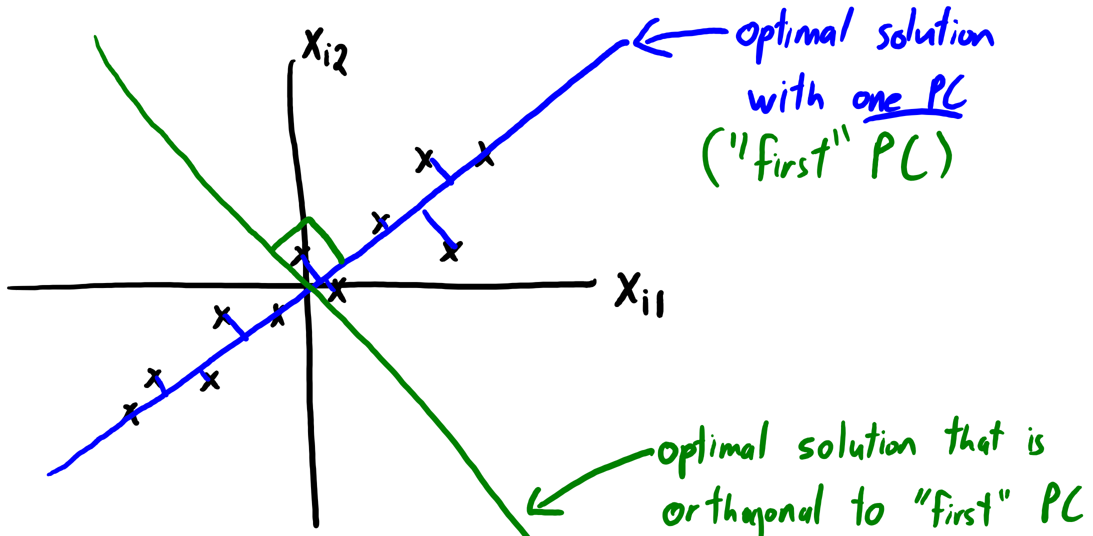
1. Non-Negative Matrix Factorization
   - Projected gradient method
2. Other Matrix Factorization Methods

Last Time: PCA with Orthogonal/Sequential Basis

- When k = 1, PCA has a scaling problem.
- When k > 1, have scaling, rotation, and label switching.
  - Standard fix: use normalized orthogonal rows w_c of 'W'.

$$\|w_c\| = 1 \quad \text{and} \quad w_c^T w_{c'} = 0 \quad \text{for } c' \neq c$$

  - And fit the rows in order:
    - First row "explains the most variance" or "reduces error the most".



Last Time: SVD and Other Methods

- SVD: linear-algebraic solution to get X = ZW
  - Enforces normalization and orthogonality
- Alternating minimization: use gradients!
  - Optimize f(W,Z) with respect to W
  - Then optimize f(W,Z) with respect to Z
  - Repeat until happy

$$\nabla_W f(W,Z) = Z^T Z W - Z^T X \quad \text{so} \quad W = (Z^T Z)^{-1}(Z^T X)$$

(writing gradient as a matrix)

$$\nabla_Z f(W,Z) = Z W W^T - X W^T \quad \text{so} \quad Z = X W^T (W W^T)^{-1}$$

These are usually invertible since k<n and k<d

6

Coming Up Next

MORE EIGENFACES

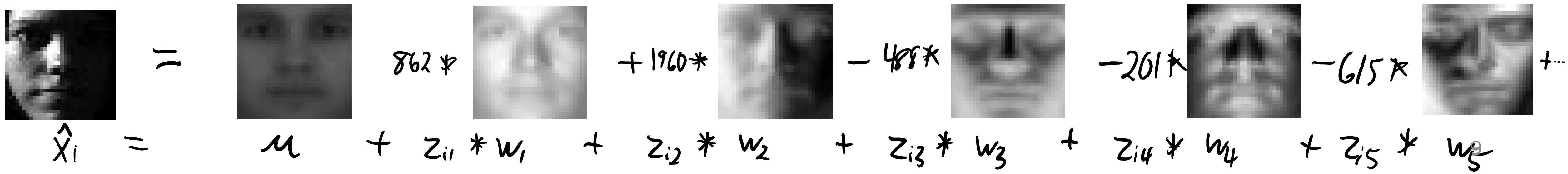
VQ vs. PCA vs. NMF

- How *should* we represent faces?
  - Vector quantization (k-means).
    - Replace face by a ________________.
    - Can't distinguish between people in the same cluster (only 'k' possible faces).
    - Almost certainly not true: too few canonical faces.

$$\hat{x}_i = z_{i1} * w_1 + z_{i2} * w_2 + z_{i3} * w_3 + z_{i4} * w_4 + z_{i5} * w_5 + z_{i6} * w_6$$

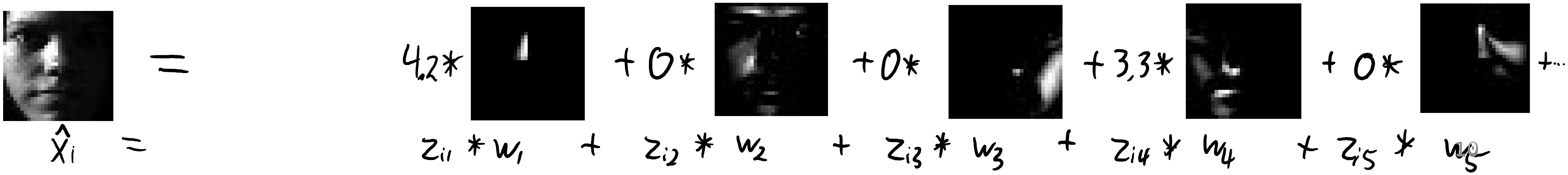
VQ vs. PCA vs. NMF

- How *should* we represent faces?
  - Vector quantization (k-means).
  - PCA (orthogonal basis).
    - Global average plus __________________ of "eigenfaces".
    - But "eigenfaces" are not intuitive ingredients for faces.
      - PCA tends to use positive/negative cancelling bases.



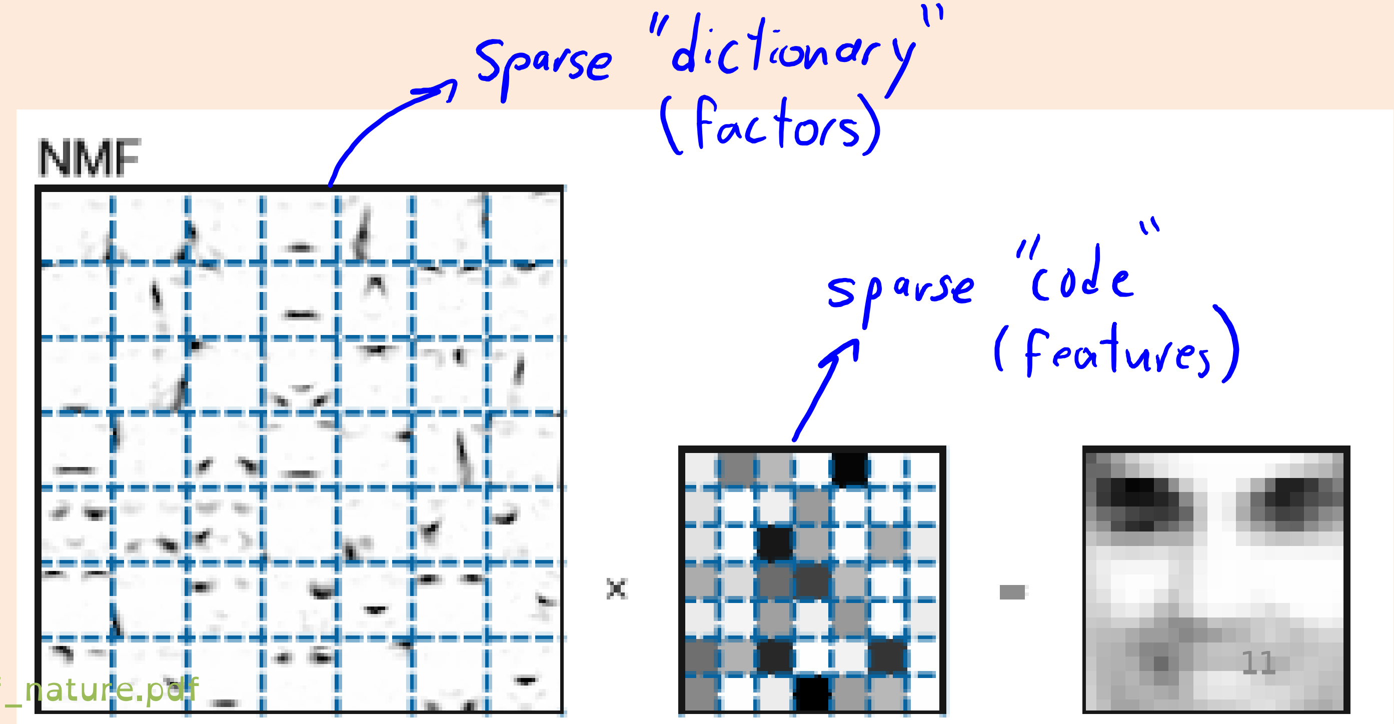
VQ vs. PCA vs. NMF

- How *should* we represent faces?
  - Vector quantization (k-means).
  - PCA (orthogonal basis).
  - NMF (non-negative matrix factorization):
    - Instead of orthogonality/ordering in W, require W and Z to be non-negative.
    - Example of "sparse coding":
      - The z_i are sparse so each face is coded by a small number of eigenfaces.
      - The w_c are sparse so eigenfaces tend to be "parts" of the face.



Why sparse coding?

- "Parts" are intuitive, and brains seem to use sparse representation.
- Energy efficiency if using sparse code.
- Increase number of concepts you can memorize
  - Some evidence in fruit fly olfactory system.



http://www.columbia.edu/~jwp2128/Teaching/W4721/papers/nmf_nature.pdf

Coming Up Next

NON-NEGATIVE MATRIX FACTORIZATION

Warm-up to NMF: Non-Negative Least Squares

- Consider our usual least squares problem:

$$f(w) = \frac{1}{2}\sum_{i=1}^{n}(w^T x_i - y_i)^2$$

- But assume y_i and elements of x_i are non-negative:
  - Could be sizes ('height', 'milk', 'km') or counts ('vicodin', 'likes', 'retweets').

Q: Does it make sense to have any $w_j < 0$?

Warm-up to NMF: Non-Negative Least Squares

$$f(w) = \frac{1}{2}\sum_{i=1}^{n}(w^T x_i - y_i)^2$$

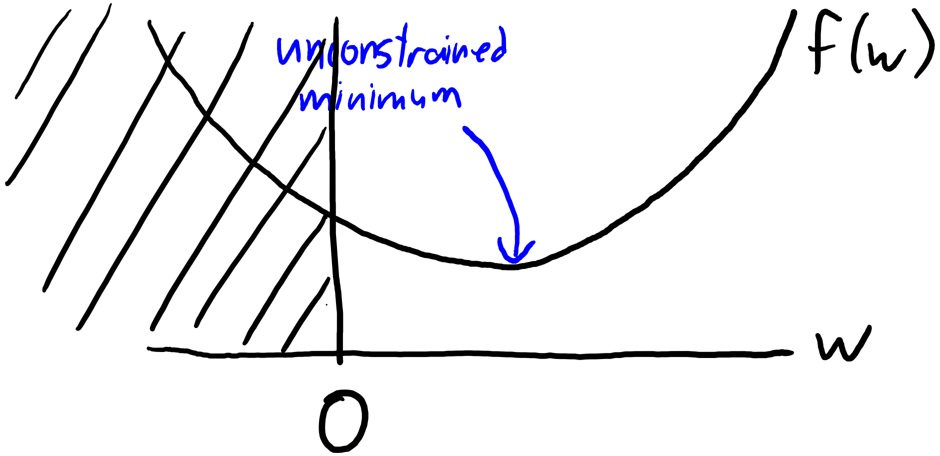
- Allow $w_j \in (-\infty, +\infty) \rightarrow$ some weights are negative to cancel out _____________ weights
- Idea: constrain $w_j \in [0, +\infty) \rightarrow$ sparsity and regularization

Sparsity and Non-Negative Least Squares

- Consider 1D non-negative least squares objective:

$$f(w) = \frac{1}{2}\sum_{i=1}^{n}(w x_i - y_i)^2 \quad \text{with} \quad w \geq 0$$

- Plotting the (constrained) objective function:



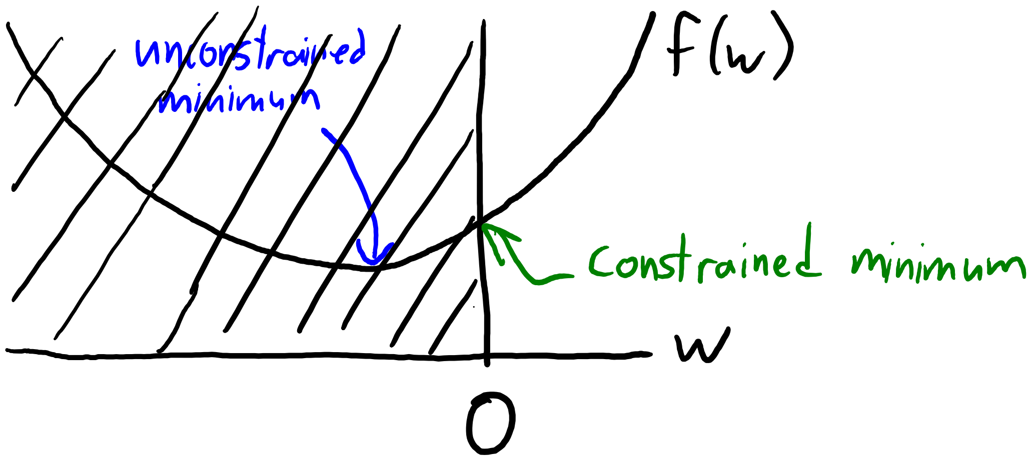
- In this case, non-negative solution is least squares solution.

Sparsity and Non-Negative Least Squares

- Consider 1D non-negative least squares objective:

$$f(w) = \frac{1}{2}\sum_{i=1}^{n}(w x_i - y_i)^2 \quad \text{with } w \geq 0$$

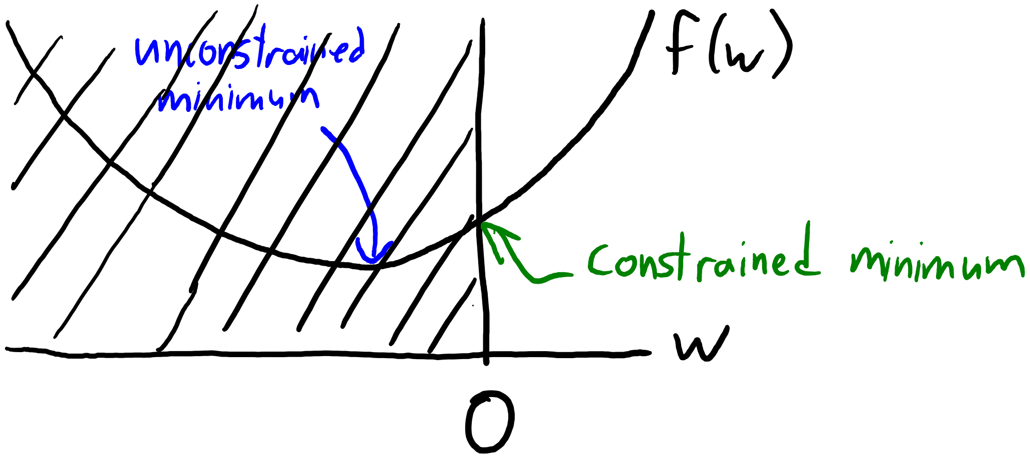
- Plotting the (constrained) objective function:



- In this case, non-negative solution is $w = 0$.

Sparsity and Non-Negativity

- Similar to L1-regularization, non-negativity leads to sparsity.
  - Also regularizes: w_j are smaller since can't "cancel" negative values.
  - Sparsity leads to cheaper predictions and often to more interpretability.
    - Non-negative weights are often also more interpretable.



Sparsity and Non-Negativity

- How can we minimize f(w) with non-negative constraints?
  - Naive approach: solve least squares problem, set negative w_j to 0.

$$\text{Compute } w = (X^T X) \backslash (X^T y)$$

$$\text{Set } w_j = \max\{0, w_j\}$$

  - This is correct when d = 1.
  - Can be worse than setting w = 0 when d ≥ 2.

Coming Up Next

PROJECTED GRADIENT

Projected Gradient

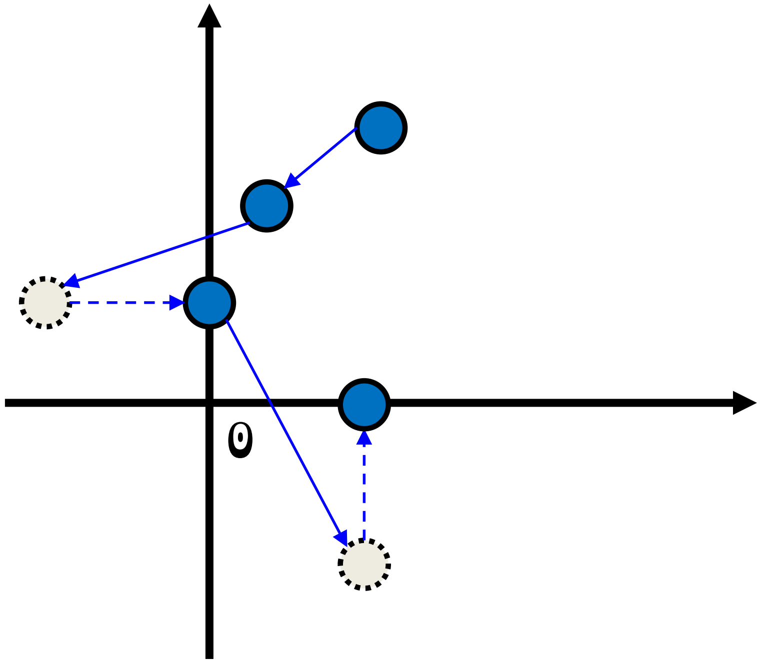
- Use projected gradient algorithm:
    - Run a gradient descent iteration:

$$w^{t+1/2} = w^t - \alpha^t \nabla f(w^t)$$

    - After each step, set negative values to 0.

$$w_j^{t+1} = \max\{0, w_j^{t+1/2}\}$$

    - Repeat.



Parameter space

Projected Gradient

- Projected gradient algorithm:

$$w^{t+1/2} = w^t - \alpha^t \nabla f(w^t) \qquad w_j^{t+1} = \max\{0, w_j^{t+1/2}\}$$

  - Similar properties to gradient descent:
    - Guarantees decrease if step size α^t is small enough.
    - Reaches local minimum under weak assumptions (global minimum for convex 'f').
      - Least squares objective is still convex when restricted to non-negative variables.
    - Solution is a "fixed point": $w^* = \max\{0, w^* - \alpha^t \nabla f(w^*)\}$.
      - Use this to decide when to stop.

  - A generalization is "proximal gradient":
    - Instead of constraints, allows non-smooth terms (OptimizerGradientDescentProximalL1).

Projected Gradient for NMF

- Back to the non-negative matrix factorization (NMF) objective:

$$f(W,Z) = \sum_{i=1}^{n}\sum_{j=1}^{d}(\langle w^j, z_i\rangle - x_{ij})^2 \quad \text{with } w_{cj} \geq 0 \text{ and } z_{ij} \geq 0$$

  - Different ways to use projected gradient:
    - Alternate between projected gradient steps on 'W' and on 'Z'.
    - Or run projected gradient on both at once.
    - Or sample a random 'i' and 'j' and do stochastic projected gradient.

Set $z_i^{t+1} = z_i^t - \alpha^t \nabla_{z_i} f(W,Z)$ and $(w^j)^{t+1} = (w^j)^t - \alpha^t \nabla_{w^j} f(W,Z)$ for selected i and j (keep other values of W and Z fixed)

Then set negative values to 0.

Projected Gradient for NMF

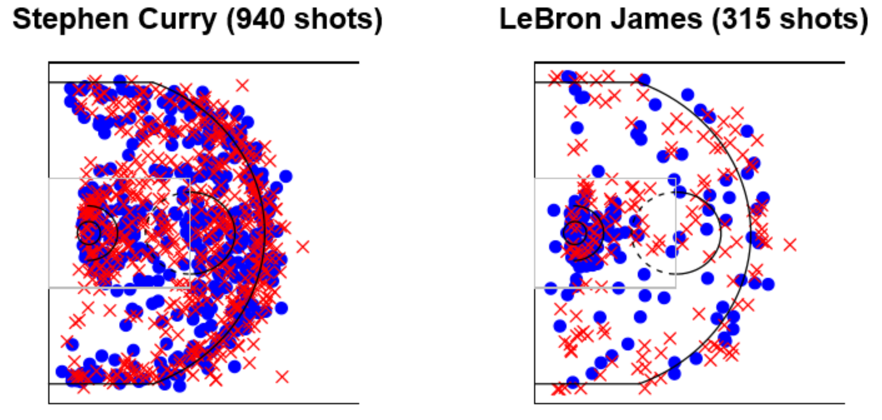
$$f(W,Z) = \sum_{i=1}^{n}\sum_{j=1}^{d}(\langle w^j, z_i\rangle - x_{ij})^2 \quad \text{with } w_{cj} \geq 0 \text{ and } z_{ij} \geq 0$$

$$\text{Set } z_i^{t+1} = z_i^t - \alpha^t \nabla_{z_i} f(W,Z) \text{ and } (w^j)^{t+1} = (w^j)^t - \alpha^t \nabla_{w^j} f(W,Z)$$

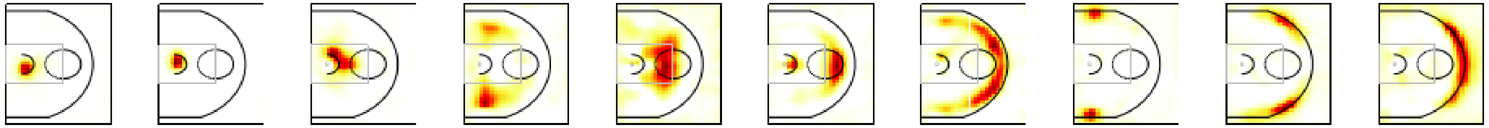
- Non-convex
- Sensitive to initialization (unlike PCA)
- Hard to find the global optimum.
  - Typically use random initialization.
  - Also, we usually don't center the data with NMF.

Application: Sports Analytics

- NBA shot charts:



- NMF (using "KL divergence" loss with k=10 and smoothed data).
  - Negative values would not make sense here.

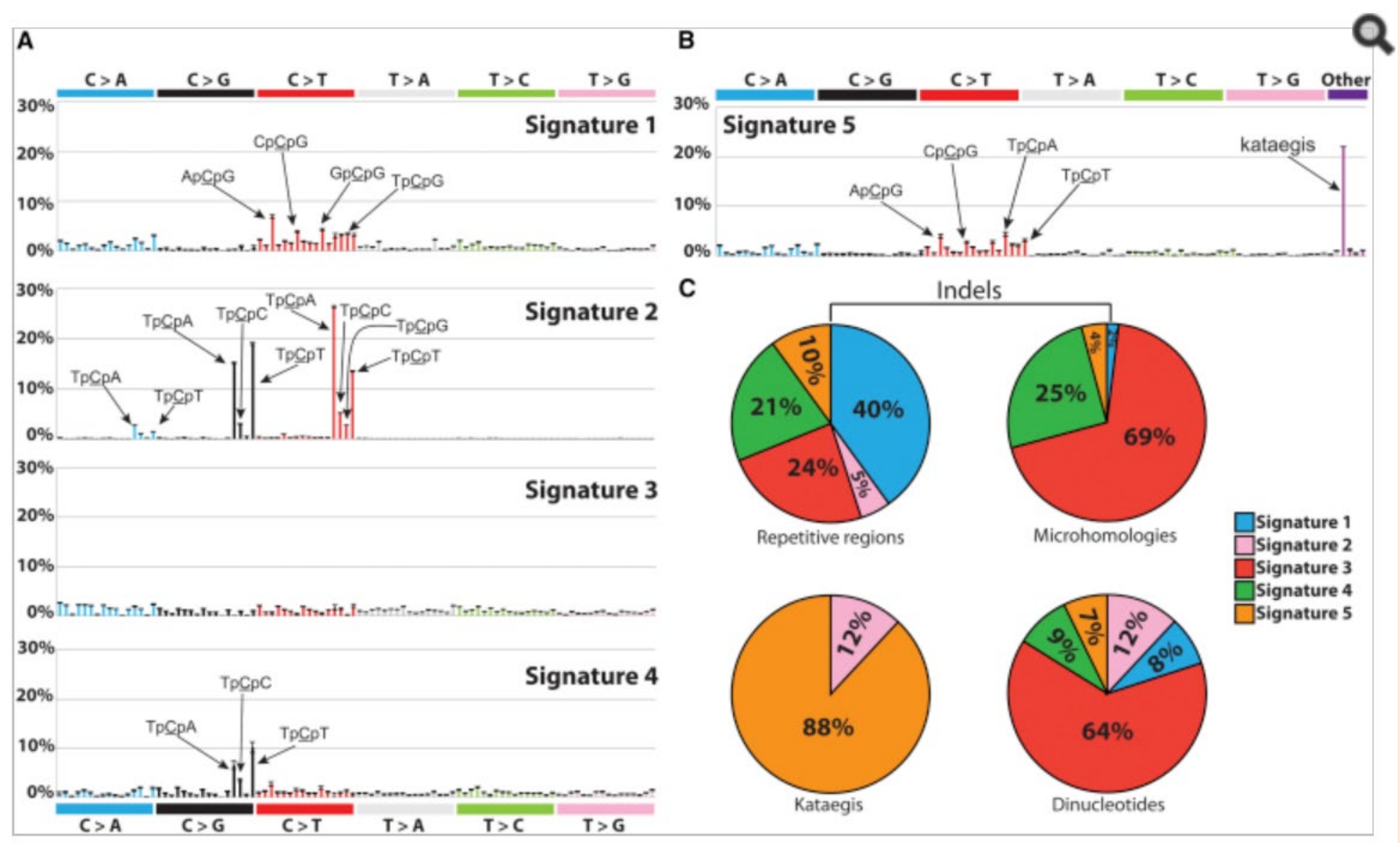


LeBron James	0.21	0.16	0.12	0.09	0.04	0.07	0.00	0.07	0.08	0.17
Brook Lopez	0.06	0.27	0.43	0.09	0.01	0.03	0.08	0.03	0.00	0.01
Tyson Chandler	0.26	0.65	0.03	0.00	0.01	0.02	0.01	0.01	0.02	0.01
Marc Gasol	0.19	0.02	0.17	0.01	0.33	0.25	0.00	0.01	0.00	0.03
Tony Parker	0.12	0.22	0.17	0.07	0.21	0.07	0.08	0.06	0.00	0.00
Kyrie Irving	0.13	0.10	0.09	0.13	0.16	0.02	0.13	0.00	0.10	0.14
Stephen Curry	0.08	0.03	0.07	0.01	0.10	0.08	0.22	0.05	0.10	0.24
James Harden	0.34	0.00	0.11	0.00	0.03	0.02	0.13	0.00	0.11	0.26
Steve Novak	0.00	0.01	0.00	0.02	0.00	0.00	0.01	0.27	0.35	0.34

http://jmlr.org/proceedings/papers/v32/miller14.pdf

Application: Cancer "Signatures"

- What are common sets of mutations in different cancers?
  - May lead to new treatment options.



https://www.ncbi.nlm.nih.gov/pmc/articles/PMC3588146/

Coming Up Next

OTHER MATRIX FACTORIZATIONS

Beyond Squared Error

- Our objective for latent-factor models (LFM):

$$f(W,Z) = \sum_{i=1}^{n} \sum_{j=1}^{d} (\langle w^j, z_i \rangle - x_{ij})^2$$

- As before, there are alternatives to squared error.

$$f(W,Z) = \sum_{i=1}^{n} \sum_{j=1}^{d} \text{loss}(\langle w^j, z_i \rangle, x_{ij})$$

Error for predicting $\langle w^j, z_i \rangle$ when true value is x_{ij}

- If X consists of +1 and -1 values, we could use logistic loss:

$$f(W,Z) = \sum_{i=1}^{n} \sum_{j=1}^{d} \log(1 + \exp(-x_{ij} \langle w^j, z_i \rangle))$$

Robust PCA (A6)

- Robust PCA methods use the absolute error:

$$f(W,Z) = \sum_{i=1}^{n} \sum_{j=1}^{d} |\langle w^j, z_i \rangle - x_{ij}|$$

- Will be robust to outliers in the matrix ‘X’.
- Encourages “residuals” r_{ij} to be ____________.
  - Non-zero r_{ij} are where the “outliers” are.

http://statweb.stanford.edu/~candes/papers/RobustPCA.pdf

Regularized Matrix Factorization

- Consider L2-regularized PCA:

$$f(W, Z) = \frac{1}{2}\|ZW - X\|_F^2 + \frac{\lambda_1}{2}\|W\|_F^2 + \frac{\lambda_2}{2}\|Z\|_F^2$$

- Replaces normalization/orthogonality/sequential-fitting.
  - Often gives lower reconstruction error on test data.
  - But requires hyper-parameters λ_1 and λ_2.

- Need to regularize both W and Z because of scaling problem.
  - If you only regularize 'W' it doesn't do anything. (WHY?)
  - Similarly, if you only regularize 'Z' it doesn't do anything.

Sparse Matrix Factorization

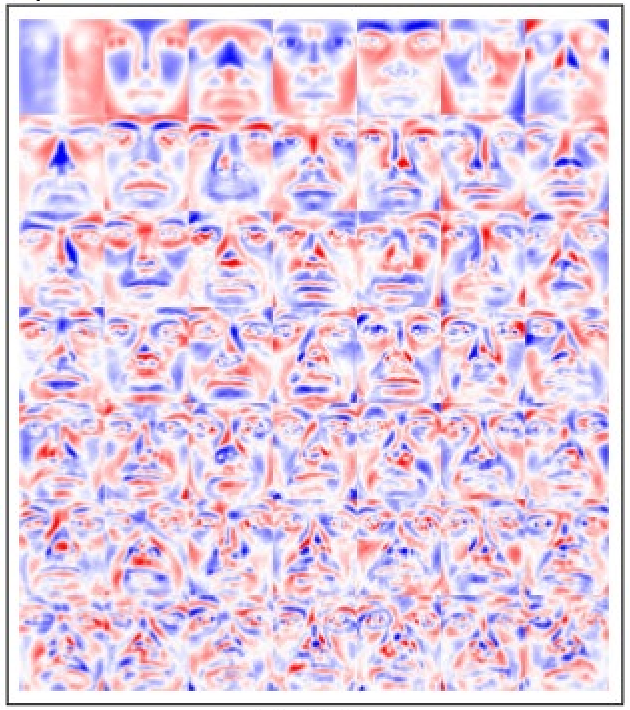
- Instead of non-negativity, we could use L1-regularization:

$$f(W,Z) = \frac{1}{2}\|ZW - X\|_F^2 + \frac{\lambda_1}{2}\sum_{i=1}^{n}\|z_i\|_1 + \frac{\lambda_2}{2}\sum_{j=1}^{d}\|w_j\|_1$$

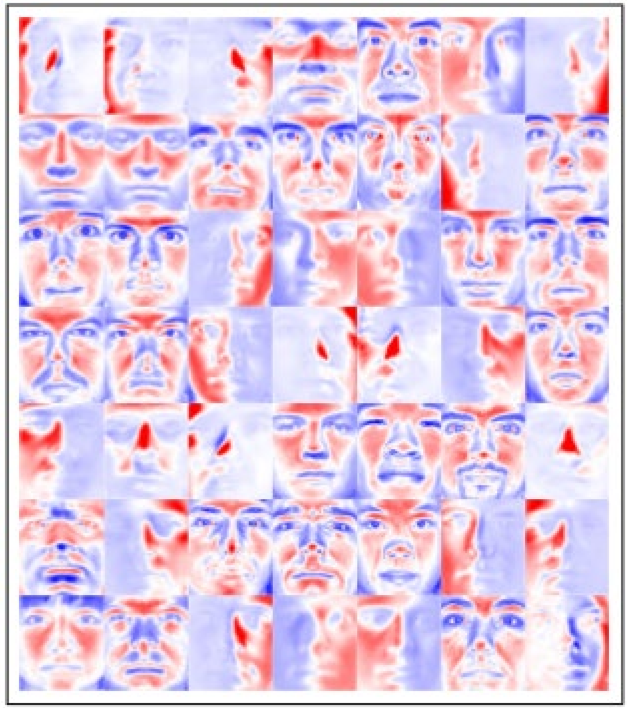
  – Called sparse coding (L1 on 'Z') or sparse dictionary learning (L1 on 'W').
- Disadvantage of using L1-regularization over non-negativity:
  – Sparsity controlled by λ_1 and λ_2 so you need to set these.
- Advantage of using L1-regularization:
  – Sparsity controlled by λ_1 and λ_2, so you can control amount of sparsity.
  – Negative coefficients often do make sense. (WHY?)

Matrix Factorization with L1-Regularization

blue: negative
red: positive

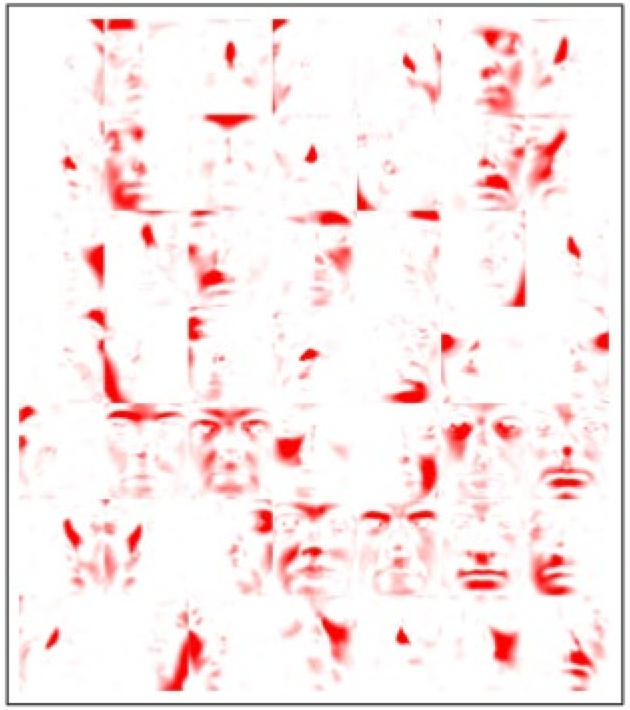


(a) PCA



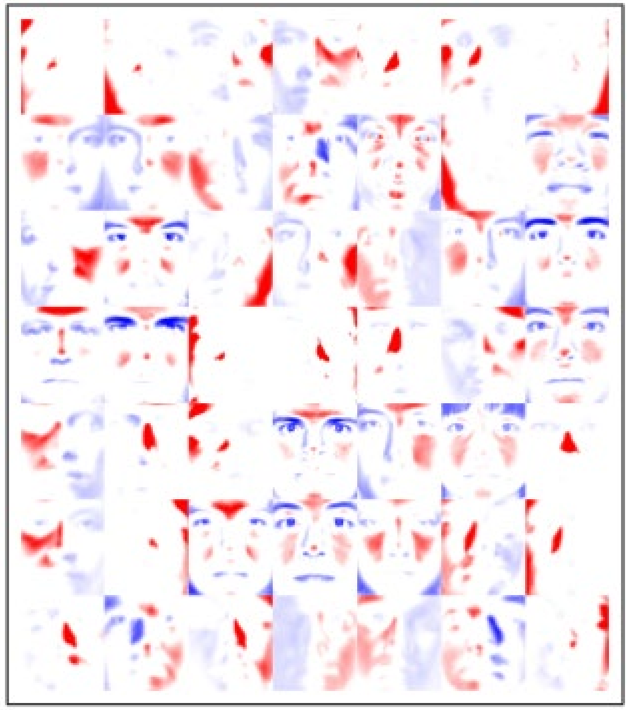
(e) Dictionary Learning

PCA without orthogonality



(c) NMF

sparsity due to non-negativity



(d) SPCA, $\tau = 30\%$

sparsity due to L_1-regularization

http://www.jmlr.org/papers/volume11/mairal10a/mairal10a.pdf

Sparse Matrix Factorization

- Instead of non-negativity, we could use L1-regularization:

$$f(W,Z) = \frac{1}{2}\|ZW - X\|_F^2 + \frac{\lambda_1}{2}\sum_{i=1}^{n}\|z_i\|_1 + \frac{\lambda_2}{2}\sum_{j=1}^{d}\|w_j\|_1$$

  – Called sparse coding (L1 on 'Z') or sparse dictionary learning (L1 on 'W').
- Many variations exist:
  – Mixing L2-regularization and L1-regularization.
    - Or normalizing 'W' (in L2-norm or L1-norm) and regularizing 'Z'.
  – K-SVD constrains each z_i to have at most 'k' non-zeroes:
    - K-means is special case where k = 1.
    - PCA is special case where k = d.

Recent Work: Structured Sparsity

- "Structured sparsity" considers dependencies in sparsity patterns.
  - Can enforce that "parts" are convex regions.

http://jmlr.org/proceedings/papers/v9/jenatton10a/jenatton10a.pdf

Summary

- Non-negative matrix factorization: LFM with no negative values.
  - Non-negativity constraints lead to sparse solution.
  - Projected gradient adds constraints to gradient descent.
- Many of our regression tricks can be used with LFMs:
  - Robust PCA uses absolute error to be robust to outliers.
  - L1-regularization leads to sparse factors/weights.

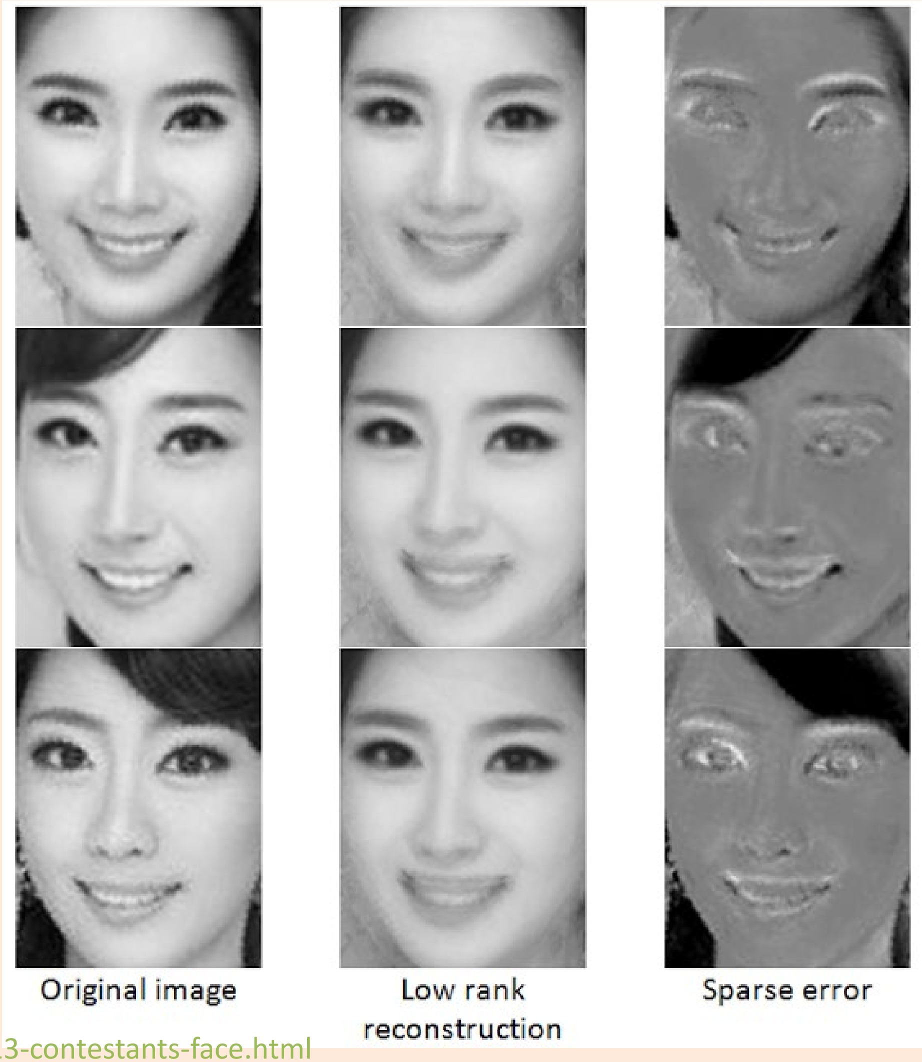
- Next time: the million-dollar Netflix challenge.

Review Questions

- Q1: How is k-means clustering an instance of latent factor methods?
- Q2: How do we encourage sparsity and regularization for Z and W without penalty terms?
- Q3: How are PCA with L1-loss and PCA with L1-regularization different?
- Q4: Why is it necessary to regularize for both Z and W for matrix factorization?
- Q5: Why would L1-regularization make negative coefficients more interpretable?

Robust PCA

- Miss Korea contestants and robust PCA:



http://jbhuang0604.blogspot.ca/2013/04/miss-korea-2013-contestants-face.html

Proof: "Synthesis" View = "Analysis" View ($WW^T = I$)

- The variance of the z_{ij} (maximized in "analysis" view):

$$\frac{1}{nk}\sum_{i=1}^{n}\|z_i - \mu_z\|^2 = \frac{1}{nk}\sum_{i=1}^{n}\|Wx_i\|^2 \quad (\mu_z = 0 \text{ and } z_i = Wx_i \text{ if } \|w_c\| = 1 \text{ and } w_c^T w_{c'} = 0)$$

$$= \frac{1}{nk}\sum_{i=1}^{n} x_i^T W^T W x_i = \frac{1}{nk}\sum_{i=1}^{n} Tr(x_i^T W^T W x_i) = \frac{1}{nk}\sum_{i=1}^{n} Tr(W^T W x_i x_i^T)$$

$$= \frac{1}{nk} Tr\left(W^T W \sum_{i=1}^{n} x_i x_i^T\right) = \frac{1}{nk} Tr(W^T W X^T X)$$

linearity of trace

$\sum_{i=1}^{n} x_i x_i^T = X^T X$

"cyclic" property of trace

- The distance to the hyper-plane (minimized in "synthesis" view):

$$\|ZW - X\|_F^2 = \|XW^T W - X\|_F^2 = Tr((XW^T W - X)^T (XW^T W - X))$$

$\|A\|_F^2 = Tr(A^T A)$

$= XW^T$

$$= Tr(W^T W X^T X W^T W) - 2Tr(W^T W X^T X) + Tr(X^T X)$$

$$= Tr(W^T \underbrace{W W^T}_{I} W X^T X) - 2Tr(W^T W X^T X) + Tr(X^T X)$$

$$= -Tr(W^T W X^T X) + (\text{constant})$$

Solved by same 'W'

Canonical Correlation Analysis (CCA)

- Suppose we have two matrices, 'X' and 'Y'.
- Want to find matrices W_X and W_Y that maximize correlation.
  - "What are the latent factors in common between these datasets?"
- Define the correlation matrices:

$$\Sigma_{XX} = \frac{1}{n}\sum_{i=1}^{n} x_i x_i^T \quad \Sigma_{YY} = \frac{1}{n}\sum_{i=1}^{n} y_i y_i^T \quad \Sigma_{XY} = \frac{1}{n}\sum_{i=1}^{n} x_i y_i^T$$

- Canonical correlation analysis (CCA) maximizes

$$Tr(W_Y^T W_X \Sigma_{XX}^{-1/2} \Sigma_{XY} \Sigma^{-1/2})$$

  - Subject to W_X and W_Y having orthogonal rows.
- Computationally, equivalent to PCA with a different matrix.
  - Using the "analysis" view that PCA maximizes $Tr(W^TWX^TX)$.

Kernel PCA

- From the "analysis" view (with orthogonal PCs) PCA maximizes:

$$Tr(W^TWX^TX)$$

- It can be shown that the solution has the form (see here):

$$\underbrace{W}_{k \times d} = \underbrace{U}_{k \times n}\underbrace{X}_{n \times l}$$

- Re-parameterizing in terms of 'U' gives a kernelized PCA:

$$Tr(X^TU^TUXX^TX) = Tr(U^TU\underbrace{XX^T}_{K}\underbrace{XX^T}_{K})$$

- It's hard to initially center data in 'Z' space,
  but you can form the centered kernel matrix (see here).

Probabilistic PCA

- With zero-mean ("centered") data, in PCA we assume that

$$x_i \approx W^T z_i$$

- In probabilistic PCA we assume that

$$x_i \sim \mathcal{N}(W^T z_i, \sigma^2 I) \qquad z_i \sim \mathcal{N}(0, I)$$

- Integrating over 'Z' the marginal likelihood given 'W' is Gaussian,

$$x_i \mid W \sim \mathcal{N}(0, W^T W + \sigma^2 I)$$

- Regular PCA is obtained as the limit of σ^2 going to 0.

Generalizations of Probabilistic PCA

- Probabilistic PCA model:

$$x_i \mid W \sim \mathcal{N}(0, W^TW + \sigma^2 I)$$

- Why do we need a probabilistic interpretation?

- Shows that PCA fits a Gaussian with restricted covariance.
  - Hope is that $W^TW + \sigma^2 I$ is a good approximation of X^TX.

- Gives precise connection between PCA and factor analysis.

Factor Analysis

- Factor analysis is a method for discovering latent factors.
- Historical applications are measures of intelligence and personality.

Trait	Description
Openness	Being curious, original, intellectual, creative, and open to new ideas.
Conscientiousness	Being organized, systematic, punctual, achievement-oriented, and dependable.
Extraversion	Being outgoing, talkative, sociable, and enjoying social situations.
Agreeableness	Being affable, tolerant, sensitive, trusting, kind, and warm.
Neuroticism	Being anxious, irritable, temperamental, and moody.

- A standard tool and widely-used across science and engineering.

https://new.edu/resources/big-5-personality-traits

PCA vs. Factor Analysis

- PCA and FA both write the matrix ‘X’ as

$$X \approx ZW$$

- PCA and FA are both based on a Gaussian assumption.

- Are PCA and FA the same?
  - Both are more than 100 years old.
  - People are still arguing about whether they are the same:
    - Doesn’t help that some packages run PCA when you call their FA method.

Google

pca vs. factor analysis

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[PDF] Principal Component Analysis versus Exploratory Factor ...
www2.sas.com/proceedings/sugi30/203-30.pdf
by DD Suhr - Cited by 118 - Related articles
1. Paper 203-30. **Principal Component Analysis vs.** Exploratory **Factor Analysis.** Diana D. Suhr, Ph.D. University of Northern Colorado. Abstract. **Principal** ...

pca - What are the differences between Factor Analysis and ...
stats.stackexchange.com/.../what-are-the-differences-between-**factor-anal**...
Aug 12, 2010 - **Principal Component Analysis** (PCA) and Common **Factor Analysis** (CFA) ..... differently one has to interpret the strength of loadings in PCA vs.

What are the differences between principal components ...
support.minitab.com/...**factor-analysis**/differences-between-**pca**-and-**facto**...
Principal Components Analysis and **Factor Analysis** are similar because both procedures are used to simplify the structure of a set of variables. However, the ...

[PDF] Principal Components Analysis - UNT
https://www.unt.edu/rss/class/.../Principal%20Components%20**Analysis**.p...
PCA vs. Factor Analysis. • It is easy to make the mistake in assuming that these are the same techniques, though in some ways exploratory factor analysis and ...

Factor analysis versus Principal Components Analysis (PCA)
psych.wisc.edu/henriques/**pca**.html
Jun 19, 2010 - **Factor analysis versus PCA**. These techniques are typically used to analyze groups of correlated variables representing one or more common ...

[PDF] Principal Component Analysis and Factor Analysis
www.stats.ox.ac.uk/~ripley/MultAnal_HT2007/PC-FA.pdf
where D is diagonal with non-negative and decreasing values and U and V ..... **Factor analysis** and PCA are often confused, and indeed SPSS has PCA as.

How can I decide between using principal components ...
https://www.researchgate.net/.../How_can_I_decide_between_using_prin...
Factor analysis (FA) is a group of statistical methods used to understand and simplify patterns ... Retrieved from http://pareonline.net/getvn.asp?v=10&n=7 ... **Principal component analysis** (PCA) is a method of factor extraction (the second step ...

[PDF] Exploratory Factor Analysis and Principal Component An...
www.lesahoffman.com/948/948_Lecture2_EFA_**PCA**.pdf
2 very different schools of thought on exploratory **factor analysis** (EFA) vs. principal components **analysis** (PCA): ➢ EFA and PCA are TWO ENTIRELY ...

Factor analysis - Wikipedia, the free encyclopedia
https://en.wikipedia.org/wiki/**Factor_analysis**
Jump to Exploratory **factor analysis versus** principal components ... - [edit]. See also: **Principal component analysis** and Exploratory **factor analysis**.

[PDF] The Truth about PCA and Factor Analysis
www.stat.cmu.edu/~cshalizi/350/lectures/13/lecture-13.pdf
Sep 28, 2009 - nents and **factor analysis**, we'll wrap up by looking at their uses and

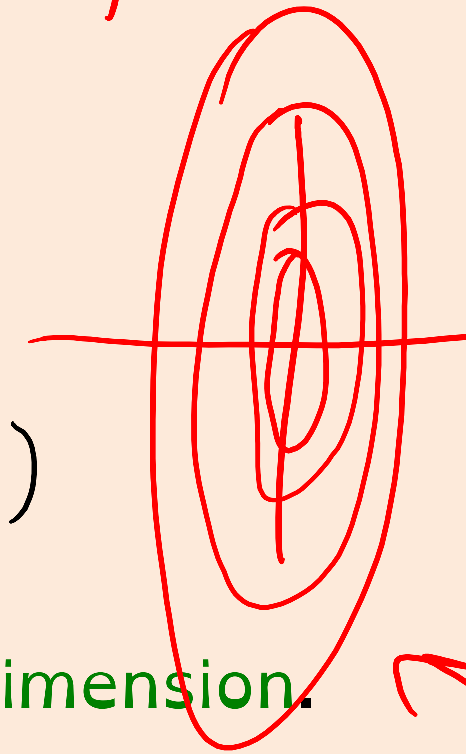
PCA vs. Factor Analysis

- In probabilistic PCA we assume:

$$x_i \sim \mathcal{N}(W^T z_i, \sigma^2 I)$$

- In FA we assume for a diagonal matrix D that:

$$x_i \sim \mathcal{N}(W^T z_i, D)$$

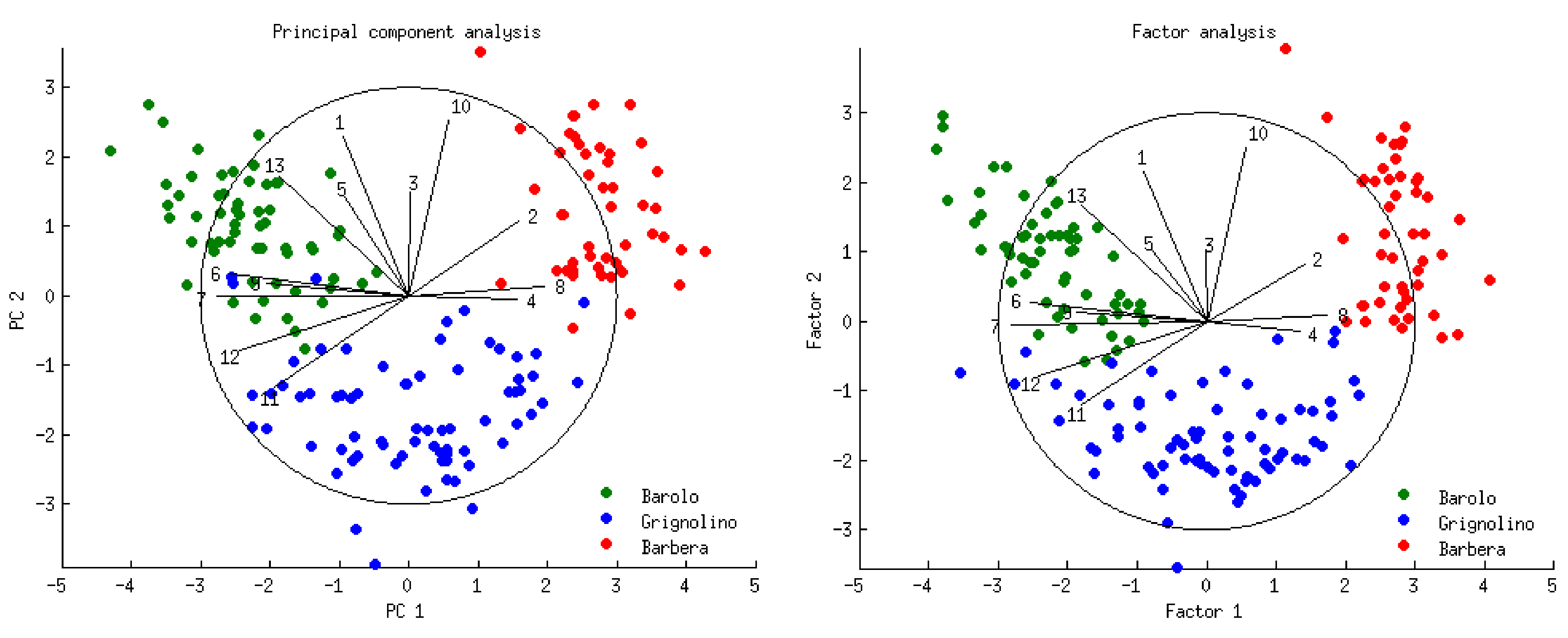


- The posterior in this case is: $x_i \mid W \sim \mathcal{N}(0, W^T W + D)$

- The difference is you have a noise variance for each dimension.
  - FA has extra degrees of freedom.

PCA vs. Factor Analysis

- In practice there often isn't a huge difference:



http://stats.stackexchange.com/questions/1576/what-are-the-differences-between-factor-analysis-and-principal-component-analysi

Factor Analysis Discussion

- Differences with PCA:
  - Unlike PCA, FA is not affected by scaling individual features.
  - But unlike PCA, it's affected by rotation of the data.
  - No nice "SVD" approach for FA, you can get different local optima.

- Similar to PCA, FA is invariant to rotation of 'W'.
  - So as with PCA you can't interpret multiple factors as being unique.

Motivation for ICA

- Factor analysis has found an enormous number of applications.
  - People really want to find the "hidden factors" that make up their data.

- But PCA and FA can't identify the factors.

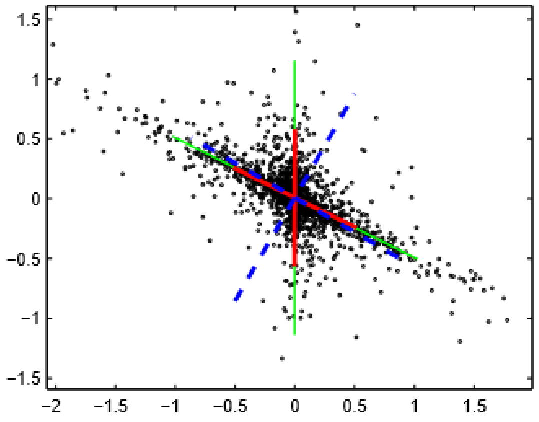


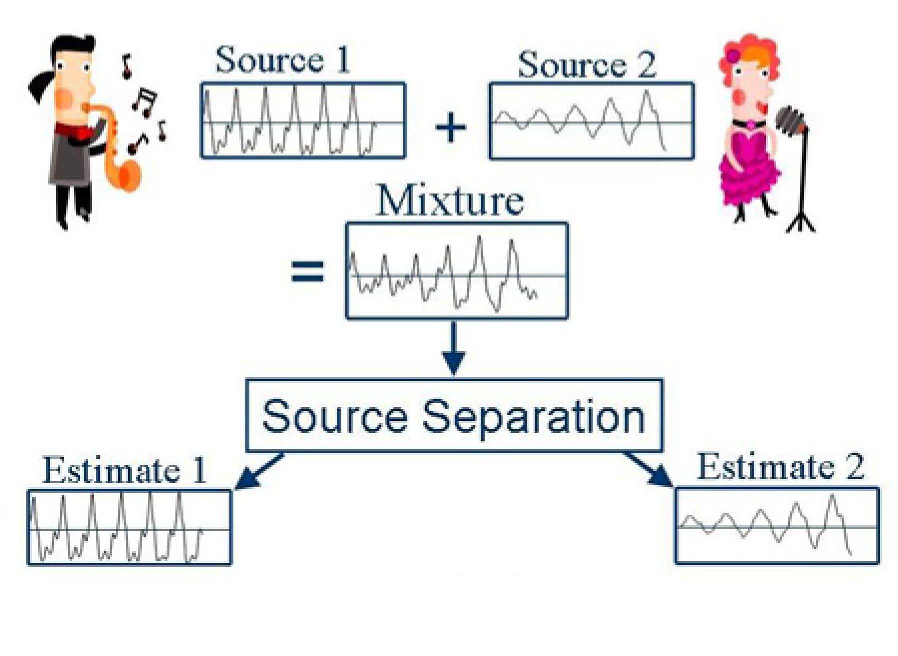
Figure : Latent data is sampled from the prior $p(x_i) \propto \exp(-5\sqrt{|x_i|})$ with the mixing matrix $\mathbf{A}$ shown in green to create the observed two dimensional vectors $\mathbf{y} = \mathbf{A}\mathbf{x}$. The red lines are the mixing matrix estimated by `ica.m` based on the observations. For comparison, PCA produces the blue (dashed) components. Note that the components have been scaled to improve visualisation. As expected, PCA finds the orthogonal directions of maximal variation. ICA however, correctly estimates the directions in which the components were independently generated.

Motivation for ICA

- Factor analysis has found an enormous number of applications.
  - People really want to find the “hidden factors” that make up their data.
- But PCA and FA can’t identify the factors.
  - We can rotate W and obtain the same model.
- Independent component analysis (ICA) is a more recent approach.
  - Around 30 years old instead of > 100.
  - Under certain assumptions it can identify factors.
- The canonical application of ICA is blind source separation.

Blind Source Separation

- Input to blind source separation:
  - Multiple microphones recording multiple sources.



- Each microphone gets different mixture of the sources.
  - Goal is reconstruct sources (factors) from the measurements.

http://music.eecs.northwestern.edu/research.php

Independent Component Analysis Applications

- ICA is replacing PCA and FA in many applications:

Some ICA applications are listed below:[1]

- optical Imaging of neurons[17]
- neuronal spike sorting[18]
- face recognition[19]
- modeling receptive fields of primary visual neurons[20]
- predicting stock market prices[21]
- mobile phone communications [22]
- color based detection of the ripeness of tomatoes[23]
- removing artifacts, such as eye blinks, from EEG data.[24]

- Recent work shows that ICA can often resolve direction of causality.

https://en.wikipedia.org/wiki/Independent_component_analysis#Applications

Limitations of Matrix Factorization

- ICA is a matrix factorization method like PCA/FA,

$$X = ZW$$

- Let's assume that $X = ZW$ for a "true" W with $k = d$.
  - Different from PCA where we assume $k \leq d$.

- There are only 3 issues stopping us from finding "true" W.

3 Sources of Matrix Factorization Non-Uniquness

- Label switching: get same model if we permute rows of W.
  - We can exchange row 1 and 2 of W (and same columns of Z).
  - Not a problem because we don't care about order of factors.

- Scaling: get same model if you scale a row.
  - If we mutiply row 1 of W by α, could multiply column 1 of Z by $1/\alpha$.
  - Can't identify sign/scale, but might hope to identify direction.

- Rotation: get same model if we rotate W.
  - Rotations correspond to orthogonal matrices Q, such matrices have $Q^TQ = I$.
  - If we rotate W with Q, then we have $(QW)^TQW = W^TQ^TQW = W^TW$.

- If we could address rotation, we could identify the "true" directions.

A Unique Gaussian Property

- Consider an independent prior on each latent features z_c.
  - E.g., in PPCA and FA we use N(0,1) for each z_c.

- If prior p(z) is independent and rotation-invariant (p(Qz) = p(z)), then it must be Gaussian (only Gaussians have this property).

- The (non-intuitive) magic behind ICA:
  - If the priors are all non-Gaussian, it isn't rotationally symmetric.
  - In this case, we can identify factors W (up to permutations and scalings).

PCA vs. ICA

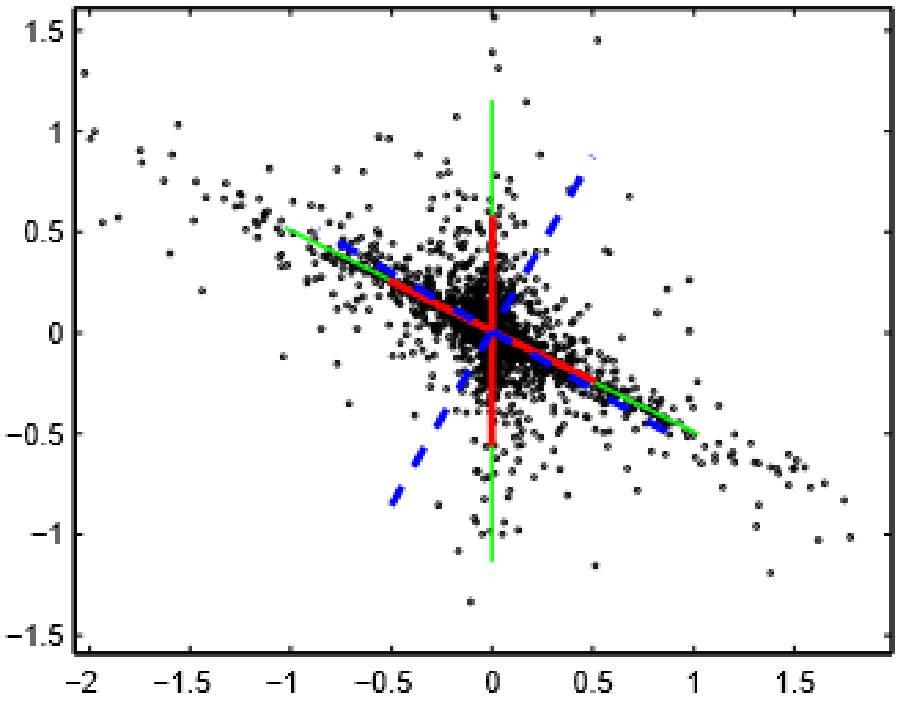


Figure : Latent data is sampled from the prior $p(x_i) \propto \exp(-5\sqrt{|x_i|})$ with the mixing matrix $\mathbf{A}$ shown in green to create the observed two dimensional vectors $\mathbf{y} = \mathbf{A}\mathbf{x}$. The red lines are the mixing matrix estimated by `ica.m` based on the observations. For comparison, PCA produces the blue (dashed) components. Note that the components have been scaled to improve visualisation. As expected, PCA finds the orthogonal directions of maximal variation. ICA however, correctly estimates the directions in which the components were independently generated.

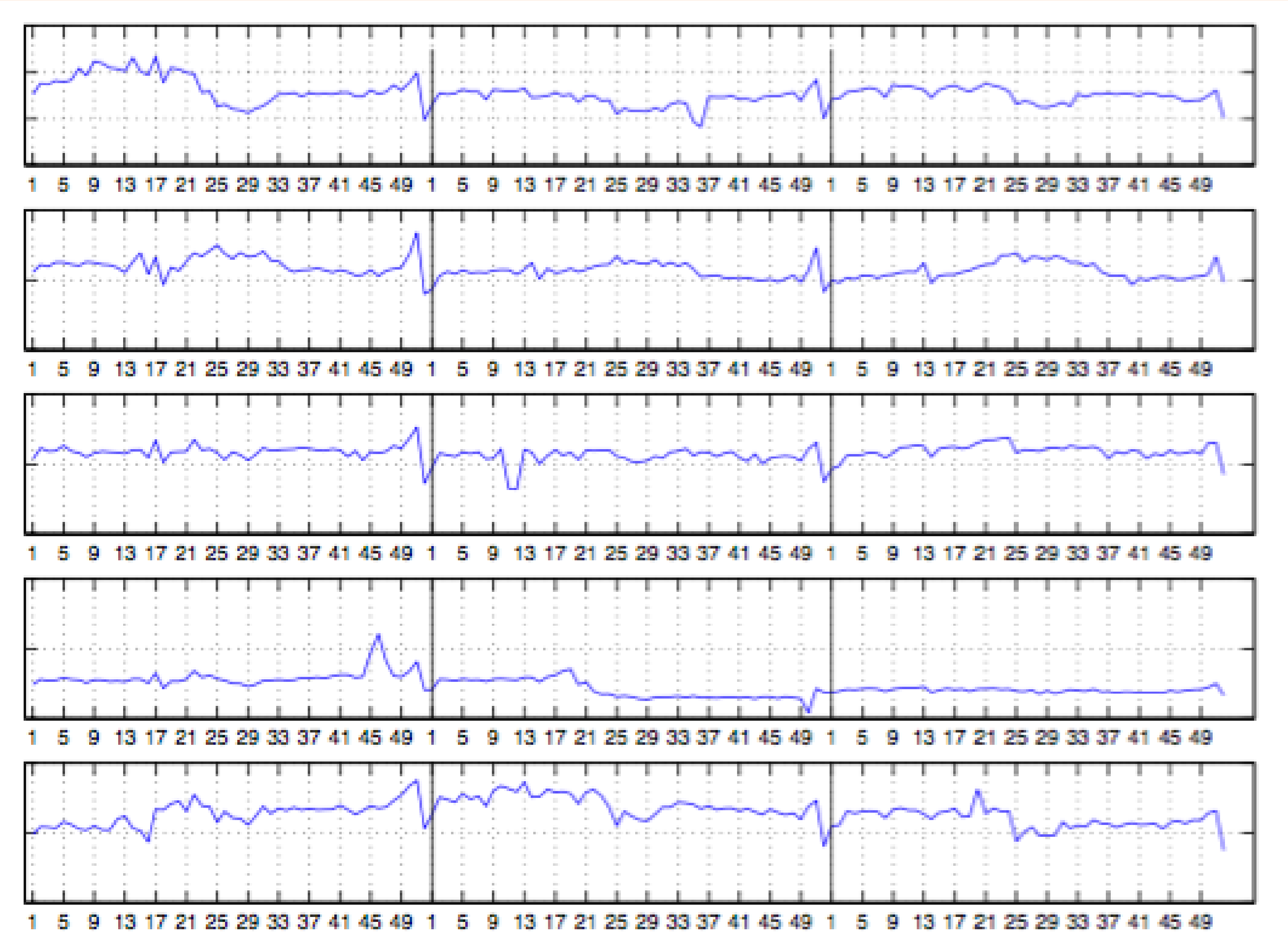
http://www.inf.ed.ac.uk/teaching/courses/pmr/lectures/ica.pdf

Independent Component Analysis

- In ICA we approximate X with ZW, assuming $p(z_{ic})$ are non-Gaussian.
- Usually we “center” and “whiten” the data before applying ICA.
- There are several penalties that encourage non-Gaussianity:
  - Penalize low kurtosis, since kurtosis is minimized by Gaussians.
  - Penalize high entropy, since entropy is maximized by Gaussians.
- The fastICA is a popular method maximizing kurtosis.

ICA on Retail Purchase Data

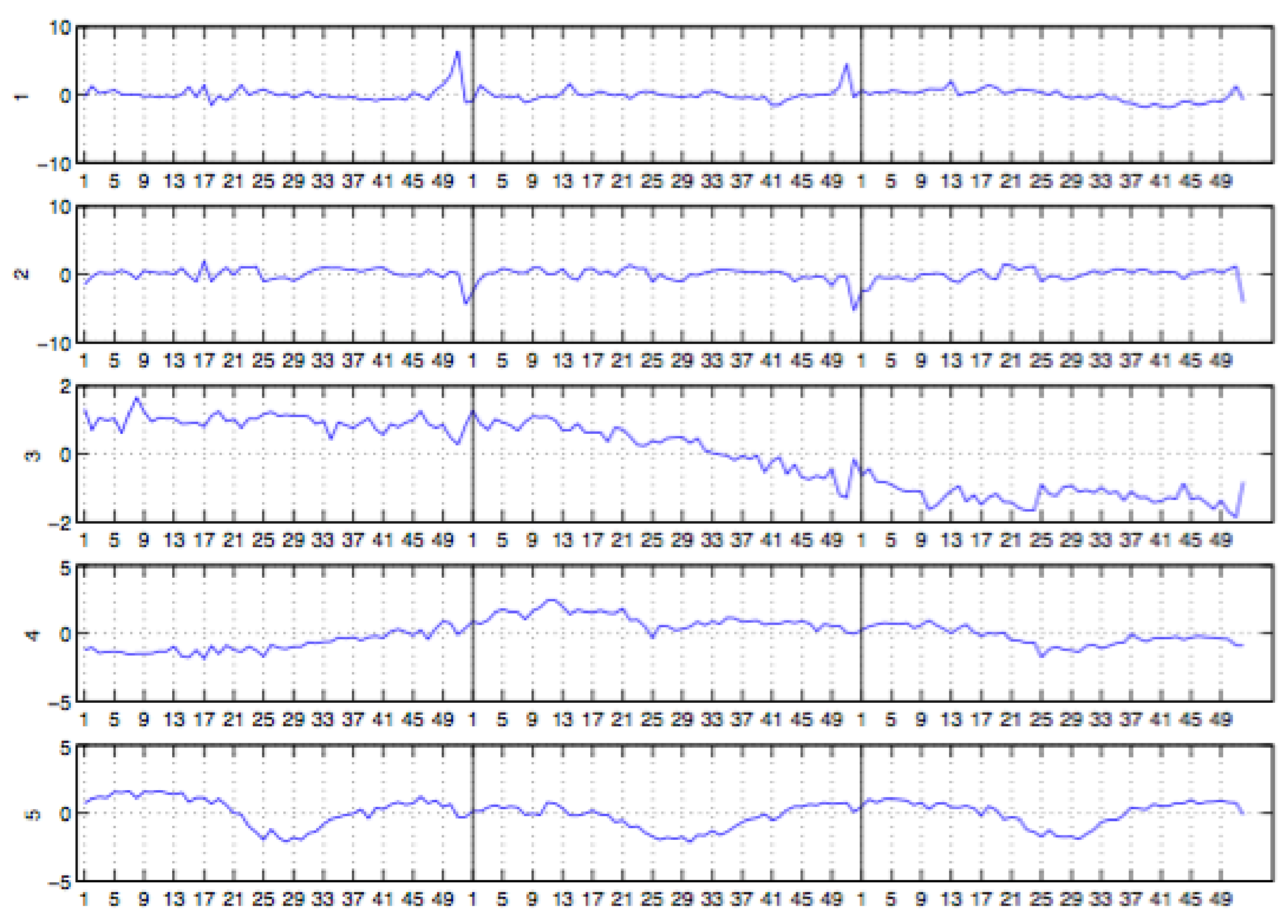
- Cash flow from 5 stores over 3 years:



http://www.stat.ucla.edu/~yuille/courses/Stat161-261-Spring14/HyvO00-icatut.pdf

ICA on Retail Purchase Data

- Factors found using ICA:



http://www.stat.ucla.edu/~yuille/courses/Stat161-261-Spring14/HyvO00-icatut.pdf