Partial Least Squares Correlation
Inter Battery Analysis
co-inertia Analysis

Hervé Abdi

Today's Topics

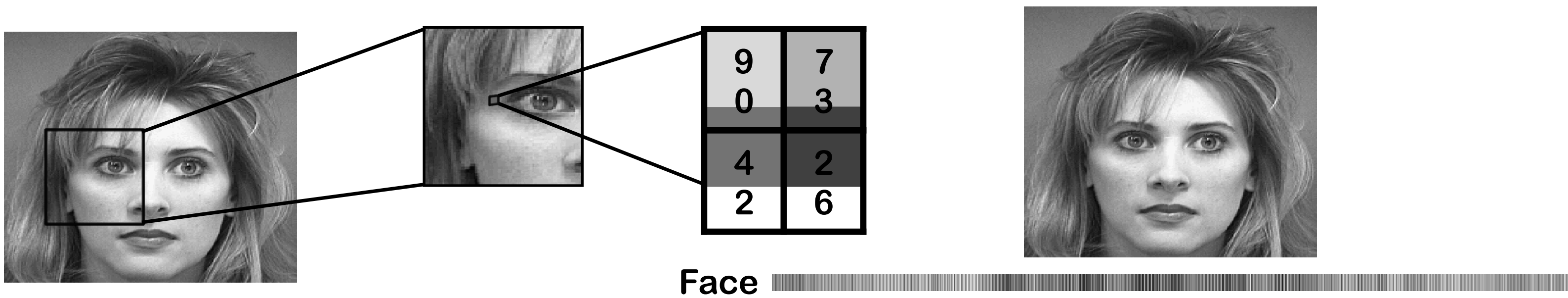
- Fast review of (PCA)
- Refresh SVD and Eigen
- Partial Least Squares Correlation (PLSC)

What are Multivariate Data?

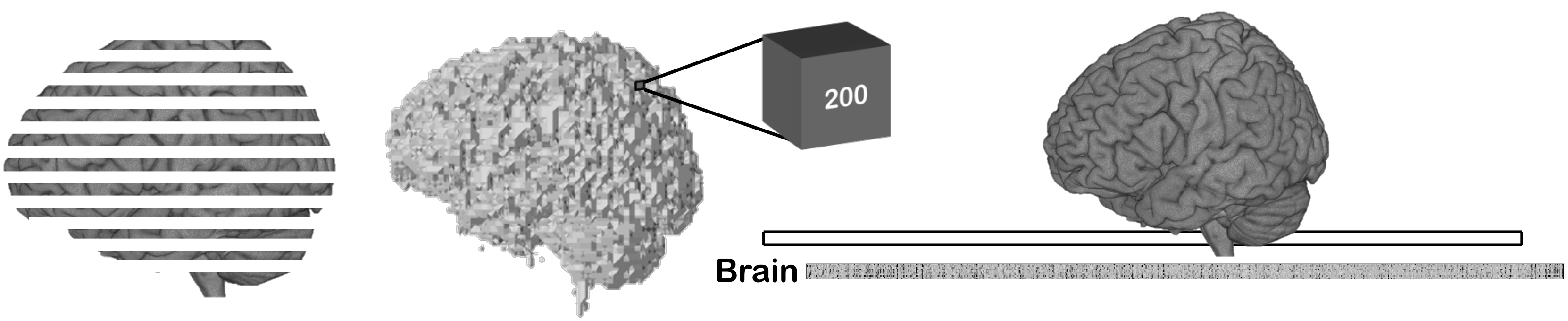
- Surveys

Personality	5	9	…	0	3	…	10	8	…	5

- Images



- Brains



Check-List

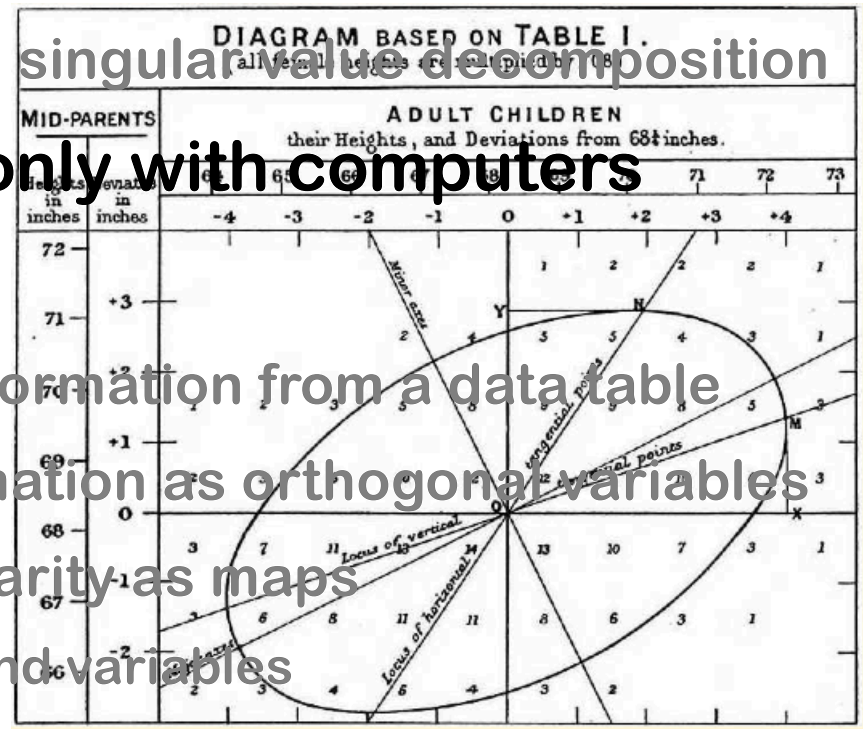
Working with Multivariate Data

- **Common characteristics**
  - Many more variables than observations (N<<P)
    - Traditional analyses cannot handle this
  - Inference: usual assumptions may not hold
- **Pre-processing**
  - Centering: subtract the mean
  - Normalizing: remove unit of measurement
- **Goal of analysis techniques**
  - Extract most important information

Principal Component Analysis

- Oldest multivariate technique
  - Idea: Cauchy (1829); Galton (1859); Pearson (1902)
  - AKA: Eigen-analysis; singular value decomposition
- But really do-able only with computers
- Goal of PCA:
  - Extract important information from a data table
  - Represent the information as orthogonal variables
  - Display pattern similarity as maps
    - Both observations and variables

Sir Francis Galton (1822-1911)



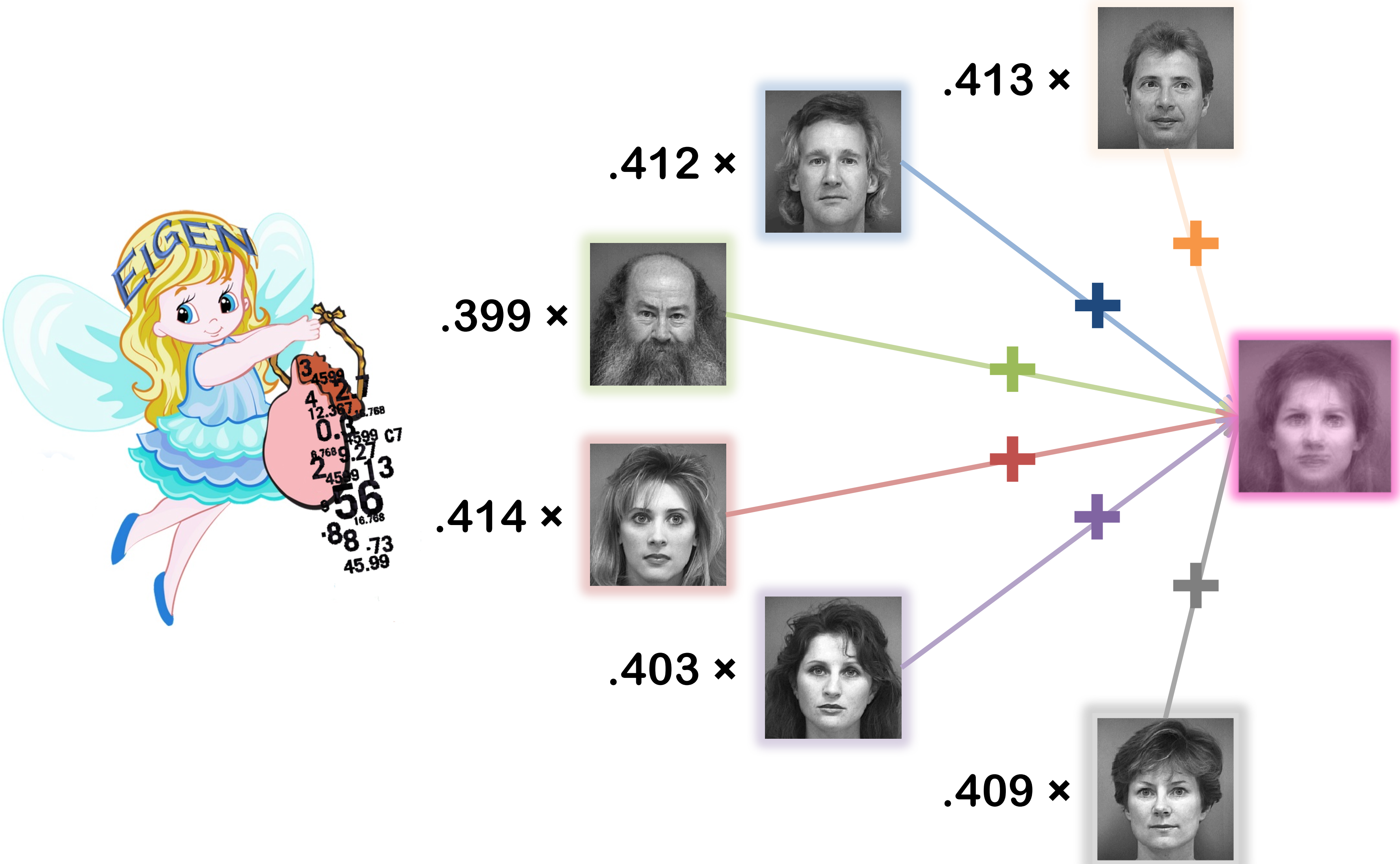
(A Kind of) PCA Comparing Mid-Parental to Adult Children Height

PCA Example with Faces

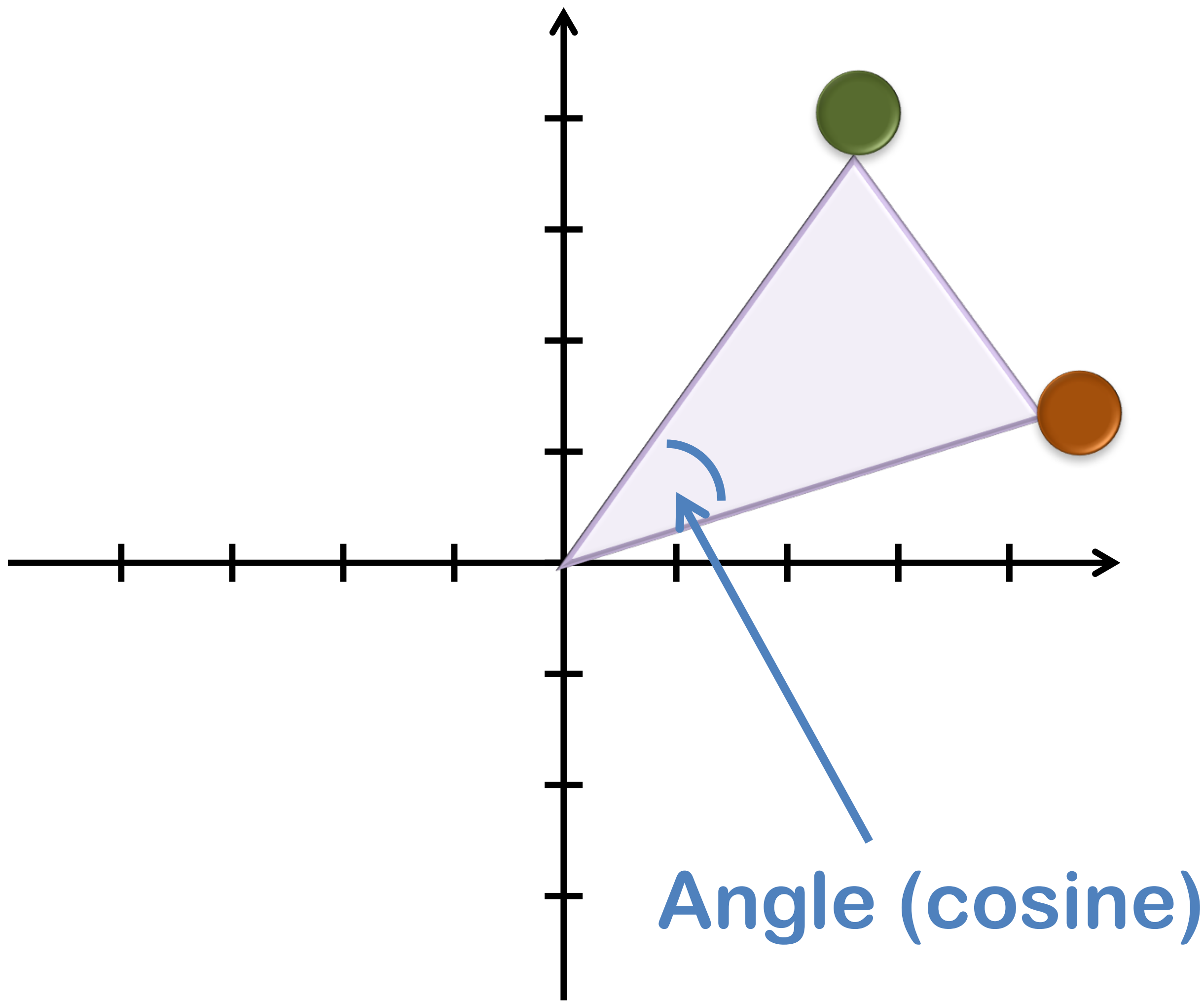
What's in a Face?

- What is common?
  - Create a mixture
- Practically
  - Weighted average
- Technically
  - Most similar face
    - To all other faces

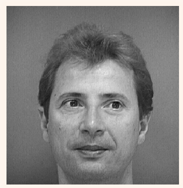
What is Most Common?

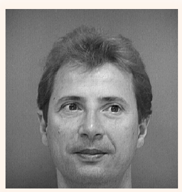
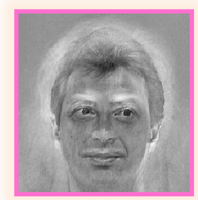


Evaluating Similarity



What Does Most Common Mean?

cos ( , ) = .98

 − .98 ×  = 

Identity!

To tell the Truth: Squared Cosines!

WHAT DO WE DO WITH AN EIGENFACE?

- **Frame it!**
  - Eigen Art
- **Subtract it!**
  - Remove commonality
- **Plot it!**
  - Pattern similarity

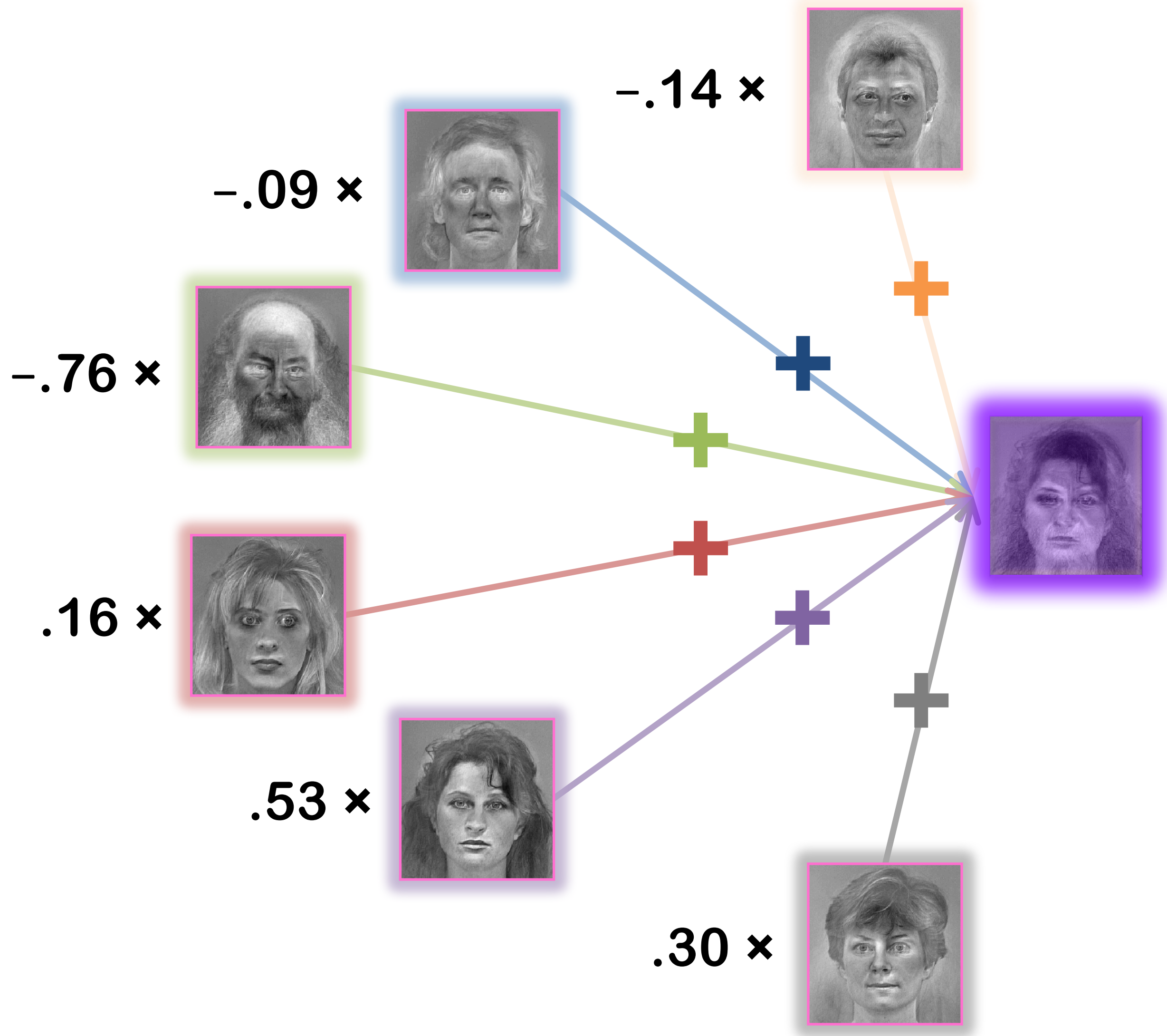
The Power of Subtraction

- Remove the first eigenface from the set
  - To get to the second eigenface
- Now, the first and second eigenfaces
  - Uncorrelated or Orthogonal
  - Explain unique variance
- Continue to find all the eigenfaces
  - When do we stop??

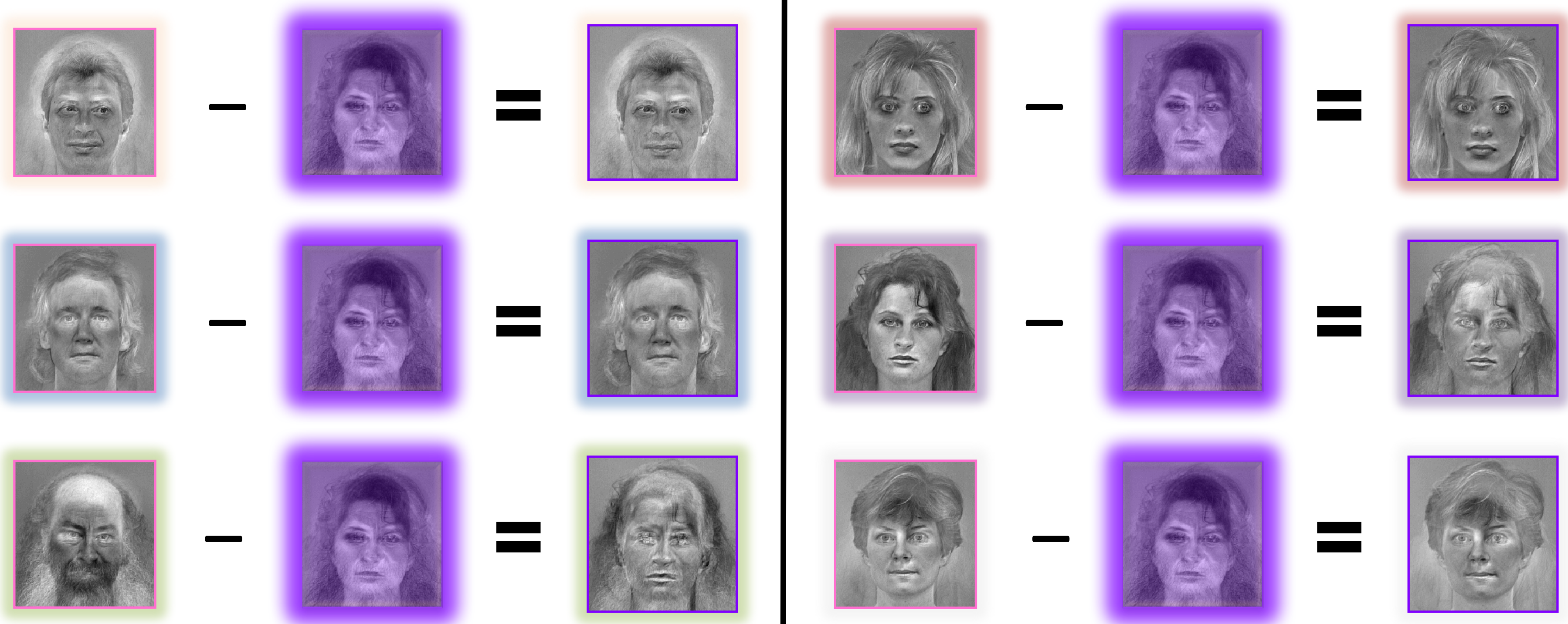
ELIMINATION BY SUBTRACTION

Extract Components

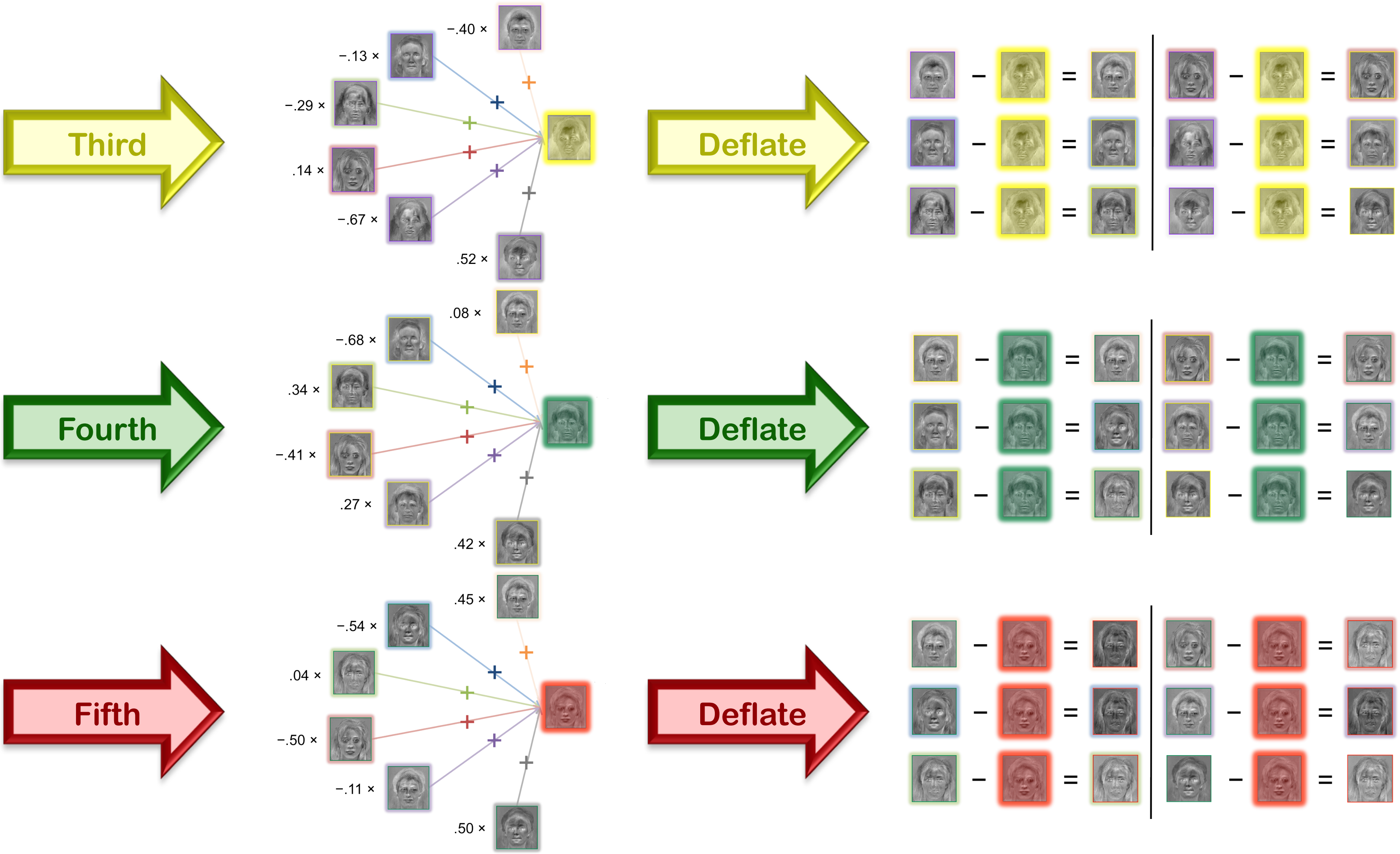
Second Eigenface



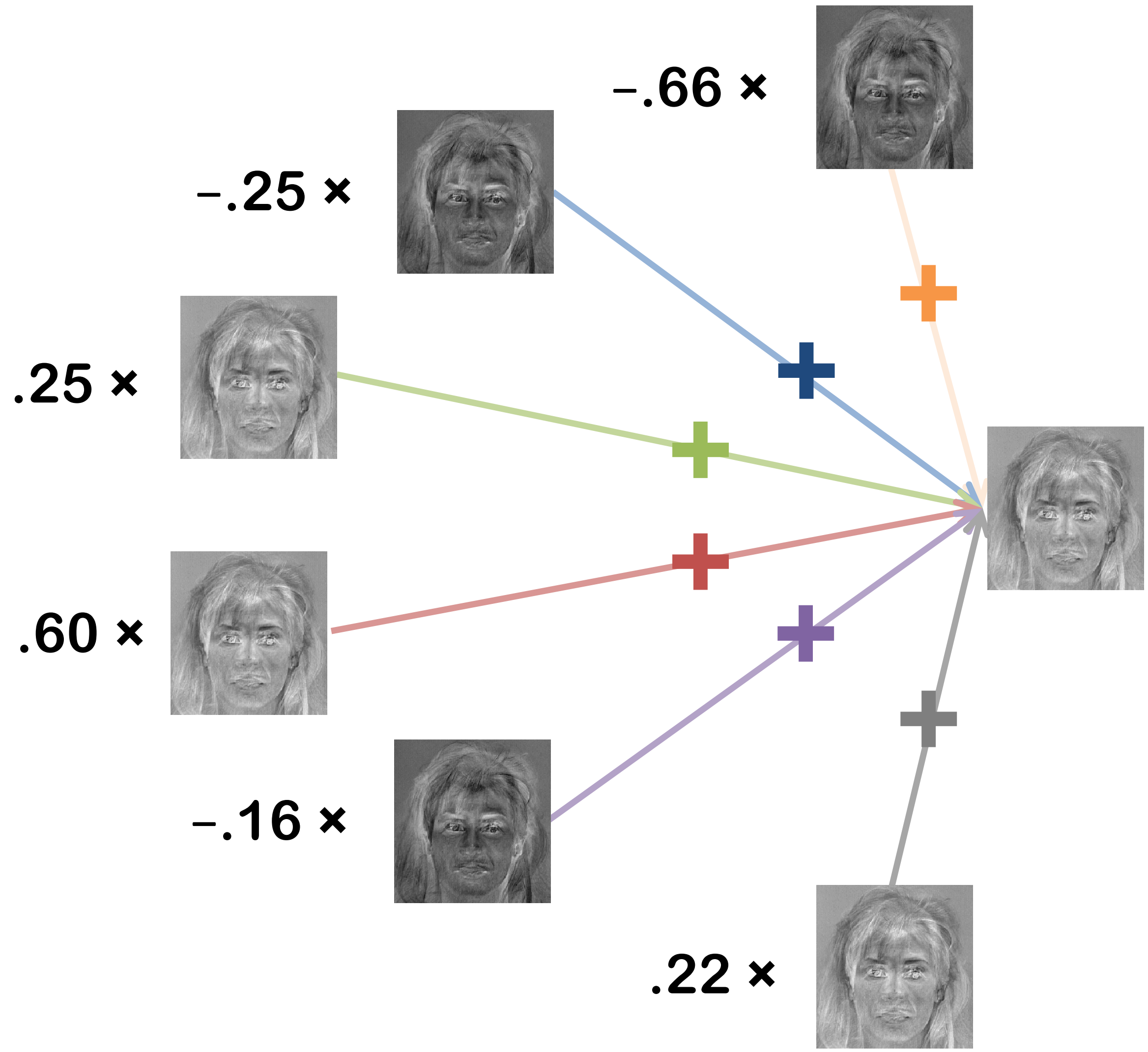
Elimination by Subtraction



And we Go On and On ...



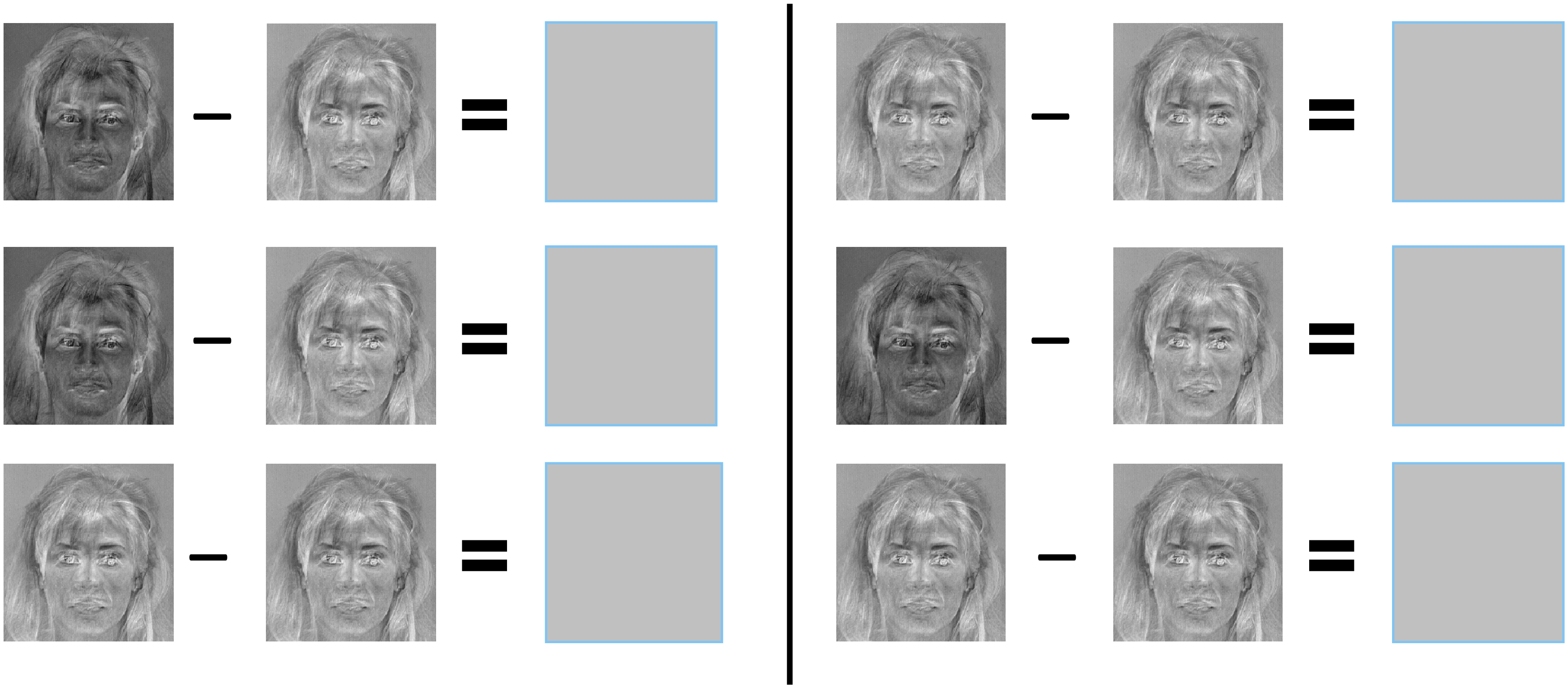
SIXTH EIGENFACE



Final Step

Elimination by Subtraction

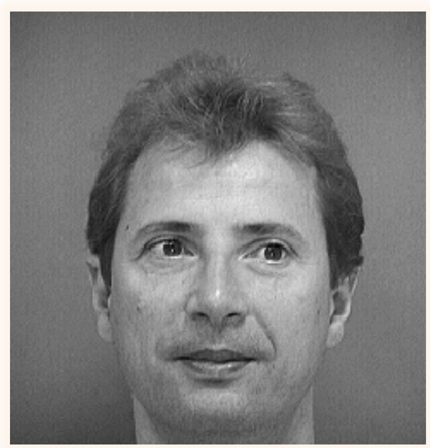
- When do we stop???



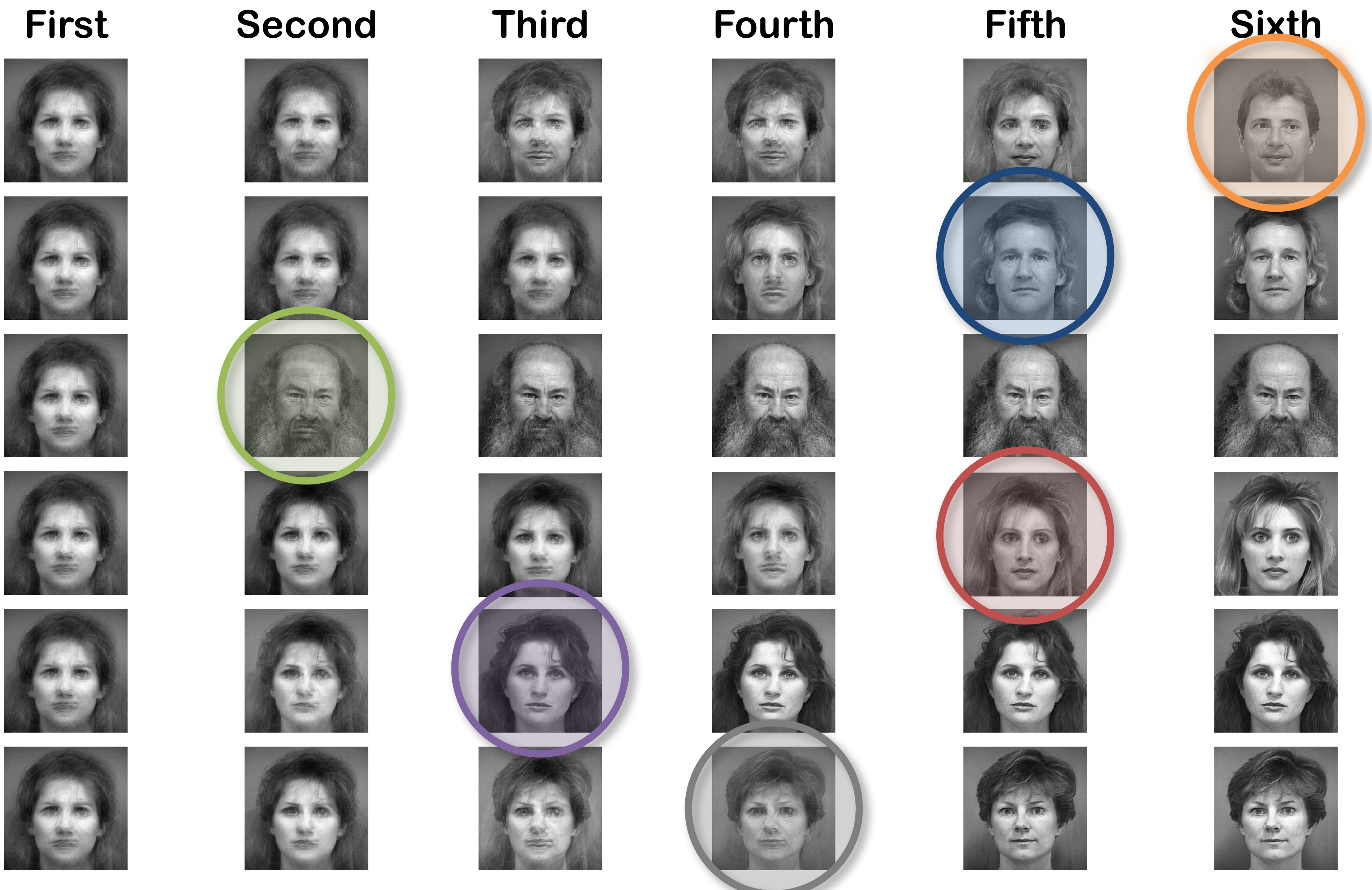
BUILDING BACK A FACE

[.98 × ] + [−.06 × ] + [.12 × ]

+ [.02 × ] + [.10 × ] + [−.12 × ]

= 

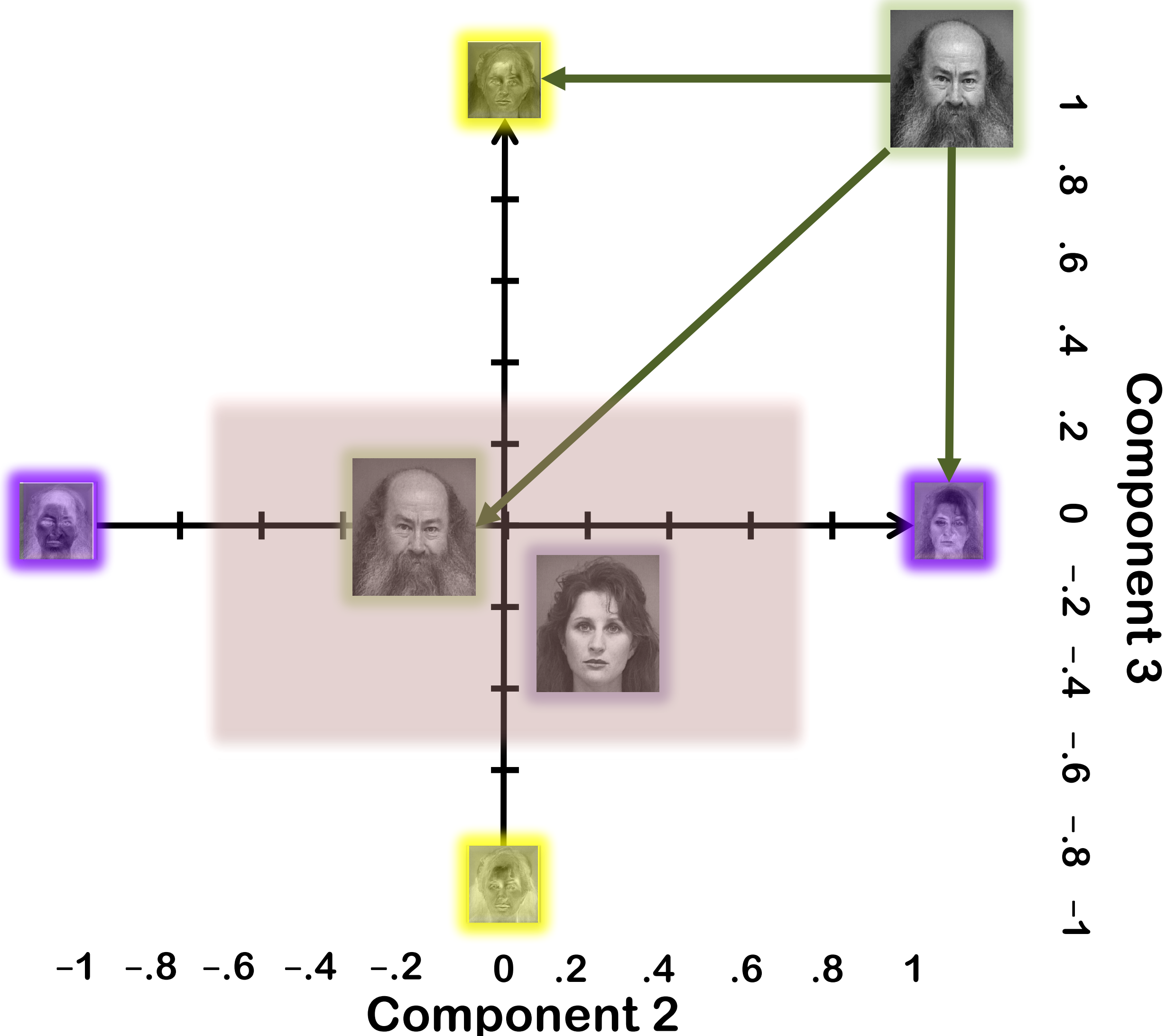
How Many Eigen Faces in a Face?



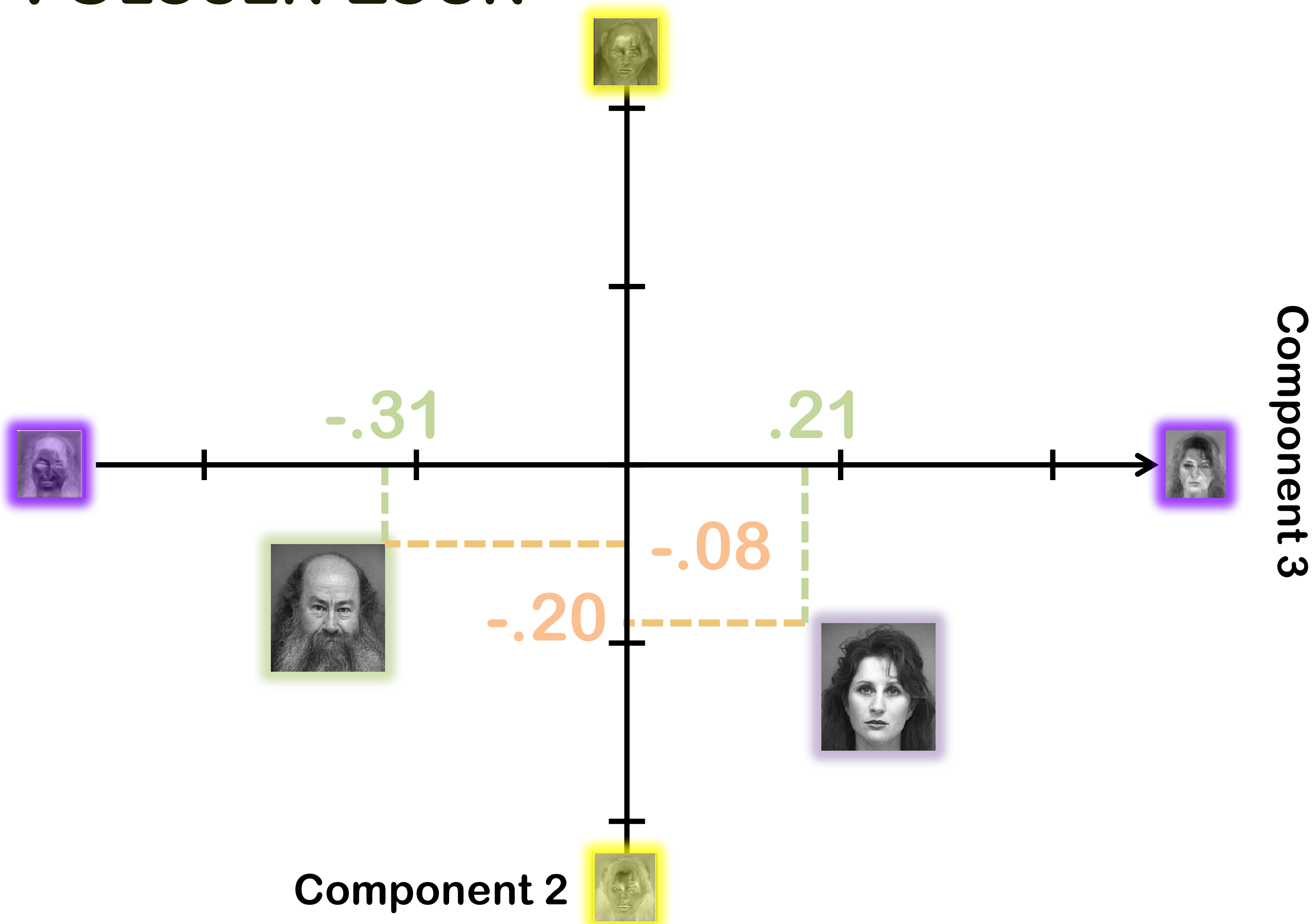
What is the Point of All This?

- Components to construct faces
  - New or original
- All information about the faces
  - 6 faces represented by 6 components
    - Instead of 55,200 pixels (per image)
- How do we examine these components?
  - Bi-dimensional plots
    - Show how these faces are related
    - We ignore the first component (average face)

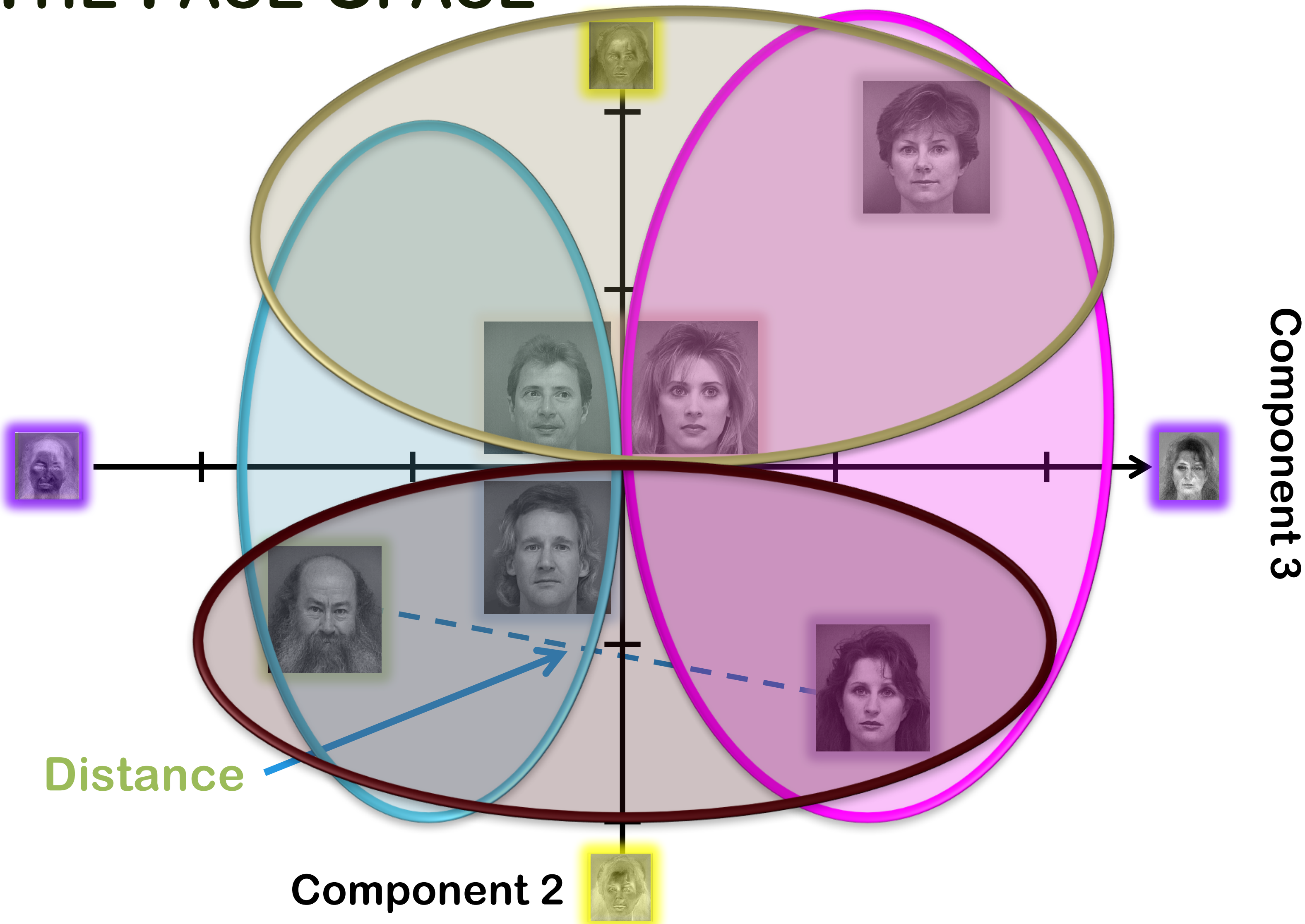
Displaying the Face Space



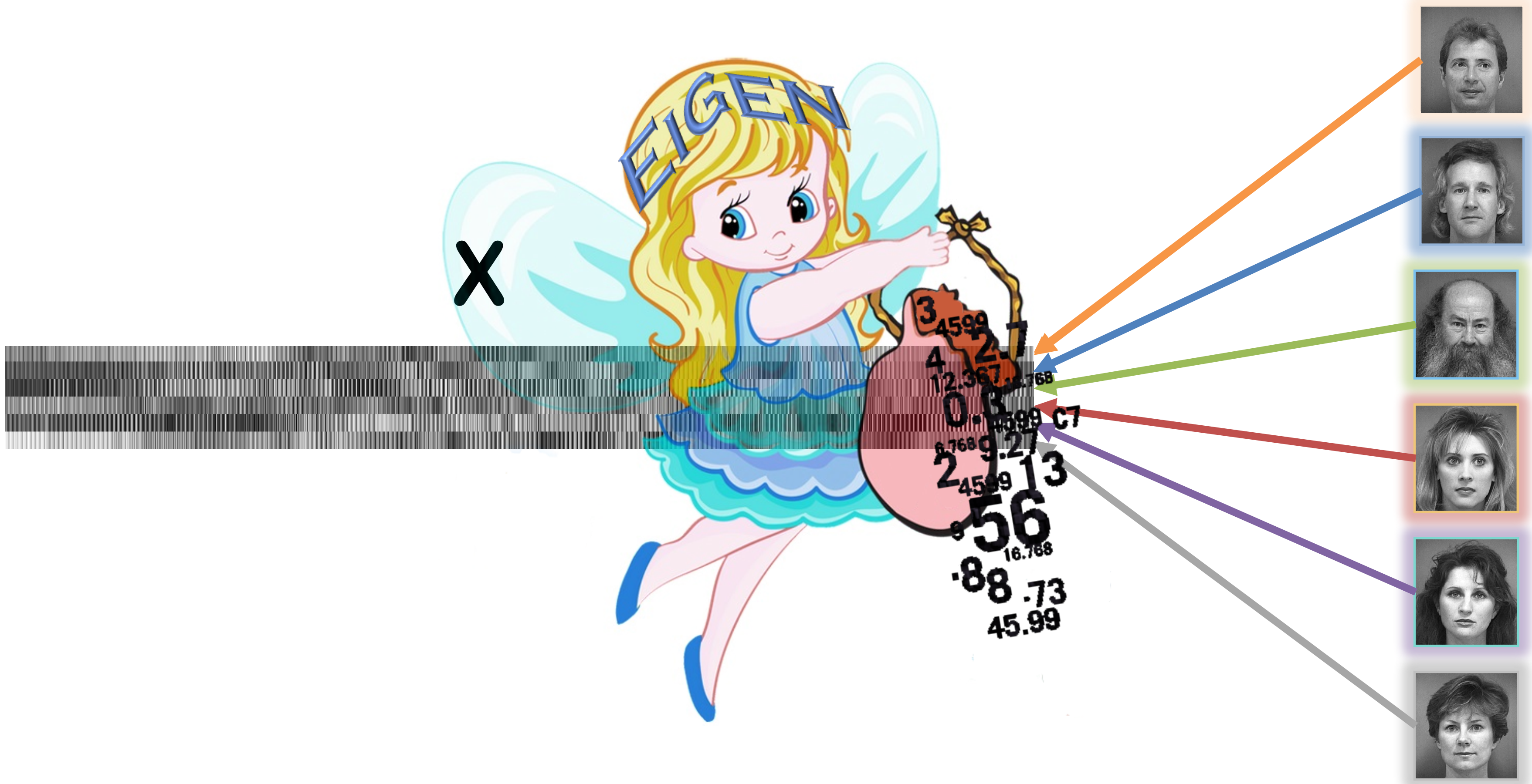
A Closer Look



The Face Space



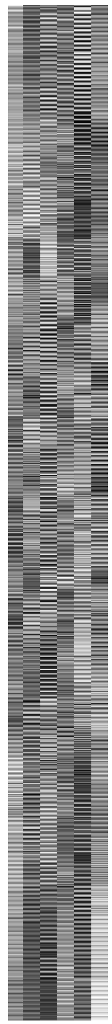
How Do We Do It?

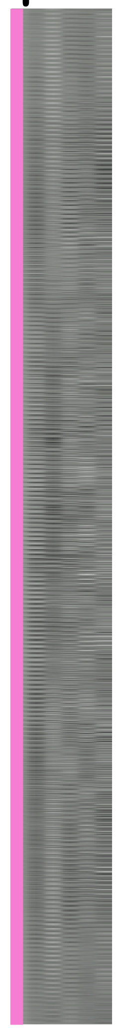


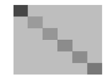
Singular Value Decomposition

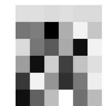
Faces Components Variance Faces

$$X = P \quad \Delta \quad Q^T$$









Pixels = Pixels

- Eig
  - E
- Co
  - Ea
- Variance
  - Each element of Δ

Explained Variance

How Good is a Component?

- How much it explains of the faces
  - Variance given by the eigenvalue
- Here:

Comp.	1	2	3	4	5	6
λ	5.61	0.16	0.09	0.06	0.05	0.03
SUM	5.61	5.78	5.82	5.92	5.97	6.00
τ (%)	5.61/6.00 = 94	3	1	1	1	1
SUM	94	97	98	99	99	100

Pause SVD

END OF SVD-EIGEN PAUSE

From One Table to Two Tables

Partial Least Squares Methods

- Partial Least Squares
  - PLS Regression – Predict performance
  - PLS Correlation – Extract commonalities
- Partial Least Squares Regression
  - Econometrics; Chemometrics
    - H. Wold (1982), M. Martens, H. Martens, S. Wold (1983)
- Partial Least Squares Correlation
  - Psychometrics; Ecology; Epidemiology
    - Tucker (1958); Dolédec & Chessel (1994); Bookstein (1982)
  - Neuroimaging
    - McIntosh, Bookstein, Haxby, & Grady (1996)

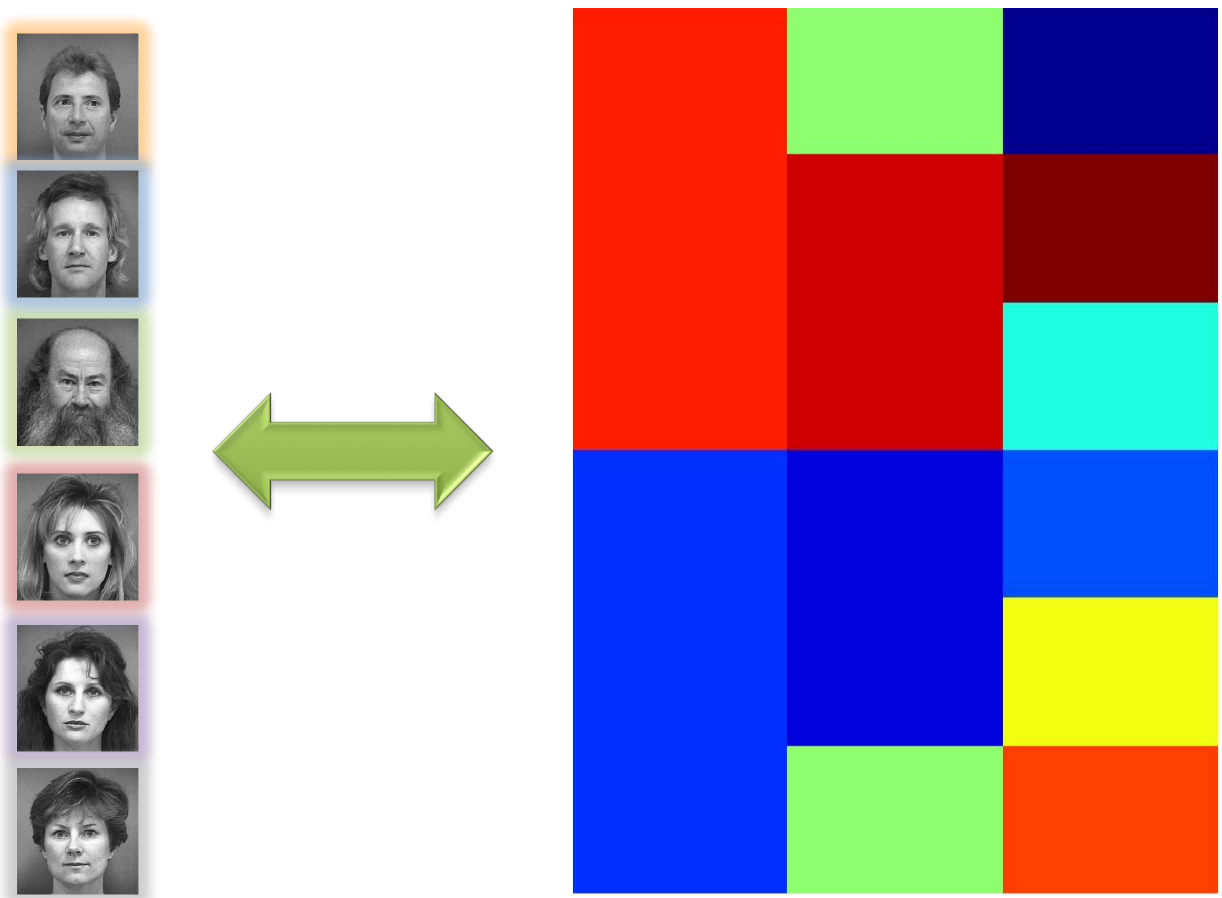
Partial Least Squares Correlation

- Goal of PLSC
  - Relate two tables
- Find commonality
  - Maximize covariance
- Components
  - "Saliences"
  - Latent variables
- Multiple versions
  - Example
    - Brain (Or Faces!)
    - Behavior

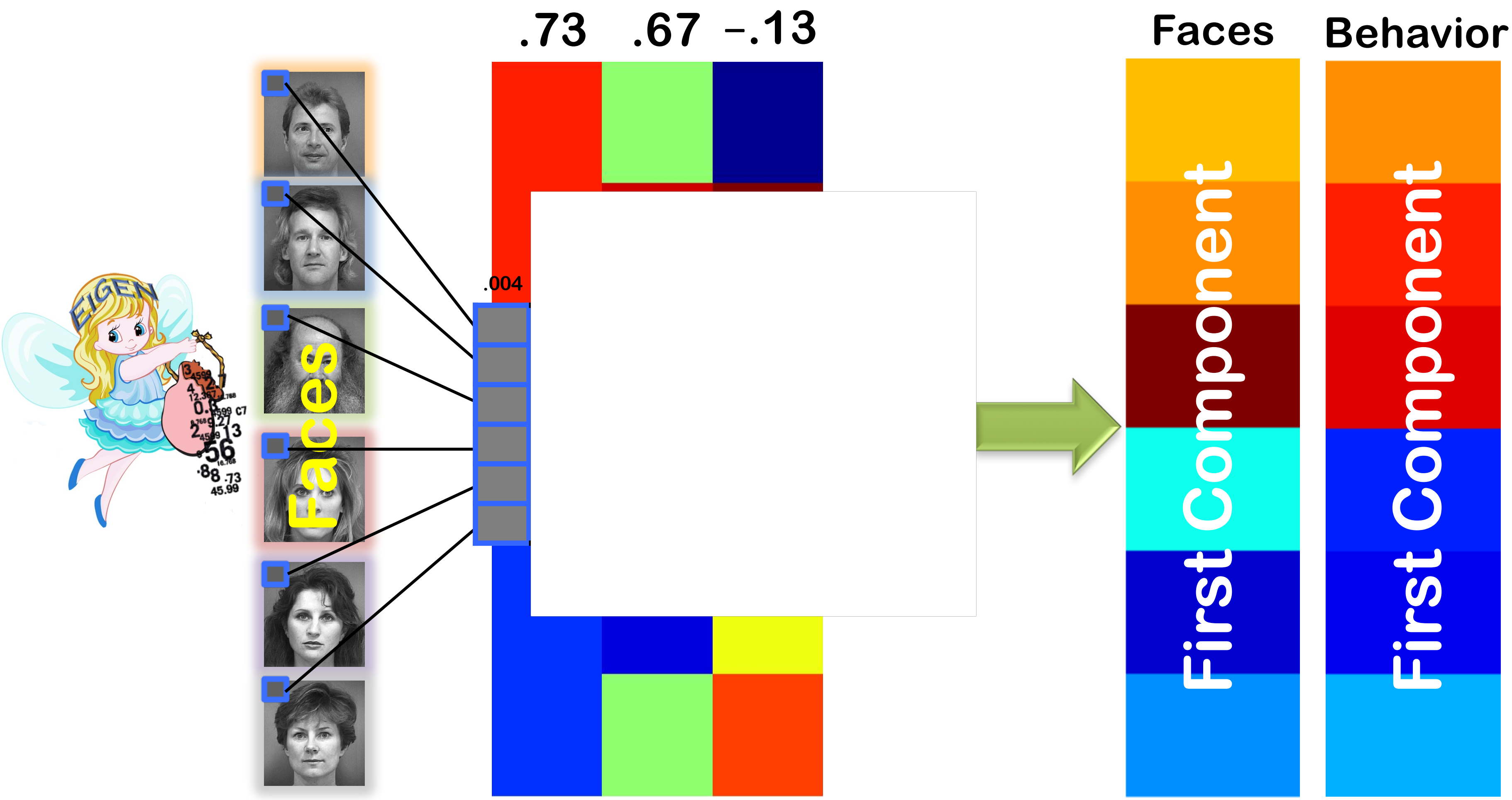
Sex	Age	Expertise
1	2	1
1	3	6
1	3	3
-1	1	2
-1	1	4
-1	2	5

QUESTION

WHAT DO WE WANT TO KNOW?



Extracting Common Information



FORMALLY

What Do we want?

One Linear Transformation of X

Called a *Latent Variable* From X

One Linear Transformation of Y

Called a *Latent Variable* From Y

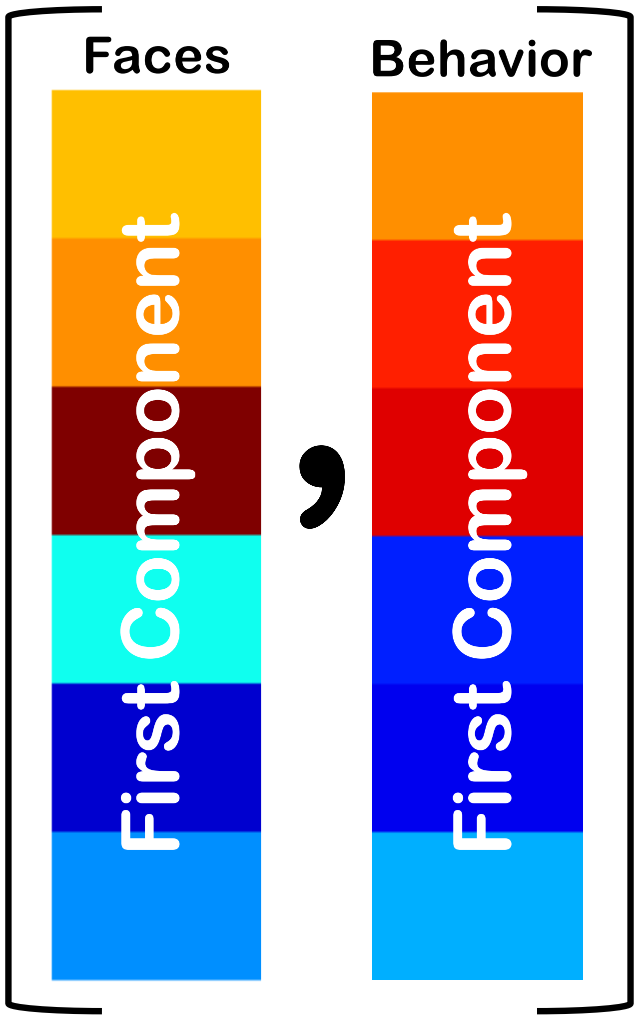
Latent variables most alike:

MAX COVARIANCE

Back to the example

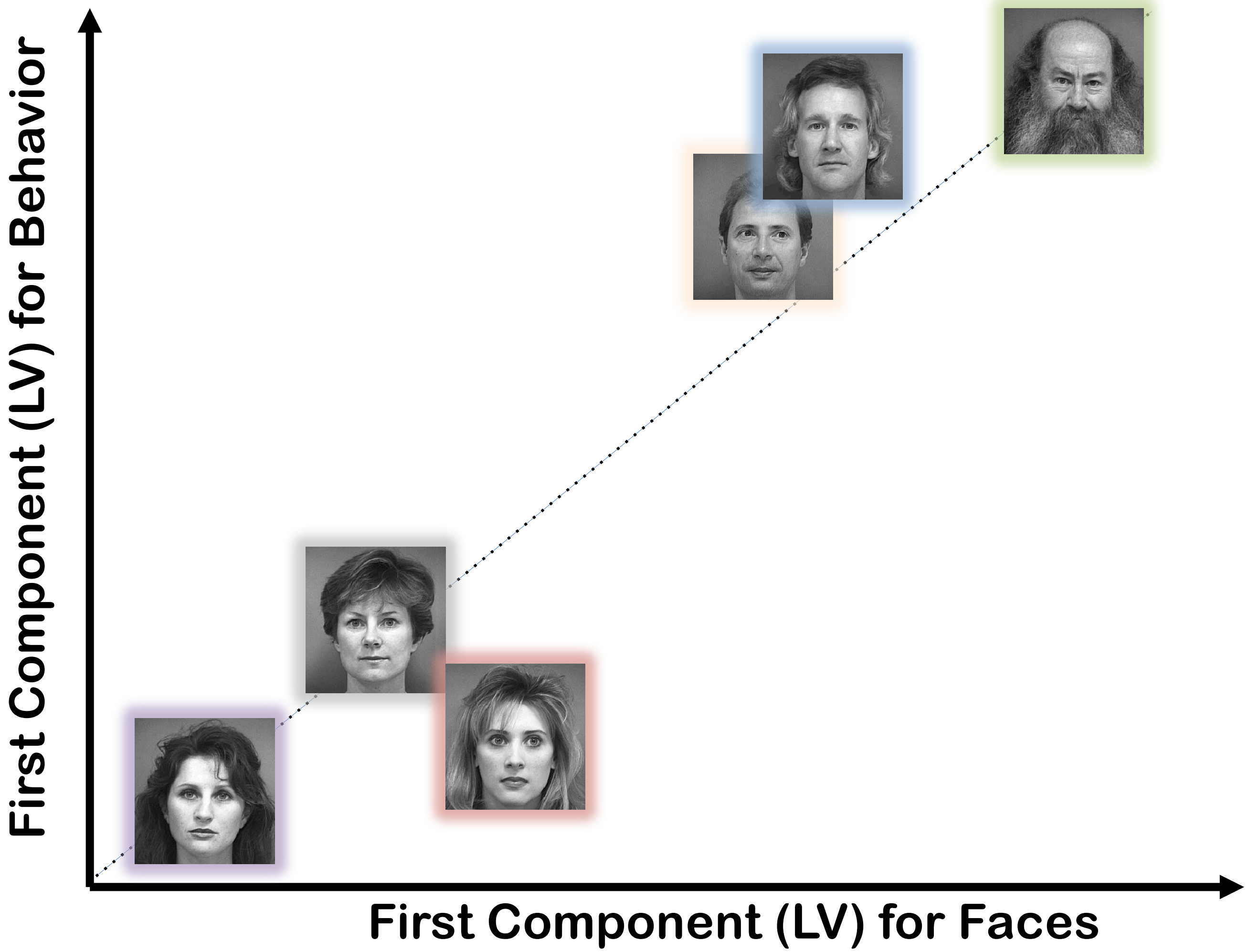
Extracting Common Information

Covariance

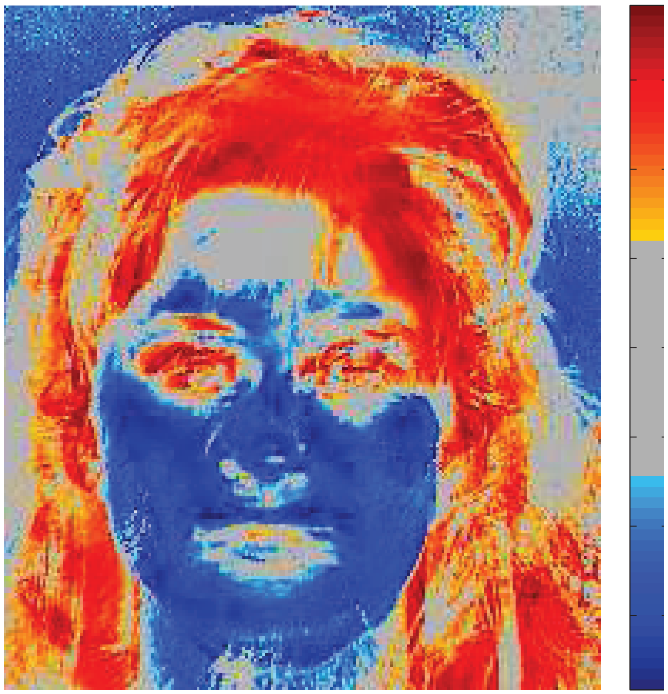


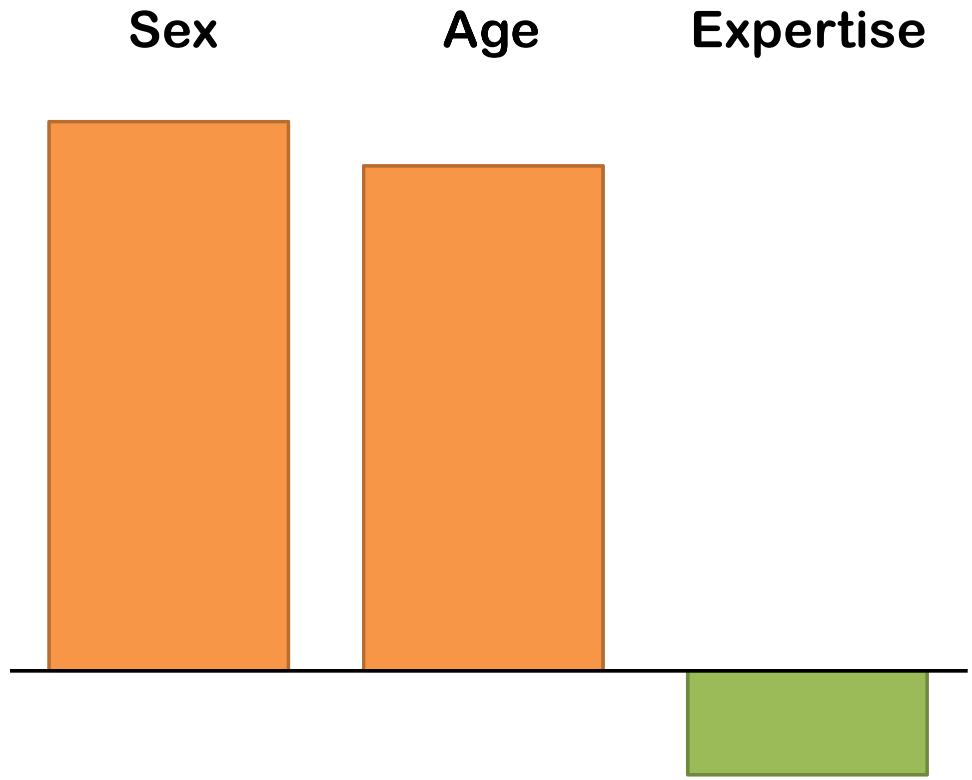
= Maximum

Understanding The First Component (LV)

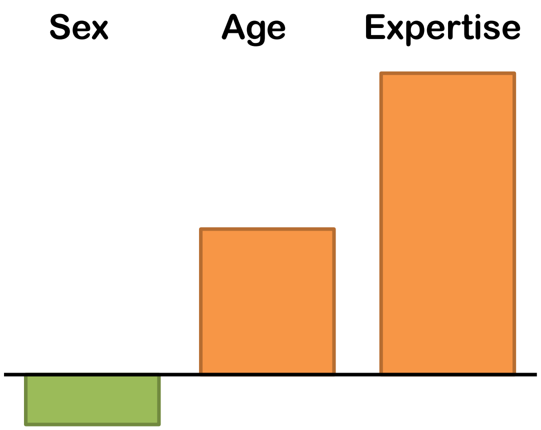


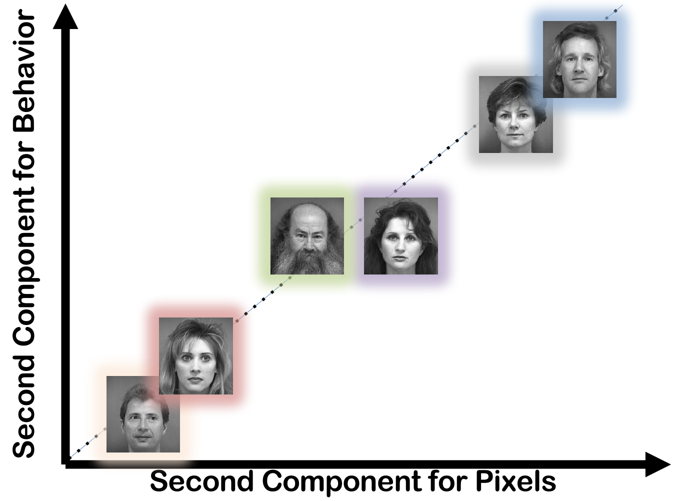
First Component: Saliences

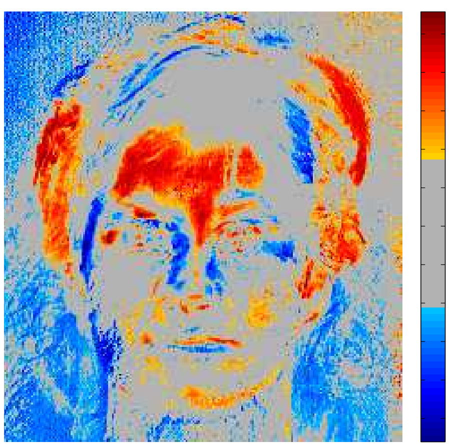


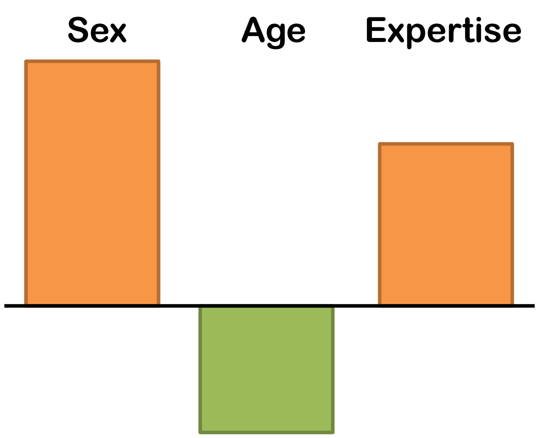


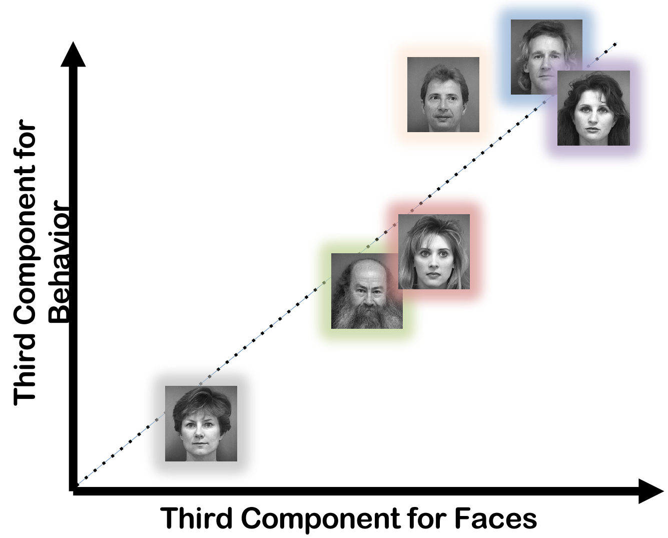
Second and Third Components



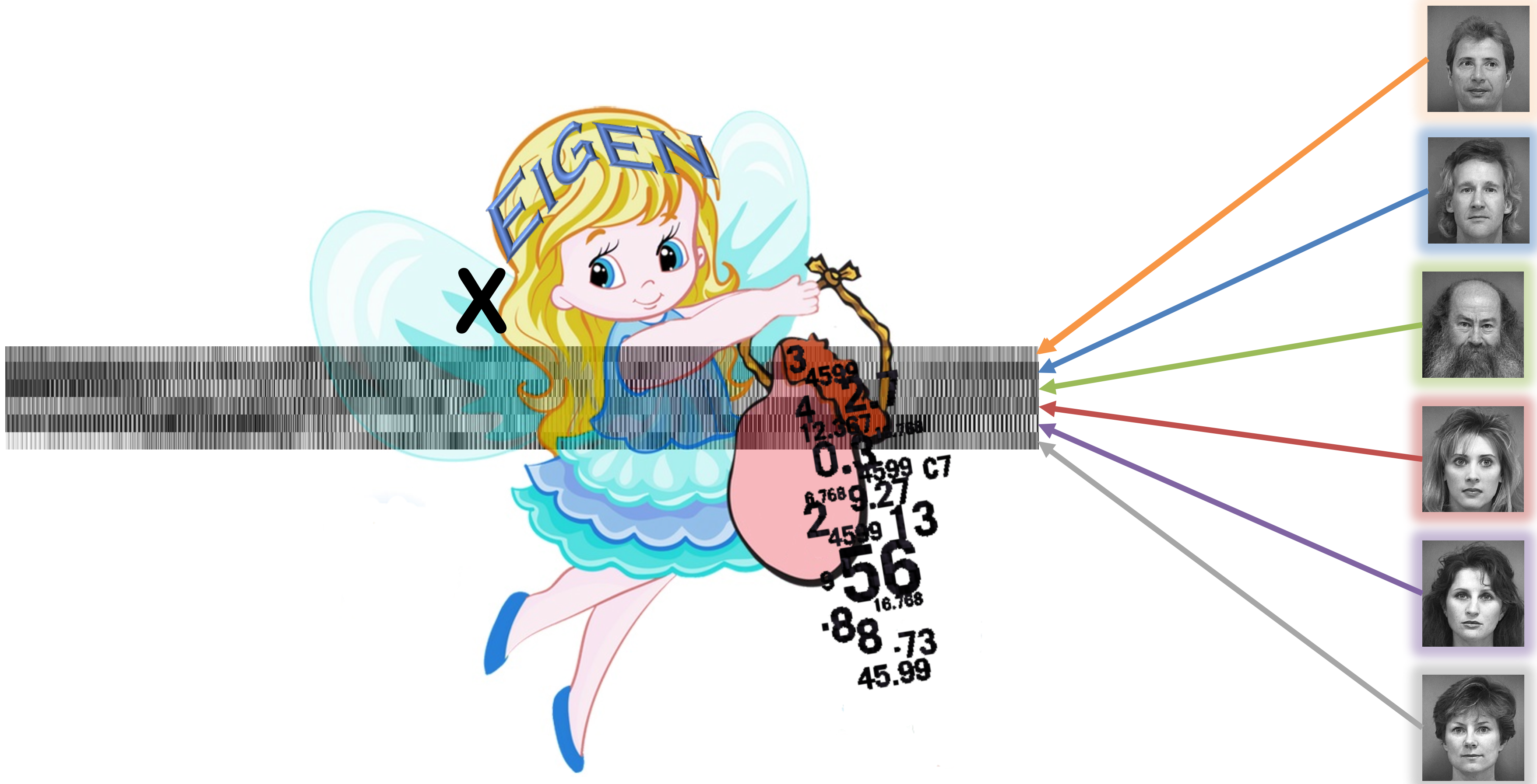




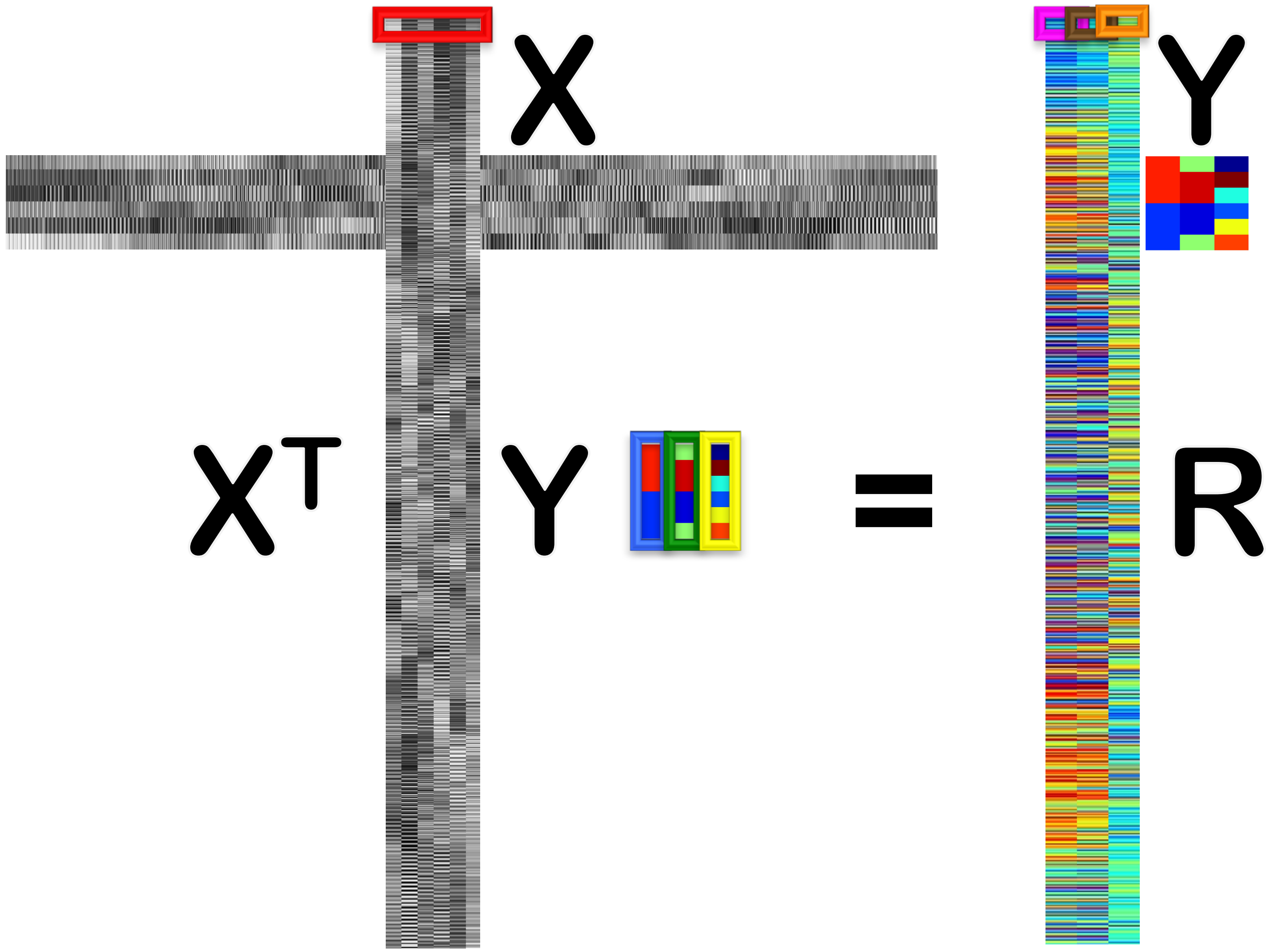




How Do We Do It?



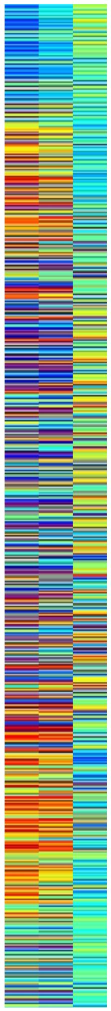
Common Information



Singular Value Decomposition

Behavior

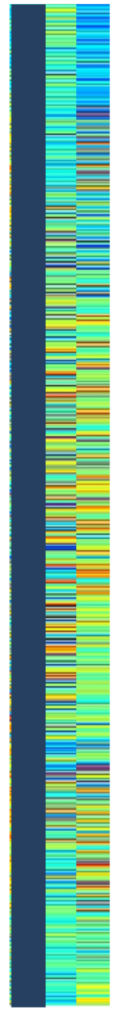
Pixels



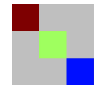
R =

=

Pixels



P

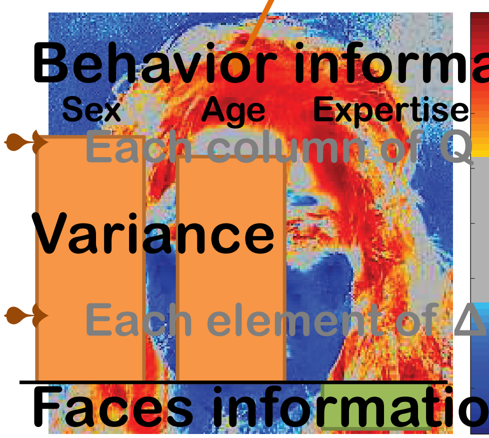


Δ

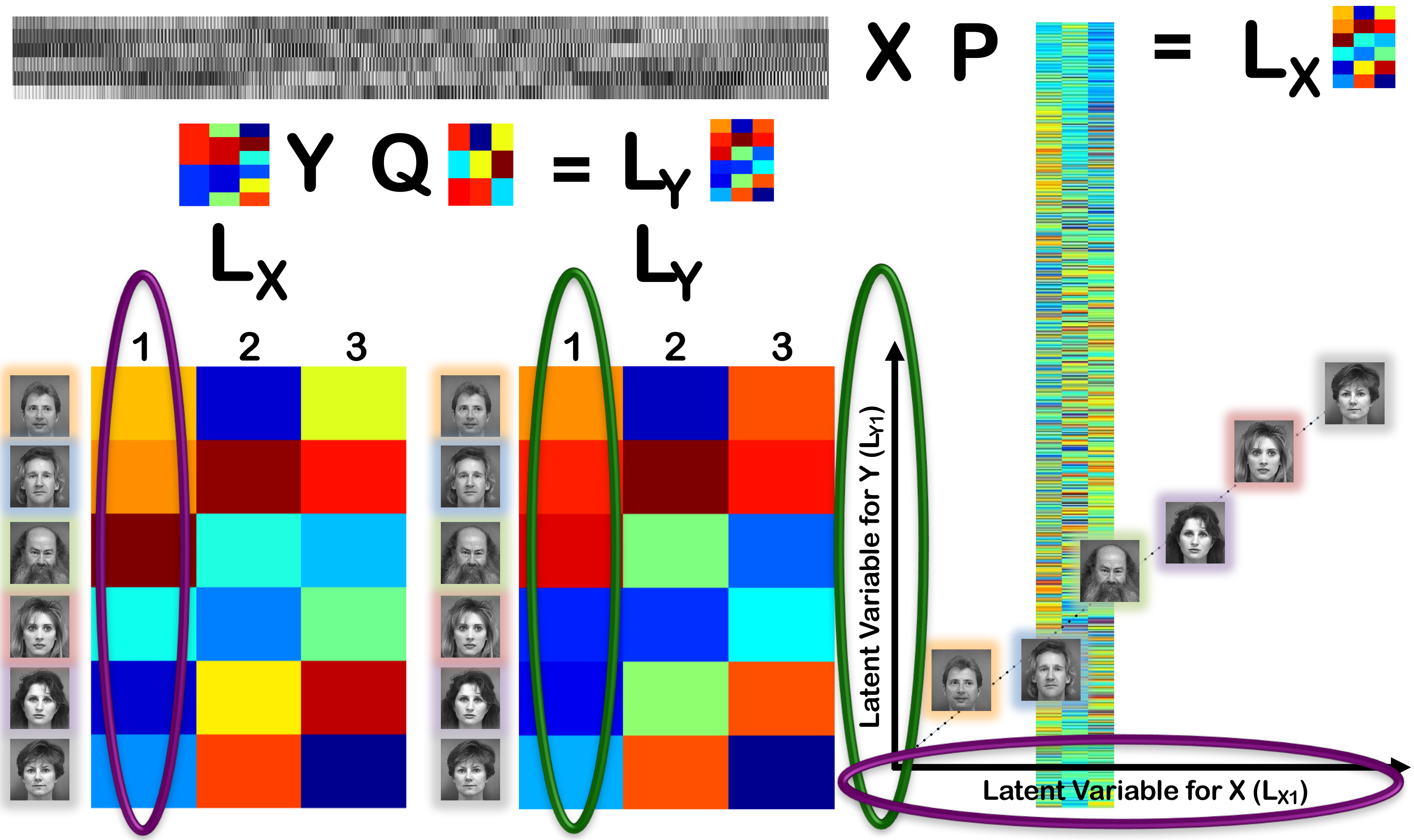
Behavior

Q^T

- Pixel information
  - Each column of P
- Behavior information
  - Each column of Q
- Variance
  - Each element of Δ
- Faces information
  - Latent variables
  - $L_X = XP$
  - $L_Y = YQ$



What is the Hidden Information?



How Good is a Component

- Saliences and latent variables
  - Look at singular values
    - Which are the square-root of eigenvalues
- Here:

Dimensions (Pairs of LVs)	1	2	3
δ	171.80	90.78	23.85
SUM	171.80	262.58	286.43
τ	60	32	8
SUM	60	92	100

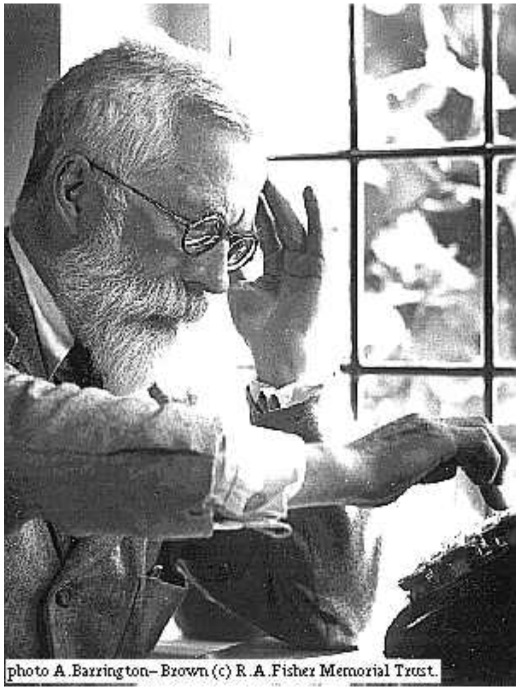
Is There Anything in the Data?

- **Are our components real?**
  - How do we find out?
    - Null hypothesis
      - Resample without replacement
    - Permutation Test
- **What are the important variables?**
  - How do we find out?
    - Determine from an infinite population
      - Resample with replacement
    - Bootstrap Test

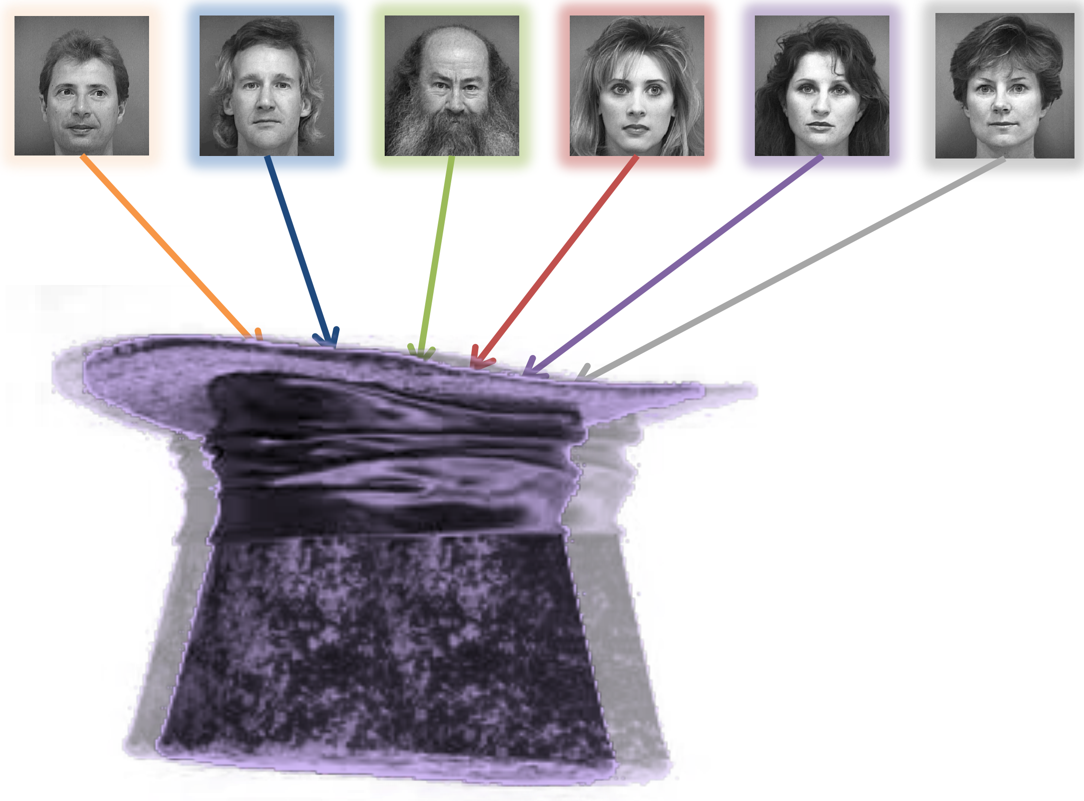
PERMUTATION TEST

William S. Gosset *aka* Student
(1876-1937)

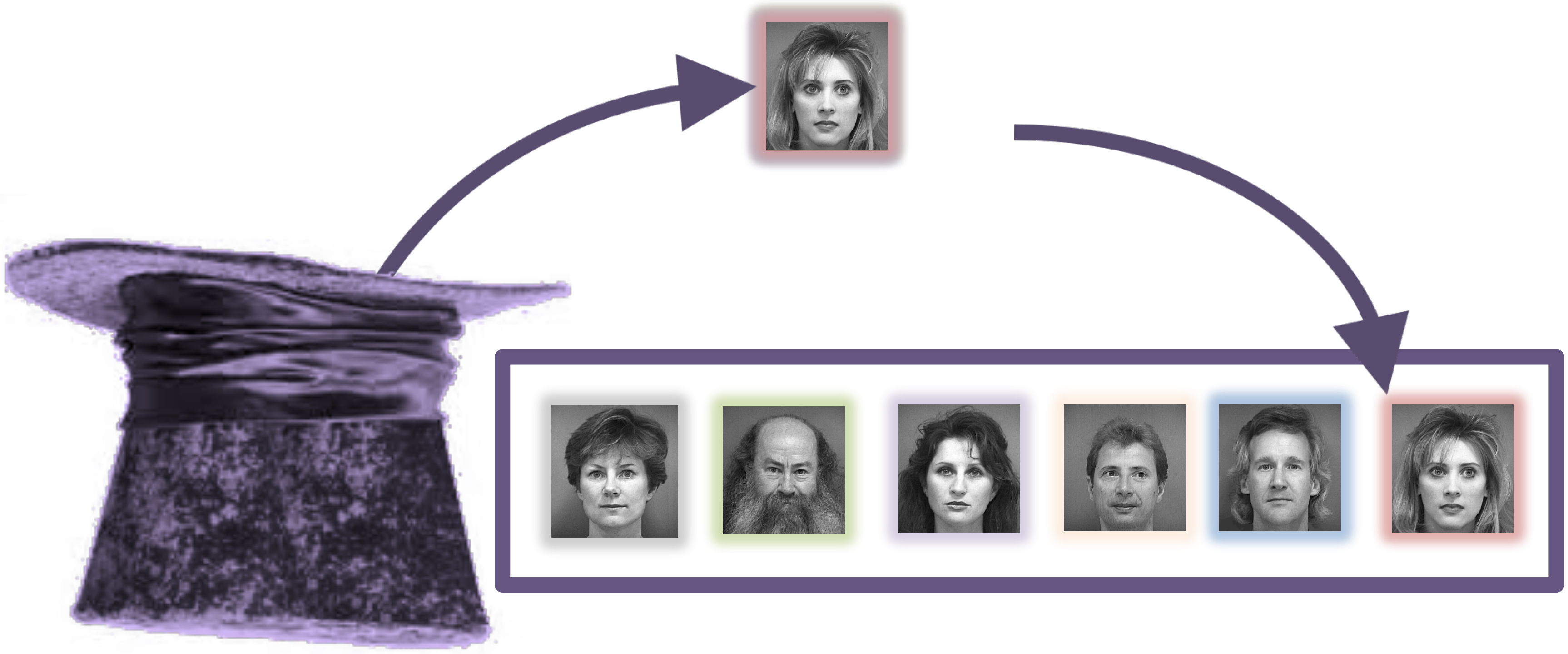
Ronald A. Fisher
(1890-1962)



Creating a Permuted Sample



Creating a Permuted Sample



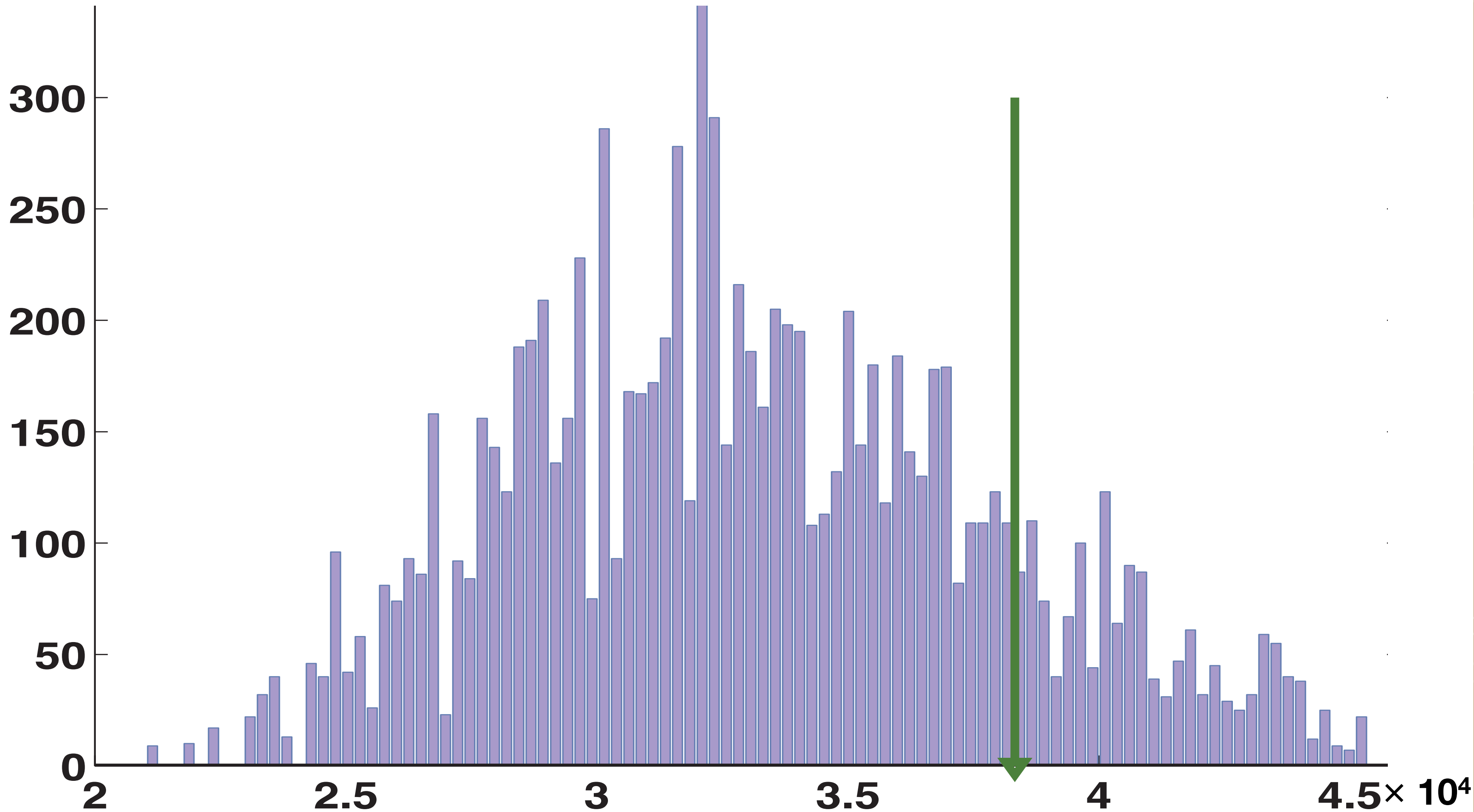
Permuted (H_0) Sample – Breaking Bonds

	Sex	Age	Expertise
Face 1/6	1	2	1
Face 2/3	1	3	6
Face 3/5	1	3	3
Face 4/1	-1	1	2
Face 5/2	-1	1	4
Face 6/4	-1	2	5

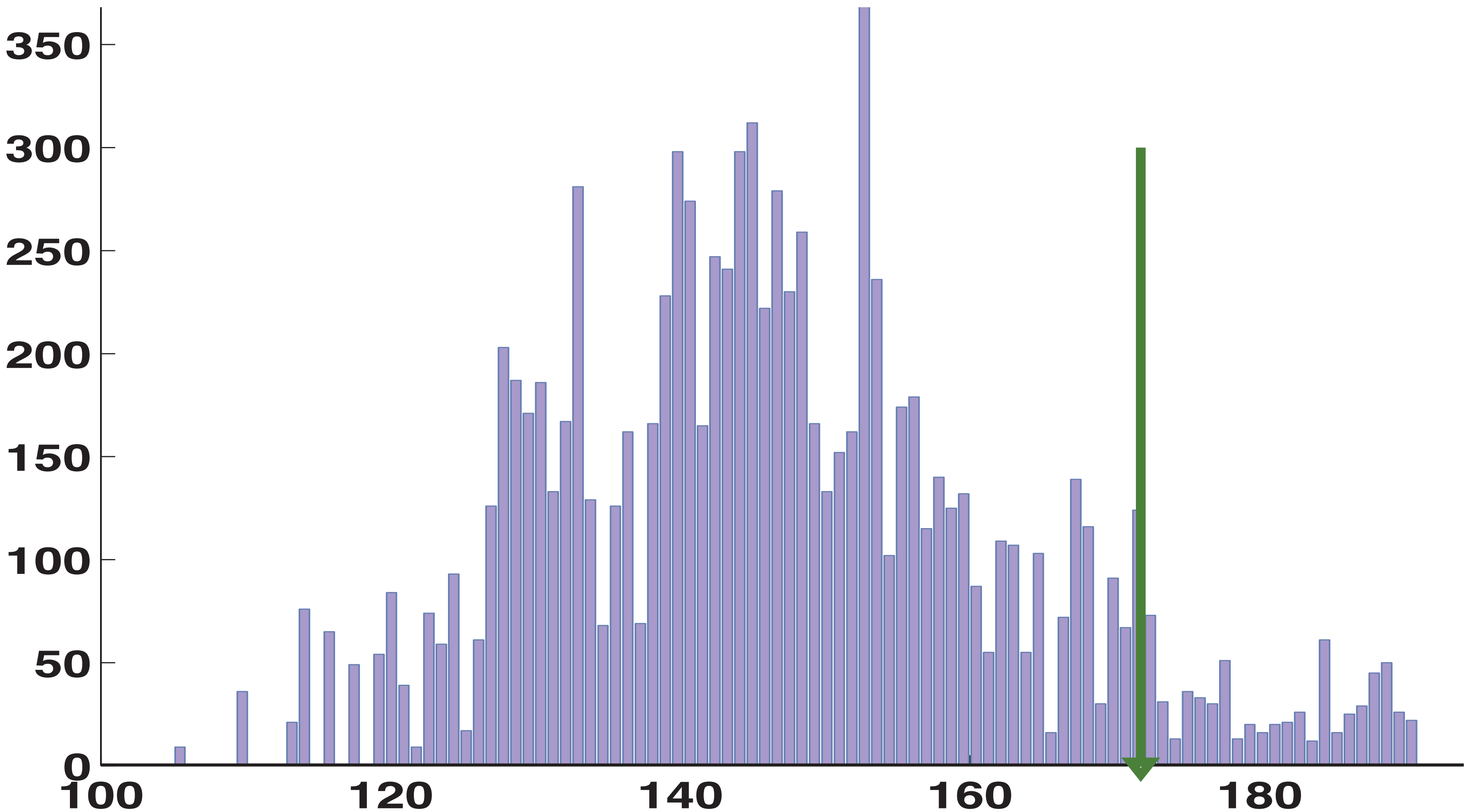
What Do We Do Next?

- Resample a lot of times!
  - Create the null distribution
- Compute a PLSC for each sample
  - Compare values from original PLSC
- Omnibus test:
  - Sum of the eigenvalues
- Specific component test:
  - Each eigenvalue

Omnibus: Approaching Significance ($p = .14$)

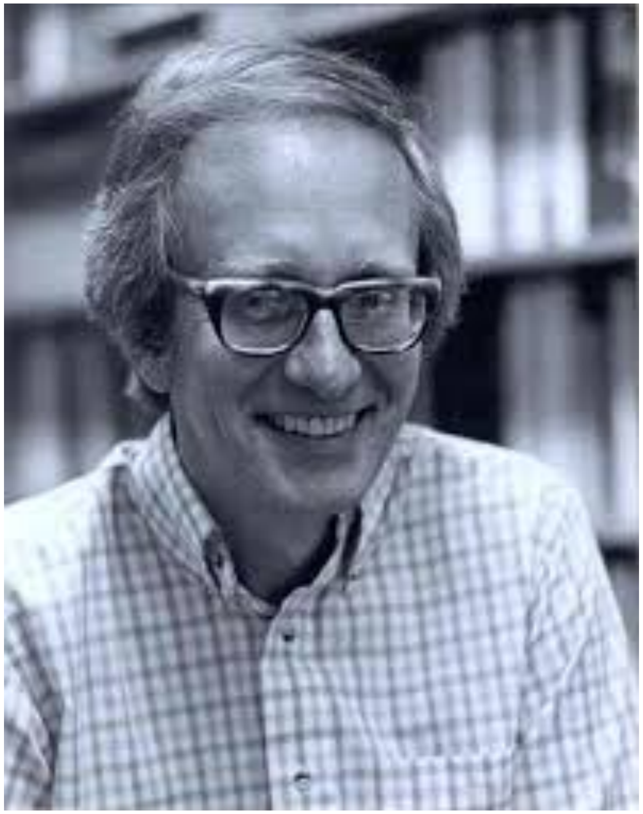


Specific Component (1st pair: p = .06)

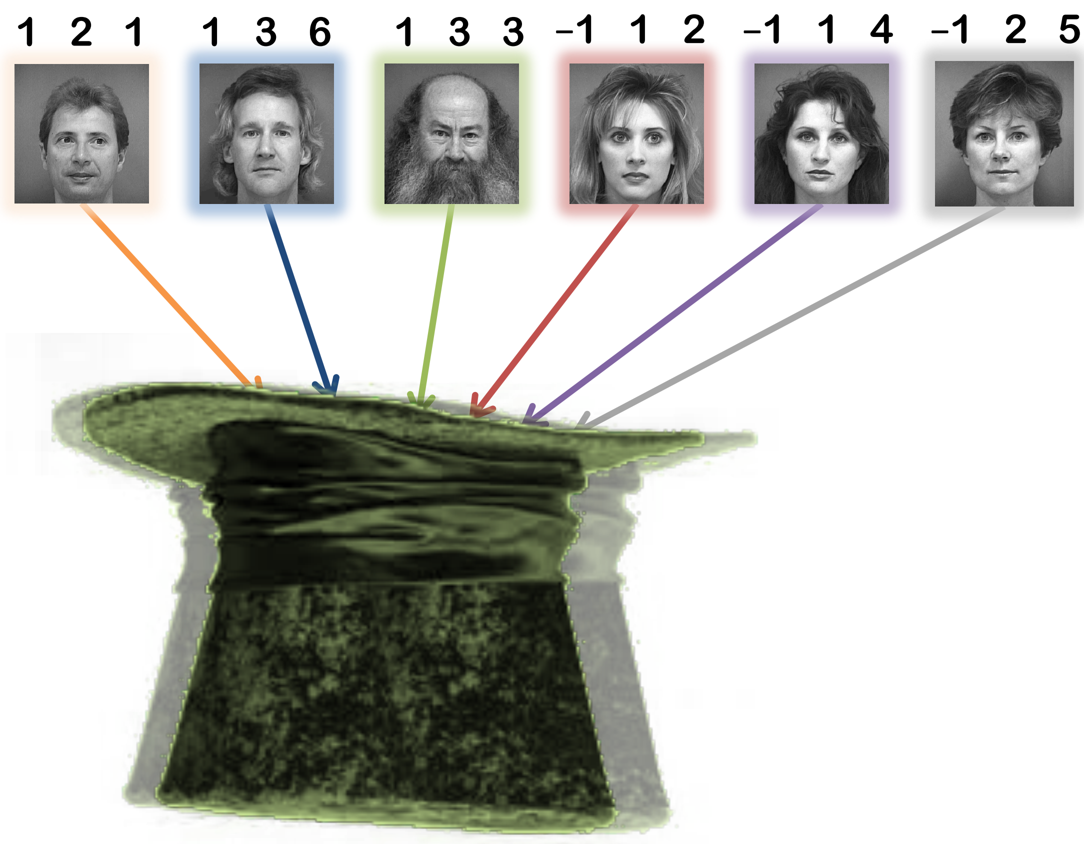


BOOTSTRAP TEST

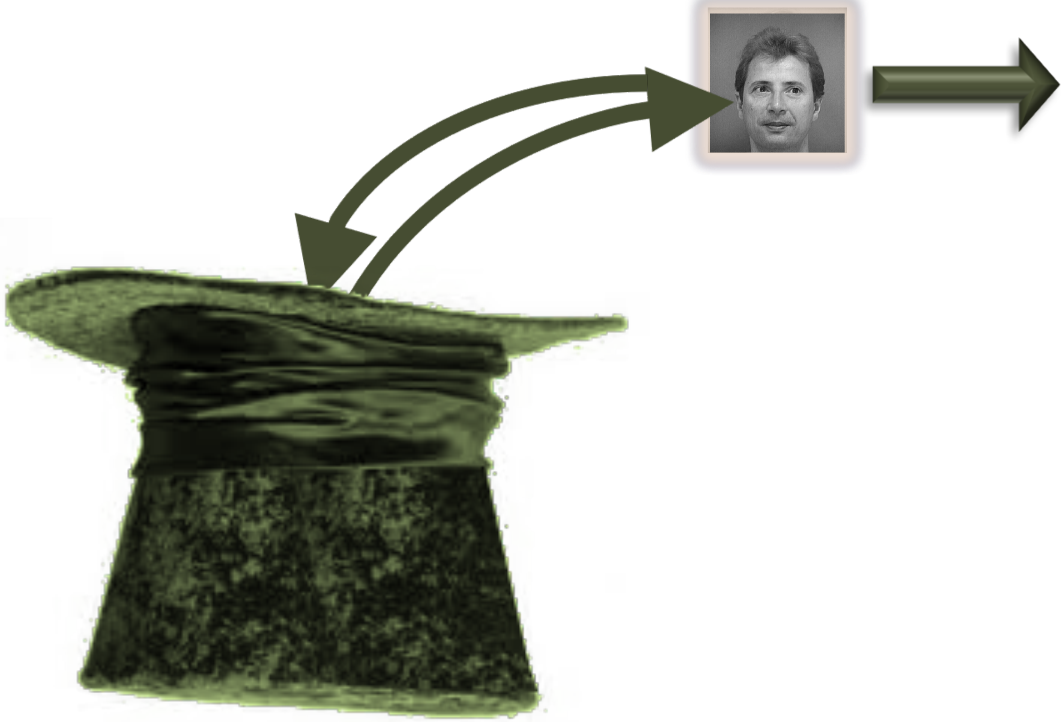
Bradley Efron



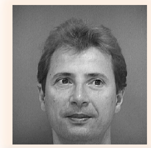
Creating a Bootstrap Sample



Creating a Bootstrap Sample



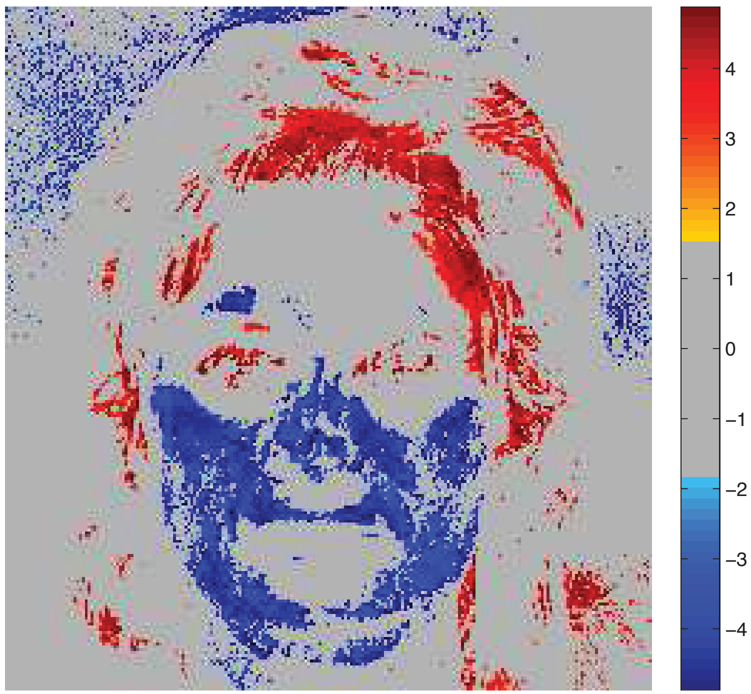
Shake!

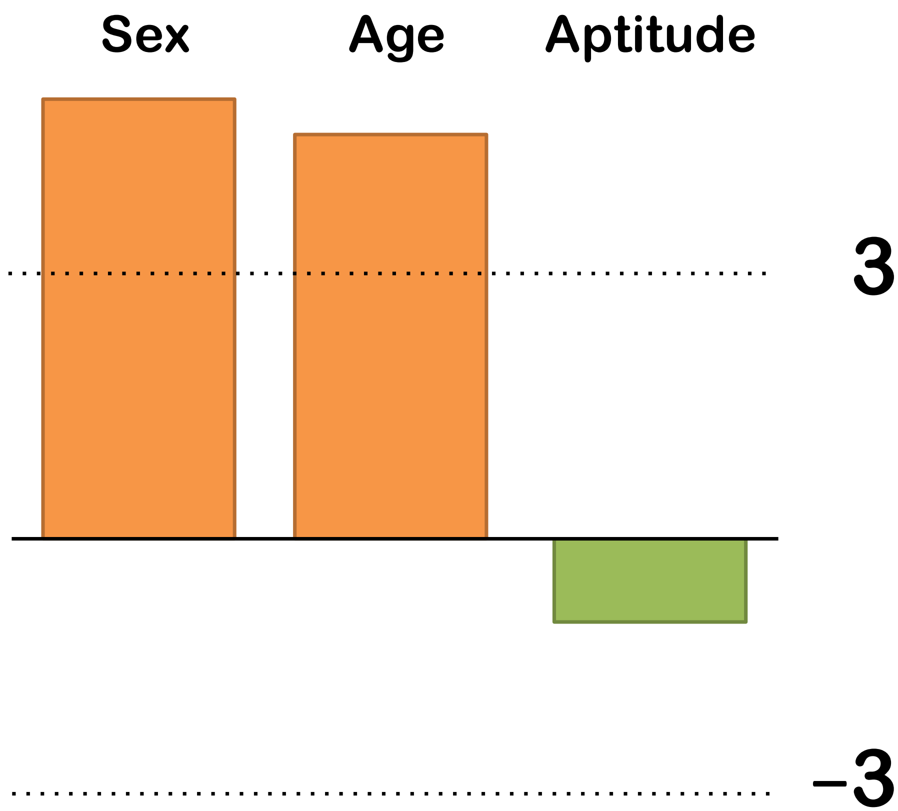
	Sex	Age	Expertise
	1	2	1
	1	3	6
	1	3	6
	−1	1	2
	−1	1	2
	−1	2	5

What Do we Do Next?

- Resample with replacement a lot of times!
- Compute a PLSC for each sample
- Compute for the variables:
  - The means (M)
  - The standard deviations (σ)
- Compute the bootstrap ratio
  - Bootstrap ratio: $t = M / \sigma$
- Display the significant variables
  - Keep only the variables with $t > 3$
  - Note that $t > 2$ is for $p < .05$

IMPORTANCE OF FIRST PAIR OF SALIENCES

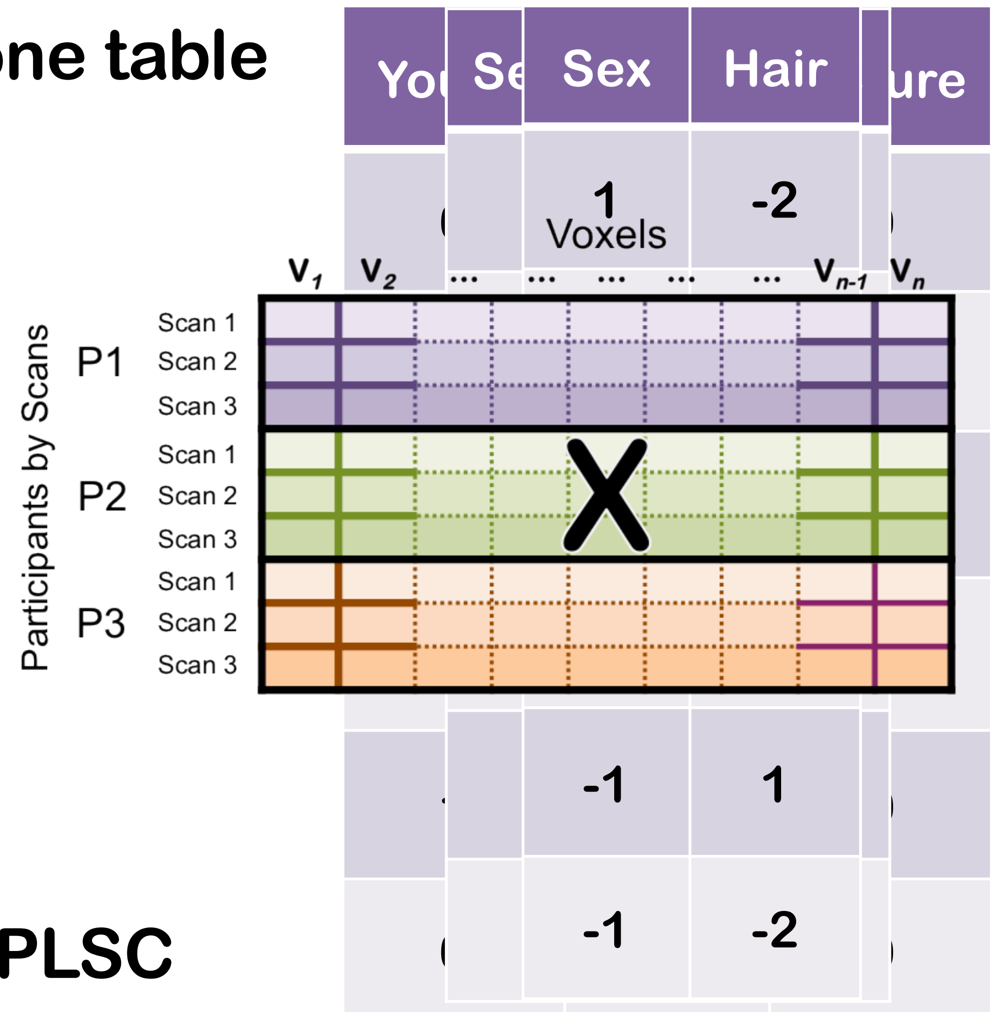




PLSC Types

Different Flavors

- Vary the data in one table
- Behavior PLSC
  - Behavior
- Task PLSC
  - Contrast
  - Mean-Centered
- Seed PLSC
  - Seed regions
- Spatio-Temporal PLSC

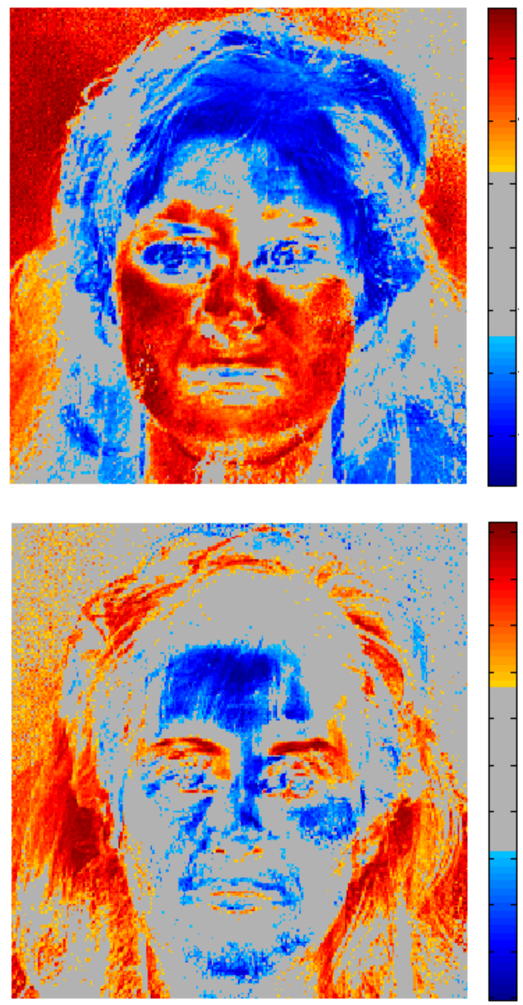


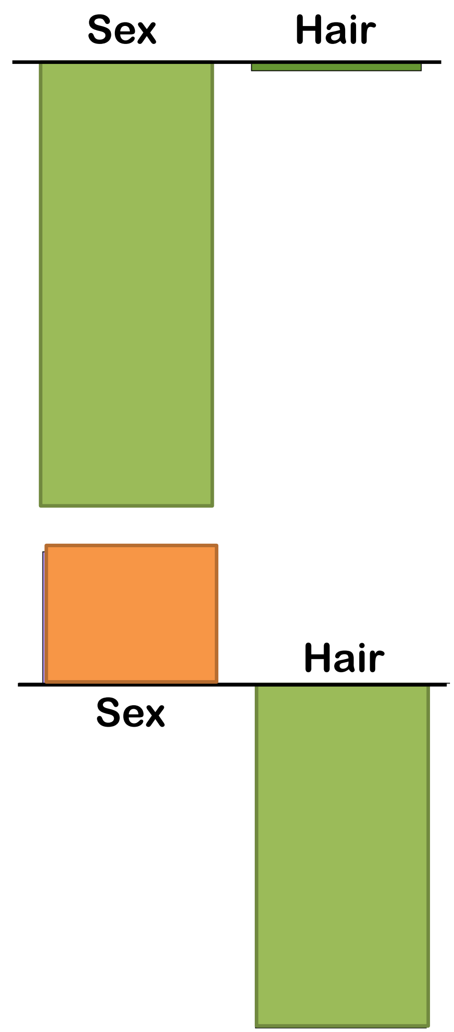
Developing PLS

- PLS for Distances
  - DISPLS Correlation
  - DISPLS Regression
- PLS for Qualitative Data
  - PLS Correspondence Analysis
- PLS for multiple data tables
  - Multi-Block PLS, DISPLS

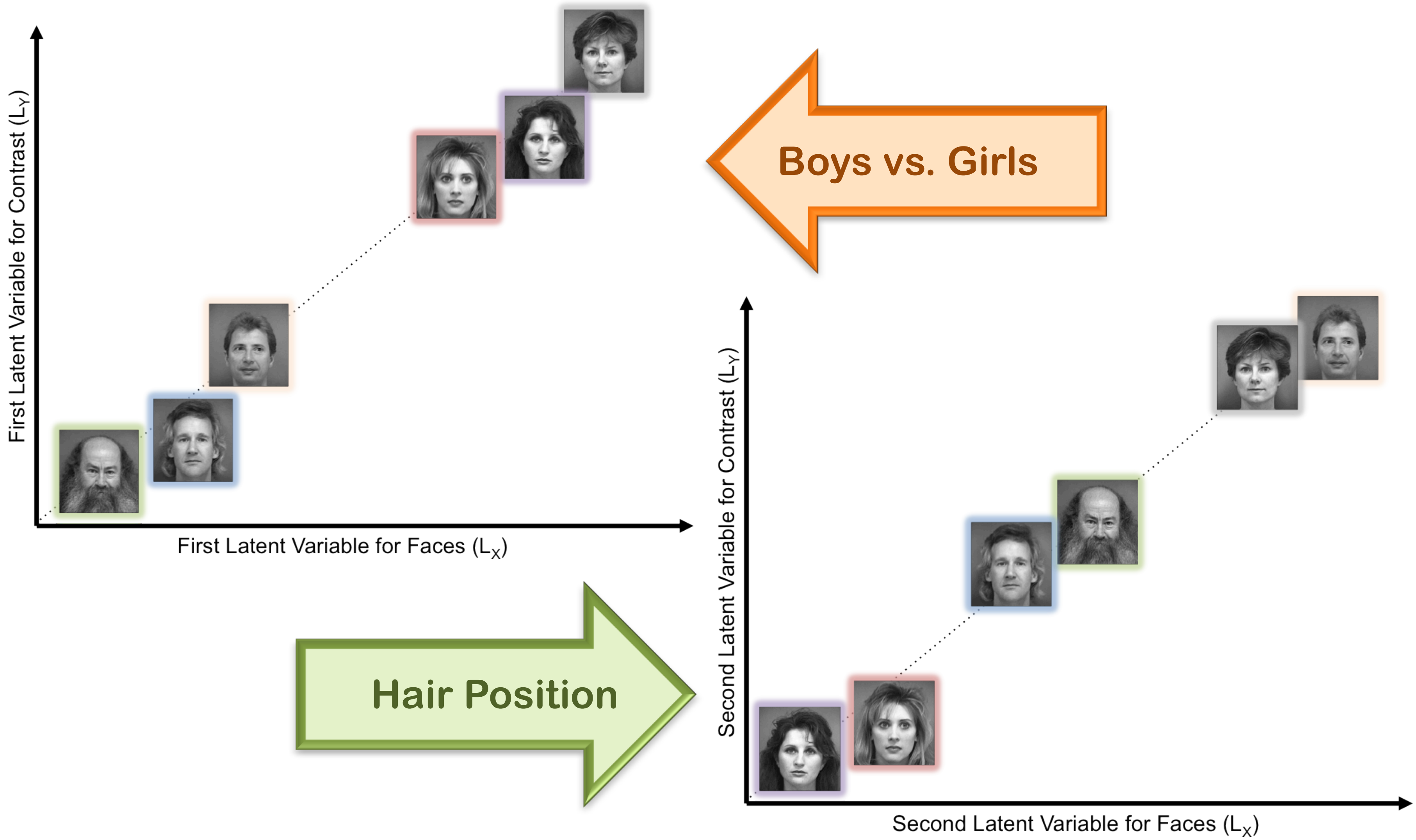
CONTRAST TASK PLSC

Sex	Hair
1	-2
1	1
1	1
-1	1
-1	1
-1	-2



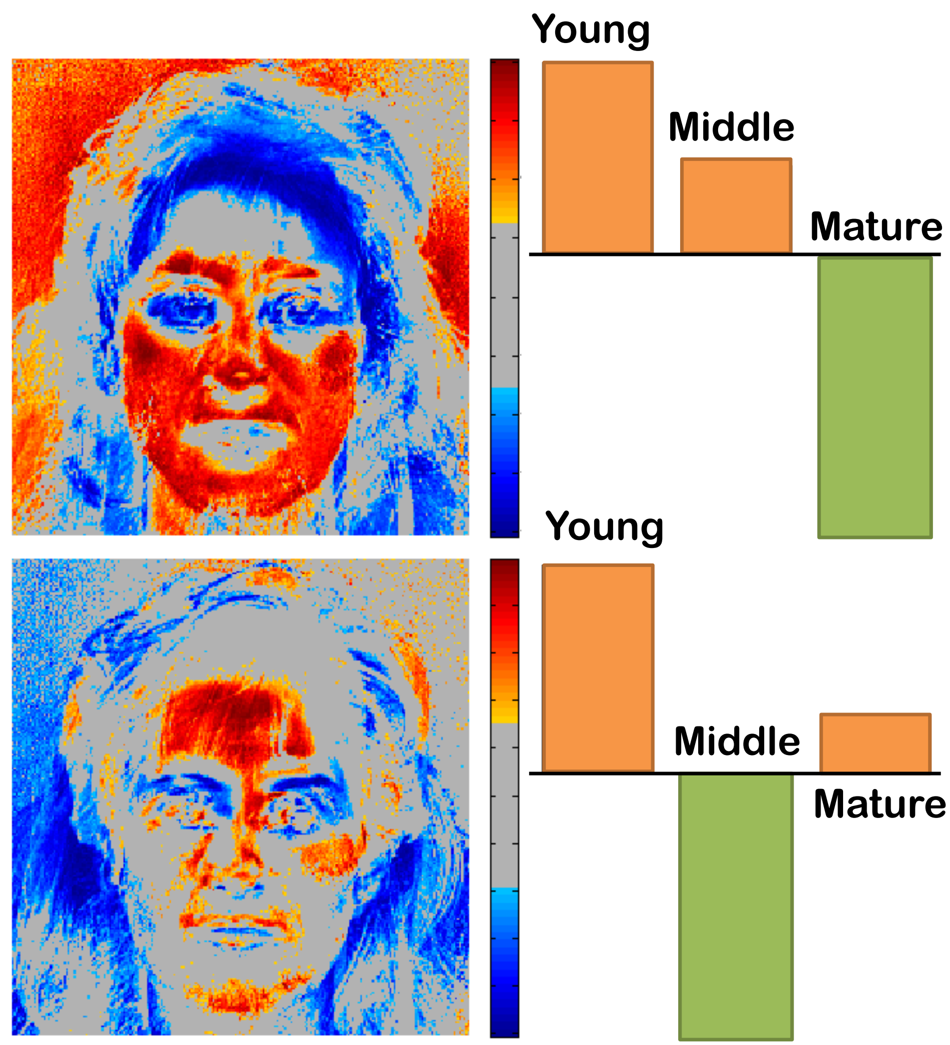


Contrast Task PLSC

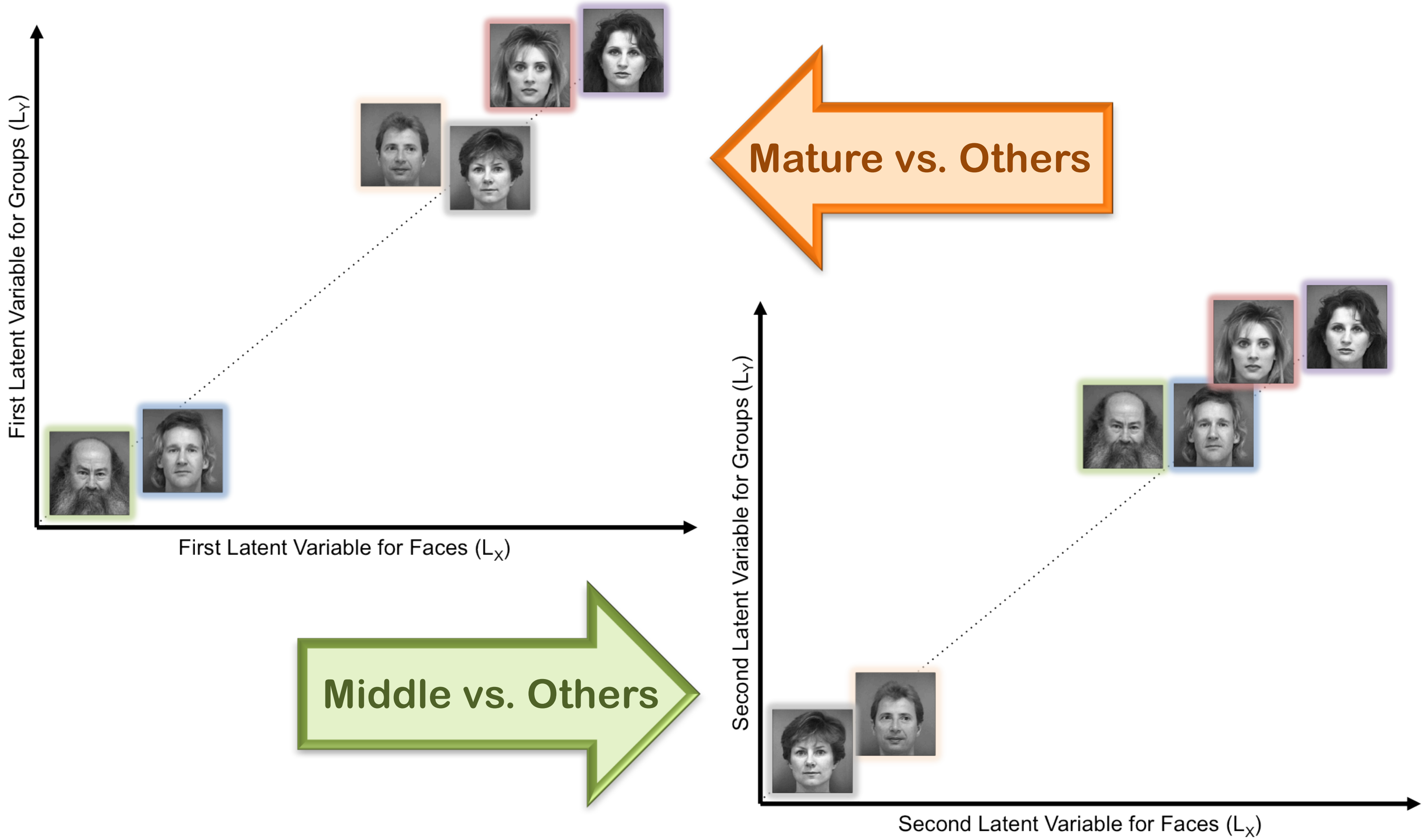


Mean-Centered Task PLSC

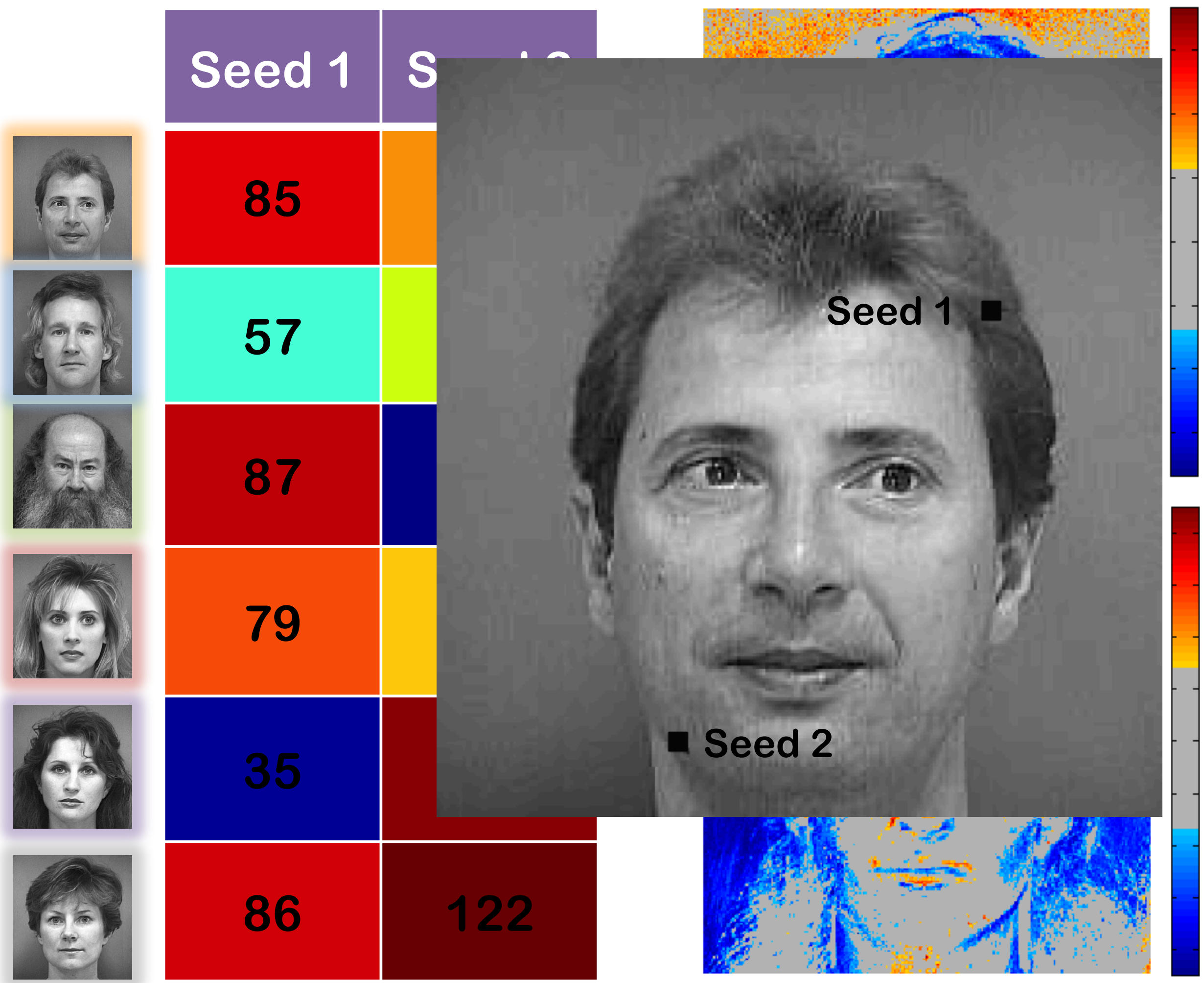
Young	Middle	Mature
0	1	0
0	0	1
0	0	1
1	0	0
1	0	0
0	1	0

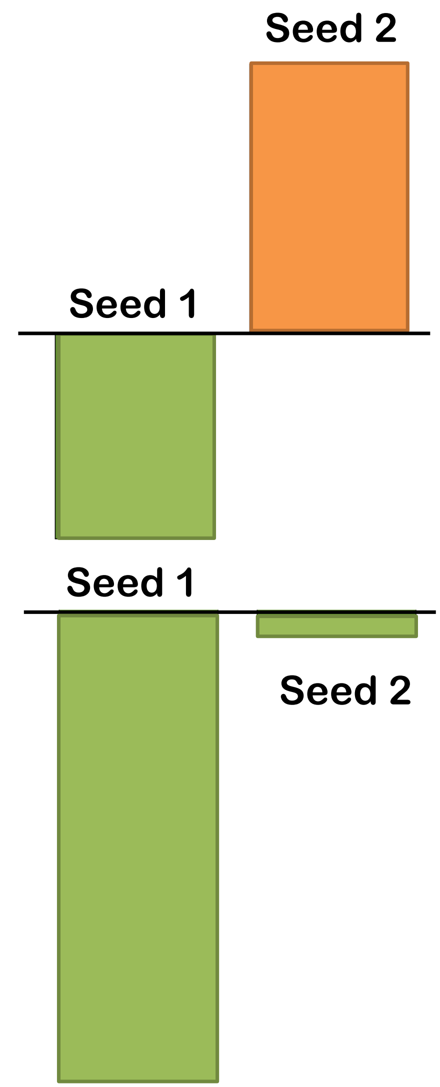


MEAN-CENTERED TASK PLSC

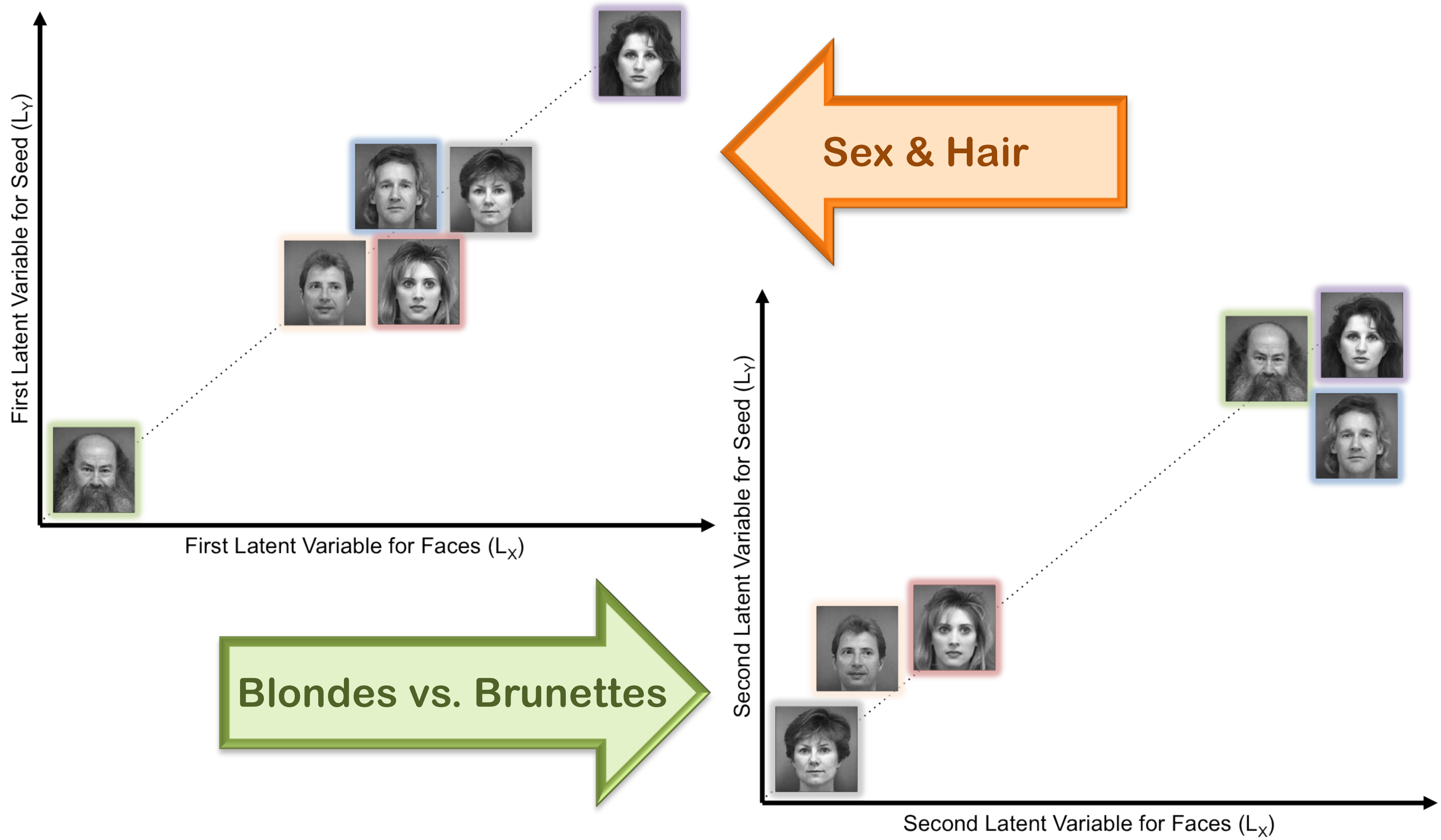


Seed PLSC


Seed 1
S
85
57
87
79
35
86
122
Seed 1
Seed 2


Seed 2
Seed 1
Seed 1
Seed 2

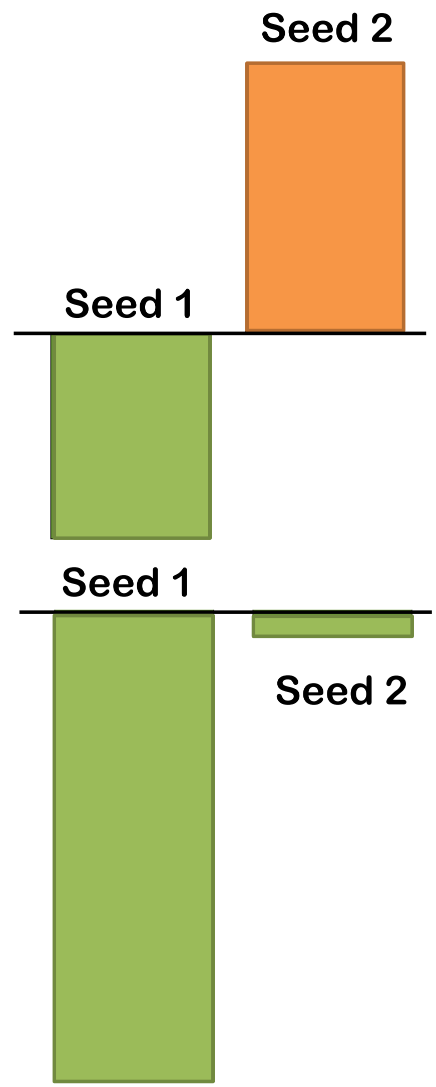
Seed PLSC


First Latent Variable for Seed (L_Y)
First Latent Variable for Faces (L_X)
Sex & Hair
Blondes vs. Brunettes
Second Latent Variable for Seed (L_Y)
Second Latent Variable for Faces (L_X)

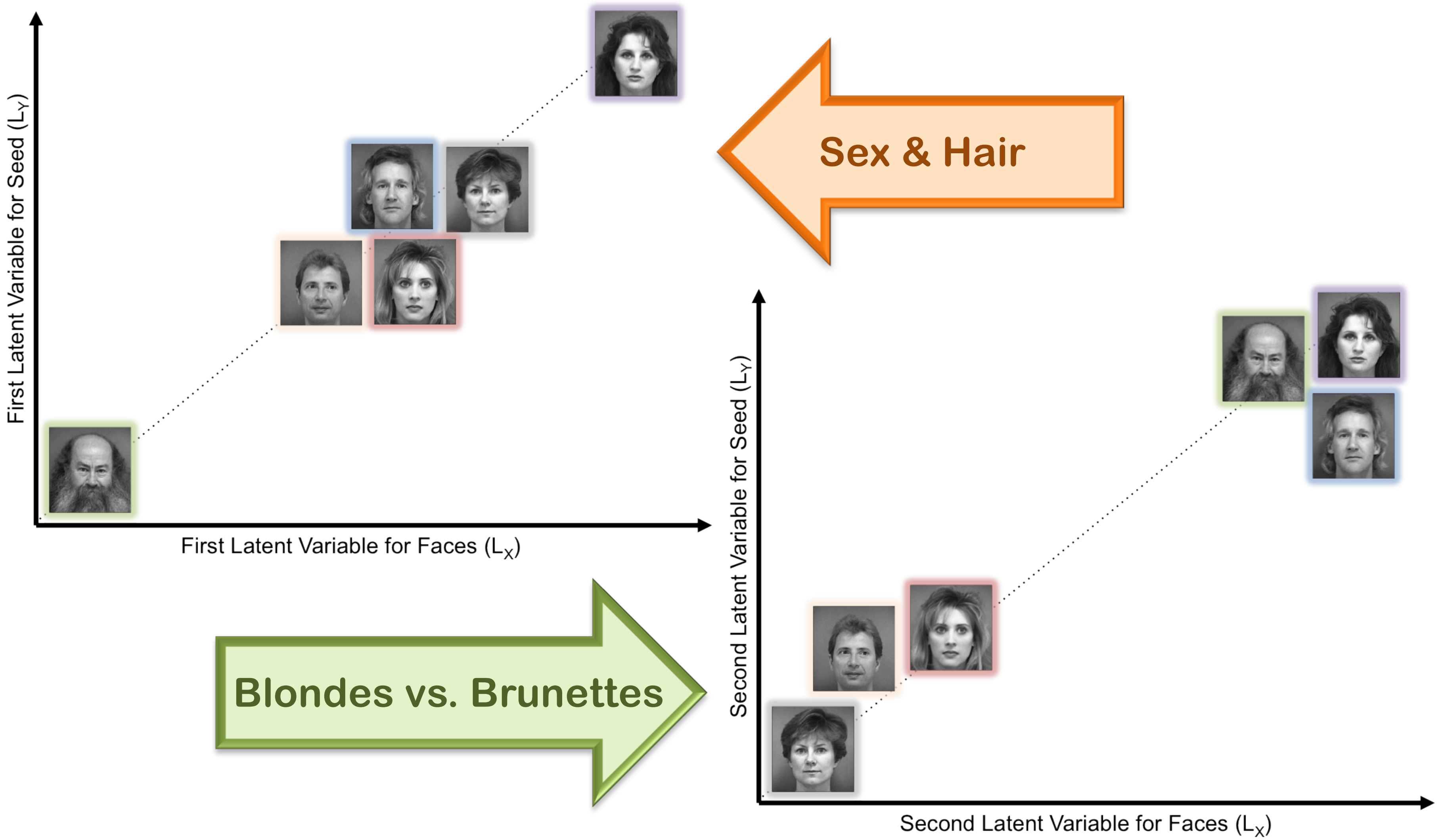
Saliences

Seed PLSC

Seed 1	S
85	
57	
87	
79	
35	
86	122

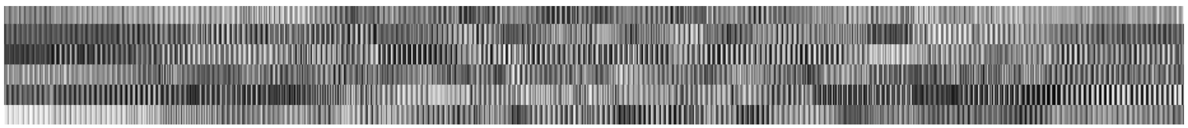


SEED PLSC

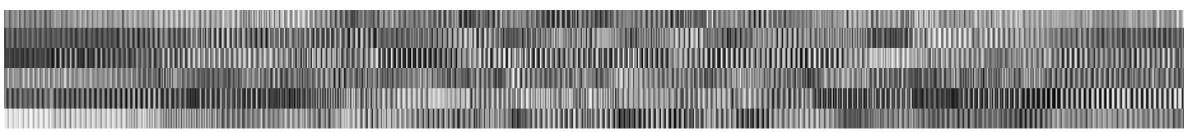

First Latent Variable for Seed (L_Y)
First Latent Variable for Faces (L_X)
Sex & Hair
Blondes vs. Brunettes
Second Latent Variable for Seed (L_Y)
Second Latent Variable for Faces (L_X)

Take Home Message

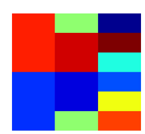
PCA



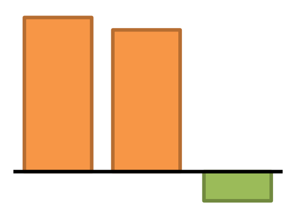
Components



PLSC



Saliences



Where to look up?

References

Krishnan, A., Williams, L. J., McIntosh, A. R., & Abdi, H. (2011). Partial Least Squares (PLS) methods for neuroimaging: a tutorial and review. *NeuroImage*, *56*, 455–475.

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