Week 6

Dimensionality Reduction

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Why Reduce Dimensionality?

1. Reduces time complexity: Less computation
2. Reduces space complexity: Less parameters
3. Saves the cost of observing the feature
4. Simpler models are more robust on small datasets
5. More interpretable; simpler explanation
6. Data visualization (structure, groups, outliers, etc) if plotted in 2 or 3 dimensions

Feature Selection vs Extraction

- Feature selection: Choosing $k<d$ important features, ignoring the remaining $d-k$

  Subset selection algorithms

- Feature extraction: Project the

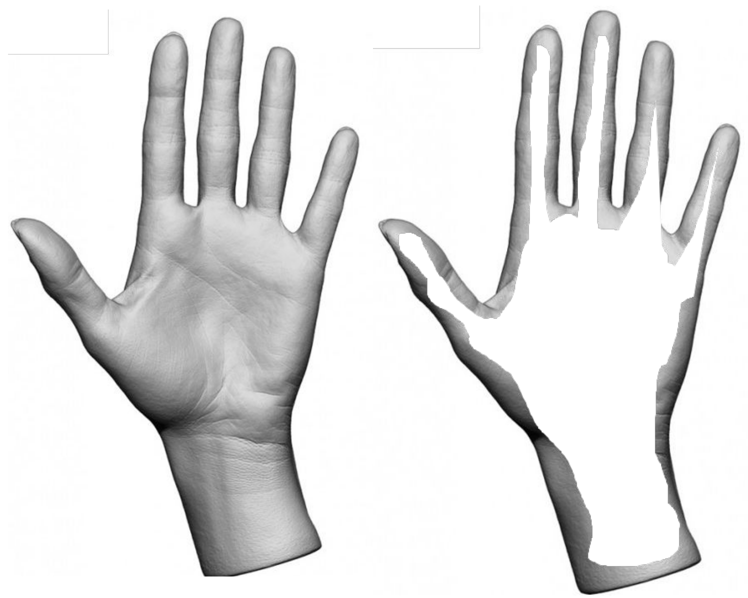
  original x_i , i =1,...,d dimensions to

  new $k<d$ dimensions, z_j , j =1,...,k

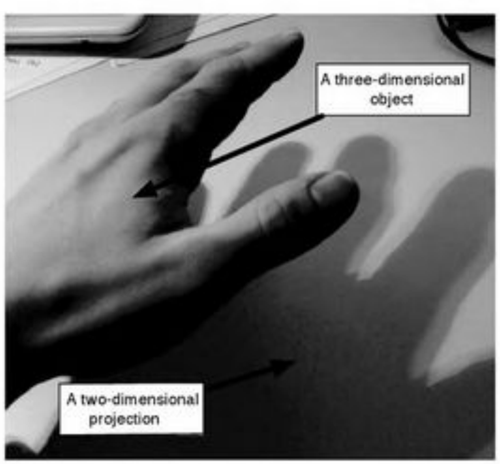
  - Principal components analysis (PCA)
  - Feature embedding
  - Factor analysis (FA)
  - Multidimensional scaling
  - Linear discriminant analysis (LDA),
  - Canonnical correlation analysis (CCA)

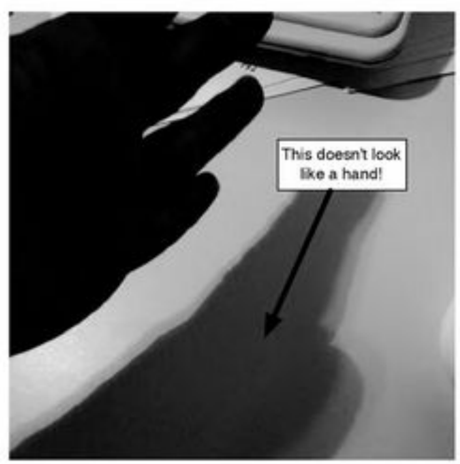
Feature Selection vs Extraction

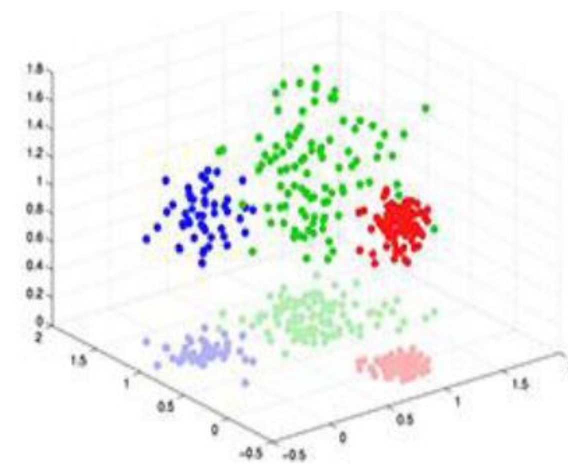
- Feature selection



- Feature extraction (through projection)







Feature Selection: Subset selection

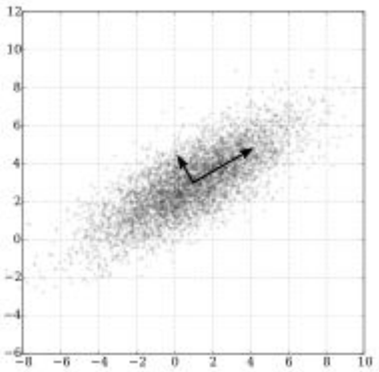
- How many subsets of *d* features?

- Forward search: Add the best feature at each step
    - Set of features F initially Ø.
    - At each iteration, find the best new feature

$$j = \text{argmin}_i \, E (F \cup x_i)$$

    - Add x_j to F if $E (F \cup x_j) < E (F)$
    - Local search! no guarantees.. why?
- O($^?$)
- Backward search: Start with all features and remove one at a time, if possible. O(?)
- Floating search (Add *k*, remove *l*)

Feature Extraction: PCA



- Principle Component Analysis
    - Unsupervised method
    - Mapping from original d-dimensional space to k-dimensional space
        - With minimum loss of information
    - Maximize the variance in k-dimensions

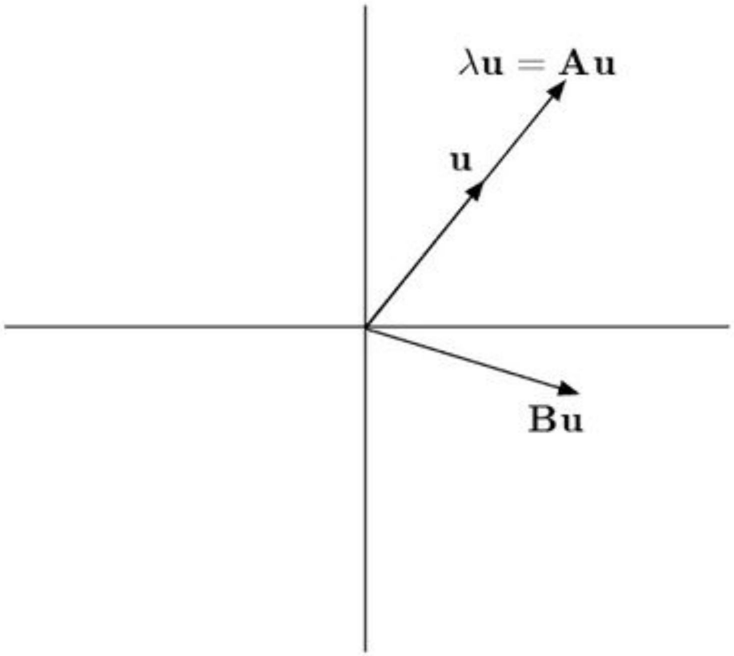
Linear algebra review

Comment 7.1 – Eigenvectors and eigen values: The eigenvector/eigenvalue equation for some square matrix $\mathbf{A}$ is given as:

$$\lambda_i \mathbf{u}_i = \mathbf{A}\mathbf{u}_i. \tag{7.4}$$

The solutions to this equation are pairs of eigenvalues (λ_i) and eigenvectors ($\mathbf{u}_i$).

The figure on the right provides some intuition for this equation. Multiplying an M-dimensional vector $\mathbf{u}$ by an $M \times M$ matrix $\mathbf{B}$ results in another M-dimensional vector. Therefore, we can consider the matrix $\mathbf{B}$ as defining a rotation of the vector $\mathbf{u}$. Different $\mathbf{B}$ matrices will produce different rotations. The solutions to Equation 7.3 for a particular matrix $\mathbf{A}$ are the vectors $\mathbf{u}$ for which applying the rotation $\mathbf{A}$ only results in a change in the length of $\mathbf{u}$. The magnitude of this change is given by the scalar λ.



$$|A| = \prod_{i=1}^{n} \lambda_i$$

Linear algebra review

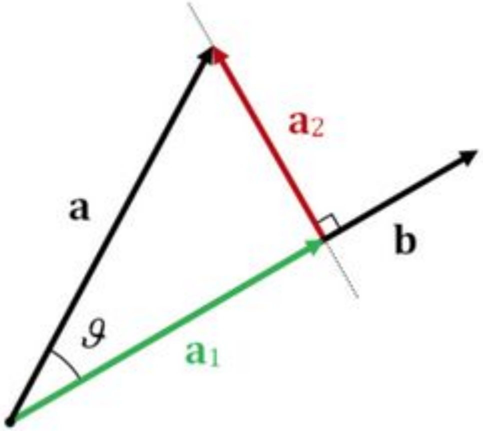
- Derivatives

$f(\mathbf{w})$	$\frac{\partial f}{\partial \mathbf{w}}$
$\mathbf{w}^\top \mathbf{x}$	$\mathbf{x}$
$\mathbf{x}^\top \mathbf{w}$	$\mathbf{x}$
$\mathbf{w}^\top \mathbf{w}$	$2\mathbf{w}$
$\mathbf{w}^\top \mathbf{C}\mathbf{w}$	$2\mathbf{C}\mathbf{w}$

$$\mathbf{A} = \begin{bmatrix} a & b \\ c & d \end{bmatrix}, \quad \mathbf{A}^{-1} = \frac{1}{ad-bc}\begin{bmatrix} d & -b \\ -c & a \end{bmatrix}$$

$$(\mathbf{X}\mathbf{w})^\top = \mathbf{w}^\top \mathbf{X}^\top$$

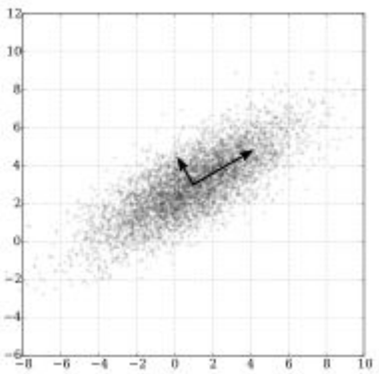
- Projection



$$\mathbf{a}_1 = a_1 \hat{\mathbf{b}}$$

$$a_1 = |\mathbf{a}| \cos\theta = \mathbf{a} \cdot \hat{\mathbf{b}} = \mathbf{a} \cdot \frac{\mathbf{b}}{|\mathbf{b}|}$$

Principle Component Analysis (PCA)

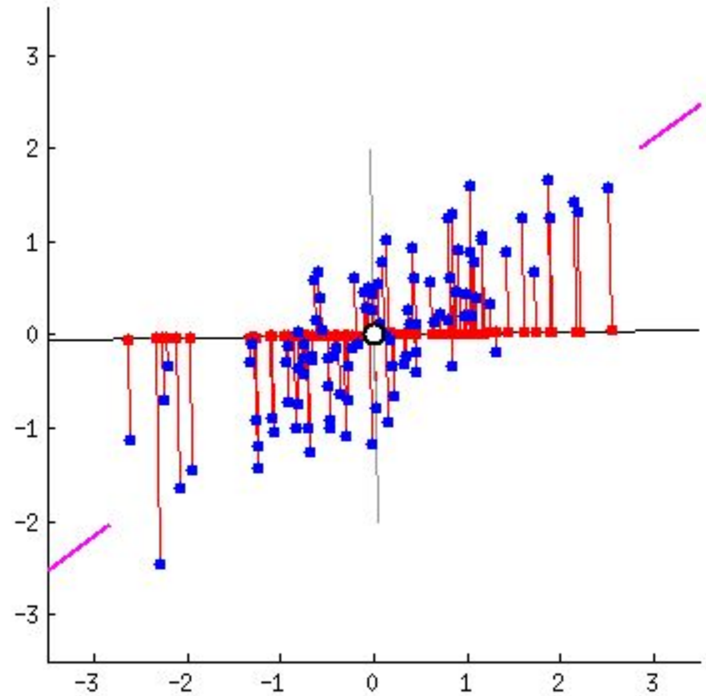


- Principle Component Analysis
  - Unsupervised method
  - Mapping from original d-dimensional space to k-dimensional space
    - With minimum loss of information
  - Maximize the variance in k-dimensions

- Assume original dimensions has zero mean
- Projection of ***x*** on the direction ***w*** is $z = \mathbf{w}^T \mathbf{x}$
- w is unit length $\|w_1\| = 1$
- Maximize the variance *Var(z)*

$$\Sigma w_1 = \alpha w_1$$

$$\Sigma w_2 = \alpha w_2$$

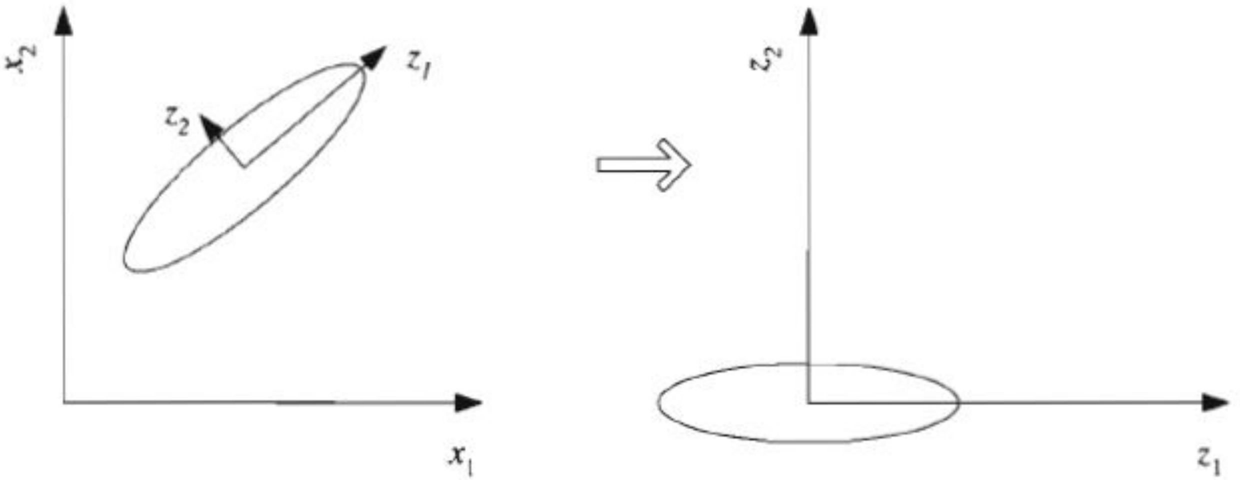

3
2
1
0
-1
-2
-3
-3
-2
-1
0
1
2
3

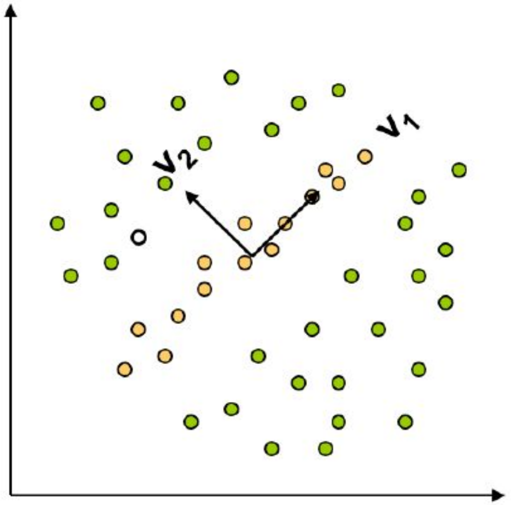
Principle Component Analysis (PCA)

- Maximize the variance

$$\Sigma w_1 = \alpha w_1$$
$$\Sigma w_2 = \alpha w_2$$
$$z = \mathbf{W}^T(\boldsymbol{x} - \boldsymbol{m})$$

where the k columns of **W** are the leading eigenvectors.
k-dimensional space: dims are the eigenvectors, and the variances over these new dimensions are equal to the eigenvalues.





Backprojection

Instance $\boldsymbol{x}^t$ is projected to the z-space as

$$\mathbf{z}^t = \mathbf{W}^T(\boldsymbol{x}^t - \boldsymbol{\mu})$$

When $\mathbf{W}$ is an orthogonal matrix such that $\mathbf{W}\mathbf{W}^T = \mathbf{I}$, it can be backprojected to the original space as

$$\hat{\boldsymbol{x}}^t = \mathbf{W}\mathbf{z}^t + \boldsymbol{\mu}$$

$$\sum_t \|\hat{\boldsymbol{x}}^t - \boldsymbol{x}\|^2$$

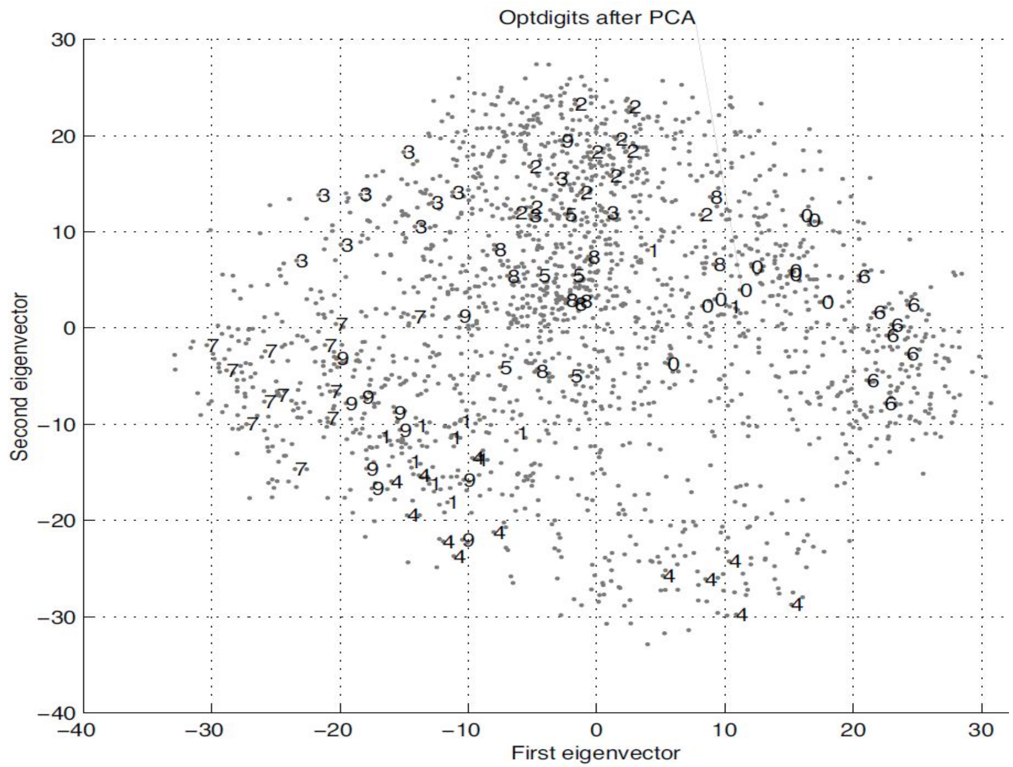
Principle Component Analysis (PCA)

- How many leading eigenvectors? Proportion of variance

$$\frac{\lambda_1 + \lambda_2 + \cdots + \lambda_k}{\lambda_1 + \lambda_2 + \cdots + \lambda_k + \cdots + \lambda_d}$$

- Reconstruction (and error) $\hat{x}^t = \mathbf{W}\mathbf{z}^t + \boldsymbol{\mu}$

- Visual analysis



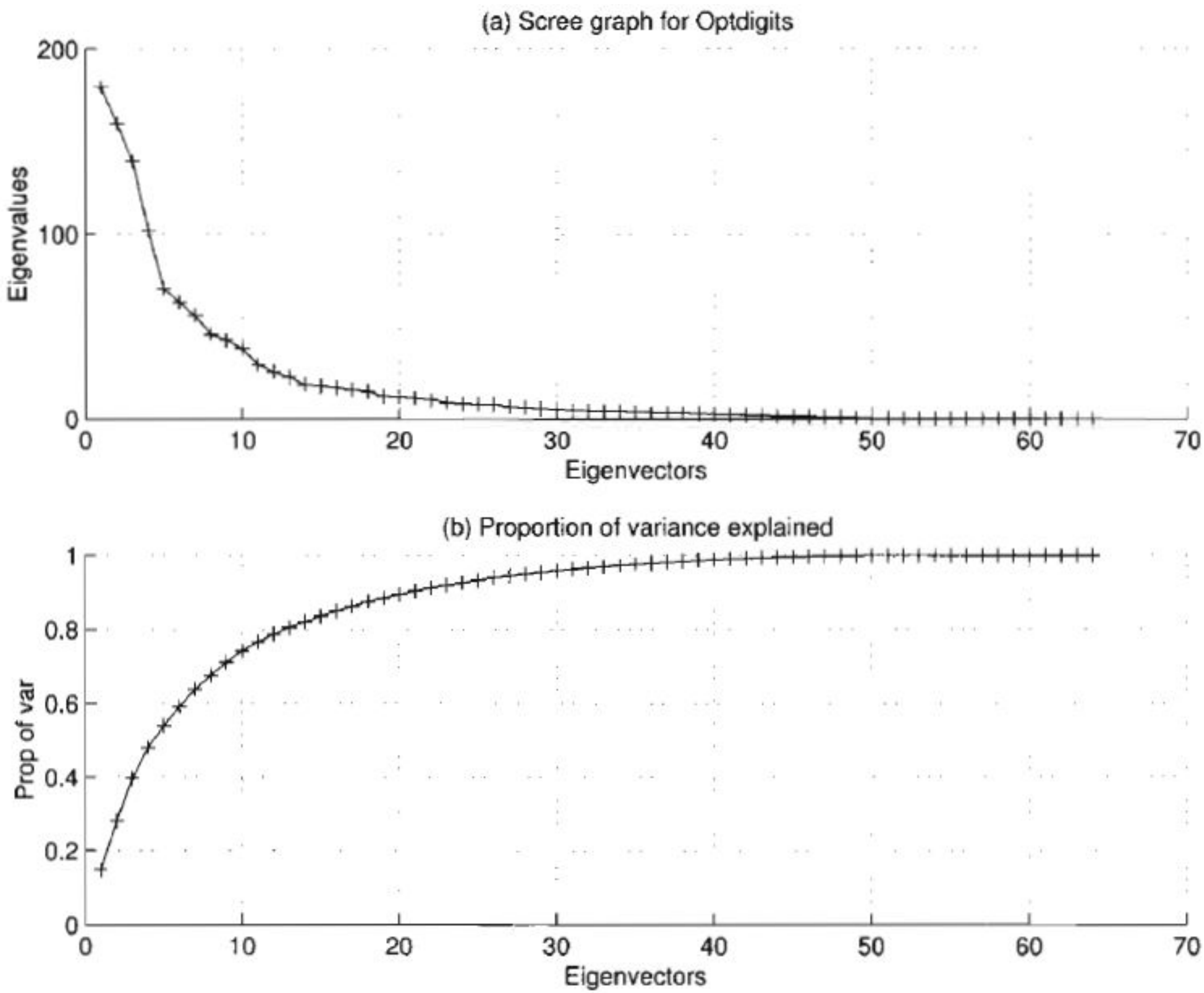
Principle Component Analysis (PCA)

- How many leading eigenvectors? Proportion of variance

$$\frac{\lambda_1 + \lambda_2 + \cdots + \lambda_k}{\lambda_1 + \lambda_2 + \cdots + \lambda_k + \cdots + \lambda_d}$$

- Visual analysis

PCA - Scree graph

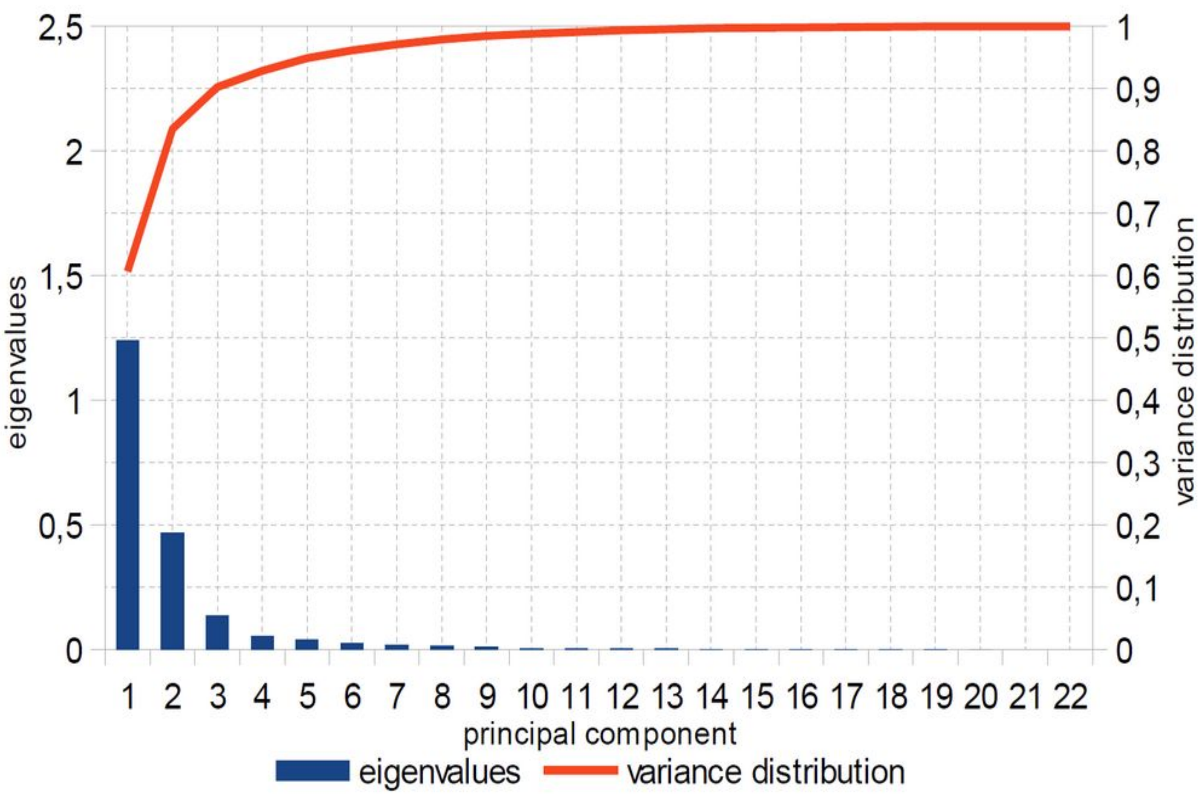


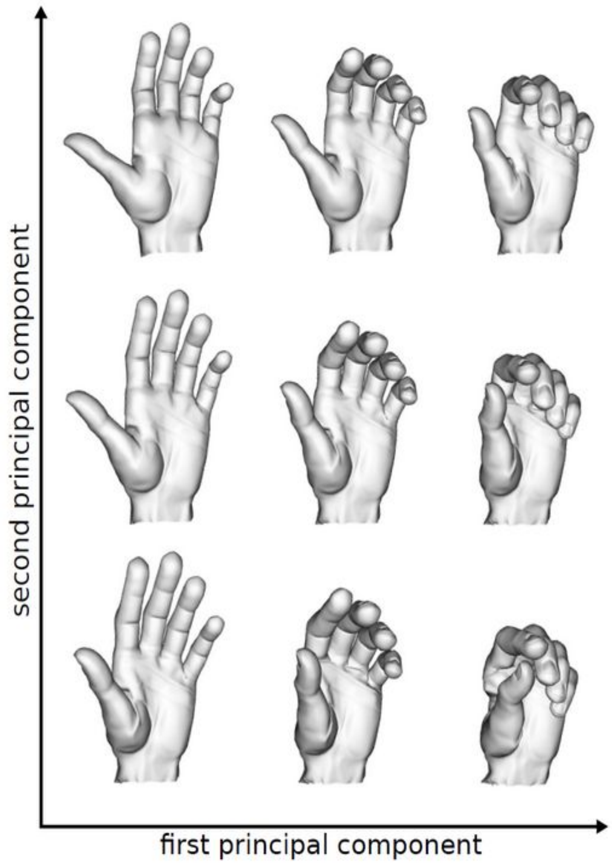
Principle Component Analysis (PCA)

- How many leading eigenvectors? Proportion of variance

- Visual analysis

$$\frac{\lambda_1 + \lambda_2 + \cdots + \lambda_k}{\lambda_1 + \lambda_2 + \cdots + \lambda_k + \cdots + \lambda_d}$$



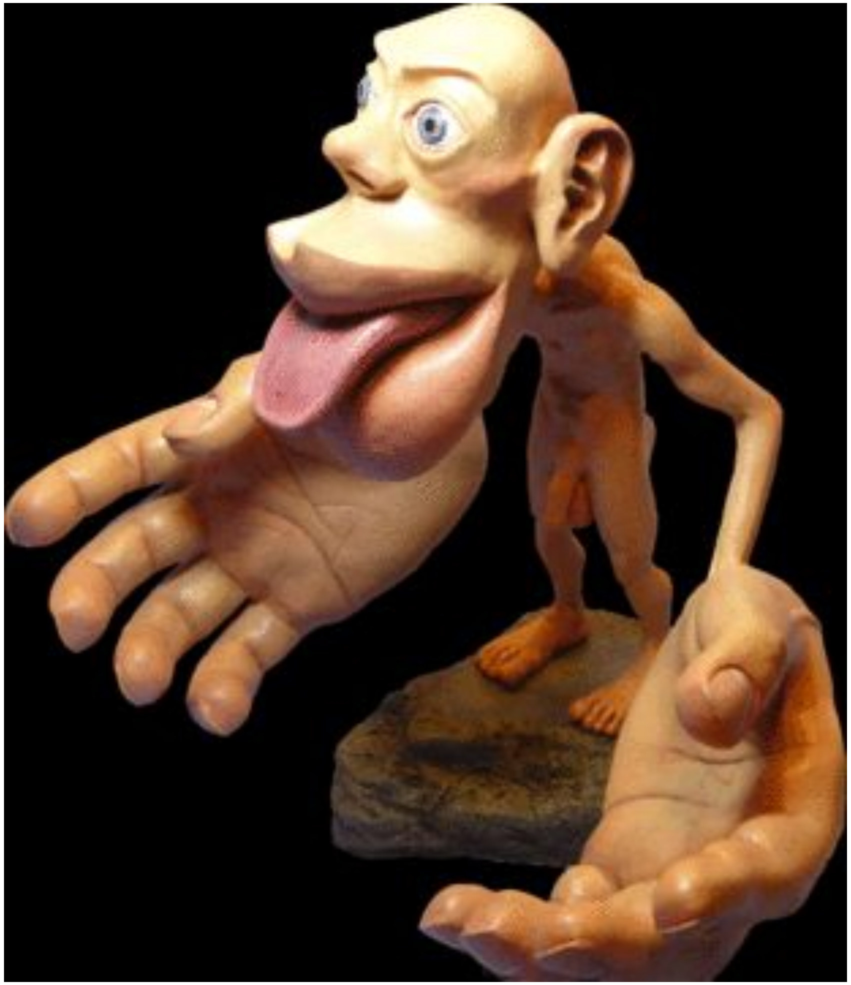


The Journal of Neuroscience, December 1, 1998, *18*(23):10105–10115

Postural Hand Synergies for Tool Use

Marco Santello, Martha Flanders, and John F. Soechting
Neuroscience Department, University of Minnesota, Minneapolis, Minnesota 55455

- Language (mouth, tongue) and tool-use capabilities separate us from animals.
- Brain region for control of hand is significant compared to other regions.
- Manipulation is challenging!



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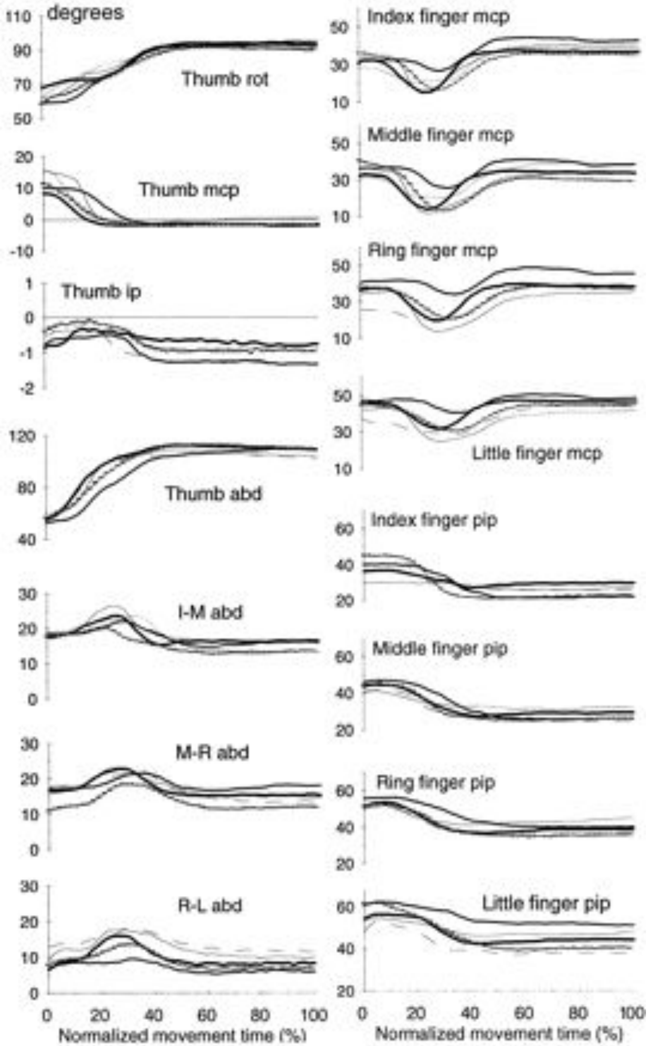
1. Apple
2. Banana
3. Baseball
4. Beer bottle
5. Beer mug
6. Brick
7. Bucket
8. Calculator
9. Chalk
10. Cherry
11. Chinese tea cup
12. Cigarette
13. Circular ashtray
14. Coffee mug
15. Comb
16. Compact disc
17. Computer mouse
18. Dictionary
19. Dinner plate
20. Dog dish
21. Door key
22. Door knob
23. Drawer handle
24. Egg
25. Espresso cup
26. Fishing rod
27. Frisbee
28. Frying pan
29. Hair dryer
30. Hammer
31. Ice cube
32. Iron
33. Jar lid
34. Kitchen knife
35. Knob of a lid
36. Knob of a stove
37. Light bulb
38. Milk carton
39. Needle
40. Notebook
41. Pen
42. Playing card
43. Rope
44. Scissors
45. Screwdriver
46. Stapler
47. Sugar cone
48. Teaspoon
49. Telephone handset
50. Tennis racket
51. Toothbrush
52. Toothpick
53. Turtle
54. Umbrella
55. Wafer
56. Wrench
57. Zipper



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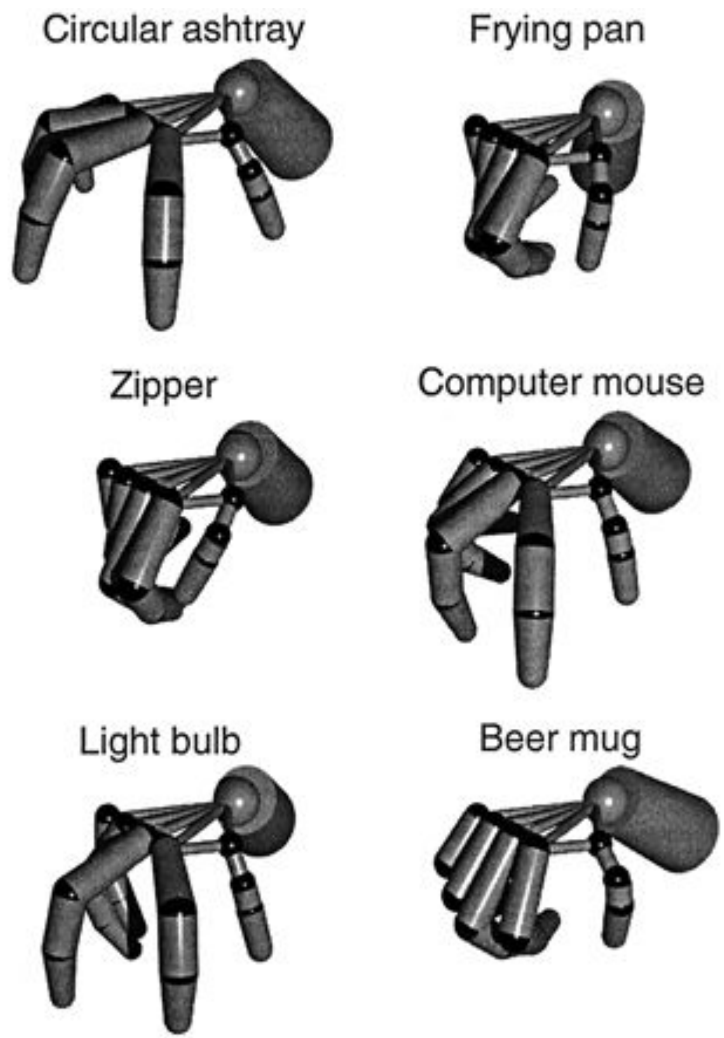

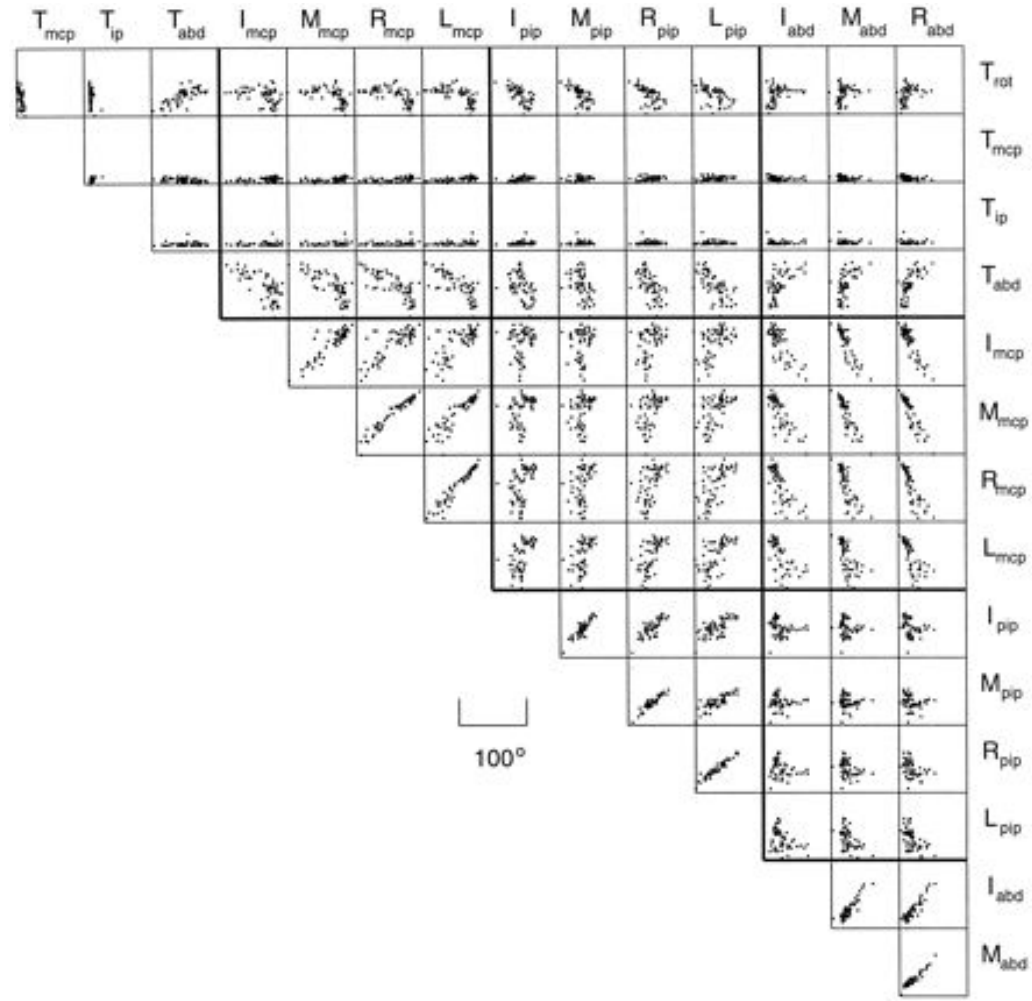

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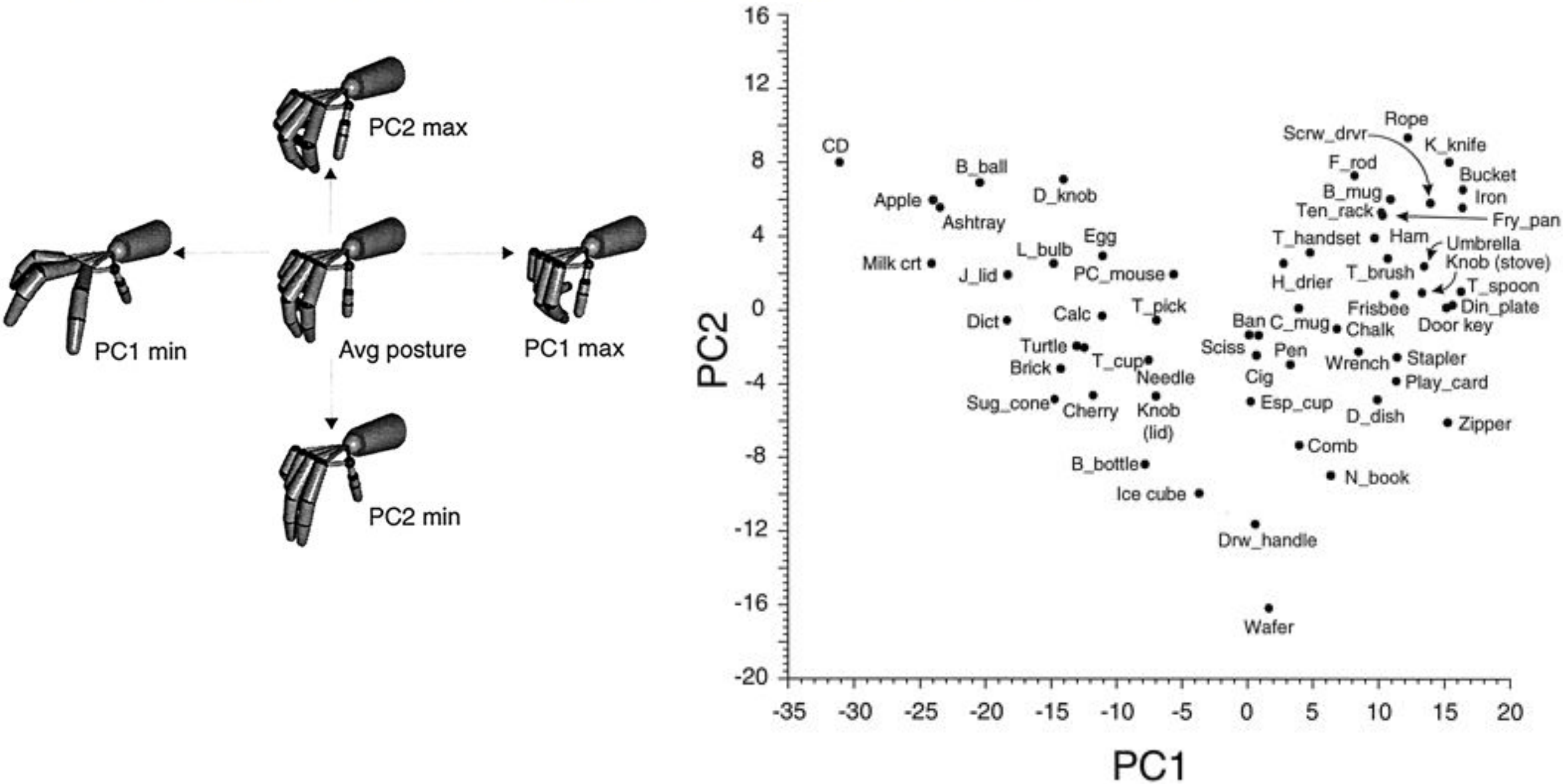

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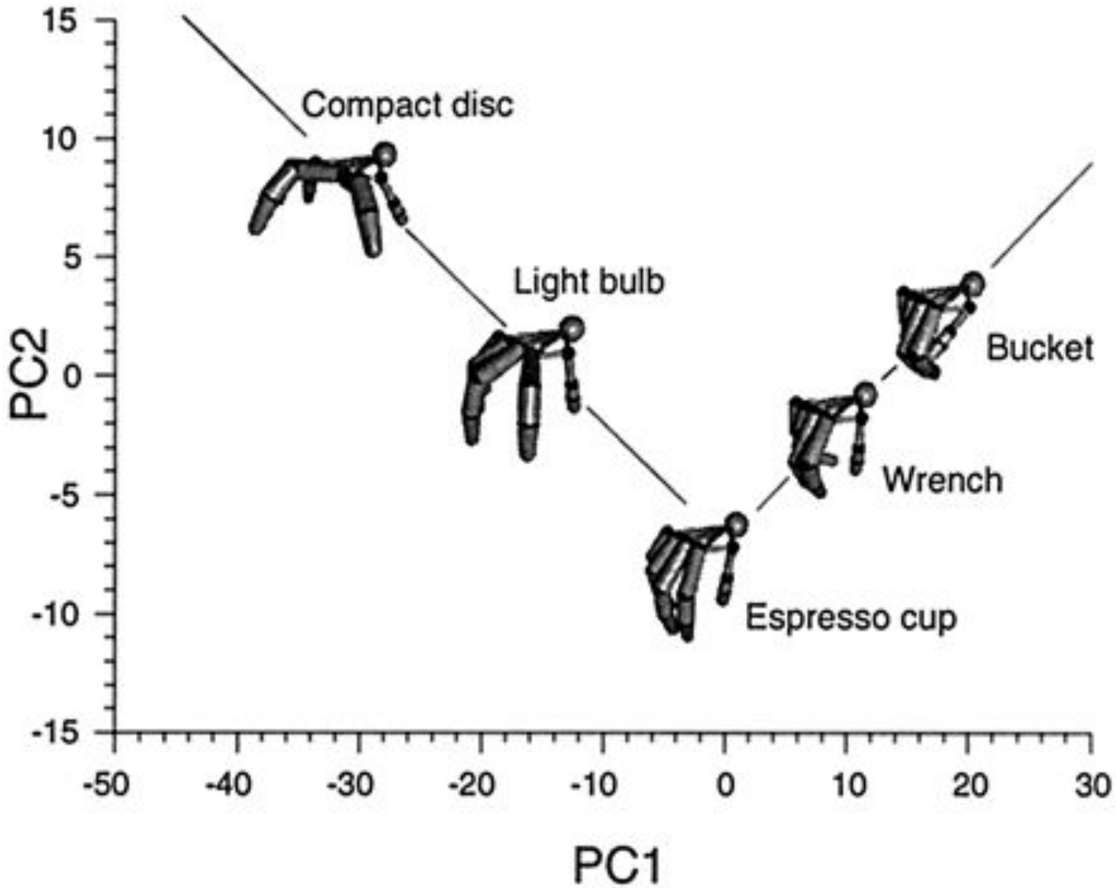
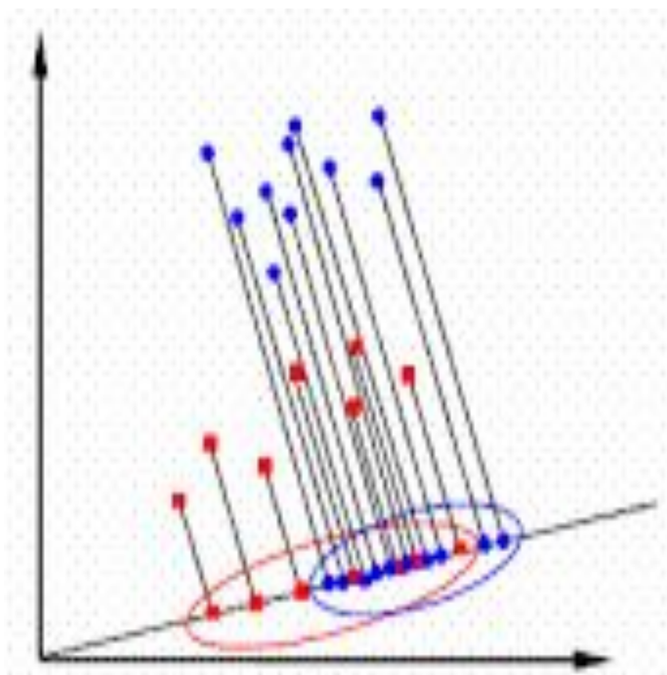


Linear Discriminant Analysis (LDA)



(a)

Linear Discriminant Analysis (LDA)

- Supervised method for dimensionality reduction
- Given samples from C_1 and C_2, find the vector **w**, when the data is projected onto **w**, examples of two classes are maximally separated.

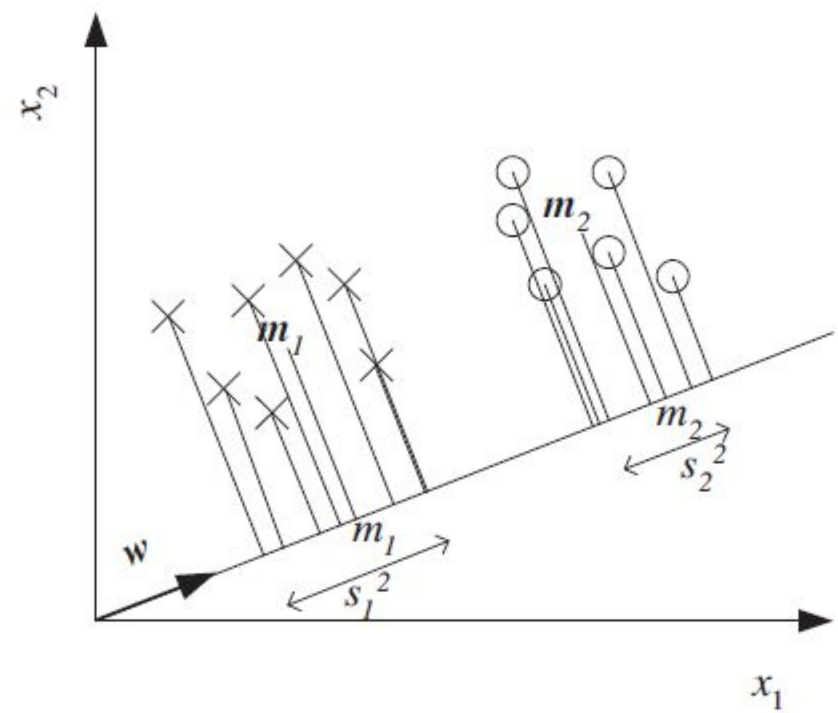
$$z = \mathbf{w}^T \mathbf{x}$$

- Find **w** that maximizes

$$J(\mathbf{w}) = \frac{(m_1 - m_2)^2}{s_1^2 + s_2^2}$$

$$m_1 = \frac{\sum_t \mathbf{w}^T \mathbf{x}^t r^t}{\sum_t r^t} = \mathbf{w}^T \mathbf{m}_1$$

$$s_1^2 = \sum_t (\mathbf{w}^T \mathbf{x}^t - m_1)^2 r^t$$



Linear Discriminant Analysis (LDA)

Take derivative of *J* wrt. **w**:

$$\mathbf{w} = c\mathbf{S}_W^{-1}(\mathbf{m}_1 - \mathbf{m}_2)$$

$$J(\mathbf{w}) = \frac{(m_1 - m_2)^2}{s_1^2 + s_2^2}$$

$$\begin{aligned}(m_1 - m_2)^2 &= (\mathbf{w}^T\mathbf{m}_1 - \mathbf{w}^T\mathbf{m}_2)^2 \\ &= \mathbf{w}^T(\mathbf{m}_1 - \mathbf{m}_2)(\mathbf{m}_1 - \mathbf{m}_2)^T\mathbf{w} \\ &= \mathbf{w}^T\mathbf{S}_B\mathbf{w}\end{aligned}$$

between-class scatter matrix

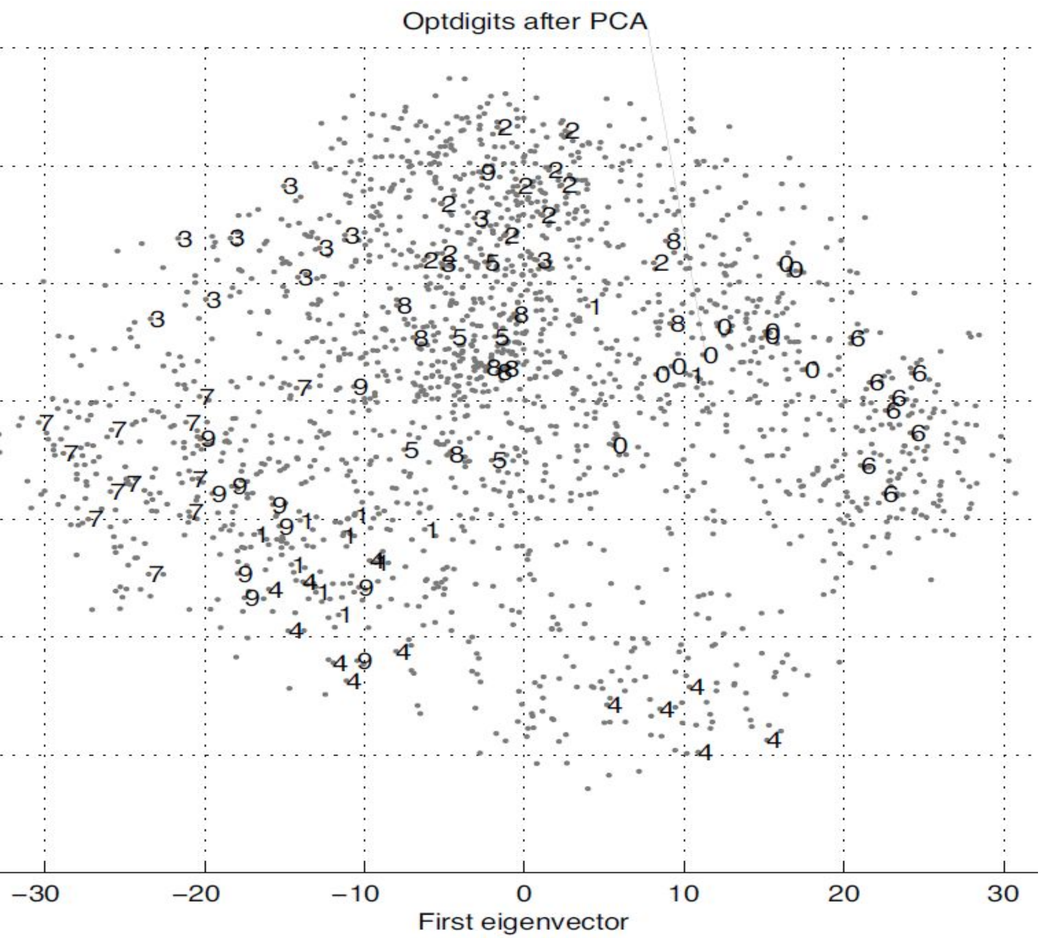
$$\sum_{i=1}^{C}\sum_{t=1}^{N}(x_t^i - \mu_i)(x_t^i - \mu_i)^T$$

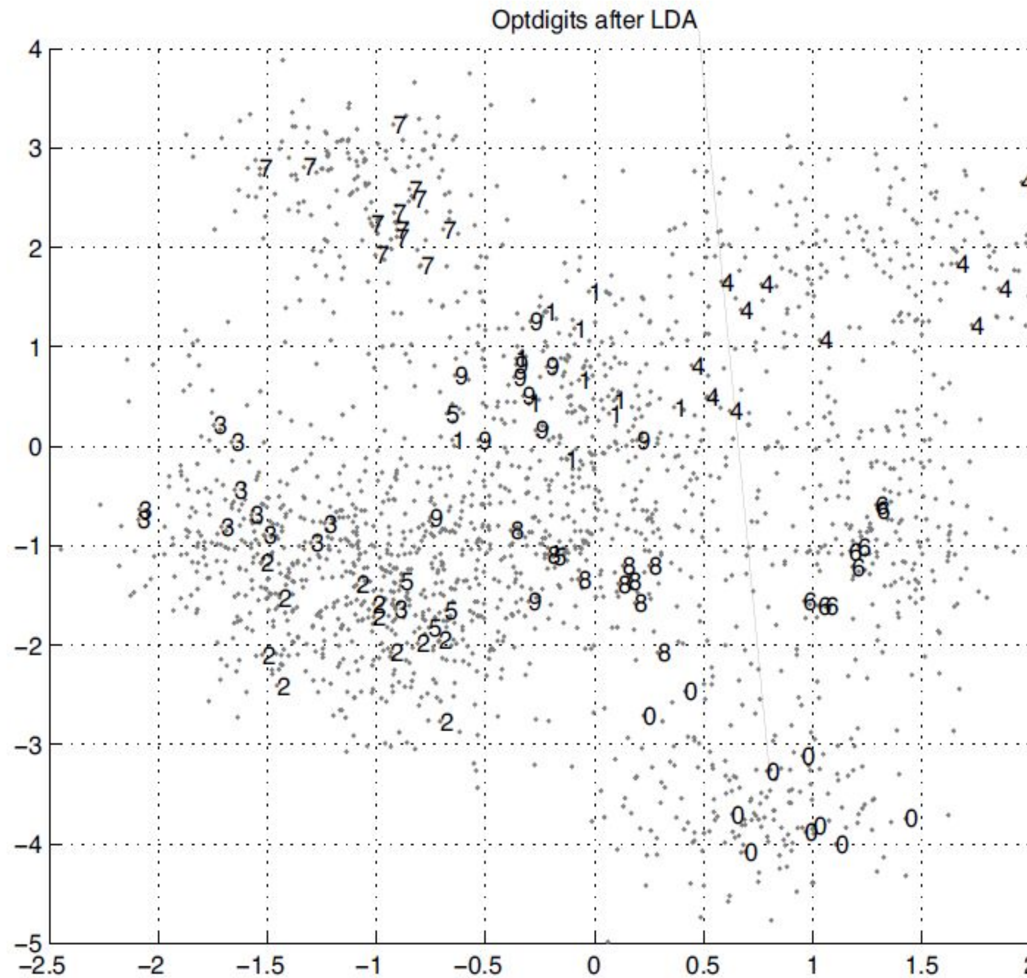
$$\begin{aligned}s_1^2 &= \sum_t (\mathbf{w}^T\mathbf{x}^t - m_1)^2 r^t \\ &= \sum_t \mathbf{w}^T(\mathbf{x}^t - \mathbf{m}_1)(\mathbf{x}^t - \mathbf{m}_1)^T\mathbf{w}r^t \\ &= \mathbf{w}^T\mathbf{S}_1\mathbf{w}\end{aligned}$$

$$\sum_{i=1}^{C} N(\mu_i - \mu)(\mu_i - \mu)^T$$

within-class scatter matrix

Linear Discriminant Analysis (LDA)





Feature embedding

- In PCA: Eigenvectors of $\mathbf{X}^T\mathbf{X}$. dxd matrix
- Feature embedding: Eigenvectors of $\mathbf{X}\mathbf{X}^T$. NxN matrix
    - If d >> N
    - Turk and Pentland 1991, 256x256 images, 40 face images

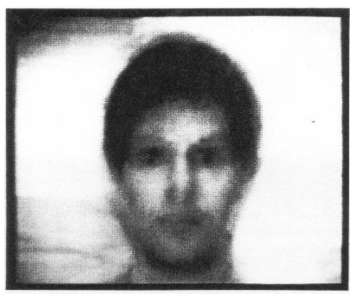


Figure 1. (b) The average face Ψ.

$$\mathbf{u}_l = \sum_{k=1}^{M} \mathbf{v}_{lk}\Phi_k,$$

New image: $\omega_k = \mathbf{u}_k^T(\Gamma - \Psi)$ $\Omega^T = [\omega_1, \omega_2 \ldots \omega_{M'}]$

Factor analysis

- Assume that there is a set of unobservable variables, *latent factors,* which when acting in combination *generate* ***x**.*
- The goal is to characterize the dependency among the observed variables by means of a smaller number of factors.
- Suppose that

  a group of variables that have high correlation among themselves and low correlation with all the other variables.

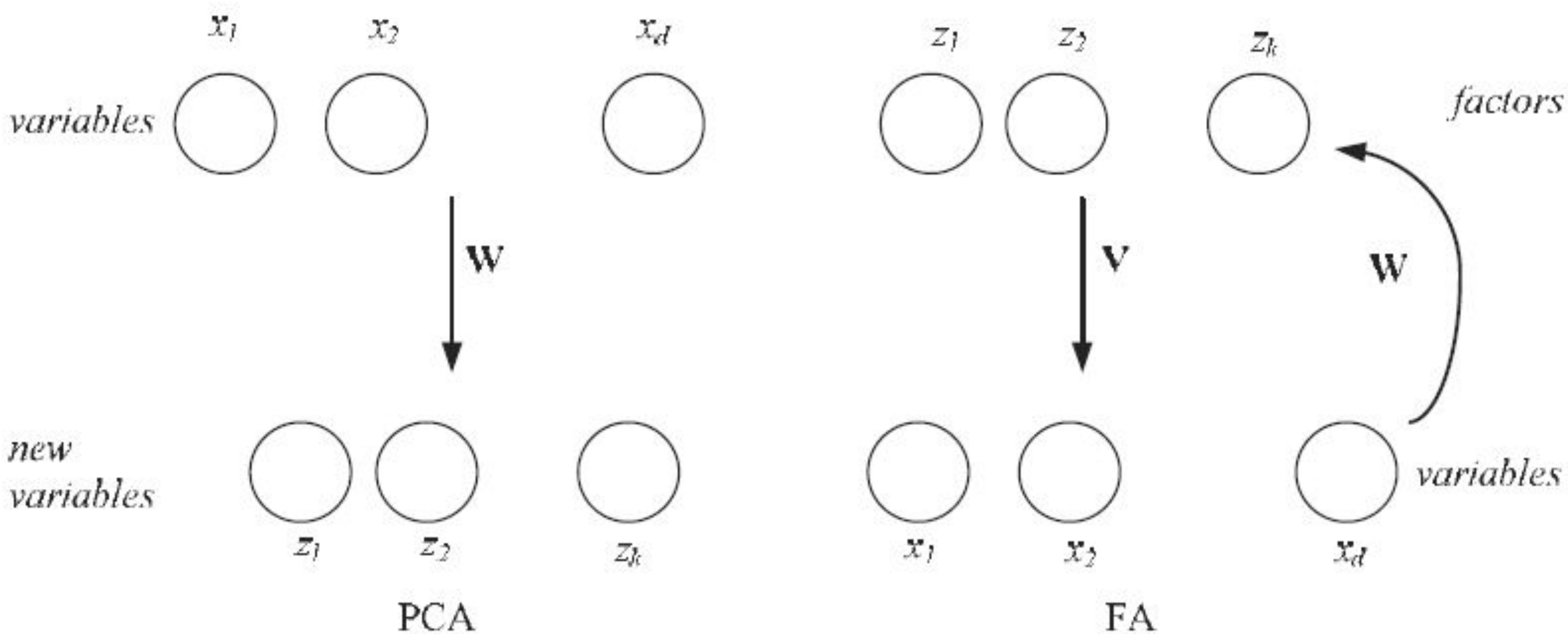
  may be a single underlying factor

- It assumes that each input dimension, x_i, can be written as a weighted sum of the $k < d$ factors, plus a residual term.

$$x_i - \mu_i = \sum_{j=1}^{k} v_{ij} z_j + \epsilon_i$$

Factor analysis

- Assume that there is a set of unobservable variables, *latent factors,* which when acting in combination *generate* ***x**.*
- The goal is to characterize the dependency among the observed variables by means of a smaller number of factors.

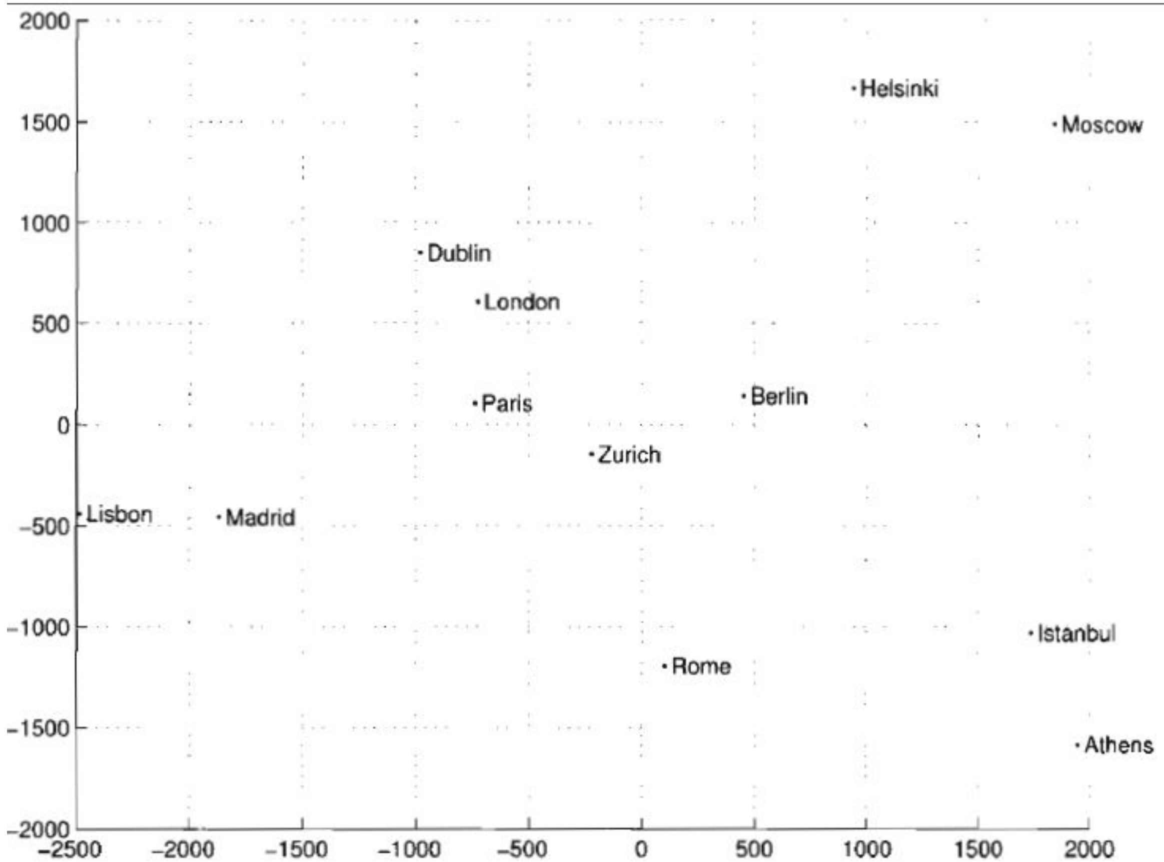


$$x_i - \mu_i = \sum_{j=1}^{k} v_{ij} z_j + \epsilon_i$$

Multidimensional scaling

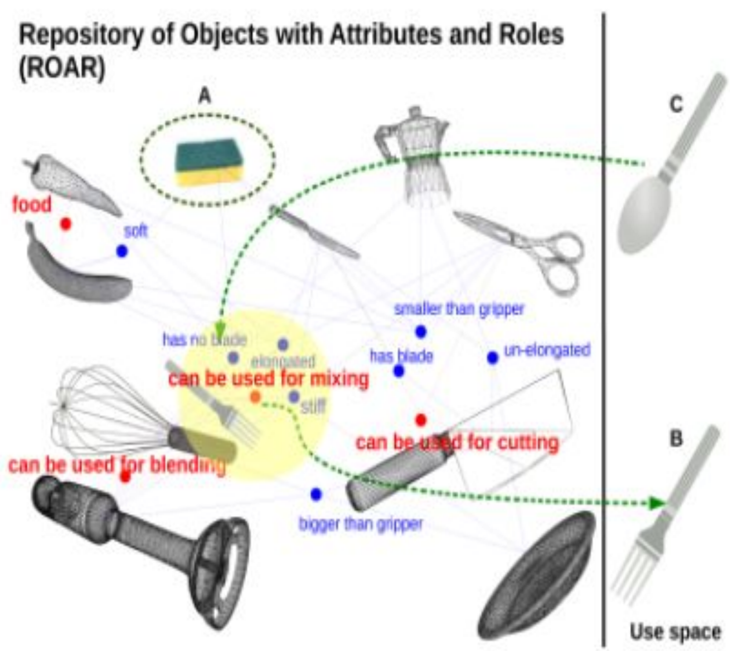
- Visualizing the level of similarity of individual cases of a dataset
- Preserve d_{ij}, the given distance in the original space.

	London	Stockholm	Lisbon	Madrid	Paris	Amsterdam	Berlin	Prague	Rome	Dublin
London	0	569	667	530	141	140	357	396	570	190
Stockholm	569	0	1212	1043	617	446	325	423	787	648
Lisbon	667	1212	0	201	596	768	923	882	714	714
Madrid	530	1043	201	0	431	608	740	690	516	622
Paris	141	617	596	431	0	177	340	337	436	320
Amsterdam	140	446	768	608	177	0	218	272	519	302
Berlin	357	325	923	740	340	218	0	114	472	514
Prague	396	423	882	690	337	272	114	0	364	573
Rome	569	787	714	516	436	519	472	364	0	755
Dublin	190	648	714	622	320	302	514	573	755	0



Multidimensional scaling

- Visualizing the level of similarity of individual cases of a dataset
- Preserve d_{ij}, the given distance in the original space.
- PCA on correlation matrix (not covariance) = MDS with Euclidean distances with each variable unit variance



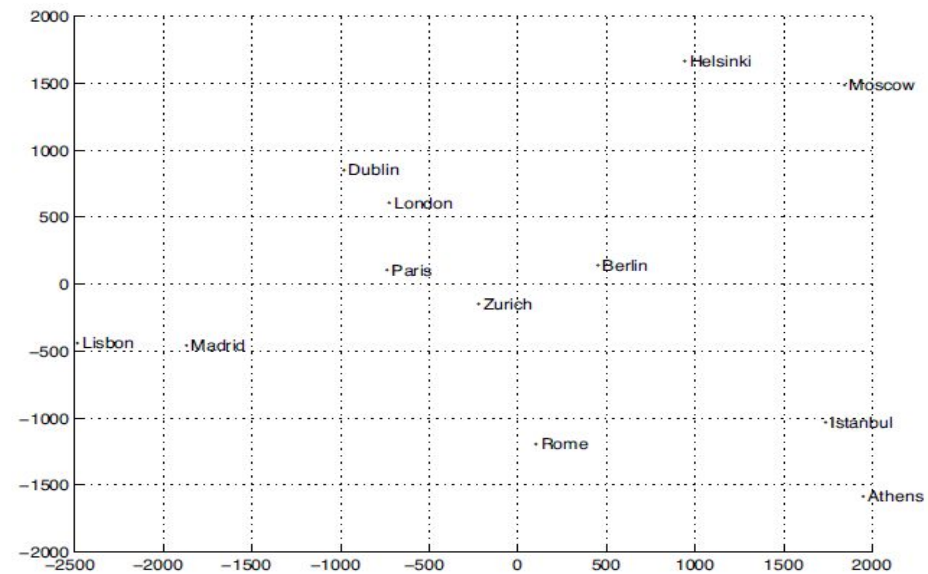
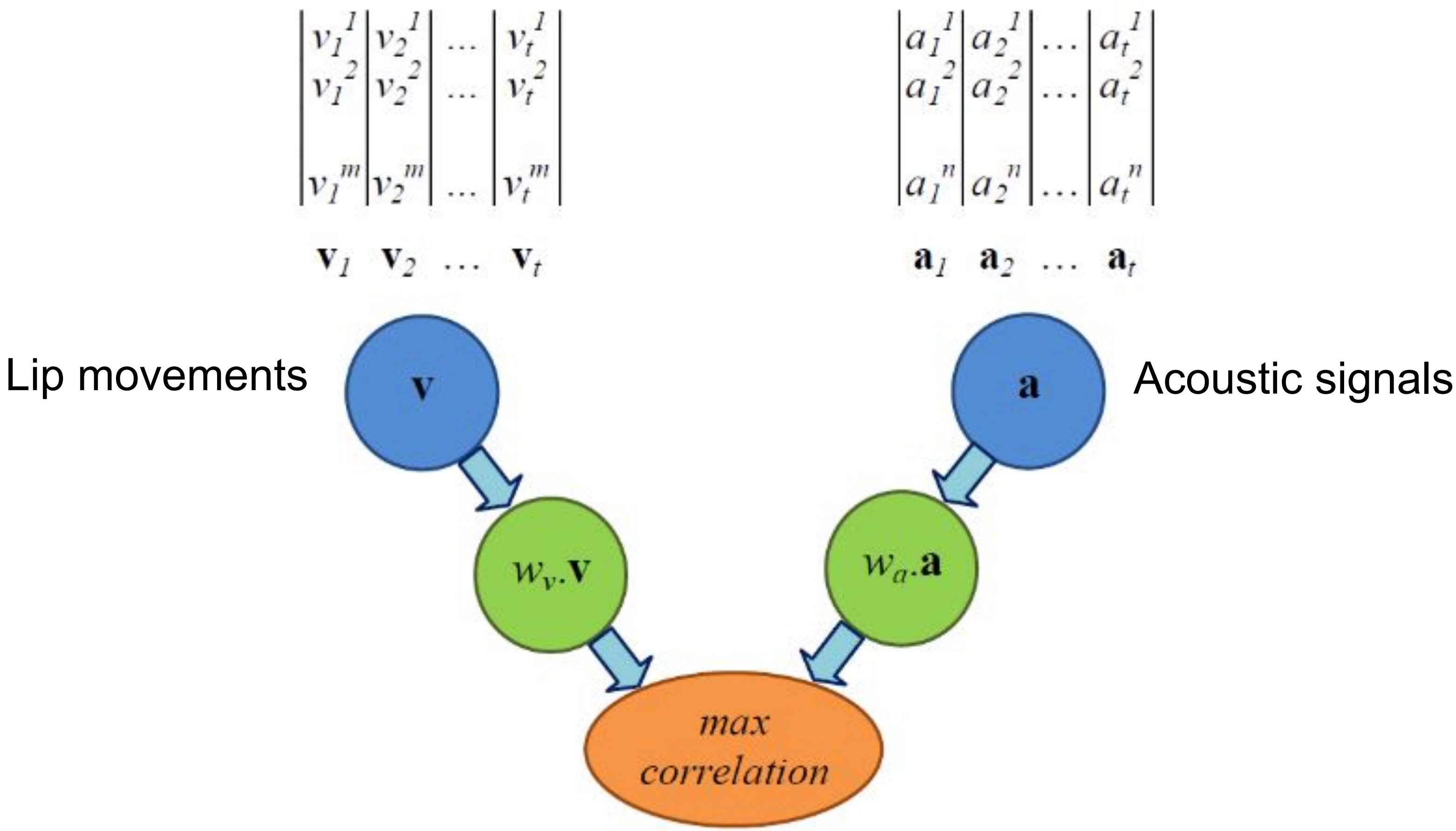


Figure 6.6 Map of Europe drawn by MDS. Pairwise road travel distances between these cities are given as input, and MDS places them in two dimensions such that these distances are preserved as well as possible.

Canonical Correlation Analysis (CCA)

- 2 sets of variables are correlated.
- Reduce dimensionality to a joint space.
- Measure the amount of correlation between **x** and **y** dimensions



Isometric feature mapping (Isomap)

- Similarity between samples may not be simply written in terms of the sum of feature differences
- Estimate geodesic distance