CS233, CME251: Geometric and Topological Data Analysis

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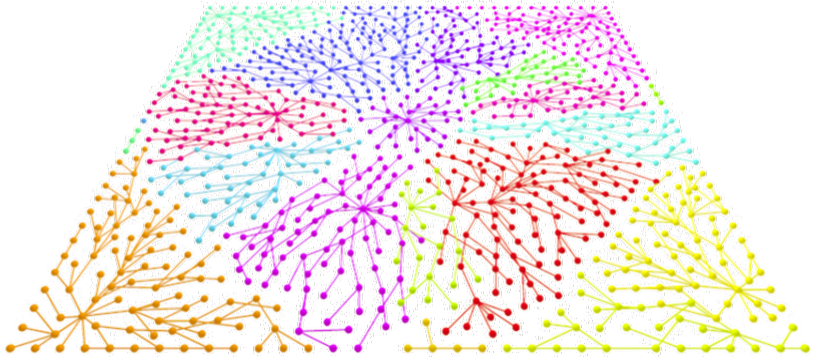
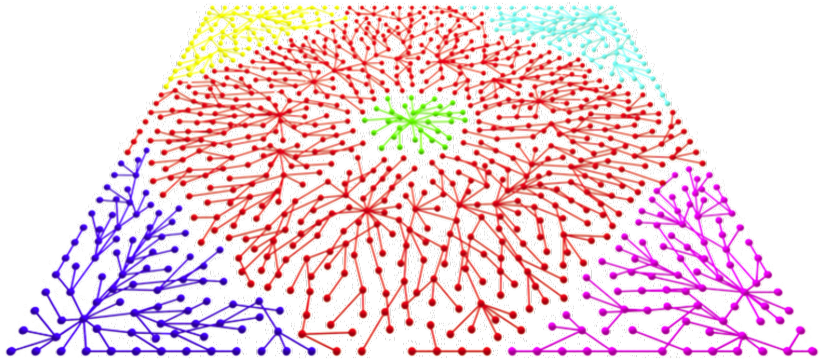
Lecture 2
30 March 2022

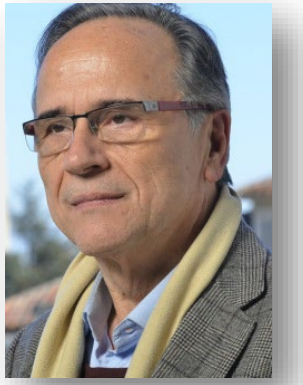




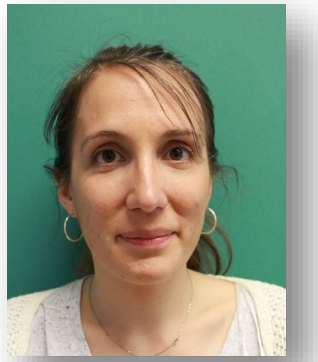
Last Time:
CS 233 Course Overview

The Principals

- Leonidas (Leo) Guibas (CS & EE)
  - Instructor
- Davis Rempe (CS)
  - Course Assistant
- Despoina Paschalidou (CS)
  - Course Assistant
- Carrie Petersen (CS)
  - Admin


Leo


Davis


Despoina


Carrie

CS233 Key Course Goals

- Cover basic tools for geometric and topological data analysis, both supervised and unsupervised
- Focus on less regular data: point clouds, graphs, meshes, simplicial complexes
- Discuss mathematical ways, based on geometry and topology, to encode and transfer knowledge about the data
- Introduce methods for joint data analysis and joint machine learning – benefiting from the “wisdom of the collection”

Course Work: Assignments

- Assignment 1: Principal Components Analysis (PCA) and Canonical Correlation analysis (CCA)
- Assignment 2: Computational Topology - Simplicial Complexes, Homology, Persistence, Mapper Algorithm
- Assignment 3: Geometry Correspondences, Shape Matching, Multi-way Alignments
- Assignment 4: Deep Learning with 3D Point-Clouds

Course Work

- Four assignments
  - modest programming in MATLAB/Python for three, one in JavaPlex
  - working in groups OK, up to three students
  - Use Google Cloud for Education coupons for deep net training
- A midterm, no final
- Each assignment and the midterm will count for 20% of the grade
- Special consideration for those taking the course credit / no credit: may omit one assignment of your choice

Class Mechanics

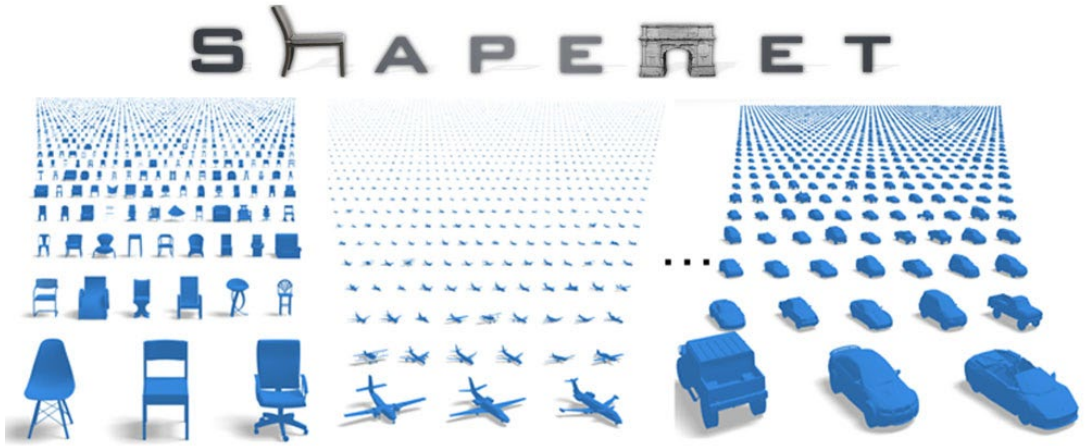
- Two weekly lectures
- Online and after class office hours
- Class web site http://cs233.stanford.edu

  http://graphics.stanford.edu/courses/cs233-22-spring

- Use Piazza (discussion group), Gradescope (for homework submissions)

Annotated DataSets: ImageNet and ShapeNet

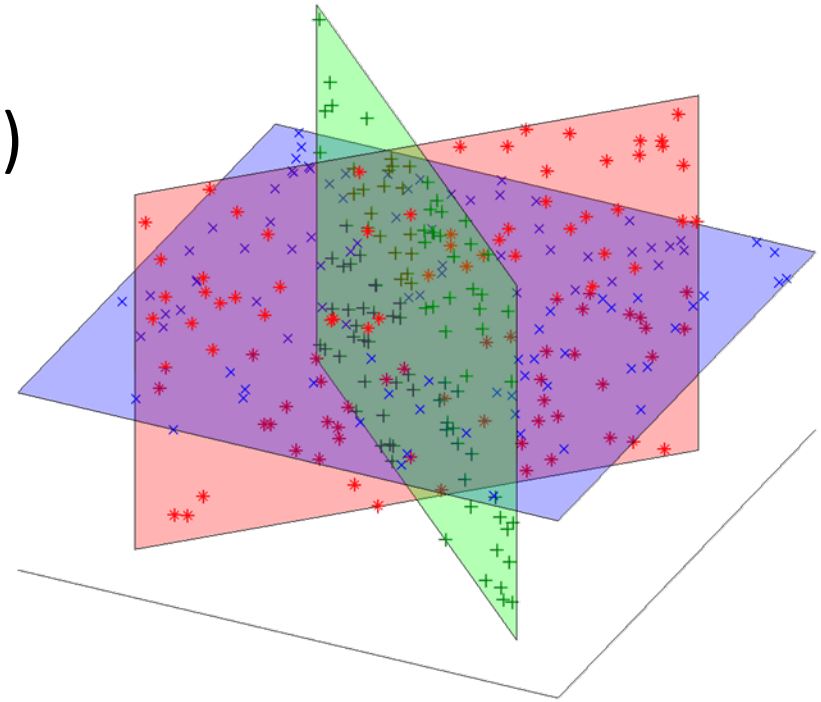
- Relate geometry and topology to data semantics
- Explain how big visual datasets including ImageNet and ShapeNet are organized
- Show the challenge of obtaining geometric annotations



Linear Space Methods

- Principal components analysis (PCA)
- Canonical correlation analysis (CCA)

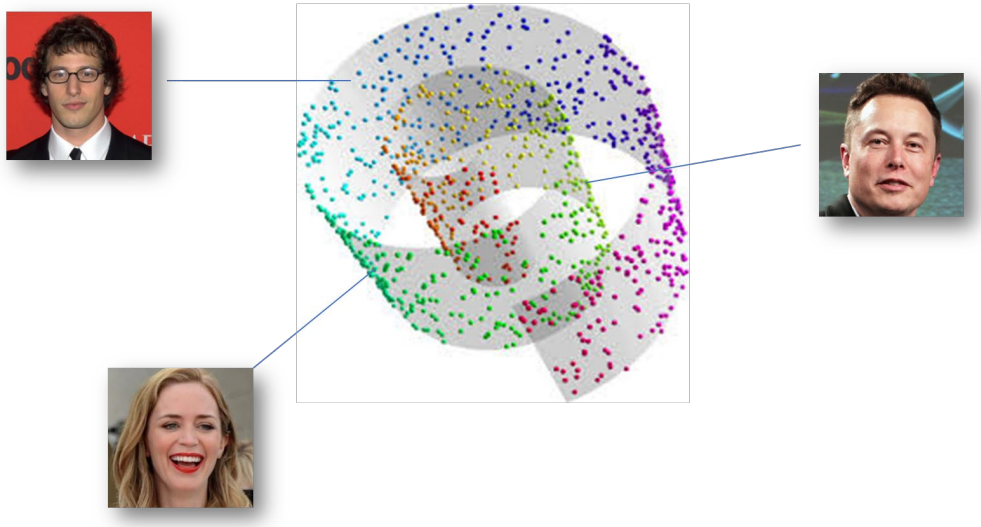
Dimensionality reduction

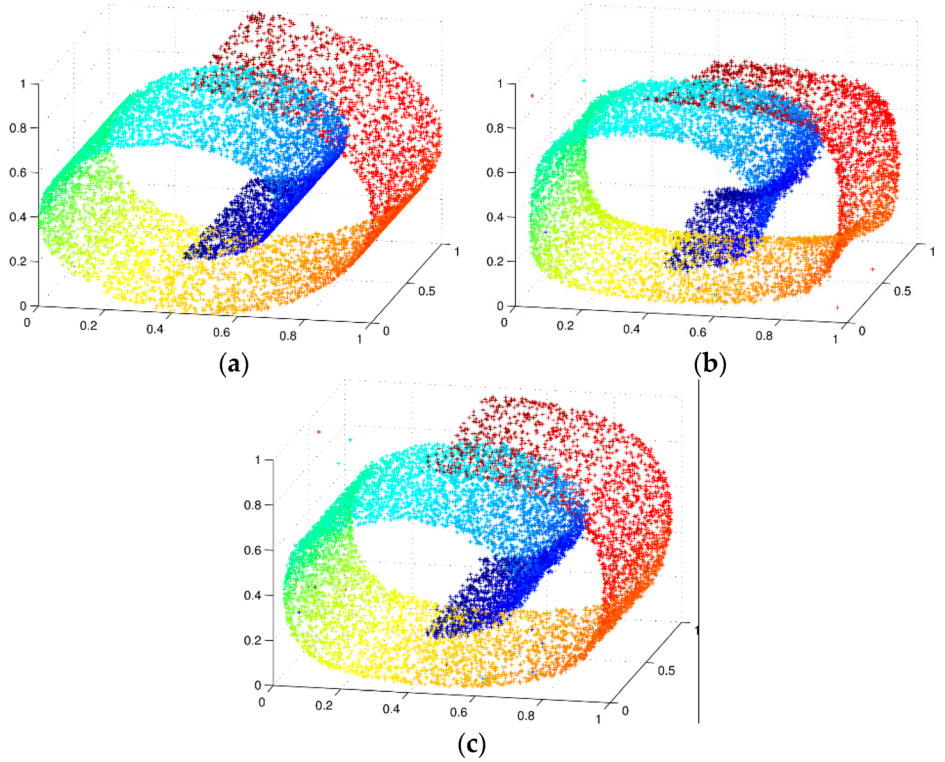


Low-d data (intrinsic dimension) living on a linear subspace, inside a high-d space (extrinsic dimension)

Data as Points on a Manifold

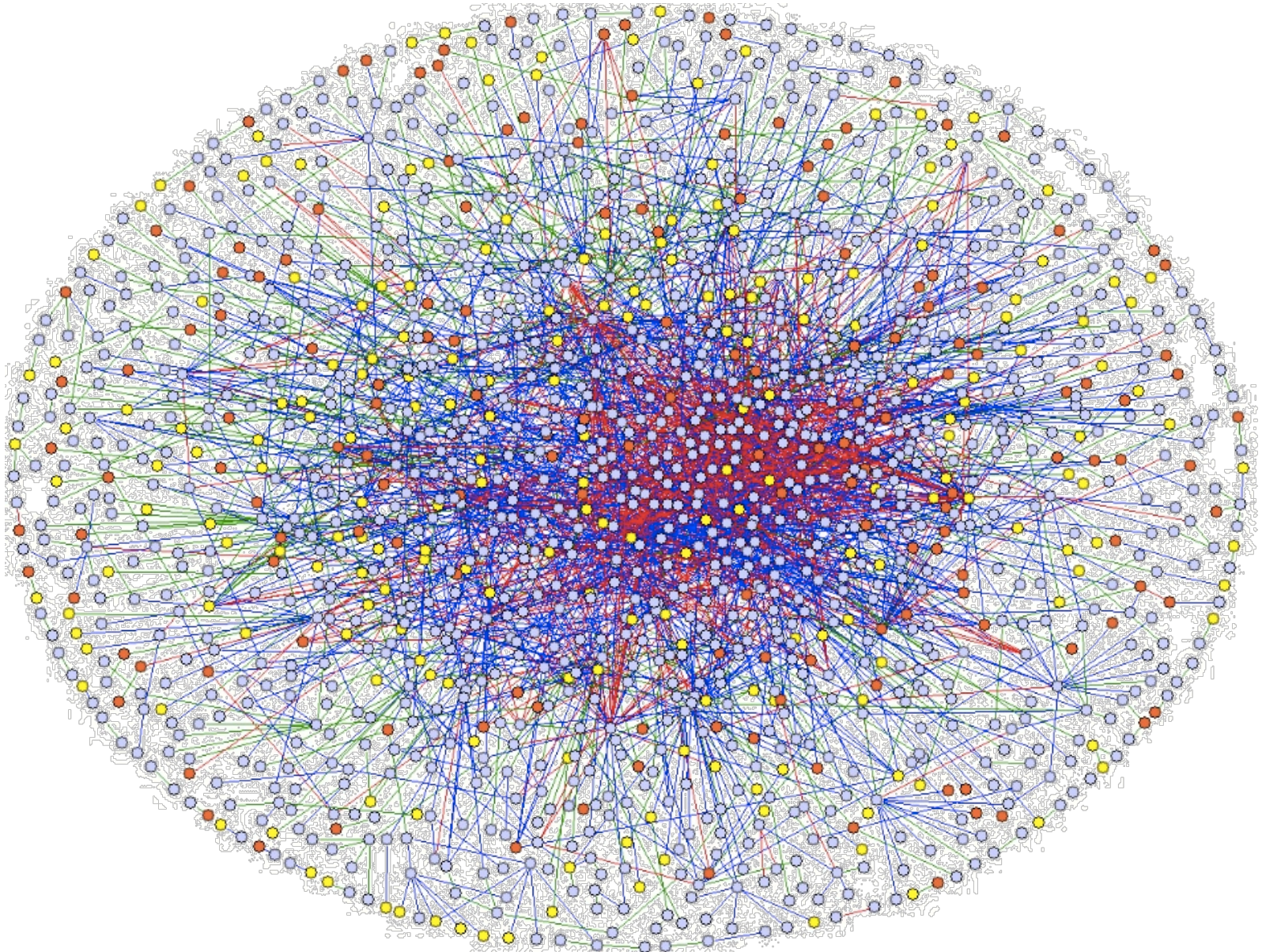
- Non-linear dimensionality reduction
- Low-d data inside high-d space may lie on a non-flat manifold





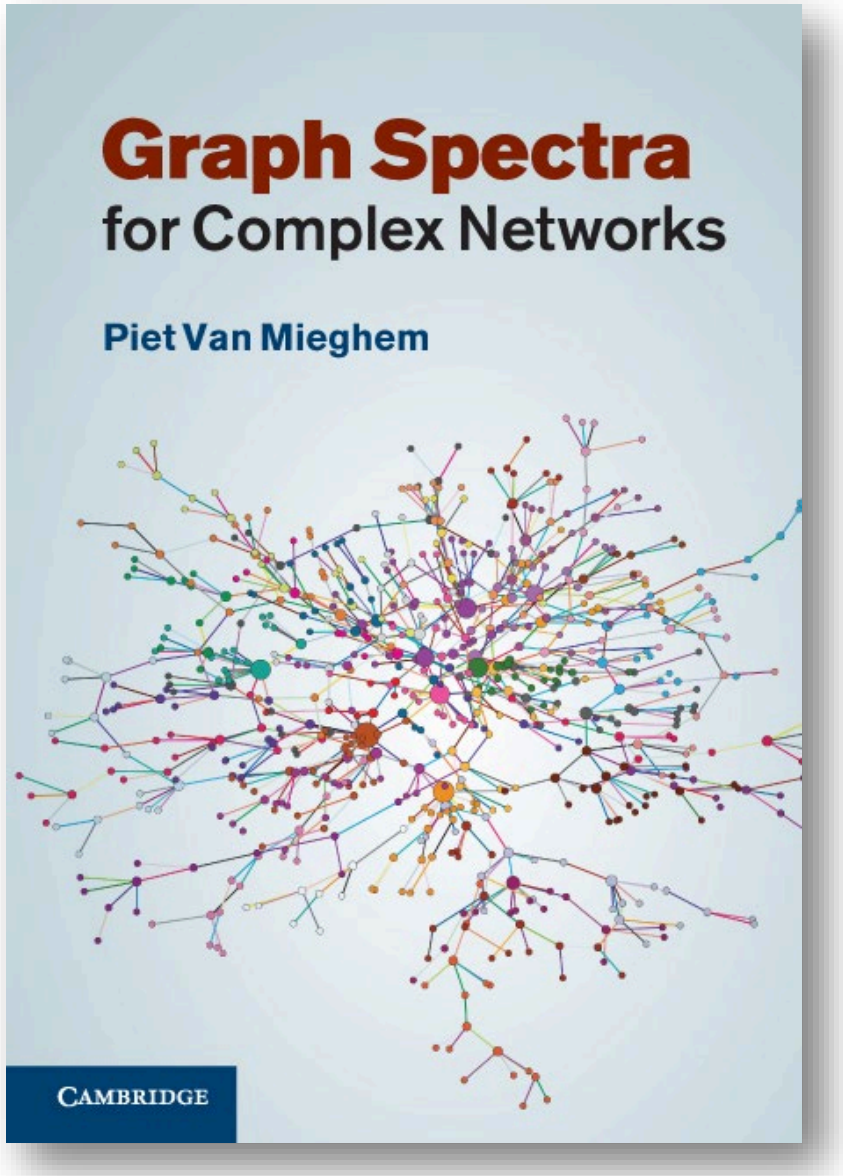
Isomap, locally linear embeddings, Laplacian eigenmaps, t-SNE

A Graph View of Data



Spectral Methods in Graph Theory

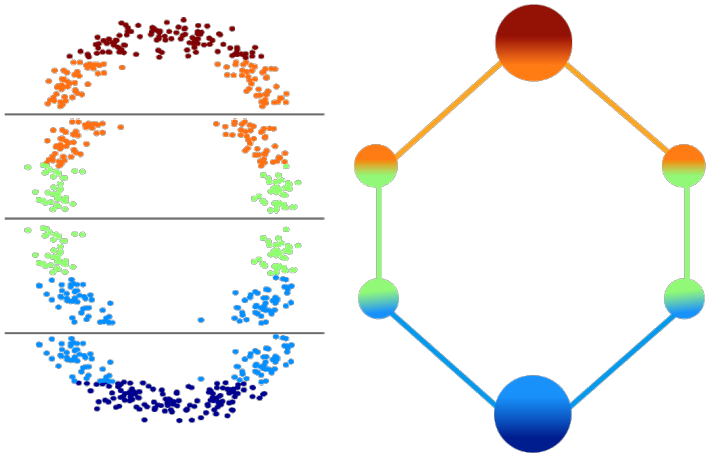
- Linking the graph-theoretic and linear algebraic view of data.



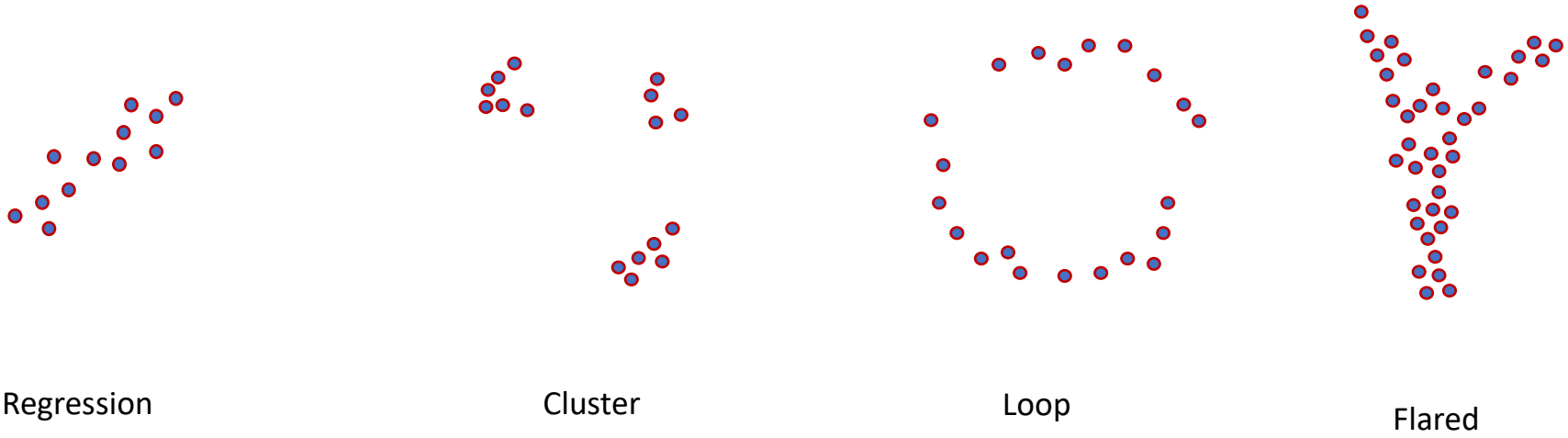
Topological Data Analysis

- Topology is the branch of mathematics that does not take distances too seriously. G. Carlsson

- Large distances (aka “similarity metrics” are often suspect …



In TDA, Sampled Spaces: “The Shape of Data”



Regression

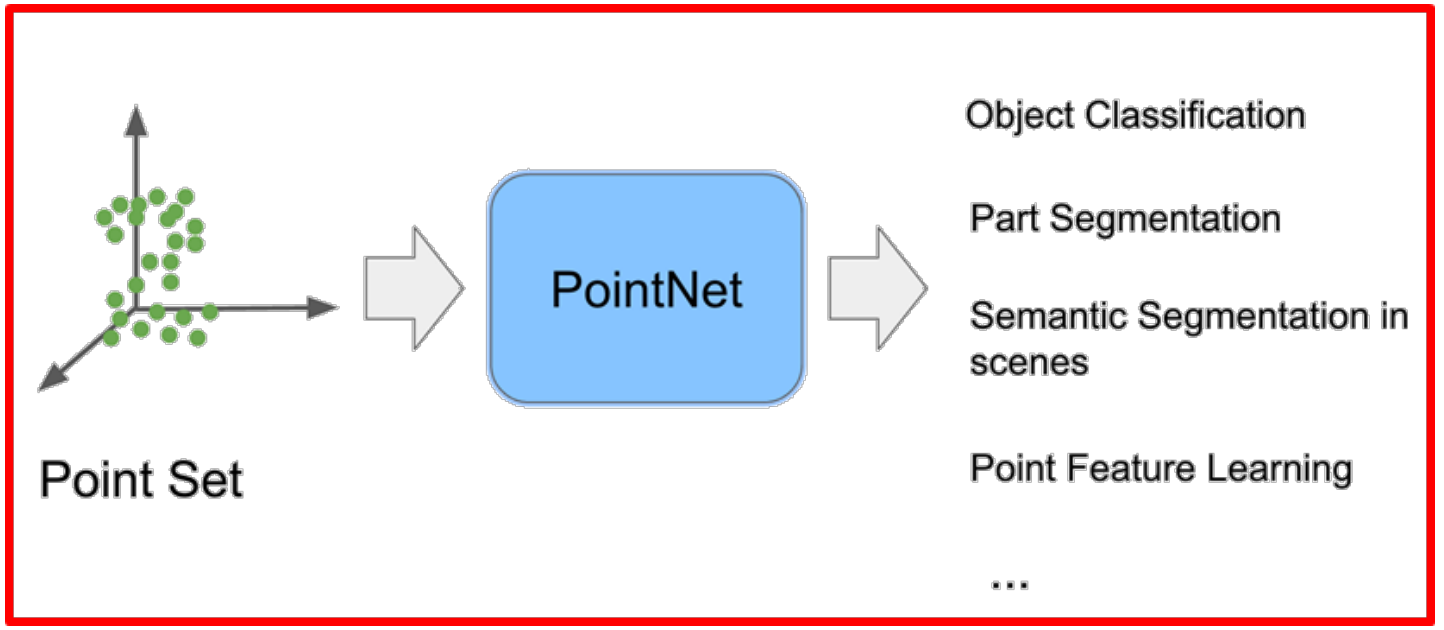
Cluster

Loop

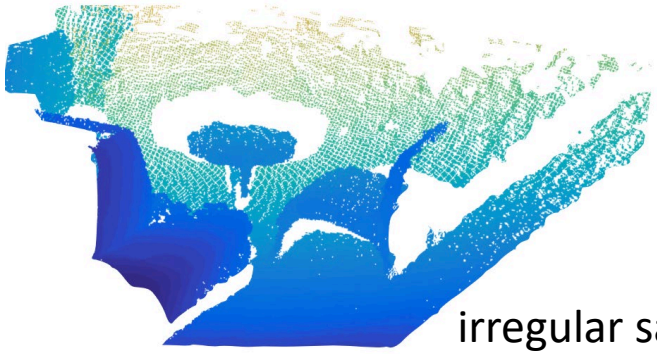
Flared

ML on Point Cloud Data

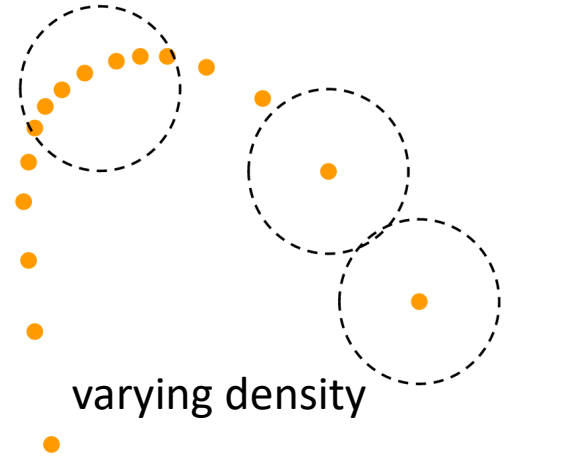
- Goal: design a NN architecture that can work directly with point clouds
- Must deal with unstructured, unordered data



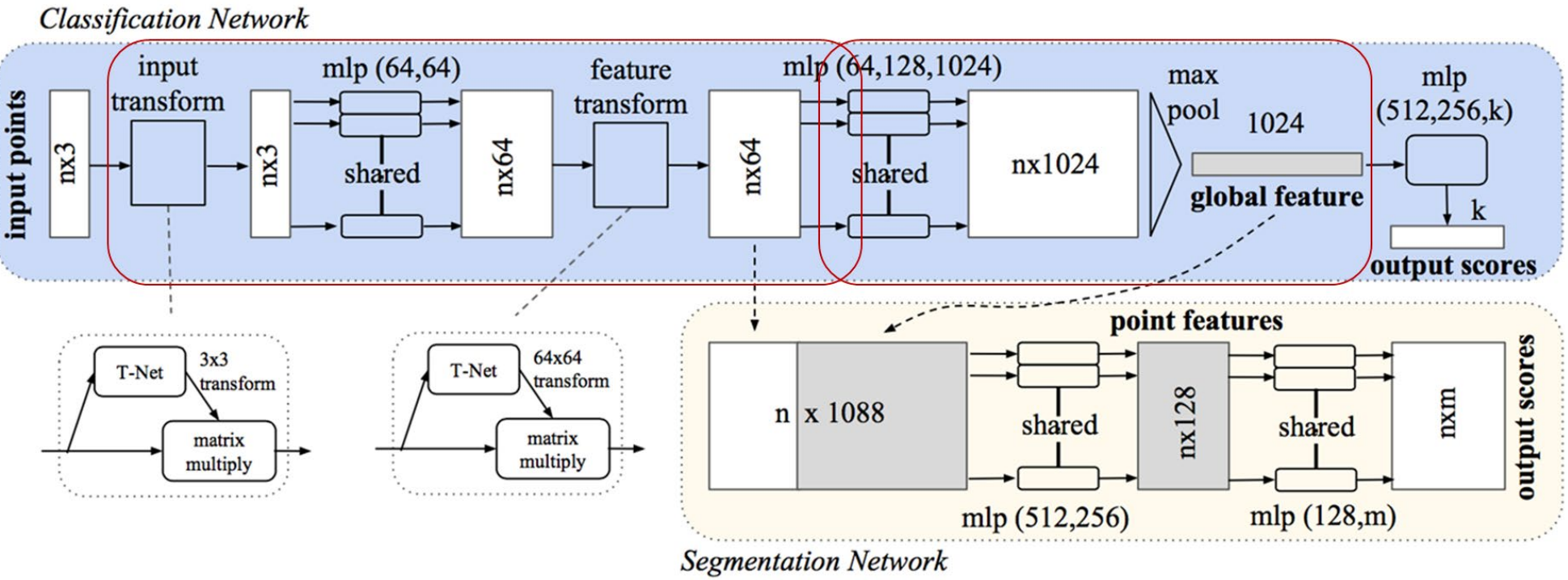
Deep Architectures: PointNet and PointNet++



irregular sampling

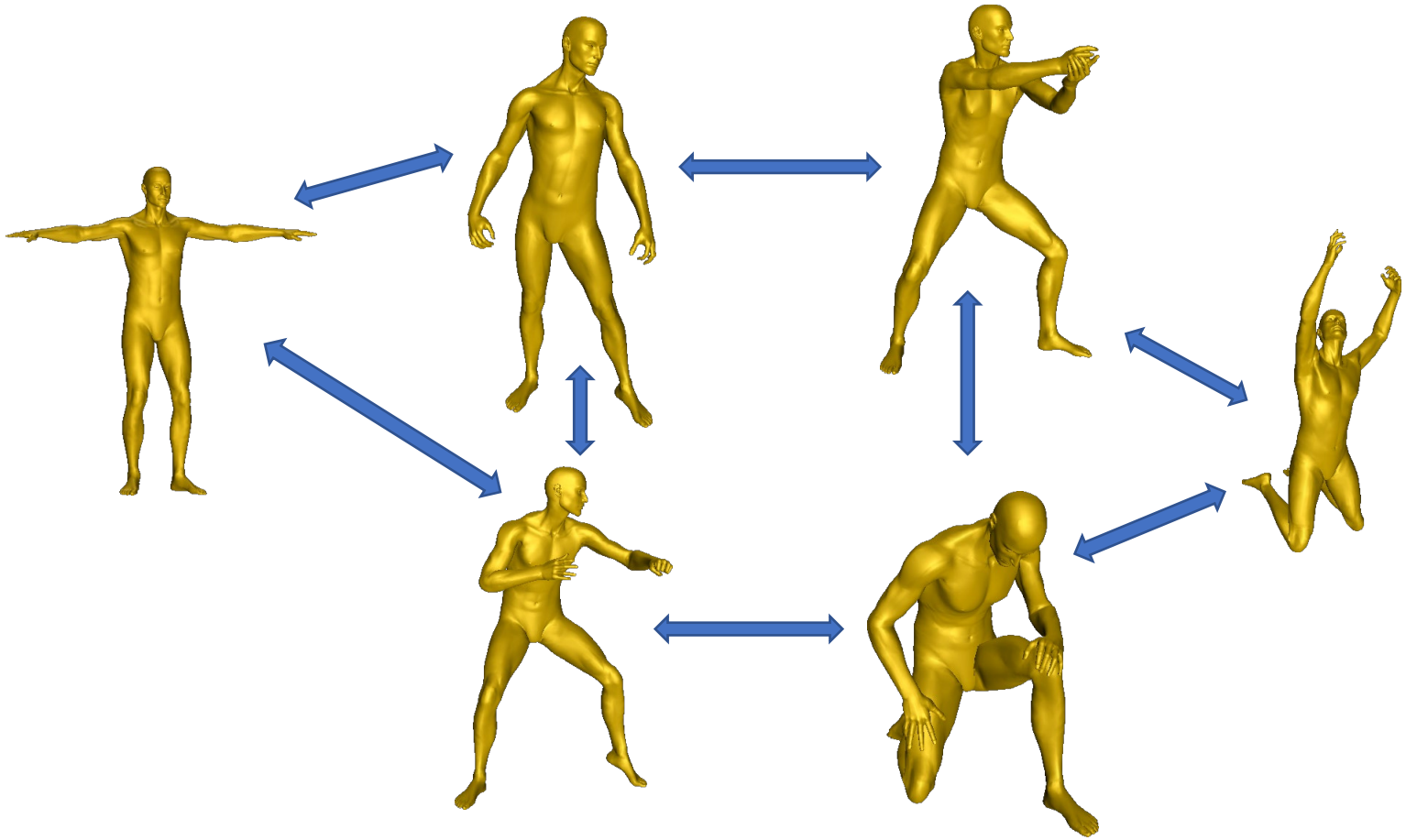


varying density

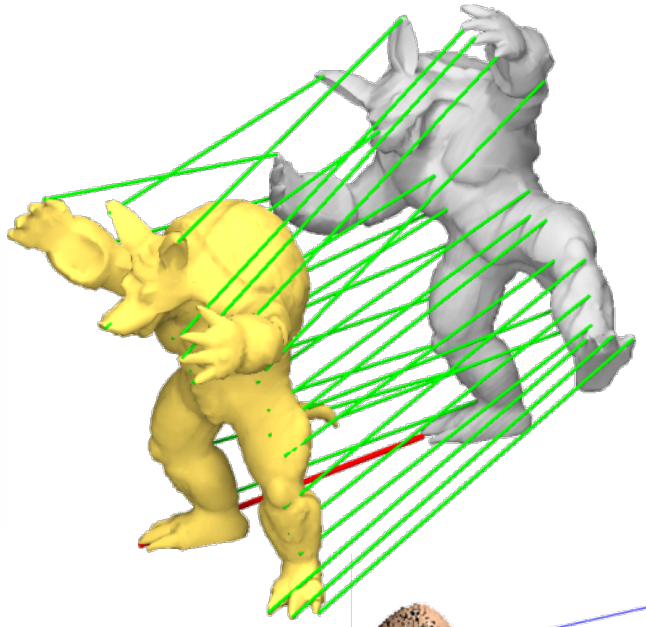


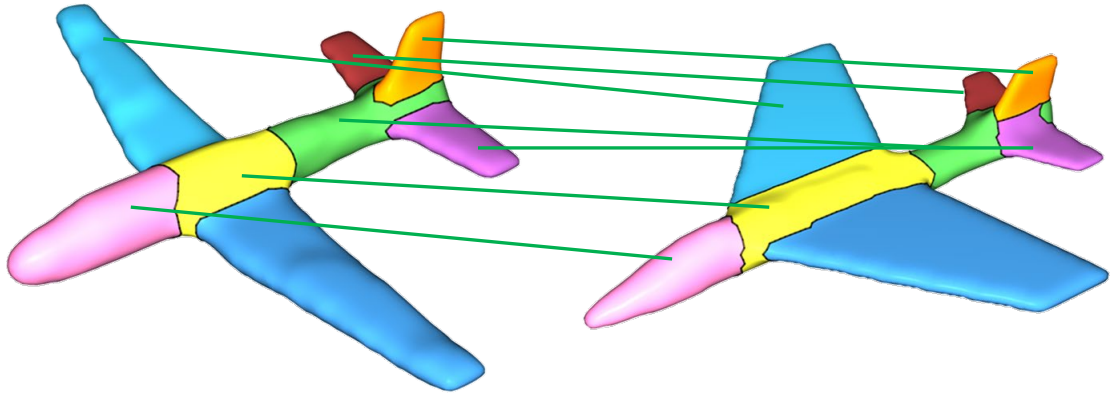
Vanilla PointNet

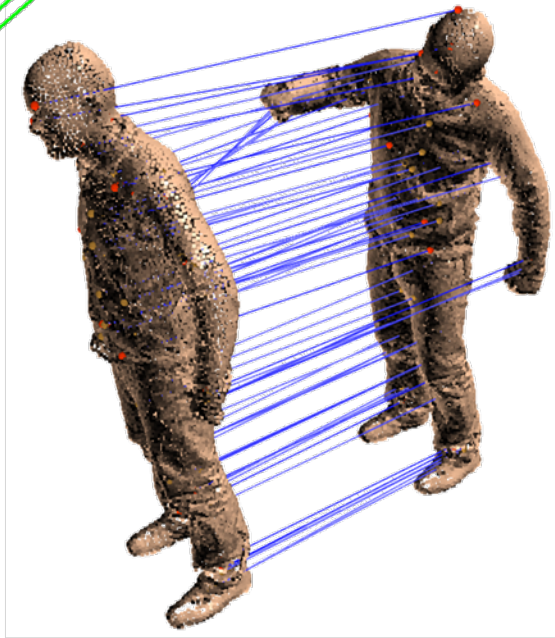
Joint Data Analysis and Correlated Data Sets



Maps and Correspondences

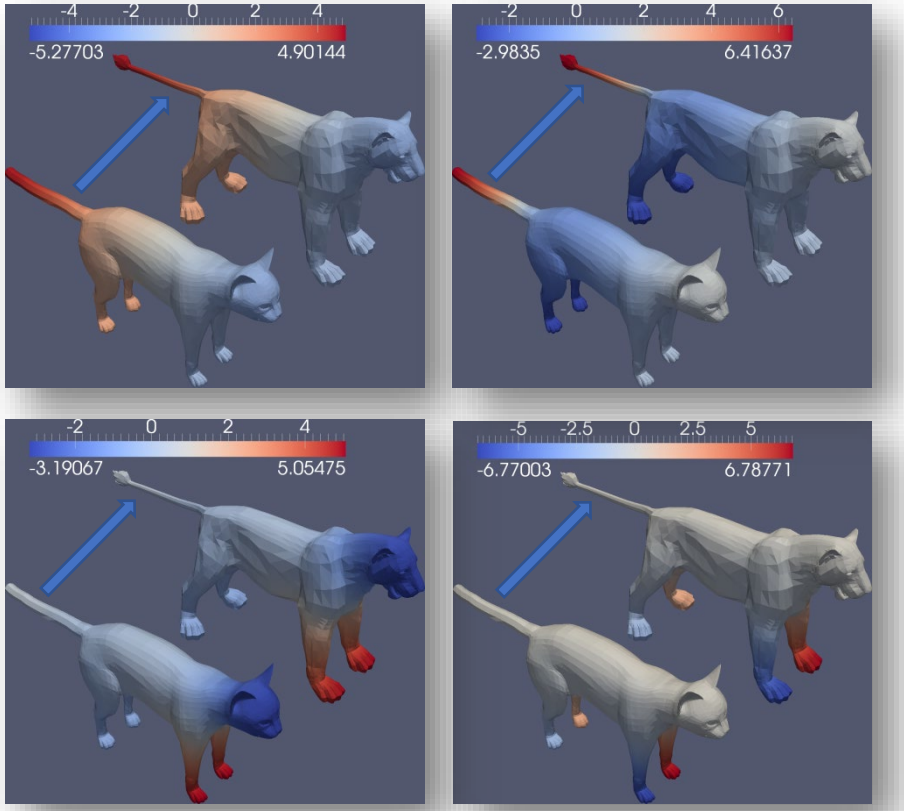




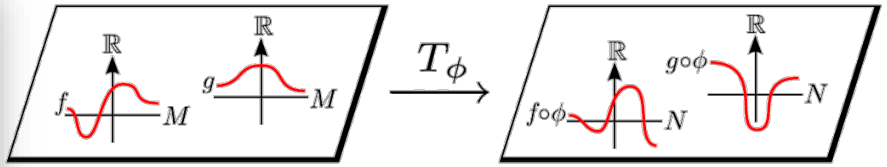


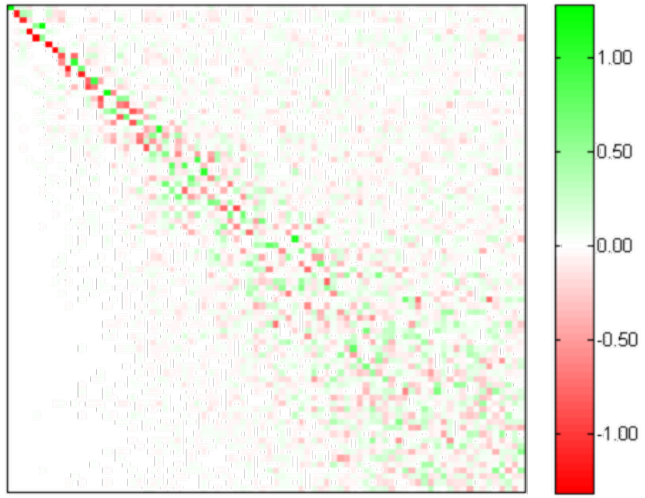
Functional Maps

from cat to lion



Functions on cat are transferred to lion using T_ϕ

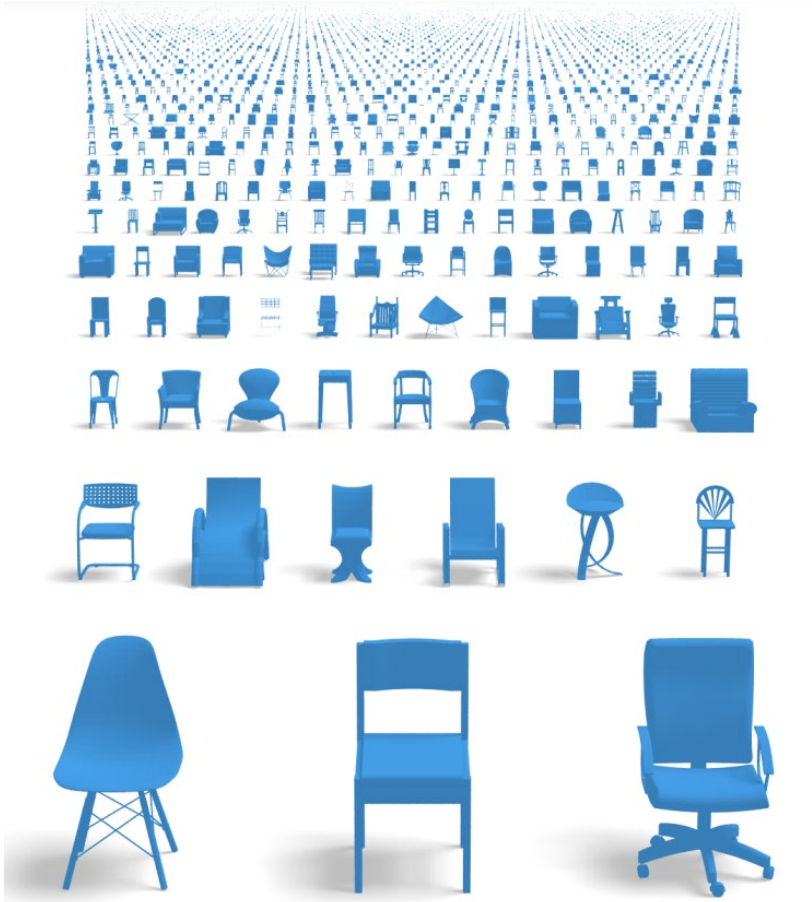




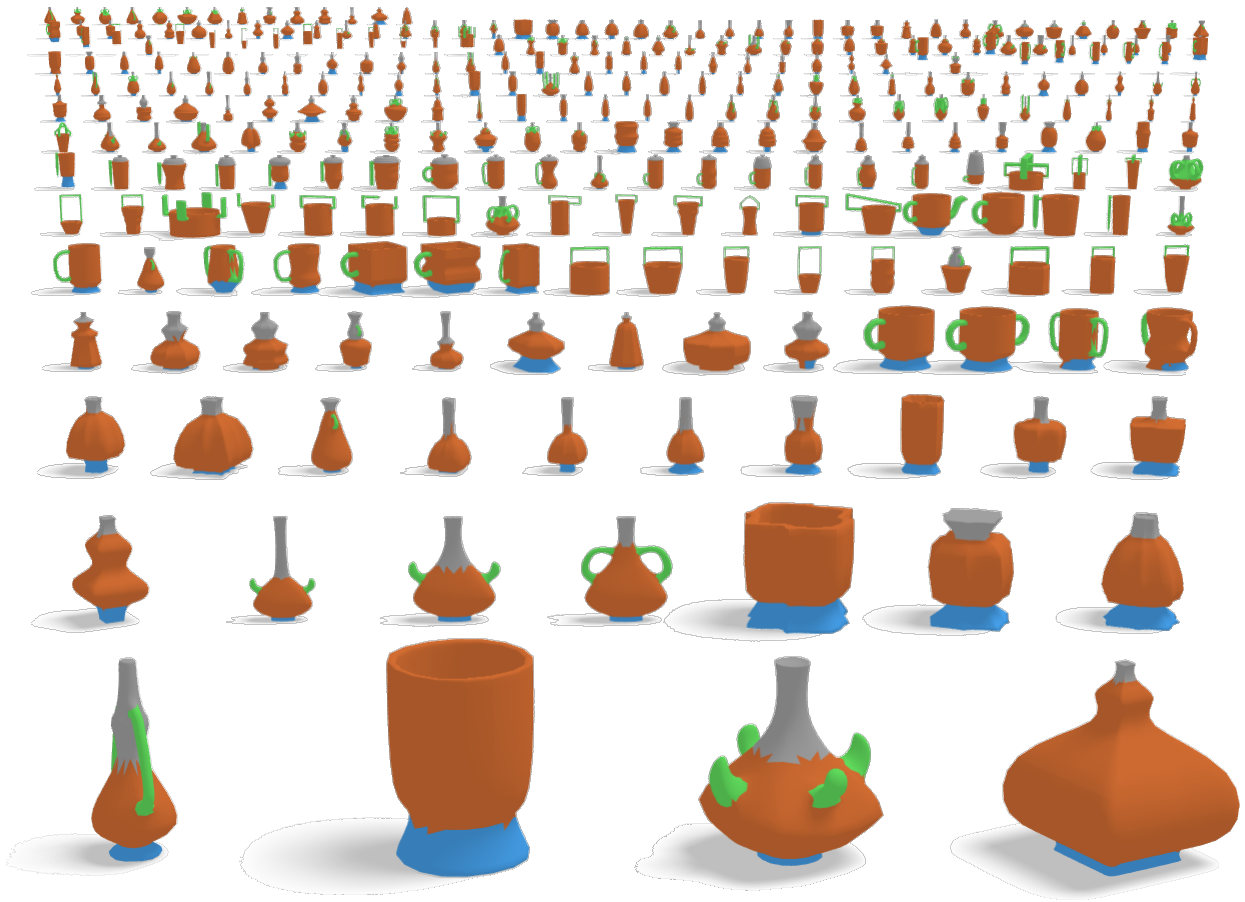
T_ϕ is a linear operator (matrix)

$$T_\phi : L^2(cat) \rightarrow L^2(lion)$$

Networks Between Data



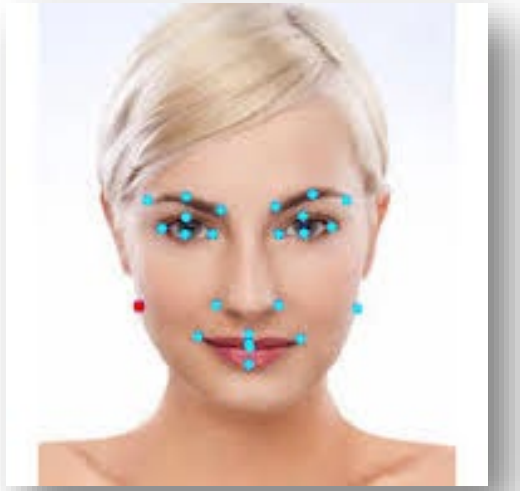
Joint Analysis: Co-Segmentation

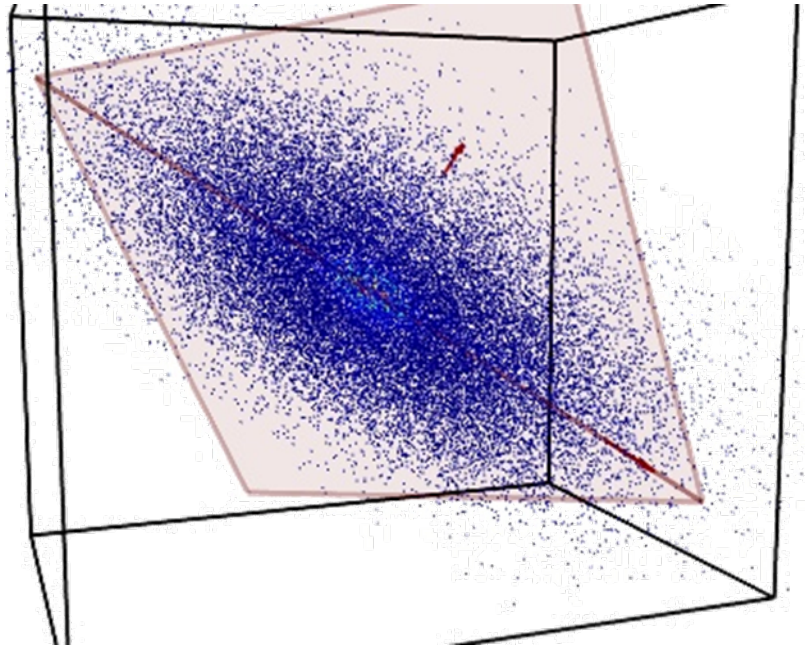


Data as Points in a Euclidean Space

Embedding Data into a Euclidean Space

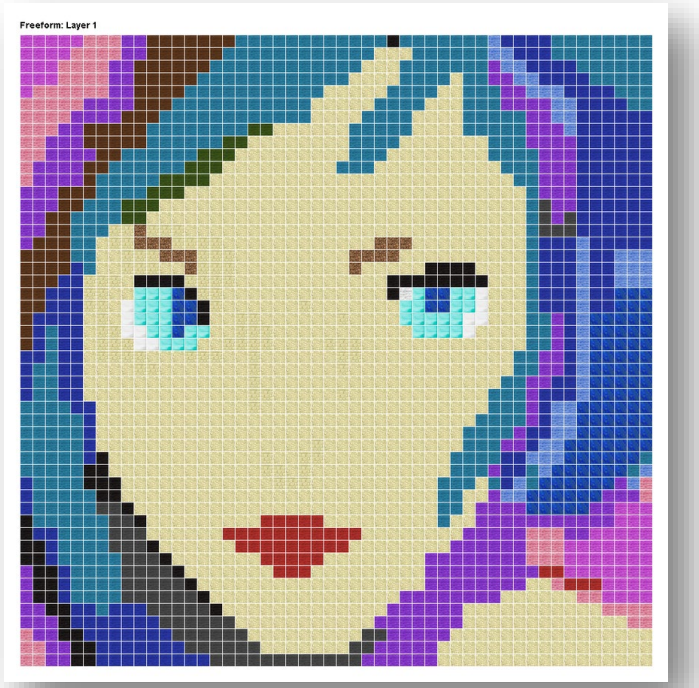
- Attributes or features can be used to map data to a Euclidean space



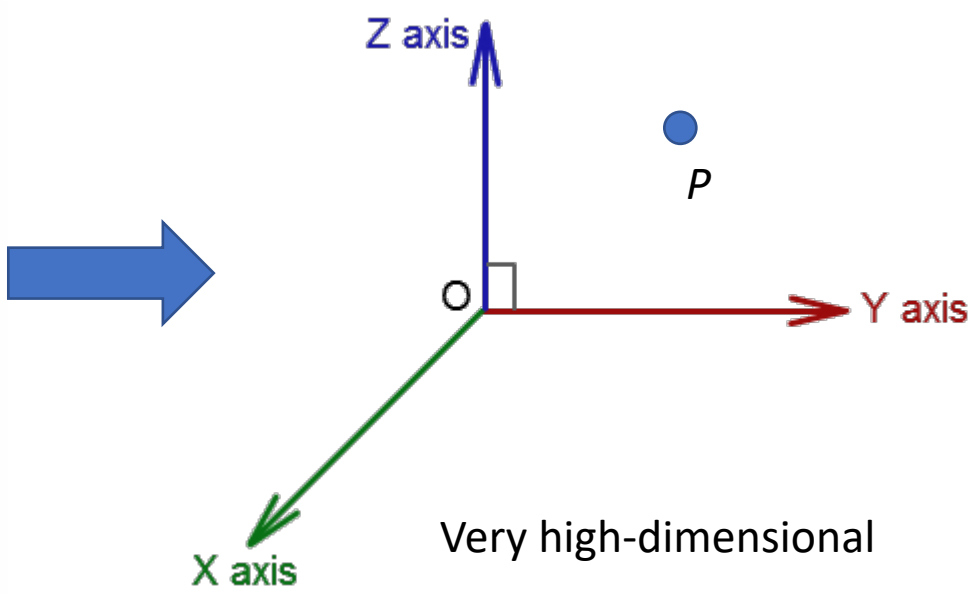


Direct Embeddings

- Input



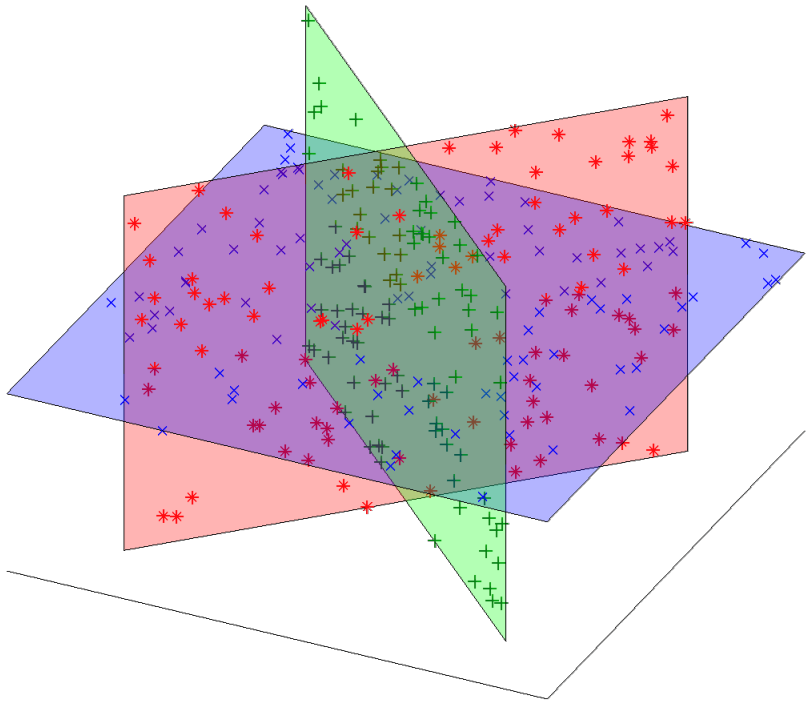
- Latent code



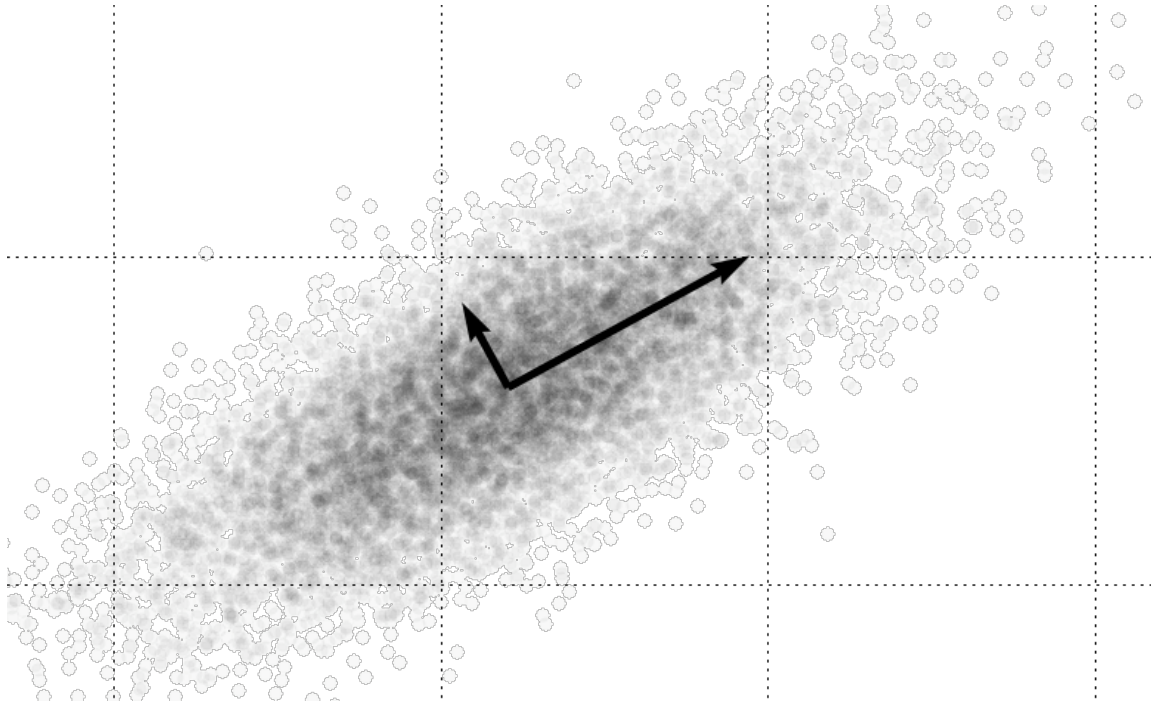
Very high-dimensional

Data as Points in a Euclidean Space

- Given a collection of objects w. many scalar “attributes” – we consider the attributes as dimensions, and therefore of the objects as points in a high dimensional Euclidean space.
- However, lower-dimensional structure is often present in the data.
- Sometimes this lower-d structure corresponds to linear subspaces within the original space.

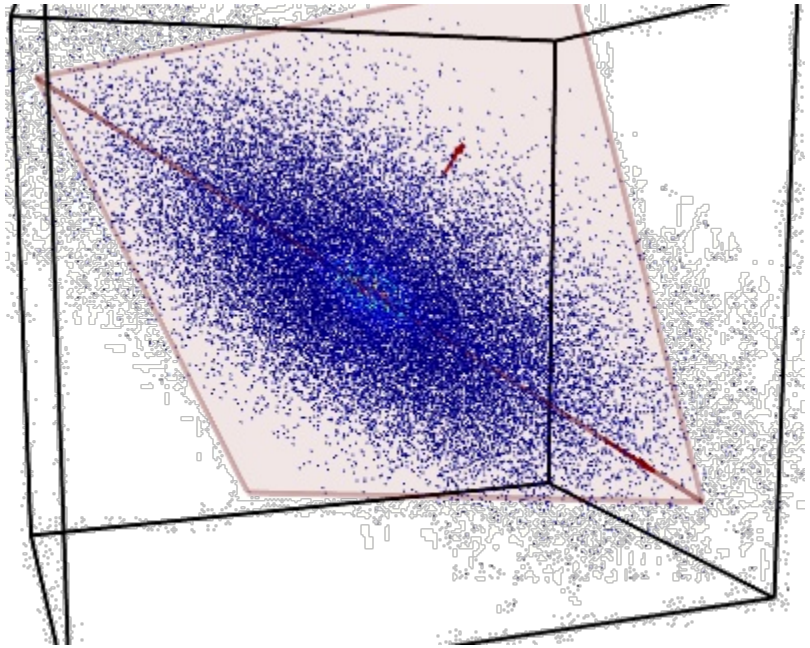


The Linear Space View of Data: Principal Components Analysis (PCA)



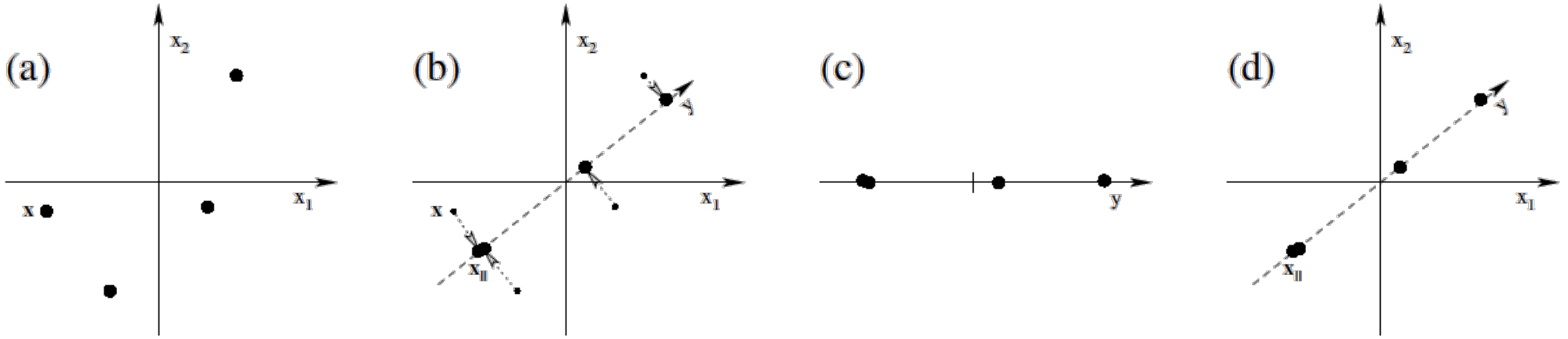
Principal Components Analysis (PCA)

- Introduced by Pearson (1901) and Hotelling (1933) to describe the variation in a set of multivariate data in terms of a set of uncorrelated variables.
- PCA looks for a single lower dimensional linear subspace that captures most of the variation in the data.
- Specifically, PCA aims to minimize the error introduced by projecting the data into this linear subspace.



Projection and Reconstruction Error

- In practice we often assume zero mean for the data (mean is at the origin, ``centered data'').
- a consequence $\rightarrow$ 2nd moment = variance
- Simple 2D to 1D example



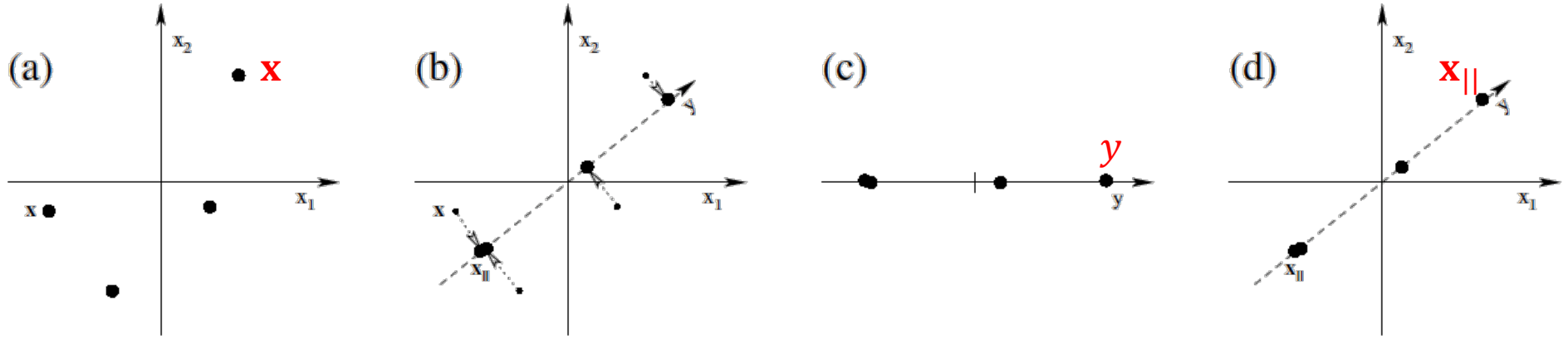
data points in 2D | projection onto 1D | data points in 1D | reconstruction in 2D

Projection and Reconstruction Error

2x1

$\mathbf{x} = (x_1, x_2)^T$ a point; $\mathbf{v}$ a unit vector normal to projection space

$y := \mathbf{v}^T \mathbf{x}$; $\mathbf{x}_{||} := \mathbf{v}\, y$; therefore $\mathbf{x}_{||} := \mathbf{v}\mathbf{v}^T \mathbf{x}$;



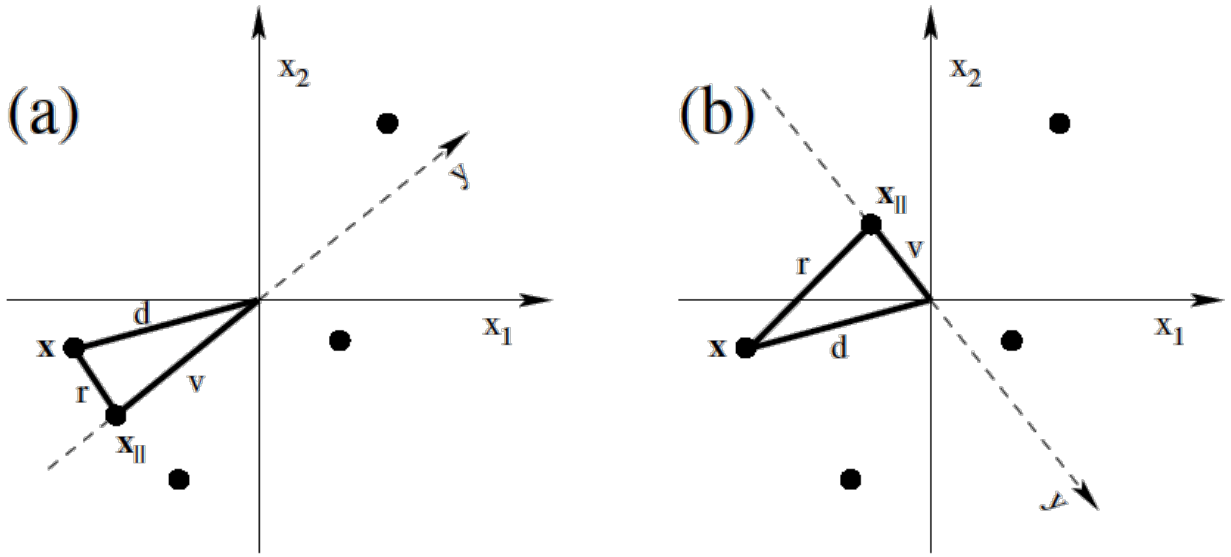
data points in 2D | projection onto 1D | data points in 1D | reconstruction in 2D

Error $E := \left\langle \left\| x^\mu - x_{||}^\mu \right\|^2 \right\rangle_\mu = \frac{1}{M} \sum_{\mu=1}^{M} \sum_{i=1}^{I} (x_i^\mu - x_{||i}^\mu)^2$

M points, *I* dimensions

Reconstruction Error and Variance

- Minimizing the reconstruction error is equivalent to maximizing the variance of the projected data.



- Remember the mean is 0

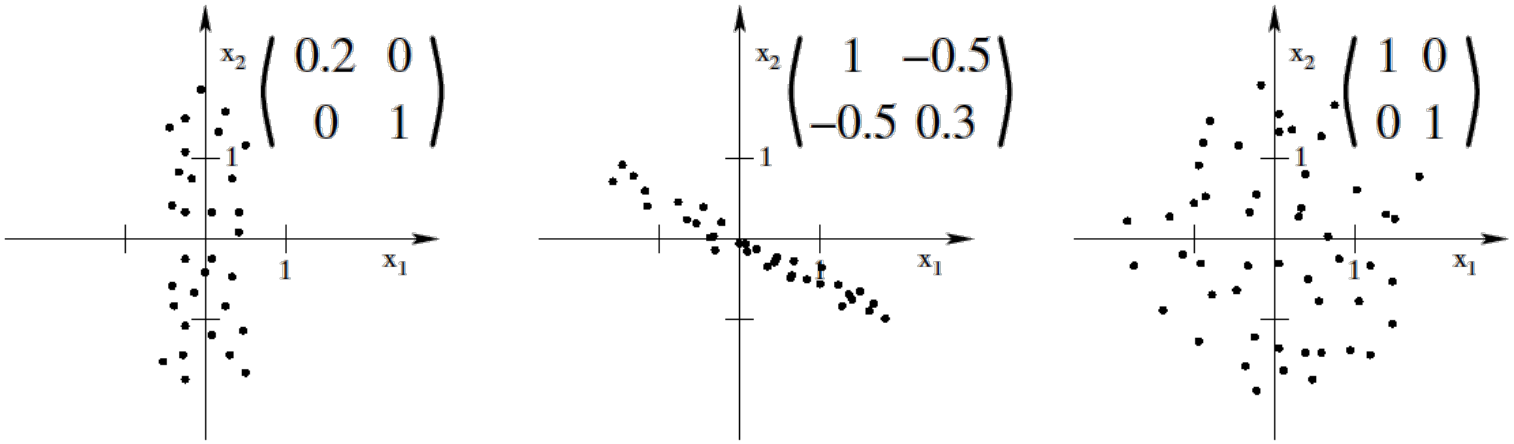
$$r^2 + v^2 = d^2$$

NB, projections of centered data are centered

Covariance Matrix

<> indicate inner products

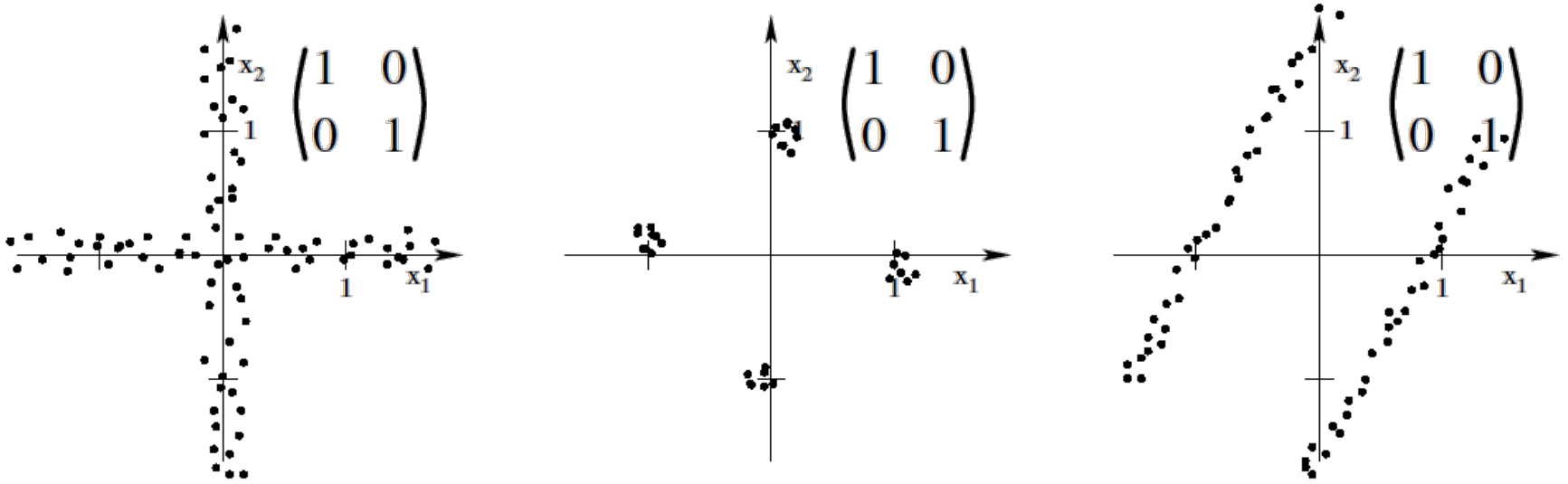
- $\mathbf{x} = (x_1, x_2)^T$, covariance $C_{12} = \langle x_1 x_2 \rangle$ [Remember: centered data]
- (Co-)variances of the 1st and 2nd components: $C_{11} = \langle x_1 x_1 \rangle$, $C_{22} = \langle x_2 x_2 \rangle$



- 2x2 covariance matrix with entries $C_{ij} = C_{ji} \coloneqq \langle x_i x_j \rangle$
- $\mathbf{C} = \begin{pmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{pmatrix}$

Covariance is Not the Full Story

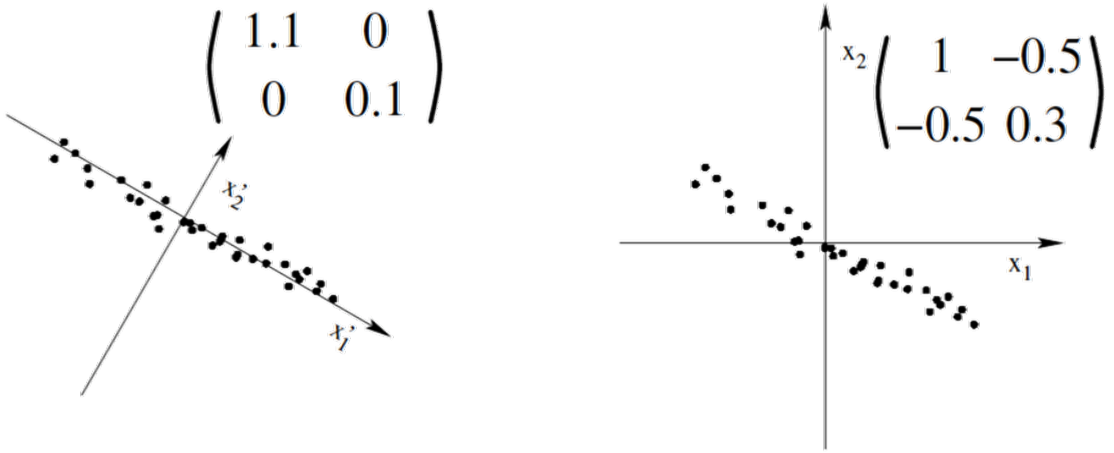
- The covariance matrix tells us about the 2nd order moments, but not about the higher-order structure of the data.



- When it comes to 1st and 2nd order moments, might as well assume a normal distribution, if all we know is the covariance matrix.

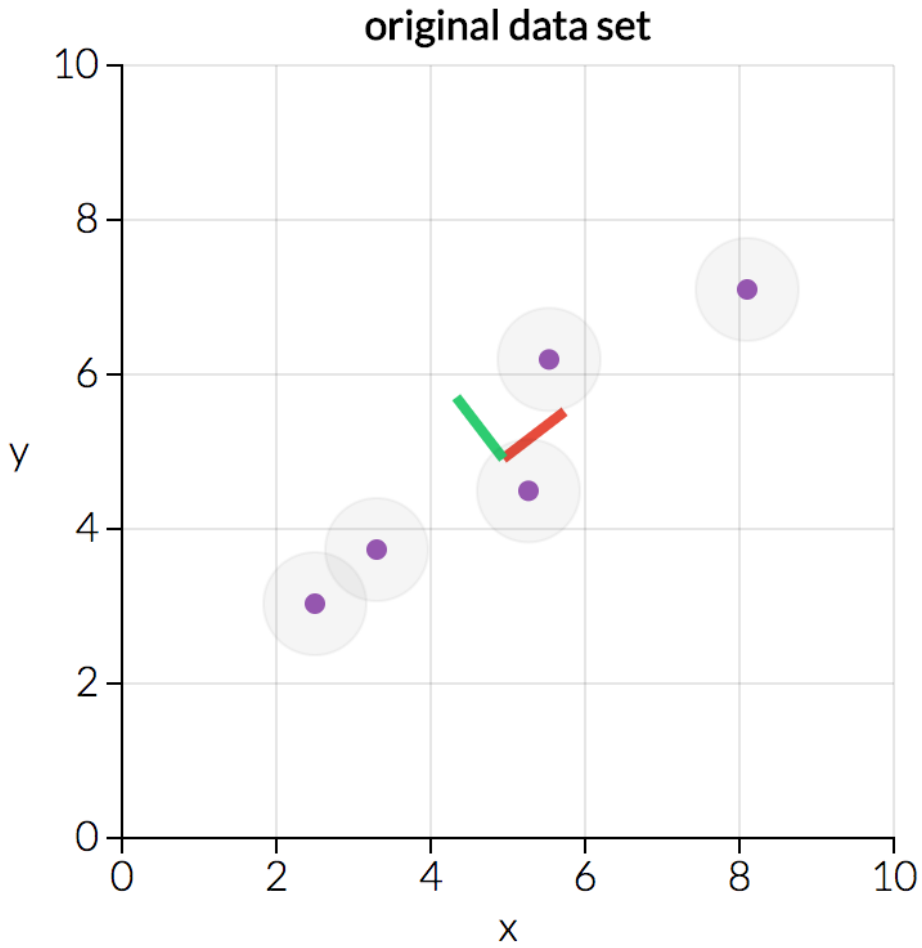
PCA by Diagonalizing the Covariance Matrix

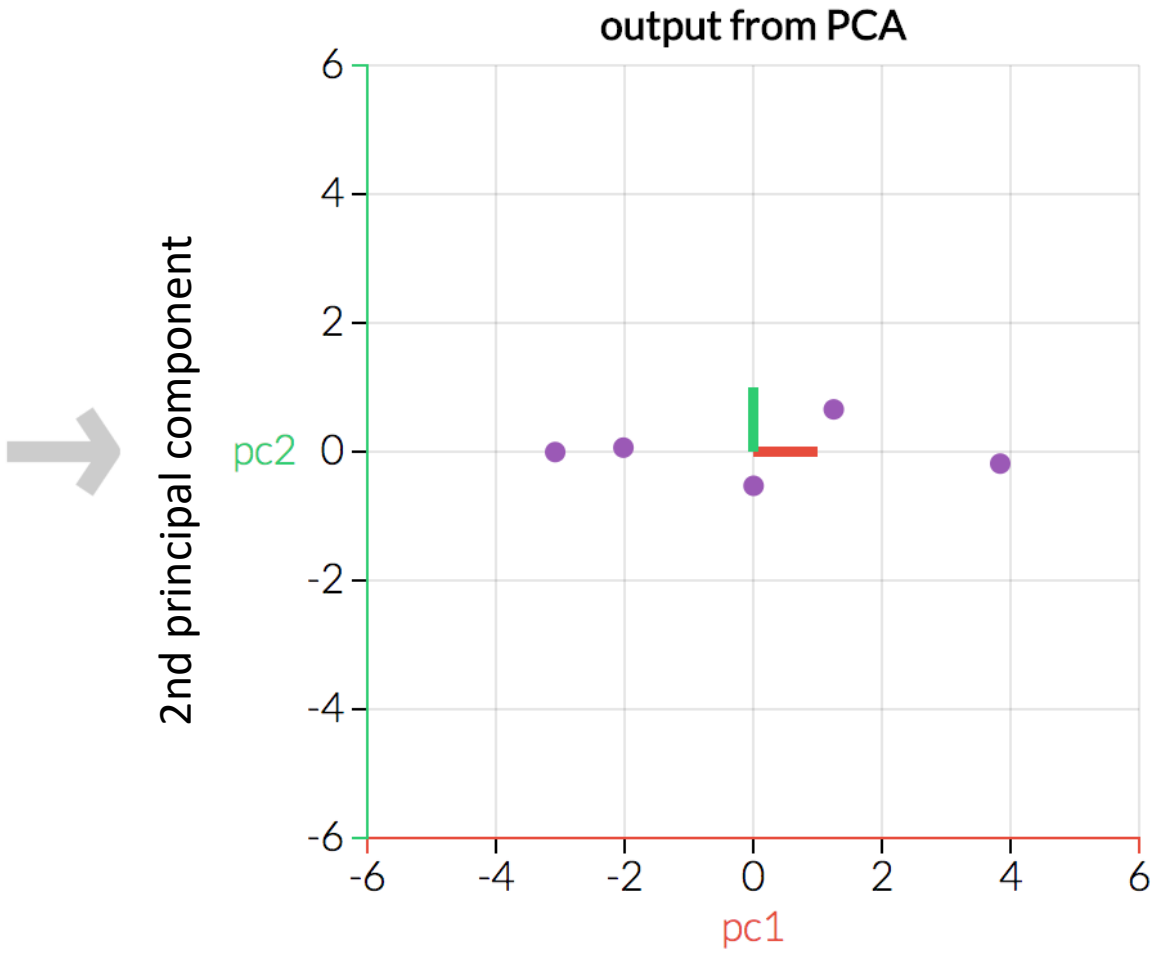
- Finding the direction of maximum variance is easy if the covariance matrix is diagonal.



- So, in general, we want to rotate the coordinate system so as to make the covariance matrix diagonal.
- This is an eigenvalue problem; the eigenvectors of the covariance matrix point in the directions of maximal and minimal variance – so we rotate the axes to align them with the directions of maximal and minimal variance.

Align Data with Variation Axes





1st principal component

Beyond 2D:
The General Case

The General PCA Problem

Principal Component Analysis (PCA): Given a set $\{\mathbf{x}^\mu : \mu = 1, ..., M\}$ **of** I**-dimensional data points** $\mathbf{x}^\mu = (x_1^\mu, x_2^\mu, ..., x_I^\mu)^T$ **with zero mean,** $\langle \mathbf{x}^\mu \rangle_\mu = \mathbf{0}_I$**, find an orthogonal matrix** $\mathbf{U}$ **with determinant** $|\mathbf{U}| = +1$ **generating the transformed data points** $\mathbf{x}'^\mu := \mathbf{U}^T\mathbf{x}^\mu$ **such that for any given dimensionality** P **the data projected onto the first** P **axes,** $\mathbf{x}'^\mu_{||} := (x'^\mu_1, x'^\mu_2, ..., x'^\mu_P, 0, ..., 0)^T$**, have the smallest**

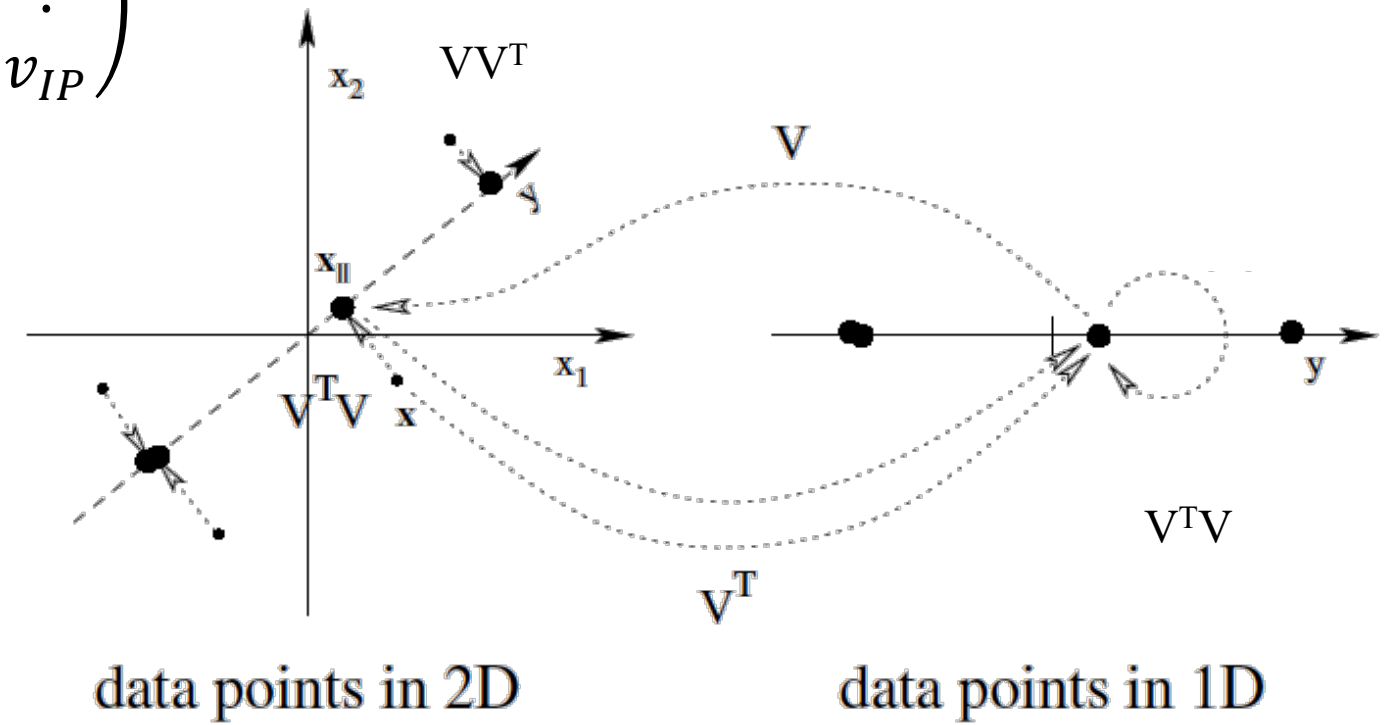
$$\text{reconstruction error} \quad E := \langle \|\mathbf{x}'^\mu - \mathbf{x}'^\mu_{||}\|^2 \rangle_\mu \tag{8}$$

among all possible projections onto a P**-dimensional subspace. The row vectors of matrix** $\mathbf{U}$ **define the new axes and are called the *principal components*.**

High-D to Low-D Projection: The Projection Matrix $\mathbf{V}^T$

- Within the large *I*-dimensional space lies a *P*-dimensional subspace spanned by *P* orthonormal vectors $\mathbf{v}_p$ ($P < I$).
- $\mathbf{v}_p^T \mathbf{v}_q = \delta_{pq} = \{1 \text{ if } p = q,\ 0 \text{ otherwise}$
- $\mathbf{V} = (\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_P) = \begin{pmatrix} v_{11} & \cdots & v_{1P} \\ \vdots & \ddots & \vdots \\ v_{I1} & \cdots & v_{IP} \end{pmatrix}$
- $\mathbf{y} = \mathbf{V}^T \mathbf{x}$

Projection, and a
new coordinate system



Low-D Inside High-D: $\mathbf{V}$

- What does $\mathbf{V}^T\mathbf{V}$ do?
- Recall $\mathbf{V} = (\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_P) = \begin{pmatrix} v_{11} & \cdots & v_{1P} \\ \vdots & \ddots & \vdots \\ v_{I1} & \cdots & v_{IP} \end{pmatrix}$
  - $\mathbf{v}_p^T\mathbf{v}_q = \delta_{pq}$
- $\boldsymbol{V^TV = I}$, simply the *p*-dimensional identity matrix

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- What does $\mathbf{V}\mathbf{V}^T$ do?
- Projection $\mathbf{x}_{||} = \mathbf{V}\mathbf{y} = \mathbf{V}\mathbf{V}^T\mathbf{x}$
- These are the original points projected in the low dimensional space (now sitting inside the high dimensional space).

The Projection Operator $\mathbf{V}\mathbf{V}^T$

- This simply projects the points of the big *I*-dimensional space onto the small *P*-dimensional space, living inside the big *I*-dimensional space

- $\mathbf{P} = \mathbf{V}\mathbf{V}^T = \sum_{p=1}^{P} \mathbf{v}_p \mathbf{v}_p{}^T$; $\mathbf{P}\mathbf{P} = (\mathbf{V}\mathbf{V}^T)(\mathbf{V}\mathbf{V}^T) = \mathbf{V}(\mathbf{V}^T\mathbf{V})\mathbf{V}^T = \mathbf{V}\mathbf{V}^T$.
- $\mathbf{P}$ is an *I*x*I* matrix
- If $P = I$, then in fact $\mathbf{P}$ is the identity matrix
- But in general $P = \sum_{p=1}^{P} \mathbf{v}_p \mathbf{v}_p{}^T$ loses information, since $P < I$

Variance and Reconstruction Error

- For a zero mean vector variance is the 2nd moment
  - $\mathrm{Var}(x) \coloneqq \sum_{i=1}^{I} \langle x_i^2 \rangle = \langle \sum_{i=1}^{I} x_i^2 \rangle = \langle \mathbf{x}^T \mathbf{x} \rangle$.

- Reconstruction error
  - Look at $\mathbf{x} - \mathbf{x}_{||}$
  - $E = \left\langle \left(\mathbf{x} - \mathbf{x}_{||}\right)^T \left(\mathbf{x} - \mathbf{x}_{||}\right) \right\rangle = \langle (\mathbf{x} - \mathbf{V}\mathbf{V}^T\mathbf{x})^T (\mathbf{x} - \mathbf{V}\mathbf{V}^T\mathbf{x}) \rangle$
  - $= \langle \mathbf{x}^T\mathbf{x} - 2\mathbf{x}^T\mathbf{V}\mathbf{V}^T\mathbf{x} + \mathbf{x}^T\mathbf{V}(\mathbf{V}^T\mathbf{V})\mathbf{V}^T\mathbf{x} \rangle$
  - $= \langle \mathbf{x}^T\mathbf{x} \rangle - \langle \mathbf{x}^T\mathbf{V}\mathbf{V}^T\mathbf{x} \rangle = \langle \mathbf{x}^T\mathbf{x} \rangle - \langle (\mathbf{V}^T\mathbf{x})^T\mathbf{V}^T\mathbf{x} \rangle$
  - $= \langle \mathbf{x}^T\mathbf{x} \rangle - \langle \mathbf{y}_{||}^T\mathbf{y}_{||} \rangle$
  - Therefore maximizing the variance of the projected data minimizes the reconstruction error.

Eigenvalues of the Covariance Matrix

- The covariance matrix $\mathbf{C}_x$
  - $\mathbf{C}_x \coloneqq \langle \mathbf{x}^T \mathbf{x} \rangle = \frac{1}{M} \sum_\mu \mathbf{x}^\mu \mathbf{x}^{\mu T}$
- Since the covariance matrix is symmetric, it always has real eigenvalues and orthogonal eigenvectors
  - $\mathbf{C}_x \mathbf{u}_i = \mathbf{u}_i \lambda_i$
  - $\lambda_i \geq \lambda_{i+1}$
  - $\mathbf{u}_i \mathbf{u}_j = \delta_{ij}$
- Now form
  - $\mathbf{U} \coloneqq (\mathbf{u}_1, \mathbf{u}_2, \ldots \mathbf{u}_I)$ – the eigenvectors of the covariance matrix
  - $\mathbf{\Lambda} \coloneqq diag(\lambda_1, \lambda_2, \ldots \lambda_I)$ – the eigenvalues of the covariance matrix

Some Useful Facts

- $\mathbf{U}^T\mathbf{U} = 1_I$
- $\mathbf{U}\mathbf{U}^T = 1_I$
- $\mathbf{C}_x\mathbf{U} = \mathbf{U}\boldsymbol{\Lambda}$
- $\mathbf{U}^T\mathbf{C}_x\mathbf{U} = \boldsymbol{\Lambda}$
- $\mathbf{C}_x = \mathbf{U}\boldsymbol{\Lambda}\mathbf{U}^T$

- The total variance of $\mathbf{x}$
  - $\langle \mathbf{x}^T\mathbf{x} \rangle = \langle \mathrm{tr}(\mathbf{x}^T\mathbf{x}) \rangle = \mathrm{tr}(\langle \mathbf{x}\mathbf{x}^T \rangle) = \mathrm{tr}(\mathbf{C}_x) = \mathrm{tr}(\mathbf{U}\mathbf{U}^T\mathbf{C}_x) = \mathrm{tr}(\mathbf{U}^T\mathbf{C}_x\mathbf{U}) = \mathrm{tr}(\boldsymbol{\Lambda}) = \sum_i \lambda_i$
  - Thus the total variance of the data is just the sum of the eigenvalues of the covariance matrix

Diagonalizing the Covariance Matrix

- Now we use orthogonal matrix **U** to transform the data so that the covariance matrix becomes diagonal

$$
\begin{aligned}
\bullet \quad \mathbf{x}' &:= \mathbf{U}^T\mathbf{x} \\
\bullet|\circ \quad \mathbf{C}'_x &:= \left\langle \mathbf{x}'\mathbf{x}'^T \right\rangle \\
\circ &\overset{(58)}{=} \left\langle (\mathbf{U}^T\mathbf{x})(\mathbf{U}^T\mathbf{x})^T \right\rangle \\
\circ &= \mathbf{U}^T \left\langle \mathbf{x}\mathbf{x}^T \right\rangle \mathbf{U} \\
\circ &\overset{(39)}{=} \mathbf{U}^T\mathbf{C}_x\mathbf{U}\,, \\
\bullet &\overset{(48)}{=} \mathbf{\Lambda}
\end{aligned}
$$

Variance for a Diagonalized Covariance Matrix

- Is this new coordinate system, which *P*-dimensional subspace minimizes the reconstruction error?
- For any $V' = (v'_1, v'_2, \ldots v'_P)$ formed from *P* orthonormal vectors

$$
\begin{aligned}
&\circ \quad \mathbf{y} \;&:=&\; \mathbf{V}'^T\mathbf{x}' \\
\circ \quad \Longrightarrow \langle \mathbf{y}^T\mathbf{y}\rangle \;&\overset{(64)}{=}\; \langle \mathbf{x}'^T\mathbf{V}'\mathbf{V}'^T\mathbf{x}'\rangle \\
&= \langle \mathrm{tr}(\mathbf{x}'^T\mathbf{V}'\mathbf{V}'^T\mathbf{x}')\rangle \quad (\text{since } s = \mathrm{tr}(s) \text{ for any scalar } s) \\
&= \langle \mathrm{tr}(\mathbf{V}'^T\mathbf{x}'\mathbf{x}'^T\mathbf{V}')\rangle \quad (\text{since } \mathrm{tr}(\mathbf{ABC}) = \mathrm{tr}(\mathbf{BCA}) \text{ if defined}) \\
\circ \quad &\overset{(59)}{=}\; \mathrm{tr}(\mathbf{V}'^T\mathbf{C}'_x\mathbf{V}') \quad (\text{since } \mathrm{tr}(\cdot) \text{ and } \langle\cdot\rangle \text{ commute}) \\
\circ \quad &\overset{(63)}{=}\; \mathrm{tr}(\mathbf{V}'^T\mathbf{\Lambda}\mathbf{V}') \\
\circ \quad &= \sum_i \lambda_i \sum_p (v'_{ip})^2 . \quad (\text{as one can work out on a sheet of paper})
\end{aligned}
$$

Variance Maximization

- To maximize the variance $< \boldsymbol{y}^T \boldsymbol{y} >$ we clearly need to put as much weight as possible on the large eigenvalues
- So the variance is maximized by using V' to project $\boldsymbol{x}'$ onto the first P eigenvectors of the covariance matrix C_x
- It is easy to check that optimal variance is $\sum_{i=1}^{P} \lambda_i$
- and that the reconstruction error is $\sum_{i=P+1}^{I} \lambda_i$

Detail

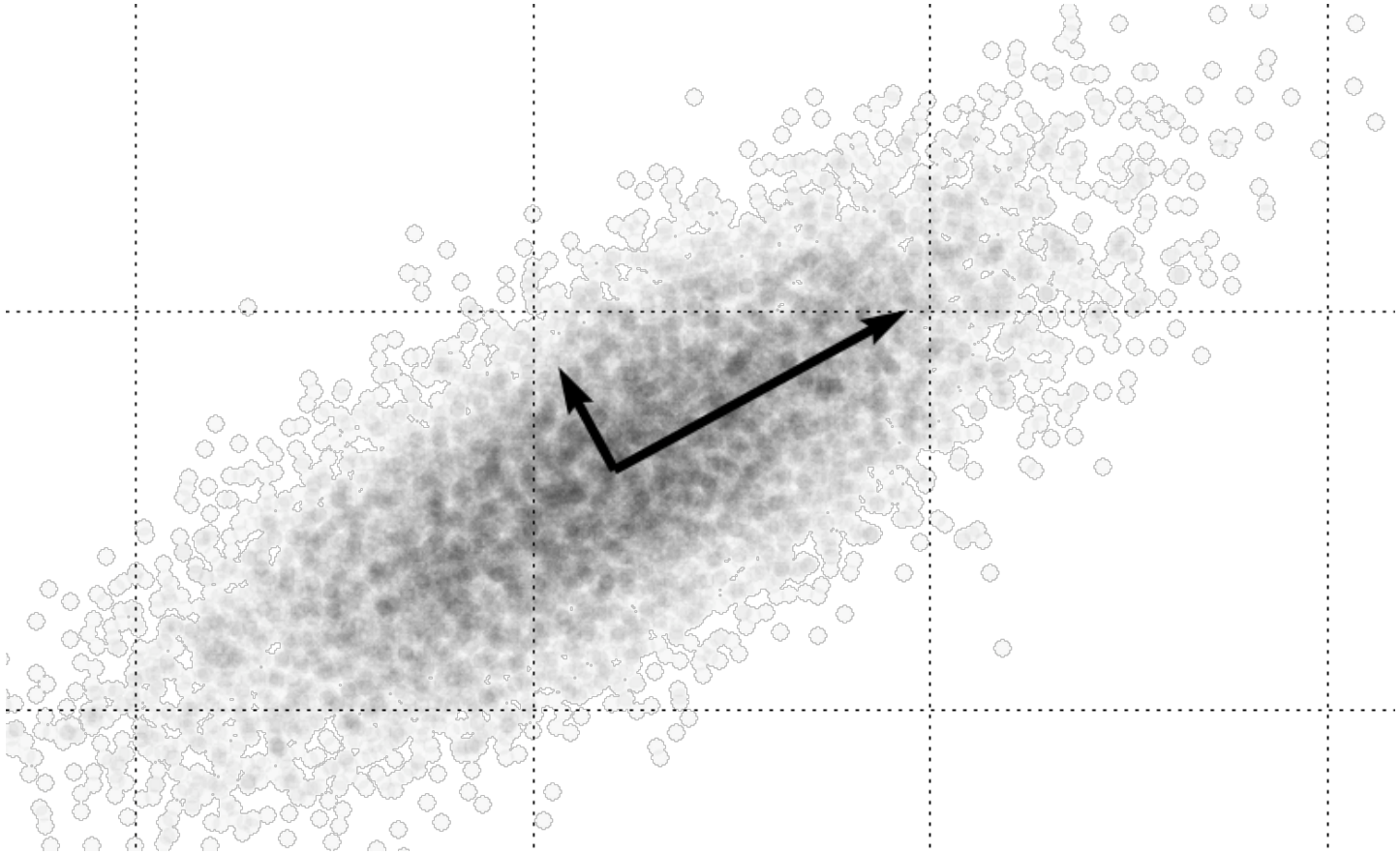
- Constraints on V'
  - $\sum_i (v'_{ip})^2 = 1$ (column vectors of $\mathbf{V}'$ have norm one),
  - $\Longrightarrow \sum_{ip} (v'_{ip})^2 = P$ (square sum over all matrix elements equals P),
  - $\sum_p (v'_{ip})^2 \leq 1$ (row vectors of $\mathbf{V}'$ have norm less or equal one).
- Best choice
  - $v'_{ip} := \delta_{ip} := \begin{cases} 1 & \text{if } i = p \\ 0 & \text{otherwise} \end{cases}$
- Since $P \leq I$

$$\sum_p (v'_{ip})^2 \overset{(74)}{=} \sum_p \delta_{ip}^2 = \left\{ \begin{array}{ll} 1 & \text{if } i \leq P \\ 0 & \text{otherwise} \end{array} \right\} \leq 1,$$

$$\sum_i (v'_{ip})^2 \overset{(74)}{=} \sum_i \delta_{ip}^2 = \delta_{pp}^2 = 1,$$

PCA Final

- For any *P*, the optimal *P*-dimensional subspace is the one spanned by the first *P* eigenvectors of the covariance matrix



PCA Examples

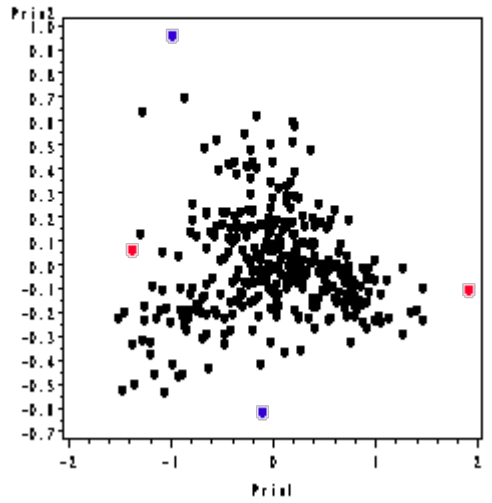
PCA Example 1: Place Ratings

- The “Places Rated Almanac” rates 329 US communities according to the following nine criteria:
  - Climate and Terrain
  - Housing
  - Health Care & the Environment
  - Crime
  - Transportation
  - Education
  - The Arts
  - Recreation
  - Economics

Places Rated

	Principal Component		
Variable	**1**	**2**	**3**
Climate	0.190	0.017	0.207
Housing	**0.544**	0.020	0.204
Health	**0.782**	**-0.605**	0.144
Crime	0.365	0.294	**0.585**
Transportation	**0.585**	0.085	0.234
Education	0.394	-0.273	0.027
Arts	**0.985**	0.126	-0.111
Recreation	**0.520**	0.402	**0.519**
Economy	0.142	0.150	0.239

PCA — Covariance Matrix — Places Rated

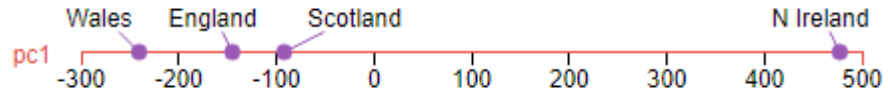


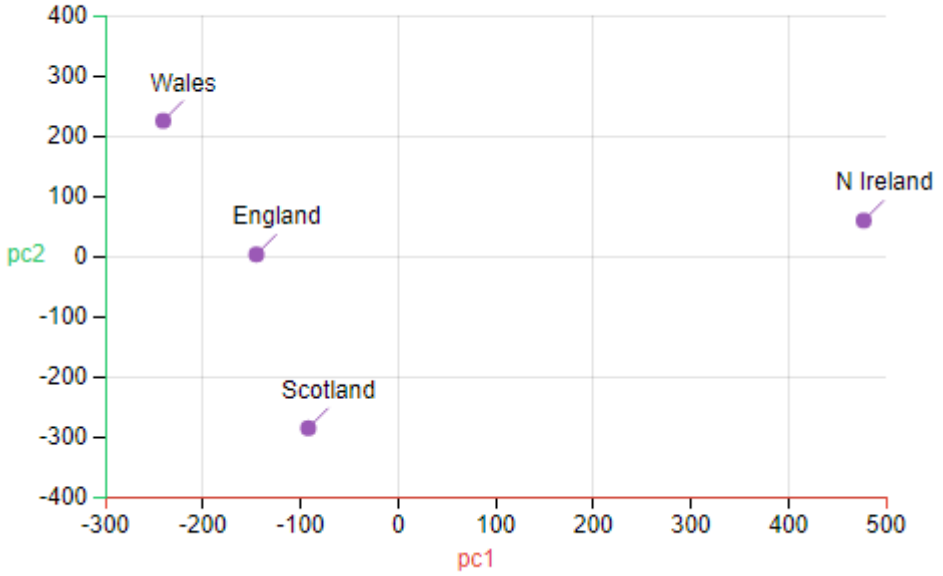
- The first principal component is strongly positively correlated with five of the original variables: Arts, Health, Transportation, Housing and Recreation scores. This suggests that these five criteria vary together. If one increases, then the remaining also increase.
- Furthermore, we see that the first principal component correlates most strongly with the Arts

PCA Ex. 2: Eating in the UK

	England	N Ireland	Scotland	Wales
Alcoholic drinks	375	135	458	475
Beverages	57	47	53	73
Carcase meat	245	267	242	227
Cereals	1472	1494	1462	1582
Cheese	105	66	103	103
Confectionery	54	41	62	64
Fats and oils	193	209	184	235
Fish	147	93	122	160
Fresh fruit	1102	674	957	1137
Fresh potatoes	720	1033	566	874
Fresh Veg	253	143	171	265
Other meat	685	586	750	803
Other Veg	488	355	418	570
Processed potatoes	198	187	220	203
Processed Veg	360	334	337	365
Soft drinks	1374	1506	1572	1256
Sugars	156	139	147	175

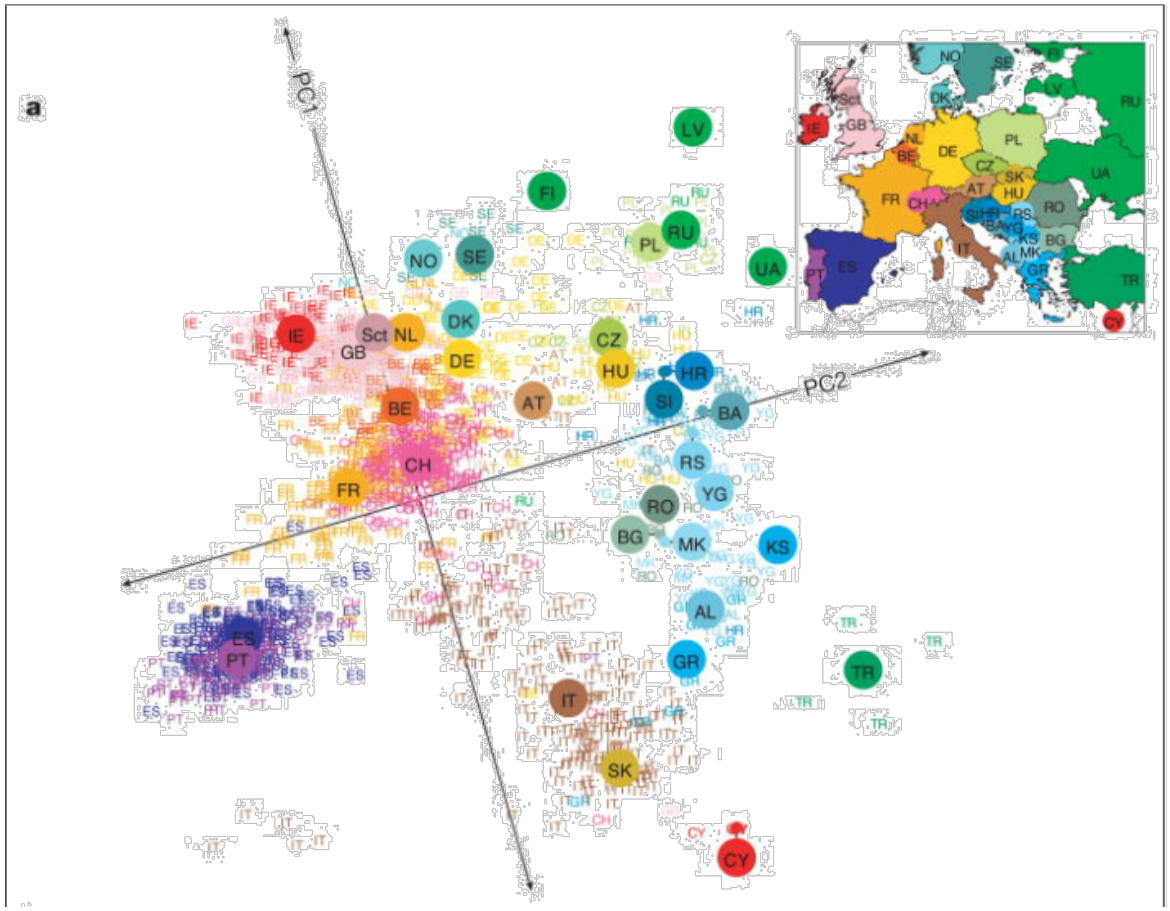
17 food groups





PCA Ex. 3: Genetic vs. Geographic Diversity in Europe

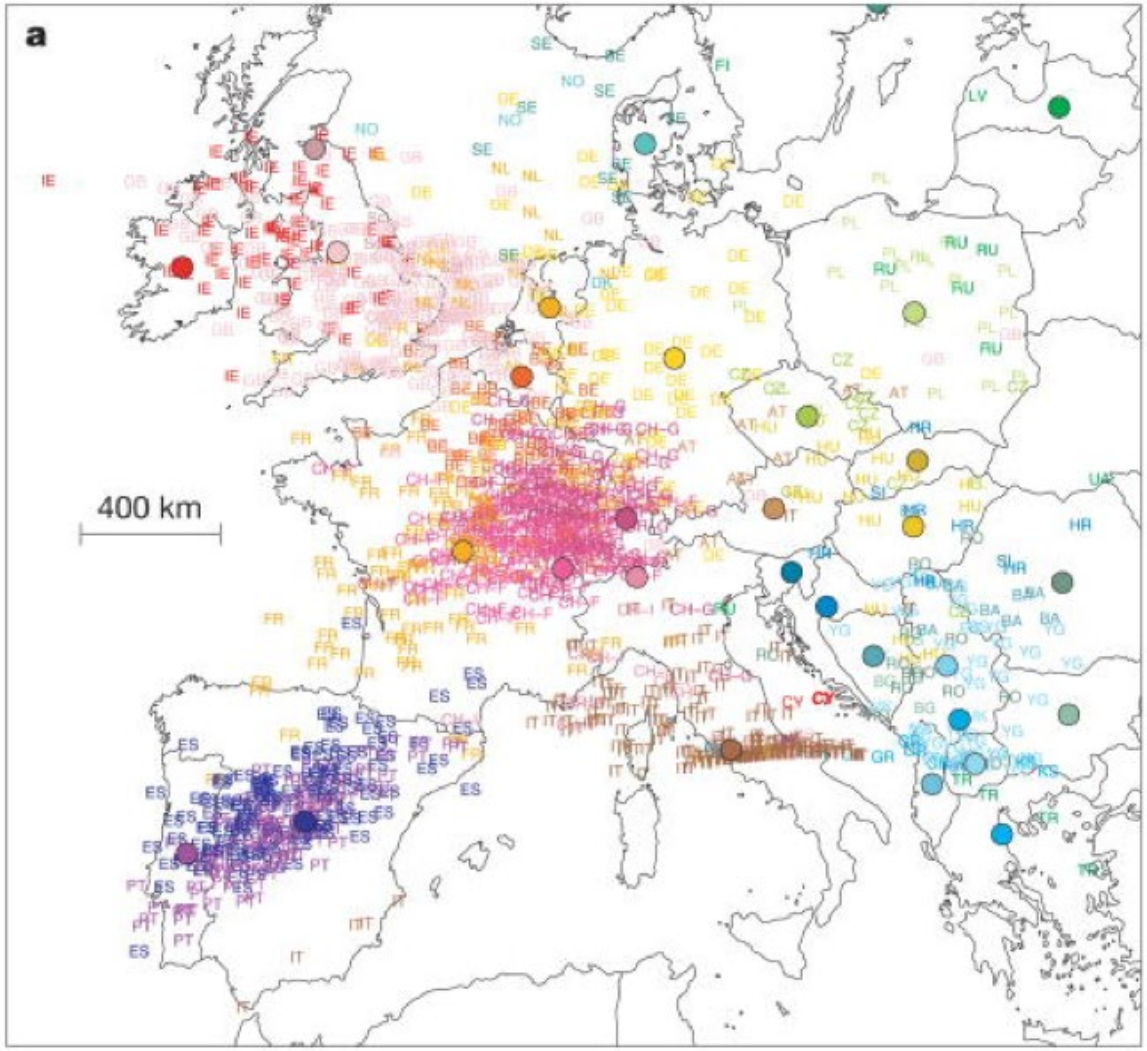
- Geonome of 3,192 individuals studied based on 197,146 SNP* loci via PCA



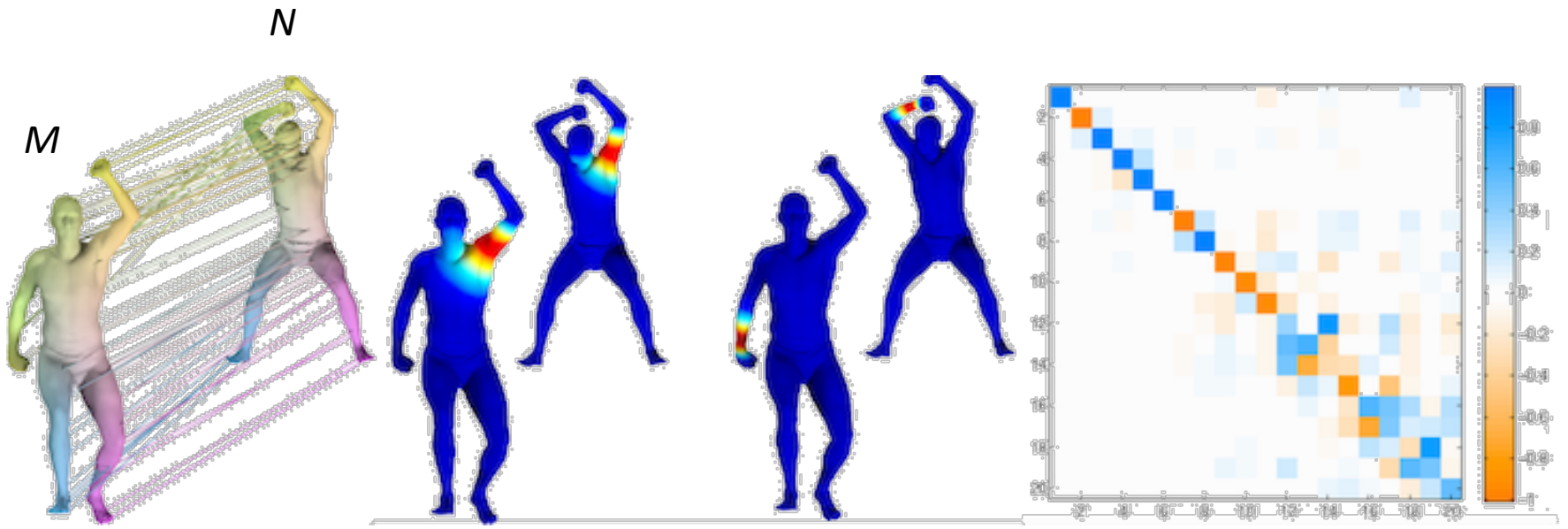
SNP = single nucleotide polymorphism

J Novembre *et al. Nature* **456**, 1-4 (2008) doi:10.1038/nature07331

Close Up



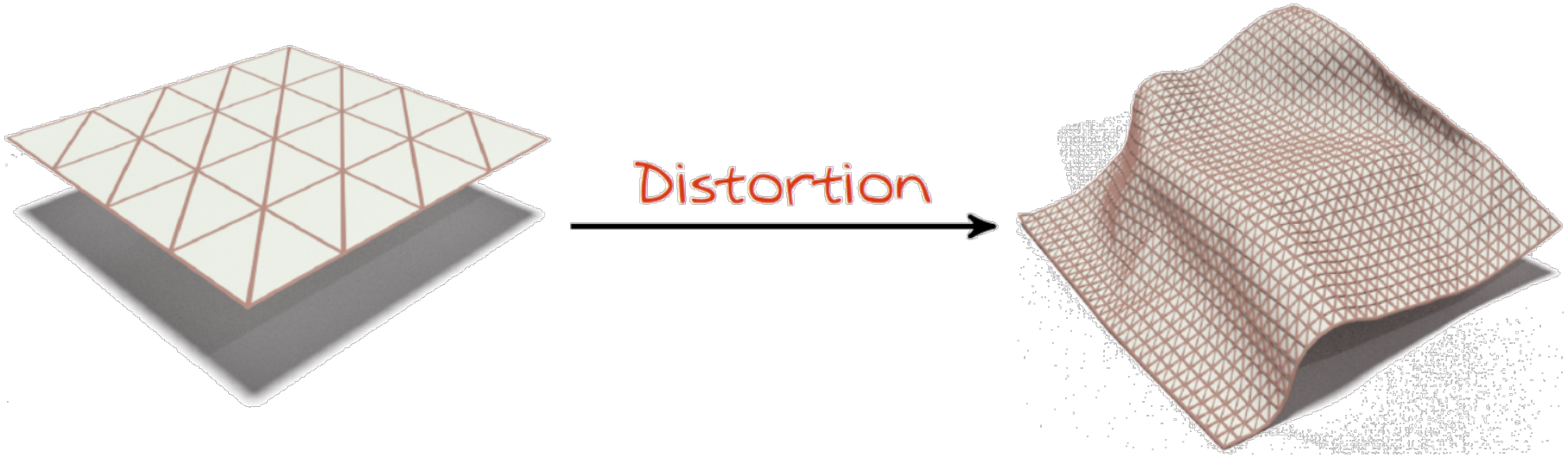
PCA Ex. 4: Shape Analysis via Functional Maps



$T : N \to M$

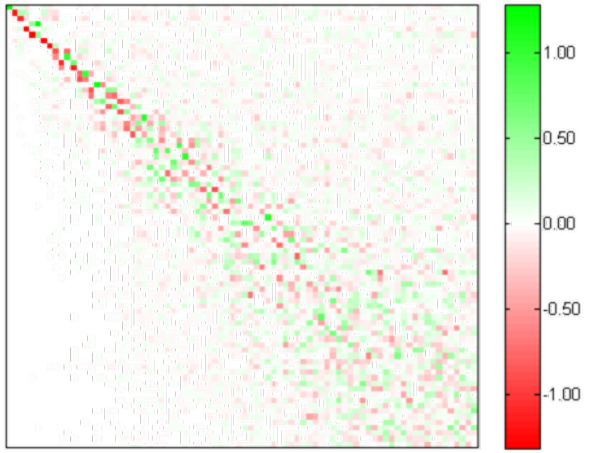
$$C_T : \begin{array}{ccc} L^2(M) & \to & L^2(N) \\ f & \mapsto & f \circ T \end{array}$$

Shape Differences



A recipe encoded as a matrix:

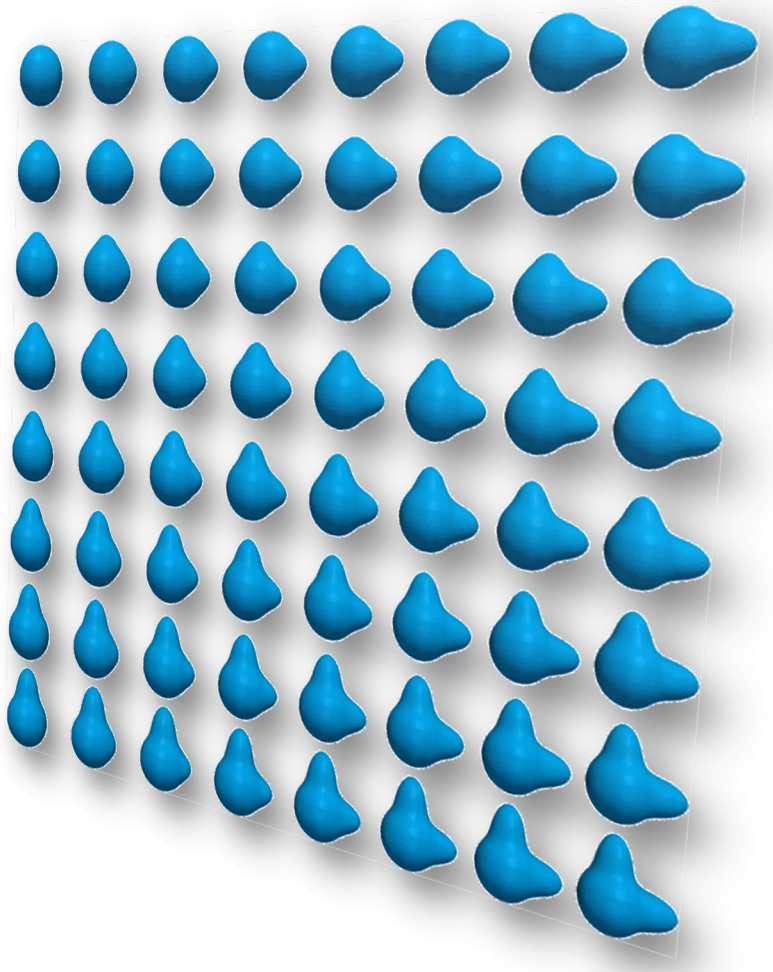
Area distortion
Conformal distortion

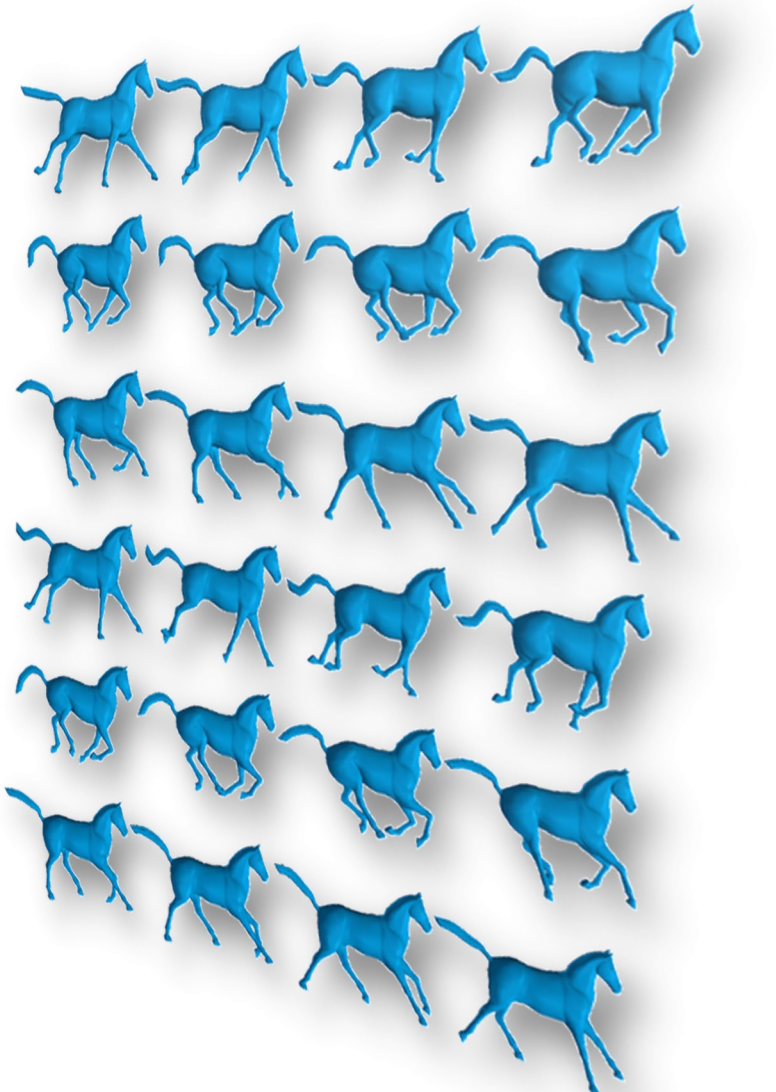


A novel type of latent space representation for 3D data

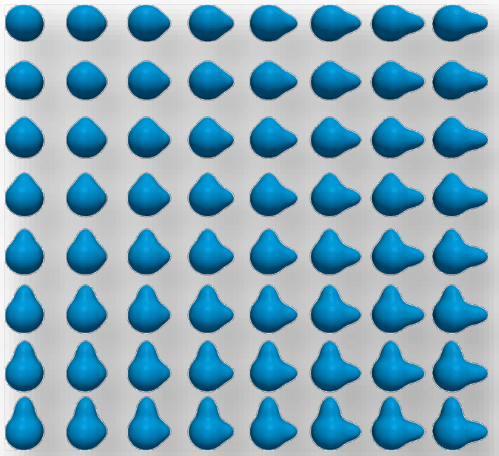
Under some conditions, lossless

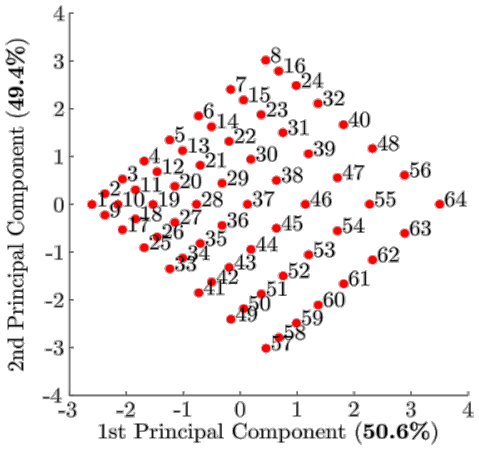
Shape Differences in Collections

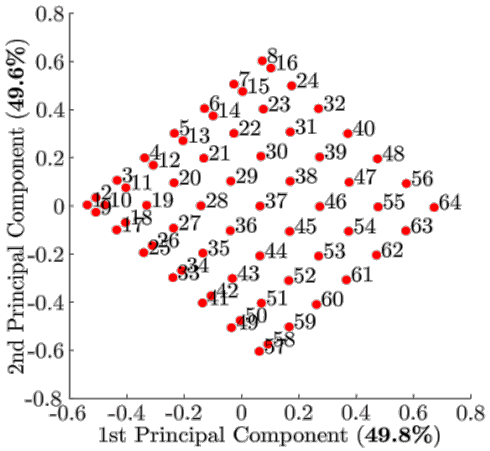


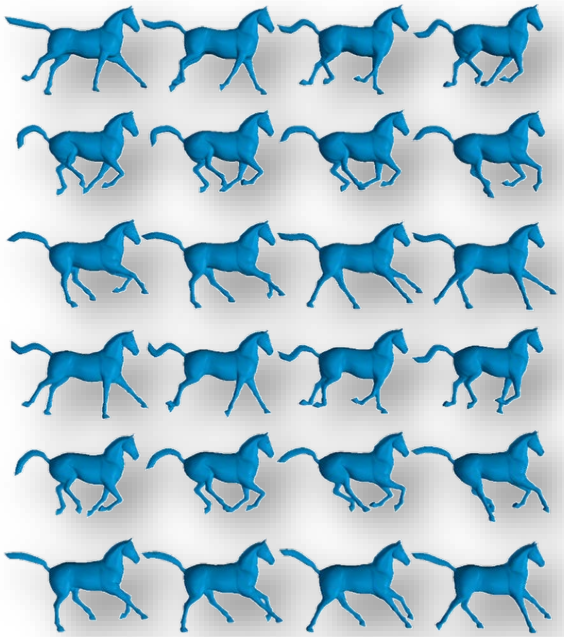


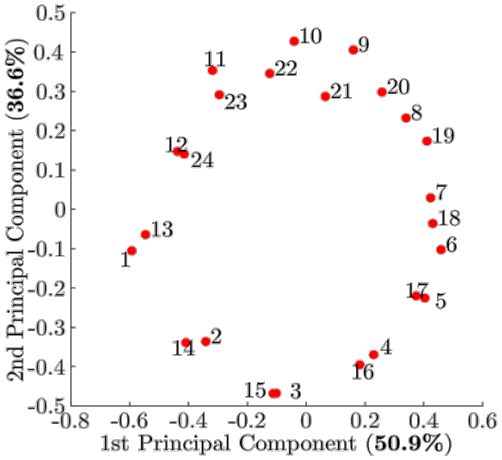
Can Be Used to Analyze Shape Collections

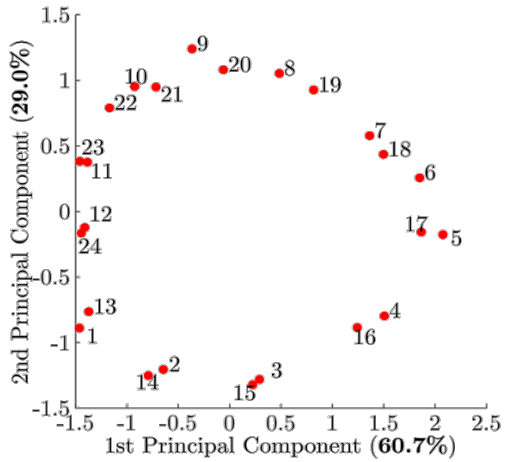












A Tidbit

Sometimes SVD to the Rescue

- What to do when we have fewer data points than dimensions ($M < I$)?

- We have, $\mathbf{X} := (\mathbf{x}^1, ..., \mathbf{x}^M)$, $\mathbf{C}_1 := \mathbf{X}\mathbf{X}^T/M$
- So

$$\begin{aligned} \mathbf{C}_1\mathbf{U}_1 &= \mathbf{U}_1\mathbf{\Lambda}_1 \\ \iff \mathbf{C}_1 &= \mathbf{U}_1\mathbf{\Lambda}_1\mathbf{U}_1^T \end{aligned}$$

- But $\mathbf{Y}_1 := \mathbf{U}_1^T\mathbf{X}$ is still high dimensional, because the eigenvectors are of dim I

Data SVD, II

- So let's transpose $\boldsymbol{X} \rightarrow \boldsymbol{X}^T$
- We get,

$$\begin{aligned} \mathbf{C}_2 &:= \mathbf{X}^T\mathbf{X}/I\,, \\ \mathbf{C}_2\mathbf{U}_2 &= \mathbf{U}_2\mathbf{\Lambda}_2 \\ \iff \mathbf{C}_2 &= \mathbf{U}_2\mathbf{\Lambda}_2\mathbf{U}_2^T\,, \\ \mathbf{Y}_2 &:= \mathbf{U}_2^T\mathbf{X}^T\,. \end{aligned}$$

- Moreover, the rows of $\mathbf{Y}_2$ are eigenvectors of $\mathbf{C}_1$

$$\begin{aligned} \mathbf{C}_1\mathbf{Y}_2^T &\overset{(100,107)}{=} (\mathbf{X}\mathbf{X}^T/M)(\mathbf{X}\mathbf{U}_2) \\ &= \mathbf{X}(\mathbf{X}^T\mathbf{X}/I)\mathbf{U}_2 I/M \\ &\overset{(104)}{=} \mathbf{X}\mathbf{C}_2\mathbf{U}_2 I/M \\ &\overset{(105)}{=} \mathbf{X}\mathbf{U}_2\mathbf{\Lambda}_2 I/M \\ &\overset{(107)}{=} \mathbf{Y}_2^T\mathbf{\Lambda}_2 I/M\,. \end{aligned}$$

- The corresponding eigenvalues are just those of $\mathbf{C}_2$ scaled by I/M.

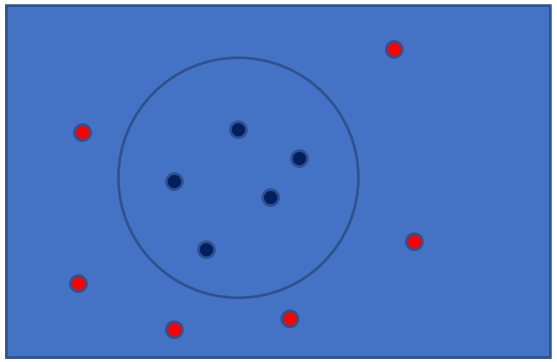
Kernels

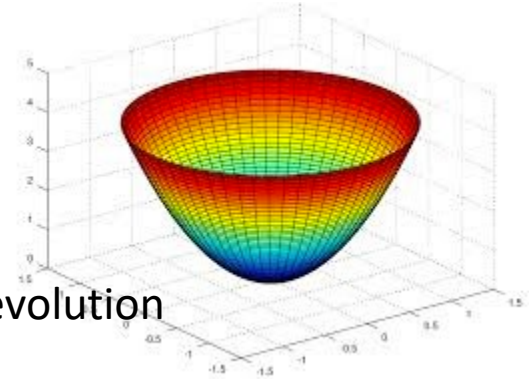
Kernel Methods – Non-Linear Relationships

- "Lifting" maps can linearize non-linear structure

- Example: circular separability in the 2D plane lifts to planar separability in 3D space, via

$$\Phi(x, y) = (x, y, x^2 + y^2)$$





paraboloid of revolution

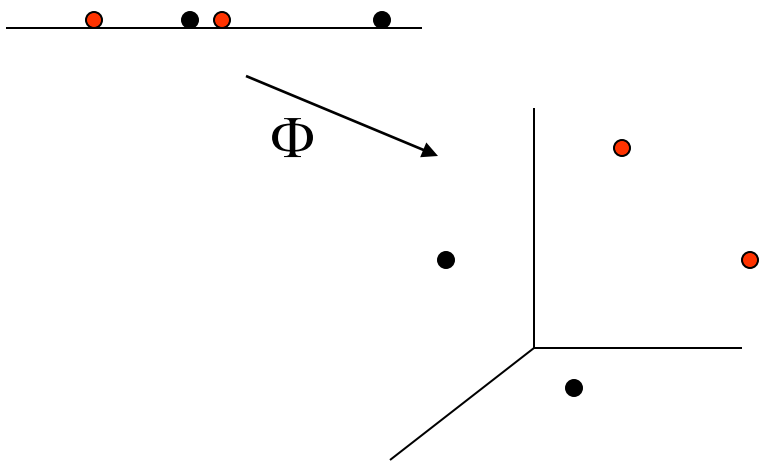
$$(x - a)^2 + (y - b)^2 \leq r^2$$

$$-2ax - 2by + x^2 + y^2 + a^2 + b^2 - r^2 \leq 0$$

Feature Spaces

- Map data to a high-dimensional feature space *F* via a non-linear mapping

$$\Phi : x \rightarrow \Phi(x), \quad R^d \rightarrow F$$



- Ex. $\Phi(x, y) = (x, y, x^2 + y^2)$
- Ex. $\Phi(x, y) = (x^2, y^2, xy)$

The Kernel Trick

- In many applications, we only need inner products (the Gram matrix) between mapped vectors for the solution (e.g., the PCA covariances)
- We do not need to compute $\Phi(x)$ directly!

$$x \rightarrow \Phi(x),$$

$$G_{ij} =< x_i, x_j > \rightarrow G_{ij}^{\Phi} =< \Phi(x_i), \Phi(x_j) >= K(x_i, x_j)$$

kernel

- If we use algorithms that only depend on the Gram-matrix *G*, then we never have to know (compute) the actual features Φ

Modularity

Kernel methods consist of several modules:

1) The lifting map
2) The choice of kernel
3) The algorithm which takes kernels as input

Modularity: Any kernel can be used with any kernel-algorithm.

some kernels:

$$k(x,y) = e^{(-\|x-y\|^2/c)} \qquad \text{RBF}$$

$$k(x,y) = (< x, y > +\theta)^d$$

$$k(x,y) = \tanh(\alpha < x, y > +\theta)$$

$$k(x,y) = \frac{1}{\sqrt{\| x-y \|^2 + c^2}}$$

some kernel algorithms:

- support vector machines
- Fisher discriminant analysis
- kernel regression
- kernel PCA
- kernel CCA

Kernel PCA

Kernel PCA (KPCA)

- Assumption behind PCA is that the data points **x** are well represented by a small-dimensional Euclidean subspace
- Often this assumption does not hold …
- However, it may still be possible that a non-linear transformation $\phi(\mathbf{x})$ "linearizes" the data -- then we can perform PCA in the space of $\phi(\mathbf{x})$
- Kernel PCA performs this "lifted" PCA; however, because of "kernel trick," it never computes the mapping $\phi(\mathbf{x})$ explicitly.

KPCA Basic Idea

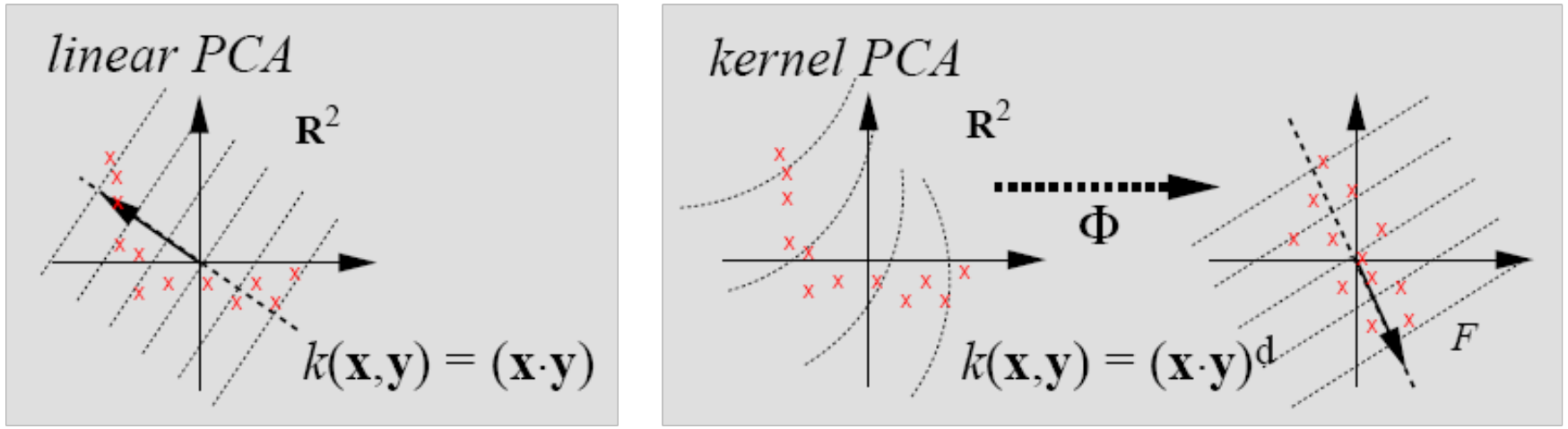


Fig. 1. Basic idea of kernel PCA: by using a nonlinear kernel function k instead of the standard dot product, we implicitly perform PCA in a possibly high–dimensional space F which is nonlinearly related to input space. The dotted lines are contour lines of constant feature value.

Kernel PCA Formulation

- We need the following fact: $C = \frac{1}{N}\sum_{i=1}^{N} \mathbf{x}_i \mathbf{x}_i^T$
- Let **v** be a eigenvector of the covariance matrix: $C = \sum_{i=1}^{N} \mathbf{x}_i \mathbf{x}_i^T$ scatter matrix
- Then **v** belongs to the linear space spanned by the data points $\mathbf{x}_i$ $I = 1, 2, \ldots N$.
- Proof:

$$C\mathbf{v} = \lambda\mathbf{v} \Rightarrow \mathbf{v} = \frac{1}{\lambda}\sum_{i=1}^{N}(\mathbf{x}_i \mathbf{x}_i^T)\mathbf{v} = \frac{1}{\lambda}\sum_{i=1}^{N}\mathbf{x}_i(\mathbf{x}_i^T \mathbf{v}) = \sum_{i=1}^{N}\alpha_i \mathbf{x}_i$$

Kernel PCA Formulation II

- Let *C* be the covariance matrix of the centered (0 mean) mapping $\phi(\mathbf{x})$:

$$C = \sum_{i=1}^{N} \phi(\mathbf{x}_i)\phi(\mathbf{x}_i)^T$$

- Let **w** be an eigenvector of *C*, then **w** can be written as a linear combination:

$$\mathbf{w} = \sum_{k=1}^{N} \alpha_k \phi(\mathbf{x}_k)$$

- Also, we have: $C\mathbf{w} = \lambda\mathbf{w}$

- Combining, we get: $$(\sum_{i=1}^{N} \phi(\mathbf{x}_i)\phi(\mathbf{x}_i)^T)(\sum_{k=1}^{N} \alpha_k \phi(\mathbf{x}_k)) = \lambda \sum_{k=1}^{N} \alpha_k \phi(\mathbf{x}_k)$$

Kernel PCA Formulation III

$$(\sum_{i=1}^{N}\varphi(\mathbf{x}_i)\varphi(\mathbf{x}_i)^T)(\sum_{k=1}^{N}\alpha_k\varphi(\mathbf{x}_k)) = \lambda\sum_{k=1}^{N}\alpha_k\varphi(\mathbf{x}_k) \Rightarrow$$

$$\sum_{i=1}^{N}\sum_{k=1}^{N}\varphi(\mathbf{x}_i)\varphi(\mathbf{x}_i)^T\varphi(\mathbf{x}_k)\alpha_k = \lambda\sum_{k=1}^{N}\alpha_k\varphi(\mathbf{x}_k) \Rightarrow$$

multiply by $\phi(x_l)^T$

$$\sum_{i=1}^{N}\sum_{k=1}^{N}\varphi(\mathbf{x}_l)^T\varphi(\mathbf{x}_i)\varphi(\mathbf{x}_i)^T\varphi(\mathbf{x}_k)\alpha_k = \lambda\sum_{k=1}^{N}\alpha_k\varphi(\mathbf{x}_l)^T\varphi(\mathbf{x}_k),\ l = 1,2,\ldots,N \Rightarrow$$

$$K^2\boldsymbol{\alpha} = \lambda K\boldsymbol{\alpha} \Rightarrow$$

$$K\boldsymbol{\alpha} = \lambda\boldsymbol{\alpha},\ \text{where}\ K_{ij} = \varphi(\mathbf{x}_i)^T\varphi(\mathbf{x}_j).$$

Kernel or Gram matrix

Kernel PCA Formulation IV

From the eigen equation $K\boldsymbol{\alpha} = \lambda\boldsymbol{\alpha}$

And the fact that the eigenvector **w** is normalized to 1, we obtain:

$$\| \mathbf{w} \|^2 = (\sum_{i=1}^{N} \alpha_i \phi(\mathbf{x}_i))^T (\sum_{i=1}^{N} \alpha_i \phi(\mathbf{x}_i)) = \boldsymbol{\alpha}^T K \boldsymbol{\alpha} = 1 \Rightarrow$$

$$\boldsymbol{\alpha}^T \boldsymbol{\alpha} = \frac{1}{\lambda}$$

The KPCA Algorithm

Step 1: Compute the Gram matrix: $K_{ij} = k(\mathbf{x}_i, \mathbf{x}_j),\ i, j = 1, \ldots, N$

Step 2: Compute (eigenvector, eigenvalue) pairs of K : $\mathbf{w}^l, \lambda_l$

Step 3: Normalize the eigenvectors: $\tilde{\boldsymbol{\alpha}}^l \leftarrow \frac{\boldsymbol{\alpha}^l}{\lambda_l}$

Thus, an eigenvector $\mathbf{w}^l$ of C is now represented as: $\mathbf{w}^l = \sum_{k=1}^{N} \alpha_k^l \varphi(\mathbf{x}_k)$

To project a test feature $\phi(\mathbf{x})$ onto $\mathbf{w}^l$ we need to compute:

$$\phi(\mathbf{x})^T \mathbf{w}^l = \phi(\mathbf{x})^T \left(\sum_{k=1}^{N} \alpha_k^l \phi(\mathbf{x}_k)\right) = \sum_{k=1}^{N} \alpha_k^l k(\mathbf{x}_k, \mathbf{x})$$

So, we never need ϕ explicitly

Feature Map Centering

So far we assumed that the feature map $\phi(\mathbf{x})$ is centered for the data points $\mathbf{x}_1, \ldots \mathbf{x}_N$

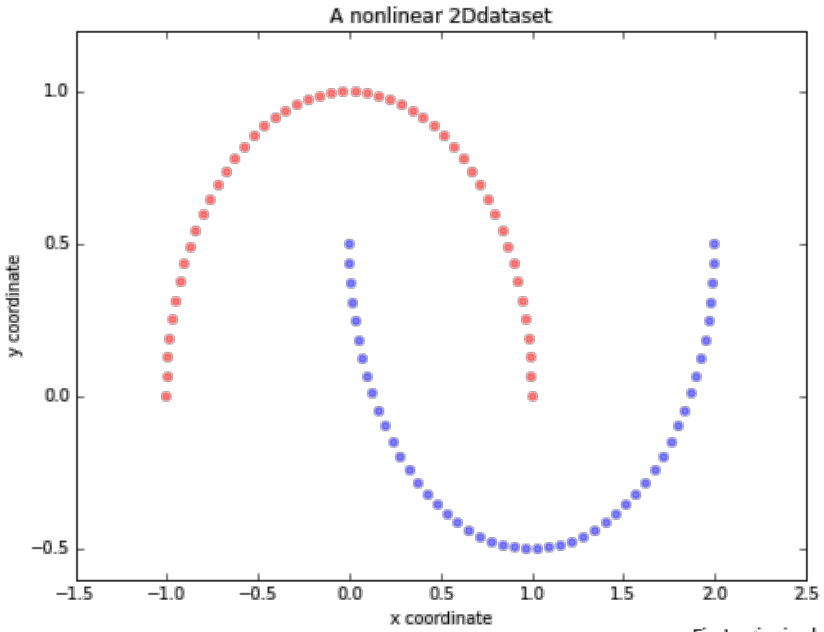
Actually, this centering can be done on the Gram matrix without ever explicitly computing the feature map $\phi(\mathbf{x})$.

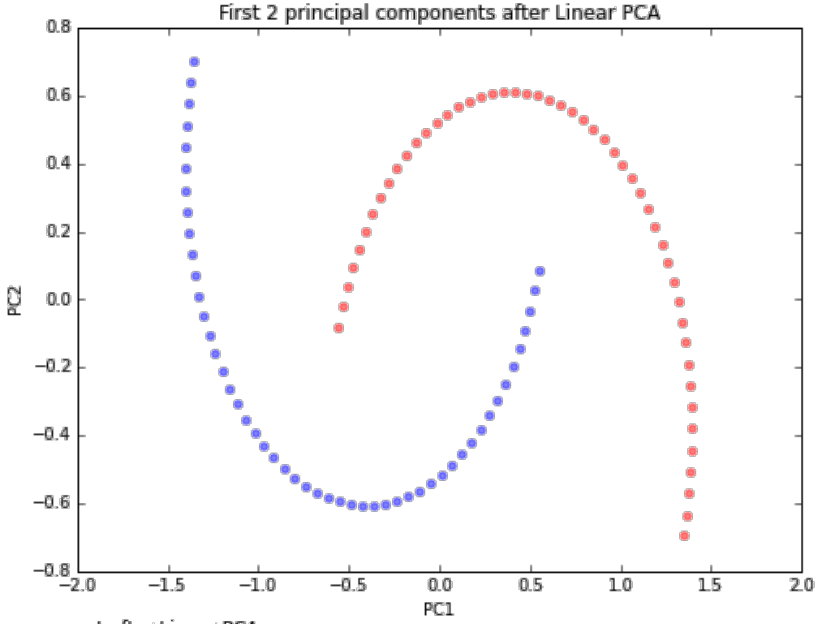
$$\tilde{K} = (I - 11^T / N) K (I - 11^T / N)$$

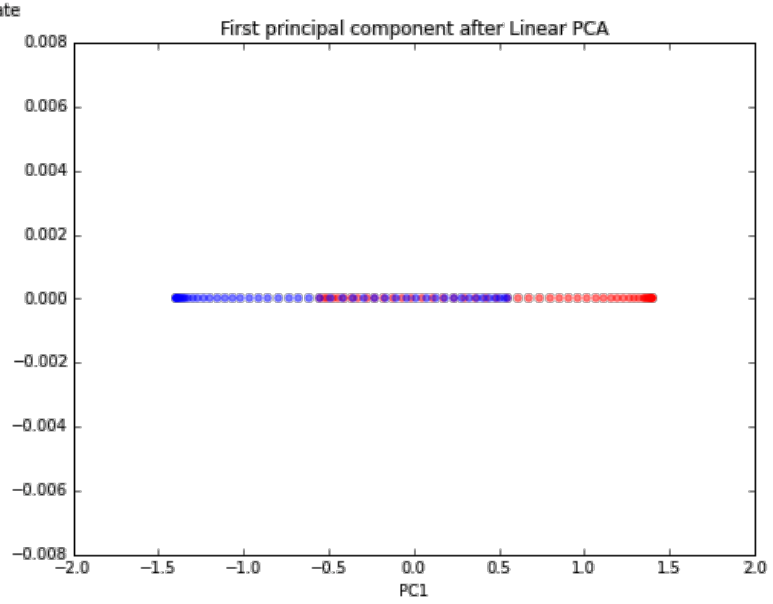
is the kernel matrix for centered features, *i.e.*, $\sum_{i=1}^{N} \phi(\mathbf{x}_i) = 0$

A similar expression exists for projecting test features on the feature eigenspace

KPCA Example

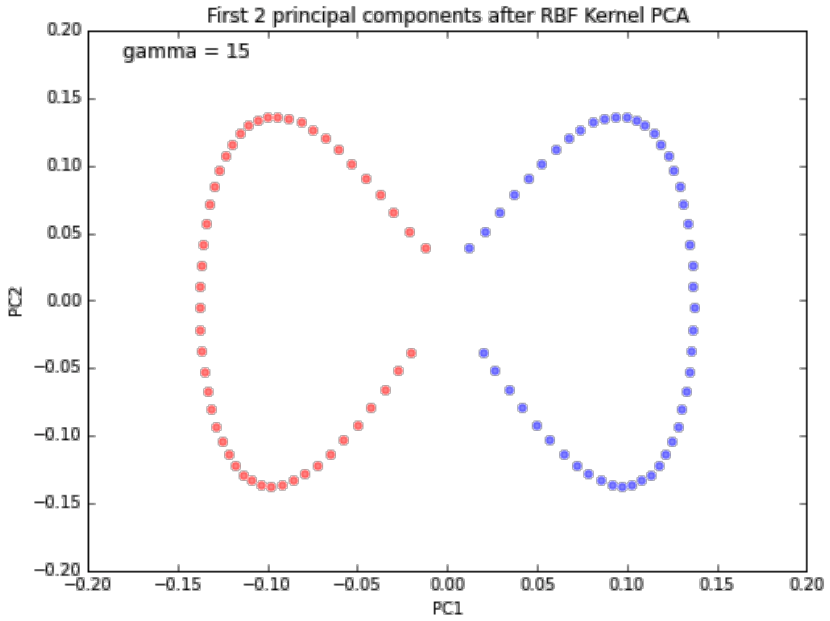


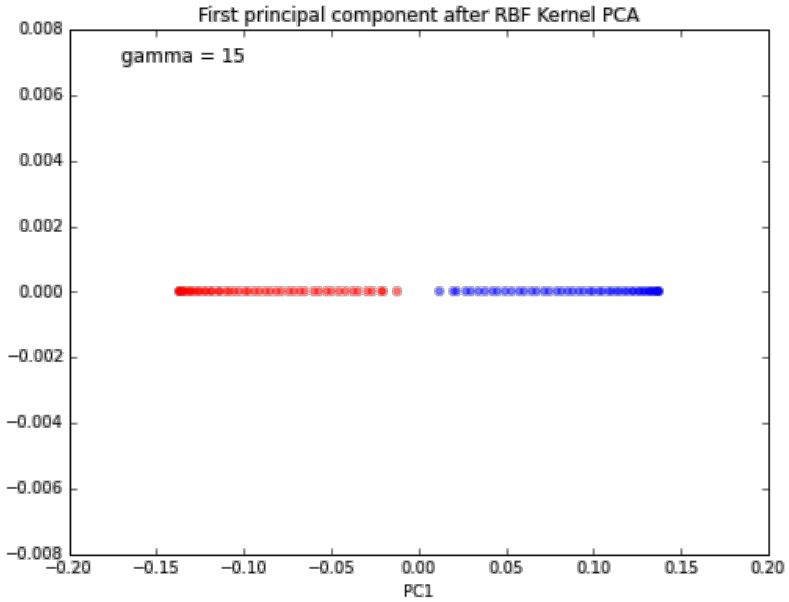




With linear PCA

KPCA Example

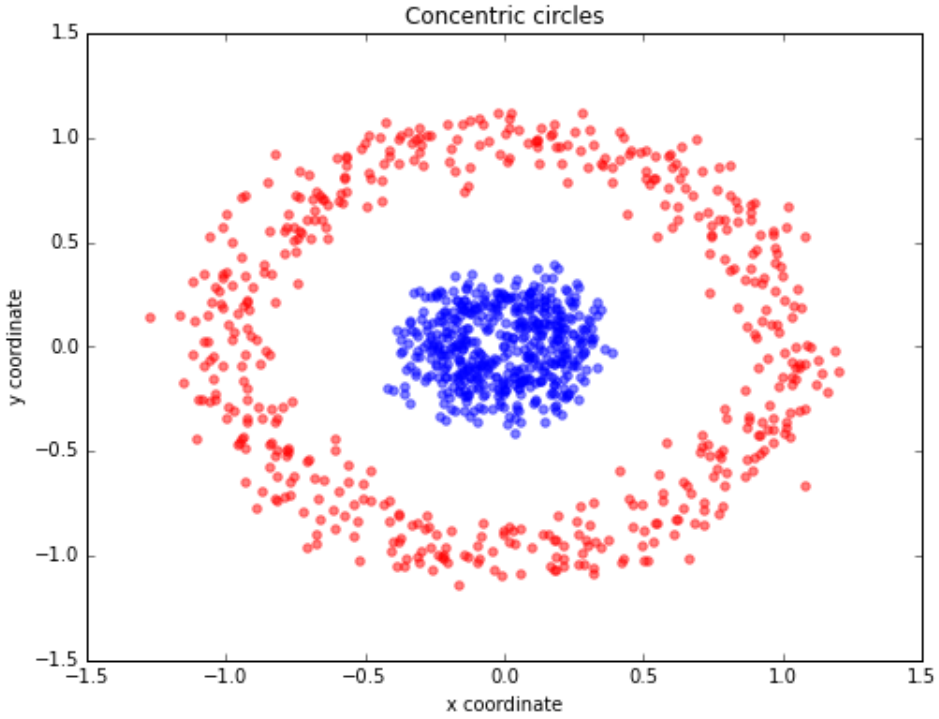


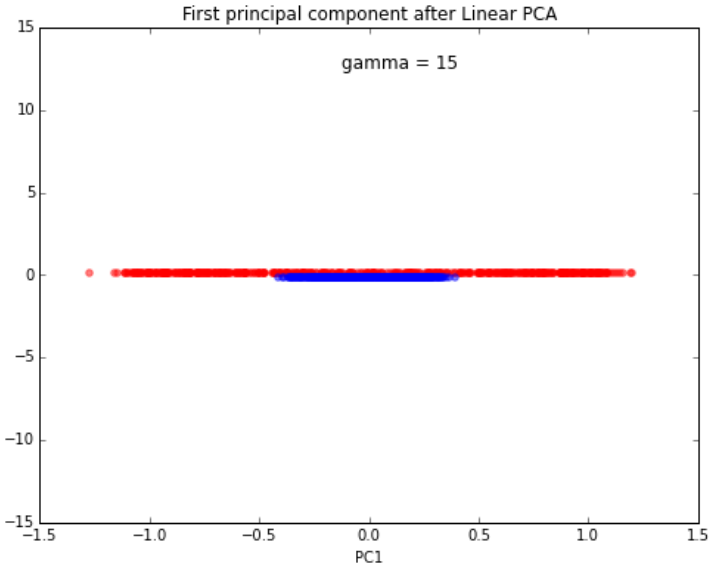


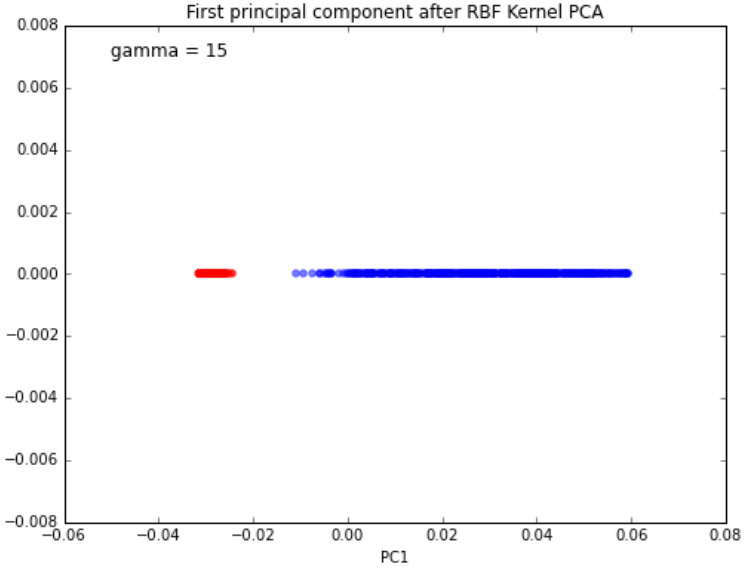
With kernel PCA,
using RBF kernel

$$K(\boldsymbol{x}_1, \boldsymbol{x}_2) = exp(-\gamma \|\boldsymbol{x}_1 - \boldsymbol{x}_2\|_2^2)$$

KPCA 2nd Example







CS233 Homework Policies

CS233 Homework Policies

- 1st homework assignments comes out next Wednesday, April 6. It will be due on Wednesday, April 20.
- Collaboration groups are allowed – in fact encouraged, of up to three students.
- A single write up per group is OK.
- Two free late periods available – after that 20% penalty for each late period, but no more than two (100% penalty after that).
- All homeworks must be submitted by the last day of the quarter, Fri, June 3, 2022

That’s All