# Algorithms

## Dimensionality reduction

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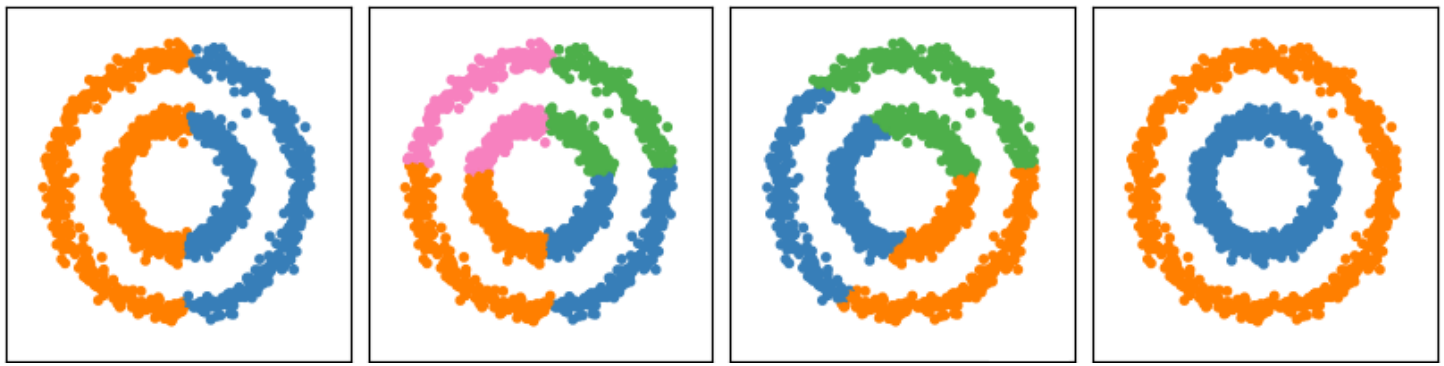
# Clustering

**Input:** data points $\{\mathbf{x}_i\}$ for $i = 1 \ldots n$.

**Output:** labeled data points $\{\mathbf{x}_{i,\ell}\}$ with $\ell = 1 \ldots k$.



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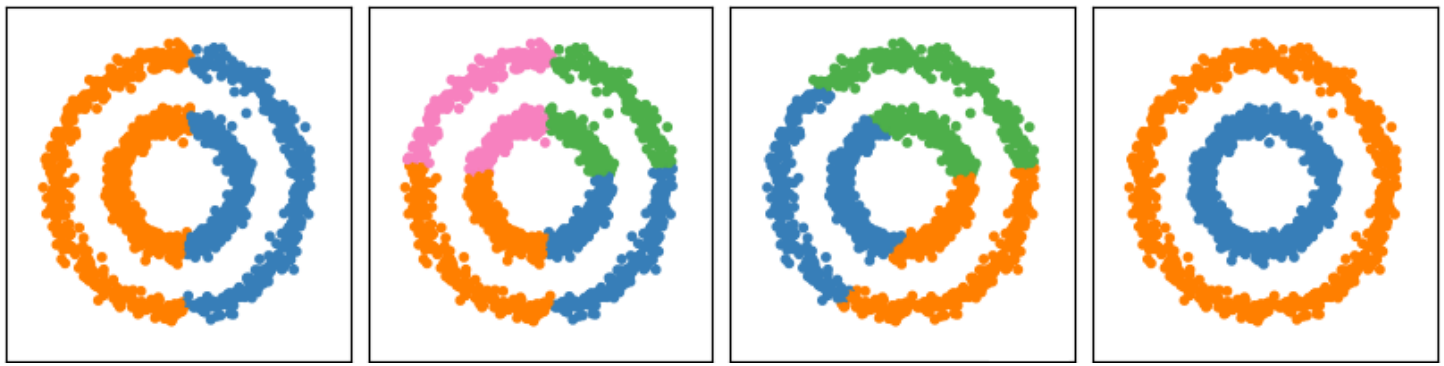
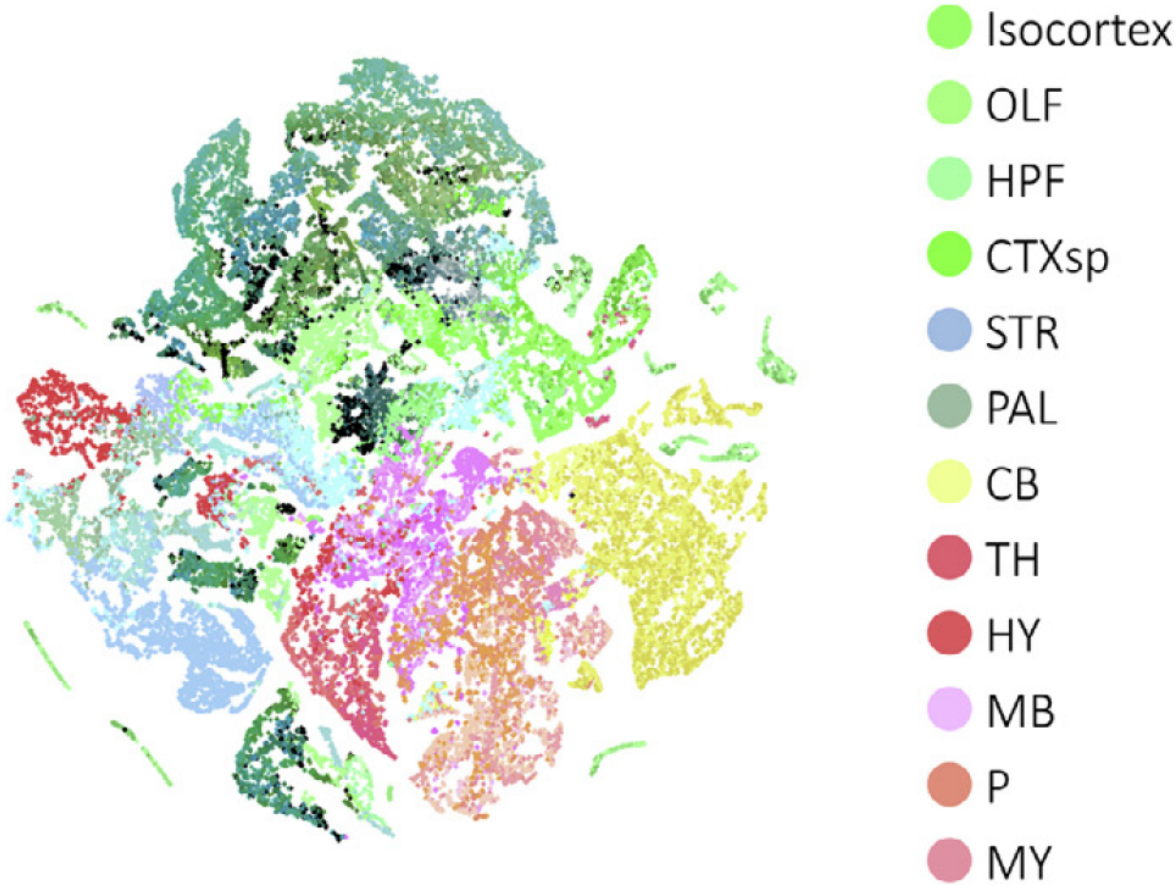


Clustering algorithms compute distances among the given points.

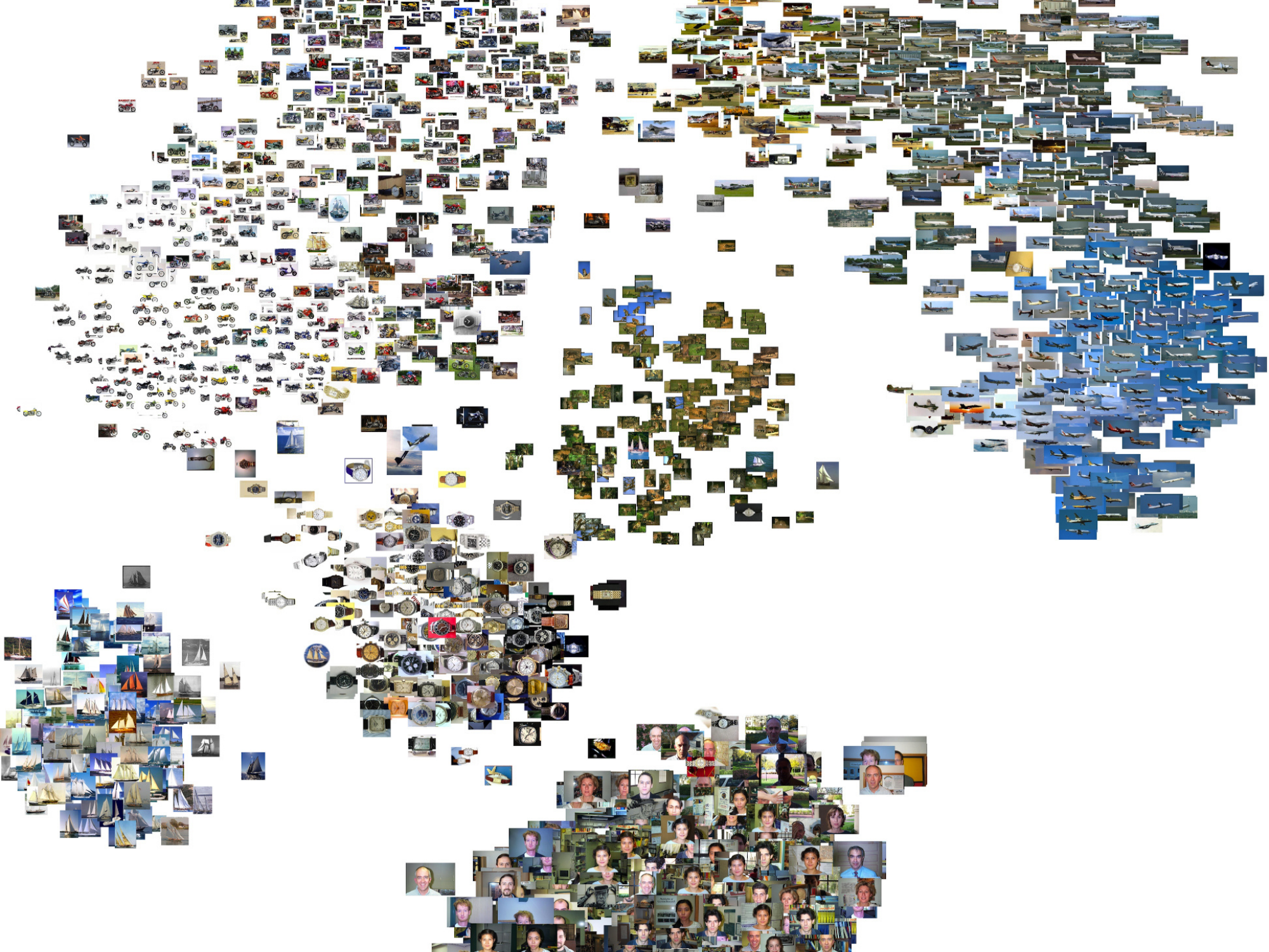
What if we only have the distances, and not the points?

# Example

Based on similarities between gene expression levels (rows of the expression matrix):




Mahfouz et al, "Visualizing the spatial gene expression organization in the brain through non-linear similarity embeddings", Methods 2015



# Distances

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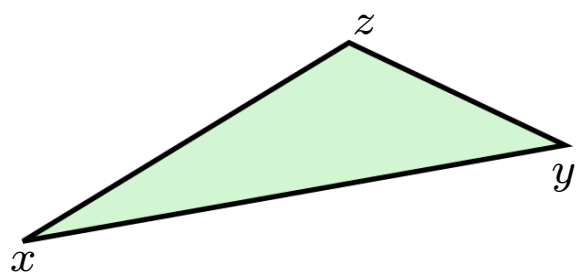
- $d(x, y) \leq d(x, z) + d(z, y)$ for any $x, y, z$ (triangle inequality)



# A cartographer's problem

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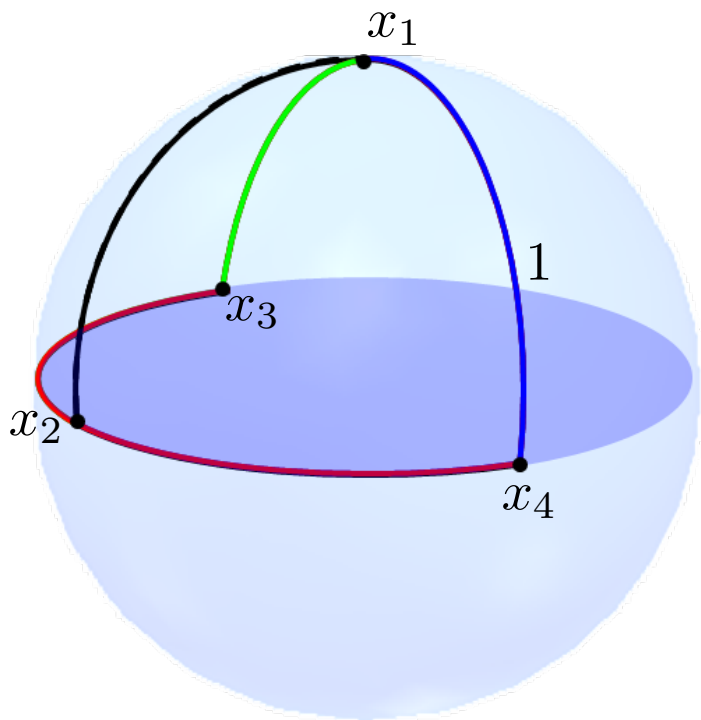
The set of points on the plane is called an embedding of the sphere in $\mathbb{R}^2$.

Any approximate solution introduces metric distortion.

# Non-embeddability of the sphere




- Consider the triangle $\Delta(x_1, x_3, x_4)$ on the plane

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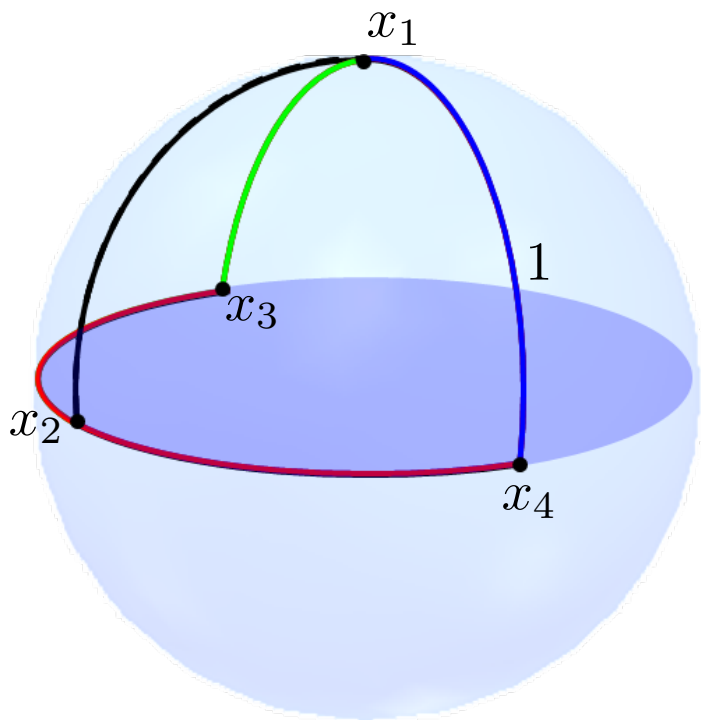


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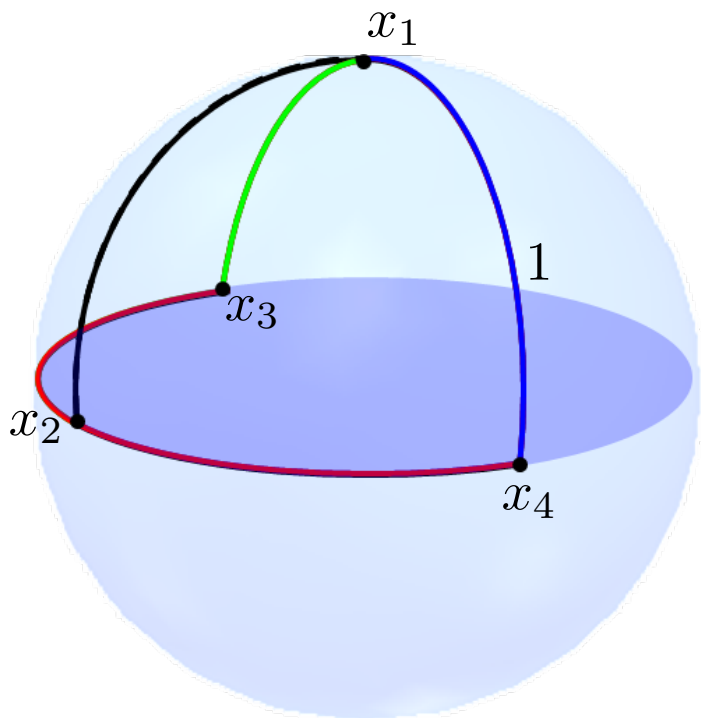


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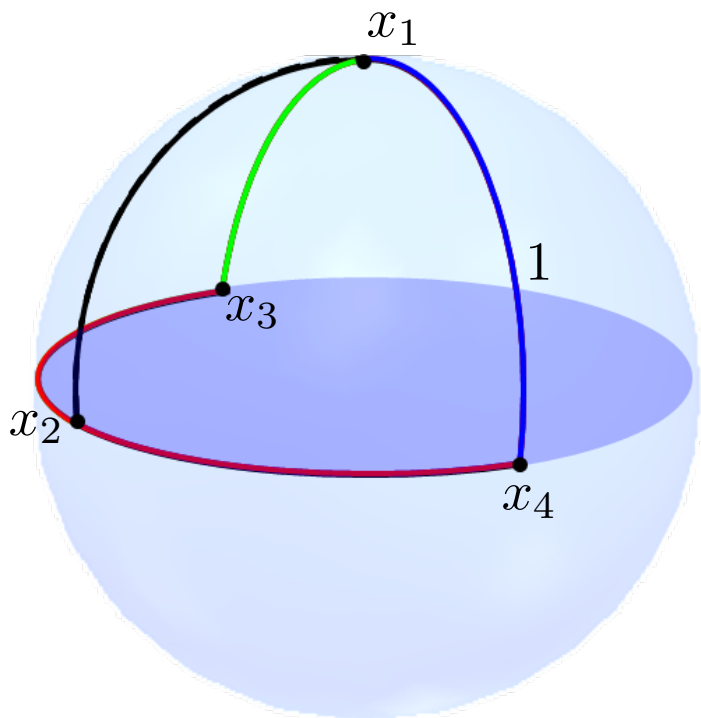


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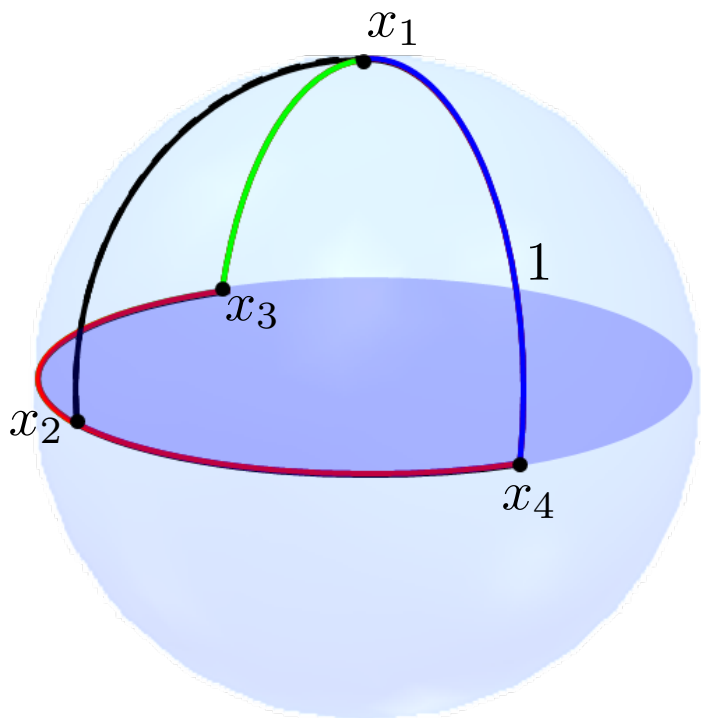


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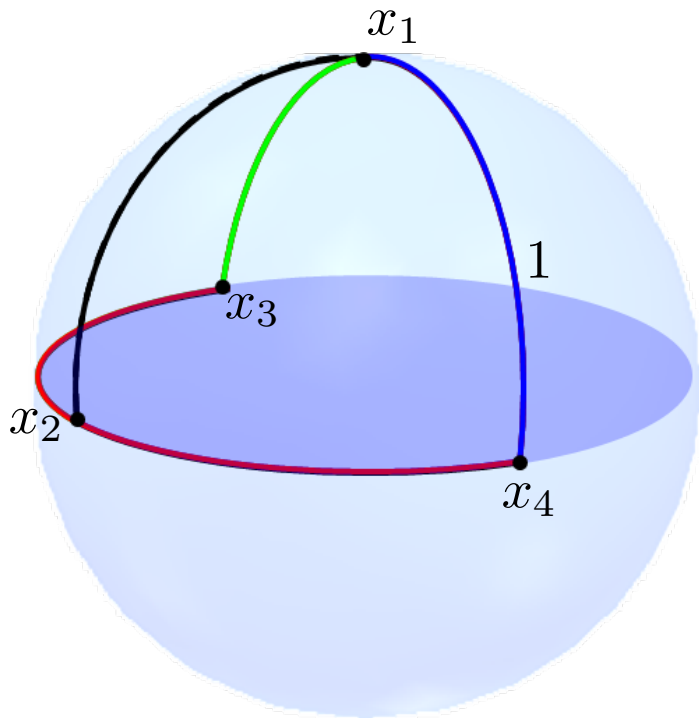


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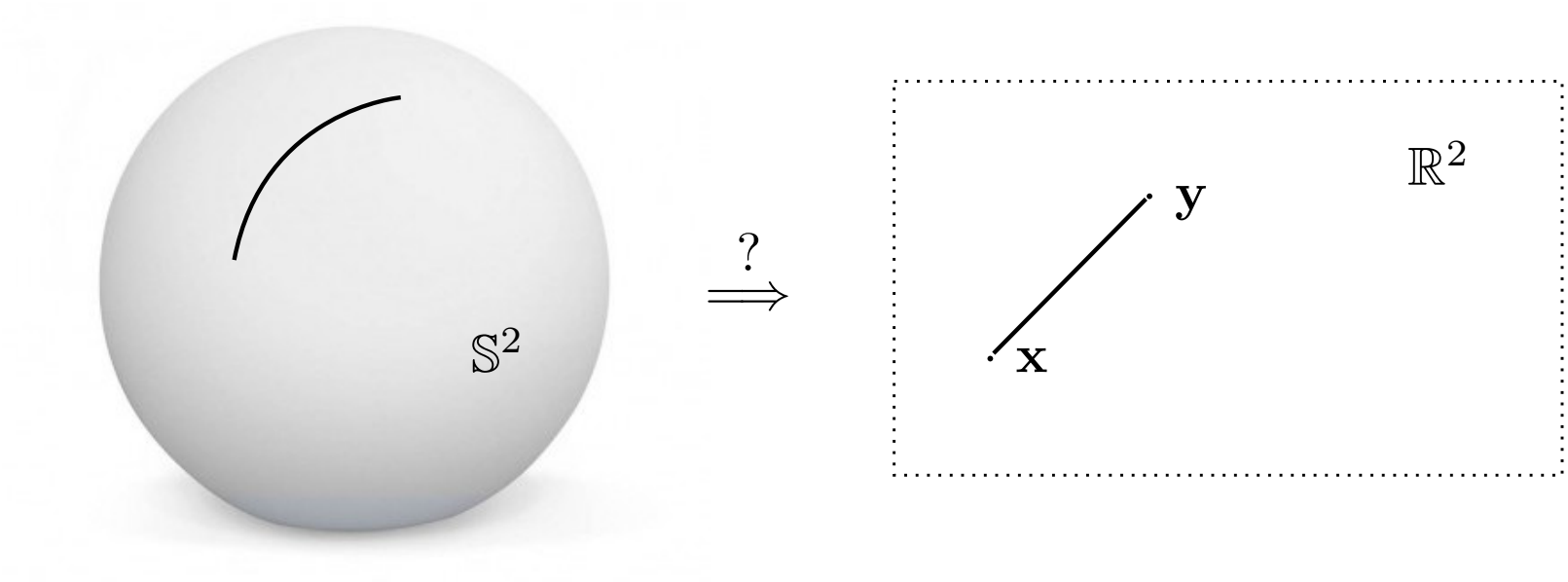
  $\Rightarrow$ The sphere cannot be embedded into $\mathbb{R}^k$ for any $k$.

# A cartographer's solution


# Minimum-distortion embeddings



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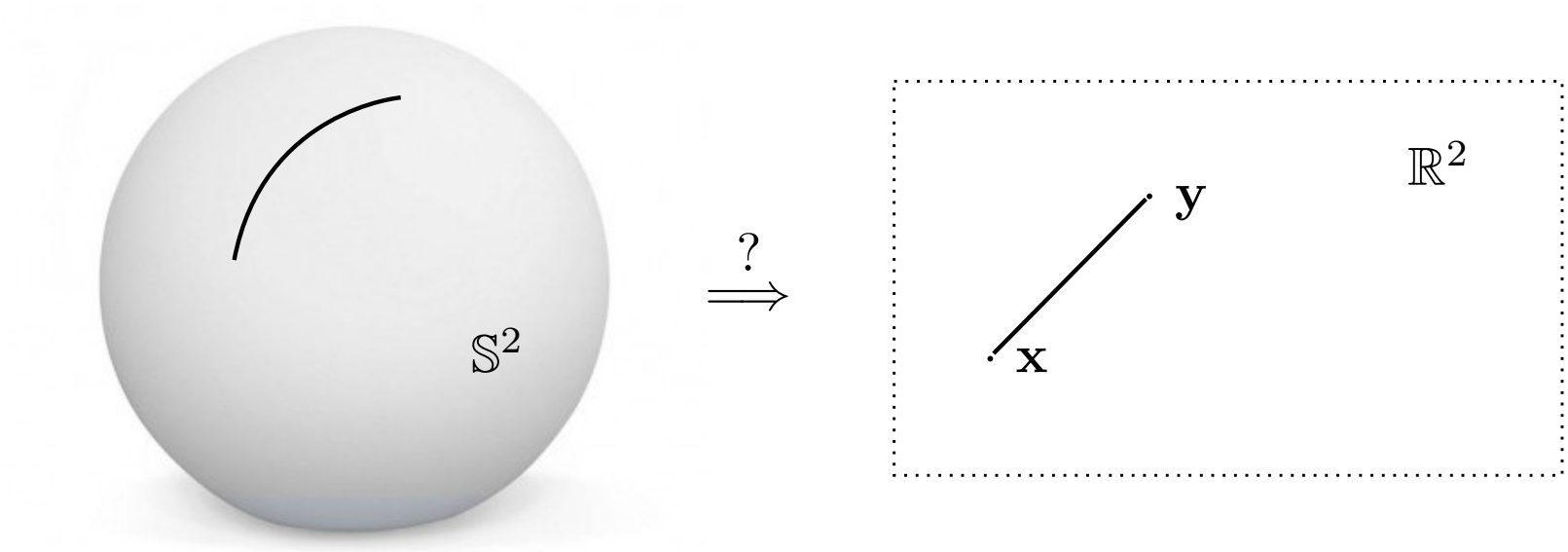


Given $d(x, y)$, find $\mathbf{x}, \mathbf{y} \in \mathbb{R}^2$ such that :

$$d(x, y) \approx \|\mathbf{x} - \mathbf{y}\|_2 \text{ for all } x, y \in \mathbb{S}^2$$

# Stress minimization

This can be cast as an optimization problem:

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The dimensionality $d$ of the points $\mathbf{x} \in \mathbb{R}^d$ is a parameter chosen by us.

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$$f(\mathbf{x}^{(0)}) \geq f(\mathbf{x}^{(1)}) \geq f(\mathbf{x}^{(2)}) \cdots$$

# Multidimensional scaling

Why "stress"?

Problems of this sort started appearing in psychology several decades ago, and are also called multidimensional scaling (MDS) problems.

> Empirical procedures of several diverse kinds have this in common: they start with a fixed set of entities and determine, for every pair of these, a number reflecting how closely the two entities are related psychologically. The nature of the psychological relation depends upon the nature of the entities. If the entities are all stimuli or all responses, we are inclined to think of the relation as one of similarity. A somewhat more objective (though less intuitive) characterization of such a relation, perhaps, is that of substitutability. The statement that stimulus $A$ is more similar to $B$ than to $C$, for example, could be interpreted to say that the psychological (or behavioral) consequences are greater when $C$, rather than $B$, is substituted for $A$. From this standpoint a natural procedure for determining similarities of stimuli or responses is by recording substitution errors during identification learning [2, 7, 12, 14, 17, 18]. In addition, though, disjunctive reaction time and sorting time have also been proposed as measures of psychological similarity [20]. Finally, of course, individuals have sometimes been instructed simply to rate each pair of stimuli, directly, on a scale of apparent similarity [1, 6]. The notion of similarity is not necessarily restricted to stimuli or responses (in the narrow sense of these words), however. Serviceable measures of similarity may also be found for concepts, attitudes, personality structures, or even social institutions, political systems, and the like.

Shepard, "The analysis of proximities: Multidimensional scaling with an unknown distance function". Psychometrika 27(2), 1962

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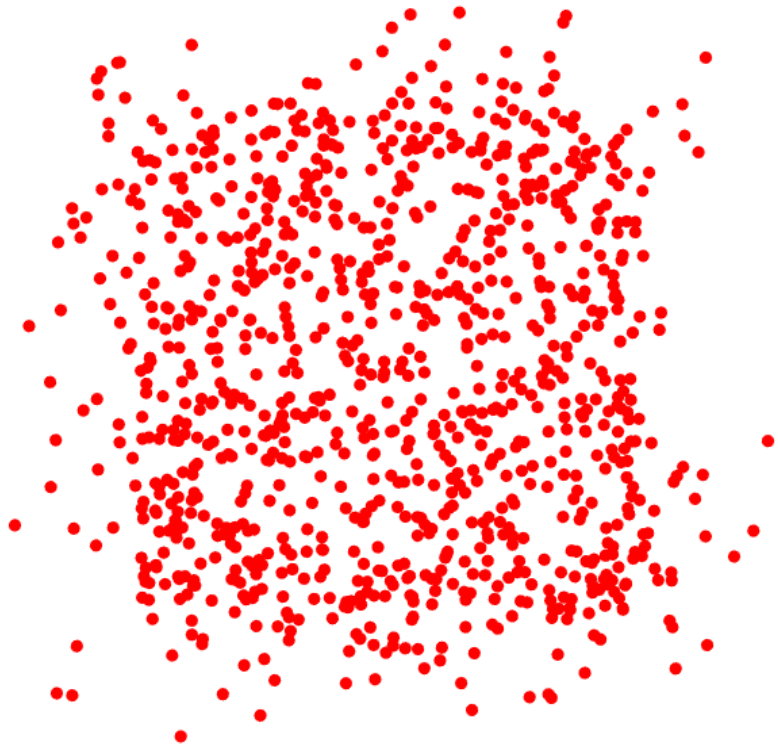

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In Python available through the scikit-learn library, together with other algorithms such as $k$-means, random forests, etc.


For stress minimization see:

`https://scikit-learn.org/stable/modules/generated/sklearn.manifold.MDS`

You are encouraged to experiment with the library!

scikit learn Install User Guide API Examples More Go

# scikit-learn

*Machine Learning in Python*

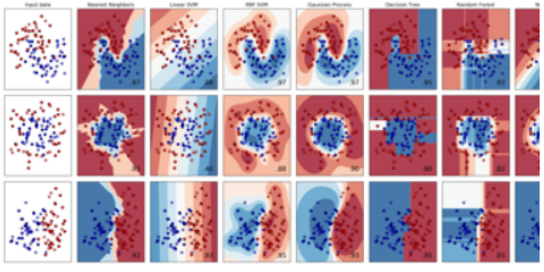
Getting Started | What's New in 0.22.2 | GitHub

- Simple and efficient tools for predictive data analysis
- Accessible to everybody, and reusable in various contexts
- Built on NumPy, SciPy, and matplotlib
- Open source, commercially usable - BSD license

## Classification

Identifying which category an object belongs to.

**Applications:** Spam detection, image recognition.
**Algorithms:** SVM, nearest neighbors, random forest, and more...

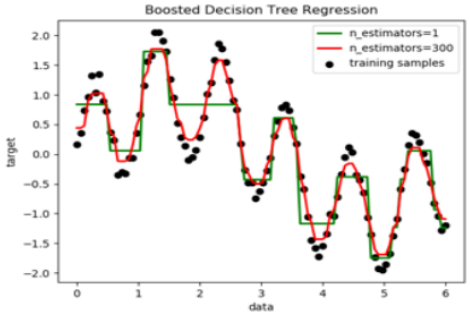


Examples

## Regression

Predicting a continuous-valued attribute associated with an object.

**Applications:** Drug response, Stock prices.
**Algorithms:** SVR, nearest neighbors, random forest, and more...

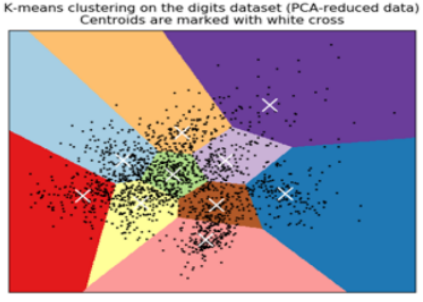



Examples

## Clustering

Automatic grouping of similar objects into sets.

**Applications:** Customer segmentation, Grouping experiment outcomes
**Algorithms:** k-Means, spectral clustering, mean-shift, and more...




Examples

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Multidimensional scaling is just one of many other Euclidean embedding techniques: T-SNE, eigenmaps, locally linear embeddings, etc.

You can experiment with others in scikit-learn:

`https://scikit-learn.org/stable/modules/generated/sklearn.manifold.TSNE`

# Dimensionality reduction: another perspective

Let us be given $n$ data points stored in matrix $\mathbf{X} \in \mathbb{R}^{d \times n}$:

$$\mathbf{X}^\top = \begin{pmatrix} — & \mathbf{x}_1^\top & — \\ & \vdots & \\ — & \mathbf{x}_n^\top & — \end{pmatrix}$$

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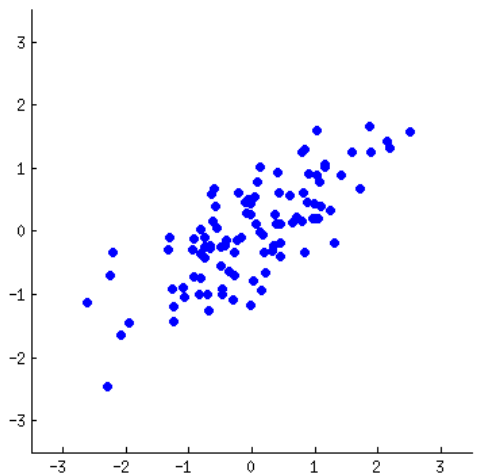

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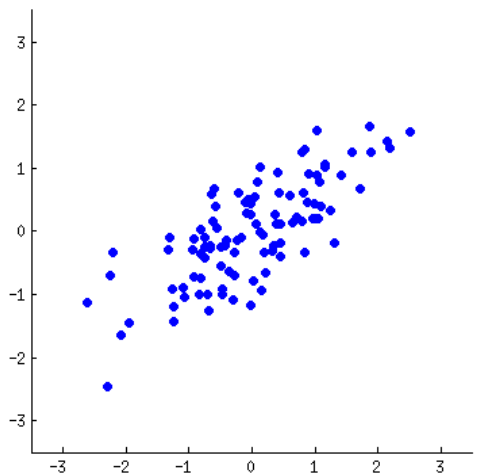
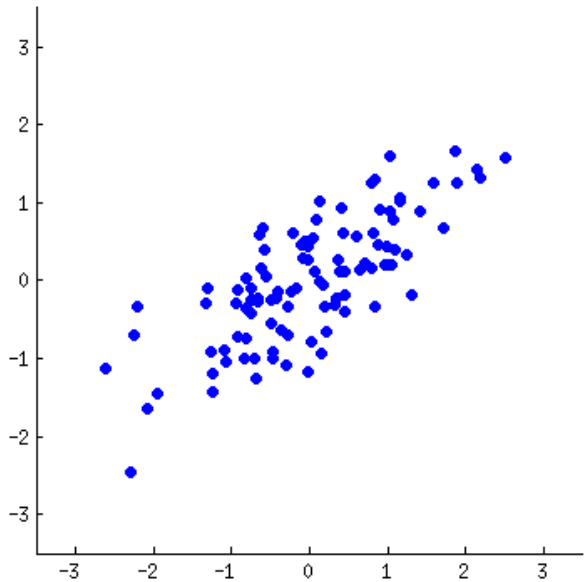
We want to replace them with a lower-dimensional approximation $\tilde{\mathbf{X}} \in \mathbb{R}^{k \times n}$, with $k \ll d$.



# Principal component analysis (PCA)

Regard our data as $n$ points in $\mathbb{R}^d$:



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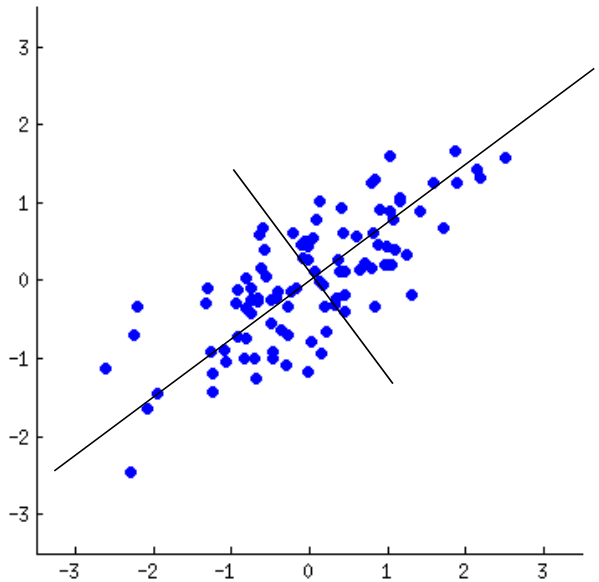


Overall idea:

- Find $k \leq d$ orthogonal directions with the most variance.
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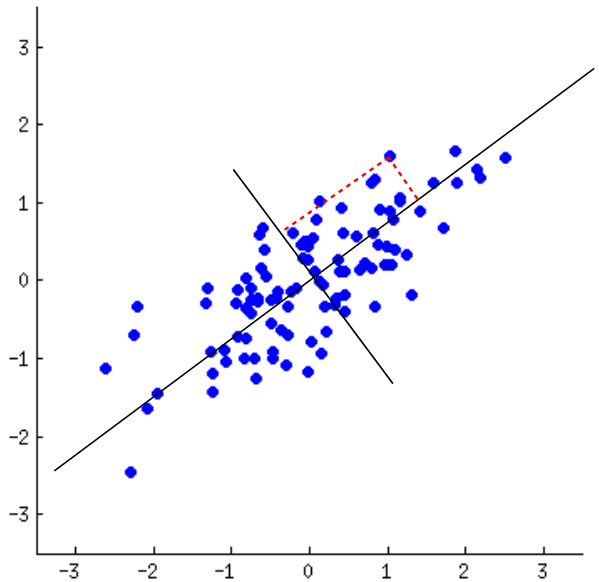


Overall idea:

- Find $k \leq d$ orthogonal directions with the most variance.
  These span a $k$-dimensional subspace of the data.
- Project all the data points onto these directions.
  This is lossy, but can be done with the smallest possible error.

# Principal component analysis (PCA)

In matrix notation:

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Assuming $\mathbf{W}^\top \mathbf{W} = \mathbf{I}$, for $k = d$ we get:

$$\mathbf{X}^\top \mathbf{W} = \mathbf{Z}^\top$$
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$$\mathbf{X}^\top \mathbf{W} = \mathbf{Z}^\top \quad \text{projection}$$
$$\mathbf{X} \approx \mathbf{W}\mathbf{Z} \quad \text{reconstruction}$$

# Principal component analysis (PCA)

In matrix notation:

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We call the columns of $\mathbf{W}$ principal components.

They are unknown and must be computed.

# Principal component analysis (PCA)

We seek the direction $\mathbf{w}$ (a column of $\mathbf{W}$) that:

- Minimizes the projection/reconstruction error.
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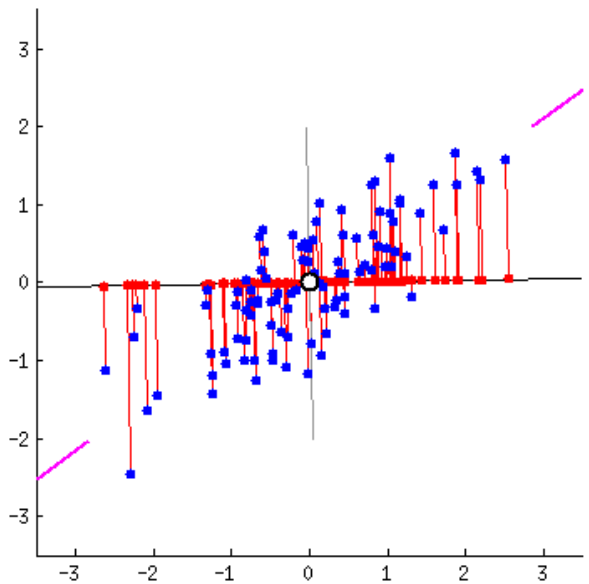

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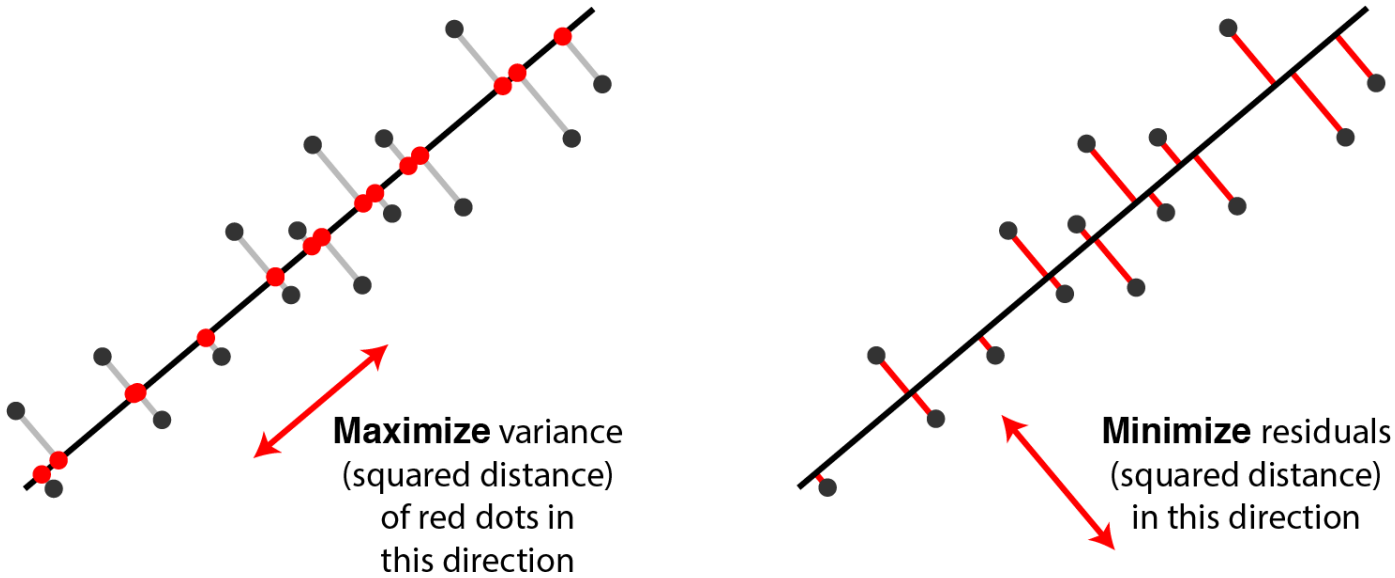

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The solution is $\mathbf{w} =$ principal eigenvector of $\mathbf{C}$ (Courant minmax principle), and the value $\mathbf{w}^\top \mathbf{C}\mathbf{w}$ is the corresponding eigenvalue.

# Principal component analysis (PCA)

After solving the problem:

$$\mathbf{w}_1 = \arg\max_{\mathbf{w}} \mathbf{w}^\top \mathbf{C}\mathbf{w}$$
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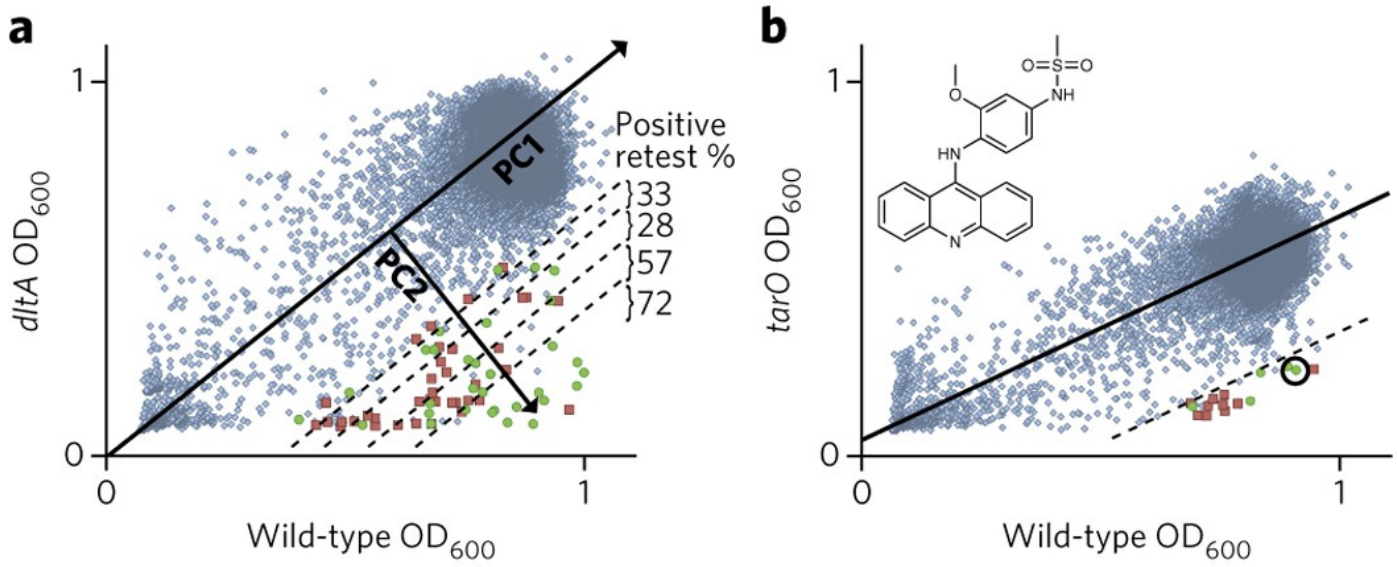
which is the second eigenvector of $\mathbf{C}$, and so on for all $\mathbf{w}_{i=2\ldots k}$.

The principal components are thus the first $k \ll d$ eigenvectors of $\mathbf{C}$, sorted by decreasing eigenvalue.

# Examples

PCA is widely used in computational biology and bioinformatics.




Suggested short reading:

Ringnér, "What is principal component analysis?", Nature Biotech. 2008 (click here)

# Exercises

Try to reproduce the examples described in:

this page (clickable link)

and in:

this page

Send me code + screenshots of your results. Feel free to experiment with other data in addition to what is used in those tutorials.