t-SNE

Jiahui Chen
Department of Mathematical Sciences
University of Arkansas

Why t-SNE and UMAP?

- Aims to solve the problems of PCA
  - Non-linear scaling to represent changes at different levels
  - Optimal separation in 2-dimensions
- T-Distributed Stochastic Neighbour Embedding (t-SNE)
- Uniform Manifold Approximation and Projection (UMAP)

Dimensionality Reduction

- The Dimensionality Reduction focus on preserving distances. A cost function should be developed to measure this reduction.
- Ideas for Dimensionality Reduction
  - Distance preservation
  - Topology preservation
  - Information preservation

tSNE is a distance-based method but tends to preserve topology

$$\mathbf{X} = \{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n \in \mathbb{R}^h\} \rightarrow \mathbf{Y} = \{\mathbf{y}_1, \mathbf{y}_2, \dots, \mathbf{y}_n \in \mathbb{R}^l\}$$

$$\min_{\mathbf{Y}} C(\mathbf{X}, \mathbf{Y})$$

Stochastic Neighbour Embedding

SNE converts Euclidean distances to similarities, that can be interpreted as probabilities. It computes pair-wise similarities.

$$p_{j|i} = \frac{\exp(-\| \mathbf{x}_i - \mathbf{x}_j \|^2 / 2\sigma_i^2)}{\sum_{k \neq i} \exp(-\| \mathbf{x}_i - \mathbf{x}_k \|^2 / 2\sigma_i^2)}$$

$$q_{j|i} = \frac{\exp(-\| \mathbf{y}_i - \mathbf{y}_j \|^2)}{\sum_{k \neq i} \exp(-\| \mathbf{y}_i - \mathbf{y}_k \|^2)}$$

$$p_{j|i} = 0, q_{j|i} = 0$$

σ_i is either set by hand or found by a binary search for the value of σ_i that makes the entropy of the distribution over neighbors equal to $\log k$

The conditional probability

- $p_{j|i} = \frac{\exp(-\|\mathbf{x}_i - \mathbf{x}_j\|^2 / 2\sigma_i^2)}{\sum_{k \neq i} \exp(-\|\mathbf{x}_i - \mathbf{x}_k\|^2 / 2\sigma_i^2)}$
- $\| \mathbf{x}_i - \mathbf{x}_j \|^2$ is the squared Euclidean distance between $\mathbf{x}_i$ and $\mathbf{x}_j$
- σ_i^2 is the variance of the Gaussian distribution centered on point $\mathbf{x}_i$
- This relationship is quantified in terms of the likelihood that one point would pick another as its neighbor under a Gaussian distribution centered on the first point
- Measure of Similarity: A higher $p_{j|i}$ indicates a stronger similarity or closeness between $\mathbf{x}_i$ and $\mathbf{x}_j$
- Local Density Adaptation: ensuring that each point has a roughly equal effective number of neighbors, which helps preserve local structures in the mapping

Kullback-Leibler Divergence

SNE converts Euclidean distances to similarities, that can be interpreted as probabilities. It computes pair-wise similarities.

$$p_{j|i} = \frac{\exp(-\|\mathbf{x}_i - \mathbf{x}_j\|^2 / 2\sigma_i^2)}{\sum_{k \neq i} \exp(-\|\mathbf{x}_i - \mathbf{x}_k\|^2 / 2\sigma_i^2)} \text{ and } q_{j|i} = \frac{\exp(-\|\mathbf{y}_i - \mathbf{y}_j\|^2)}{\sum_{k \neq i} \exp(-\|\mathbf{y}_i - \mathbf{y}_k\|^2)}$$

$P_i = \{p_{1|i}, p_{2|i}, \ldots, p_{n|i}\}$ and $Q_i = \{q_{1|i}, q_{2|i}, \ldots, q_{n|i}\}$ are the distributions on the neighbors of datapoint i.

Kullback-Leibler Divergence (KL) compares two distributions

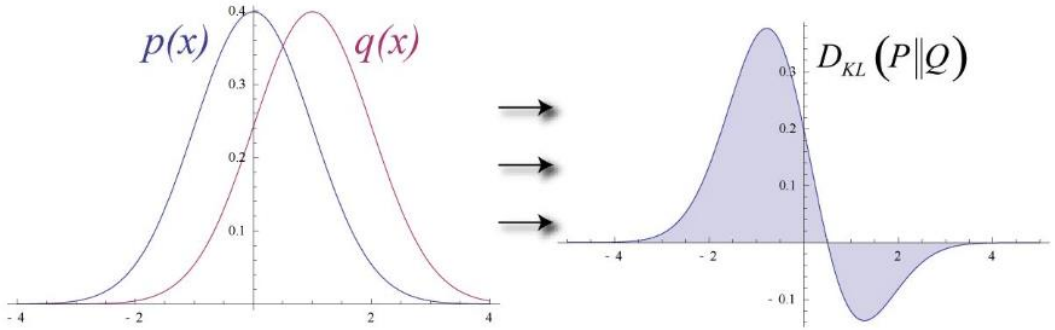
$$C = \sum_i KL(P_i \parallel Q_i) = \sum_i \sum_j p_{j|i} \log \frac{p_{j|i}}{q_{j|i}}$$

Minimization

KL divergence is asymmetric and always positive

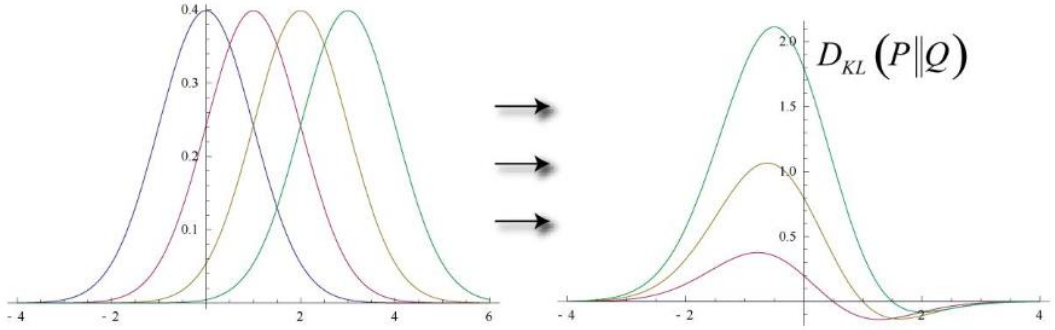
$$\frac{\mathrm{d}C}{\mathrm{d}\mathbf{y}_i} = 2 \sum_j (p_{j|i} - q_{j|i} + p_{i|j} - q_{i|j})(\mathbf{y}_i - \mathbf{y}_j)$$

Kullback-Leibler Divergence



Original Gaussian PDF's

KL Area to be Integrated

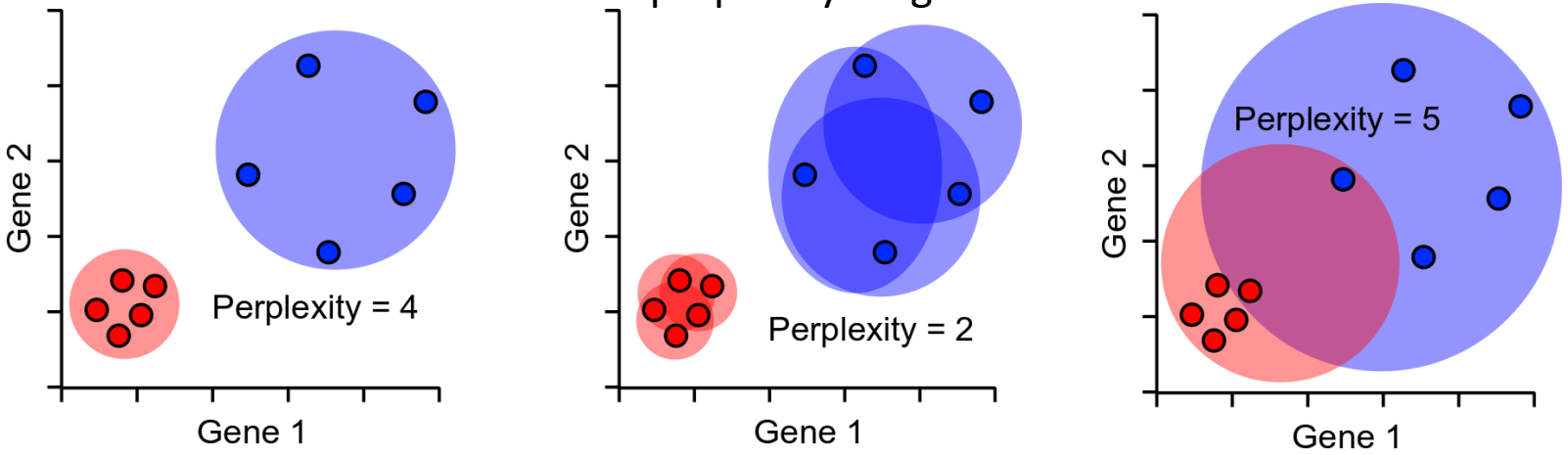


$$D_{\mathrm{KL}}(P\|Q) = \sum_i P(i)\,\log\frac{P(i)}{Q(i)}.$$

Measures the similarity between two probability distributions & it is asymmetric

Perplexity

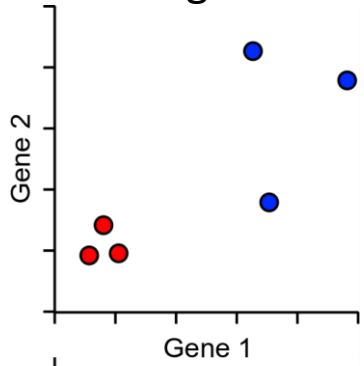
- σ_i is either set by hand or found by a binary search for the value of σ_i that makes the entropy of the distribution over neighbors equal to $\log k$
- Perplexity = expected number of neighbours within a cluster. It can be thought of as a guess about the number of close neighbours each point has.
- Distances scaled relative to perplexity neighbours

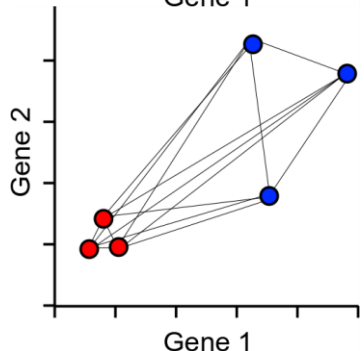


[Simon Andrews, 2024]

Perplexity

For the distance $d_{ij}^2 = \| \mathbf{x}_i - \mathbf{x}_j \|^2 / 2\sigma_i^2$ in $p_{j|i}$, σ_i is either set by hand or found by a binary search for the value of σ_i that makes the entropy of the distribution over neighbors equal to $\log k$.



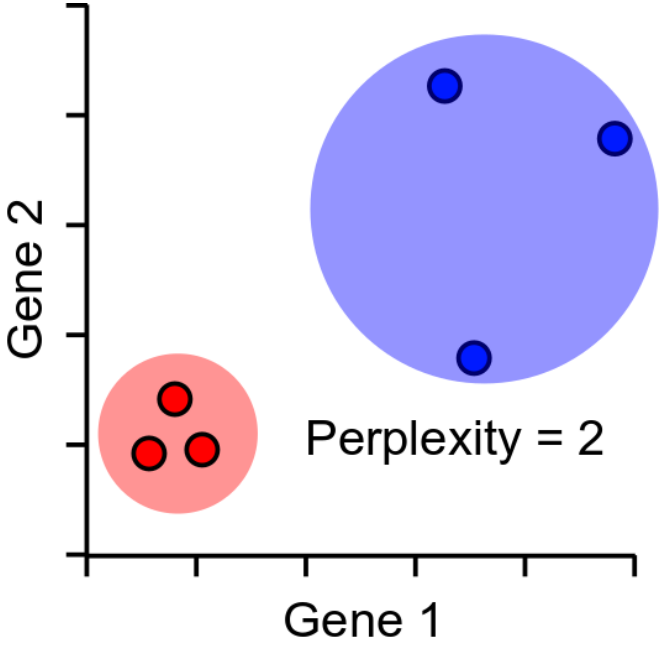


	0	10	10	295	158	153
	9	0	1	217	227	213
	1	8	0	154	225	238
	205	189	260	0	23	45
	248	227	246	44	0	54
	233	176	184	41	36	0

[Simon Andrews, 2024]

Perplexity

For the distance $d_{ij}^2 = \| \mathbf{x}_i - \mathbf{x}_j \|^2 / 2\sigma_i^2$ in $p_{j|i}$, σ_i is either set by hand or found by a binary search for the value of σ_i that makes the entropy of the distribution over neighbors equal to $\log k$.



	0	4	6	586	657	836
	4	0	4	815	527	776
	9	3	0	752	656	732
	31	28	29	0	4	7
	31	24	25	4	0	7
	40	37	32	8	8	0

[Simon Andrews, 2024]

Shannon entropy

For the distance $d_{ij}^2 = \| \mathbf{x}_i - \mathbf{x}_j \|^2 / 2\sigma_i^2$ in $p_{j|i}$, σ_i is either set by hand or found by a binary search for the value of σ_i that makes the entropy of the distribution over neighbors equal to $\log k$.

Here, k - is the effective number of local neighbors or "perplexity" and is chosen by hand.

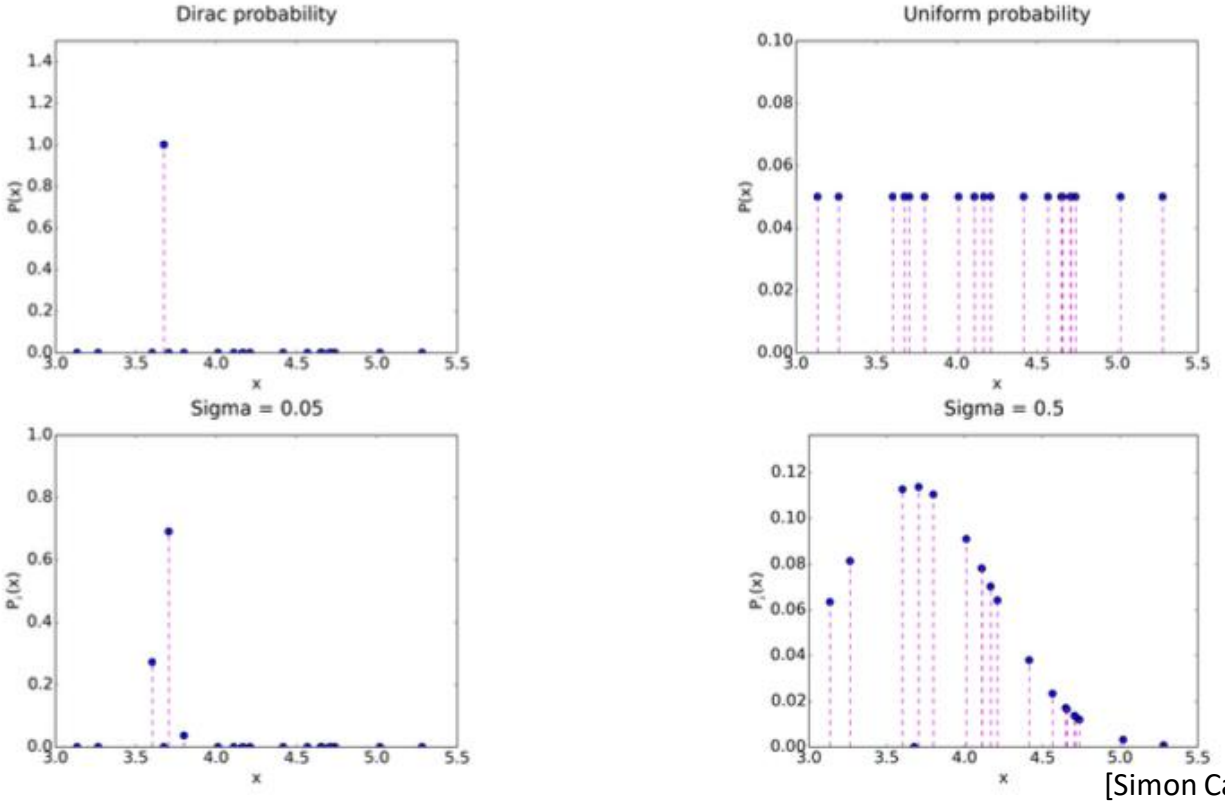
$$\text{Perplexity}(P_i) = 2^{H(P_i)}$$

where $H(P_i)$ is the Shannon entropy of the conditional probability distribution P_i

$$H(P_i) = -\sum_j p_{j|i} \log_2 p_{j|i}$$

Shannon entropy

$$\text{Perplexity}(P_i) = 2^{H(P_i)}, H(P_i) = -\sum_j p_{j|i} \log_2 p_{j|i}$$



[Simon Carbonnelle, 2016]

Perplexity and Shannon Entropy

- perplexity is a measure of how well a probability distribution predicts a sample
- quantify the effective number of neighbors for a point in datasets
- Shannon entropy measures the uncertainty or randomness of a probability distribution
- High entropy -> a uniform distribution -> high uncertainty
- Low entropy -> a peaked distribution (Dirarc) -> low uncertainty
- Perplexity is a function of Shannon entropy, providing a quantifiable measure of how concentrated or dispersed a probability distribution is, in the sense of predicting neighbors in data analysis contexts.

Shannon entropy

For the distance $d_{ij}^2 = \| \mathbf{x}_i - \mathbf{x}_j \|^2 / 2\sigma_i^2$ in $p_{j|i}$, σ_i is either set by hand or found by a binary search for the value of σ_i that makes the entropy of the distribution over neighbors equal to $\log k$.

Here, k - is the effective number of local neighbors or “perplexity” and is chosen by hand.

The binary search adjusts σ_i until the perplexity of the conditional distribution P_i is approximately equal to the user-defined perplexity.

If the entropy is too high (the distribution is too spread out), σ_i needs to be decreased, leading to a less dispersed distribution.

Conversely, if the entropy is too low, σ_i needs to be increased.

Symmetric SNE

- Kullback-Leiber Divergence of SNE

$$C = \sum_i KL(P_i \parallel Q_i) = \sum_i \sum_j p_{j|i} \log \frac{p_{j|i}}{q_{j|i}}$$

where, $p_{j|i} = \frac{\exp(-\|\mathbf{x}_i - \mathbf{x}_j\|^2 / 2\sigma_i^2)}{\sum_{k \neq i} \exp(-\|\mathbf{x}_i - \mathbf{x}_k\|^2 / 2\sigma_i^2)}$ and $q_{j|i} = \frac{\exp(-\|\mathbf{y}_i - \mathbf{y}_j\|^2)}{\sum_{k \neq i} \exp(-\|\mathbf{y}_i - \mathbf{y}_k\|^2)}$

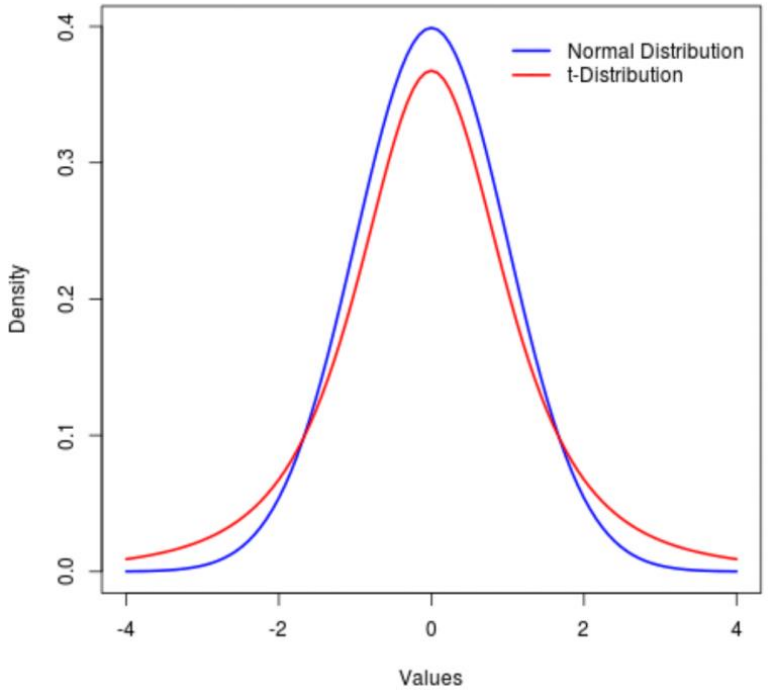
- Asymmetric -> Symmetric, HOW?
- $p_{j|i} = \frac{\exp(-\|\mathbf{x}_i - \mathbf{x}_j\|^2 / 2\sigma_i^2)}{\sum_{k \neq i} \exp(-\|\mathbf{x}_i - \mathbf{x}_k\|^2 / 2\sigma_i^2)} \rightarrow p_{ij} = \frac{p_{j|i} + p_{i|j}}{2n}$ and $q_{j|i} \rightarrow q_{ji}$
- $C = KL(P \parallel Q)$, and $\frac{\mathrm{d}C}{\mathrm{d}\mathbf{y}_i} = 4 \sum_j (p_{ij} - q_{ij})(\mathbf{y}_i - \mathbf{y}_j)$
- Faster Computation

t-SNE

- Use heavier tail distribution than Gaussian in low-dim space (t-Distribution)

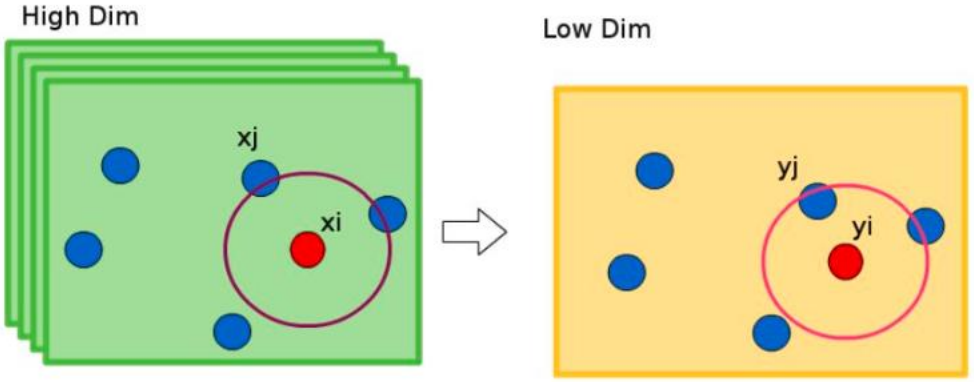
$$q_{ji} \propto (1 + \| \mathbf{y}_i - \mathbf{y}_j \|^2)^{-1}$$

- Why Student-t Distribution?



Student-t Distribution

- The crowding problem: when embedding neighbors from a high-dim space into a low-dim space, there is too little space near a point for all of its close-by neighbors.
- Suppose data is intrinsically high dimensional
- We try to model the local structure of this data in the map
- Result: Dissimilar points have to be modeled as too far apart in the map!



UNIVERSITY OF ARKANSAS

t-SNE

- Use heavier tail distribution than Gaussian in low-dim space (t-Distribution)

$$q_{ij} \propto (1 + \| \mathbf{y}_i - \mathbf{y}_j \|^2)^{-1}$$

- $p_{ij} = \frac{p_{j|i} + p_{i|j}}{2n}$ and $q_{ij} = \frac{(1+\|\mathbf{y}_i - \mathbf{y}_j\|^2)^{-1}}{\sum_{k \neq i}(1+\|\mathbf{y}_i - \mathbf{y}_k\|^2)^{-1}}$
- The gradient: $\frac{\mathrm{d}C}{\mathrm{d}\mathbf{y}_i} = 4 \sum_j (p_{ij} - q_{ij})(\mathbf{y}_i - \mathbf{y}_j)(1 + \| \mathbf{y}_i - \mathbf{y}_j \|^2)^{-1}$
- Even Faster Computation
- Better Behavior

Gradient Descent in t-SNE

- **Initial Low-Dimensional Embedding**

t-SNE starts with an initial, often random, low-dimensional representation of each high-dimensional data point.

- **KL Divergence**

The KL divergence measures how well the low-dimensional distribution of points matches the high-dimensional distribution.

- **Updating Points**

$$\mathbf{y}_i = \mathbf{y}_i - lr\frac{\mathrm{d}C}{\mathrm{d}\mathbf{y}_i} \text{ where } \frac{\mathrm{d}C}{\mathrm{d}\mathbf{y}_i} = 4\sum_j (p_{ij} - q_{ij})(\mathbf{y}_i - \mathbf{y}_j)\,(1 + \| \mathbf{y}_i - \mathbf{y}_j \|^2)^{-1}$$

- **Iterative Optimization**: This process of calculating the gradient and updating the positions of the points is repeated iteratively.

Discussion

- tSNE aims to maintain the local structure of the data by preserving the local neighbor relationships.
- PCA is a linear algorithm that projects the data onto a new coordinate system such that the greatest variance by some projection of the data comes to lie on the first coordinate.

References

- Simon Andrews, Babraham Bioinformatics
- Simon Carbonnelle, Universit´e Catholique de Louvain, ICTEAM