IFT 4030/7030,
Machine Learning for Signal Processing
Week5: Machine Learning 2, Non-linear Dimensionality Reduction

Cem Subakan

SpeechBrain

UNIVERSITÉ LAVAL

Mila

Admin

- Homework 1 is out, due on October 24th !!!
  - Notez que le devoir 1 est publié, dû à l'octobre 24!
- How are projects going? I will share the access information for the cluster soon.
  - Comment vont les projets? On va partager les infos pour le cluster bientot.

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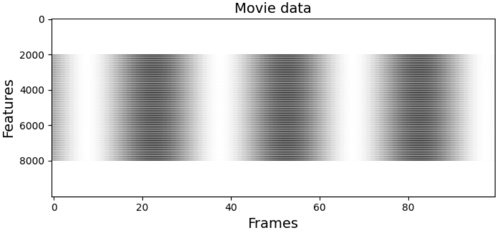
- Non-linear dimensionality reduction
  - Au'jourdhui: Reduction de dimensionalité non-linéaire

Why dimensionality reduction

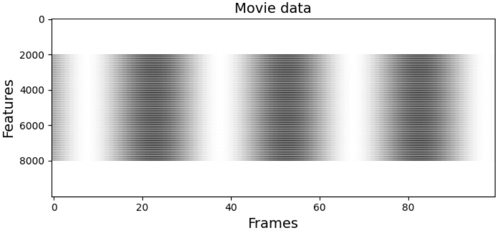
- How many real dimensions in this video? (We have 100 x 100 x 100 dimensions that we can see)
  - Combien de dimensions effectifs dans cette vidéo?

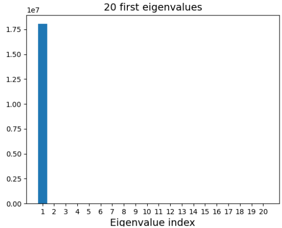
`Watch the video.`

Very low dimensionality



Very low dimensionality





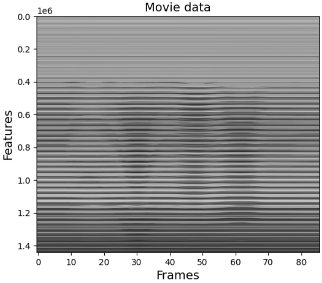
We only need one pixel to convey the same information / On a besoin d'un seul pixel pour le convoi de meme info!

How about this video?

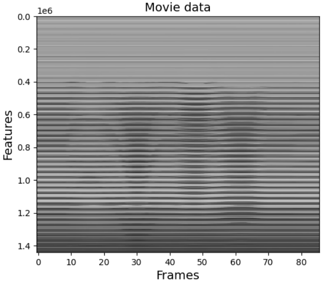
- What is the dimensionality now? / Quelle est la dimensionalité maintenant?
  - Large: $87 \times 800 \times 600 \times 3$.

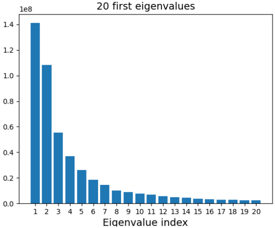
`Watch the video.`

More dimensions?



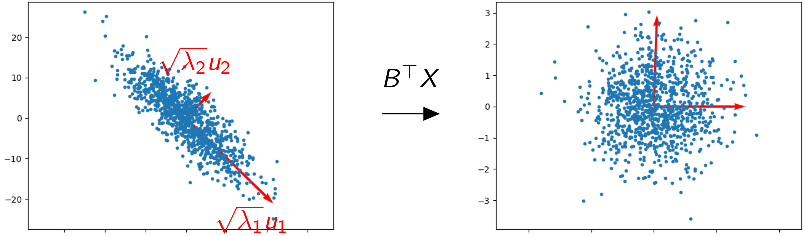
More dimensions?





We have more active dimensions according to PCA, but I think it should be less (4 could do it) / On a plus de dimensions qui sont actives selon PCA, mais je pense 4 serait suffisant.

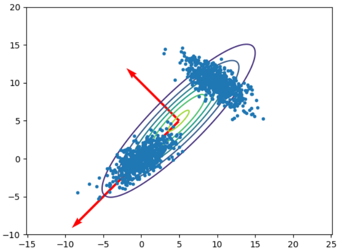
PCA on easy data



$$B^\top = \mathrm{diag}([\sqrt{\lambda_1}, \sqrt{\lambda_2}])^{-1} U^\top.$$

PCA on harder data

- Principal components are not really meaningful here / Les composants principaux n'ont pas du sense nécessairement içi!



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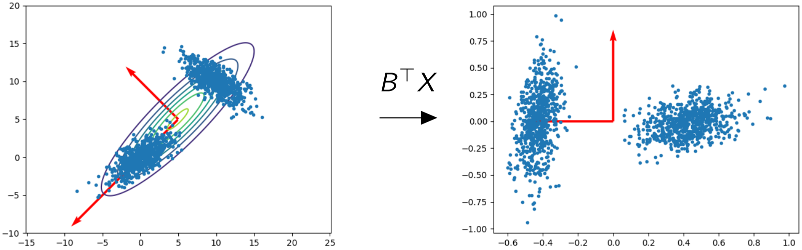

What's wrong with PCA?

- Principal components are linear, assume Gaussian distribution.
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- Data is not always (often not in fact) Gaussian.
  - Les données ne sont pas souvent Gaussienné.
- Can we define non-linear components?
  - Peut-on définir des composants non-linéaires?

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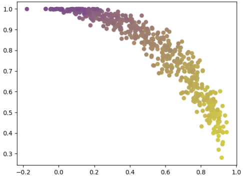
Linearizing the data

- Can we find a feature transformation $\phi()$ such that the data is more Gaussian?
  - Peut-on trouver une transformation $\phi()$ pour que les données sont plus Gaussiennes?



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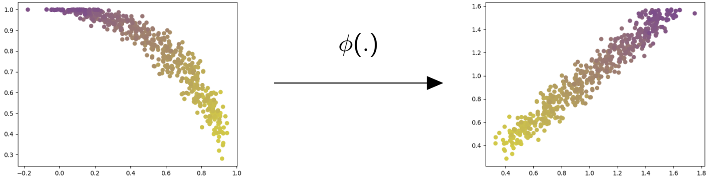

- Now we can do PCA! / Maintenant on peut faire PCA!

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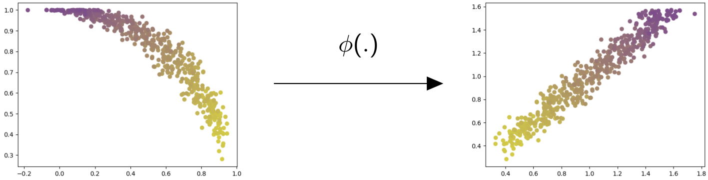

- Now we can do PCA! / Maintenant on peut faire PCA!
- Note that we can use a $\Phi(.)$ function that increases the dimensionality as well. / Notez qu'on peut aussi utiliser une fonction $\Phi(.)$ qui augmente la dimensionnalité.

From PCA to Kernel PCA

- In regular PCA we do / Dans le PCA régulier on fait:

$$C = \text{cov}(X)$$
$$Cu_i = \lambda_i u_i$$

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$$C = \text{cov}(X)$$
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- In Kernel PCA we will do / Dans Kernel PCA on fera:

$$C := \text{cov}(\phi(x))$$
$$Cu_i = \lambda_i u_i$$

Why do we call it 'Kernel' PCA?

- Let's do some thinking / Réflechissons sur le sujet

$$C = \frac{1}{N} \sum_{n=1}^{N} \phi(x_n)\phi(x_n)^\top$$

  - Let's get the eigenvectors into the picture / Mettons les valeurs propres dans les équations

$$Cu_i = \frac{1}{N} \sum_{n=1}^{N} \phi(x_n) \left(\phi(x_n)^\top u_i \right) = \lambda_i u_i$$

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- We kinda see that $u_i = \sum_n a_{in}\phi(x_n)$. Let's substitute! / On fait cette observation, substitions!

$$\frac{1}{N}\sum_{n=1}^{N}\phi(x_n)\phi(x_n)^\top\sum_{n'}a_{in'}\phi(x_{n'}) = \lambda_i\sum_n a_{in}\phi(x_n)$$

Why do we call it 'Kernel' PCA? (continued)

- Let's multiply both sides by $\phi(l)^\top$, and re-arrange. Multiplions avec $\phi(l)^\top$ de deux cotés et re-arrengons:

$$\frac{1}{N}\sum_{n=1}^{N}\phi(x_l)\phi(x_n)^\top\sum_{n'}a_{in'}\phi(x_n)\phi(x_n') = \lambda_i\sum_{n}a_{in}\phi(x_l)\phi(x_n)^\top$$
$$\rightarrow \frac{1}{N}\sum_{n=1}^{N}k(x_l,x_n)\sum_{n'}a_{in'}k(x_n,x_n') = \lambda_i\sum_{n}a_{in}k(x_l,x_n)$$

- Let's switch to array notation: (remember from lecture 1 that we can do it) / Switchons à la notation d'array (souvenez le cours 1)

$$K^2 a_i = \lambda_i N K a_i$$
$$K a_i = \lambda_i N a_i$$

- We can therefore simply find the eigenvectors of K. Assuming that $\phi(x)$ is zero mean! If not, we need to do more work to remove the mean.
  - On peut alors tout simplement trouver les vecteurs propres de K. Mais notez qu'on a supposé que $\phi(x)$ est zero-mean! On doit travailler davantage si on veut substraitre le moyen.

Projection on to principal components

- Let's think about projection on to eigenvalue v_i of cov($\phi(x)$ / Considérons la projection sur la valeur propre v_i de cov($\phi(x)$).

$$w_i(x) = \phi(x)^\top u_i$$

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$$\begin{aligned} w_i(x) &= \phi(x)^\top u_i \\ &= \sum_n a_{in} \phi(x) \phi(x_n)^\top \end{aligned}$$

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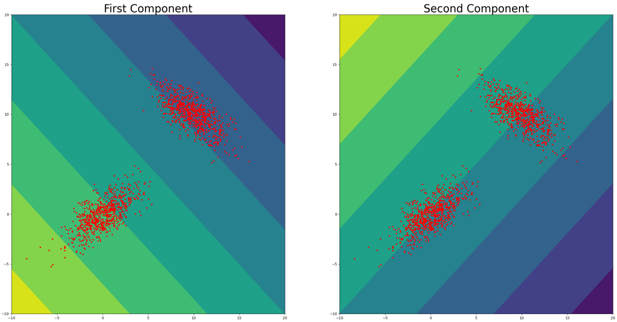
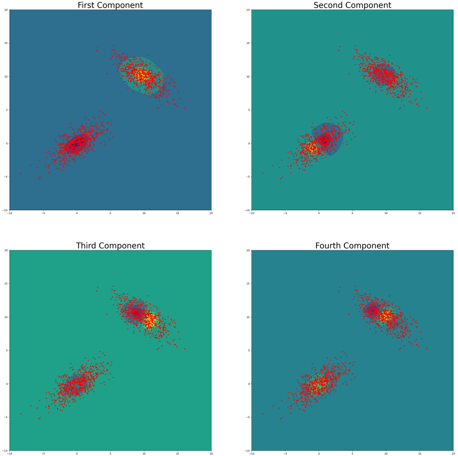
- Notice that the $i'th$ eigenvector a_i of K is of length N, and K is of size $N \times N$, (as opposed to $\text{cov}(x)$ which is $L \times L$). For large datasets this is a limiting factor.
  - Notez que la valeur propre i de K est de longeur N, et K est de taille $N \times N$. (Notez que $\text{cov}(x)$ est de taille $L \times L$) Pour des datasets qui sont large, c'est quelque chose limitante.

Regular PCA components are not very informative



The contours show/ Les contours montre $w_i^\top \begin{bmatrix} x \\ y \end{bmatrix}$.

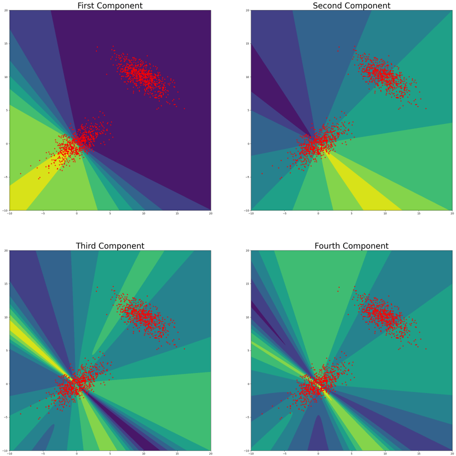
Kernel PCA components



The contours show/ Les contours montre $w_i^\top K\left(\begin{bmatrix} x \\ y \end{bmatrix}, X\right)$.

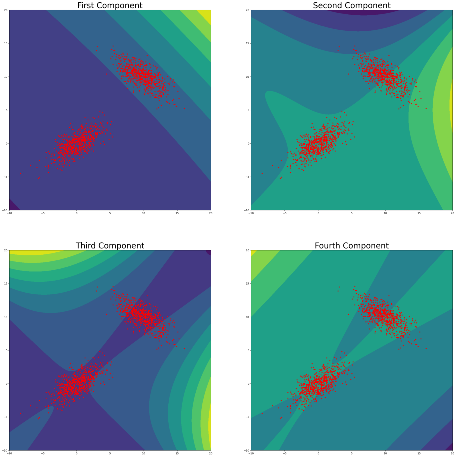
$K = \exp(-\gamma\|x-y\|^2)$ is rbf kernel.

Kernel PCA components



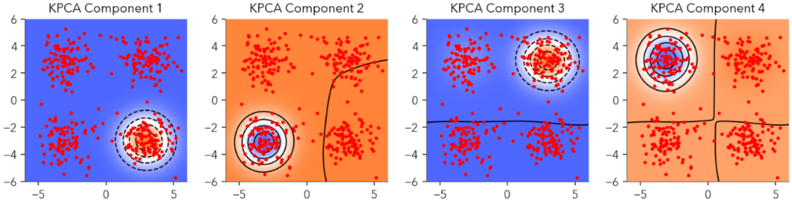
The contours show/ Les contours montre $w_i^\top K\left(\begin{bmatrix} x \\ y \end{bmatrix}, X\right)$. K is sigmoid kernel.

Kernel PCA components



The contours show/ Les contours montre $w_i^\top K\left(\begin{bmatrix}x\\y\end{bmatrix}, X\right)$. K is polynomial kernel.

Kernel PCA Better Performance



with / avec RBF Kernel
Taken from UIUC MLSP class

Kernel PCA Summary

- Performance is highly dependent on the Kernel. / La performance est dependent sur le choix du noyau.

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- Kernel PCA reveals more interesting variations in the data if the Kernel choice is good / Kernel PCA rèvele des variations plus intéssentes dans les données, si le choix du Kernel est bon.

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- Kernel PCA reveals more interesting variations in the data if the Kernel choice is good / Kernel PCA rèvele des variations plus intéssentes dans les données, si le choix du Kernel est bon.
- Kernel PCA is more expensive and not suitable for large datasets / Kernel PCA est computationnalement cher large datasets.

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Multi Dimensional Scaling (MDS)

- MDS tries to find a low dimensional embedding such that the pairwise-distances are preserved.
  - MDS trouve un embedding à bas dimension telle que les distances pairwises sont préservés.
- We construct a matrix of pairwise distances / On construit une matrice des distances pairwises

$$d_{i,j} = \|x_i - x_j\|^2$$

- We want to estimate $\widehat{x}$ such that / on veut estimer $\widehat{x}$ telle que

$$\|\widehat{x}_i - \widehat{x}_j\| \approx d_{ij}$$

- How do we do it? / Comment est-ce qu'on fait ça?

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- How do we do it? / Comment est-ce qu'on fait ça?
  - Eigenvectors / Vecteurs Propres

Let's write it out

- $d_{i,j} = \|x_i - x_j\|^2 = x_i^\top x_i + x_j^\top x_j - 2x_i^\top x_j$
- In matrix form / Dans la forme matricielle

$$D = \underbrace{\text{diag}(X^\top X)1_N^\top}_{\text{copy across columns}} + \underbrace{1_N\text{diag}(X^\top X)^\top}_{\text{copy across rows}} - 2X^\top X$$

- Next we make the columns and rows zero mean
  - On fait les colonnes et les lignes zero-moyenne $Z := I_N - 1_N 1_N^\top / N$
  - DZ removes mean column, ZD removes mean row.
  - We apply this on D, and we can show that / On applique ça sur D et on peut montrer que
- $ZDZ = -2ZX^\top XZ = -2(XZ)^\top(XZ) = -2(X - \mathbb{E}[x])^\top(X - \mathbb{E}[x])$

In other words

- Or define the similarity matrix / définissions la matrice de similarité

$$S := -\frac{1}{2}ZDZ = -\frac{1}{2}\left(D - \frac{1}{N}1_{N\times N}D - \frac{1}{N}D1_{N\times N} + \frac{1}{N^2}1_{N\times N}D1_{N\times N}\right)$$

- Then do an eigen decomposition on $S = (X - \mathbb{E}[x])^\top (X - \mathbb{E}[x]) = U\Lambda U^\top$, Set $\widehat{X} = \Lambda^{-1/2}U^\top$, which is an embedding / qui est un embedding.
- For low-dim embeddings, just use low dimensional version of $\widehat{X}$.

MDS with 3dims

Pretty good!

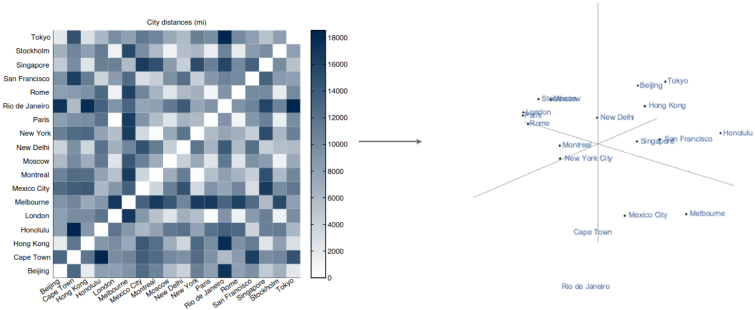

Image taken from UIUC MLSP class

MDS with 2dims

Still pretty good!

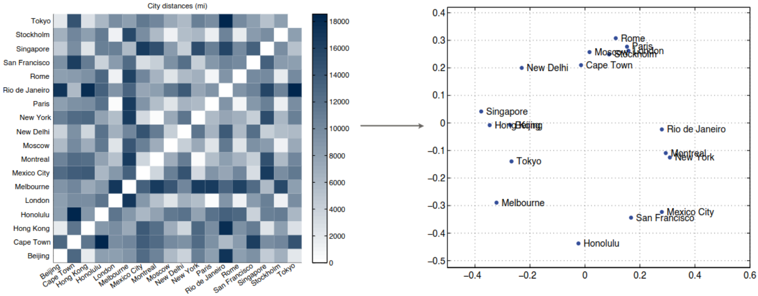

Image taken from UIUC MLSP class

MDS variants

- MDS which uses cosine similarity instead of distances
  - MDS qui utilise la similarité cosinus au lieu de distances
- MDS which uses ranking
  - MDS qui utilise des rankings
- MDS which uses a kernel
  - MDS qui utilise un noyau
- Using only local data
  - Juste usage des données locales

Why MDS?

- MDS finds the implied geometry of the dataset
  - MDS trouve la géometrie de notre dataset.
    - Not obvious in large dimensions / Pas évident si le donnée a beaucoup de dimensions.
- Sort of like PCA
  - Decompose $X^\top X$ au lieu de $XX^\top$.
- Sort of like kPCA also
  - Decompose $X^\top X$
- It's a linear decomposition in the end like PCA and kPCA.
  - Fin de la journée c'est une décomposition linéaire comme PCA et kPCA.

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Actual dimensionality can be misleading

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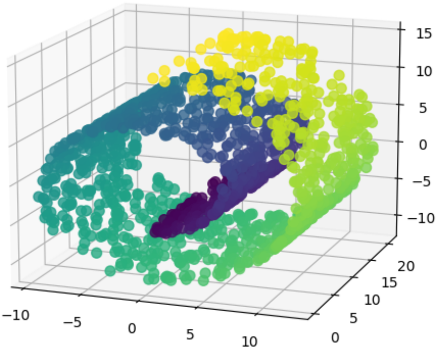
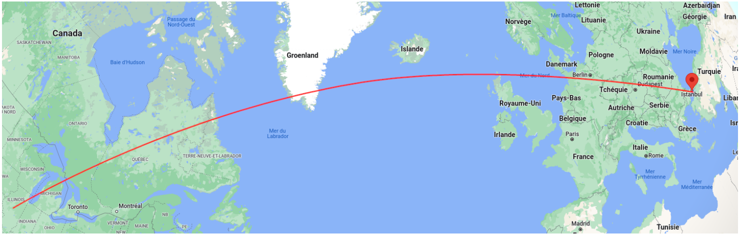


Local vs Global



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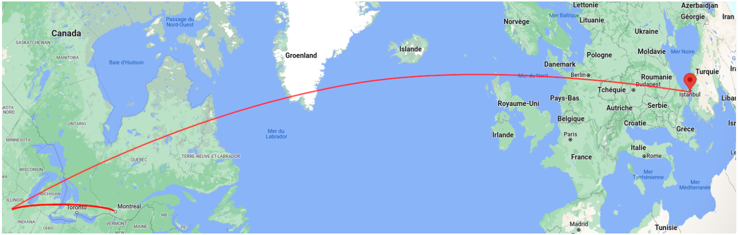
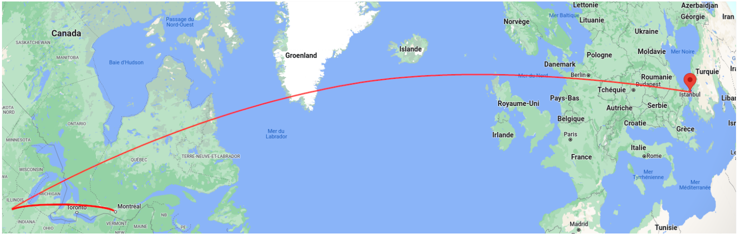


Earth is round, but locally flat (/flatter)! / La terre est ronde mais localement plate ou plus plate

Local vs Global



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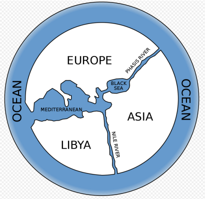
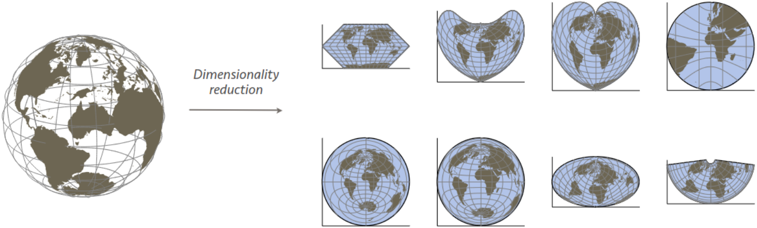


I DON'T MEAN THIS

Map projections

- Many ways to go from 3D to 2D / Plusieurs façons de réduire la dimensionnalité de 3 à 2.



Taken from UIUC MLSP class

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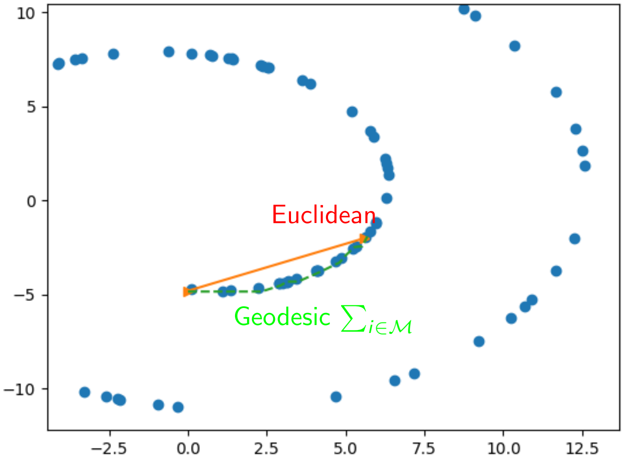
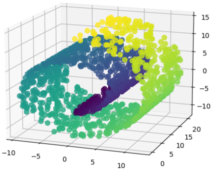
Euclidean vs Geodesic Distance

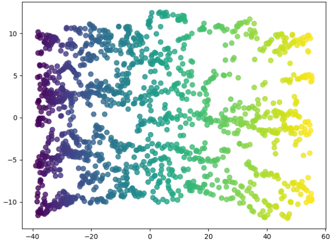


ISOMAP

- MDS with geodesic distances / MDS avec des distances géodesiques.
- Results in embeddings that are more structure aware / Comme ça on obtiens des embeddings qui sont plus consients des structure du manifold.

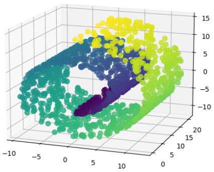
Unroll the swiss roll - ISOMAP

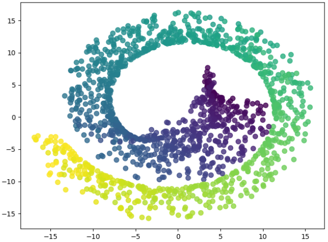




- Pretty good! Maps the geodesic distances well into the euclidean space
  - On est capable de mapper les distances géodesic bien à l'espace euclidienne.

Unroll the swiss roll - MDS





- This doesn't map as well / Ici ça ne map pas aussi bon.

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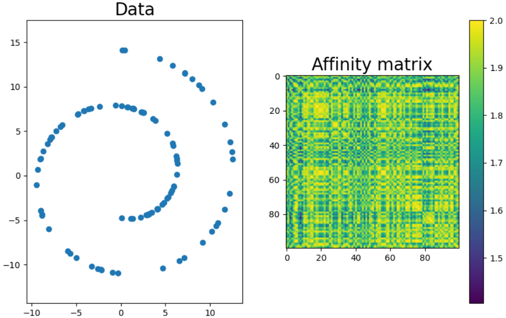
Neighborhood Approach

- Make a note of N nearby points and supress the rest, / Trouve N points qui sont plus proches, ignore les autres.



- Affinity Matrix $w_{i,j} = \exp(-\|x_i - x_j\|)$

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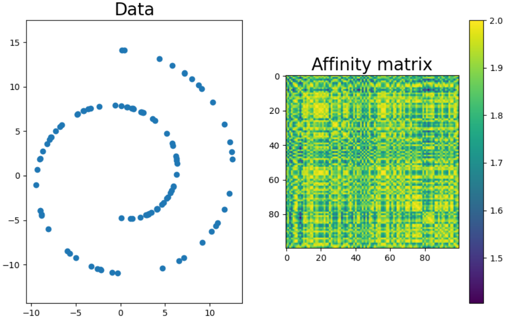

- Affinity Matrix $w_{i,j} = \exp(-\|x_i - x_j\|)$
- (The data is not ordered / Le data n'est pas en ordre)

Laplacian Eigenmap

- Minimize / Minimisons:

$$E_{LE} = \min_{y} \sum_{i,j} \|y_i - y_j\|^2 w_{i,j}$$

- We want / On veut:

	Large $\|y_i - y_j\|$	Small $\|y_i - y_j\|$
Large w_{ij}	**Bad**	Good
Small w_{ij}	Good	Don't care

- In matrix form / Dans la forme matricielle:

$$E_{LE} = 2Y^\top LY$$
$$L = \underbrace{W - \text{diag}(1^\top W)}_{\text{Graph Laplacian}} = W - R$$

Laplacian Eigenmap Solution

- The solution (Note that we normalize the Laplacian) / Notez qu'on normalise la Laplacienne.

$$\min_Y Y^\top \underbrace{R^{-1/2} L R^{-1/2}}_{\text{normalized Laplacian}} Y$$

$$s.t.\ Y^\top R^2 T = I$$

- What will be the solution? / C'est quoi la solution? (On a déjà vu des choses similaires)

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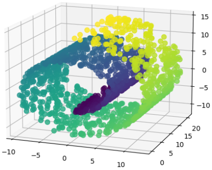
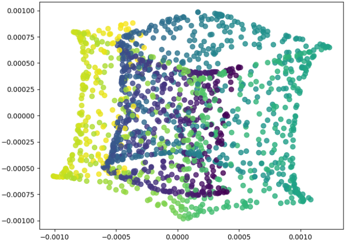
- What will be the solution? / C'est quoi la solution? (On a déjà vu des choses similaires)
- $\widehat{L} = U \Sigma U^\top$. $\widehat{Y} = U \Sigma^{-1/2}$.
- But this time we take the smallest eigenvalues. (We are minimizing)
  - Mais cette fois on prends les valeur propres qui sont petits. (On est en train de minimiser)

Unroll the swiss roll - Laplacian Eigenmap





- The Kernel distance isn't as good as geodesic distance / La distance de Kernel n'est pas aussi bon pour le problème.

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TSNE

- This is a very popular visualization tool / Un outil très populaire
- The idea is to define inter-sample similarity metrices in high and low dimensional spaces / L'idée est de définir des mésures de similarités dans l'espace originale et la projection

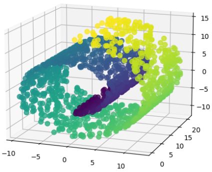
$$\text{Original space} \rightarrow p_{i,j} \approx \frac{\exp(-\|x_i - x_j\|^2/2\sigma_i^2)}{\sum_{k\neq i}\exp(-\|x_i - x_j\|^2/2\sigma_i^2)}$$

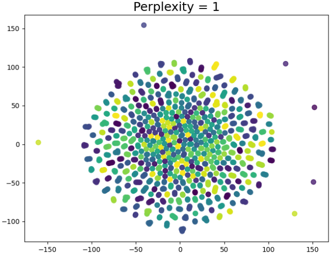
$$\text{Low-dim space } \rightarrow q_{i,j} \approx \frac{(1+\|y_i - y_j\|^2)^{-1}}{\sum_k \sum_{l\neq k}(1+\|y_l - y_k\|^2)^{-1}}$$

- Minimize via gradient descent wrt y: / Minimisons pour y avec gradient descent:

$$KL(p||q(y)) = \sum_{i\neq j} p_{ij} \log \frac{p_{ij}}{q_{ij}(y)}$$

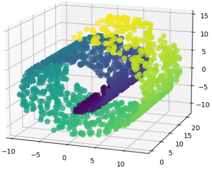
Unroll the swiss roll - TSNE

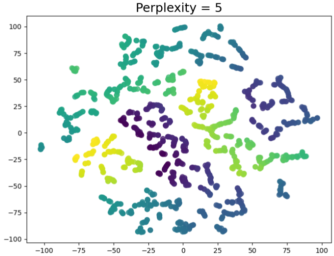




- Perplexity ((σ_i) related to number of neighbors) changes results a lot! / Perplexité (lié à la taille du voisinage) affecte les résultats beaucoup!

Unroll the swiss roll - TSNE





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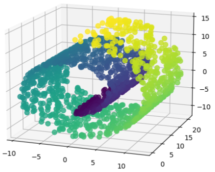

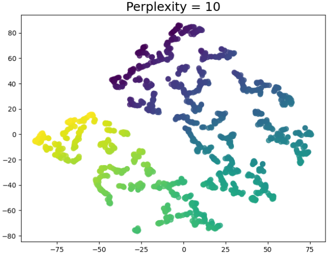

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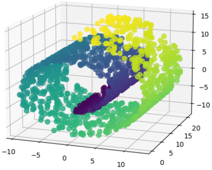

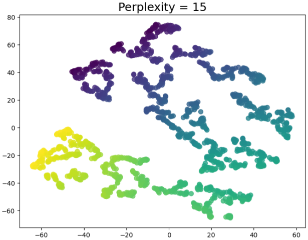

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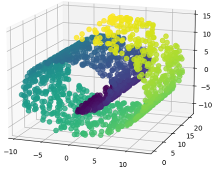

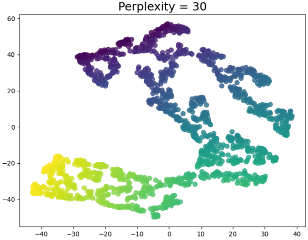

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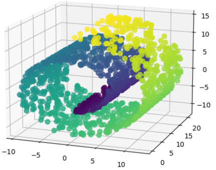

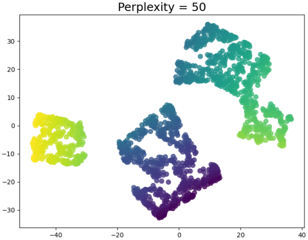

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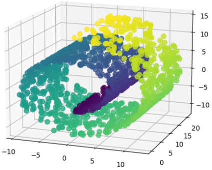

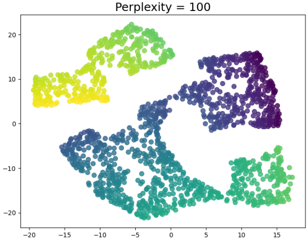

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Table of Contents

Locally Linear Embedding

- Consider local neighboorhood of each point / Considérons le voisinage locale des points
  - Assume each neihborhood is linear / Supposons que le chaque voisinage est linéaire

$$x_i \approx \sum_{j \in \mathcal{N}(i)} w_{ij} x_j$$

- Then we solve the following problem / Puis on résouds la problème suivante:

$$\min_W \sum_i \|x_i - \sum_{j \in \mathcal{N}(i)} w_{ij} x_j\|^2$$
$$s.t. \sum_j w_{ij} = 1$$

- It's a convex problem, and can be solved easily.

Locally Linear Embedding - Finding y

- The weights will work just as well / Les poids qu'on avait trouvé fonctionnera dans faible dimensionnalité aussi
- We fix w_{ij}, and then solve, / On fixe w_{ij} et pis résouds,

$$\min_y \sum_i \|y_i - \sum_{j \in \mathcal{N}(i)} w_{ij} y_j\|^2$$

Locally Linear Embedding - Finding y

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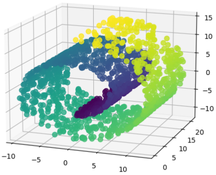
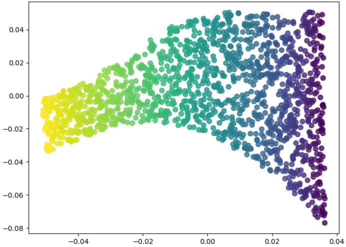
$$\min_y \sum_i \|y_i - \sum_{j \in \mathcal{N}(i)} w_{ij} y_j\|^2$$

- And (not surprisingly) , the solution is an eigendecomposition problem. / La solution est encore une fois décomposition des valeurs propres.
- We eigendecompose $(I - W)^\top (I - W)$, and take the eigenvectors that correspond to the smallest eigenvalues.... / On decompositionne $(I - W)^\top (I - W)$, pis prends les vecteurs propres qui correspond aux valeurs propres plus petits.

Unroll the swiss roll - LLE

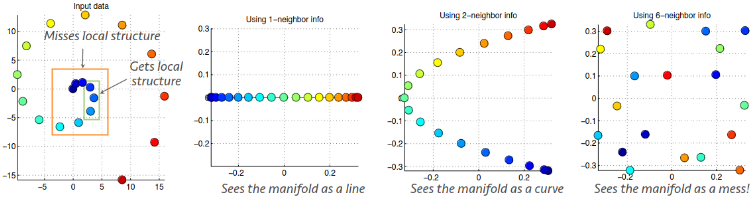




- Not that bad! / Pas si mauvais!

A note on the manifold methods

- Modeling the local structure is important! If you use too large neighborhoods, you will lose the structure.
  - C'est important d'etre capable à modéliser la structure locale. Si on utilise des voisinages qui sont trop larges, on perdra la structure.



Taken from UIUC MLSP class

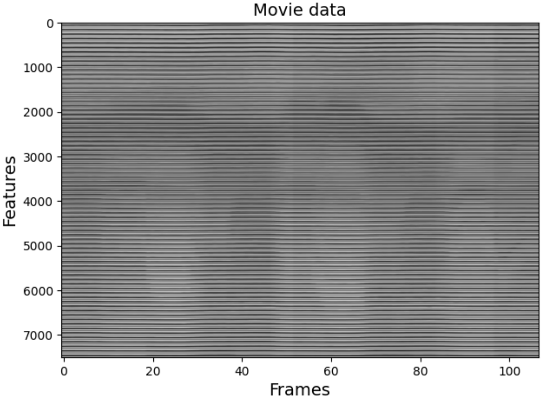
A video example

- High dimensional input $100 \times 75 = 7500$ dimensions / Une entrée à haute dimensions.
- Low dimensional structure, Moving lips around
  - Structure de petite dimensionnalité. Je bouge les levres.
- Can we simplify this? Peut-on simplifier cela?

`Watch`

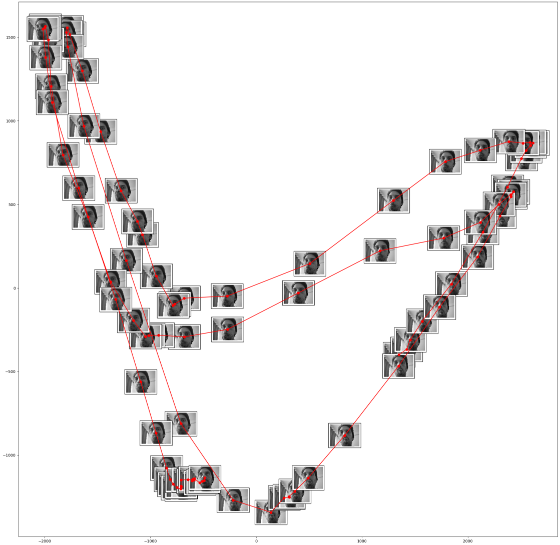
Frames

Unraveled

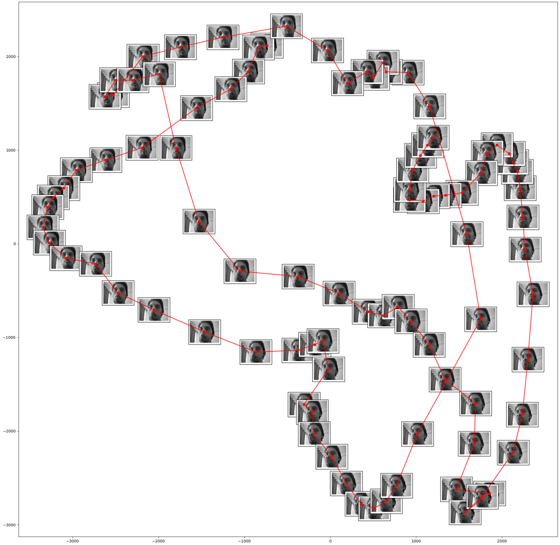


Movie data
Features
Frames
0
1000
2000
3000
4000
5000
6000
7000
0
20
40
60
80
100

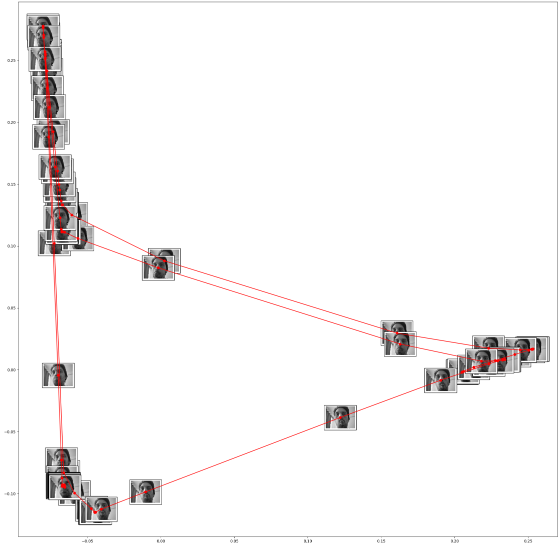
PCA



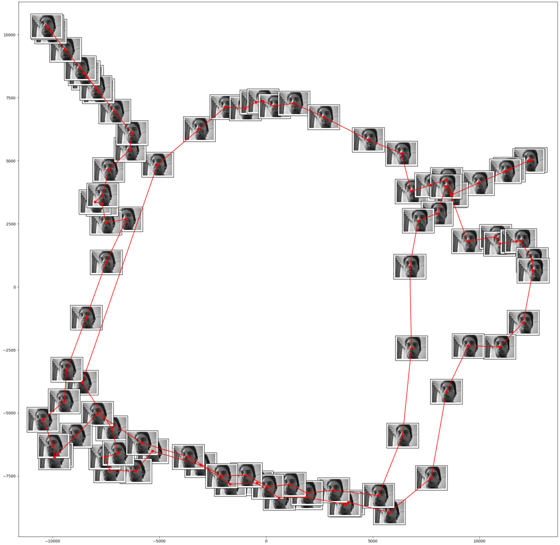
MDS



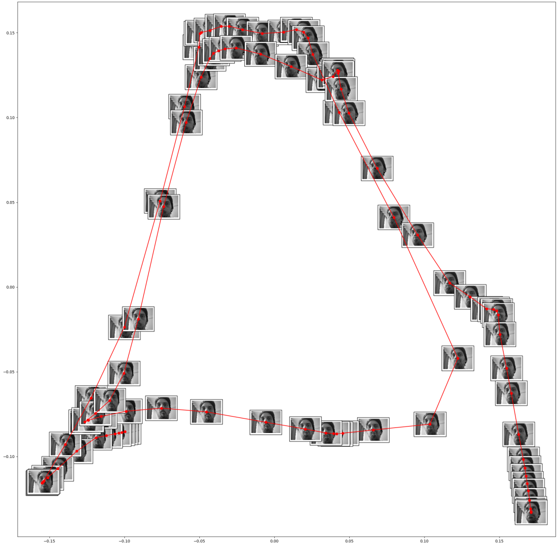
Laplacian Eigenmaps



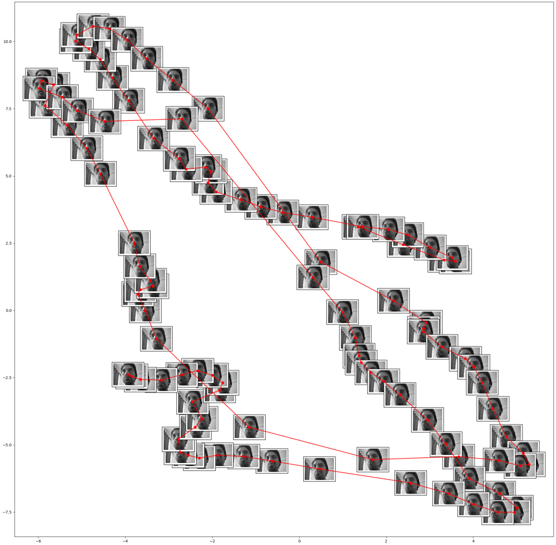
ISOMAP



LLE



TSNE

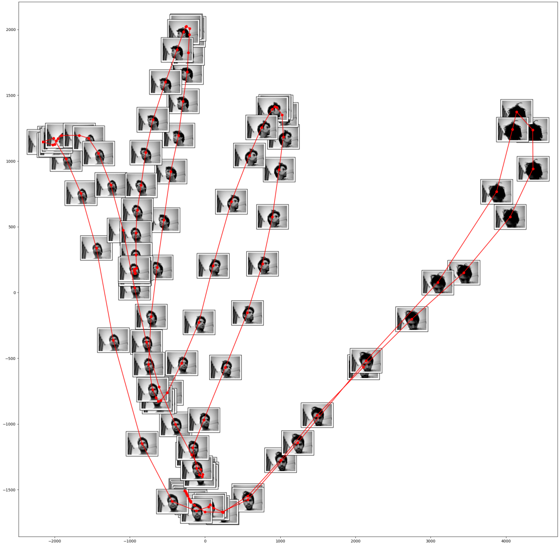


Another example

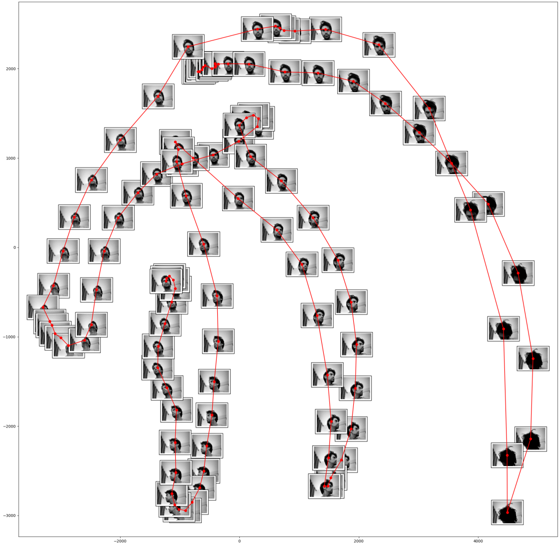
- This time we have distinct axes, left,right,up,down head movements
  - Cette fois-ci on a des mouvements distinctes, gauche, droite, haut, bas

Watch

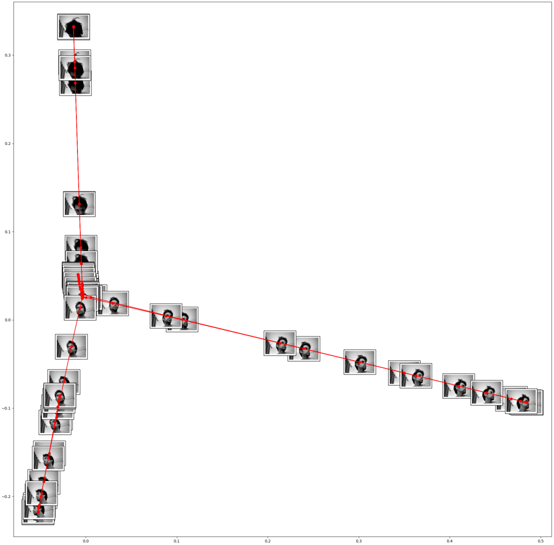
PCA


2000
1500
1000
500
0
−500
−1000
−1500
−2000
−1000
0
1000
2000
3000
4000

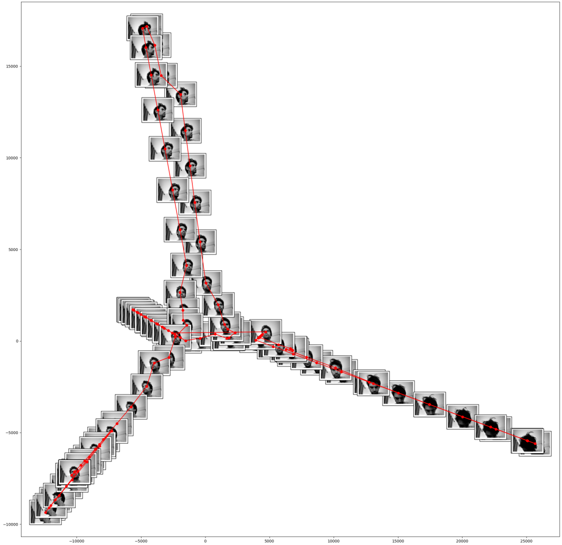
MDS



Laplacian Eigenmaps



ISOMAP



15000
10000
5000
0
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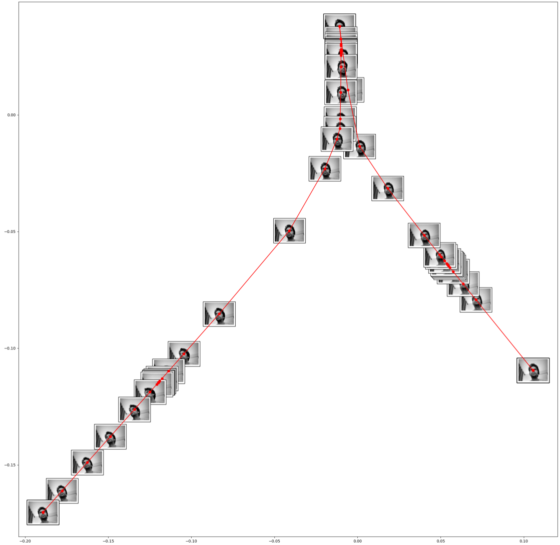
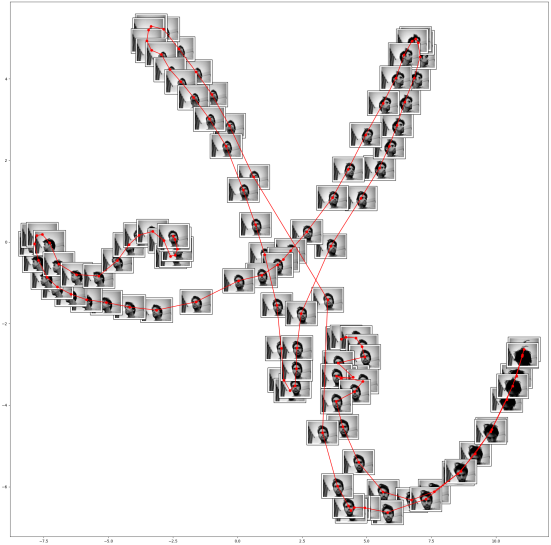
−10000
−10000
−5000
0
5000
10000
15000
20000
25000

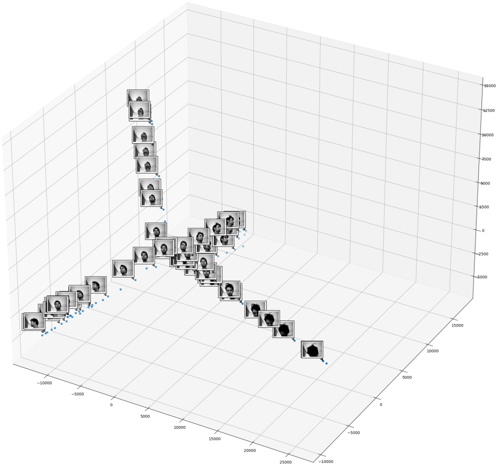
LLE



TSNE



ISOMAP



Even better! – learns 4 axes. / on apprend 4 axes

So, which method do we use?

- It depends. Pays off to experiment with different hyperparameters.
    - Ça depends. C'est bien d'experimenter avec différents approches.

Recap

- Kernel PCA: Map to another space where things are more appropriate for PCA. / On map à une autre espace plus approprié pour PCA.
- MDS: A transform which presevers pairwise distances.
- Manifolds
  - ISOMAP
  - Laplacian Eigenmaps
    - Locally Linear Embeddings

Suggested Reading

- LLE: https://cs.nyu.edu/~roweis/lle/papers/lleintro.pdf
- Kernel PCA: Bishop Chapter 12, https://citeseerx.ist.psu.edu/viewdoc/download;jsessionid=476974F6AA53BD038615E67656102714?doi=10.1.1.128.7613&rep=rep1&type=pdf
- Laplacian Eigenmaps: https://papers.nips.cc/paper/2001/file/f106b7f99d2cb30c3db1c3cc0fde9ccb-Paper.pdf

Next class

- Classification / Deep Learning (this time for real)