IFT 4030/7030, Machine Learning for Signal Processing

Week4: Machine Learning 1, Decompositions

Cem Subakan

Admin

- Did you have a chance to read the project proposal document?
  - Avez-vous regardé le document sur les proposals de projets?
- The deadline for the labs will be strict from lab 2 on.
  - On aura un deadline stricte pour les labos en commançant par labo 2.
- The first homework will be released soon!
  - Le devoir 1 va sortir bientot!

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- Today: We are starting with machine learning.
  - Aujourd'hui on commence avec l'apprentissage automatique.

This week

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- Today, our aim is to build the foundation for training machine learning models.
- Au'jourdhui le but est de batir le fondation pour l'entrainement des modèles.
- More specifically, we will build a framework around learnable decompositions.
  - Plus spécifiquement on va batir un framework autour des decompositions appris.

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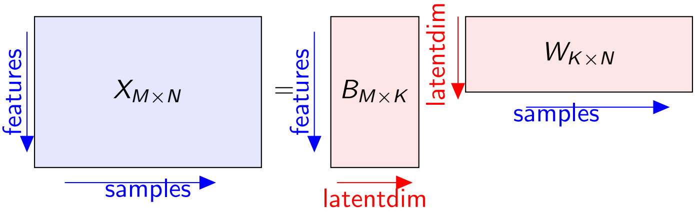
The framework

$$\underbrace{X}_{\substack{\text{Data}\\\text{Matrix}}} = \underbrace{B}_{\text{Bases}} \times \underbrace{W}_{\substack{\text{Activations}\\\text{(Embeddings)}}}$$



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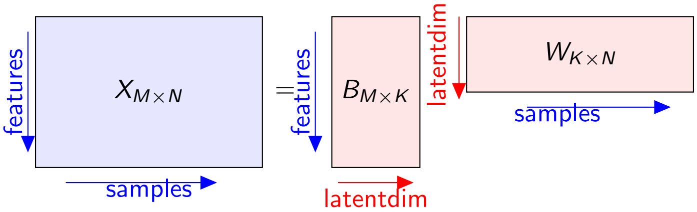

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  - Notez qu'on est en train de trouver un embedding de K dimensions pour un data qui a M dimensions.

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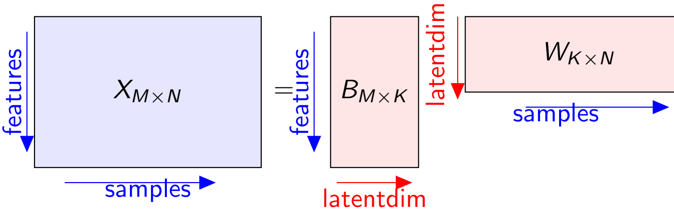

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  - Notez qu'on est en train de trouver un embedding de K dimensions pour un data qui a M dimensions.
- We embed X, in the space defined by the columns of B.
  - On embed X dans une espace definit par les colonnes de B.

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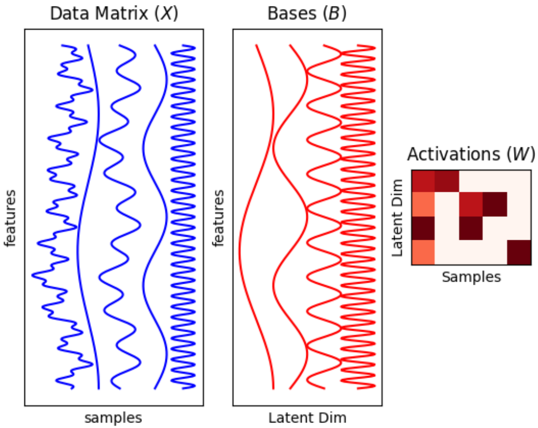
Example

- Remember this from last week?
  - Vous-vous en souvenez ça de la semaine passée?



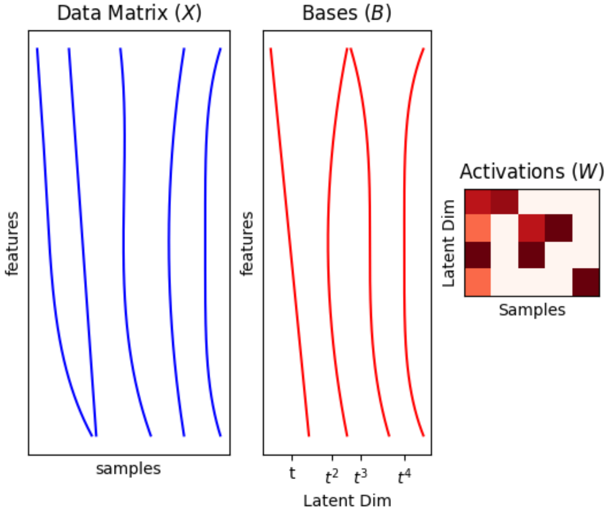
The goal

- We are trying to build a framework that can effectively reduce dimensionality, to explain data in a concise way.
  - On essaie de batir un framework qui peut effectivement reduire la dimensionalité et expliquer les données de manière parsimonieux.

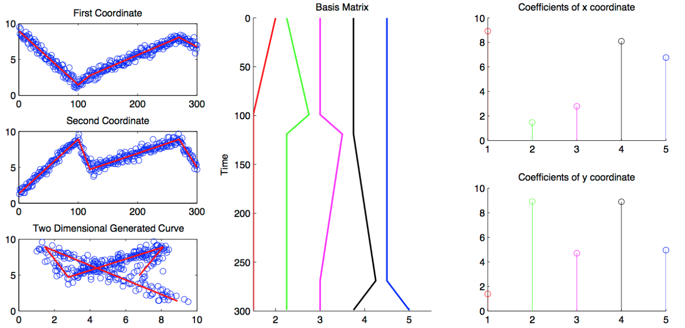
The goal

- We are trying to build a framework that can effectively reduce dimensionality, to explain data in a concise way.
  - On essaie de batir un framework qui peut effectivement reduire la dimensionalité et expliquer les données de manière parsimonieux.
- We can use basis functions other than sinusoids!
  - On peut utiliser des bases autres que les sinusoids!

Non-sinusoids (finally)

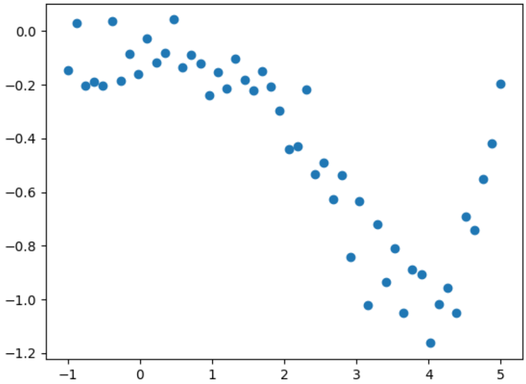


Piece-wise functions!!



But why, I still don't get it?

- One application might be do to regression.
  - On peut faire de la regression avec ce framework.



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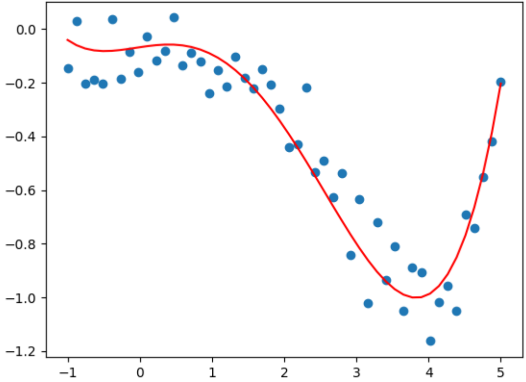
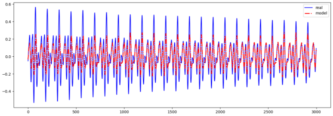
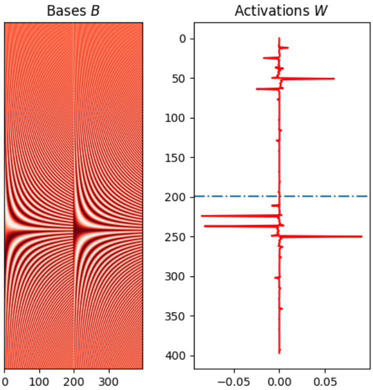


Something a bit more real

- Modeling a guitar string `Listen Real`, `Listen the Model`
  - Modélisons un corde de guitare





Visualizing the model ingredients

$$\underbrace{\begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_T \end{bmatrix}}_{\mathrm{x}} = \underbrace{\begin{bmatrix} b_1(1) & b_2(1) & \dots & b_K(1) \\ b_1(2) & b_2(2) & \dots & b_K(2) \\ \vdots & \vdots & \ddots & \vdots \\ b_1(T) & b_2(T) & \dots & b_K(T) \end{bmatrix}}_{B} \underbrace{\begin{bmatrix} w_1 \\ w_2 \\ \vdots \\ w_K \end{bmatrix}}_{\mathrm{w}}$$

- $b_k(t)$ is the k'th basis function in the basis (design) matrix B.
  - $b_k(t)$ est la fonction de base k'eme dans la matrice de base.
- The output is a linear combination of the basis functions such that
  - La sortie du modèle est la combination linéaire des bases:

$$x_t = \sum_{k=1}^{K} w_k b_k(t) = w_1 b_1(t) + w_2 b_2(t) + \cdots + w_K b_K(t).$$

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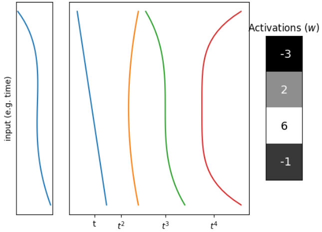
- Here's an example design matrix with polynomial basis functions. This particular choice is also called a Vandermonde matrix.
  - Voici un matrice de desin exemplaire avec fonctions de bases polynomiel. On appele ce choix la matrice Vandermonde.



Even autoregressive modeling

Autoregressive Modeling

$$\underbrace{\begin{bmatrix} x_{K+1} \\ x_{K+2} \\ \vdots \\ x_T \end{bmatrix}}_{y} = \underbrace{\begin{bmatrix} x_K & x_{K-1} & \cdots & x_2 & x_1 \\ x_{K+1} & x_K & \cdots & x_3 & x_2 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ x_{t-2} & x_{t-3} & \cdots & x_{t-K+2} & x_{t-K+1} \\ x_{t-1} & x_{t-2} & \cdots & x_{t-K+1} & x_{t-K} \end{bmatrix}}_{B} \underbrace{\begin{bmatrix} w_1 \\ w_2 \\ \vdots \\ w_K \end{bmatrix}}_{\mathrm{w}}$$

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Autoregressive Modeling **LLM:Linear Language Model** (I am joking)

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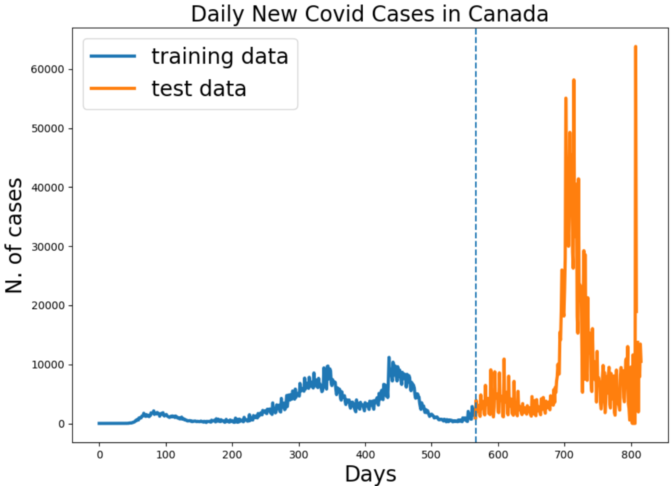
Btw, do see that we have a series of convolutions? / En passant, vous voyez vous qu'on fait des convolutions?

Real Real-life data

- We try to fit a regression model with autoregressive design matrix on nbr. of cases data with $K = 3$. / On utilise un matrice de design qui est autoregressive. On utilise un filtre de $K = 3$.



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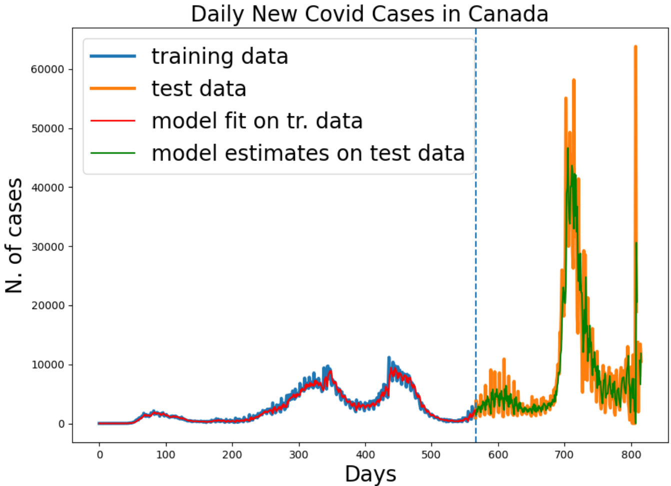

How to learn W?

- Consider the following model (Linear Regression):
  - Considérons la modèle suivante (Regression Linéaire):

$$\begin{aligned} w_n &\sim \mathcal{N}(\mathrm{w}_n; 0, \sigma_0^2 I) \\ x_{t,n} | w_n &\sim \mathcal{N}(x_t; B(t)\mathrm{w}_n, \sigma^2 I) \end{aligned}$$

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- Let's write the model likelihood / Écrivons le likelihood du modèle,

$$\begin{aligned} \mathcal{L} := \log p(x_{1:T,n}, \mathrm{w}_n) &= \sum_t p(x_{t,n}|\mathrm{w}_n) + \log p(\mathrm{w}_n) \\ &= \sum_t \log \mathcal{N}(x_t; B(t)\mathrm{w}_n, \sigma^2 I) + \log \mathcal{N}(\mathrm{w}_n; 0, \sigma_0^2 I) \end{aligned}$$

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$$

- What should we do next to estimate $\mathrm{w}_{1:N}$?
  - Qu-est qu'on fait maintenant pour estimer $\mathrm{w}_{1:N}$?

Finding the best w_n

- Now, we will take the gradient of $\mathcal{L}$ with respect to w_n, set it equal to zero and solve for w_n. We switch to matrix-vector notation, and drop the n index to reduce clutter.

$$
\begin{aligned}
\mathcal{L} &\propto (B\mathrm{w}-\mathrm{x})^\top (B\mathrm{w}-\mathrm{x}) \\
&= -\frac{1}{2\sigma^2}\left(\mathrm{w}^\top B^\top B\mathrm{w} - 2\mathrm{w}^\top B^\top \mathrm{x} + \mathrm{x}^\top \mathrm{x}\right) - \frac{1}{2\sigma_0^2}\left(\mathrm{w}^\top w\right)
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- And the gradient,

$$\frac{\partial \mathcal{L}}{\partial \mathrm{w}} = -\frac{1}{\sigma^2}\left(\mathrm{B}^\top \mathrm{B}\mathrm{w} - \mathrm{B}^\top \mathrm{x}\right) - \frac{1}{\sigma_0^2}\mathrm{w} \tag{1}$$

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$$

- Solve for w,

$$
\begin{aligned}
\frac{1}{\sigma^2}\left(B^\top B\mathrm{w} - \mathrm{B}^\top \mathrm{x}\right) - \frac{1}{\sigma_0^2}\mathrm{w} =& 0 \\
\left(B^\top B + \frac{\sigma^2}{\sigma_0^2} I\right)\mathrm{w} =& B^\top \mathrm{x} \\
\rightarrow \widehat{w} = \left(B^\top B\mathrm{w} + \frac{\sigma^2}{\sigma_0^2} I\right)^{-1} & B^\top \mathrm{x}
\end{aligned}
$$

The MAP solution for w_n

- Note this is the MAP solution for w_n for $n \in \{1, \ldots, N\}$ that we saw before:
  - Notez que c'est la solution MAP pour w_n, $n \in \{1, \ldots, N\}$:

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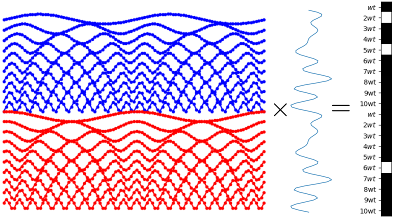
- Ok, but were we doing this last week? Is this optimal?
- D'accord, on faisait ça la semaine denière? Est-ce optimale?



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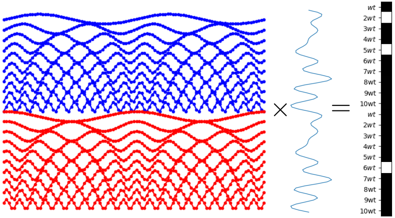

- **Yes!/Oui!**

Fourier Transform Maximizes Gaussian Likelihood

- Let's see / Voyons:

$$\widehat{\mathrm{w}}_n = \left(B^\top B\right)^{-1} B^\top$$

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$$\widehat{w}_n = \underbrace{\left(B^\top B\right)^{-1} B^\top}_{B^\dagger} x$$

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- We can then deduce that DFT maximizes the Gaussian Likelihood under this linear regression / decomposition model! (or minimizes $l2$ error)
  - On peut alors déduire que DFT maximise le likelihood Gaussian sous ce modèle. (ou il minimise l'erreur $l2$.)

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Let's learn B too!

- Note that earlier we were only learning the activations W for a fixed basis matrix B:
  - On apprenait juste les activations W pour des bases fixes B:

$$\min_{W} \|X - BW\|$$

  - But, we can learn B too!
  - Mais, on peut apprendre B aussi!

$$\min_{B,W} \|X - BW\|$$

But how?

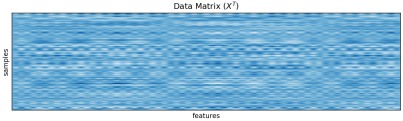
- We can alternate the least squares solution such that,
  - On peut juste alterner entres les solutions least-squares,

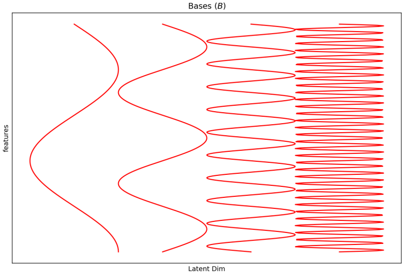
Algorithm 1 Alternating Least Squares

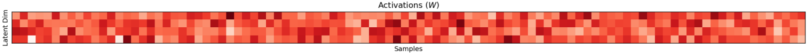
procedure ALTERNATING LEAST SQUARES
Input: Input Data Matrix X. Threshold value ϵ.
Output: Estimated Basis and Activation Matrices $\widehat{B}$, $\widehat{W}$.
    Initialize $\widehat{B}$, $\widehat{W}$.
    while $\|X - \widehat{B}\widehat{W}\| \geq \epsilon$ **do**
        $\widehat{W} = \widehat{B}^{\dagger}X$
        $\widehat{B} = X\widehat{W}^{\dagger}$
    end while
end procedure

Alternating Least Squares Dataset

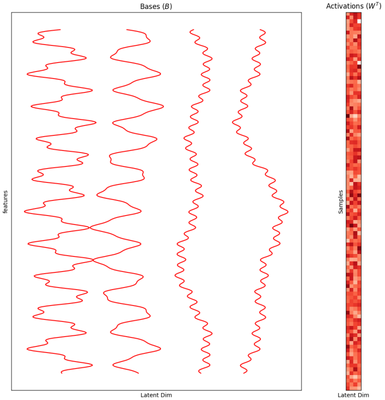
- Let's try alternating least squares on this dataset
  - Essayong cet methode sur ce dataset







The result



- Kinda good, but we can do better.
  - Ça fait quelque chose, mais pas idéale.

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- We want to find an orthogonal transformation $B^\top B = I$, so that $W = B^\top X$.
  - On veut trouver une transformation orthogonale.
- Let's calculate:

$$\begin{aligned}
\mathrm{covar}(w) =& \mathrm{covar}(B^\top x) \\
=& B^\top \underbrace{\mathbb{E}[(x - \mathbb{E}[x])(x - \mathbb{E}[x])^\top]}_{:=C} B
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- So basically want to solve for B such that $B^\top C B = I$, that is C is whitened.
  - Dans le fond on veut blanchir C.

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- Let's calculate:

$$\begin{aligned}\mathrm{covar}(w) =& \mathrm{covar}(B^\top x) \\ =& B^\top \underbrace{\mathbb{E}[(x - \mathbb{E}[x])(x - \mathbb{E}[x])^\top]}_{:=C} B\end{aligned}$$

- So basically want to solve for B such that $B^\top C B = I$, that is C is whitened.
  - Dans le fond on veut blanchir C.
- Any ideas? (Ei.. SV.. ?)

Eigenvectors to the rescue

- Consider the SVD of C, s.t. $C = U\Sigma U^\top$. **(Same as eigenvalue decomp. why?)**
  - Considérons le SVD de C.

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$$B^\top U\Sigma U^\top B = I$$

- We can easily see that $B = U\Sigma^{-1/2}$ does the job!
  - On a trouvé la solution $B = U\Sigma^{-1/2}$!

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$$B^\top U\Sigma U^\top B = I$$

- We can easily see that $B = U\Sigma^{-1/2}$ does the job!
  - On a trouvé la solution $B = U\Sigma^{-1/2}$!
- The columns of U are the eigenvectors of C!
  - Les colonnes de U sont les vecteurs propres de C.

A note on variance

- Note that this way we maximize the variance along the direction of b_1. / Cette solution maximise la variance sur la direction de b_1.

$$\mathcal{V} := \mathrm{var}(b_1^\top x) = b_1^\top \mathbb{E}[(x - \mathbb{E}[x])(x - \mathbb{E}[x])^\top] b_1$$

- Let's maximize this variance such that $b_1^\top b_1 = 1$. / Maximisons la variance telle que b_1 est de norme unitaire.

$$\begin{aligned}\mathcal{V} =& b_1^\top C b_1 - \lambda b_1^\top b_1 \\ \frac{\partial \mathcal{V}}{\partial b_1} =& 2Cb_1 - \lambda b_1 \\ \rightarrow Cb_1 =& \lambda b_1\end{aligned}$$

- So, we have the definition of an eigenvector... / Donc c'est la définition du vecteur propre de C.

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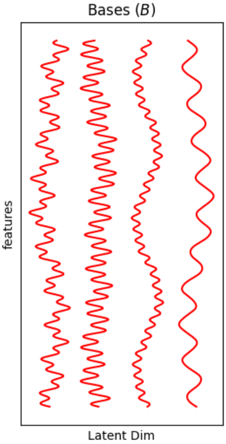
- So, we have the definition of an eigenvector... / Donc c'est la définition du vecteur propre de C.
- Similarly the other principal components are found..
  - Similairement, les autres components principaux sont trouvés..

The recipe for PCA

- $X - \mathbb{E}[x] = U\Sigma V^\top$
- $(X - \mathbb{E}[x])(X - \mathbb{E}[x])^\top = C = U\Sigma^2 U^\top$.
- We said that we need the eigenvectors of C, which are the columns of U. / On a besoin de calculer les vecteurs propres de C, qui sont les colonnes de U.
- We also note that the left singular vectors of $X - \mathbb{E}[x]$ also give the same result.
  - On note aussi que les vecteurs singulaires gauche de $X - \mathbb{E}[x]$ donnent la meme resultat.

PCA on our sinusoid basis problem

- A bit better!



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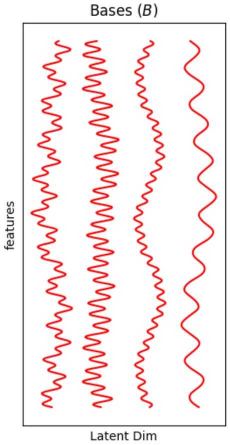
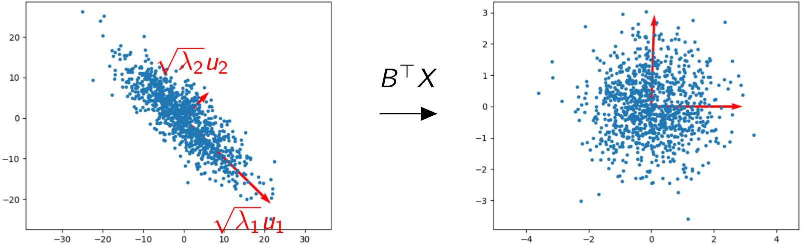


- We can improve this! (more on this later ICA)
  - On peut améliorer ça. (On verra)

Interpretation of PCA



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

Dimensionality Reduction with PCA

- Note that PCA makes the following decomposition / On fait la décomposition suivante:

$$\mathrm{var}(X) = \sum_{k=1}^{K} \lambda_k u_k u_k^\top$$

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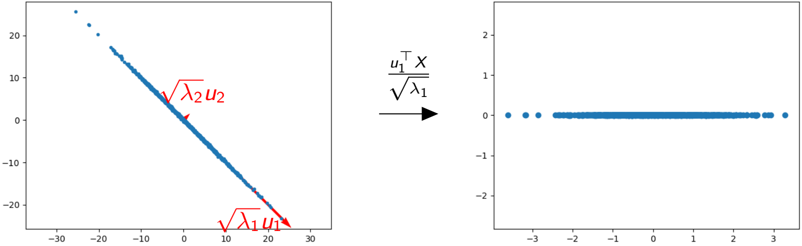

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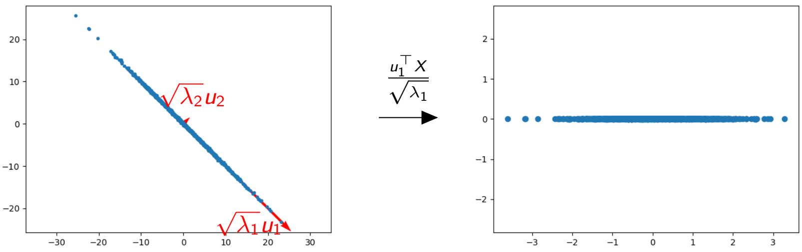
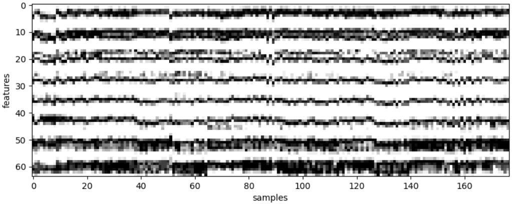


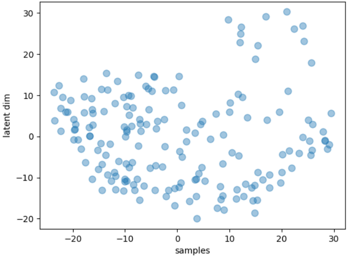
- $\lambda_1 = 10$, $\lambda_2 = 0.1$. Most of the variance is along one direction. We can only use one dim. / La variance est sur une direction. On peut s'en débarrasser d'une direction.

Embedding digits in 2 dimensions

- We only keep two dimensions / On garde juste 2 dimensions



$B^\top(X - \mathbb{E}[x])$



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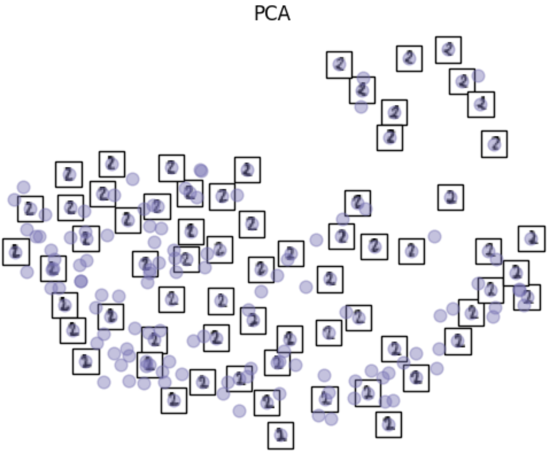
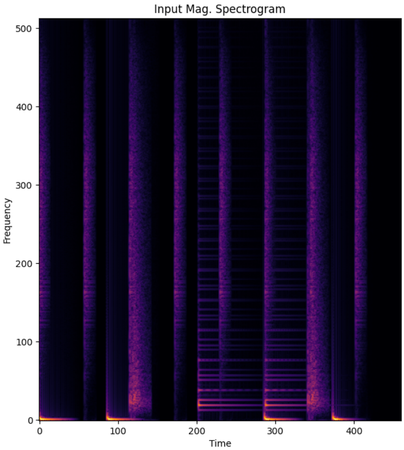
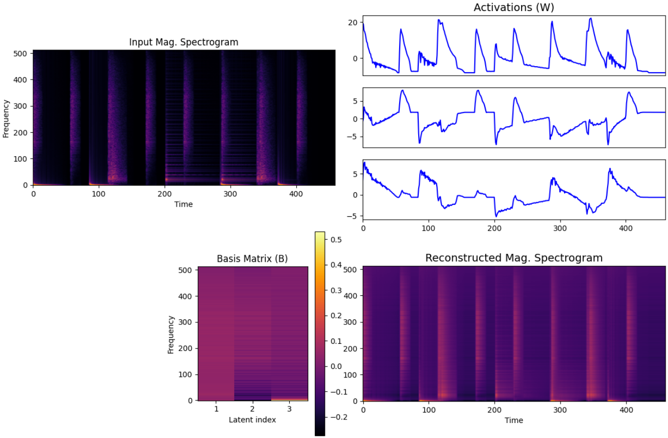


Embedding spectra

- Let's embed this spectrogram into a 3 dim. space / On va embedder ce spectrogram dans un 3 dim. espace. `Listen`



Embedding spectra with PCA



PCA on time-series

- Let's apply PCA on local windows of a time series / Appliqueons PCA on des fenetres d'un time series

$$x_1, x_2, \dots, x_T$$

- Pack in a data matrix as follows

$$X = \begin{bmatrix} x_1 & x_{1+s} & x_{1+2s} & \dots \\ x_2 & x_{2+s} & x_{2+2s} & \dots \\ \vdots & \vdots & \vdots & \ddots \\ x_N & x_{N+s} & x_{N+2s} & \dots \end{bmatrix}$$

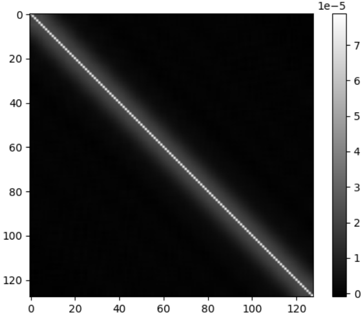
- Note that if we do $W = FX$, this is equal to Short-Time-Fourier-Transform that we saw last week.
  - Notez que si on utilise les bases de Fourier ça donne STFT.
    - s is the hopsize we saw for STFT. / s est le hopsize, meme que STFT.

But let's do PCA instead

- Let's consider this process / Considerons cette processus

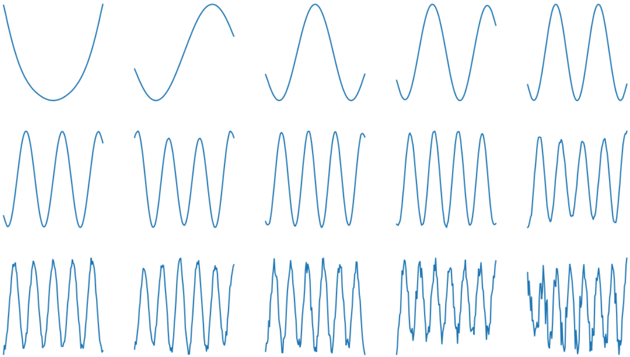
$$x_t = x_{t-1} + 0.825x_{t-2} + 0.65x_{t-3} + 0.475x_{t-4} + 0.3x_{t-5} + n$$

  - $n \sim \mathcal{N}(0, 0.008^2)$
- The covariance matrix



  - A circulant matrix! / Une matrice circulante!

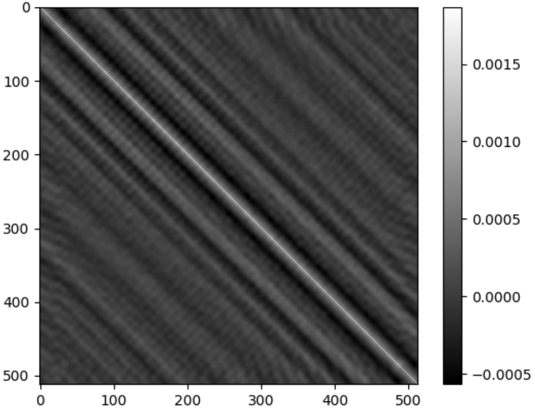
Sinusoids!



Sinusoids (DCT bases are eigenvectors of circulant matrices) .. / Les bases sinusoids sont les vecteurs propres des matrices circulants.

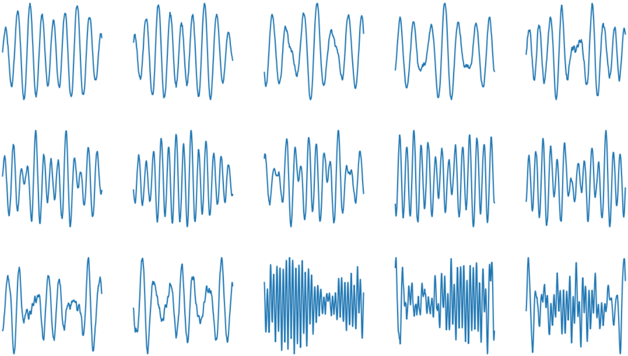
Same thing on speech

- And here's the covariance matrix for a 14sec long speech signal.
  - Matrice de covariance pour un parole de 14secondes.



- Seems like we have high covariance in the neighborhood, then some periodicity.
  - Haut covariance locale, et un peu de périodicité.

Sinusoids!



Listen
So, it seems sinusoidal bases are kinda statistically optimal for local covariance as well.. / Les bases sinusoids sont optimale si on a une covariance locale!.

Table of Contents

Independent Component Analysis (ICA)

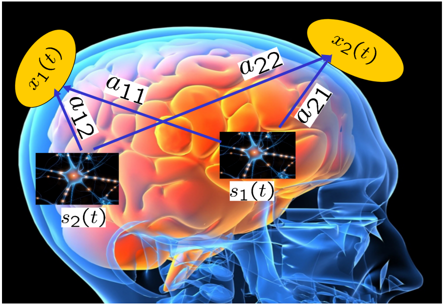
- ICA estimates a square mixing matrix $B \in \mathbb{R}^{K \times K}$, such that,
  - ICA estime un matrice carré B, telle que,

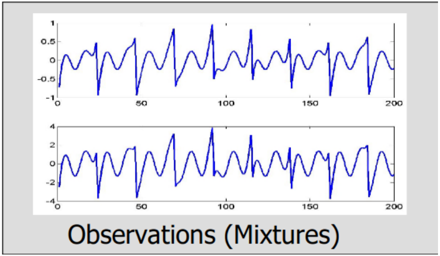
$$x = Bw + n$$

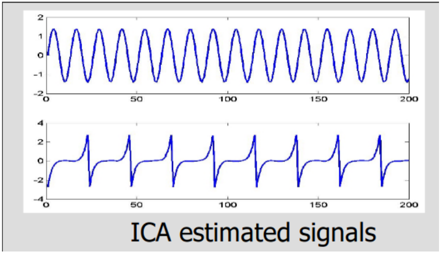
  the elements of $w \in \mathbb{R}^K$ are statistically independent. / les élements du vecteur w sont statisquement indépendent.

- We want to achieve $p(w) = p(w_1)p(w_2)\dots p(w_K)$.
  - On veut que le probabilité joint $p(s)$ se factorise.

ICA Application

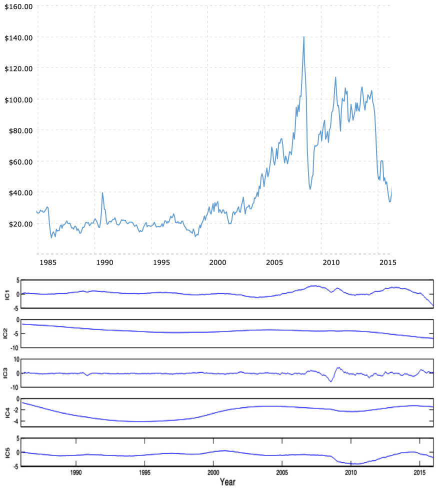






[images taken from `https://www.cs.cmu.edu/~bapoczos/other_presentations/ICA_26_10_2009.pdf`]

Source Separation for Financial Data



- In the paper Factor analysis of financial time series using EEMD-ICA based approach the authors decompose oil prices using an ICA variant.
- They claim:
  - IC1 is correlated to USD.
  - IC2 is correlated to oil suppy and demand.
  - IC3 is correlated to political and extreme events.
  - IC4 reflects cyclical nature of oil prices.
  - IC5 is correlated with stock, gold markets.

Methods to solve ICA (high-level)

- Non linear decorrelation $\mathbb{E}[f(w_i)g(w_j)]$, for fixed f, g.
  - Decorrelation non-linéaire pour $\mathbb{E}[f(w_i)g(w_j)]$, f, g sont fixes..
    - Cichocki-Unbehauen algorithm

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- Higher order diagonalization.
  - Diagonalize

$$Q(s) := \mathbb{E}[w_i w_j w_k w_l] - \mathbb{E}[w_i w_j]\mathbb{E}[w_k w_l] - \mathbb{E}[w_i w_k]\mathbb{E}[w_j w_l] - \mathbb{E}[w_i w_l]\mathbb{E}[w_j w_k]$$

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- Info-theoretic approach

$$\min \mathrm{KL}(p(w) \| p(w_1)p(w_2)\dots p(w_K)) = \min \int p(w) \log \frac{p(w)}{\prod_k p(w_k)}$$

  - We try to make the product of marginals become the joint / on essaie de faire la produit de marginales égale à joint.

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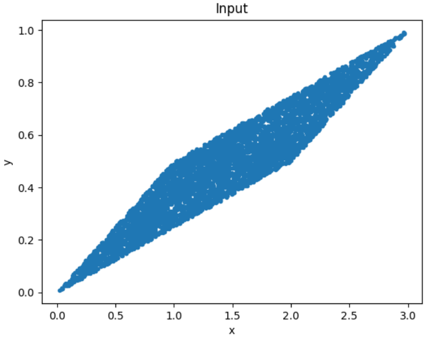
  - We try to make the product of marginals become the joint / on essaie de faire la produit de marginales égale à joint.
- More: FastICA, Neural Nets, Negentropy (Measure of non-gaussianity), More...

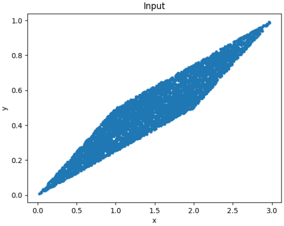
PCA vs ICA

- Let's consider this toy example

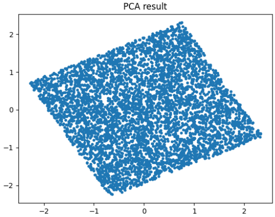
$$
\begin{aligned}
r_1, r_2 \sim & \mathcal{U}(0,1) \\
x = & r_1 + r_2 \\
y = & 2r_1 + r_2
\end{aligned}
$$



PCA vs ICA



PCA



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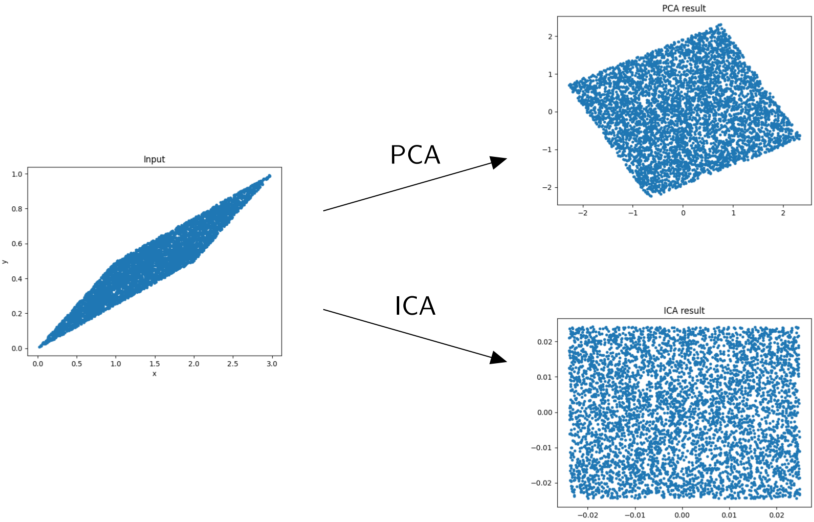


PCA's uncorrelatedness criterion is not enough in this case / La décorrelation de PCA n'est pas suffisante ici!

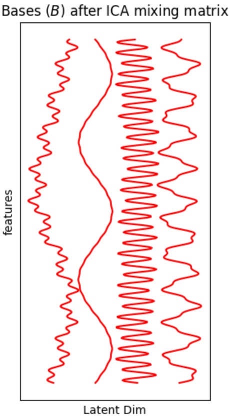
PCA on steroids

- We were doing the decomposition / On faisait la décomposition,

$$X = BW$$

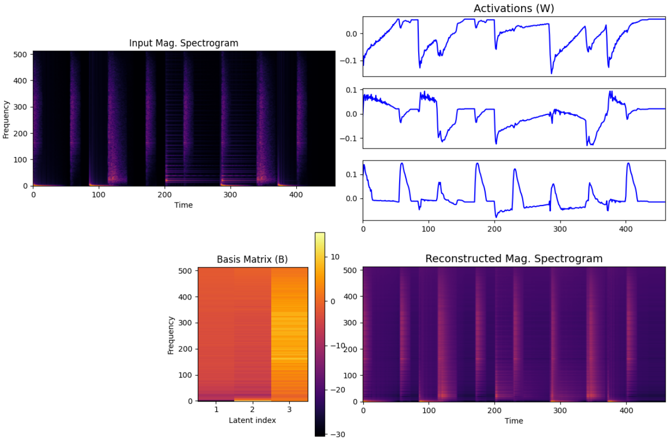
- We can apply ICA to obtain / On peut appliquer ICA pour obtenir

$$X = BB_I W_I = \tilde{B} W_I$$



- Closer to sinusoids!

Embedding spectra with ICA



Bit better but we can do better..

ICA Summary

- PCA assumes that everything is Gaussian. (For Gaussian data it does return independent dimensions)
  - PCA suppose que le monde est Gaussienne.
- iCA does not assume Gaussian, and try to achieve independence.
  - ICA essaie d'obtenir l'independence.
- Most ICA estimators are approximate
  - La majorité des estimateurs ICA sont approximatives.
- We don't have an important ordering of components, so no dim. reduction
  - On n'a pas un ordering des composant, donc on ne peut faire une reduction de dimensions.
    - We can however combine it PCA to improve it. / On peut le combiner avec PCA pour l'améliorer.

Table of Contents

Non-Negative Matrix Factorization

- We want to again optimize for B, W, but for $W \geq 0$, $W \geq 0$. i

$$\min_{B,W} \|X - BW\|$$
$$s.t. B \geq 0, W \geq 0.$$

- First proposed in 1999 Nature paper. / Proposé dans un papier Nature en 1999.
- Works pretty well on data non-négative. Fonctionne magiquement bien sur le data non-negative.
- We often work with non-negative data. (counts, pixels, energy...) / On travaille souvent avec du data non-négative.

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- We often work with non-negative data. (counts, pixels, energy...) / On travaille souvent avec du data non-négative.
- If we have negative values in our estimates, they cancel out, harm interpretability. / Si on a des values négatives dans les parameters, ça nuit l'interpretabilité.

But how?

- We can alternate the least squares solutions and also project such,
  - On peut juste alterner entres les solutions least-squares avec une addition des projetions,

---

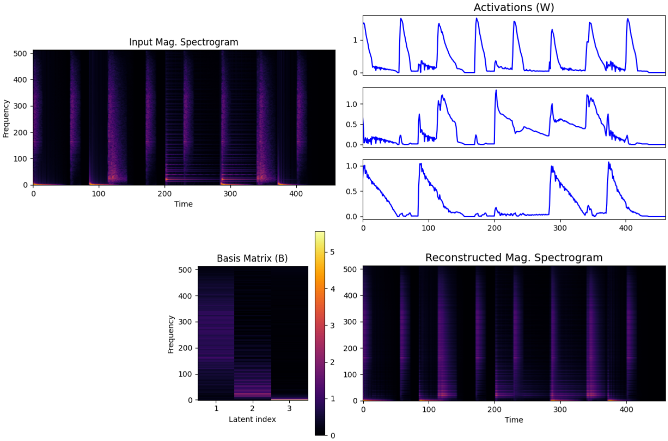
Algorithm 2 Alternating Least Squares for NMF

---

procedure ALTERNATING LEAST SQUARES FOR NMF
Input: Input Data Matrix X. Threshold value ϵ.
Output: Estimated Basis and Activation Matrices $\widehat{B}$, $\widehat{W}$.
  Initialize $\widehat{B} \geq 0$, $\widehat{W} \geq 0$.
  while $\|X - \widehat{B}\widehat{W}\| \geq \epsilon$ **do**
    $\widehat{W} = \widehat{B}^{\dagger}X$; $\widehat{W} = \max(0, \widehat{W})$
    $\widehat{B} = X\widehat{W}^{\dagger}$; $\widehat{B} = \max(0, \widehat{B})$
  end while
end procedure

- There are also other algos. (e.g. Multiplicative Updates, probabilitic versions..)
  - Y a des autres algos. aussi.

NMF to rescue



PCA, NMF or ICA?

- It depends. / Ça depends.
- PCA is great for dim. reduction / PCA est très utile pour réduire la dimensionnalité.
- ICA gives more sparse/independent embeddings / ICA donne des embeddings plus parsimonieux.
- NMF gives interpretable results, but only for non-negative / NMF donne des résultats interpretables, mais juste pour des données non-negatives.

Recap

- We have introduced a framework that handles fixed basis regression, and learnable-basis regression.
  - On a introduit un framework qui peut gérer la regression avec des bases fixés, et regression avec des bases apprises.
- We have talked about very important latent variable methods such as PCA, ICA, NMF.
  - On a parlé des méthodes importants de variables latents comme PCA, ICA et NMF.

Suggested Reading

- Chapters 4, 12, Bishop
- The NMF Nature paper
  `https://www.nature.com/articles/44565/`
- Eigenfaces `https://en.wikipedia.org/wiki/Eigenface`

Next Week

- What if we want to learn non-linear embeddings? Manifold methods!
    - Qu'est-ce qu'on fait si on veut apprendre des embeddings non-linéaires? Méthodes de manifolds!