Advanced Data Analysis: Projection Pursuit (1)

Masashi Sugiyama (Computer Science)

W8E-406, sugi@cs.titech.ac.jp

http://sugiyama-www.cs.titech.ac.jp/~sugi

I.i.d. Samples

- Independent and identically distributed (i.i.d.) samples:

$$\boldsymbol{x}_i \overset{i.i.d.}{\sim} P(\boldsymbol{x})$$

  - Independent: the joint probability is the product of each probability
  - Identically distributed: each variable follow the identical distribution

$$P(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n) = P(\boldsymbol{x}_1) \times \cdots \times P(\boldsymbol{x}_n)$$

Gaussian Distribution

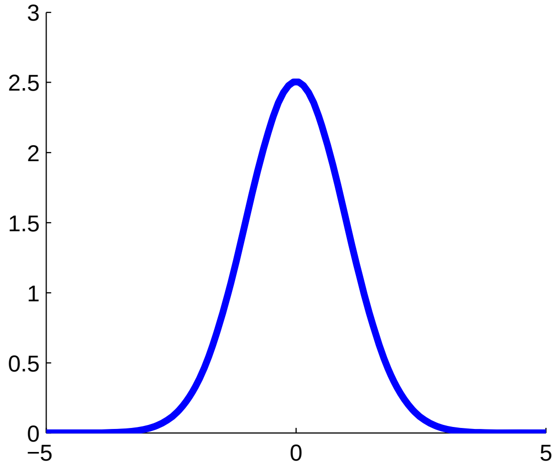
- Gaussian distribution: the probability density function is given by

$$\phi_{\boldsymbol{\mu},\boldsymbol{\Sigma}}(\boldsymbol{x}) = \frac{1}{(2\pi)^{\frac{d}{2}}|\boldsymbol{\Sigma}|^{\frac{1}{2}}} \exp\left(-\frac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1}(\boldsymbol{x}-\boldsymbol{\mu})\right)$$

- $\boldsymbol{\mu}, \boldsymbol{\Sigma}$:mean, covariance

$$\mathbb{E}[\boldsymbol{x}] = \boldsymbol{\mu}$$

$$\mathbb{E}[(\boldsymbol{x}-\boldsymbol{\mu})(\boldsymbol{x}-\boldsymbol{\mu})^\top] = \boldsymbol{\Sigma}$$

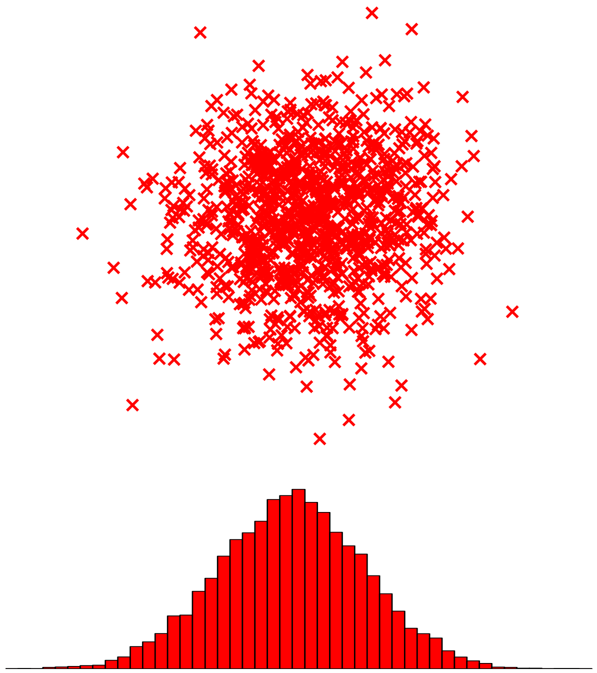


- When one-dimensional,

$$\phi_{\mu,\sigma^2}(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)$$

Interesting Directions for Data Visualization

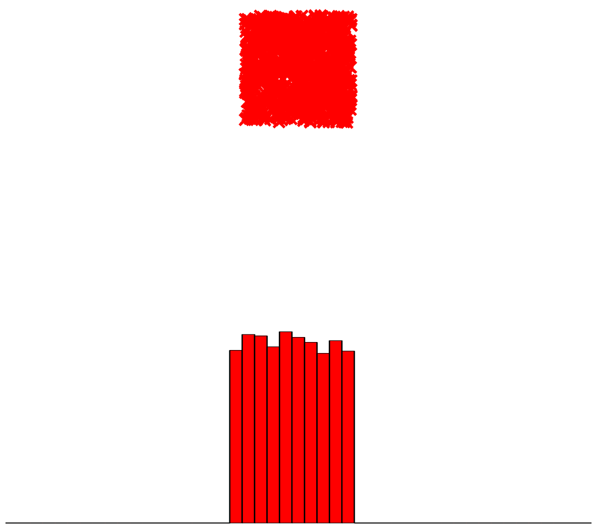
- Which distribution is interesting to visualize?
- If data follows the Gaussian distribution, samples are spherically distributed.
- Visualizing spherically distributed samples is not so interesting.
- What about "non-Gaussian" data?



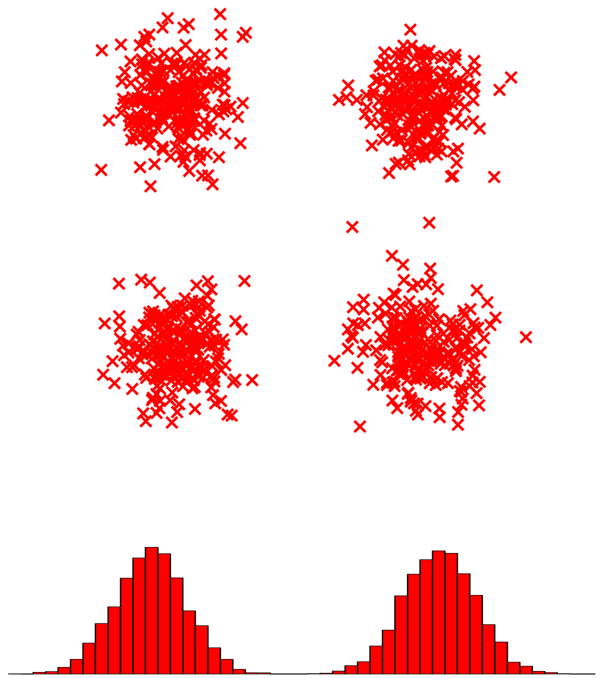
Non-Gaussian Distributed Data

- Non-Gaussian data look more interesting than Gaussian!

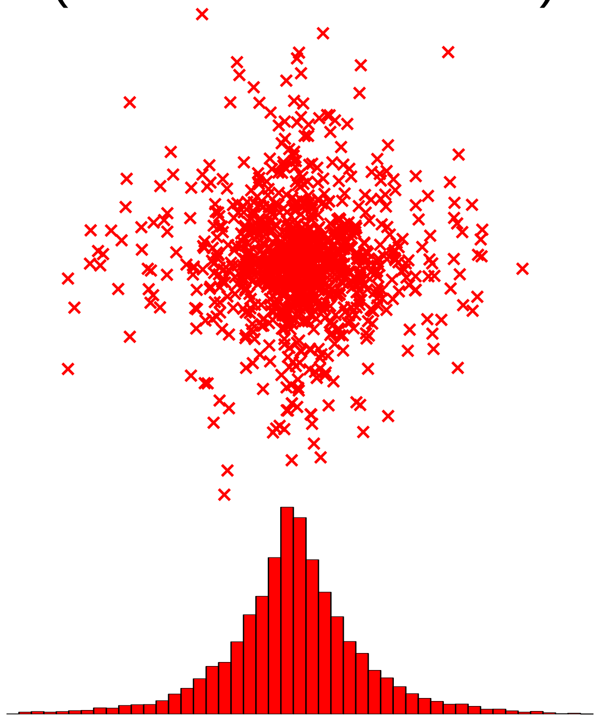
Uniform
(sharp edge)



Gaussian mixture
(cluster structure)



Laplacian
(existence of outliers)



Projection Pursuit

- Idea: Find the most non-Gaussian direction in the data
- For this purpose, we need a criterion to measure non-Gaussianity of data as a function of projection directions.

Kurtosis

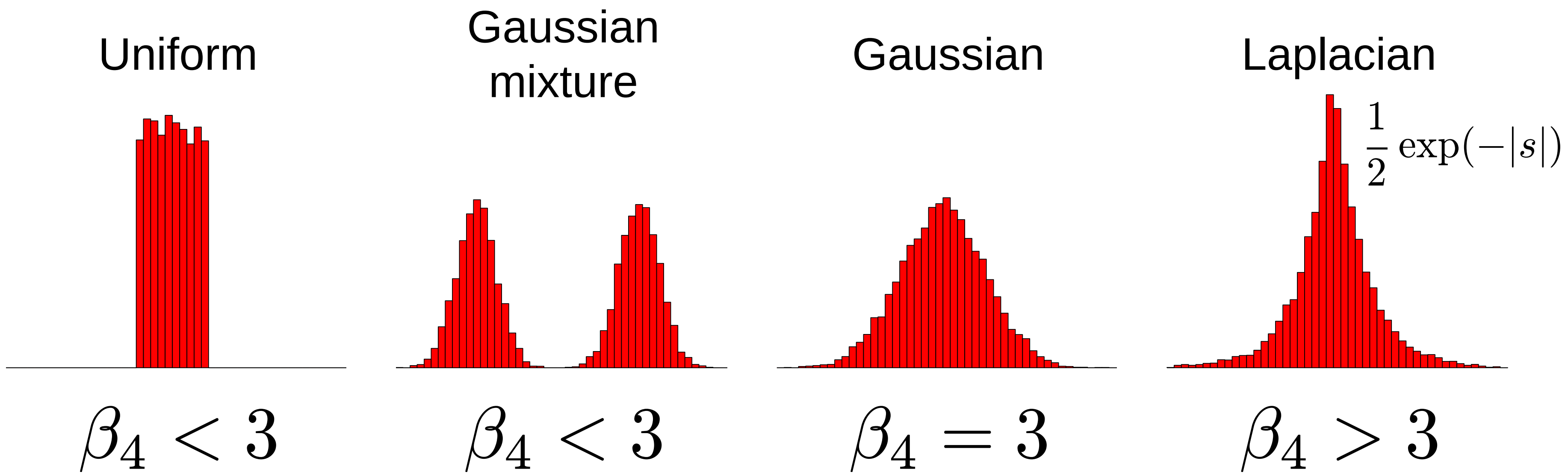
- Kurtosis for a one-dimensional random variable s:

$$\beta_4 = \frac{\mathbb{E}[(s - \mathbb{E}[s])^4]}{(\mathbb{E}[(s - \mathbb{E}[s])^2])^2} \quad (> 0)$$

- Kurtosis measures the "sharpness" of distributions.
- If tails of distribution are
  - Heavy ⇒ β_4 is large
  - Light ⇒ β_4 is small

Kurtosis (cont.)

- $\beta_4 = 3$: Gaussian distribution
- $\beta_4 < 3$: Sub-Gaussian distribution
- $\beta_4 > 3$: Super-Gaussian distribution



Kurtosis-Based Non-Gaussianity Measure

$$\beta_4 = \frac{\mathbb{E}[(s - \mathbb{E}[s])^4]}{(\mathbb{E}[(s - \mathbb{E}[s])^2])^2}$$

- Non-Gaussianity is strong if $(\beta_4 - 3)^2$ is large.
- Non-Gaussianity of data for direction $\boldsymbol{b}$ can be measured by letting $s = \langle \boldsymbol{b}, \boldsymbol{x} \rangle$ and $\|\boldsymbol{b}\| = 1$.

PP Criterion

- In practice, we use empirical approximation:

$$J_{PP}(\boldsymbol{b}) = \left(\frac{\frac{1}{n}\sum_{i=1}^{n}(s_i - \overline{s})^4}{(\frac{1}{n}\sum_{i=1}^{n}(s_i - \overline{s})^2)^2} - 3 \right)^2$$

$$s_i = \langle \boldsymbol{b}, \boldsymbol{x}_i \rangle$$

$$\overline{s} = \frac{1}{n}\sum_{i=1}^{n} s_i$$

- PP criterion:

$$\boldsymbol{\psi} = \mathop{\mathrm{argmax}}_{\boldsymbol{b} \in \mathbb{R}^d} J_{PP}(\boldsymbol{b})$$

$$\text{subject to } \|\boldsymbol{b}\| = 1$$

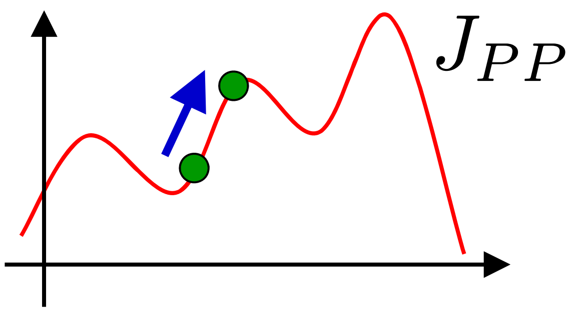
- There is no known method for analytically solving this optimization problem.
- We resort to numerical methods.

Gradient Ascent Approach

- Repeat until convergence:
  - Update $\boldsymbol{b}$ to increase J_{PP} :

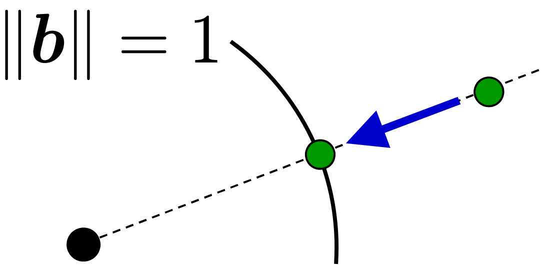
$$\boldsymbol{b} \longleftarrow \boldsymbol{b} + \varepsilon \frac{\partial J_{PP}}{\partial \boldsymbol{b}}$$

$$(\varepsilon > 0)$$



  - Modify $\boldsymbol{b}$ to satisfy $\|\boldsymbol{b}\| = 1$:

$$\boldsymbol{b} \longleftarrow \boldsymbol{b}/\|\boldsymbol{b}\|$$



Data Centering and Sphering

- Centering:

$$\overline{\boldsymbol{x}}_i = \boldsymbol{x}_i - \frac{1}{n}\sum_{j=1}^{n} \boldsymbol{x}_j$$

- Sphering (or pre-whitening):

$$\widetilde{\boldsymbol{x}}_i = \left(\frac{1}{n}\sum_{i=1}^{n} \overline{\boldsymbol{x}}_i \overline{\boldsymbol{x}}_i^\top\right)^{-\frac{1}{2}} \overline{\boldsymbol{x}}_i$$

- In matrix,

$$\widetilde{\boldsymbol{X}} = (\frac{1}{n}\boldsymbol{X}\boldsymbol{H}^2\boldsymbol{X}^\top)^{-\frac{1}{2}}\boldsymbol{X}\boldsymbol{H}$$

$$\widetilde{\boldsymbol{X}} = (\widetilde{\boldsymbol{x}}_1|\widetilde{\boldsymbol{x}}_2|\cdots|\widetilde{\boldsymbol{x}}_n)$$

$$\boldsymbol{X} = (\boldsymbol{x}_1|\boldsymbol{x}_2|\cdots|\boldsymbol{x}_n)$$

$$\boldsymbol{H} = \boldsymbol{I}_n - \frac{1}{n}\boldsymbol{1}_{n\times n}$$

$\boldsymbol{I}_n$: n-dimensional identity matrix

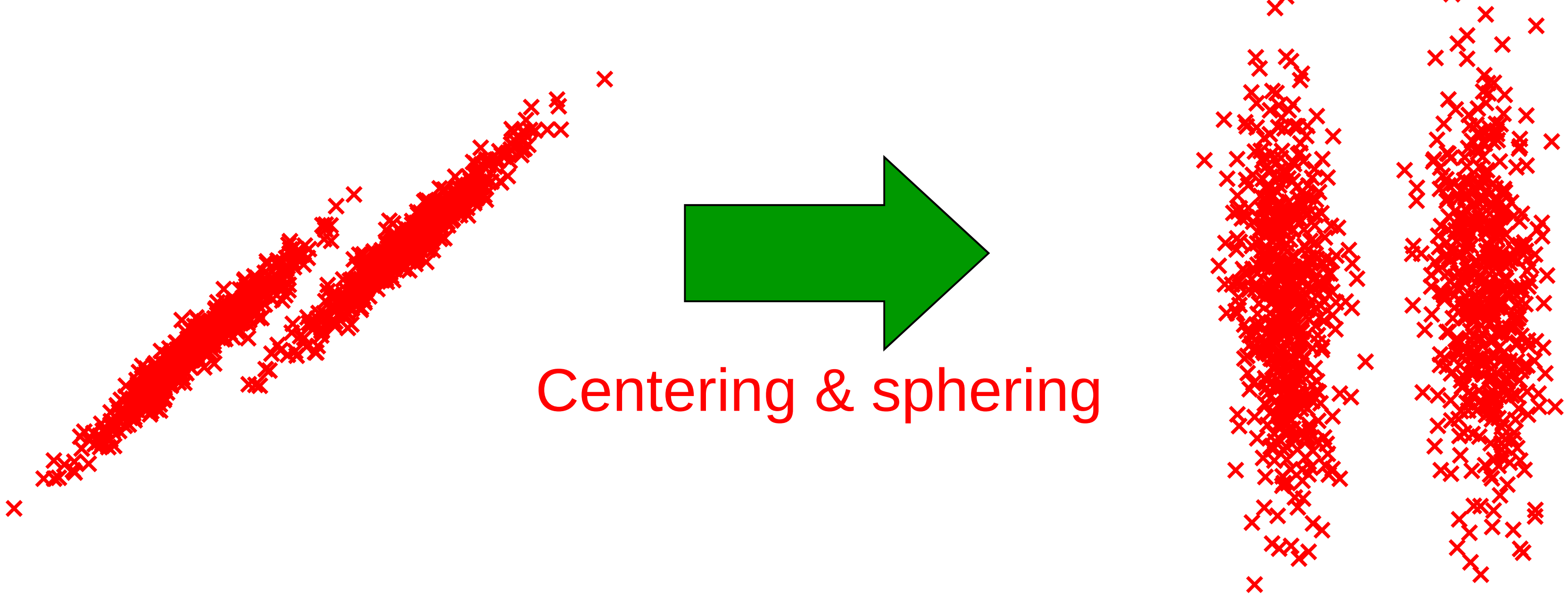
$\boldsymbol{1}_{n\times n}$: $n \times n$ matrix with all ones

Data Centering and Sphering

- By centering and sphering, the covariance matrix becomes identity:

$$\frac{1}{n}\sum_{i=1}^{n}\widetilde{\boldsymbol{x}}_i\widetilde{\boldsymbol{x}}_i^{\top} = \boldsymbol{I}_d$$

Homework: Prove it!



Simplification for Sphered Data

- For centered and sphered samples $\{\widetilde{\boldsymbol{x}}_i\}_{i=1}^n$,

$$J_{PP}(\boldsymbol{b}) = \left(\frac{1}{n}\sum_{i=1}^{n}\langle \boldsymbol{b}, \widetilde{\boldsymbol{x}}_i\rangle^4 - 3\right)^2$$

$$\frac{\partial J_{PP}}{\partial \boldsymbol{b}} = 2\left(\frac{1}{n}\sum_{i=1}^{n}\langle \boldsymbol{b}, \widetilde{\boldsymbol{x}}_i\rangle^4 - 3\right)\left(\frac{4}{n}\sum_{i=1}^{n}\widetilde{\boldsymbol{x}}_i\langle \boldsymbol{b}, \widetilde{\boldsymbol{x}}_i\rangle^3\right)$$

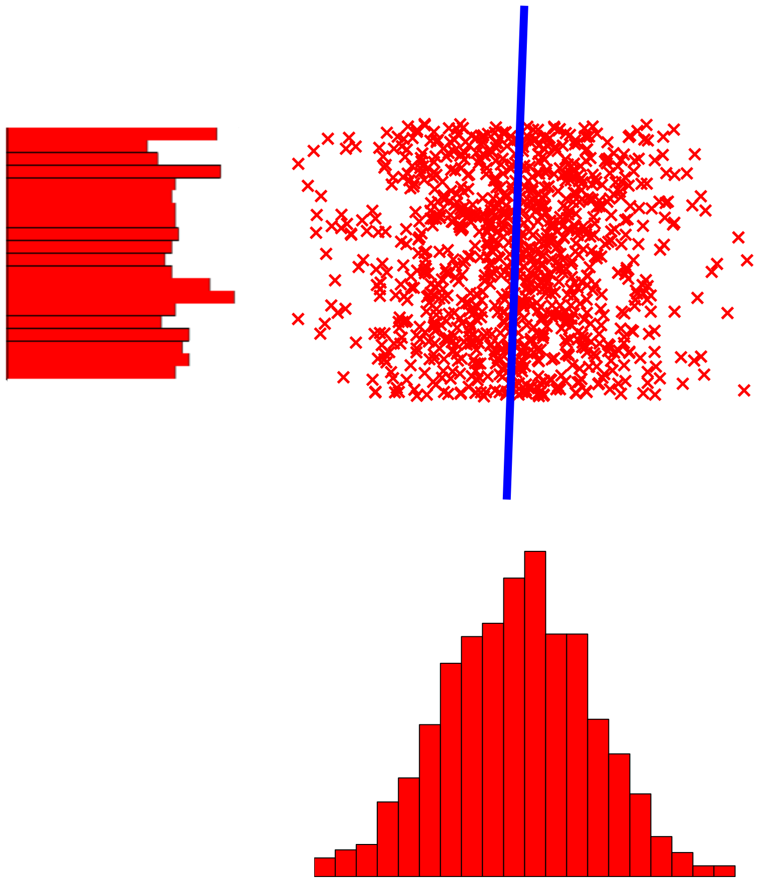
- The gradient update rule is

$$\boldsymbol{b} \longleftarrow \boldsymbol{b} + \varepsilon\left(\frac{1}{n}\sum_{i=1}^{n}\langle \boldsymbol{b}, \widetilde{\boldsymbol{x}}_i\rangle^4 - 3\right)\frac{1}{n}\sum_{i=1}^{n}\widetilde{\boldsymbol{x}}_i\langle \boldsymbol{b}, \widetilde{\boldsymbol{x}}_i\rangle^3$$

- Don't forget normalization: $\boldsymbol{b} \longleftarrow \boldsymbol{b}/\|\boldsymbol{b}\|$
- Homework: Derive the gradient update rule!

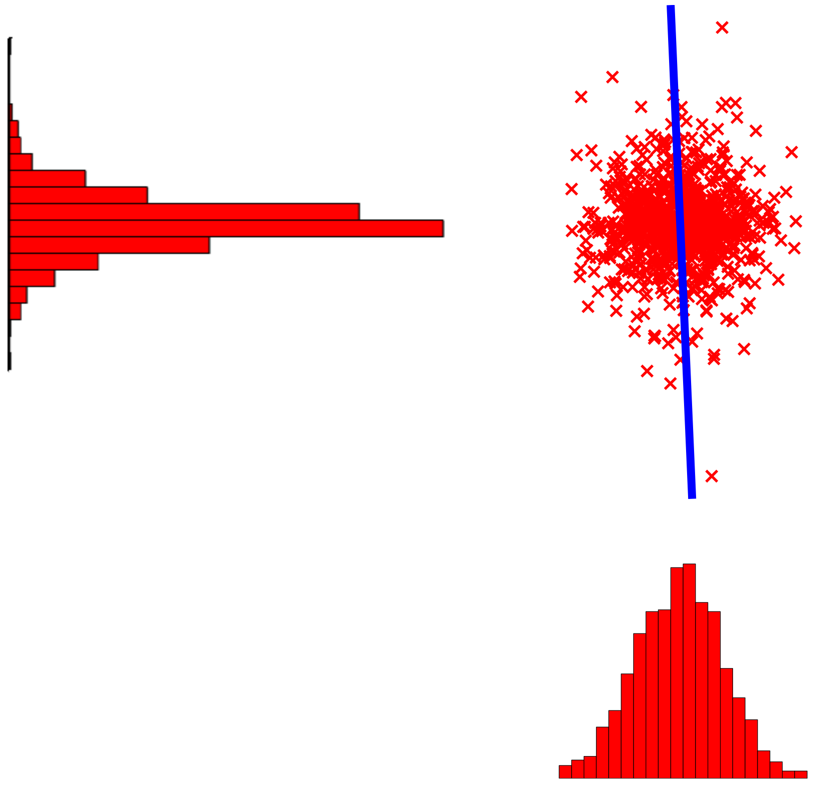
Examples

- $d = 2, \quad m = 1, \quad n = 1000$
- $\boldsymbol{x} = \begin{pmatrix} s \\ t \end{pmatrix}$
- $s \sim N(0,1)$
- $t \sim U(-\sqrt{3}, \sqrt{3})$



Examples (cont.)

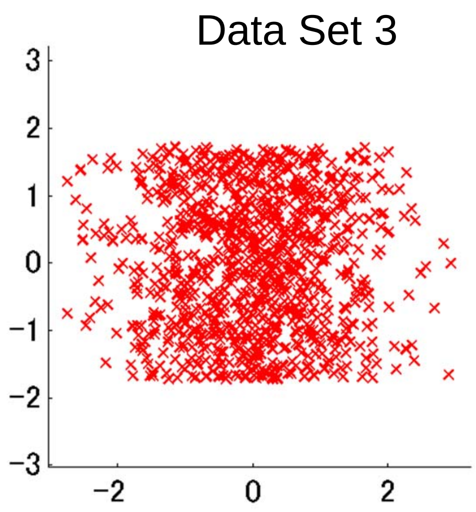
- $d = 2, \quad m = 1, \quad n = 1000$
- $\boldsymbol{x} = \begin{pmatrix} s \\ t \end{pmatrix}$
- $s \sim N(0, 1)$
- $t \sim Lap(0, 1)$

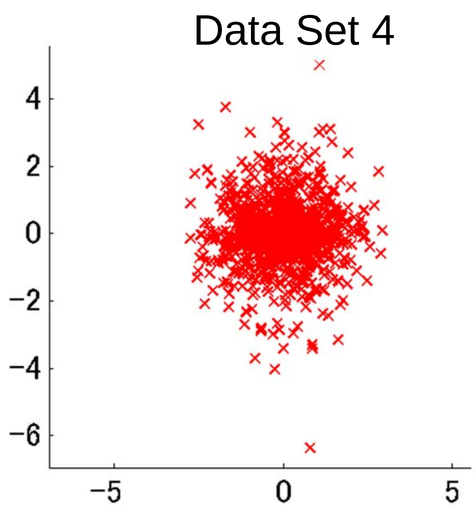


Homework

1. Implement PP and reproduce the 2-dimensional examples shown in the class.

http://sugiyama-www.cs.titech.ac.jp/~sugi/data/DataAnalysis





You may create similar (and more interesting) data sets by yourself.

Homework (cont.)

2. Prove the following for centered and sphered samples $\{\widetilde{\boldsymbol{x}}_i\}_{i=1}^n$:

A) Covariance matrix is given by

$$\frac{1}{n}\sum_{i=1}^{n}\widetilde{\boldsymbol{x}}_i\widetilde{\boldsymbol{x}}_i^\top = \boldsymbol{I}_d$$

B) J_{PP} under $\|\boldsymbol{b}\| = 1$ is given by

$$J_{PP}(\boldsymbol{b}) = \left(\frac{1}{n}\sum_{i=1}^{n}\langle\boldsymbol{b},\widetilde{\boldsymbol{x}}_i\rangle^4 - 3\right)^2$$

C) Gradient $\partial J_{PP}/\partial\boldsymbol{b}$ is given by

$$\frac{\partial J_{PP}}{\partial\boldsymbol{b}} = 2\left(\frac{1}{n}\sum_{i=1}^{n}\langle\boldsymbol{b},\widetilde{\boldsymbol{x}}_i\rangle^4 - 3\right)\left(\frac{4}{n}\sum_{i=1}^{n}\widetilde{\boldsymbol{x}}_i\langle\boldsymbol{b},\widetilde{\boldsymbol{x}}_i\rangle^3\right)$$

Notification of Final Assignment

- Data Analysis: Apply dimensionality reduction or clustering techniques to your own data set and “mine” something interesting!

- Deadline: July 31st (Wed) 17:00
  - Bring your printed report to W8E-406.
  - E-mail submission is also possible (though not recommended).

Mini-Conference on Data Analysis

- On July 16th and 23rd, we have a mini-conference on data analysis.
- Some of the students may present their data analysis results.
- Those who give a talk at the conference will have very good grades!

Mini-Conference on Data Analysis

- Application procedure: On June 25th, just say to me "I want to give a talk!".
- Presentation: approx. 10 min (?)
  - Description of your data
  - Methods to be used
  - Outcome
- Slides should be in English.
- Better to speak in English, but Japanese may also be allowed (perhaps your friends will provide simultaneous translation!).

Schedule

- June 18th: Preparation for Mini-Conference
- June 25th: Projection Pursuit (2)
  - Application Deadline to Mini-Conference
- July 2nd: Independent Component Analysis
- July 9th: Preparation for Mini-Conference
- July 16th: Mini-Conference Day 1
- July 23rd: Mini-Conference Day 2