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Introduction to ML and AI Methods (Part I)

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Day 1 - August 29th, 2022

2022 ELEDIA@ICAM PhD Summer Schools
Machine Learning & AI Methods
Theory, Techniques, and Advanced Engineering Applications
29 Aug. - 02 Sept. 2022, Trento, Italy (Onsite and Online)

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Notation Guidelines

Text Style

- ***Question***
- **Definition**
- **Positive Outcome**
- **Positive observation**
- **Negative Outcome**
- **Negative observation**
- **Neutral Outcome**
- **Neutral observation**
- **Final Result**
- **Theorem [1]**
- ***Hypotheses* [1]**
- **Open Issue/Drawback**
- **Technique/Approach**
- Key-parameters (Test cases)
- **Problem Statement**
- **Other important sentence**

Slide Background

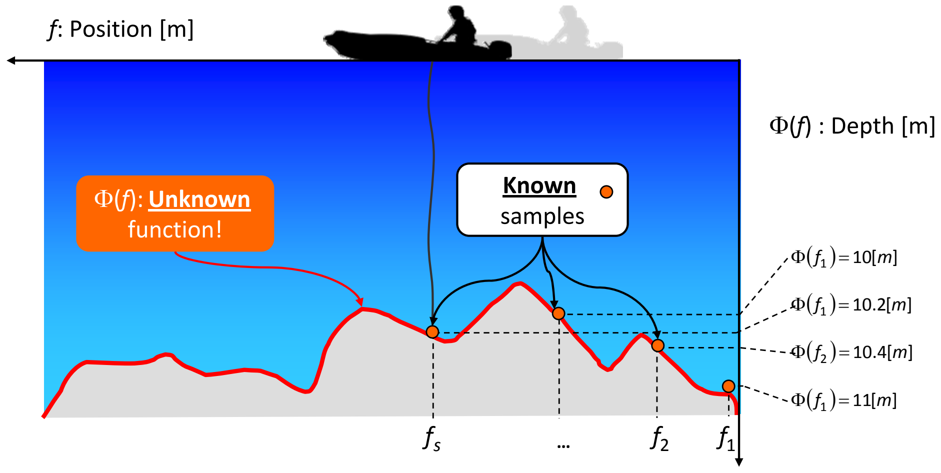
Light YELLOW – Numerical Examples	Light GRAY – Proofs/Maths
Light GREEN – Rules-of-Thumb	Light GBLU – Redundant
Light PINK – Resume/Shortening	Light ORANGE – Repetitions/Reminder
Light VIOLET – Glossary/Math Defs/Key	Light RED – Alternative Flow

Outline

- Introduction and Motivation
- Prediction Through **Interpolation Techniques**
  - ***Nearest Neighbor Interpolation***
  - ***Linear Interpolation***
- **3-Steps Learning-by-Examples** (***LBE***) Framework
  - Step 1: ***Dimensionality Reduction***
    - ***Sequential Feature Selection (SFT)***
    - ***Principal Component Analysis (PCA)***
    - ***Sammon Mapping***
    - ***Partial Least Squares (PLS)***

Introduction & Motivation (1/2)

What A men on a boat wants to measure **how deep** is a lake



How He can **measure the depth** in a discrete number of **S positions**

$$\Rightarrow \{[f_i, \Phi(f_i)], i = 1, \dots, S\}$$

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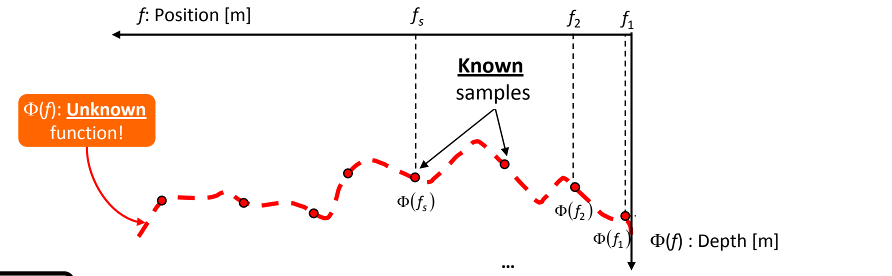
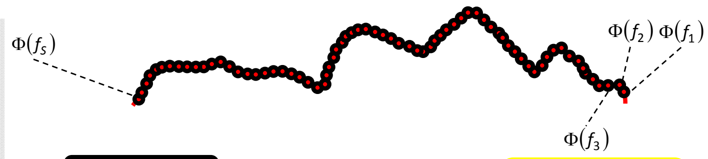
Introduction & Motivation (1/2)

How can he retrieve the depth $\Phi(f)$ for every position f ?



Approach Take **a lot** of very close consecutive **samples** of $\Phi(f)$

EXAMPLE:
Sample distance: 5 cm
Covered distance: 100 m
Required samples: 2000
Time per sample: 2 min
Total time: 2.78 days!!



➡ **Issue** **Too expensive**!!

Faster Approach?

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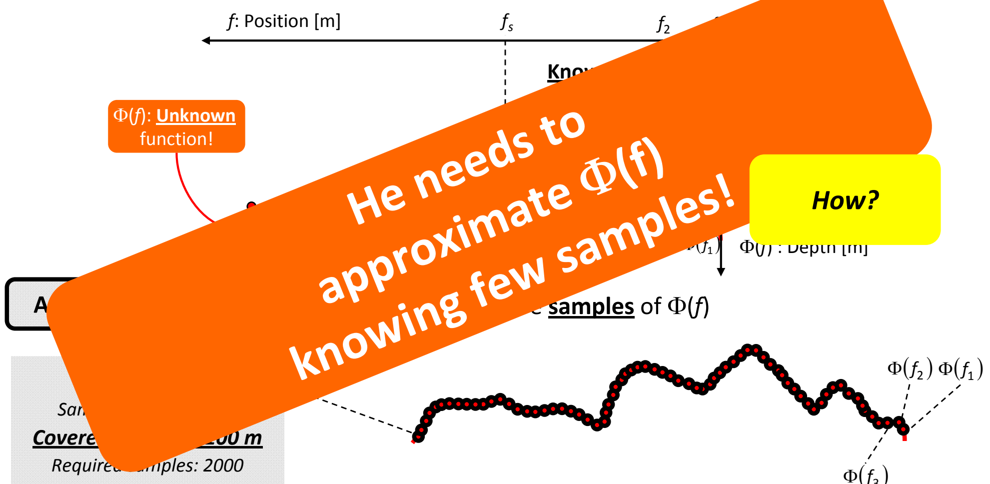
Introduction & Motivation (1/2)

How can he retrieve the depth $\Phi(f)$ for every position f ?



➡ **Issue** **Too expensive**!!

Faster Approach?

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Efficient Evaluation of $\Phi(f)$

Open Issue Computationally-efficient methods

Fast Direct Solvers (small-medium problems)

- customized solvers with **limited** range of application ↓
- **no "training"** needed ↑
- can be applied for **small-medium** problems ↓

Approximate $\Phi(f)$ computation (large problems)

- $\Phi(f)$ is **predicted** ↑
- need of a **"training"** phase ↓
- can be applied **whatever** the problem size ↑

Which Approaches?

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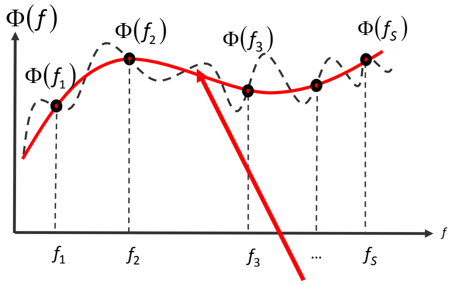
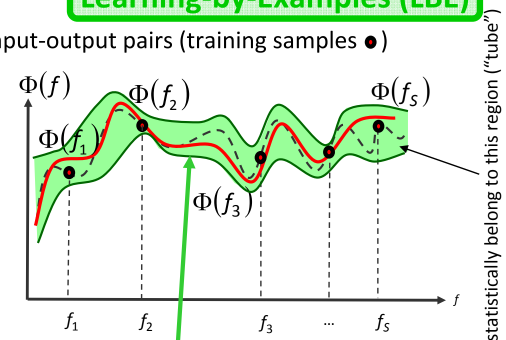
Efficient Evaluation of $\Phi(f)$

Approximate Φ(f) computation through a predictor ("Surrogate Model")

Interpolation | **Learning-by-Examples (LBE)**

$[\mathbf{f}_i; \Phi(\mathbf{f}_i)]\ i = 1,...,S$: Set of S **known** input-output pairs (training samples ●)





Approximation given by a **parametric function** with form is **postulated in advance** (e.g., polynomials, splines, ecc..)

Often implies exact fit at training points

Doesn't assume a parametric function a-priori but "**understands**" the **statistical behavior** of the underlying function.

Exact fit at training points not mandatory

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Efficient Evaluation of $\Phi(f)$

Approximate Φ(f) computation through a predictor (large problems)

Interpolation

- Simple and efficient strategies ↑
- Requires to *a-priori* know/estimate functional dependency (e.g.: polynomial, exponential, etc.) ↓
- Low generalization capabilities ↓
- *Examples: **nearest neighbor interpolation**, **linear interpolation**, polynomial interpolation, spline interpolation*

Learning-by-Examples (LBE)

- Numerically efficient ↑
- No *a-priori* knowledge required ↑
- Good generalization capabilities ↑
- *Examples: Support Vector Machines (SVM), Artificial Neural Networks (ANN), Gaussian Processes (GP), Radial Basis Function (RBF)*

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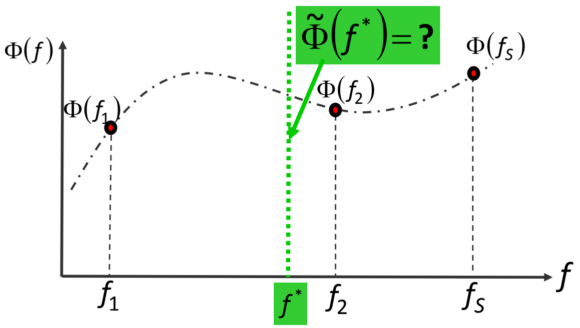
Prediction Through Interpolation

Given the function value $\Phi(f)$ at S N-dimensional samples, how to estimate the function value at f*?

EXAMPLE:
Number of variables: N=1



Solution **Interpolate** available data ("easiest" prediction)

How?
- **Nearest Neighbor (NN) interpolation** (A)
- Linear interpolation (B)

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(A) Nearest Neighbor (NN) Interpolation

Approach The function value in **f*** is equal to the value assumed by the **nearest** training sample

Steps

(1) Compute the **Euclidean distance** between **f*** and $\mathbf{f}_i$, i=1,...,S

$$d(\mathbf{f}^*, \mathbf{f}_i) = \sqrt{\sum_{n=1}^{N} (f_{n,i} - f_n^*)^2}$$

N-dimensional

(2) Predict at **f***

$$\boxed{\tilde{\Phi}(\mathbf{f}^*)} = \Phi(\mathbf{f}_i) \quad \text{if} \quad d(\mathbf{f}^*, \mathbf{f}_i) < d(\mathbf{f}^*, \mathbf{f}_j) \quad \forall i, j = 1,...,S \quad i \neq j$$

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(A) NN Interpolation - 1D Case

$$\tilde{\Phi}\left(\mathbf{f}^*\right)=\Phi\left(\mathbf{f}_i\right) \quad \text{if} \quad d\left(\mathbf{f}^*,\mathbf{f}_i\right)<d\left(\mathbf{f}^*,\mathbf{f}_j\right) \quad \forall i,j=1,\dots,S \quad i\neq j$$

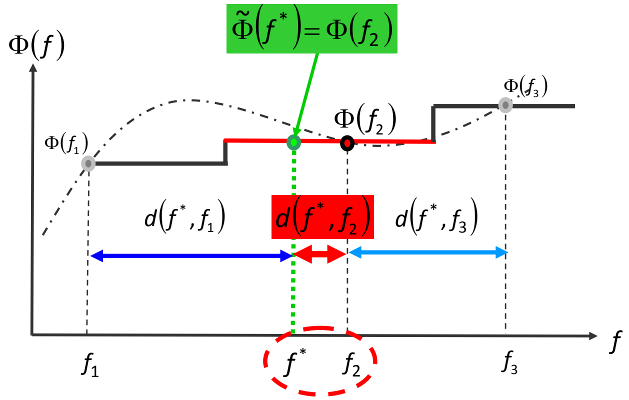
EXAMPLE:
Number of variables: N=1

$d\left(f^*,f_2\right)<d\left(f^*,f_1\right)$

$d\left(f^*,f_2\right)<d\left(f^*,f_3\right)$

The **nearest neighbor** of f^* is f_2

$\tilde{\Phi}\left(f^*\right)=\Phi\left(f_2\right)$



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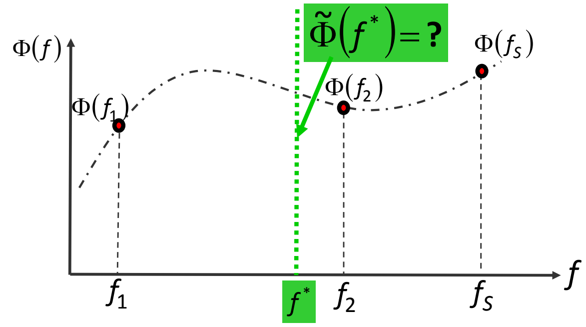
Prediction Through Interpolation

Given the function value $\Phi(f)$ at S N-dimensional samples, how to estimate the function value at f*?

EXAMPLE:
Number of variables: N=1



Solution **Interpolate** available data ("easiest" prediction)

How?
- **Nearest Neighbor (NN) interpolation** (A)
- Linear interpolation (B)

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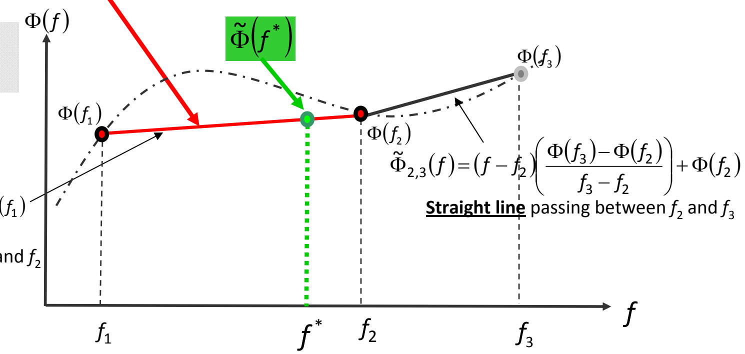
(B) Linear Interpolation - 1D Case

Approach The function value in f^* is given by the equation of the **straight line** passing between the two neighboring points

EXAMPLE:
Number of variables: N=1



$\tilde{\Phi}_{1,2}(f)=\left(f-f_1\right)\left(\frac{\Phi(f_2)-\Phi(f_1)}{f_2-f_1}\right)+\Phi(f_1)$

Straight line passing between f_1 and f_2

$\tilde{\Phi}_{2,3}(f)=\left(f-f_2\right)\left(\frac{\Phi(f_3)-\Phi(f_2)}{f_3-f_2}\right)+\Phi(f_2)$

Straight line passing between f_2 and f_3

$$\boxed{\tilde{\Phi}\left(f^*\right)=\left(f^*-f_1\right)\left(\frac{\Phi(f_2)-\Phi(f_1)}{f_2-f_1}\right)+\Phi(f_1)}$$

...And for N>1?

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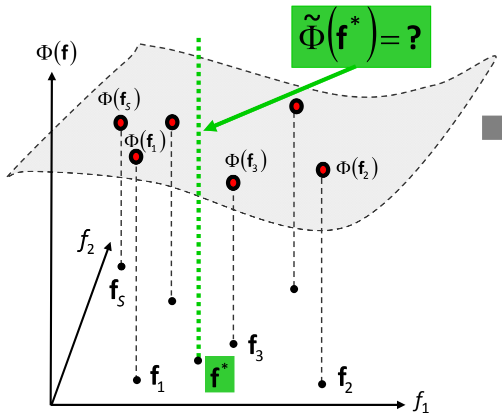
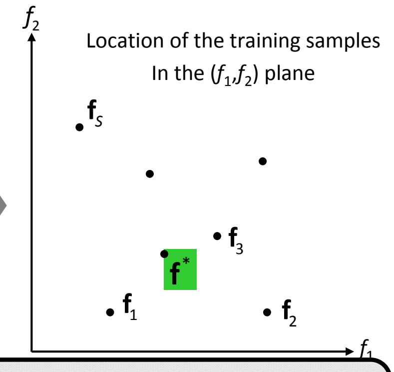
(B) Linear Interpolation - ND Case

Let be given a set of *S N*-dimensional training samples $\left[\mathbf{f}_i;\Phi\left(\mathbf{f}_i\right)\right] i=1,\dots,S$ •

EXAMPLE:
Number of variables: N=2





The prediction at f* will depend on the values assumed by its neighboring points

How to identify?

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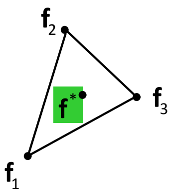
B ND Linear Interpolation - Steps

Approach The function value in **f*** is given by the **weighted sum** of its **neighboring points**

- Create the **Voronoi Diagram** $\mathcal{V}$(S)
- Create the **dual graph** $\mathcal{G}$(S) of $\mathcal{V}$(S)
- Convert $\mathcal{G}$ (S) to the **Delaunay diagram** $\mathcal{D}$ (S)
- Compute the **weights** α_i i=1,..,N+1
- Compute $\tilde{\Phi}(\mathbf{f}^*)$

Determine the **N+1 neighboring points** of **f***



Predict: $\tilde{\Phi}(\mathbf{f}^*) = \sum_{i=1}^{N+1} \alpha_i \Phi(\mathbf{f}_i)$

How?

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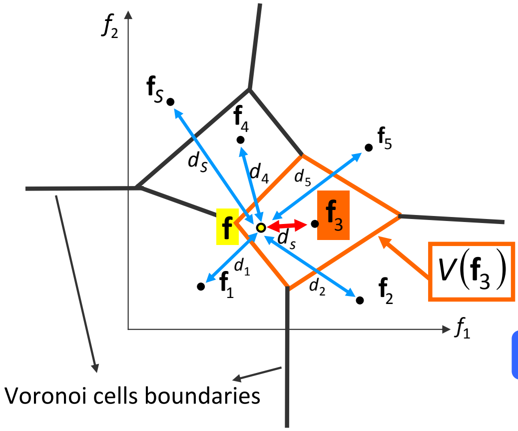
B Voronoi Cells/Diagrams

Def. **Voronoi cell** V($\mathbf{f}_i$) associated to sample $\mathbf{f}_i$:
Region of points whose Euclidean distance to $\mathbf{f}_i$ is lower than the distance to all other samples

EXAMPLE:
Number of variables: N=2

$$V(\mathbf{f}_i) = \{\mathbf{f} \mid d(\mathbf{f}, \mathbf{f}_i) \leq d(\mathbf{f}, \mathbf{f}_j)\, \forall i, j = 1, \dots, S\; i \neq j\}$$



f is closer to $\mathbf{f}_3$ than to all the other samples

$d_S < d_i \quad \forall i \neq 3$

$\Rightarrow \mathbf{f}_S \in V(\mathbf{f}_3)$

Def. **Voronoi diagram** $\mathcal{V}(S)$:
Complete set of S Voronoi cells

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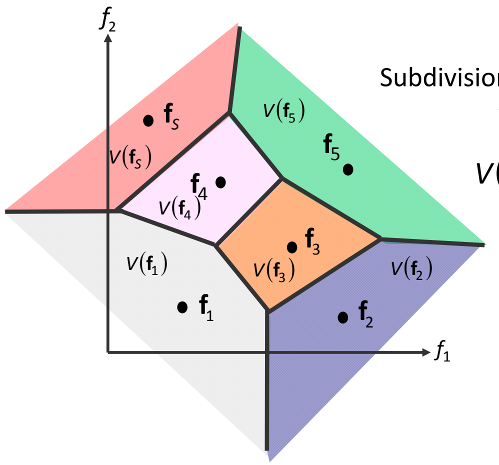
B ND Linear Interpolation - Step 1/5

- Create the **Voronoi Diagram** $\mathcal{V}$(S)
- Create the **dual graph** $\mathcal{G}$(S) of $\mathcal{V}$(S)
- Convert $\mathcal{G}$ (S) to the **Delaunay diagram** $\mathcal{D}$ (S)
- Compute the **weights** α_i i=1,..,N+1
- Compute $\tilde{\Phi}(\mathbf{f}^*)$

1 Create **Voronoi Diagram** $\mathcal{V}(S)$

EXAMPLE:
Number of variables: N=2



Subdivision of the plane into S Voronoi cells

$V(\mathbf{f}_i)\, \forall i = 1, \dots, S$

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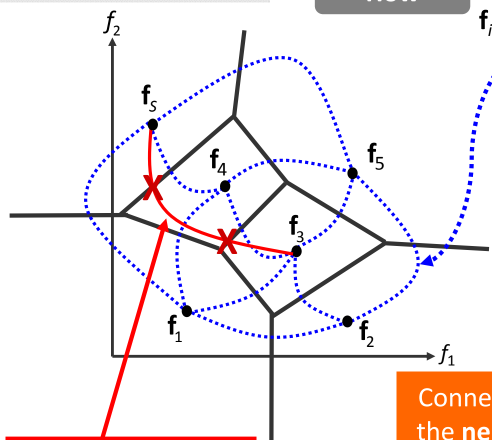
B ND Linear Interpolation - Step 2/5

- Create the **Voronoi Diagram** $\mathcal{V}$(S)
- Create the **dual graph** $\mathcal{G}$(S) of $\mathcal{V}$(S)
- Convert $\mathcal{G}$ (S) to the **Delaunay diagram** $\mathcal{D}$ (S)
- Compute the **weights** α_i i=1,..,N+1
- Compute $\tilde{\Phi}(\mathbf{f}^*)$

2 Create the **dual graph** $\mathcal{G}(S)$ of the Voronoi Diagram $\mathcal{V}(S)$

EXAMPLE:
Number of variables: N=2

How Connect two samples $\mathbf{f}_i$ and $\mathbf{f}_j$ if there exist a path crossing **only one Voronoi cell boundary**



Connection not allowed

(2 Voronoi buondaries crossed)

Connections will identify the **neighboring** samples for a given point **f***…

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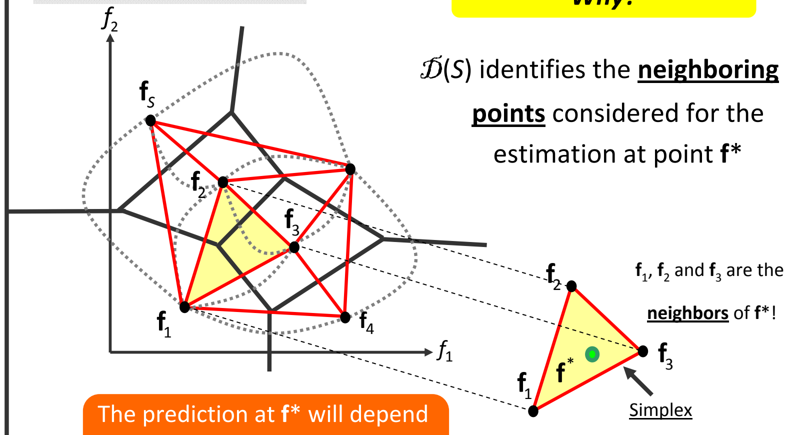
ⓑ ND Linear Interpolation - Step 3/5

- Create the **Voronoi Diagram** $\mathcal{V}(S)$
- Create the **dual graph** $\mathcal{G}(S)$ of $\mathcal{V}(S)$
- Convert $\mathcal{G}(S)$ to the **Delaunay diagram** $\mathcal{D}(S)$
- Compute the **weights** α_i i=1,..,N+1
- Compute $\tilde{\Phi}(\mathbf{f}^*)$

③ Create the **Delaunay Diagram** $\mathcal{D}(S)$: convert curved paths to **straight lines**

EXAMPLE:
Number of variables: N=2



Why?

$\mathcal{D}(S)$ identifies the **neighboring points** considered for the estimation at point **f***

The prediction at **f*** will depend on the values assumed by its **neighboring points**

ⓑ ND Linear Interpolation - Step 4/5

- Create the **Voronoi Diagram** $\mathcal{V}(S)$
- Create the **dual graph** $\mathcal{G}(S)$ of $\mathcal{V}(S)$
- Convert $\mathcal{G}(S)$ to the **Delaunay diagram** $\mathcal{D}(S)$
- Compute the **weights** α_i i=1,..,N+1
- Compute $\tilde{\Phi}(\mathbf{f}^*)$

④ Approximate the function at **f*** as a **weighted sum** of **N+1 independent samples** belonging to the same N-dimensional "simplex"

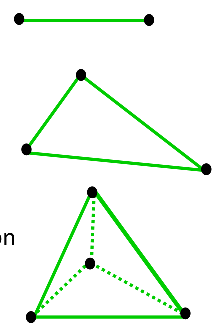
Prediction at **f***:

$$\tilde{\Phi}(\mathbf{f}^*) = \sum_{i=1}^{N+1} \alpha_i \Phi(\mathbf{f}_i) = \alpha_1 \Phi(\mathbf{f}_1) + \cdots + \alpha_{N+1} \Phi(\mathbf{f}_{N+1})$$

weights

Simplex

- N=1: Line
- N=2: Triangle
- N=3: Tetrahedron
- ...



How to **compute** the **weigths** α_n n=1,...,N+1?

ⓑ ND Linear Interpolation - Step 5/5

Weights Computation (1/2)

Def. **Volume** of a N-dimensional simplex: $Vol(\mathbf{f}_1,\ldots,\mathbf{f}_{N+1}) = \det\begin{pmatrix} \mathbf{f}_1 & \cdots & \mathbf{f}_{N+1} \\ 1 & \cdots & 1 \end{pmatrix}$

EXAMPLE:

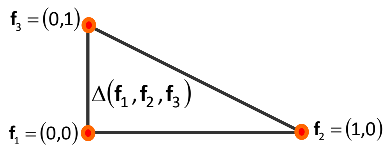
N=1

$$Vol(f_1,f_2) = \det\begin{pmatrix} f_1 & f_2 \\ 1 & 1 \end{pmatrix} = \boxed{f_1 - f_2} = -1$$

For N=1 volume = length

Signs depends on the ordering of the 2 points

N=2



$$Area(\Delta(\mathbf{f}_1,\mathbf{f}_2,\mathbf{f}_3)) = \frac{Base \cdot Height}{2} = \frac{1}{2}$$

$$Vol(\mathbf{f}_1,\mathbf{f}_2,\mathbf{f}_3) = \det\begin{pmatrix} \mathbf{f}_1 & \mathbf{f}_2 & \mathbf{f}_3 \\ 1 & 1 & 1 \end{pmatrix} = \det\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 1 & 1 \end{pmatrix} = -1$$

$$Vol(\mathbf{f}_1,\mathbf{f}_2,\mathbf{f}_3) = \boxed{\pm 2 Area(\Delta(\mathbf{f}_1,\mathbf{f}_2,\mathbf{f}_3))}$$

Signs depends on the ordering of the 3 points

For N>1 volume ∝ area

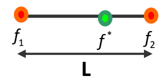
ⓑ ND Linear Interpolation - Step 5/5

Weights Computation (2/2)

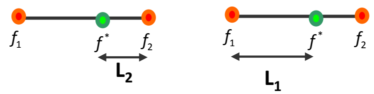
Weight for *i*-th neighbor $\mathbf{f}_i$: $\alpha_i = \dfrac{Vol(\mathbf{f}_1,\ldots,\mathbf{f}_{i-1},\mathbf{f}^*,\mathbf{f}_{i+1},\ldots,\mathbf{f}_{N+1})}{Vol(\mathbf{f}_1,\ldots,\mathbf{f}_{N+1})}$

EXAMPLE:

N=1



$$\alpha_1 = \frac{Vol(\mathbf{f}^*,\mathbf{f}_2)}{Vol(\mathbf{f}_1,\mathbf{f}_2)} = \frac{L_2}{L} \qquad \alpha_2 = \frac{Vol(\mathbf{f}_1,\mathbf{f}^*)}{Vol(\mathbf{f}_1,\mathbf{f}_2)} = \frac{L_1}{L}$$

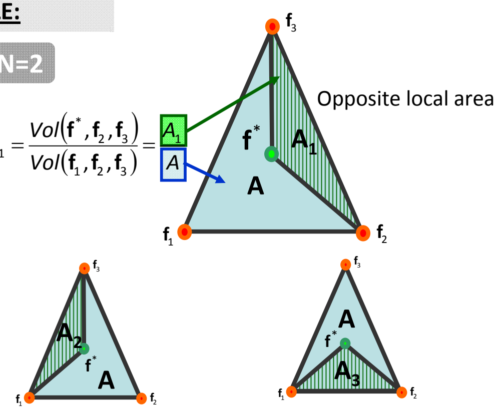


$$\boxed{\alpha_2 > \alpha_1}$$

$\tilde{\Phi}(f^*)$ will depend more on $\Phi(f_2)$

N=2

$$\alpha_1 = \frac{Vol(\mathbf{f}^*,\mathbf{f}_2,\mathbf{f}_3)}{Vol(\mathbf{f}_1,\mathbf{f}_2,\mathbf{f}_3)} = \frac{A_1}{A}$$



$$\alpha_2 = \frac{Vol(\mathbf{f}_1,\mathbf{f}^*,\mathbf{f}_3)}{Vol(\mathbf{f}_1,\mathbf{f}_2,\mathbf{f}_3)} = \frac{A_2}{A} \qquad \alpha_3 = \frac{Vol(\mathbf{f}_1,\mathbf{f}_2,\mathbf{f}^*)}{Vol(\mathbf{f}_1,\mathbf{f}_2,\mathbf{f}_3)} = \frac{A_3}{A}$$

B Linear Interpolation - Example

N=1

1. Volume calculation

$$Vol(\mathbf{f}_1,\mathbf{f}_2)=Vol(f_1,f_2)=\left|\det\begin{pmatrix} f_1 & f_2 \\ 1 & 1\end{pmatrix}\right|=f_2-f_1$$

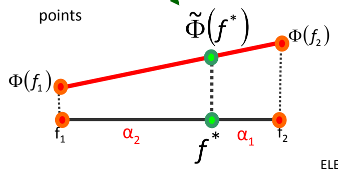
2. Weights calculation

$$\alpha_1=\frac{Vol(f^*,f_2)}{Vol(f_1,f_2)}=\frac{f_2-f^*}{f_2-f_1}\quad \alpha_2=\frac{Vol(f_1,f^*)}{Vol(f_1,f_2)}=\frac{f^*-f_1}{f_2-f_1}$$

3. Function approximation

$$\boxed{\tilde{\Phi}(f^*)}=\alpha_1\Phi(f_1)+\alpha_2\Phi(f_2)=(f^*-f_1)\left(\frac{\Phi(f_2)-\Phi(f_1)}{f_2-f_1}\right)+\Phi(f_1)$$

equation of a straight line passing between two points



N=2

1. Volume calculation

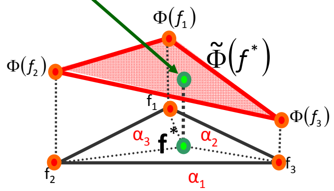
$$Vol(\mathbf{f}_1,\mathbf{f}_2,\mathbf{f}_3)=\left|\det\begin{pmatrix} \mathbf{f}_1 & \mathbf{f}_2 & \mathbf{f}_3 \\ 1 & 1 & 1\end{pmatrix}\right|=2Area(\Delta(\mathbf{f}_1,\mathbf{f}_2,\mathbf{f}_3))$$

2. Weights calculation

$$\alpha_1=\frac{Vol(\mathbf{f}^*,\mathbf{f}_2,\mathbf{f}_3)}{Vol(\mathbf{f}_1,\mathbf{f}_2,\mathbf{f}_3)}\quad \alpha_2=\frac{Vol(\mathbf{f}_1,\mathbf{f}^*,\mathbf{f}_3)}{Vol(\mathbf{f}_1,\mathbf{f}_2,\mathbf{f}_3)}\quad \alpha_3=\frac{Vol(\mathbf{f}_1,\mathbf{f}_2,\mathbf{f}^*)}{Vol(\mathbf{f}_1,\mathbf{f}_2,\mathbf{f}_3)}$$

3. Function approximation

$$\boxed{\tilde{\Phi}(\mathbf{f}^*)}=\alpha_1\Phi(\mathbf{f}_1)+\alpha_2\Phi(\mathbf{f}_2)+\alpha_3\Phi(\mathbf{f}_3)$$



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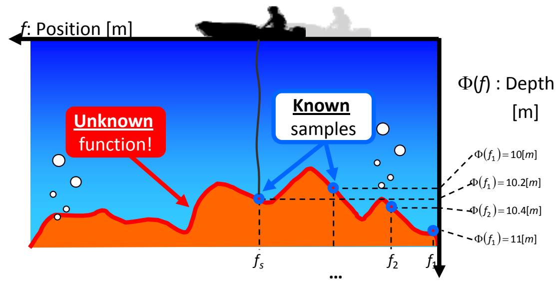
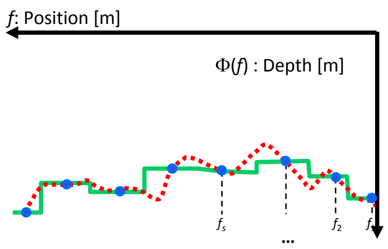
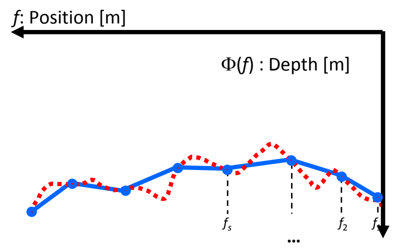
Nearest Neighbor Vs. Linear Interpolation (1/2)



Nearest Neighbor



Linear Interpolation



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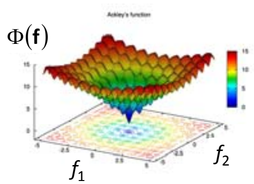
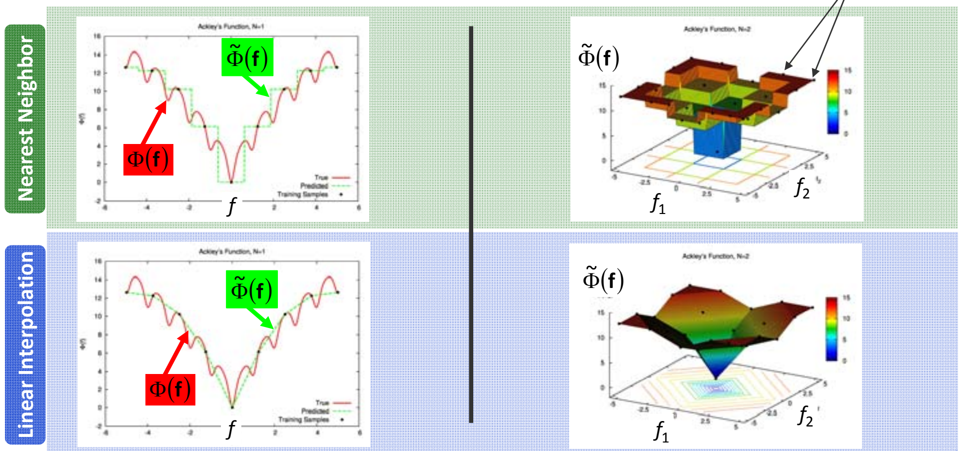
Nearest Neighbor Vs. Linear Interpolation (2/2)

Function: "Ackley"



N=1, S=9 **N=2, S=25**

Training samples



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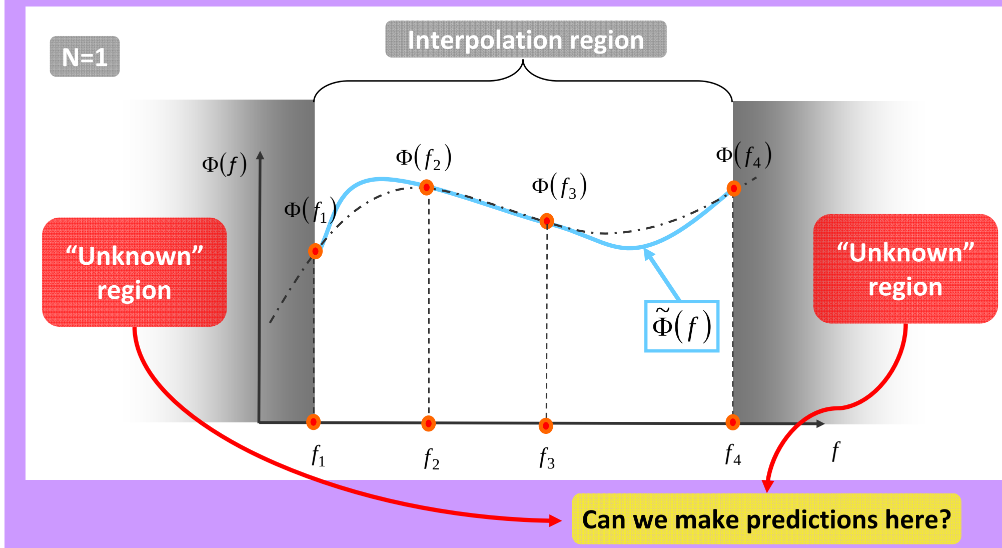
Interpolation Vs. Extrapolation (1/2)

Interpolation Predict $\tilde{\Phi}(f)$ **between** observed points



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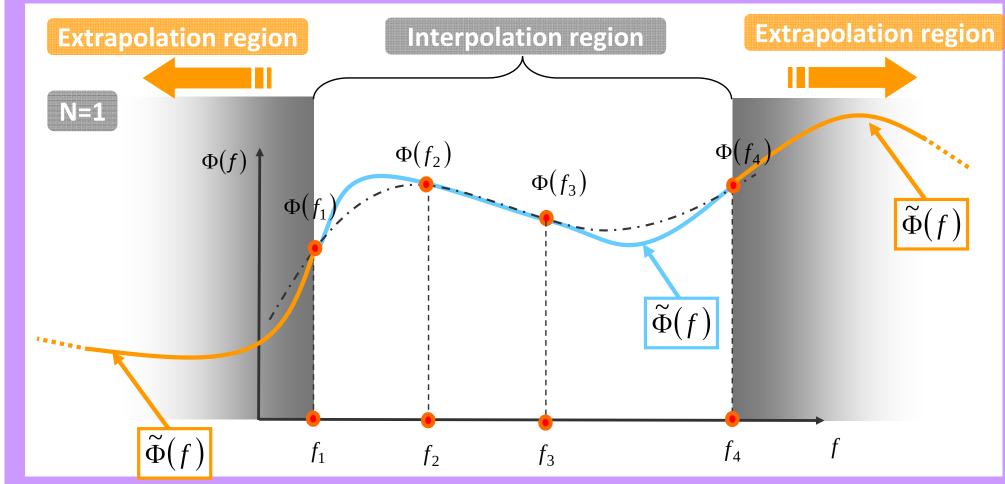
Interpolation Vs. Extrapolation (2/2)

Extrapolation Predict $\tilde{\Phi}(f)$ **beyond** observed points



Always possible?

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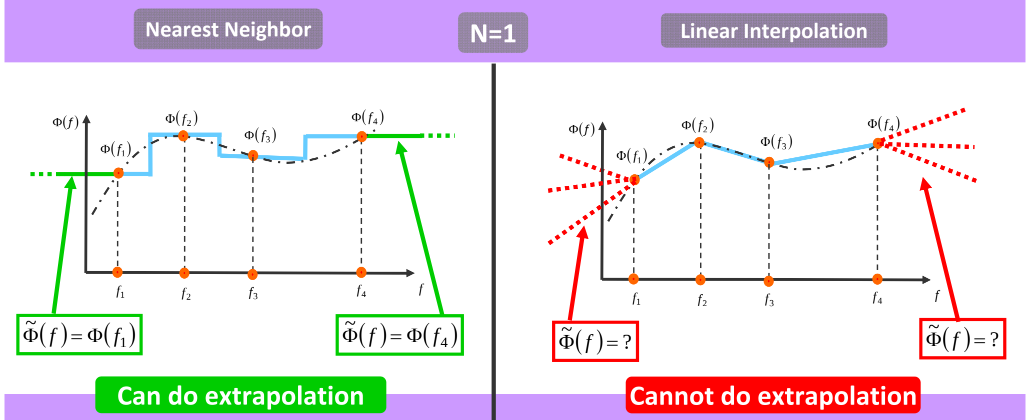
Extrapolation Capabilities



How to extrapolate?
- Nearest neighbor
- Extend the external straight lines

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Efficient Evaluation of $\Phi(f)$

Approximate Φ(f) computation through a predictor (large problems)

Interpolation

- Simple and efficient strategies ↑
- Requires to *a-priori* know/estimate functional dependency (e.g.: polynomial, exponential, etc.) ↓
- Low generalization capabilities ↓
- *Examples: **nearest neighbor interpolation**, **linear interpolation**, polynomial interpolation, spline interpolation*

Learning-by-Examples (LBE)

- Numerically efficient ↑
- No *a-priori* knowledge required ↑
- Good generalization capabilities ↑
- *Examples: Support Vector Machines (SVM), Artificial Neural Networks (ANN), Gaussian Processes (GP), Radial Basis Function (RBF)*

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How do LBE Methods Work?

Learning-By-Example Methods are formulated as two-step approaches

1 **Training** — Offline

f (known) → **LBE Algorithm** → Φ(f) (known)

Objective

Give the LBE method a set of known input-output relations (**[f, Φ(f)]** computed pairs) to train it

2 **Testing** — Online

f (known) → **LBE Algorithm** → Φ(f) (unknown)

Objective

Give the LBE method a set of inputs [**f**] and let it predict the output [**Φ(f)**]

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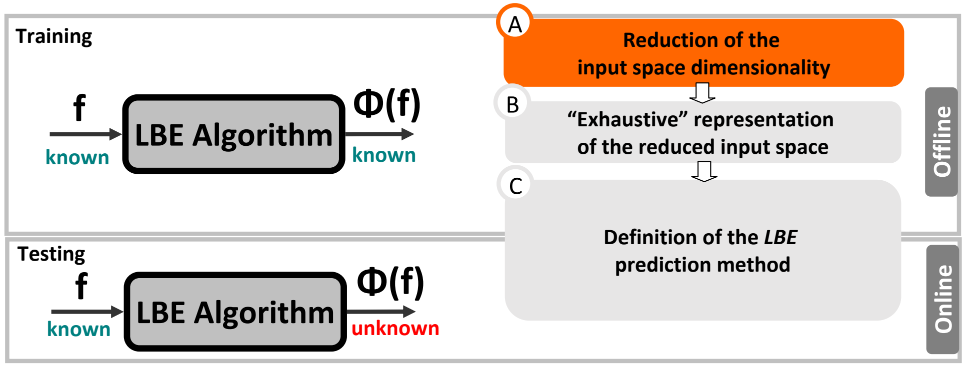
The 3-Steps LBE Framework



Problem How to deal with a <u>large number of variables</u> (N)?

Solution <u>**Reduce the DoFs of the functional space:**</u>
Look for the H<N variables showing the largest impact on the output ("*sensitivity analysis*")

How?

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Reduction of the DoFs

Why? If the <u>**number of variables N is large**</u>, the number of required training samples <u>**S must be large**</u>

"Curse of dimensionality"

$N\uparrow \Rightarrow S\uparrow\uparrow\uparrow$

Num variables — Training size

- High <u>cost</u> of training phase
- High <u>learning complexity</u>

The number of required I/O samples (*S*) increases <u>**much faster**</u> than *N*!

How to mitigate it?

Map the N variables to a lower dimensionality space to reduce their number (and therefore, reduce S)

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Mapping Samples to a Lower Dimensional Space

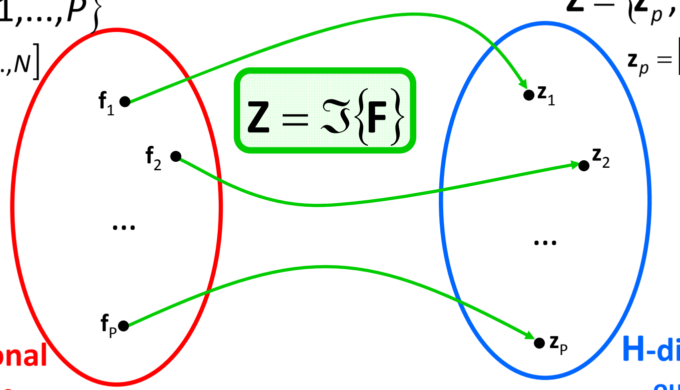
Approach Map P <u>**N-dimensional**</u> samples into P <u>**H-dimensional**</u> samples with **H<N**

$\mathbf{F}=\{\mathbf{f}_p, p=1,\ldots,P\}$

$\mathbf{f}_p=[f_{p,n}, n=1,\ldots,N]$

$\mathbf{Z}=\{\mathbf{z}_p, p=1,\ldots,P\}$

$\mathbf{z}_p=[z_{p,h}, h=1,\ldots,H]$



N-dimensional input space

H-dimensional output space

H<N

How to map?

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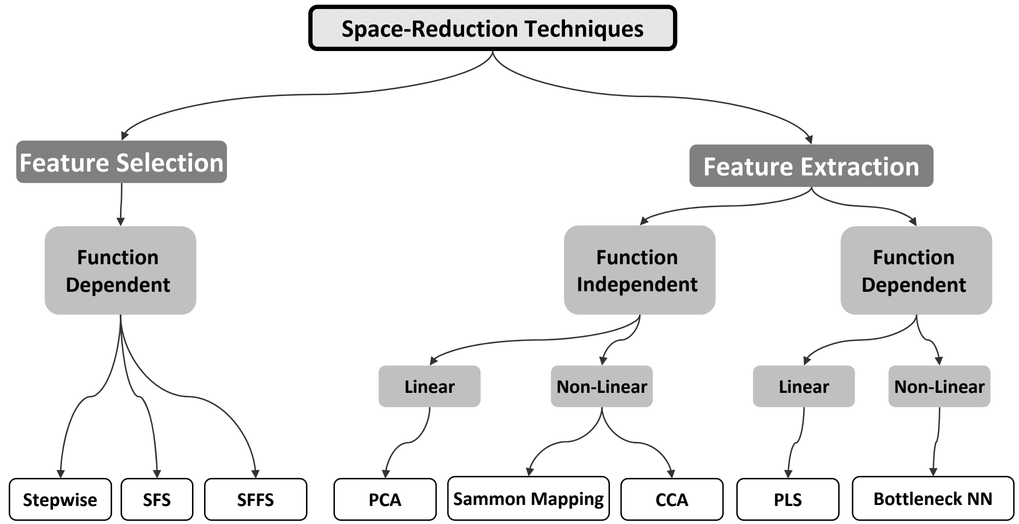
Space-Reduction: Overview



Selection Vs. Extraction?
Function Dependent Vs. Independent?
Linear Vs. Non-Linear?

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Feature Selection vs. Feature Extraction

Feature Selection

Goal **Select** a **subset** of H < N **most relevant** variables (on Φ)

$$\mathbf{f}_p = \left[f_{p,1}, f_{p,2}, f_{p,3}, f_{p,4}, \ldots, f_{p,n}, \ldots f_{p,N} \right]$$

Less relevant on Φ | Less relevant on Φ

More relevant (informative) on Φ

$$\mathbf{z}_p = \left[z_{p,1}, z_{p,2}, \ldots, z_{p,h}, \ldots z_{p,H} \right]$$

Most informative measured features are kept

Sensitivity analysis required to understand which features must be selected

Feature Extraction

Goal **Generate** H **new variables** as a **combination** of the original ones

$$\mathbf{f}_p = \left[f_{p,1}, f_{p,2}, f_{p,3}, f_{p,4}, \ldots, f_{p,n}, \ldots f_{p,N} \right]$$

Feature "combination" $\mathbf{z}_p = \Im\left\{ \mathbf{f}_p \right\}$

$$\mathbf{z}_p = \left[z_{p,1}, z_{p,2}, \ldots, z_{p,h}, \ldots z_{p,H} \right]$$

All measured features used to extract ***new features***

No sensitivity analysis required

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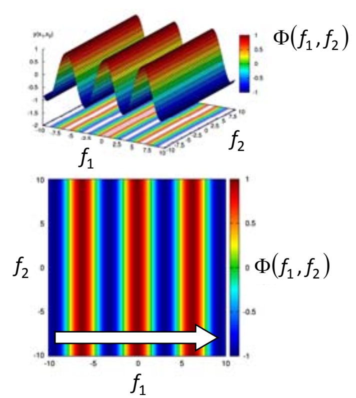
When Feature Selection and When Extraction?

Feature Selection

Example $\Phi(f_1, f_2) = \cos(f_1)$



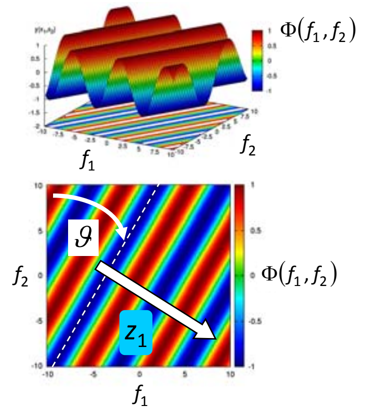
$\Phi(f_1, f_2)$ **depends only** on f_1

$\Phi(f_1, f_2) = \Phi(f_1)$

$$z_1 = f_1$$

Feature Extraction

Example $\Phi(f_1, f_2) = \cos\{f_1 \cos(\vartheta) - f_2 \sin(\vartheta)\}$



$\Phi(f_1, f_2)$ **can be expressed** as $\Phi(z_1)$

$$z_1 = \Im\{f_1, f_2\} = f_1 \cos(\vartheta) - f_2 \sin(\vartheta)$$

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Function Independent vs. Function Dependent

Function Independent

Idea Reduction of the DoFs is based only on the **analysis** of the **input** samples

$\mathbf{F} = \{\mathbf{f}_p, p = 1, \ldots, P\}$ Old input variables

$$\mathbf{Z} = \Im\{\mathbf{F}\}$$

Most suitable for enhancing visualization of input data

Function Dependent

Idea Reduction of the DoFs is based on the **analysis** of the **input-output relationship**

Old input variables: $\mathbf{F} = \{\mathbf{f}_p, p = 1, \ldots, P\}$

Corresponding output: $\mathbf{\Phi} = \{\Phi(\mathbf{f}_p), p = 1, \ldots, P\}$

$$\mathbf{Z} = \Im\{\mathbf{F}; \mathbf{\Phi}\}$$

Most suitable for the prediction of Φ

$$\mathbf{f}_p = \left[f_{p,n}, n = 1, \ldots, N \right]$$
$$\mathbf{z}_p = \left[z_{p,h}, h = 1, \ldots, H \right]$$
$$\mathbf{Z} = \{\mathbf{z}_p, p = 1, \ldots, P\}$$

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Linear vs. Non-Linear Feature Extraction

Linear Feature Extraction

Def. The new H variables are **linear combinations** of the old N variables

New variables / Old variables

$$\mathbf{Z} = \mathbf{F}\mathbf{W}$$

$[P \times H]$ $[P \times N]$ $[N \times H]$

Linear transformation matrix

Non-Linear Feature Extraction

Def. The new H variables are NOT linear combinations of the old N variables

New variables / Old variables

$$\mathbf{Z} = \Im\{\mathbf{F}\}$$

$[P \times H]$ $[P \times N]$

Non-linear transformation function

h-th component of *p*-th transformed sample

$$z_{p,h} = \sum_{n=1}^{N} f_{p,n} w_{n,h}$$

Linear combination of the old N variables

$$z_{p,h} = \Im\{f_{p,n}; n = 1 \ldots, N\}$$

P: Number of transformed samples

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Sequential Feature Selection (SFS)

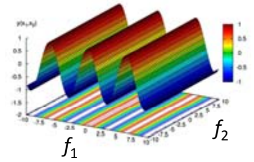
- Space-Reduction Techniques
  - **Feature Selection**
    - Function Dependent
      - Stepwise
      - **SFS**
      - SFFS
  - Feature Extraction
    - Function Independent
      - Linear
        - PCA
      - Non-Linear
        - Sammon Mapping
        - CCA
    - Function Dependent
      - Linear
        - PLS
      - Non-Linear
        - Bottleneck NN

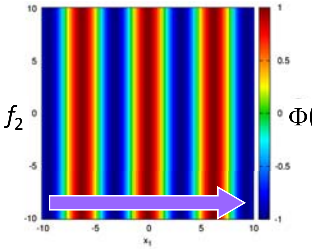
Sequential Feature Selection (SFS) - Basic Idea

Idea Given a set of N variables, select the subset of **H<N** variables having the largest impact on the function

Example $\Phi(f_1, f_2) = \cos(f_1)$

$\Phi(f_1, f_2)$ **depends only** on f_1 $\boxed{\Phi(f_1, f_2) = \Phi(f_1)}$





Select only f_1

$z_1 = f_1$

How to select f_1?

SFS – Block Diagram

Idea Given a set of N variables, select the subset of **H<N** variables having the largest impact on the function

Start from an empty set of selected variables

↓ q=0

Add the variable that optimizes singularly the selected criterion

↓ q=1

Add the variable that, together with those already selected, optimizes the selected criterion

↓ q=q+1

q==H? — NO → back to "Add the variable that, together with those already selected…"; YES → STOP

q=Number of selected variables

H=Number of variables to select

SFS – How to Select Variables (1/4)

Start from an empty set of selected variables

↓ q=0

Add the variable that optimizes singularly the selected criterion

↓ q=1

Add the variable that, together with those already selected, optimizes the selected criterion

↓ q=q+1

q==H? — NO → back; YES → STOP

EXAMPLE:

Dimension of the input space : N = 4

Number of variables to select: H = 3

$\Phi(f_1, f_2, f_3, f_4) = 10 f_2 + f_3 + \cos(f_4) + 0.1 f_1$

Less relevant on Φ | More relevant on Φ

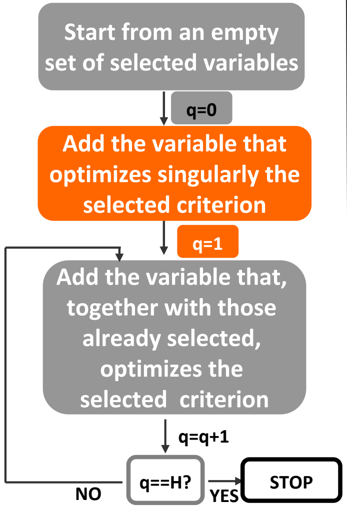
$\underbrace{f_1 \quad f_2 \quad f_3 \quad f_4}_{\text{Consider all possible variables}}$

Number of selected variables: q=0

$\mathbf{z} = \{\ \}$

Which is the first variable to select?

SFS – How to Select Variables (2/4)

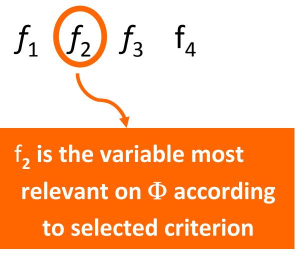


EXAMPLE:

Dimension of the input space : N = 4

Number of variables to select: H = 3

$$\Phi(f_1, f_2, f_3, f_4) = 10 f_2 + f_3 + \cos(f_4) + 0.1 f_1$$



q=1

$$\mathbf{z} = \{f_2\}$$

How to select the remaining H-1 variables?

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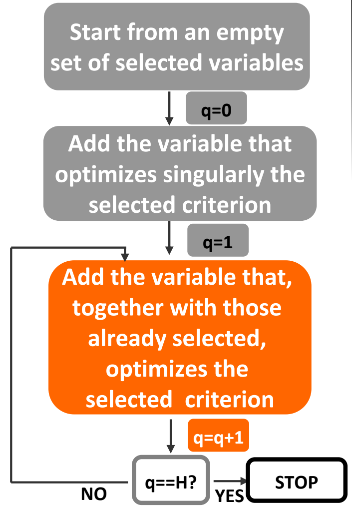
SFS – How to Select Variables (3/4)

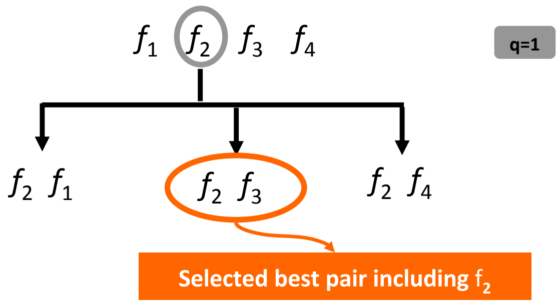


EXAMPLE:

Dimension of the input space : N = 4

Number of variables to select: H = 3

$$\Phi(f_1, f_2, f_3, f_4) = 10 f_2 + f_3 + \cos(f_4) + 0.1 f_1$$



q=2

$$\mathbf{z} = \{f_2, f_3\}$$

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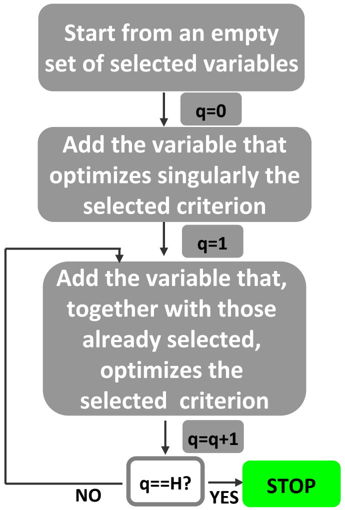
SFS – How to Select Variables (4/4)

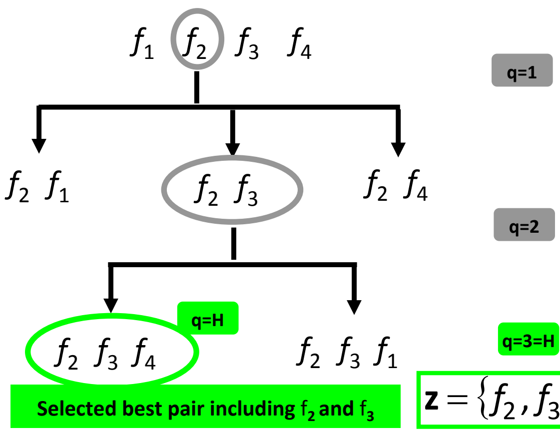


EXAMPLE:

Dimension of the input space : N = 4

Number of variables to select: H = 3

$$\Phi(f_1, f_2, f_3, f_4) = 10 f_2 + f_3 + \cos(f_4) + 0.1 f_1$$



$$\mathbf{z} = \{f_2, f_3, f_4\}$$

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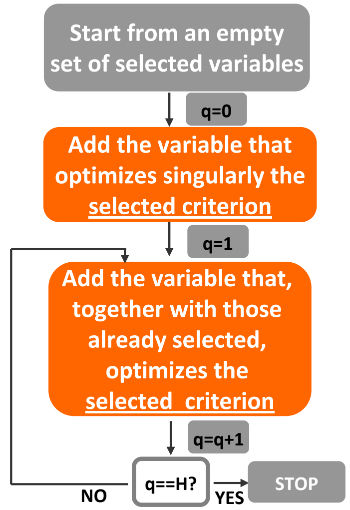
SFS – Selection Criterion?

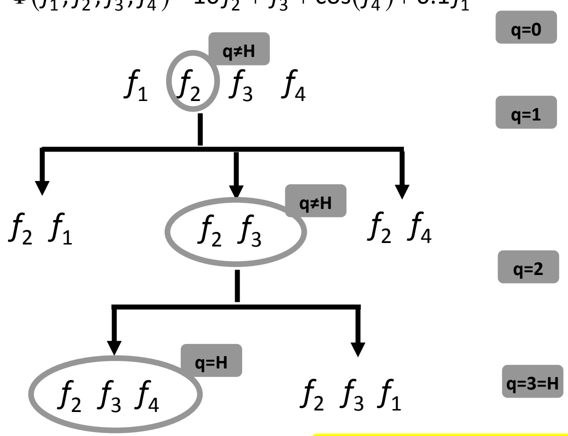


EXAMPLE:

Dimension of the input space : N = 4

Number of variables to select: H = 3

$$\Phi(f_1, f_2, f_3, f_4) = 10 f_2 + f_3 + \cos(f_4) + 0.1 f_1$$



Which criterion?

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Feature Selection: Minimization of Criterion J(·)

EXAMPLE:
Dimension of the input space : N = 4
Number of variables to select: H = 3

$$\Phi(f_1, f_2, f_3, f_4) = 10 f_2 + f_3 + \cos(f_4) + 0.1 f_1$$

$\mathbf{f} = [f_1, f_2, f_3, f_4]$ → $\mathbf{z}_a = [f_1, f_2, f_3]$

$\mathbf{f} = [f_1, f_2, f_3, f_4]$ → $\mathbf{z}_b = [f_1, f_2, f_4]$

$\mathbf{f} = [f_1, f_2, f_3, f_4]$ → $\mathbf{z}_c = [f_1, f_3, f_4]$

$\mathbf{f} = [f_1, f_2, f_3, f_4]$ → $\mathbf{z}_d = [f_2, f_3, f_4]$

Criterion

$J(\mathbf{z}_a) = 7.5 \times 10^{-2}$ $\quad J(\mathbf{z}_b) = 5.4 \times 10^{-2}$ $\quad J(\mathbf{z}_c) = 8.9 \times 10^{-2}$ $\quad J(\mathbf{z}_d) = 3.6 \times 10^{-2}$

Lowest value of J(.)

$$\mathbf{z}_{opt} = \arg\left\{ \min_{\mathbf{z}_a, \mathbf{z}_b, \mathbf{z}_c, \mathbf{z}_d} (J(\mathbf{z})) \right\} = \mathbf{z}_d$$

How to comupte J(·)?

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Feature Selection: How to Evaluate J(·)?

Goal

Compute the **<u>prediction error</u>** when using only the set of selected variables **z**

$$\mathbf{f} = [f_1, f_2, f_3, f_4]$$

$$\mathbf{z}_d = [f_2, f_3, f_4]$$

Prediction error obtained when considering variables f_2,f_3,f_4 and discarding variable f_1

$$J(\mathbf{z}_d) = 3.6 \times 10^{-2}$$

Approach: Cross-Validation

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Computation of Prediction Error: Cross-Validation

Let's consider *P* *H*-dimensional samples, where $\mathbf{z}_p = \underbrace{[f_{p,2}, f_{p,3}, f_{p,4}]}_{\text{Example}}; p = 1,\dots,P$

1. Subdivide the P samples into **V subsets** of T samples

$$\mathbf{Z} = \underbrace{\begin{bmatrix} f_{1,2} & f_{1,3} & f_{1,4} \\ f_{2,2} & f_{2,3} & f_{2,4} \\ \vdots & \vdots & \vdots \\ f_{P,2} & f_{P,3} & f_{P,4} \end{bmatrix}}_{[P \times H]} \underbrace{\begin{bmatrix} \Phi_1 \\ \Phi_2 \\ \vdots \\ \Phi_P \end{bmatrix}}_{[P \times 1]}$$

SUBSET 1 (T samples) — **USE FOR VALIDATION**

SUBSET V-1 (T samples)
SUBSET V (T samples) — **USE FOR TRAIN**

2. For each v-th subset train a predictor using the remaining V-1 subsets

3. Use the resulting model to check prediction accuracy on the v-th subset of selected samples

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Computation of Prediction Error: Cross-Validation

4. Compute Mean Squared Error (η) of the feature subset **z**

For each v-th validation subset (v=1,...,V)

$$\eta_v(\mathbf{z}) = \frac{1}{T} \sum_{i=1}^{T} \left\{ \Phi_{i,v} - \underbrace{\tilde{\Phi}_{i,v}(\mathbf{z})}_{\text{Predicted output}} \right\}^2$$

Example

$$\underbrace{\mathbf{z} = \{f_2, f_3, f_4\}}_{\text{Selected features}}$$

5. Average Mean Squared Error over all V validation subsets

Final criterion (to be minimized)

$$J(\mathbf{z}_d) = \underbrace{\boxed{\frac{1}{V} \sum_{v=1}^{V}}}_{\text{Average over all V subsets}} \frac{1}{T} \sum_{i=1}^{T} \left\{ \Phi_{i,v} - \tilde{\Phi}_{i,v}(\mathbf{z}) \right\}^2$$

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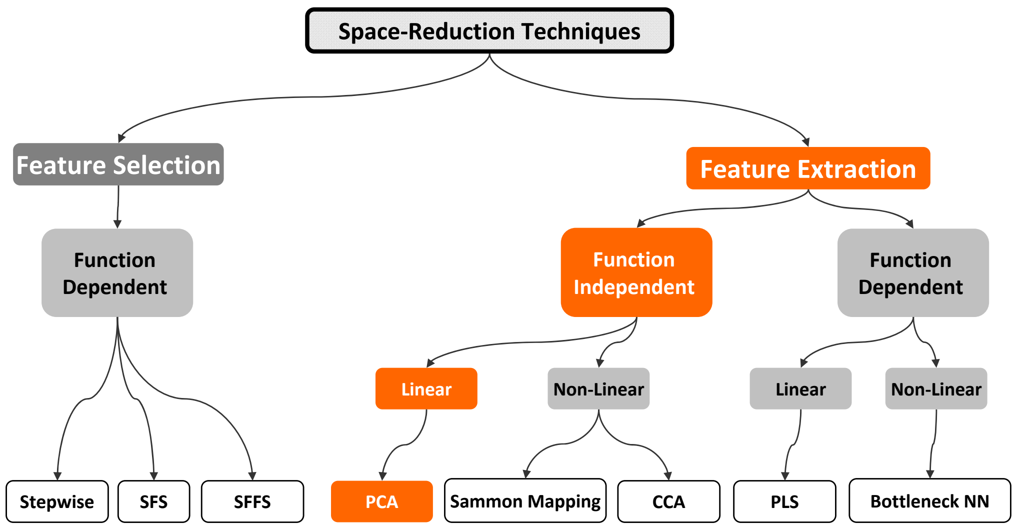
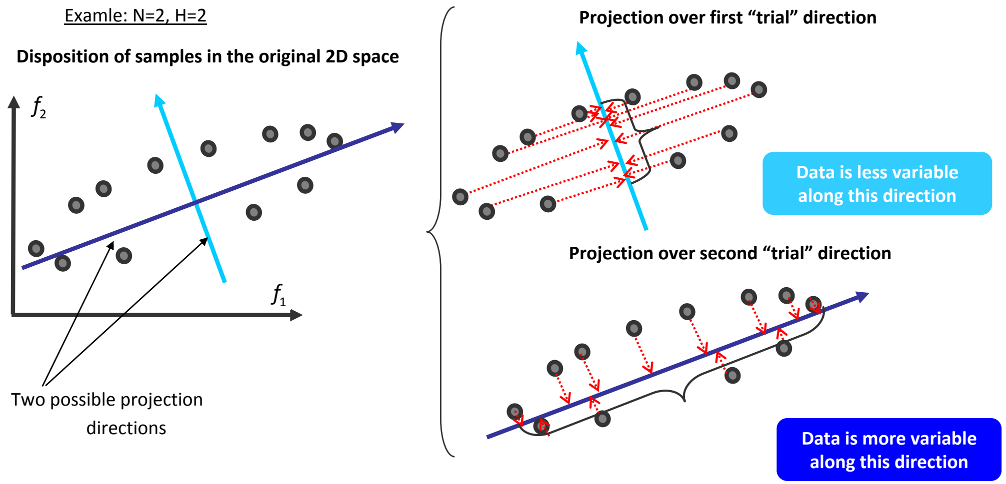
Principal Component Analysis (PCA)



PCA - Basic Idea (1/2)

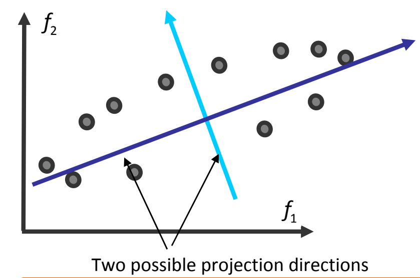
Idea Given P N-dimensional samples $\mathbf{F}=\{\mathbf{f}_p, p=1,\dots,P\}$ find the $H \le N$ **principal components** of data, i.e., the **directions** where there is the **largest variance**



PCA - Basic Idea (2/2)

Idea Given P N-dimensional samples $\mathbf{F}=\{\mathbf{f}_p, p=1,\dots,P\}$ find the $H \le N$ principal components of data, i.e., the **directions** where there is the **most variance**

Disposition of samples in the original 2D space



Which directions?

Compute the **N eigenvectors** of the **covariance matrix** in the original input space

How much variance?

Compute the **eigenvalues** associated to each eigenvector: larger eigenvalue means larger variance

Feature extraction: Project input samples onto the H<N eigenvectors {$\underline{W}_h$, h=1,…,H} showing the largest eigenvalues (the principal components)

$\underline{W}_h; h=1,\dots,H$ Basis of the J-dimensional subspace ***How to compute?***

PCA – Computation of The Basis

Linear Transformation

New variables, Old variables, Basis

$$\underset{[P\times H]}{\mathbf{Z}} = \underset{[P\times N]}{\mathbf{F}} \times \underset{[N\times H]}{\mathbf{W}} \qquad \underline{W} = \begin{bmatrix} w_{1,1} & w_{2,1} & \cdots & w_{H,1} \\ w_{1,2} & w_{2,2} & \cdots & w_{H,2} \\ \vdots & \vdots & \cdots & \vdots \\ w_{1,N} & w_{2,N} & \cdots & w_{H,N} \end{bmatrix}$$

$\underline{W}_1 \quad \underline{W}_2 \quad \dots \quad \underline{W}_H$

How to Compute? The basis vectors {$\underline{W}_h$; h=1,…,H} are the **eigenvectors** of the **covariance matrix** associated to the H **highest eigenvalues**

Covariance Matrix

$$\mathbf{C} = \frac{1}{P-1}\sum_{p=1}^{P}\left(\mathbf{f}_p - \overline{\mathbf{f}}\right)\left(\mathbf{f}_p - \overline{\mathbf{f}}\right)^T$$

Average vector

$$\overline{\mathbf{f}} = \frac{1}{S}\sum_{s=1}^{S}\mathbf{f}_p$$

Properties

- {$\underline{W}_h$; h=1,…,H} are called **principal components**
- {$\underline{W}_h$; h=1,…,H} are mutually **orthogonal**
- $\underline{W}_1$ has the **largest possible variance** (followed by $\underline{W}_2$, …, $\underline{W}_H$)

Covariance Matrix

$$\mathbf{C}=\begin{bmatrix} \mathrm{var}(f_1) & \mathrm{cov}(f_1,f_2) & \cdots & \mathrm{cov}(f_1,f_N) \\ \mathrm{cov}(f_2,f_1) & \mathrm{var}(f_2) & \cdots & \mathrm{cov}(f_2,f_N) \\ \vdots & \ddots & \ddots & \vdots \\ \mathrm{cov}(f_N,f_1) & \cdots & \mathrm{cov}(f_N,f_{N-1}) & \mathrm{var}(f_N) \end{bmatrix}$$

Diagonal: Variance of i-th (i=1,…,N) variables

$$\mathrm{var}(f_i)=\frac{1}{P-1}\sum_{p=1}^{P}\left(f_{p,i}-\bar{f}_i\right)^2$$

Average of i-th variable

$$\bar{f}_i=\frac{1}{P}\sum_{p=1}^{P}f_{p,i}$$

Off-Diagonal: Covariance between i-th and j-th variables

$$\mathrm{cov}(f_i,f_j)=\frac{1}{P-1}\sum_{p=1}^{P}\left(f_{p,i}-\bar{f}_i\right)\left(f_{p,j}-\bar{f}_j\right)$$

$\mathrm{cov}(f_i,f_j)=\mathrm{cov}(f_j,f_i) \Rightarrow$ **C** is symmetric

Meaning of cov(f_i,f_j)?

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Covariance Between Two Variables

Covariance between i-th and j-th variables

$$\mathrm{cov}(f_i,f_j)=\frac{1}{P-1}\sum_{p=1}^{P}\left(f_{p,i}-\bar{f}_i\right)\left(f_{p,j}-\bar{f}_j\right) \qquad \mathrm{cov}(f_i,f_j)=\mathrm{cov}(f_j,f_i)$$

Meaning Measure of how much two variables f_i and f_j **change together**

- If f_j assumes **larger values** when f_i **increases**, covariance is **posivive**
- If f_j assumes **lower values** when f_i **increases**, covariance is **negative**

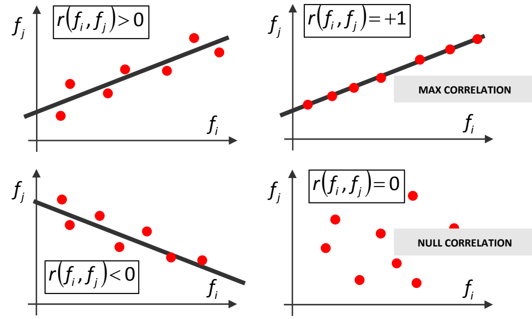
Correlation Coefficient r (Normalized Covariance)

$$r(f_i,f_j)=r(f_j,f_i)=\frac{\mathrm{cov}(f_i,f_j)}{std(f_i)\,std(f_j)}$$

$$-1\le r(f_i,f_j)\le +1$$

$$std(f_i)=\sqrt{\frac{1}{P-1}\sum_{p=1}^{P}\left(f_{p,i}-\bar{f}_i\right)^2}$$

Stadard deviation of i-th variable



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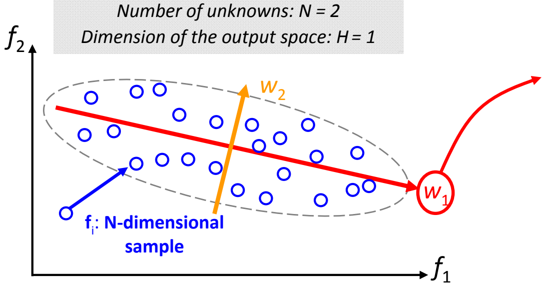
PCA – 2-D Example

EXAMPLE:

Number of unknowns: N = 2

Dimension of the output space: H = 1

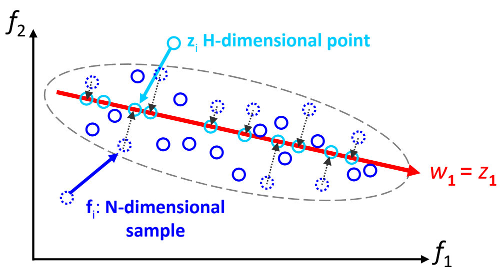


Eigenvector $\mathbf{w}_1$ corresponds to the highest eigenvalue

Greatest variance of the data lies on the first principal component $\mathbf{w}_1$

Project samples onto the principal component $\mathbf{w}_1$

- The total number of eigenvectors is equal to N
- The eigenvectors are mutually orthogonal



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PCA - Example (1/7)

EXAMPLE:

Number of unknowns: N = 2

Number of samples: P = 10

Compute the covariance matrix C

↓

Compute the eigenvalues of C

↓

Compute the eigenvectors of C

↓

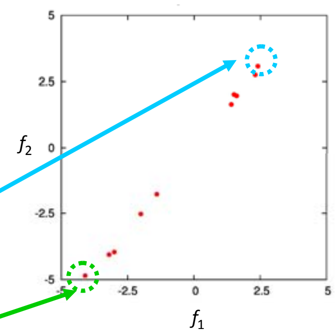
Project samples onto eigenvectors

Input 2-dimensional samples

$\mathbf{F} = [P\times N]$

Sample Index, *p*	f_1	f_2
1	1.4	1.65
2	1.6	1.975
3	-1.4	-1.775
4	-2.0	-2.525
5	-3.0	-3.95
6	2.4	3.075
7	1.5	2.025
8	2.3	2.75
9	-3.2	-4.05
10	-4.1	-4.85

Disposition of samples in the original space



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PCA - Example (2/7)

EXAMPLE:
Number of unknowns: N = 2
Number of samples: P = 10

Compute the covariance matrix C → Compute the eigenvalues of C → Compute the eigenvectors of C → Project samples onto eigenvectors

$$\underset{[N\times N]}{\mathbf{C}}=\begin{bmatrix} Var(f_1) & Cov(f_1,f_2) \\ Cov(f_2,f_1) & Var(f_2) \end{bmatrix}$$

Variance of *i*-th variable

$$Var(f_i)=\frac{1}{P-1}\sum_{p=1}^{P}\left(f_{p,i}-\bar{f}_i\right)^2$$

Average of *i*-th variable

$$\bar{f}_i=\frac{1}{P}\sum_{p=1}^{P}f_{p,i}$$

Covariance between variables f_1 and f_2

$$Cov(f_1,f_2)=Cov(f_2,f_1)=\frac{1}{P-1}\sum_{p=1}^{P}\left(f_{p,1}-\bar{f}_1\right)\left(f_{p,2}-\bar{f}_2\right)$$

$$\bar{f}_1=-0.45 \qquad \bar{f}_2=-0.5675$$

$$Var(f_1)=6.4228$$
$$Var(f_2)=9.9528$$
$$Cov(f_1,f_2)=Cov(f_2,f_1)=7.9876$$

$$\Rightarrow \quad \mathbf{C}=\begin{bmatrix} 6.4228 & 7.9876 \\ 7.9876 & 9.9528 \end{bmatrix}$$

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PCA - Example (3/7)

EXAMPLE:
Number of unknowns: N = 2
Number of samples: P = 10

Compute the covariance matrix C → **Compute the eigenvalues of C** → Compute the eigenvectors of C → Project samples onto eigenvectors

Find the eigenvalues of **C** by solving

$$\det\left(\mathbf{C}-\lambda\mathbf{I}\right)=0$$

$$\det\left(\mathbf{C}-\lambda\mathbf{I}\right)=\det\begin{bmatrix} Var(f_1)-\lambda & Cov(f_1,f_2) \\ Cov(f_2,f_1) & Var(f_2)-\lambda \end{bmatrix}=0$$

$$\mathbf{C}=\begin{bmatrix} 6.4228 & 7.9876 \\ 7.9876 & 9.9528 \end{bmatrix} \qquad Var(f_1)=6.4228 \quad Var(f_2)=9.9528$$

$$\lambda_1=16.368$$
$$\lambda_2=0.00746$$

Eigenvalues of the covariance matrix

Note The sum of the eigenvalues equals the sum of the variances

$$\lambda_1+\lambda_2=16.3756=Var(f_1)+Var(f_2)$$

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PCA - Example (4/7)

EXAMPLE:
Number of unknowns: N = 2
Number of samples: P = 10

Compute the covariance matrix C → Compute the eigenvalues of C → **Compute the eigenvectors of C** → Project samples onto eigenvectors

For each *i*-th eigenvalue solve

$$\begin{cases} \left(\mathbf{C}-\lambda_i\mathbf{I}\right)\times\mathbf{w}_i=0 \Rightarrow \begin{bmatrix} Var(f_1)-\lambda_i & Cov(f_1,f_2) \\ Cov(f_2,f_1) & Var(f_2)-\lambda_i \end{bmatrix}\begin{bmatrix} w_{i,1} \\ w_{i,2} \end{bmatrix}=0 \\ \text{Subject to} \\ w_{i,1}^2+w_{i,2}^2=1 \end{cases}$$

Eigenvector associated to the *i*-th eigenvalue

$(\mathbf{C}-\lambda_1\mathbf{I})$ $\quad \lambda_1=16.368$

$$\begin{bmatrix} -9.9453 & 7.9876 \\ 7.9876 & -6.4153 \end{bmatrix}\begin{bmatrix} w_{1,1} \\ w_{1,2} \end{bmatrix}=0 \Rightarrow$$

First principal component

$$\underline{W}_1=\begin{bmatrix} 0.6262 \\ 0.7790 \end{bmatrix}$$

$$\begin{bmatrix} 6.41534 & 7.9876 \\ 7.9876 & 9.94534 \end{bmatrix}\begin{bmatrix} w_{2,1} \\ w_{2,2} \end{bmatrix}=0 \Rightarrow$$

$(\mathbf{C}-\lambda_2\mathbf{I})$ $\quad \lambda_2=0.00746$

Second principal component

$$\underline{W}_2=\begin{bmatrix} -0.7790 \\ 0.6262 \end{bmatrix}$$

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PCA - Example (5/7)

EXAMPLE:
Number of unknowns: N = 2
Number of samples: P = 10

Compute the covariance matrix C → Compute the eigenvalues of C → Compute the eigenvectors of C → **Project samples onto eigenvectors**

Eigenvectors of the covariance matrix

$$\mathbf{Z}=\mathbf{F}_0\mathbf{W}=\left(\mathbf{F}-\bar{\mathbf{F}}\right)\left[\mathbf{w}_1 \quad \mathbf{w}_2\right]$$

Projected samples

Zero-mean input samples

$$\underset{[P\times H]}{\mathbf{Z}}=$$

$f_1-\bar{f}_1$	$f_2-\bar{f}_2$
1.85	2.2175
2.05	2.5425
-0.95	-1.2075
-1.55	-1.9575
-2.55	-3.3825
2.85	3.6425
1.95	2.5925
2.75	3.3175
-2.75	-3.4825
-3.65	-4.2825

×

$\mathbf{w}_1$	$\mathbf{w}_2$
0.6262	-0.7797
0.7797	0.6262

=

Projected samples

z_1	z_2
2.8874	-0.0538
3.2660	-0.0062
-1.5363	-0.0154
-2.4968	-0.0173
-4.2340	-0.1299
4.6246	0.0589
3.2424	0.1031
4.3086	-0.0667
-4.4372	-0.0366
-5.6245	0.1641

$[P\times H]$

$$\bar{f}_1=-0.45 \qquad \bar{f}_2=-0.5675$$

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PCA - Example (6/7)

EXAMPLE:
Number of unknowns: N = 2
Number of samples: P = 10

$$\mathbf{Z} = \mathbf{F}_0\mathbf{W} = \left(\mathbf{F} - \overline{\mathbf{F}}\right)\left[\mathbf{w}_1 \quad \mathbf{w}_2\right]$$

Eigenvectors of the covariance matrix

Projected samples

Zero-mean input samples

Compute the covariance matrix C → Compute the eigenvalues of C → Compute the eigenvectors of C → **Project samples onto eigenvectors**

Z =

z_1	z_2
2.8874	-0.0538
3.2660	-0.0062
-1.5363	-0.0154
-2.4968	-0.0173
-4.2340	-0.1299
4.6246	0.0589
3.2424	0.1031
4.3086	-0.0667
-4.4372	-0.0366
-5.6245	0.1641

Projected samples

Note

$$Var(z_1) = 16.368 = \lambda_1$$
$$Var(z_2) = 0.00746 = \lambda_2$$

The variance of the projections onto the principal components is equal to the eigenvalues of the covariance matrix

The first eigenvector expresses around 99% of total variance

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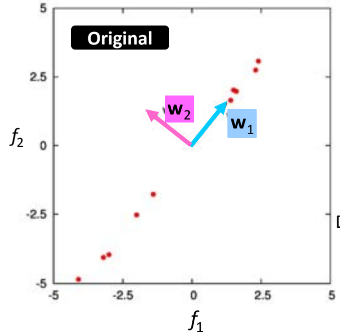
PCA - Example (7/7)

EXAMPLE:
Number of unknowns: N = 2
Number of samples: P = 10

Compute the covariance matrix C → Compute the eigenvalues of C → Compute the eigenvectors of C → **Project samples onto eigenvectors**

Disposition of samples in the original space (N=2)

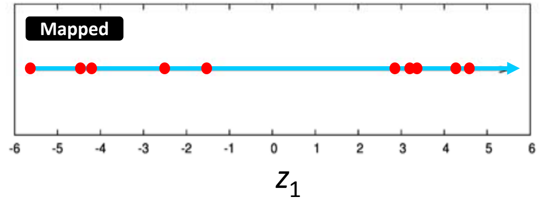


$\mathbf{w}_1$ is the **direction of maximum variance**

→ $\lambda_1 = 16.368$
$\lambda_2 = 0.00746$

Data have a very limited variance along $\mathbf{w}_2$

Disposition of samples after projection onto first principal component (H=1)



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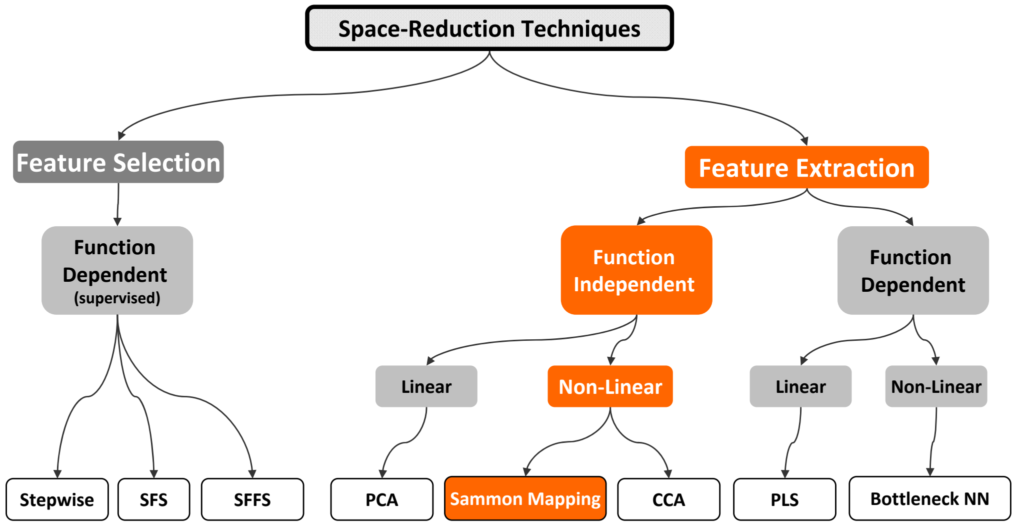
Sammon Mapping



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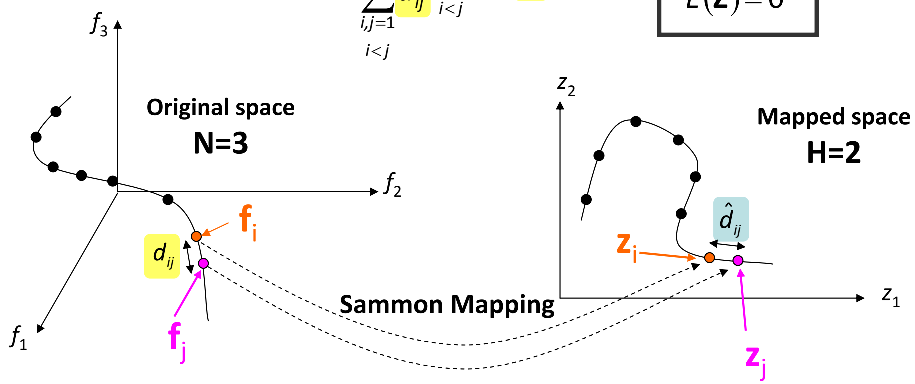
Sammon Mapping – Basic Idea

Goal **Preserve** the topological structure (**distance between samples**) between the two N-dimensional and H-dimensional (H<N) spaces

Mismatch between the distances in the two spaces (to be minimized)

$$E(\mathbf{Z}) = \frac{1}{\sum_{\substack{i,j=1 \\ i<j}}^{P} d_{ij}} \sum_{\substack{i,j=1 \\ i<j}}^{P} \frac{\left(d_{ij} - \hat{d}_{ij}\right)^2}{d_{ij}}$$

if $d_{ij} = \hat{d}_{ij}$ ⬇ $E(\mathbf{Z}) = 0$



$$d_{ij} = \sqrt{\sum_{n=1}^{N}\left(f_{n,i} - f_{n,j}\right)^2}$$

$$\hat{d}_{ij} = \sqrt{\sum_{h=1}^{H}\left(z_{h,i} - z_{h,j}\right)^2}$$

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Sammon Mapping – Minimization of E(Z)

Goal **Minimize** the mismatch E(**Z**): $\mathbf{z}^{opt} = \arg\min_{\mathbf{z}} \{E(\mathbf{z})\} = \arg\min_{\mathbf{z}} \left\{ \frac{1}{\sum_{\substack{i,j=1\\ i<j}}^{P} d_{ij}} \sum_{\substack{i,j=1\\ i<j}}^{P} \frac{\left(d_{ij} - \hat{d}_{ij}\right)^2}{d_{ij}} \right\}$

How Gradient Descent Optimization

Initialization

$k=0 \quad \mathbf{Z}^{(0)}$

$k = k+1$

Update

$\mathbf{Z}^{(k+1)} = \mathbf{Z}^{(k)} + \Delta\mathbf{Z}$

How to Choose Z $\boldsymbol{^{(0)}}$***?***

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Sammon Mapping - Initialization

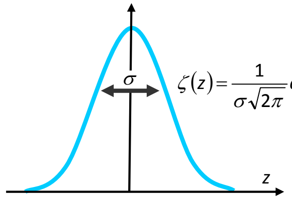
Initialization strategies for setting $\mathbf{Z}^{(0)}$

Random Initialization

Normal distribution with zero mean and variance equal to one

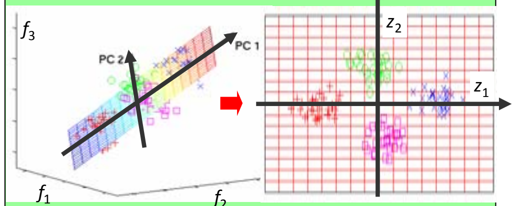
$$z_{p,h}^{(0)} = \mathcal{N}\left(\mu = 0; \sigma^2 = 1\right)$$

$h = 1,\ldots,H; \quad p = 1,\ldots,P$



$$\zeta(z) = \frac{1}{\sigma\sqrt{2\pi}} e^{\frac{-(z-\mu)^2}{2\sigma^2}}$$

Principal Component Analysis (PCA) Initialization



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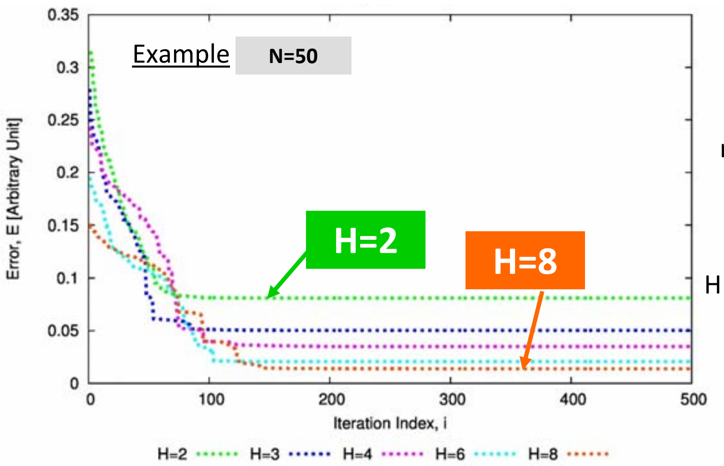
Sammon Mapping – Minimization of E(Z)

Goal **Minimize** the mismatch E(**Z**): $\mathbf{z}^{opt} = \arg\min_{\mathbf{z}} \{E(\mathbf{z})\} = \arg\min_{\mathbf{z}} \left\{ \frac{1}{\sum_{\substack{i,j=1\\ i<j}}^{P} d_{ij}} \sum_{\substack{i,j=1\\ i<j}}^{P} \frac{\left(d_{ij} - \hat{d}_{ij}\right)^2}{d_{ij}} \right\}$

How Gradient Descent Optimization



If H tends to N, the mismatch E tends to zero

H tipically user-defined

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Partial Least Squares (PLS)

Space-Reduction Techniques

- **Feature Selection**
  - **Function Dependent** (supervised)
    - **Stepwise**
    - **SFS**
    - **SFFS**
- **Feature Extraction**
  - **Function Independent**
    - **Linear**
      - **PCA**
    - **Non-Linear**
      - **Sammon Mapping**
      - **CCA**
  - **Function Dependent**
    - **Linear**
      - **PLS**
    - **Non-Linear**
      - **Bottleneck NN**

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PLS – Goal (1/2)

Goal Find a **new** set of **variables Z** such that the **input-output** relationship is **linearized** as much as possible

Zero-mean output · New variables · **Linear Approximation** $\tilde{\Phi}_0$

$$\Phi_0 = ZQ^T + E$$

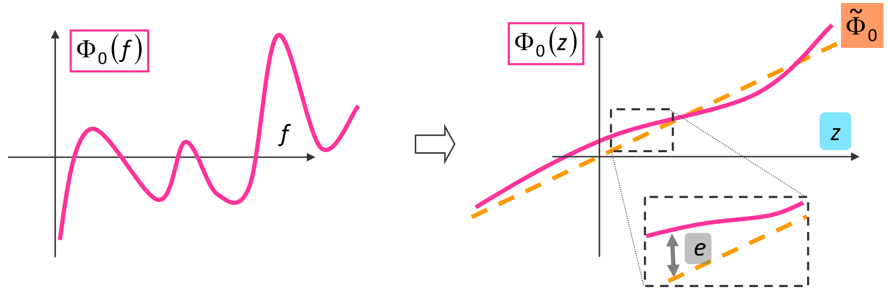
$$[P\times V] \quad [P\times H] \quad [H\times V] \quad [P\times V]$$

Approximation error $E = \Phi_0 - \tilde{\Phi}_0$

The lower the error, the better the approximation

P: Number of samples
H: # of new variables
V: Dimension of the output

Example: N=1, V=1, H=1



Input-output relation is **non-linear** w.r.t. the "old" variable f

Input-output relation is **almost linear** w.r.t. the "new" variable z

PLS – Goal (2/2)

Goal Find a **new** set of **variables Z** such that the **input-output** relationship is **linearized** as much as possible

Zero-mean output · New variables · **Linear Approximation** $\tilde{\Phi}_0$

$$\Phi_0 = ZQ^T + E$$

$$[P\times V] \quad [P\times H] \quad [H\times V] \quad [P\times V]$$

Approximation error $E = \Phi_0 - \tilde{\Phi}_0$

P: Number of samples
H: # of new variables
V: Dimension of the output

$$\begin{bmatrix} (\Phi_{1,1}-\bar{\Phi}_1) & (\Phi_{1,2}-\bar{\Phi}_2) & \cdots & (\Phi_{1,V}-\bar{\Phi}_V)\\ (\Phi_{2,1}-\bar{\Phi}_1) & (\Phi_{2,2}-\bar{\Phi}_2) & \cdots & (\Phi_{2,V}-\bar{\Phi}_V)\\ \vdots & \ddots & (\Phi_{p,v}-\bar{\Phi}_v) & \vdots\\ (\Phi_{P,1}-\bar{\Phi}_1) & \cdots & \ddots & (\Phi_{P,V}-\bar{\Phi}_V)\end{bmatrix} = \underbrace{\begin{bmatrix} z_{1,1} & z_{1,2} & \cdots & z_{1,H}\\ z_{2,1} & z_{2,1} & \cdots & z_{2,H}\\ \vdots & \ddots & z_{p,h} & \vdots\\ z_{P,1} & \cdots & \ddots & z_{P,H}\end{bmatrix}}_{H:\ \#\ \text{new variables}} \begin{bmatrix} q_{1,1} & q_{1,2} & \cdots & q_{1,V}\\ q_{2,1} & q_{2,1} & \cdots & q_{2,V}\\ \vdots & \ddots & q_{h,v} & \vdots\\ q_{H,1} & \cdots & \ddots & q_{H,V}\end{bmatrix} + \begin{bmatrix} e_{1,1} & e_{1,2} & \cdots & e_{1,V}\\ e_{2,1} & e_{2,1} & \cdots & e_{2,V}\\ \vdots & \ddots & e_{p,v} & \vdots\\ e_{P,1} & \cdots & \ddots & e_{P,V}\end{bmatrix}$$

v-th component of the function value for the p-th sample

$$\Phi_{p,v} - \bar{\Phi}_v = [\Phi_0(\mathbf{f}_p)]_v = \left(\sum_{h=1}^{H} z_{p,h} q_{h,v}\right) + e_{p,v}$$

Goal **Minimize** the approximation error **E**

How to find Z?

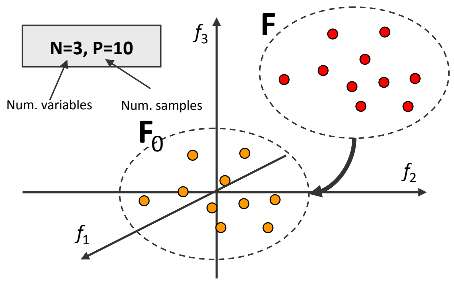
Centering F and Φ

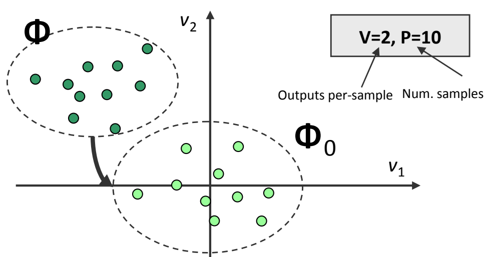
Centered input samples (N dimensional)

$$F_0 = (F - \bar{F}) = \{[(f_{p,n} - \bar{f}_n), n=1,\dots,N], p=1,\dots,P\}$$

Centered output values (V dimensional)

$$\Phi_0 = (\Phi - \bar{\Phi}) = \{[(\Phi_{p,v} - \bar{\Phi}_v), v=1,\dots,V], p=1,\dots,P\}$$





$$F_0 = \begin{bmatrix} (f_{1,1}-\bar{f}_1) & (f_{1,2}-\bar{f}_2) & \cdots & (f_{1,N}-\bar{f}_N)\\ (f_{2,1}-\bar{f}_1) & (f_{2,2}-\bar{f}_2) & \cdots & (f_{2,N}-\bar{f}_N)\\ \vdots & \ddots & (f_{p,n}-\bar{f}_n) & \vdots\\ (f_{P,1}-\bar{f}_1) & \cdots & \ddots & (f_{P,N}-\bar{f}_N)\end{bmatrix}$$

$$\Phi_0 = \begin{bmatrix} (\Phi_{1,1}-\bar{\Phi}_1) & (\Phi_{1,2}-\bar{\Phi}_2) & \cdots & (\Phi_{1,V}-\bar{\Phi}_V)\\ (\Phi_{2,1}-\bar{\Phi}_1) & (\Phi_{2,2}-\bar{\Phi}_2) & \cdots & (\Phi_{2,V}-\bar{\Phi}_V)\\ \vdots & \ddots & (\Phi_{p,v}-\bar{\Phi}_v) & \vdots\\ (\Phi_{P,1}-\bar{\Phi}_1) & \cdots & \ddots & (\Phi_{P,V}-\bar{\Phi}_V)\end{bmatrix}$$

Average of i-th variable (i=1,...,N) over P samples

$$\bar{f}_i = \frac{1}{P}\sum_{p=1}^{P} f_{p,i}$$

Average of v-th output (v=1,...,V) over P samples

$$\bar{\Phi}_v = \frac{1}{P}\sum_{p=1}^{P} \Phi_{p,v}$$

PLS – Extract The New Variables (Z)

Idea Find a **linear** transformation matrix $W = \Psi\{F;\Phi\}$ such that

Input · Output

(Zero-mean) old variables

New variables

$$Z = F_0 W$$

$$[P\times H] \quad [P\times N] \quad [N\times H]$$

P: Number of transformed samples
N: # old variables
H: # new variables

$$F_0 = (F - \bar{F}) = \{[(f_{p,n} - \bar{f}_n), n=1,\dots,N], p=1,\dots,P\}$$

Average of each n-th variable (n=1,...,N)

Such that the input-output relationship becomes **linear** w.r.t. **Z**

Value of the h-th new variable for the p-th sample

$$z_{p,h} = \sum_{n=1}^{N} f^0_{p,n} w_{n,h}$$

Value of the n-th old variable for the p-th sample (zero-mean)

The new variables are linear combinations of the old ones

How to find W?

Linear Decomposition of Input and Output Matrices

Basic HP Both input ($\mathbf{F}_0$) and output ($\mathbf{\Phi}_0$) can be expressed by **linear approximations**

Input

$$\underset{[P\times N]}{\mathbf{F}_0} = \underset{[P\times H]}{\mathbf{Z}}\underset{[H\times N]}{\mathbf{A}^T} + \underset{[P\times N]}{\mathbf{L}}$$

Output

$$\underset{[P\times V]}{\mathbf{\Phi}_0} = \underset{[P\times H]}{\mathbf{U}}\underset{[H\times V]}{\mathbf{Q}^T} + \underset{[P\times V]}{\mathbf{G}}$$

Errors made by the linear approximation

W is such that the transformed variables **(Z)** have **maximum correlation** with the transformed output **(U)**

⇓

If **Z** and **U** are **correlated**, we will be able to estimate the output directly from **Z**

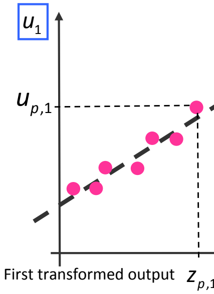
$$\mathbf{\Phi}_0 = \mathbf{Z}\mathbf{Q}^T + \mathbf{E}$$

PLS – Approach

Approach **Maximize** the **covariance** between corresponding columns of **Z** and **U**

Input $\mathbf{F}_0 = \mathbf{Z}\mathbf{A}^T + \mathbf{L}$

Output $\mathbf{\Phi}_0 = \mathbf{U}\mathbf{Q}^T + \mathbf{G}$



$\mathbf{z}_1$ has maximum covariance with $\mathbf{u}_1$,

$\mathbf{z}_2$ has maximum covariance with $\mathbf{u}_2$,

...

$\mathbf{z}_1$ First transformed variable

$\mathbf{u}_1$ First transformed output

$$\mathbf{Z} = \begin{bmatrix} z_{1,1} & z_{1,2} & \cdots & z_{1,H} \\ z_{2,1} & z_{2,2} & \cdots & z_{2,H} \\ \vdots & & \ddots & \vdots \\ z_{P,1} & \cdots & \ddots & z_{P,H} \end{bmatrix} \qquad \mathbf{U} = \begin{bmatrix} u_{1,1} & u_{1,2} & \cdots & u_{1,H} \\ u_{2,1} & u_{2,2} & \cdots & u_{2,H} \\ \vdots & & \ddots & \vdots \\ u_{P,1} & \cdots & \ddots & u_{P,H} \end{bmatrix}$$

P: # of samples

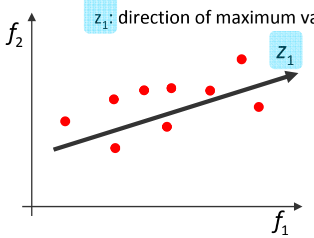
Difference w.r.t PCA?

PLS vs. PCA

PCA

PCA finds the **directions of maximum variation** in **F**

z_1: direction of maximum variance in **F**

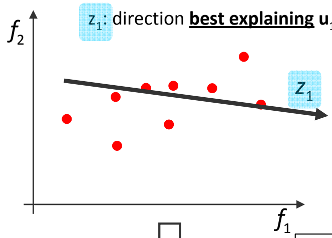


If applied to **Φ** it would find the directions of maximum variation in **Φ**

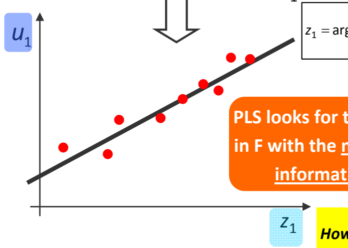
PLS

PLS finds the **directions** in **F** **best predicting** the output value **Φ**

z_1: direction **best explaining** $\mathbf{u}_1$



⇓



$$z_1 = \arg\left\{\max_{z_1}\left[r(z_1,u_1)\right]\right\}$$

PLS looks for the directions in F with the **most relevant information on Φ**

How to compute W?

Eigenvalue Decopomposition Algorithm (1/6)

- **Initialization: set h=0, Compute $\mathbf{F}_0$ and $\mathbf{\Phi}_0$**
- h=h+1
- **Compute the h-th column of W ($\mathbf{w}_h$)**
- **Compute the h-th column of Z ($\mathbf{z}_h$)**
- **Compute the h-th column of U ($\mathbf{u}_h$)**
- ***h==H?*** yes → **END**; no → **Update $\mathbf{F}_{h-1}$ and $\mathbf{\Phi}_{h-1}$** → h=h+1

Variables of the first sample $\mathbf{f}_1$

$$\mathbf{F} = \begin{bmatrix} f_{1,1} & f_{1,2} & \cdots & f_{1,N} \\ f_{2,1} & f_{2,2} & \cdots & f_{2,N} \\ \vdots & \ddots & & \vdots \\ f_{P,1} & \cdots & \ddots & f_{P,N} \end{bmatrix} \quad [P\times N]$$

Number of samples — Number of variables

Outputs of the first sample $\mathbf{\Phi}(\mathbf{f}_1)$

$$\mathbf{\Phi} = \begin{bmatrix} \Phi_{1,1} & \Phi_{1,2} & \cdots & \Phi_{1,V} \\ \Phi_{2,1} & \Phi_{2,2} & \cdots & \Phi_{2,V} \\ \vdots & \ddots & & \vdots \\ \Phi_{P,1} & \cdots & \ddots & \Phi_{P,V} \end{bmatrix} \quad [P\times V]$$

Number of outputs per sample

Average of *i*-th variable

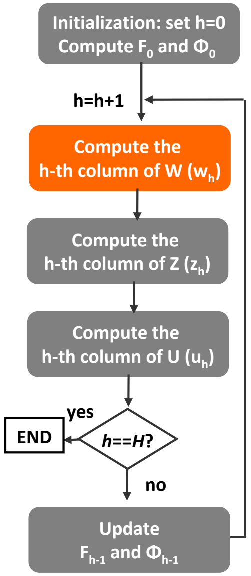
$$\bar{f}_i = \frac{1}{P}\sum_{p=1}^{P} f_{p,i} \Longrightarrow \mathbf{F}_0 = \mathbf{F} - \bar{\mathbf{F}} = \begin{bmatrix} (f_{1,1}-\bar{f}_1) & (f_{1,2}-\bar{f}_2) & \cdots & (f_{1,N}-\bar{f}_N) \\ (f_{2,1}-\bar{f}_1) & (f_{2,2}-\bar{f}_2) & \cdots & (f_{2,N}-\bar{f}_N) \\ \vdots & & \ddots & \vdots \\ (f_{P,1}-\bar{f}_1) & \cdots & \ddots & (f_{P,N}-\bar{f}_N) \end{bmatrix}$$

Subtract the average from both input and ouput

Average of *v*-th output

$$\bar{\Phi}_v = \frac{1}{P}\sum_{p=1}^{P} \Phi_{p,v} \Longrightarrow \mathbf{\Phi}_0 = \mathbf{\Phi} - \bar{\mathbf{\Phi}} = \begin{bmatrix} (\Phi_{1,1}-\bar{\Phi}_1) & (\Phi_{1,2}-\bar{\Phi}_2) & \cdots & (\Phi_{1,V}-\bar{\Phi}_V) \\ (\Phi_{2,1}-\bar{\Phi}_1) & (\Phi_{2,2}-\bar{\Phi}_2) & \cdots & (\Phi_{2,V}-\bar{\Phi}_V) \\ \vdots & & (\Phi_{p,v}-\bar{\Phi}_v) & \vdots \\ (\Phi_{P,1}-\bar{\Phi}_1) & \cdots & \ddots & (\Phi_{P,V}-\bar{\Phi}_V) \end{bmatrix}$$

Eigenvalue Decopomposition Algorithm (2/6)



At iteration *h*:

(1) Compute the matrix

$$\mathbf{M}_{h-1} = \mathbf{F}_{h-1}^T \mathbf{\Phi}_{h-1} \mathbf{\Phi}_{h-1}^T \mathbf{F}_{h-1}$$

$$[N\times N] \quad [N\times P] \quad [P\times V] \quad [V\times P] \quad [P\times N]$$

(2) Compute and sort the eigenvalues of $\mathbf{M}_{h-1}$

Solve $\det\left(\mathbf{M}_{h-1} - \lambda\mathbf{I}\right) = 0 \Rightarrow \lambda(M_{h-1})_1 > \lambda(M_{h-1})_2 > \ldots > \lambda(M_{h-1})_N$

(3) Compute $\mathbf{w}_h$ as the **eigenvector** associated to the **highest eigenvalue** ($\lambda(M_{h-1})_1$)

Solve $\left[\mathbf{M}_{h-1} - \lambda\left(\mathbf{M}_{h-1}\right)_1\right]\boxed{\mathbf{w}_h} = 0$

(4) Store $\mathbf{w}_h$ as the h-th column of matrix $\mathbf{W}$

$$\mathbf{W} = \begin{bmatrix} w_{1,1} & \cdots & w_{1,h} & \cdots \\ w_{2,1} & \ddots & w_{2,h} & \\ \vdots & & \vdots & \\ w_{N,1} & \cdots & w_{N,h} & \cdots \end{bmatrix}$$

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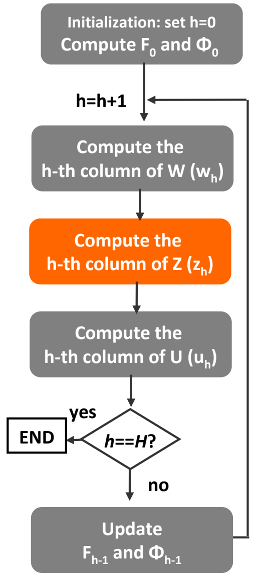
Eigenvalue Decopomposition Algorithm (3/6)



At iteration *h*:

(5) Compute the vector $\mathbf{z}_h$

$$\mathbf{z}_h = \mathbf{F}_{h-1}\mathbf{w}_h$$

$$\begin{bmatrix} z_{1,h} \\ z_{2,h} \\ \vdots \\ z_{P,h} \end{bmatrix} = \mathbf{F}_{h-1} \begin{bmatrix} w_{1,h} \\ w_{2,h} \\ \vdots \\ w_{P,h} \end{bmatrix}$$

(6) Store $\mathbf{z}_h$ as the h-th column of matrix $\mathbf{Z}$

$$\mathbf{Z} = \begin{bmatrix} z_{1,1} & \cdots & z_{1,h} & \cdots \\ z_{2,1} & \ddots & z_{2,h} & \\ \vdots & & \vdots & \\ z_{P,1} & \cdots & z_{P,h} & \cdots \end{bmatrix}$$

Values of the *h*-th new variable for the *P* input samples

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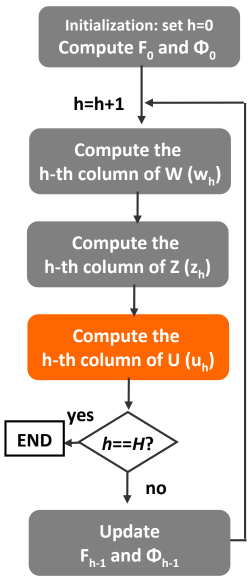
Eigenvalue Decopomposition Algorithm (4/6)



At iteration *h*:

(7) Compute the matrix

$$\mathbf{N}_{h-1} = \mathbf{\Phi}_{h-1}^T \mathbf{F}_{h-1} \mathbf{F}_{h-1}^T \mathbf{\Phi}_{h-1}$$

$$[V\times V] \quad [V\times P] \quad [P\times N] \quad [N\times P] \quad [P\times V]$$

(8) Compute and sort the eigenvalues of $\mathbf{N}_{h-1}$

Solve $\det\left(\mathbf{N}_{h-1} - \lambda\mathbf{I}\right) = 0 \Rightarrow \lambda(\mathbf{N}_{h-1})_1 > \lambda(\mathbf{N}_{h-1})_2 > \ldots > \lambda(\mathbf{N}_{h-1})_N$

(9) Compute $\mathbf{c}_h$ as the **eigenvector** associated to the **highest eigenvalue** ($\lambda(\mathbf{N}_{h-1})_1$)

Solve $\left[\mathbf{N}_{h-1} - \lambda\left(\mathbf{N}_{h-1}\right)_1\right]\mathbf{c}_h = 0$

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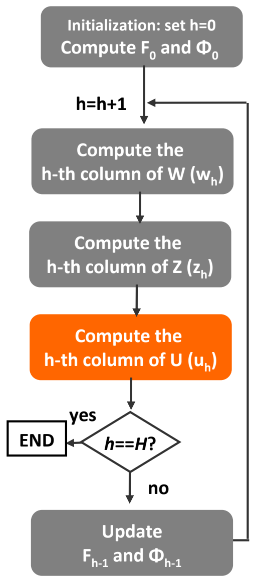
Eigenvalue Decopomposition Algorithm (5/6)



At iteration *h*:

(10) Compute the vector $\mathbf{u}_h$

$$\mathbf{u}_h = \mathbf{\Phi}_{h-1}\mathbf{c}_h$$

$$\begin{bmatrix} u_{1,h} \\ u_{2,h} \\ \vdots \\ u_{P,h} \end{bmatrix} = \mathbf{\Phi}_{h-1} \begin{bmatrix} c_{1,h} \\ c_{2,h} \\ \vdots \\ c_{V,h} \end{bmatrix}$$

(11) Store $\mathbf{u}_h$ as the h-th column of matrix $\mathbf{U}$

$$\mathbf{U} = \begin{bmatrix} u_{1,1} & \cdots & u_{1,h} & \cdots \\ u_{2,1} & \ddots & u_{2,h} & \\ \vdots & & \vdots & \\ u_{P,1} & \cdots & u_{P,h} & \cdots \end{bmatrix}$$

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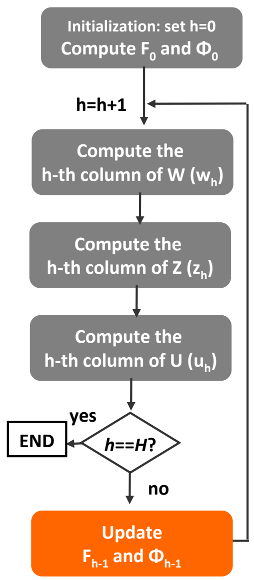
Eigenvalue Decopomposition Algorithm (6/6)



At iteration *h*:

(12) Update $\mathbf{F}_{h-1}$

$$\mathbf{F}_h = \mathbf{F}_{h-1} - \mathbf{z}_h \mathbf{z}_h^T \mathbf{F}_{h-1}$$

(13) Update $\mathbf{\Phi}_{h-1}$

$$\mathbf{\Phi}_h = \mathbf{\Phi}_{h-1} - \mathbf{z}_h \mathbf{z}_h^T \mathbf{\Phi}_{h-1}$$

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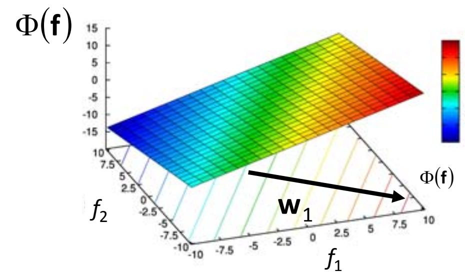
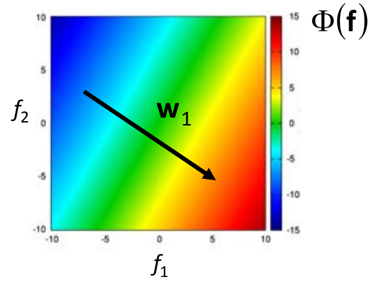
PLS Example (1/8)

EXAMPLE:
Number of variables: N = 2
Number of samples: P = 10
Dimension of the output: V=1
Number of new variables: H=1

"Rotated plane"

$$\Phi(f_1, f_2) = f_1 \cos(\vartheta_r) - f_2 \sin(\vartheta_r) \qquad \vartheta_r = 30[\text{deg}]$$





Observation Direction $\mathbf{w}_1$ is sufficient for computing $\Phi(\mathbf{f})$ univocally

Goal Find $\mathbf{w}_1$ to **reduce the number of variables** from **N=2** to **H=1**

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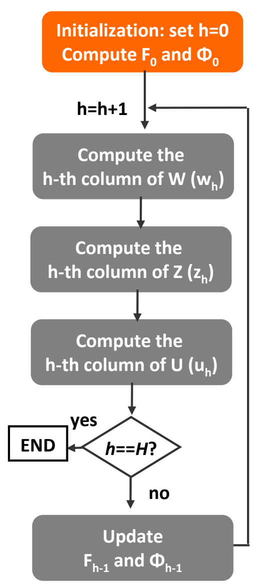
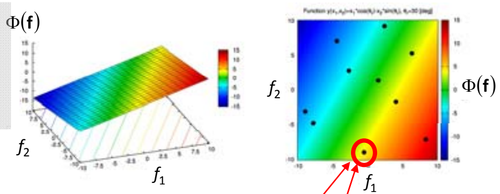
PLS Example (2/8)



EXAMPLE:
Number of variables: N = 2
Number of samples: P = 10
Dimension of the output: V=1
Number of new variables: H=1



$$\Phi(f_1, f_2) = f_1 \cos(\vartheta_r) - f_2 \sin(\vartheta_r)$$

$\mathbf{F} =$

f_1	f_2
-4.46	7.09
4.04	-1.72
-2.73	2.75
1.50	1.35
-9.00	-3.12
8.45	-7.13
2.40	9.24
-4.79	-8.97
6.34	5.30
-7.82	-4.80

$\mathbf{\Phi} =$

$\Phi(f_1,f_2)$
-7.40
4.36
-3.74
0.62
-6.24
10.88
-2.55
4.07
2.84
-4.38

Samples of the function

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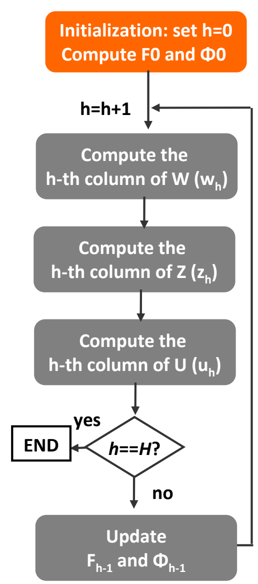
PLS Example (3/8)



EXAMPLE:
Number of variables: N = 2
Number of samples: P = 10
Dimension of the output: V=1
Number of new variables: H=1

$$\bar{f}_1 = -0.178 \qquad \bar{\Phi} = -0.15$$
$$\bar{f}_2 = -0.002$$

Centered (zero-mean) version of both input and output samples

$\mathbf{F}_0 =$

$f_1 - \bar{f}_1$	$f_2 - \bar{f}_2$
-4.28	7.09
4.22	-1.71
-2.56	2.75
1.67	1.35
-8.83	-3.11
8.63	-7.13
2.57	9.23
-0.30	-8.97
6.51	5.30
-7.65	-4.80

$\mathbf{\Phi}_0 =$

$\Phi - \bar{\Phi}$
-7.25
4.51
-3.59
0.78
-6.09
11.04
-2.39
4.23
2.99
-4.22

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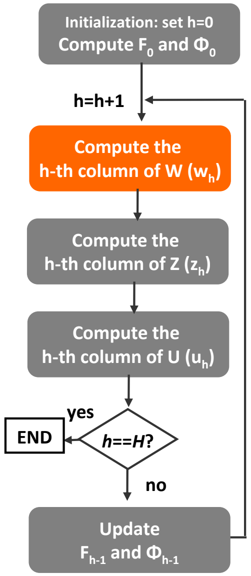
PLS Example (4/8)



EXAMPLE:
Number of variables: N = 2
Number of samples: P = 10
Dimension of the output: V=1
Number of new variables: H=1

Iteration h=1

1. Compute the matrix $\mathbf{M}_0 = \mathbf{F}_0^T \mathbf{\Phi}_0 \mathbf{\Phi}_0^T \mathbf{F}_0$

$$\underset{[N\times N]}{\mathbf{M}_0} = 10^4 \begin{bmatrix} 6.44 & -3.85 \\ -3.85 & 2.30 \end{bmatrix}$$

2. Compute and sort the eigenvalues of $\mathbf{M}_0$

Highest eigenvalue

Solve $\det(\mathbf{M}_0 - \lambda \mathbf{I}) = 0 \Rightarrow \lambda(M_0)_1 = 8.74 \times 10^4$

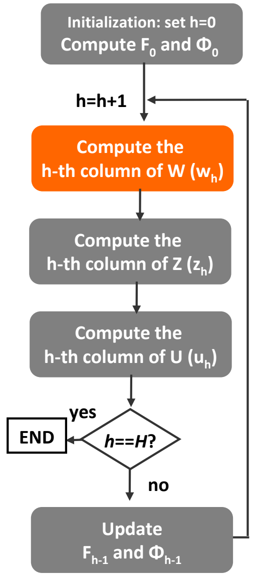
3. Compute $\mathbf{w}_1$ as the **eigenvector** associated to the **highest eigenvalue**

Solve $[\mathbf{M}_0 - \lambda(\mathbf{M}_0)_1]\mathbf{w}_1 = 0 \Rightarrow \mathbf{w}_1 = \begin{bmatrix} 0.86 \\ -0.51 \end{bmatrix}$

4. Store $\mathbf{w}_1$ as the 1-st column of matrix $\mathbf{W}$

$$\mathbf{W} = \begin{bmatrix} 0.86 & \cdots \\ -0.51 & \cdots \end{bmatrix}$$

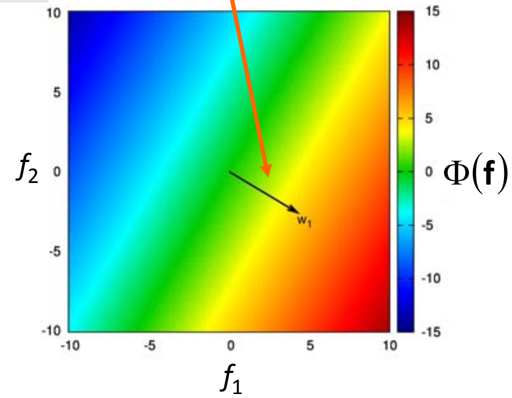
PLS Example (5/8)



EXAMPLE:
Number of variables: N = 2
Number of samples: P = 10
Dimension of the output: V=1
Number of new variables: H=1

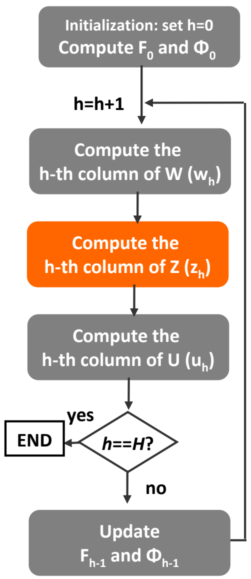
w1 is the direction we were looking for!

$$\mathbf{w}_1 = \begin{bmatrix} 0.86 \\ -0.51 \end{bmatrix}$$



$\Phi(\mathbf{f})$ is **linear** w.r.t. this direction!

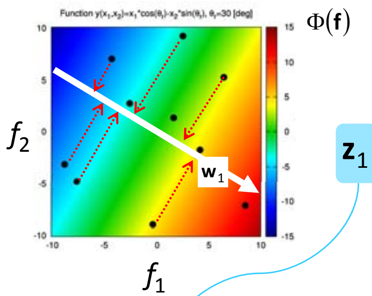
PLS Example (6/8)



EXAMPLE:
Number of variables: N = 2
Number of samples: P = 10
Dimension of the output: V=1
Number of new variables: H=1

Iteration h=1

5. Project samples onto $\mathbf{w}_1$: compute the vector $\mathbf{z}_1$



$\mathbf{z}_1 = \mathbf{F}_0 \mathbf{w}_1 =$

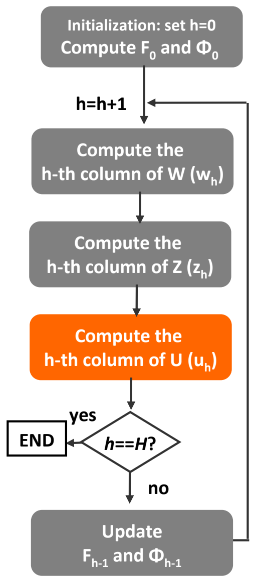
-7.31
4.50
-3.60
0.75
-5.98
11.06
-2.53
4.34
2.88
-4.11

6. Store $\mathbf{z}_1$ as the 1-st column of matrix $\mathbf{Z}$

$$\mathbf{Z} = \begin{bmatrix} z_{1,1} & \cdots & \cancel{z_{1,h}} & \cdots \\ z_{2,1} & \ddots & \cancel{z_{2,h}} & \\ \vdots & & \cancel{\vdots} & \\ z_{P,1} & \cdots & \cancel{z_{N,h}} & \cdots \end{bmatrix}$$

Knowledge of $z_{p,1}$ is **sufficient** for computing $\Phi(\mathbf{f})$

PLS Example (7/8)



EXAMPLE:
Number of variables: N = 2
Number of samples: P = 10
Dimension of the output: V=1
Number of new variables: H=1

Iteration h=1

7. Compute the matrix

$$\underset{[V\times V]}{\mathbf{N}_0} = \mathbf{\Phi}_0^T \mathbf{F}_0 \mathbf{F}_0^T \mathbf{\Phi}_0 = 8.74 \times 10^4$$

In this case V=1

8. Compute and sort the eigenvalues of $\mathbf{N}_0$

Solve $\det(\mathbf{N}_0 - \lambda \mathbf{I}) = 0 \Rightarrow \lambda(\mathbf{N}_{h-1})_1 = 8.74 \times 10^4$

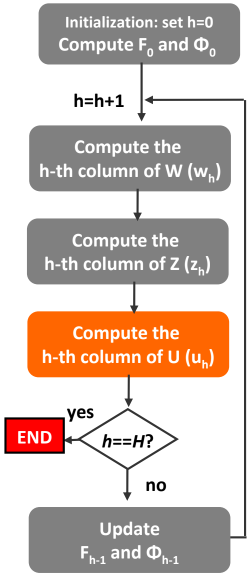
9. Compute $\mathbf{c}_1$ as the **eigenvector** associated to the **highest eigenvalue**

Solve $[\mathbf{N}_0 - \lambda(\mathbf{N}_0)_1]\mathbf{c}_1 = 0 \Rightarrow \mathbf{c}_1 = 1$

10. Compute the vector $\mathbf{u}_1$

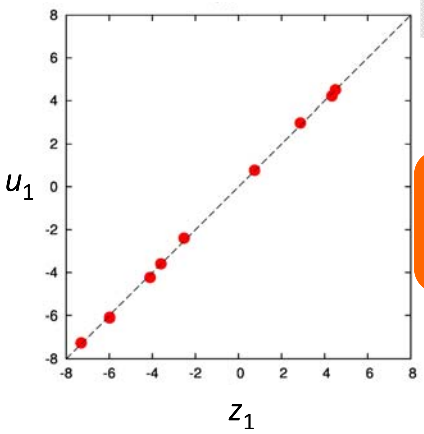
$$\mathbf{u}_1 = \mathbf{\Phi}_0 \mathbf{c}_1 = \mathbf{\Phi}_0$$

PLS Example (8/8)



Iteration h=1

EXAMPLE:
Number of variables: N = 2
Number of samples: P = 10
Dimension of the output: V=1
Number of new variables: H=1



Correlation between z_1 and u_1 is maximized

$$r(z_1,u_1)\approx 0.99$$

We can **use the new variable z_1 instead of f_1 and f_2** to compute/predict Φ

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Conclusions

- Introduction and Motivation
- Prediction Through **Interpolation Techniques**
  - ***Nearest Neighbor Interpolation***
  - ***Linear Interpolation***
- **3-Steps Learning-by-Examples** (***LBE***) Framework
  - Step 1: ***Dimensionality Reduction***
    - ***Sequential Feature Selection (SFT)***
    - ***Principal Component Analysis (PCA)***
    - ***Sammon Mapping***
    - ***Partial Least Squares (PLS)***

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Introduction to ML and AI Methods (Part I)

Dr. Marco SALUCCI

Day 1 - August 29th, 2022

2022 ELEDIA@ICAM PhD Summer Schools
Machine Learning & AI Methods
Theory, Techniques, and Advanced Engineering Applications
29 Aug. - 02 Sept. 2022, Trento, Italy (Onsite and Online)

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