Estimation of Mars surface physical properties from hyperspectral images using the SIR method

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Source: ESA

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INRIA RHÔNE-ALPES

Outline

I. Context
   - Hyperspectral image data
   - Inverse problem

II. Dimension reduction
   - PCA
   - SIR

III. Regularization and estimation
   - Zhong et al., 2005
   - Tikhonov

IV. Validation on simulations

V. Application to the south polar cap of Mars

VI. Conclusion and future work

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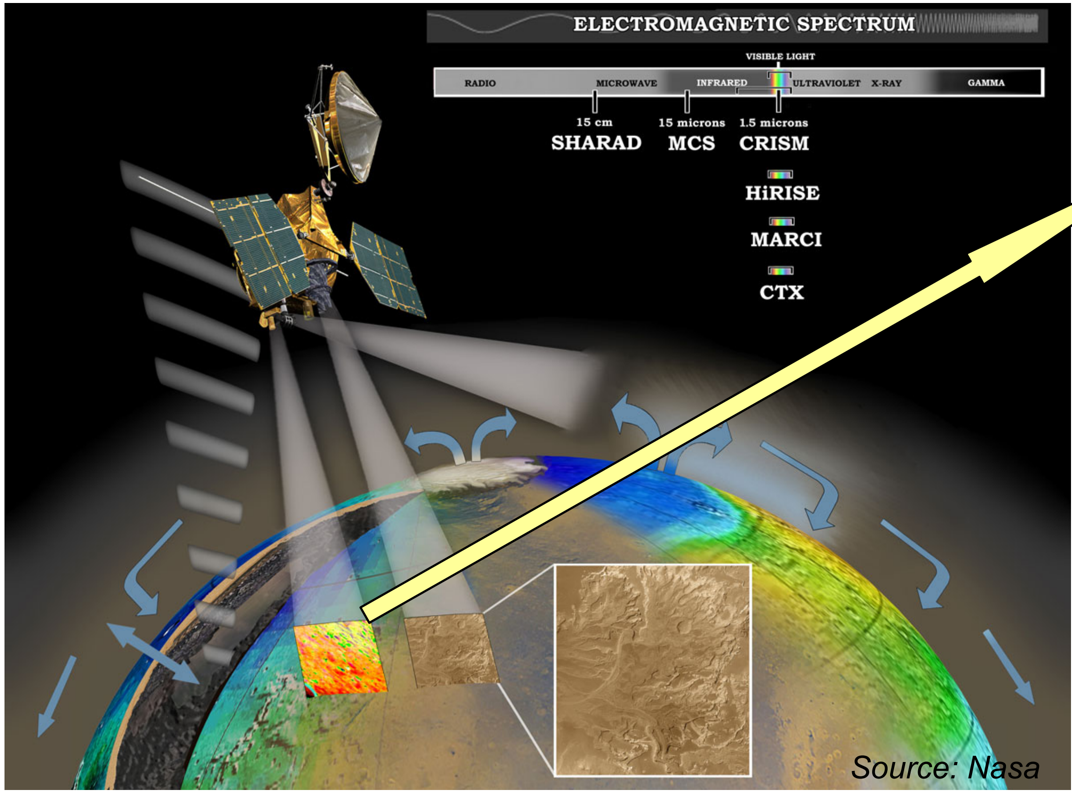
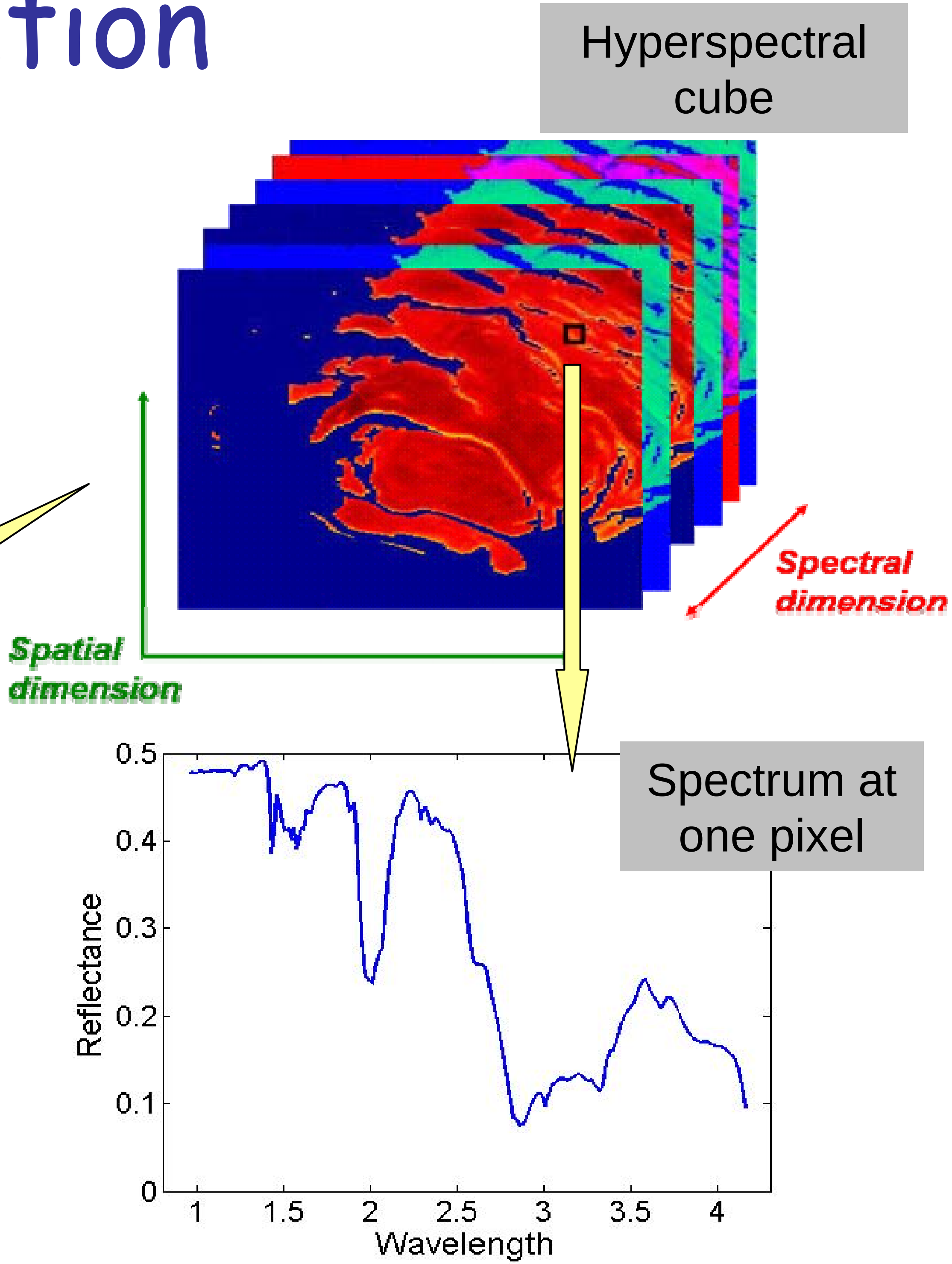
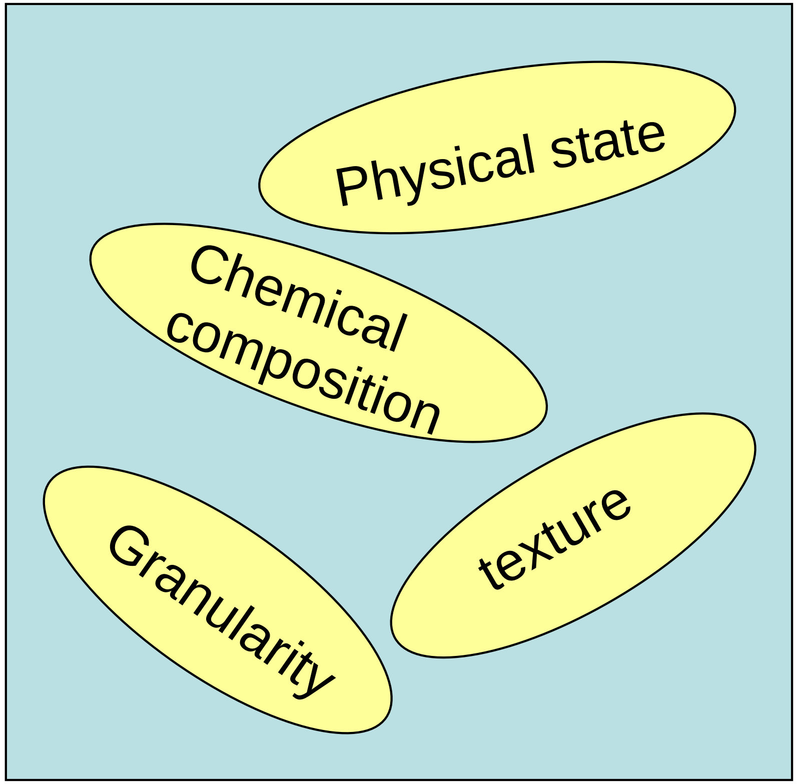
Introduction

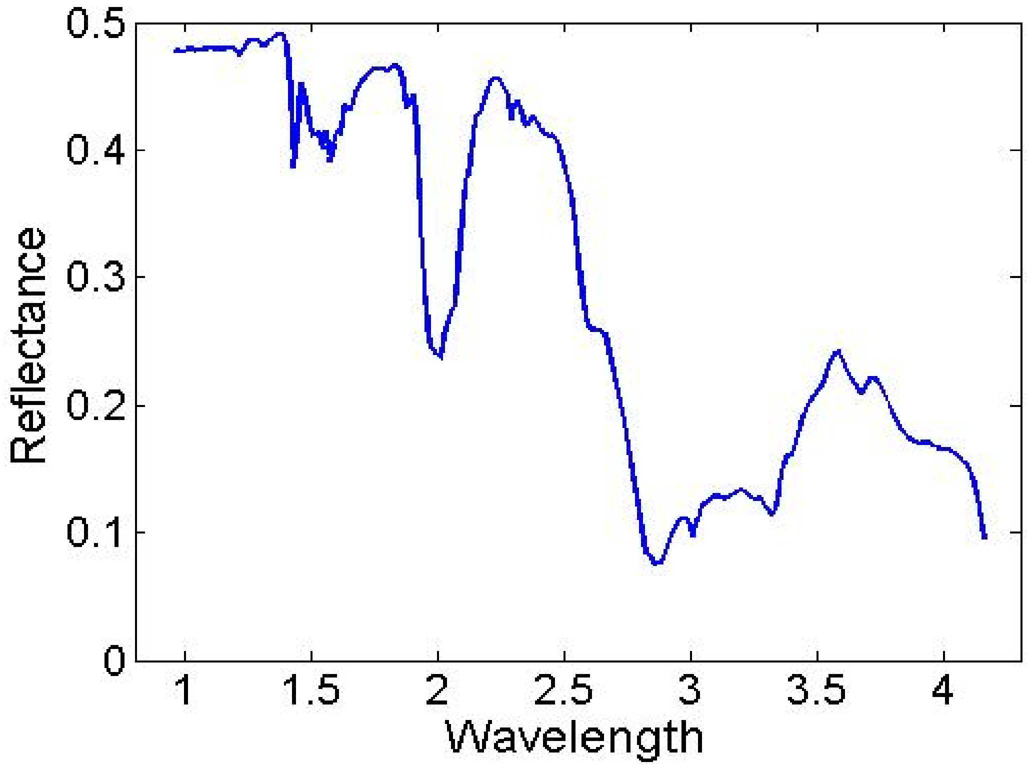
Spectrometer





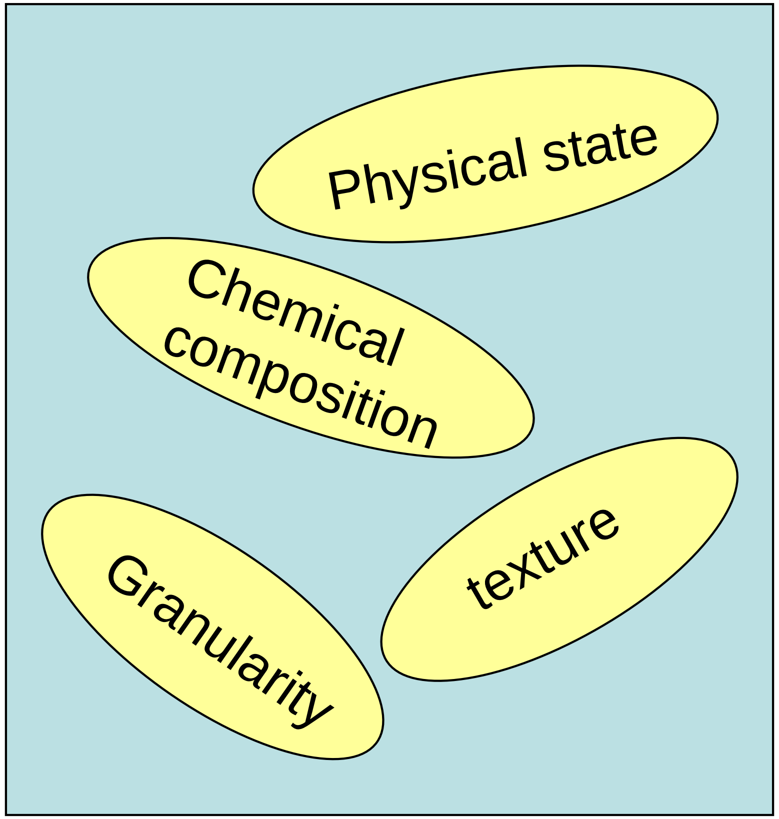
Radiative transfer model

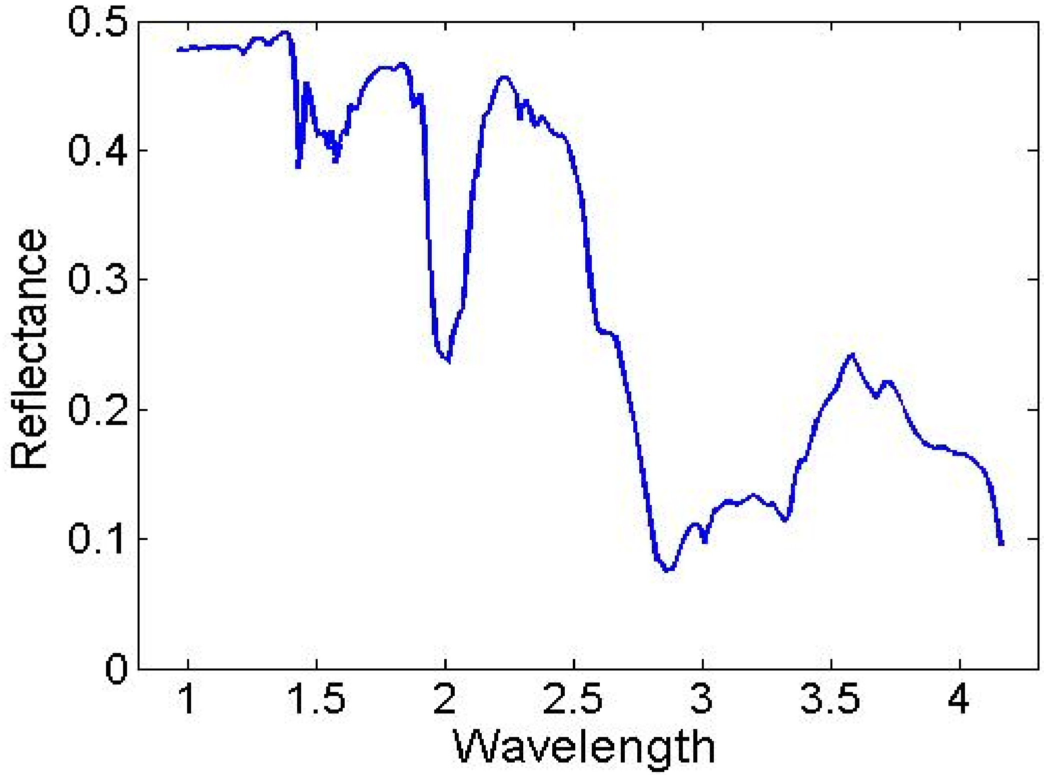




RADIATIVE TRANSFER MODEL: evaluates direct link between parameters and spectra. Allows the construction of a training data

Inverse problem

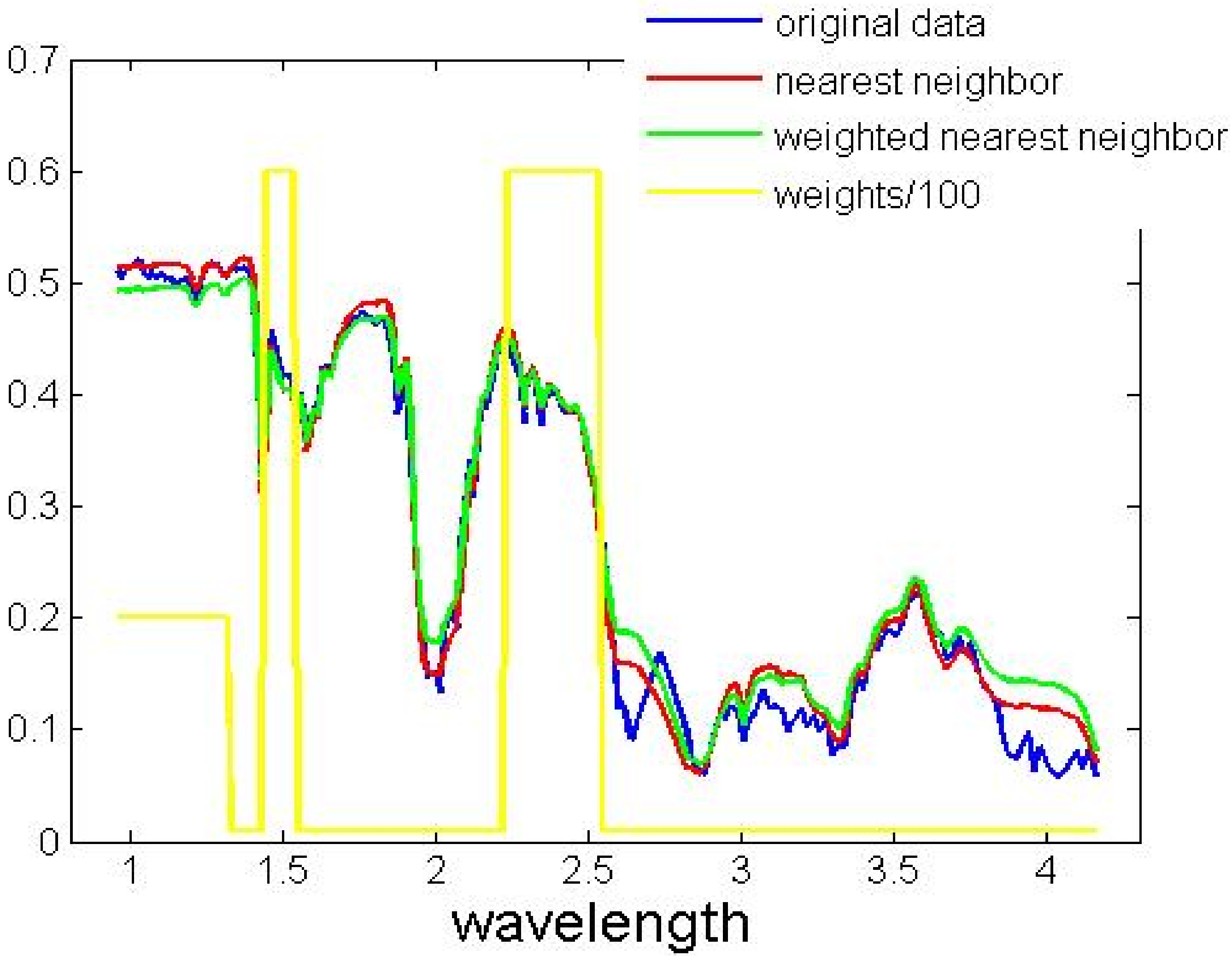




INVERSE PROBLEM: evaluates the properties of atmospheric and surface materials from the spectra

Usual methods

- Nearest neighbor
- Weighted Nearest neighbor



Aim

- To establish functional relationships between:
  - Spectra $x \in \mathbb{R}^p$ (p=184) from Mars Express mission
  - Physical parameter $y \in \mathbb{R}$: proportion of water, proportion of dust, grain size…
  - Construct *f* in order to estimate parameters:

$$
\begin{aligned}
f : \mathbb{R}^p &\longrightarrow \mathbb{R} \\
x &\longrightarrow y
\end{aligned}
$$

Difficulties

- Curse of dimensionality (184 wavelengths): dimension of *x* has to be reduced
- Find projection axis $a \in \mathbb{R}^p$ (here, only the first axis will be retained)
- Instead of estimating f such as $y = f(x)$, we will suppose there exists $g : \mathbb{R} \to \mathbb{R}$ exists such that:

$$y = g(< a, x >, \varepsilon)$$

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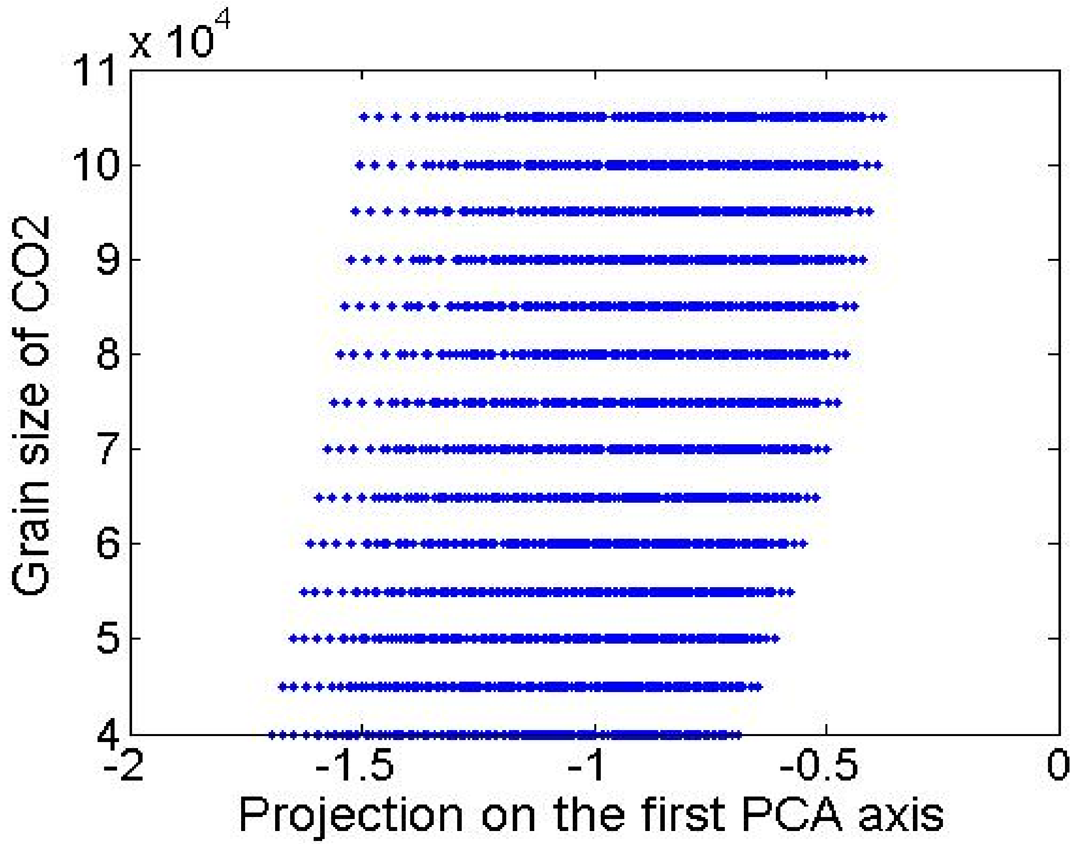
Principal component analysis

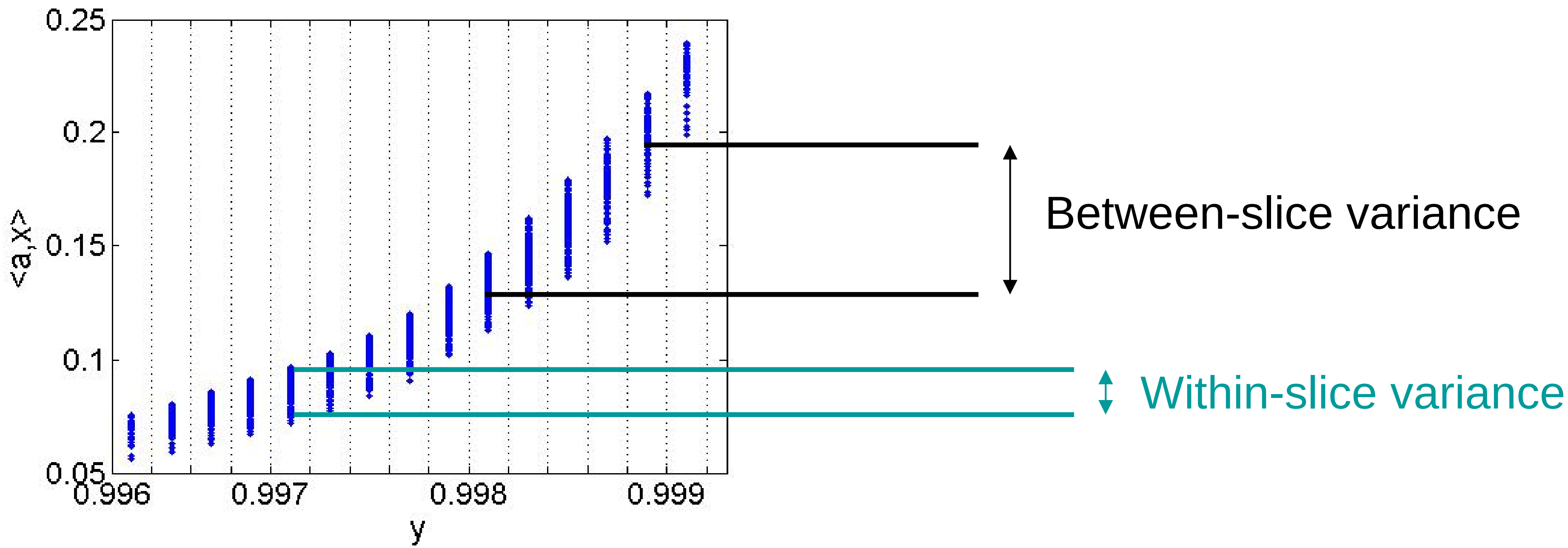
- **Maximizes the variance** of the projections of the observations *x*
- Does not take into account *y*



Sliced inverse regression

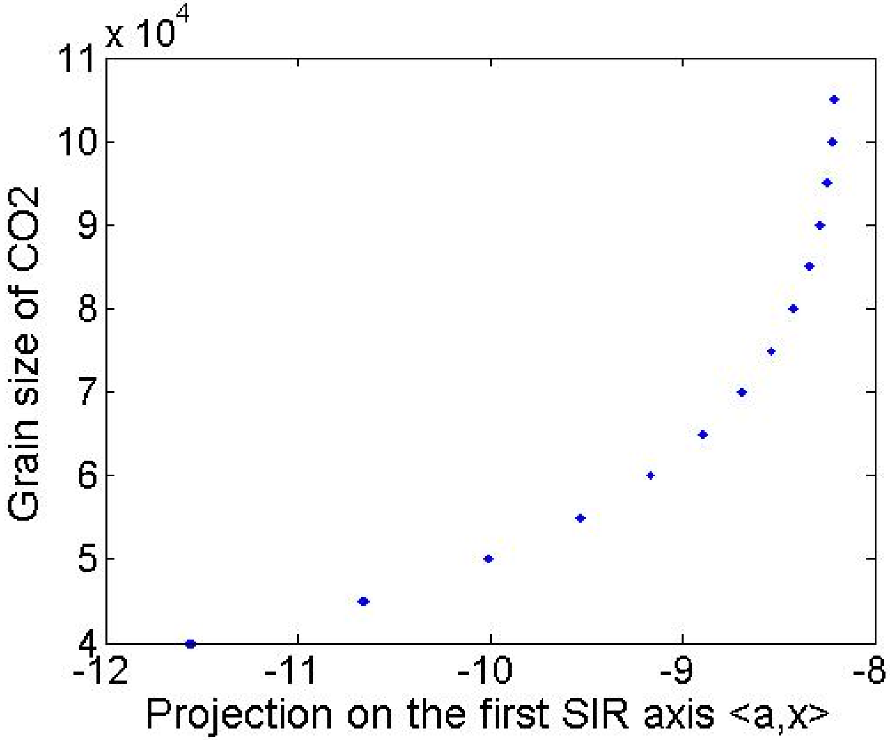
- Proposed by Li (1991)
- Maximizes the between-slice variance of projections
- PCA of E(*X*/*Y*) with $Z = \Sigma^{-1/2} X$
- Eigenvectors of $\Sigma^{-1}\Gamma$ with $\Gamma = \mathrm{var}(E(X/Y))$

  $\Sigma = \mathrm{var}(X)$

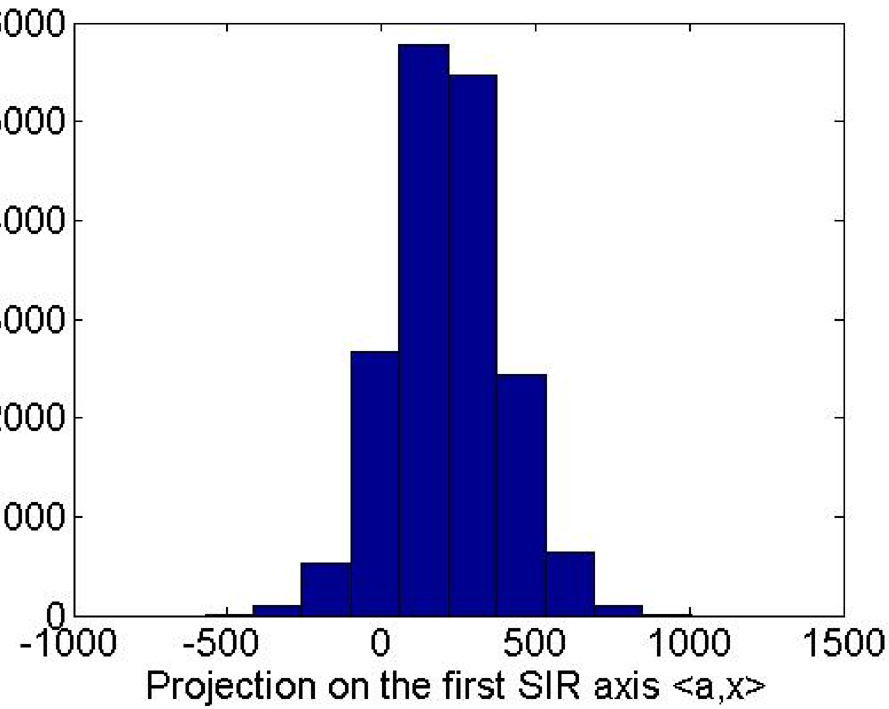


Application of SIR

TRAINING DATA



OBSERVED DATA



Problem

- Covariance matrix is ill-conditioned
  - Bad estimations of the directions
  - Sensitivity to noise
- Can be solved using regularization

DATA (x , y)

⇩

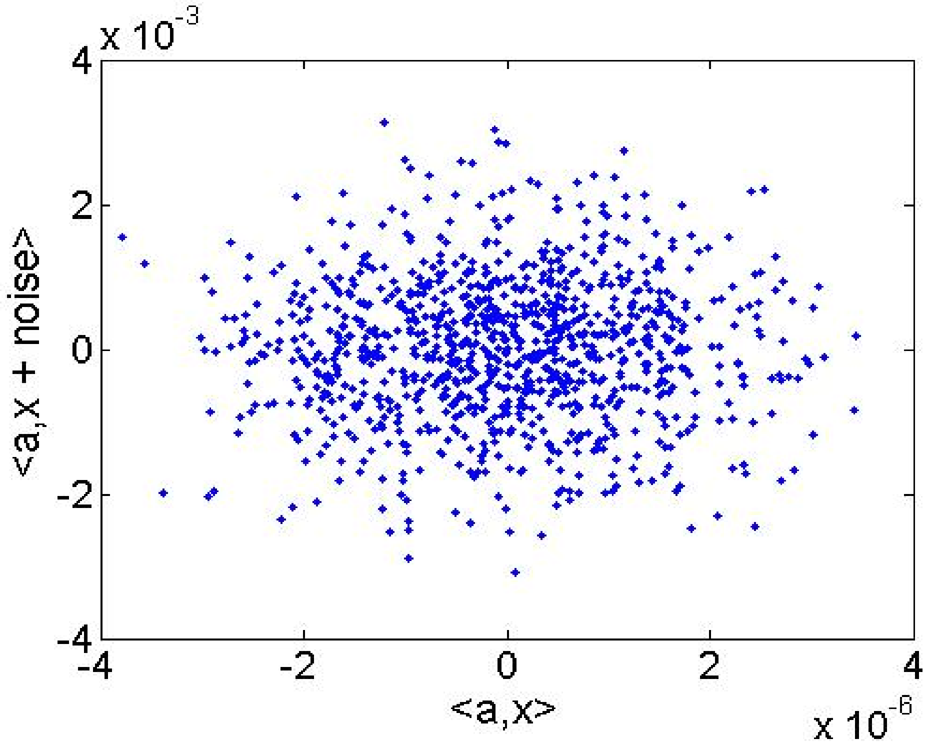
SLICED INVERSE REGRESSION

⇩

AXIS a

↙ ↘

< a, x > | < a , x + noise >



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Regularization (1)

- Usual SIR:
  - eigenvectors of $\Sigma^{-1}\Gamma$
- Regularized SIR:
  - Zhong et al., 2005: eigenvectors of

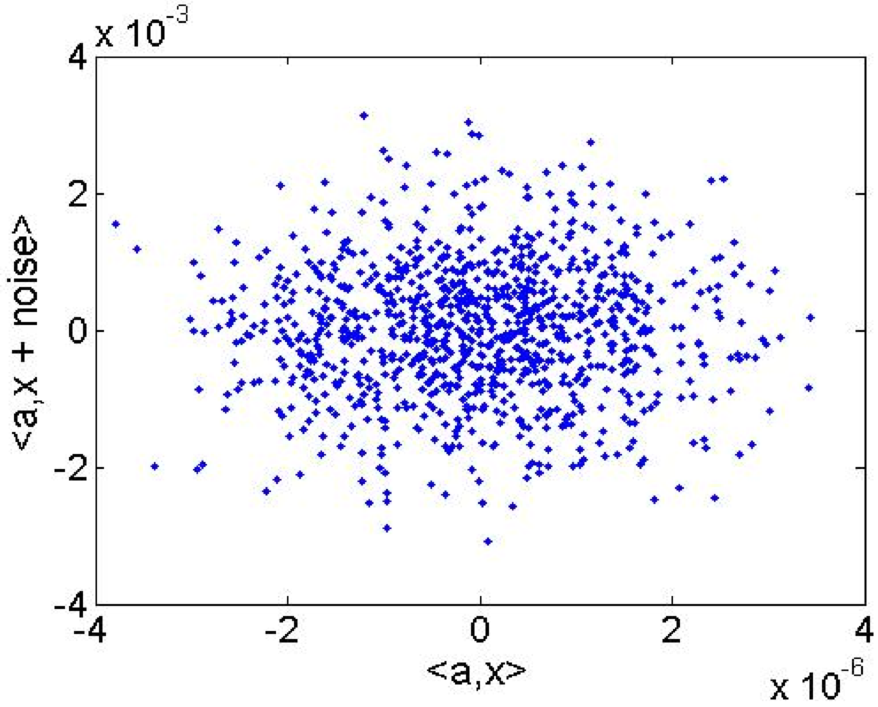
$$\left(\Sigma + \lambda Id\right)^{-1}\Gamma$$

  - Tikhonov regularization: eigenvectors of

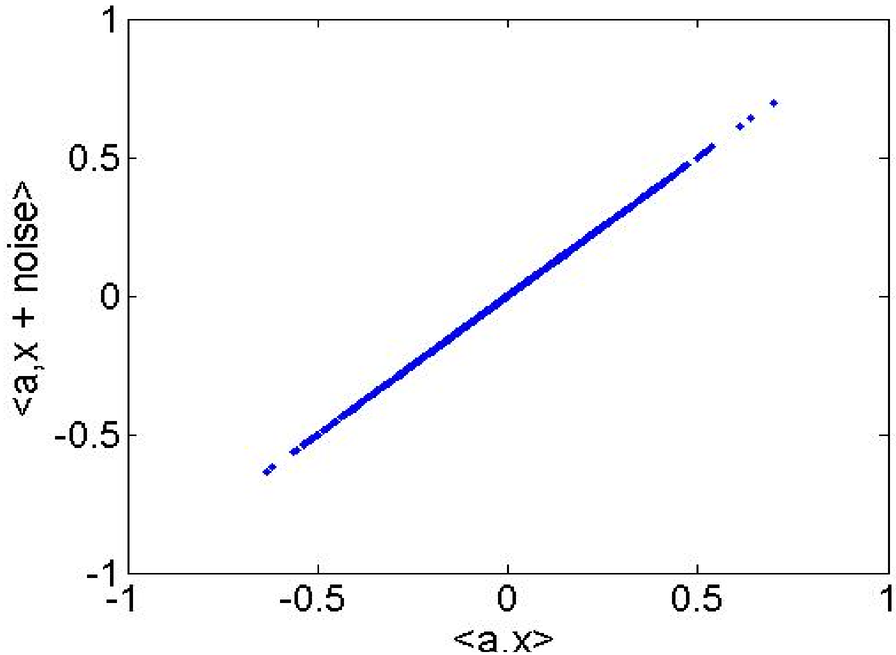
$$\left(\Sigma^2 + \lambda Id\right)^{-1}\Sigma\,\Gamma$$

Regularization (2)

Usual SIR



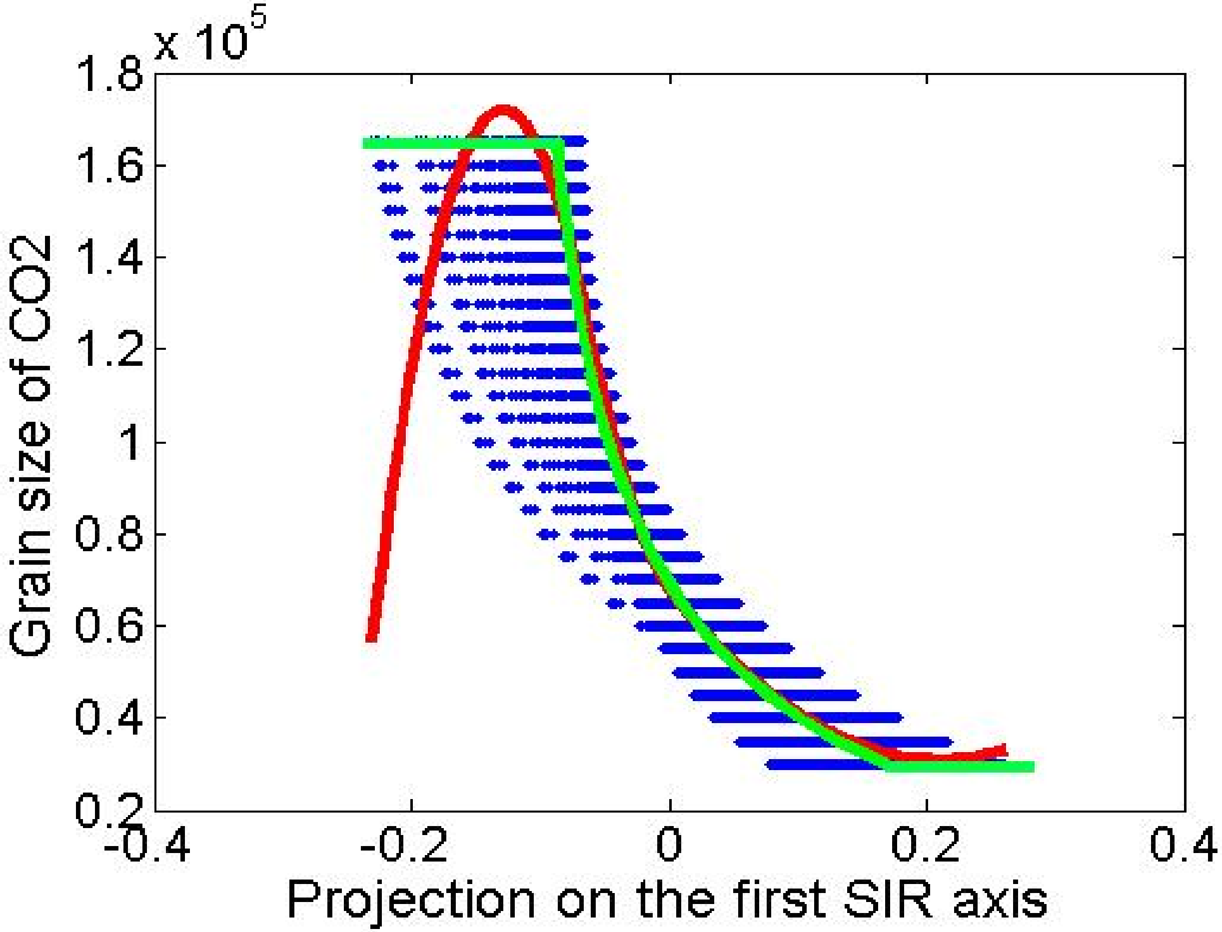
Regularized SIR (Tikhonov)



- *Depends on the regularization parameter λ*
- *The condition number of the matrix decreases when λ increases*
- *The estimation bias increases when λ increases*

Estimation

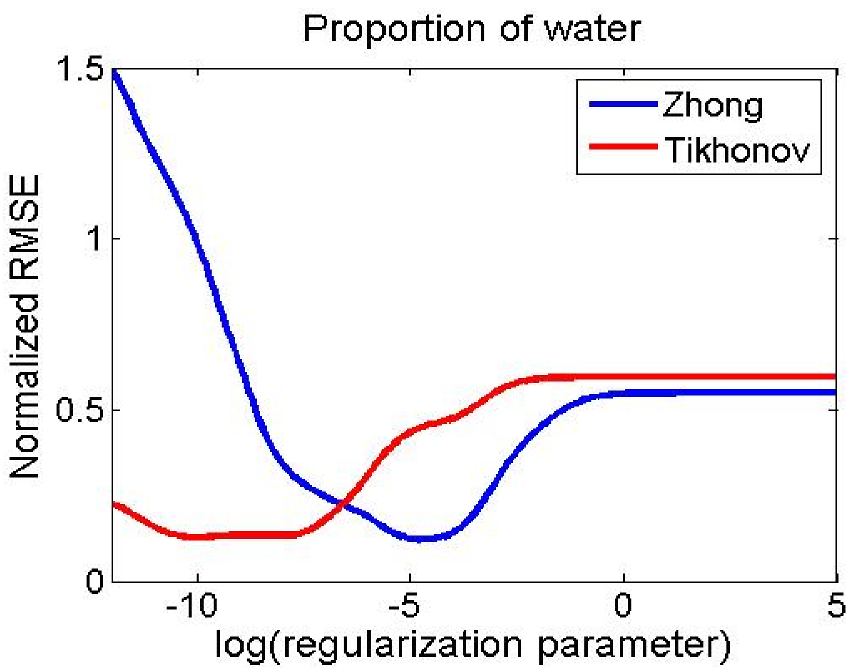
- Nearest neighbors (quite long!)
- Spline functions (choice of new parameters, boundaries)
- **Linear interpolation**

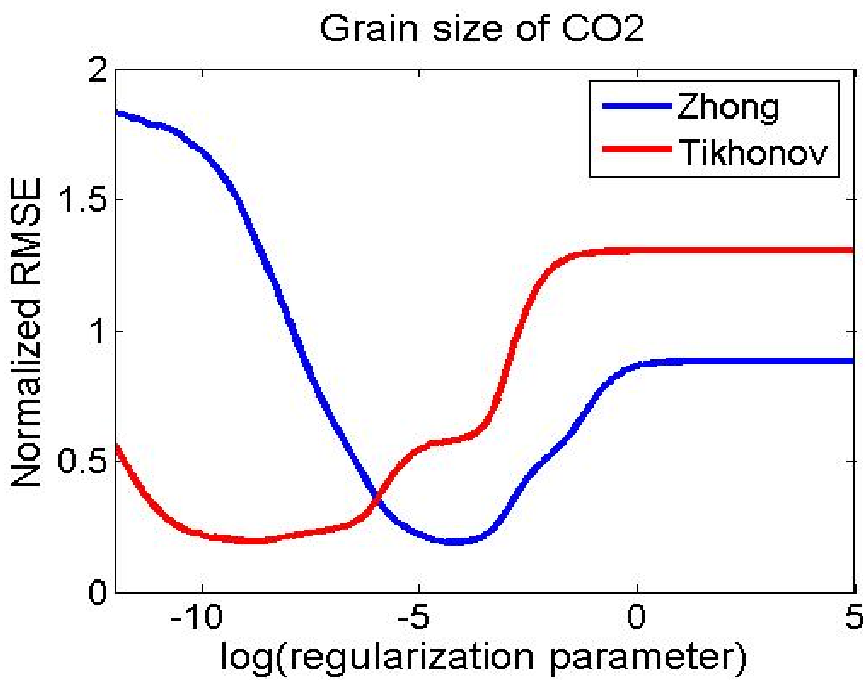


Choice of the regularization parameter

- By minimization of “Normalized RMSE” criterion

$$\frac{\|\hat{y}-y\|}{\|y-\bar{y}\|}=\frac{\text{Residuals sum of square}}{\text{Total sum of square}}$$





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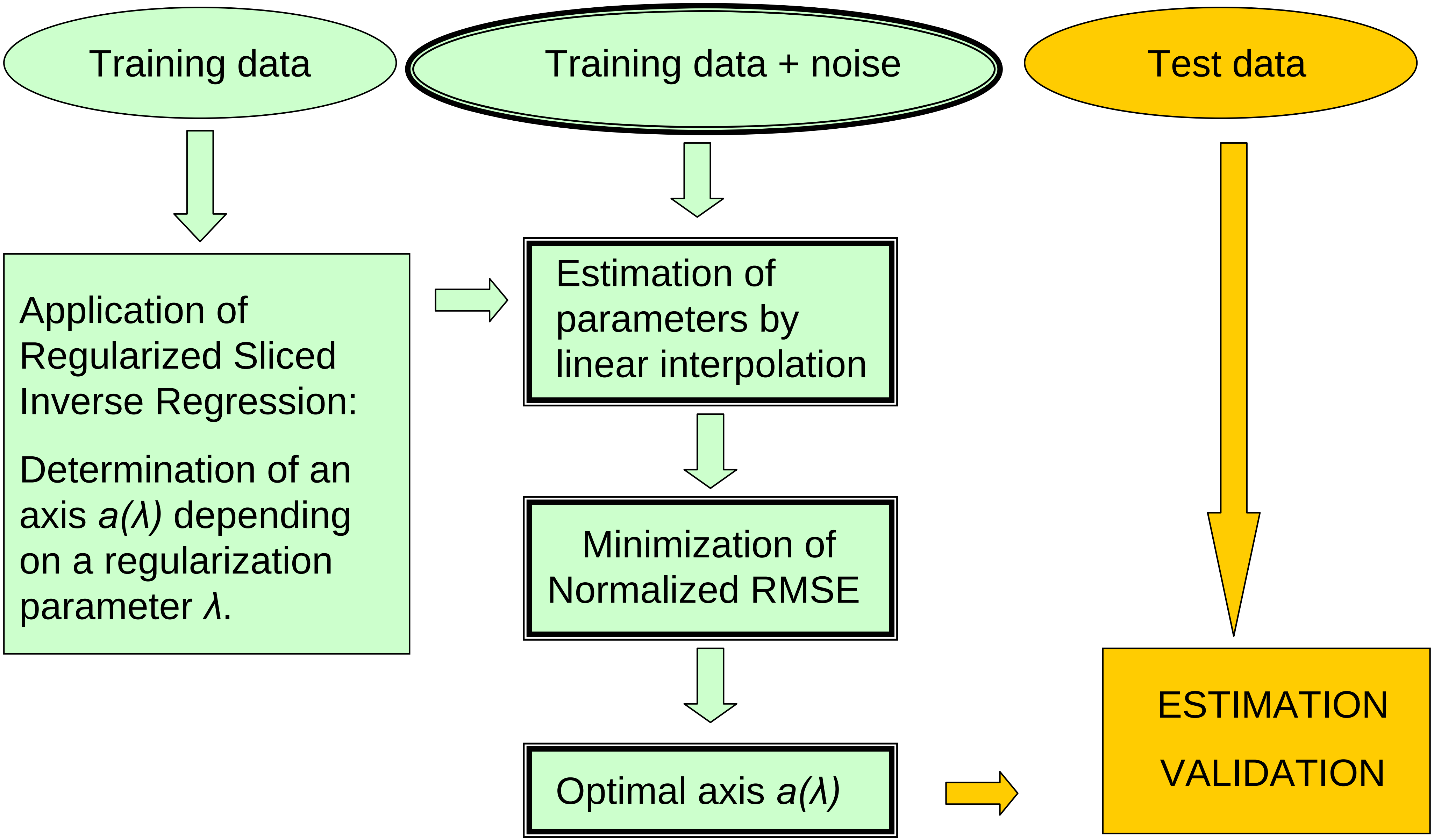
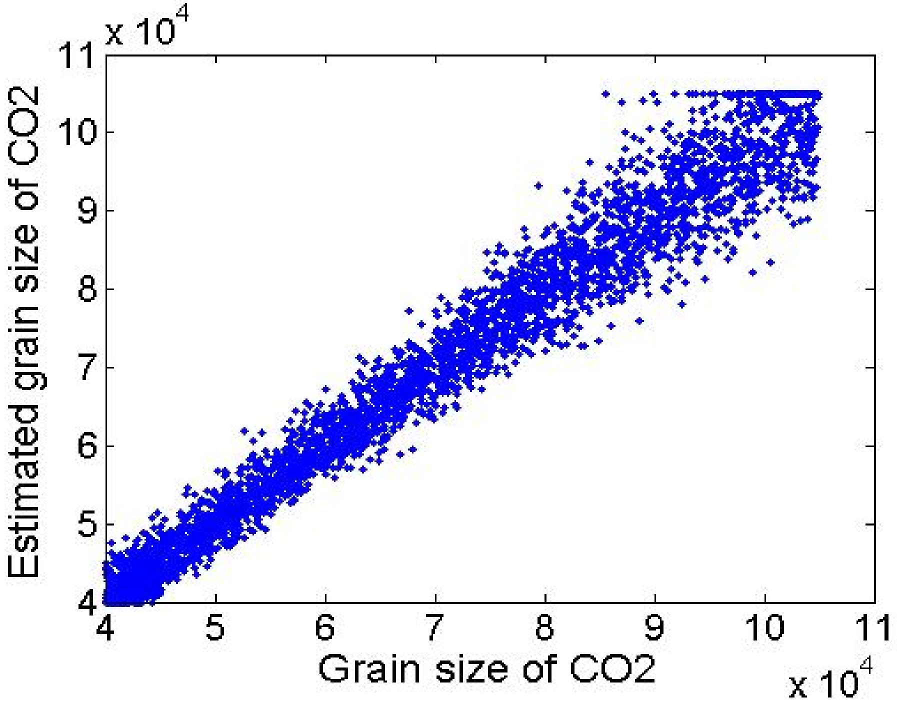
Validation (1)

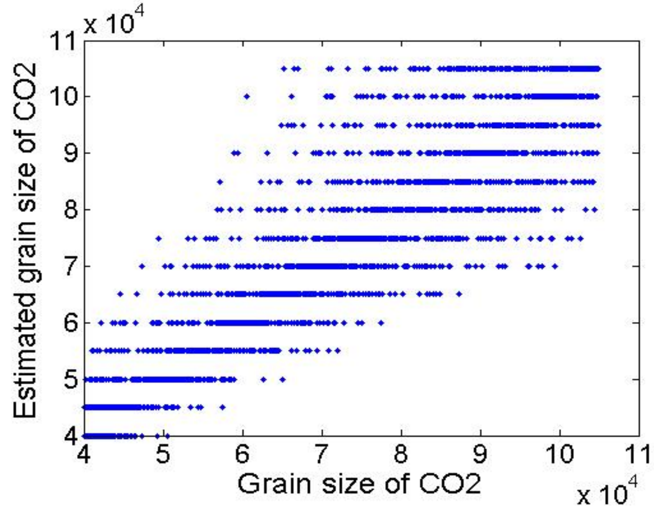


Validation (2)

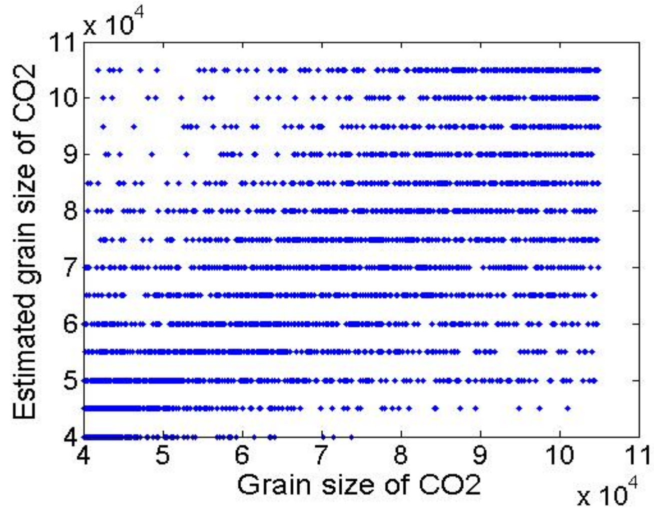
Regularized Sliced inverse regression (Tikhonov)



Nearest neighbors



Weighted nearest neighbors



Validation (3)

Normalized RMSE criterion:

$$\frac{\|\hat{y}-y\|}{\|y-\bar{y}\|} = \frac{\text{Residuals sum of square}}{\text{Total sum of square}}$$

Better when close to 0

SIR criterion:

$$\frac{{}^t a\,\Gamma\,a}{{}^t a\,\Sigma\,a} = \frac{\text{between-slice variance}}{\text{total variance}}$$

Better when close to 1

		Tikhonov		Zhong		Nearest neighbor	Weighted nearest neighbor
Parameter	**Variation interval**	$\frac{\|\hat{y}-y\|}{\|y-\bar{y}\|}$	$\frac{{}^t a\,\Gamma\,a}{{}^t a\,\Sigma\,a}$	$\frac{\|\hat{y}-y\|}{\|y-\bar{y}\|}$	$\frac{{}^t a\,\Gamma\,a}{{}^t a\,\Sigma\,a}$	$\frac{\|\hat{y}-y\|}{\|y-\bar{y}\|}$	$\frac{\|\hat{y}-y\|}{\|y-\bar{y}\|}$
Proportion of dust	[0.0006 0.002]	0.33	0.92	0.33	0.92	0.56	0.53
Proportion of CO2	[0.9960 0.9988]	0.27	0.96	0.23	0.94	0.56	0.54
Proportion of water	[0.0006 0.002]	0.13	1.00	0.12	1.00	0.27	0.28
Grain size of water	[100 400]	0.37	0.92	0.38	0.87	0.40	0.68
Grain size of CO2	[40000 105000]	0.19	0.99	0.18	0.98	0.38	0.82

- SIR gives better results than nearest neighbor classification
- Tikhonov and Zhong regularizations are equivalent
- With Tikhonov regularization, minimal normalized RMSE is reached on a larger interval than with Zhong's.

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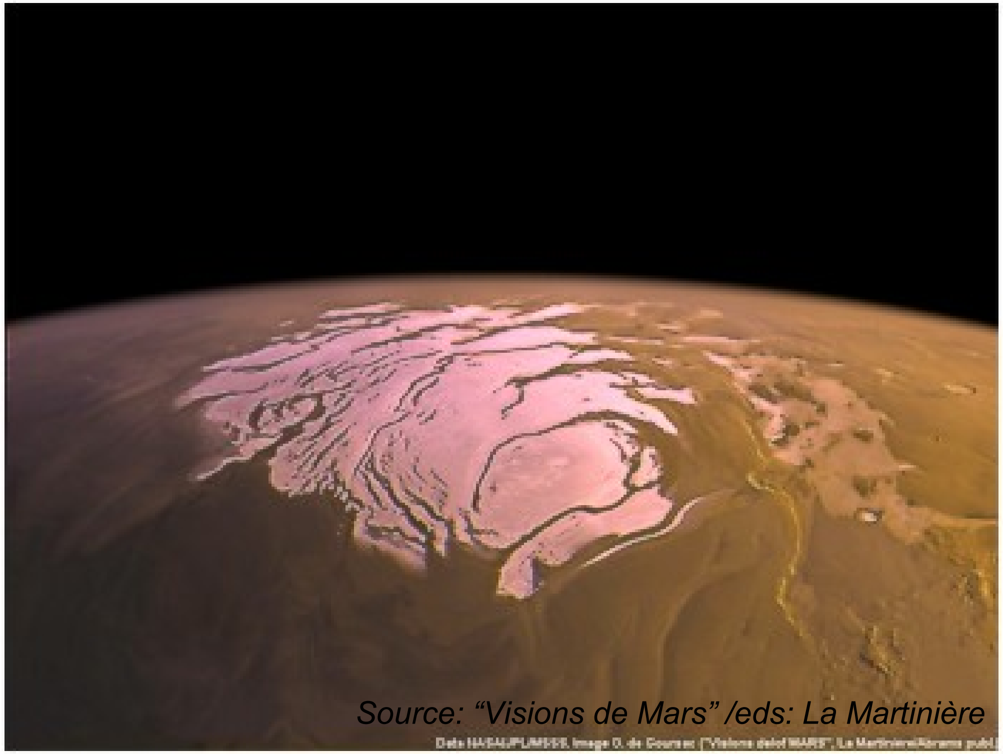
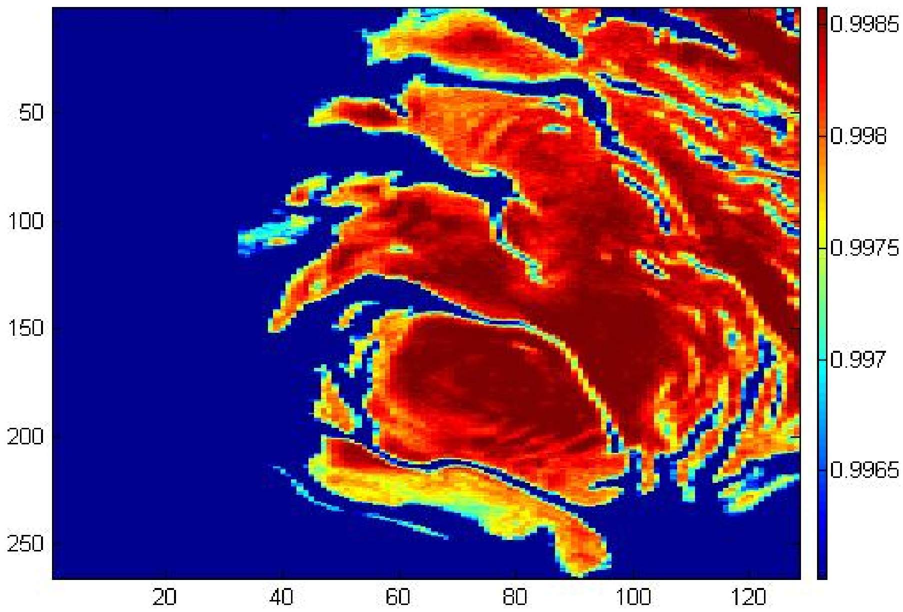
Application to south polar cap of Mars


Source: “Visions de Mars” /eds: La Martinière

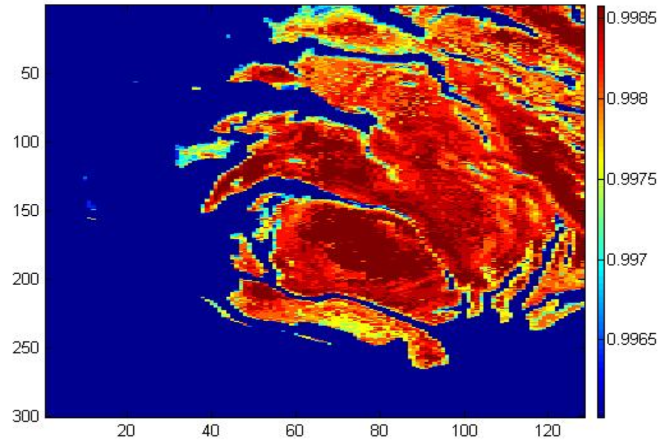
- Model determined by physicists (water + CO_2 + dust)
- 17753 spectra
- 184 wavelengths
- Training data simulated by radiative transfer model
- 5 parameters to study : proportions of water, dust and CO_2, grain sizes of CO_2 and water.

Proportion of CO2

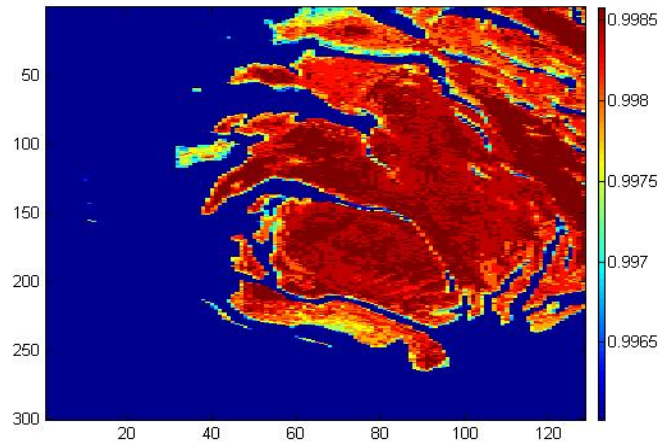
Regularized Sliced Inverse Regression (Tikhonov)



Nearest neighbors

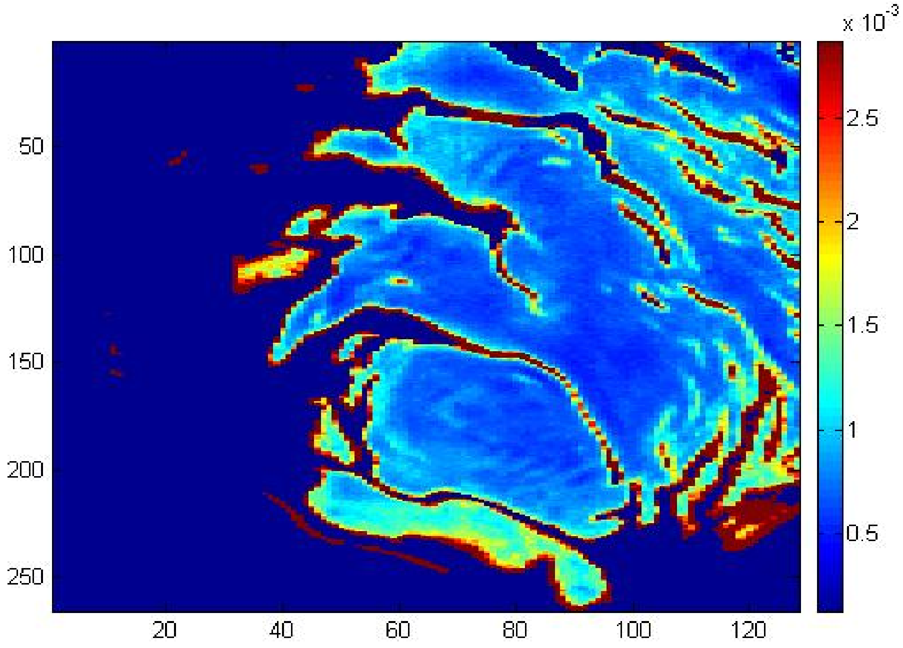


Weighted nearest neighbors

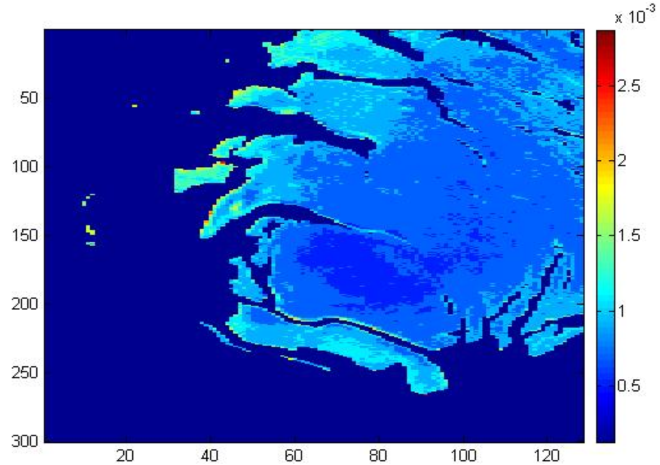


Proportion of water

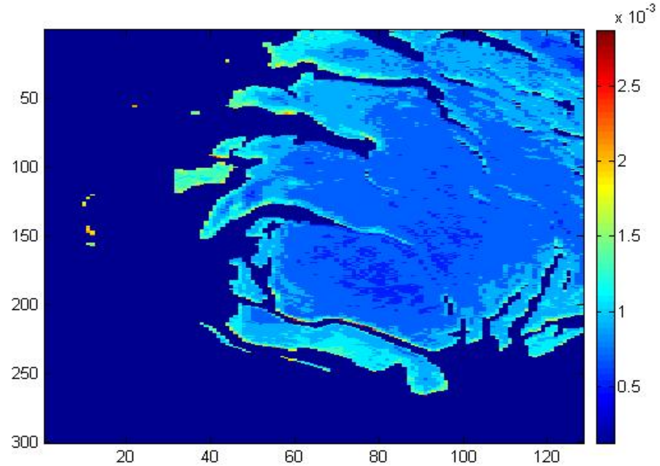
Regularized Sliced Inverse Regression (Tikhonov)



Nearest neighbors



Weighted nearest neighbors



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Conclusion and further work

- Good results on simulations.
- Realistic results on real data.
- Validation is difficult because of the lack of ground measurements.
- SIR for data streams.

SIR for data streams

- We consider data arriving sequentially by blocks in a stream.
- Each data block $j = 1, \ldots, J$ is a n-sample from the regression model $y = g(< a, x >, \varepsilon)$.
- **Goal** : Update the estimation of the direction a at each arrival of a new block of observations.

Joint work with team CQFD, INRIA Bordeaux Sud-Ouest

Method

- Compute the **individual directions** $\hat{a}_j$ on each block $j = 1, \ldots, J$ using regularized SIR.
- Compute a **common direction** as

$$\hat{a} = \underset{||a||=1}{\operatorname{argmax}} \sum_{j=1}^{J} \cos^2(\hat{a}_j, a) \cos^2(\hat{a}_j, \hat{a}_J).$$

Idea : If $\hat{a}_j$ is close to $\hat{a}_J$ then $\hat{a}$ should be close to $\hat{a}_j$.
Explicit solution : $\hat{a}$ is the eigenvector associated to the largest eigenvalue of

$$M_J = \sum_{j=1}^{J} \hat{a}_j \hat{a}_j^t \cos^2(\hat{a}_j, \hat{a}_J).$$

Advantages of SIRdatastream

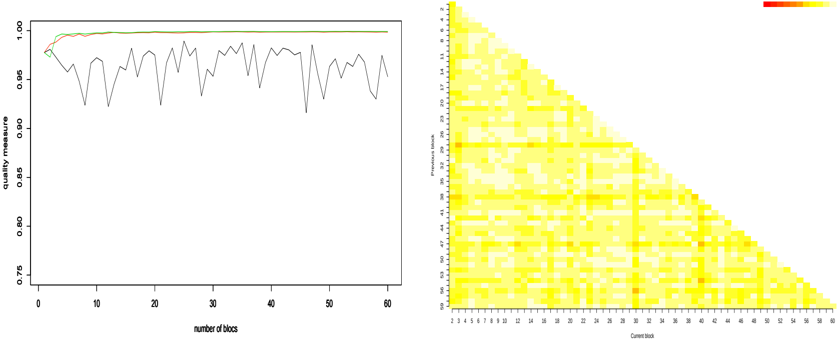
- Computational complexity $O(Jnp^2)$ v.s. $O(J^2np^2)$ for the brute-force method which would consist in applying regularized SIR on the union of the j first blocks for $j = 1, \dots, J$.
- Data storage $O(np)$ v.s. $O(Jnp)$ for the brute-force method.

(under the assumption $n >> \max(J, p)$).

- Interpretation of the weights $\cos^2(\hat{a}_j, \hat{a}_J)$.

Illustration on simulations

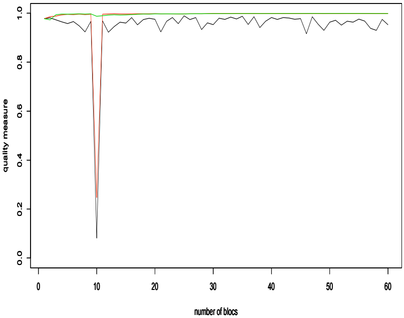
Scenario 1 : A common direction in all the 60 blocks.



Left : $\cos^2(\hat{a}, a)$ for SIRdatastream, SIR brute-force and SIR estimators at each time t. *Right :* $\cos^2(\hat{a}_j, \hat{a}_J)$. The lighter (yellow) is the color, the larger is the weight. Red color stands for very small squared cosines.

Illustration on simulations

Scenario 2 : The 10th block is an outlier.



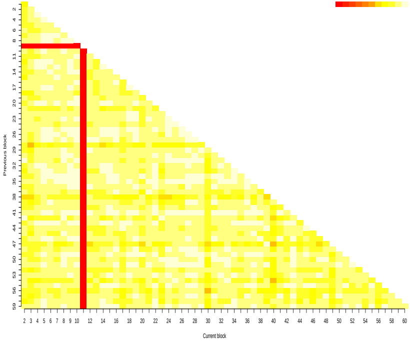


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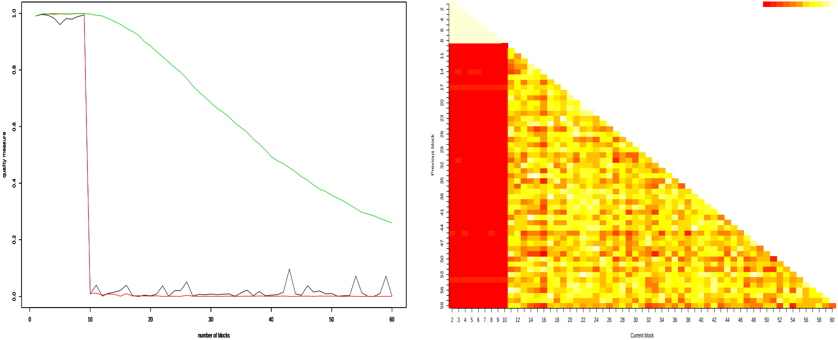
Illustration on simulations

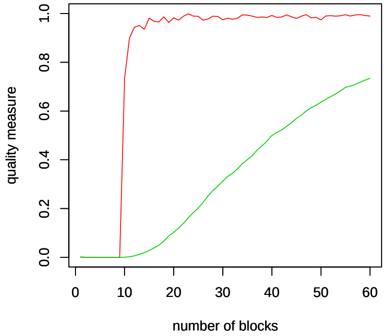
Scenario 3 : A drift occurs from the 10th block (a to a')

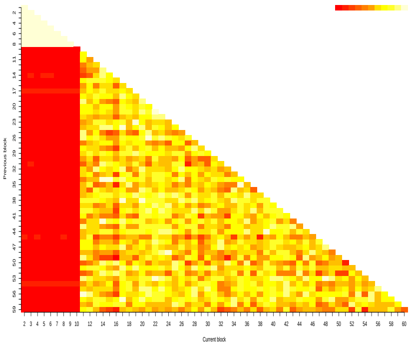


Left : $\cos^2(\hat{a}, a)$ for SIRdatastream, SIR brute-force and SIR estimators at each time t. *Right :* $\cos^2(\hat{a}_j, \hat{a}_J)$. The lighter (yellow) is the color, the larger is the weight. Red color stands for very small squared cosines.

Illustration on simulations

Scenario 3 (cont'd) : A drift occurs from the 10th block (a to a')

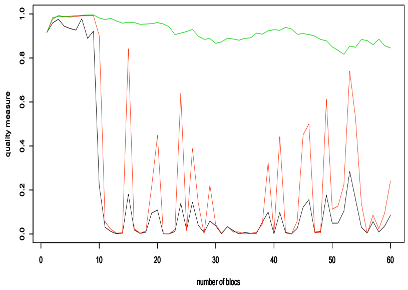


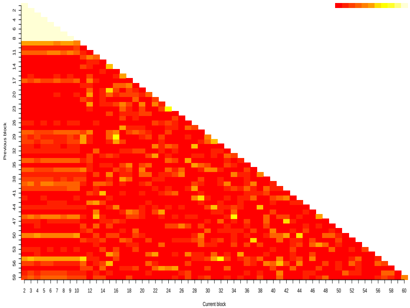


Left : $\cos^2(\hat{a}, a')$ for SIRdatastream and SIR brute-force. *Right :* $\cos^2(\hat{a}, a')$

Illustration on simulations

Scenario 4 : From the 10th block to the last one, there is no common direction.





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Related research themes in Mistis

Dimension reduction

- Dimension reduction for regression (this talk),
- Unsupervised dimension reduction (nonlinear PCA),
- Dimension reduction for classification and clustering.

Classification

- Robust classification and outlier detection,
- Classification with missing data,
- Classification of spatial data,
- Classification of heterogeneous data.

References on SIR

- [Li, 1991] Li, K.C. (1991). Sliced inverse regression for dimension reduction. *Journal of the American Statistical Association*, **86**, 316–327.
- [Cook, 2007]. Cook, R.D. (2007). Fisher lecture : Dimension reduction in regression. *Statistical Science*, **22**(1), 1–26.
- [Zhong et al, 2005] : Zhong, W., Zeng, P., Ma, P., Liu, J.S. and Zhu, Y. (2005). RSIR : Regularized Sliced Inverse Regression for motif discovery. *Bioinformatics*, **21**(22), 4169–4175.
- [Chiaromonte et al, 2002] : Chiaromonte, F. and Martinelli, J. (2002). Dimension reduction strategies for analyzing global gene expression data with a response. *Mathematical Biosciences*, **176**, 123–144.

References on this work

- Bernard-Michel, C., Douté, S., Fauvel, M., Gardes, L. et Girard, S. (2009). Retrieval of Mars surface physical properties from OMEGA hyperspectral images using Regularized Sliced Inverse Regression. *Journal of Geophysical Research - Planets*, **114**, E06005
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