

## Variational approach to

## time series analysis

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### Hidden Regimes and Model Reduction

- overwiev of the standard clustering methods, their problems
- *variational approach*: regularized model distance functional
- *finite element* approach to *clustering problem*
- manifold clustering
- toy examples
- <u>Applications:</u>
  - analysis of weather data (*regimes*, *prediction*)
  - computational finance (*portfolio theory*)
  - compression of 3D *turbulence simulation data*

## Hidden Regimes and Model Reduction





Let  $x(t): \mathbf{R}^1 \to \Psi \subset \mathbf{R}^n$  be the observed process  $t \in [0, T]$ 

Define  $\mathbf{K}$  local models by a *model distance functional*:

$$g(x, \theta_i)$$
 :  $\Psi \times \Omega \to [0, \overline{g}], \quad 0 < \overline{g} < +\infty,$   
 $\theta_1, \dots, \theta_{\mathbf{K}} \in \Omega \subset \mathbf{R}^d$ 

**Examples** 

• Geometrical clustering:  $\theta_i \in \Psi$  - cluster centers  $g(x, \theta_i) = ||x - \theta_i||^2$ ,





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**Examples** 

• Geometrical clustering:  $\theta_i \in \Psi$  - cluster centers  $g(x, \theta_i) = ||x - \theta_i||^2$ ,

• Gaussian clustering:  $\theta_i = (\mu_i, \Sigma_i)$  - Gaussian parameters  $g(x, \theta_i) = ||x - \mu_i||_{\Sigma_i^{-1}}^2$ 





### What is "clustering"?

Find 
$$\Gamma(t) = (\gamma_1(t), \dots, \gamma_{\mathbf{K}}(t))$$
 such that for each  $t$ :

$$\sum_{i=1}^{\mathbf{K}} \gamma_i(t) g\left(x, \theta_i\right) \quad \to \quad \min_{\Gamma(t), \Theta},$$

subjected to constraints:

$$\sum_{i=1}^{\mathbf{K}} \gamma_i(t) = 1, \quad \forall t \in [0, T]$$
$$\gamma_i(t) \geq 0, \quad \forall t \in [0, T], i = 1, \dots, \mathbf{K}$$





Find  $\Gamma(t) = (\gamma_1(t), \dots, \gamma_{\mathbf{K}}(t))$  such that for each t:

$$\mathbf{L}(\Theta, \Gamma(t)) = \int_0^T \sum_{i=1}^{\mathbf{K}} \gamma_i(t) g\left(x_t, \theta_i\right) \to \min_{\Gamma(t), \Theta},$$

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Numerical Method: Subspace Iteration (splitting scheme)

No global convergence (non-convex optimization, simulated annealing)





Geometrical distance:  $heta_i \in \Psi$  - time-independent cluster centers

$$g(x, \theta_i) = || x - \theta_i ||^2,$$

$$t_j, j = 1, \dots, n \in [0, T]$$

$$\sum_{i=1}^{K} \sum_{j=1}^{n} \gamma_i(t_j) || x_{t_j} - \theta_i ||^2 \rightarrow \min_{\Gamma(t),\Theta} \qquad (Bezdek1981, Hoppner et.al. 1999)$$

Iteration number (l):

$$\begin{split} \gamma_i^{(l)}(t_j) &= \begin{cases} 1 & i = \arg\min \| x_{t_j} - \theta_i^{(l-1)} \|^2, \\ 0 & \text{otherwise}, \end{cases} \\ \theta_i^{(l)} &= \frac{\sum_{j=1}^n \gamma_i^{(l)}(t_j) x_{t_j}}{\sum_{j=1}^n \gamma_i^{(l)}(t_j)}. \end{split}$$

"Sharp" assigment : problem for overlapping data



## K-Means clustering: Toy Example I











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Problems:

- 1. Euclidean distance may be not appropriate
- 2. geometrical clustering gets no use of temporal information





Problem 1: 
$$\mathbf{L}(\gamma_i(t), \mathbf{T}_i, \mu_i) \to \min$$
  
 $g(x, \theta_i) = ||x - \mathcal{T}_i \mathcal{T}_i^{\mathbf{T}} x ||^2$ 







Problem 1: 
$$\mathbf{L}(\gamma_i(t), \mathbf{T}_i, \mu_i) \to \min$$
  
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<u>Idea</u>: Essential manifold can be appproximated by *linear attractive manifolds+switching* 







Geometrical distance:  $\theta_i \in \Psi$  - time-independent cluster centers,

$$\sum_{i=1}^{\mathbf{K}} \sum_{j=1}^{n} \gamma_{i}^{m}(t_{j}) \parallel x_{t_{j}} - \theta_{i} \parallel^{2} \rightarrow \min_{\Gamma(t),\Theta|}$$
(Bezdek1987)  
$$\mathbf{I}_{x_{t_{j}}} = \{ p \in \{1, \dots, \mathbf{K}\} \mid \parallel x_{t_{j}} - \theta_{p}^{(l-1)} \parallel^{2} = 0 \}$$







## **Exercise 1**: proof that this formulas are true

$$\begin{split} \gamma_i^{(l)}(t_j) &= \begin{cases} \frac{1}{\sum_{p=1}^{\mathsf{K}} \left(\frac{\|x_{t_j} - \theta_i^{(l-1)}\|^2}{\|x_{t_j} - \theta_p^{(l-1)}\|^2}\right)^{\frac{1}{m-1}}} & \text{if } \mathbf{I}_{x_{t_j}} \text{ is empty}, \\ \sum_{r \in \mathbf{I}_{x_{t_j}}} \gamma_r^{(l)}(t_j) &= 1 & \text{if } \mathbf{I}_{x_{t_j}} \text{ is not empty}, i \in \mathbf{I}_{x_{t_j}}, \\ 0 & \text{if } \mathbf{I}_{x_{t_j}} \text{ is not empty}, i \notin \mathbf{I}_{x_{t_j}}, \\ \theta_i^{(l)} &= \frac{\sum_{j=1}^n \gamma_i^{(l)}(t_j) x_{t_j}}{\sum_{j=1}^n \gamma_i^{(l)}(t_j)}. \end{split}$$





Geometrical distance:  $\theta_i \in \Psi$  - time-independent cluster centers,

$$\sum_{i=1}^{K} \sum_{j=1}^{n} \gamma_i^m(t_j) \parallel x_{t_j} - \theta_i \parallel^2 \rightarrow \min_{\Gamma(t),\Theta}$$
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			F	uzzy	y c–Mean	s (m=1.	5)			
				- Contraction of the Contraction						
0	50	100	150	200	0 250 Time	300	350	400	450	50





*Geometrical distance*:  $\theta_i \in \Psi$  - *time-independent* cluster centers,

$$\sum_{i=1}^{K} \sum_{j=1}^{n} \gamma_{i}^{m}(t_{j}) \parallel x_{t_{j}} - \theta_{i} \parallel^{2} \rightarrow \min_{\Gamma(t),\Theta}$$
(Bezdek1987)







Geometrical distance:  $\theta_i \in \Psi$  - time-independent cluster centers,

introduce the "fuzzifier" m > 1

$$\sum_{i=1}^{K} \sum_{j=1}^{n} \gamma_i^m(t_j) \parallel x_{t_j} - \theta_i \parallel^2 \rightarrow \min_{\Gamma(t),\Theta}$$
(Bezdek1987)



Just to "fuzzify" is not enough!



### Problem 2: <u>identification of "persistent states"</u>

Let  $\gamma_i(\cdot)$  on  $t \in [0, T], i = 1, \dots, \mathbf{K}$  be differentiable and  $\partial_t \gamma_i \in \mathcal{L}_2(0,T)$  , i. e. :  $\mathbf{L}(\Theta, \Gamma(t)) = \int_0^T \sum_{i=1}^{\mathbf{K}} \gamma_i(t) g(x_t, \theta_i) \to \min_{\Gamma(t), \Theta},$  $\gamma(t)$  $\gamma(t_{k-2}) \gamma(t_{k-3})$ Num<u>ber Of Jump</u>s Time Interval  $=\sum \frac{(\gamma_i(t_{k+1}) - \gamma_i(t_k))^2}{\Delta t}$  $\gamma(t_{\rm k})$ n





## Problem 2: incorporation of temporal information

Let  $\gamma_i(\cdot)$  on  $t \in [0, T], i = 1, ..., \mathbf{K}$  be differentiable and  $\partial_t \gamma_i \in \mathcal{L}_2(0, T)$ , i. e. :  $\mathbf{L}(\Theta, \Gamma(t)) = \int_0^T \sum_{i=1}^{\mathbf{K}} \gamma_i(t) g(x_t, \theta_i) \to \min_{\Gamma(t), \Theta},$ 

subjected to

$$|\gamma_i|_{\mathcal{H}^1(0,T)} = \| \partial_t \gamma_i(\cdot) \|_{\mathcal{L}_2(0,T)} = \int_0^T \left( \partial_t \gamma_i(t) \right)^2 dt \le C_\epsilon^i < +\infty,$$

Regularized clustering functional:

$$\mathbf{L}^{\epsilon}(\Theta, \Gamma(t), \epsilon^{2}) = \mathbf{L}(\Theta, \Gamma(t)) + \epsilon^{2} \sum_{i=1}^{\mathbf{K}} \int_{0}^{T} \left(\partial_{t} \gamma_{i}\left(t\right)\right)^{2} dt \to \min_{\Gamma(t), \Theta}$$

(H. 08, to appear in SISC)



Regularized clustering functional: (H. 08, to appear in SISC)  $\mathbf{L}^{\epsilon}(\Theta, \Gamma(t), \epsilon^{2}) = \mathbf{L}(\Theta, \Gamma(t)) + \epsilon^{2} \sum_{i=1}^{\mathbf{K}} \int_{0}^{T} \left(\partial_{t} \gamma_{i}(t)\right)^{2} dt \to \min_{\Gamma(t), \Theta}$ 



Regularized clustering functional: (H. 08, to appear in SISC)  $\mathbf{L}^{\epsilon}(\Theta, \Gamma(t), \epsilon^{2}) = \mathbf{L}(\Theta, \Gamma(t)) + \epsilon^{2} \sum_{i=1}^{\mathbf{K}} \int_{0}^{T} \left(\partial_{t} \gamma_{i}\left(t\right)\right)^{2} dt \to \min_{\Gamma(t), \Theta}$ 

Galerkin-Ansatz:

$$\gamma_{i}(t) = \tilde{\gamma}_{i}(t) + \delta_{N}$$
$$= \sum_{k=1}^{N} \tilde{\gamma}_{i}^{(k)} v_{k}(t) + \delta_{N}$$

where  $\tilde{\gamma}_{i}^{(k)} = \int_{0}^{T} \gamma_{i}(t) v_{k}(t) dt$ , and  $\mathbf{L}^{\epsilon} = \tilde{\mathbf{L}}^{\epsilon} + \mathcal{O}(\delta_{N}) \rightarrow \min_{\tilde{\gamma}_{i}(t),\Theta},$  $\tilde{\mathbf{L}}^{\epsilon} = \sum_{i=1}^{K} \int_{0}^{T} [\tilde{\boldsymbol{z}}_{i}(t) - (\boldsymbol{z}_{i}) + \boldsymbol{z}_{i}^{2}(0) \tilde{\boldsymbol{z}}_{i}(t)]$ 

$$\tilde{\mathbf{L}}^{\epsilon} = \sum_{i=1} \int_{0} \left[ \tilde{\gamma}_{i}(t) g(x_{t}, \theta_{i}) + \epsilon^{2} \left( \partial_{t} \tilde{\gamma}_{i}(t) \right)^{2} \right] dt$$





(H. 08, to appear in SISC)

$$\tilde{\mathbf{L}}^{\epsilon} = \sum_{i=1}^{\mathbf{K}} \left[ a^{\mathbf{T}}(\theta_i) \bar{\gamma}_i + \epsilon^2 \bar{\gamma}_i^{\mathbf{T}} \mathbf{H} \bar{\gamma}_i \right] \to \min_{\bar{\gamma}_i, \Theta}$$

subjected to

 $\mathbf{K}$ 

i=1

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$$\sum \tilde{\gamma}_i^{(k+1)} = 1, \quad \forall k = 1, \dots, N,$$

$$\tilde{\gamma}_i^{(k+1)} \geq 0, \quad \forall k = 1, \dots, N; i = 1, \dots, \mathbf{K}.$$

ative Subspace Minimization sparse QP can be used

where 
$$a(\theta_i) = \left( \int_{t_1}^{t_2} v_1(t) g(x_t, \theta_i) dt, \dots, \int_{t_{N-1}}^{t_N} v_N(t) g(x_t, \theta_i) dt \right)$$

is a vector of *FEM-discretized model distances* and  $\mathbf{H}$  is

a mass-matrix of the FEM-basis





**Theorem** Let for a given observed time series  $x(t) : \mathbf{R}^1 \to \Psi \subset \mathbf{R}^n$ , the model distance functional is chosen such that it satisfies (2),  $\Psi$  and  $\Omega$  are compact,  $g(x_t, \cdot)$  is continuously differentiable function of  $\theta$  and

$$\frac{\partial}{\partial \Theta} \tilde{\mathbf{L}}^{\epsilon} \left( \Theta^*, \bar{\gamma} \right) = 0,$$

has a unique solution  $\Theta^* = (\theta_1^*, \dots, \theta_K^*), \theta_i^* \in \Omega$  for any fixed  $\bar{\gamma}$  satisfying (18-19) and  $\frac{\partial^2}{\partial \Theta^2} \tilde{\mathbf{L}}^{\epsilon}(\Theta^*, \bar{\gamma})$ is positive definite. Then for any  $\epsilon^2 \geq 0$  and any finite continuous non-negative finite elements set  $\{v_1(t), v_2(t), \dots, v_N(t)\} \in \mathcal{L}_2(0, T)$  such that the respective mass-matrix  $\mathcal{H}$  is positive definite, the above algorithm is monotonous, *i. e.*, for any  $j \geq 1$ 

$$ilde{\mathrm{L}}^\epsilon \left( \Theta^{[j+1]}, ar{\gamma}^{[j+1]}_i 
ight) \hspace{.1in} \leq \hspace{.1in} ilde{\mathrm{L}}^\epsilon \left( \Theta^{[j]}, ar{\gamma}^{[j]}_i 
ight).$$

### Convergence to a local optimum only!

(coupling to some *global opimizer* necessary)



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## Toy Example I

$$\mathbf{L}(\gamma_i(t), \mathbf{T}_i, \mu_i) \to \min_{g(x, \theta_i)} g(x, \theta_i) = \| x - \theta_i \|^2,$$









## Toy Example I

$$\mathbf{L}(\gamma_i(t), \mathbf{T}_i, \mu_i) \to \min$$
$$g(x, \theta_i) = \| x - \theta_i \|^2,$$









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$$\mathbf{L}(\gamma_i(t), \mathbf{T}_i, \mu_i) \to \min$$
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How to determine the optimal K: probabilistic model assumptions a posteriory

$$g(x,\theta_i) = ||x - \theta_i||^2,$$







How to determine the optimal ε: standard L-Curve approach from Tikhonov-regularized linear least-squares problems (Cullum(79), Hansen(99))





Toy Example II







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### Error of FEM-Based Clustering









### Effect of Regularization



the distributions identified by  $\mathbf{L}(\gamma_i(t), \mathbf{T}_i, \mu_i) \to \min$  $g(x, \theta_i) = ||x - \mathcal{T}_i \mathcal{T}_i^{\mathbf{T}} x ||^2$ 

## Application: meteorology (cooperation with R. Klein)





# Wind Jets transport moisture from US to Europe

Jet-Blocking











Jet-Blocking results in "indian summer" and "blackberry cold" in Europe





Weather Data in Europe: 29x20 grid (44 years) (Data from H.Osterle, PIK) Up to 4 hidden states are statistically separable







Weather Data in Europe: 29x20 grid (44 years) (Data from H.Osterle, PIK) Up to 4 hidden states are statistically separable



Comparison with Lejenas-Okland blocking index

Hidden State 4: Jet Blocking Situation



 $\mathbf{L}(\gamma_i(t), \mathbf{T}_i, \mu_i) \rightarrow \min : \mathsf{K}=4$ 



Reduced dynamical description

Stochastic Prediction: Markov+SDEs (H./Klein/Dolaptchiev/Schütte, SIAM MMS 06, H., JAS 08, H./Dolaptchiev/Eliseev/Mokhov/Klein, JAS 08)



$$z(t) = \mathbf{T}_i^{\mathsf{T}} (x_t - \mu_i)$$
  
$$\dot{z}(t) = F_i (z(t) - \bar{\mu}_i) + \Sigma_i \dot{W}(t)$$





### Weather Data in Europe: 29x20 grid (44 years) (Data from H.Osterle, PIK) Up to 4 hidden states are statistically separable

1 Day temperature predictions



 $z(t) = \mathbf{T}_i^{\mathsf{T}} (x_t - \mu_i)$  $\dot{z}(t) = F_i (z(t) - \bar{\mu}_i) + \Sigma_i \dot{W}(t)$ 







**Optimal Portfolio:** Maximize Yield and Minimize Risk

(H. Markowitz 1952, Nobel Price 1990)

#### Mathematical Analysis of available Financial Information









Given a probability space  $(\Omega, \mathcal{F}, P)$ , a **stochastic process** (or **random process**) with state space X is a collection of X-valued random variables indexed by a set T ("time"). That is, a stochastic process F is a collection

$$\{F_t: t \in T\}$$

where each Ft is an X-valued random variable.

Probability Density Function:  $Pr(4.3 \le X \le 7.8) = \int_{4.3}^{7.8} f(x) dx$ 

Expectation Value:  

$$E(X) = \int_{\Omega} X \, dP \qquad \mu = \int x \, p(x) \, dx$$
Variance:  

$$Var(X) = \int (x - \mu)^2 \, p(x) \, dx$$







Let  $P_s(T) \in \mathbf{R}^n$  be a stochastic price process and  $x \in \mathbf{R}^n$  is a portfolio, then  $c(T,x) = \langle P_s(T),x \rangle$  the portfolio price

Maximize Yield	and	Minimize Risk





Let  $P_s(T) \in \mathbf{R}^n$  be a stochastic price process and  $x \in \mathbf{R}^n$ is a portfolio, then  $c(T, x) = \langle P_s(T), x \rangle$  the portfolio price  $\mathbf{E}(c) - \alpha \mathbf{V}ar^-(c - \mathbf{E}(c)) \rightarrow \max_{x \in \mathbf{R}}$ 



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Let  $P_s(T) \in \mathbf{R}^n$  be a stochastic price process and  $x \in \mathbf{R}^n$  is a portfolio, then  $c(T,x) = \langle P_s(T),x \rangle$  the portfolio price

$$\mathbf{E}(c) - \alpha \mathbf{V}ar^{-}(c - \mathbf{E}(c)) \rightarrow \max_{x}$$

#### Numerical solution possible

**Exercise 3**: write the above maximization problem in vector-matrix form. What kind of constraints on x will be meaningful? Under which conditions on  $\partial P_s(t)/\partial t$  does this constrained maximization problem have a unique solution for a fixed  $\alpha$ 





#### Persistent Regimes in Financial Data: Market Phases

*Market Phases* are hidden in *multiple*, *noisy* data-series



I. Horenko, Ch. Schütte, <u>German Patent</u> 10 2007 014 921.4 on 22.03.2007





#### Persistent Regimes in Financial Data: Market Phases



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Identification of *hidden market phases* reduces the *portfolio risk* 

 $\mathbf{L}(\gamma_i(t), \mathbf{T}_i, \mu_i) \to \min$  $g(x, \theta_i) = \| x - \mathcal{T}_i \mathcal{T}_i^{\mathbf{T}} x \|^2$ 



## http://www.portfolio-calculator.com



http://www.portfolio–calculator.com

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and the bare and benchmanner		

 $\mathbf{L}(\gamma_i(t), \mathbf{T}_i, \mu_i) \to \min$  $g(x, \theta_i) = \| x - \mathcal{T}_i \mathcal{T}_i^{\mathbf{T}} x \|^2$ 

## Example: analysis of DNS data (with R.Klein)





0.5 >

fine-grid spatial patterns  $\Leftrightarrow$  coarse-grid stencil data

#### Issues (1st phase):

- Structure of fluctuations
- Fluctuations vs. mean flow
- Coarse-grid dynamics



DNS by G. Gassner (IAG, Uni Stuttgart)

*Aim:* construction of *reduced stochastic models* for subscale phenomena

based on available DNS data or data-based model reduction





#### **DNS Data: Compression**

#### Fluid Flow in 3D 1.2 TB Data (Data from R.Klein/M.Uhlmann, FU)



15 x 80 GB ≈ 2.000 EUR

1 USB with 2 GB  $\approx$  20 EUR

1 CD ≈ 0.2 EUR

$$z(t) = \mathbf{T}_i^{\mathsf{T}} (x_t - \mu_i)$$
  
$$\dot{z}(t) = F_i (z(t) - \bar{\mu}_i) + \Sigma_i \dot{W}(t)$$

# Take–Home-Messages :

- 1. Variational approach to time series analysis. No explicit probabilistic assumptions needed (difference to GMM/HMM)
- 2. Probabilistic assumptions can be done a posteriory (determination of  $\boldsymbol{K}$ )
- 3. *Regularization* controls the *persistence* of regimes.







### Thank you for attention!