
Numerics of Stochastic Processes VII

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„Mathematics in key technologies“





Model Distance Functional

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

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

$$g(x, \theta_i) : \Psi \times \Omega \rightarrow [0, \bar{g}], \quad 0 < \bar{g} < +\infty,$$

$$\theta_1, \dots, \theta_{\mathbf{K}} \in \Omega \subset \mathbf{R}^d$$

Examples

- *Geometrical clustering*: $\theta_i \in \Psi$ - cluster centers

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

- *Gaussian clustering*: $\theta_i = (\mu_i, \Sigma_i)$ - Gaussian parameters

$$g(x, \theta_i) = \|x - \mu_i\|_{\Sigma_i^{-1}}^2$$



Averaged Clustering Functional



Find $\Gamma(t) = (\gamma_1(t), \dots, \gamma_K(t))$ such that for each t :

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

subjected to constraints:

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

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

Numerical Method: Subspace Iteration (splitting scheme)

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



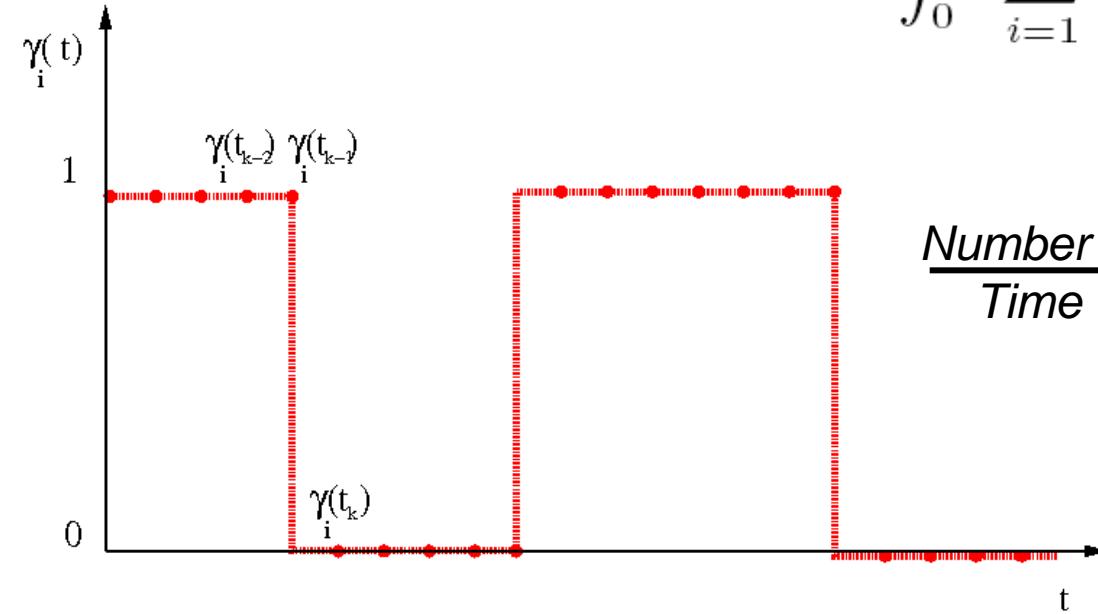
Incorporation of Temporal Information

Problem 2: identification of “*persistent states*“

Let $\gamma_i(\cdot)$ on $t \in [0, T], i = 1, \dots, K$ be differentiable and

$\partial_t \gamma_i \in \mathcal{L}_2(0, T)$, i.e.:

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



$$\frac{\text{Number Of Jumps}}{\text{Time Interval}} =$$

$$= \sum_{k=1} \frac{(\gamma_i(t_{k+1}) - \gamma_i(t_k))^2}{\Delta t}$$



Tikhonov-type Regularization

Problem 2: incorporation of temporal information

Let $\gamma_i(\cdot)$ on $t \in [0, T], i = 1, \dots, K$ be differentiable and

$\partial_t \gamma_i \in \mathcal{L}_2(0, T)$, i.e.:

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

subjected to

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

Regularized clustering functional:

$$\mathbf{L}^\epsilon(\Theta, \Gamma(t), \epsilon^2) = \mathbf{L}(\Theta, \Gamma(t)) + \epsilon^2 \sum_{i=1}^K \int_0^T (\partial_t \gamma_i(t))^2 dt \rightarrow \min_{\Gamma(t), \Theta}$$

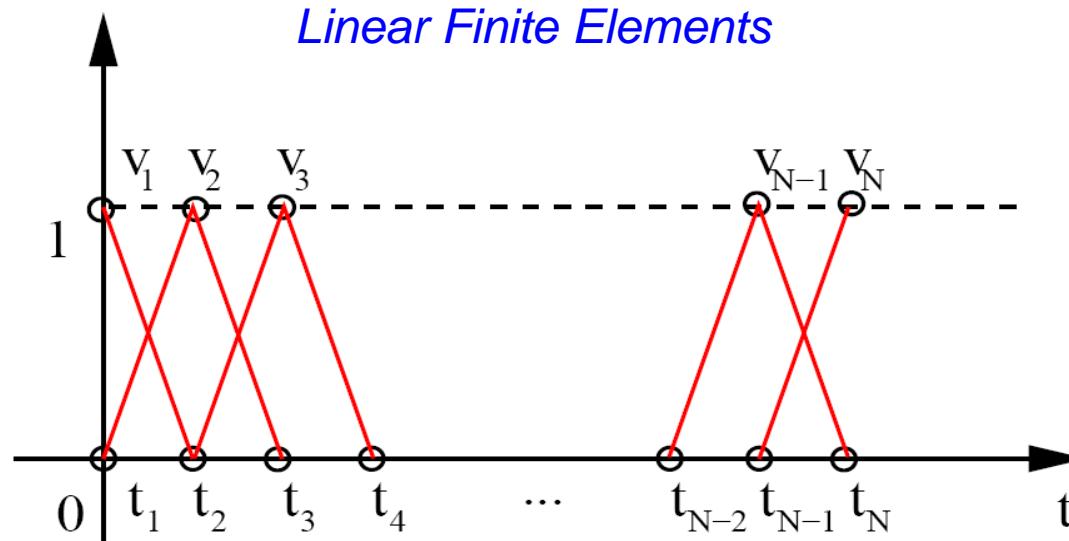
(H. 08, to appear in SISC)



FEM: Time Discretization

Let $\{0 = t_1, t_2, \dots, t_{N-1}, t_N = T\}$. We define a set of continuous functions on $[0, T]$, or finite elements set $\{v_1(t), v_2(t), \dots, v_N(t)\} \in \mathcal{L}_2(0, T)$ with local support.

Example:





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FEM: Regularized Clustering Functional

Regularized clustering functional: (H. 08, to appear in SISC)

$$\mathbf{L}^\epsilon(\Theta, \Gamma(t), \epsilon^2) = \mathbf{L}(\Theta, \Gamma(t)) + \epsilon^2 \sum_{i=1}^K \int_0^T (\partial_t \gamma_i(t))^2 dt \rightarrow \min_{\Gamma(t), \Theta},$$



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$$\mathbf{L}^\epsilon(\Theta, \Gamma(t), \epsilon^2) = \mathbf{L}(\Theta, \Gamma(t)) + \epsilon^2 \sum_{i=1}^K \int_0^T (\partial_t \gamma_i(t))^2 dt \rightarrow \min_{\Gamma(t), \Theta},$$

Galerkin-Ansatz :

$$\begin{aligned}\gamma_i(t) &= \tilde{\gamma}_i(t) + \delta_N \\ &= \sum_{k=1}^N \tilde{\gamma}_i^{(k)} v_k(t) + \delta_N\end{aligned}$$

where $\tilde{\gamma}_i^{(k)} = \int_0^T \gamma_i(t) v_k(t) dt$, and

$$\mathbf{L}^\epsilon = \tilde{\mathbf{L}}^\epsilon + \mathcal{O}(\delta_N) \rightarrow \min_{\tilde{\gamma}_i(t), \Theta},$$

$$\tilde{\mathbf{L}}^\epsilon = \sum_{i=1}^K \int_0^T \left[\tilde{\gamma}_i(t) g(x_t, \theta_i) + \epsilon^2 (\partial_t \tilde{\gamma}_i(t))^2 \right] dt.$$



FEM-Discretized Clustering Functional

(H. 08, to appear in SISC)

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

subjected to

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

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

Iterative 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*



Algorithm: monotony conditions

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

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

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 $j \geq 1$

$$\tilde{\mathbf{L}}^\epsilon \left(\Theta^{[j+1]}, \bar{\gamma}_i^{[j+1]} \right) \leq \tilde{\mathbf{L}}^\epsilon \left(\Theta^{[j]}, \bar{\gamma}_i^{[j]} \right).$$

Convergence to a local optimum only!

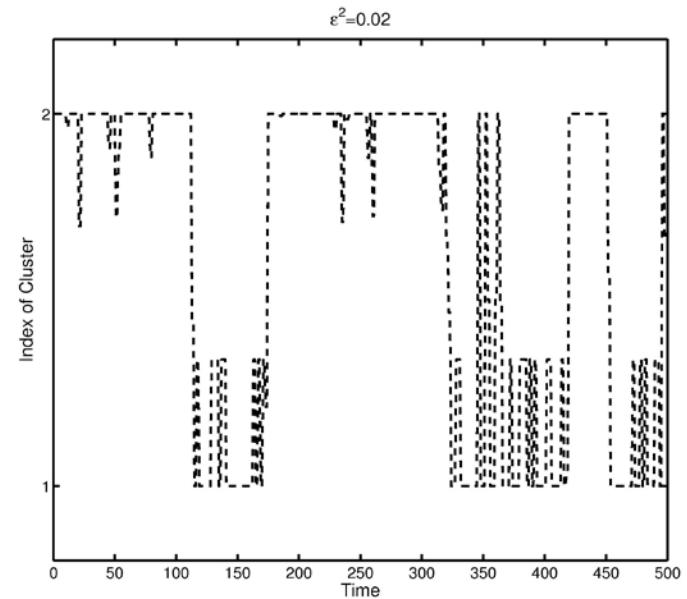
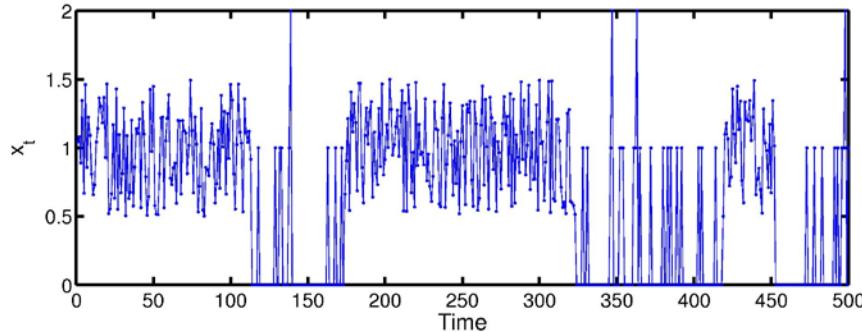
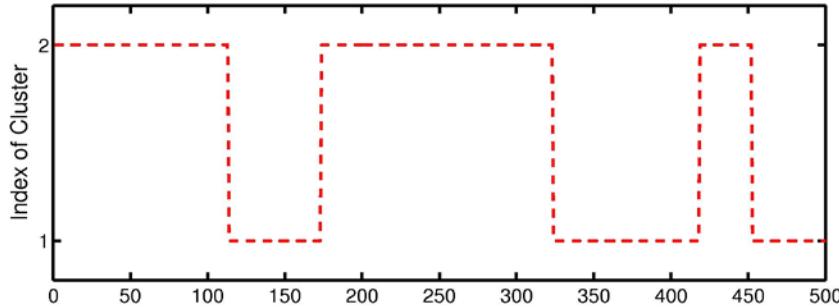
(coupling to some *global optimizer* necessary)



Toy Example I

$$\mathbf{L}(\gamma_i(t), \mathbf{T}_i, \mu_i) \rightarrow \min$$

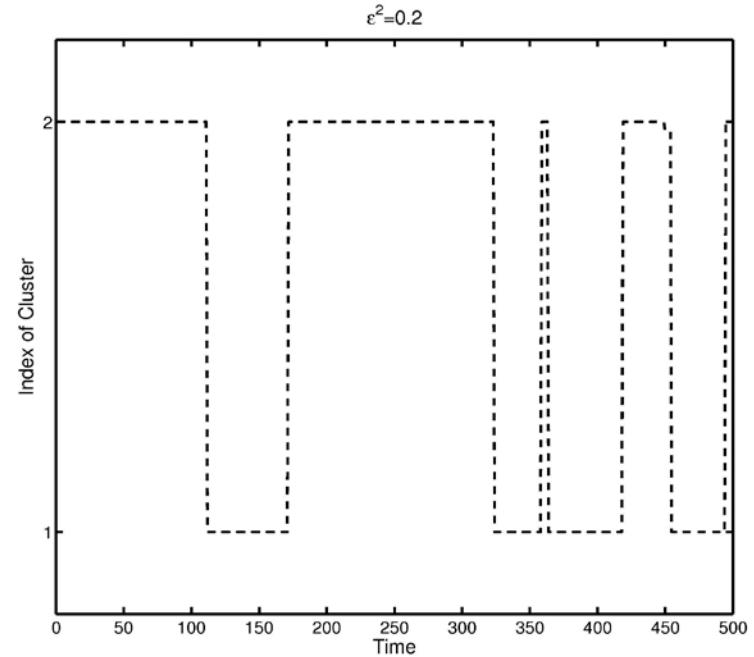
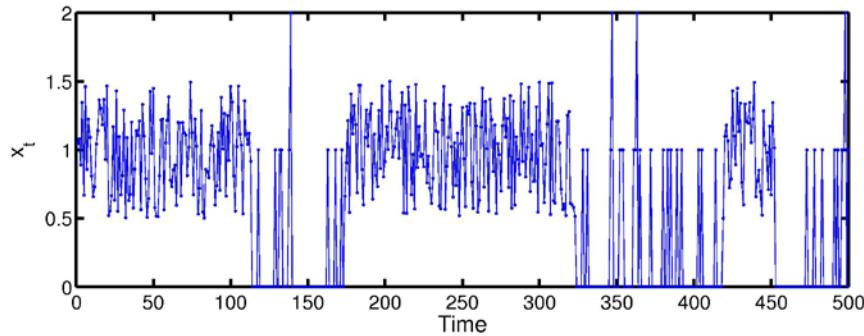
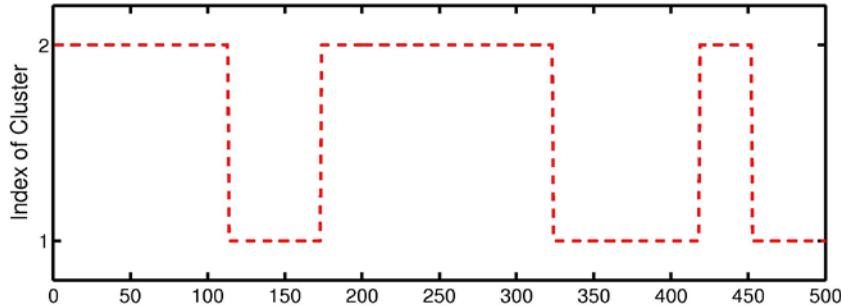
$$g(x, \theta_i) = \|x - \theta_i\|^2,$$





Toy Example I

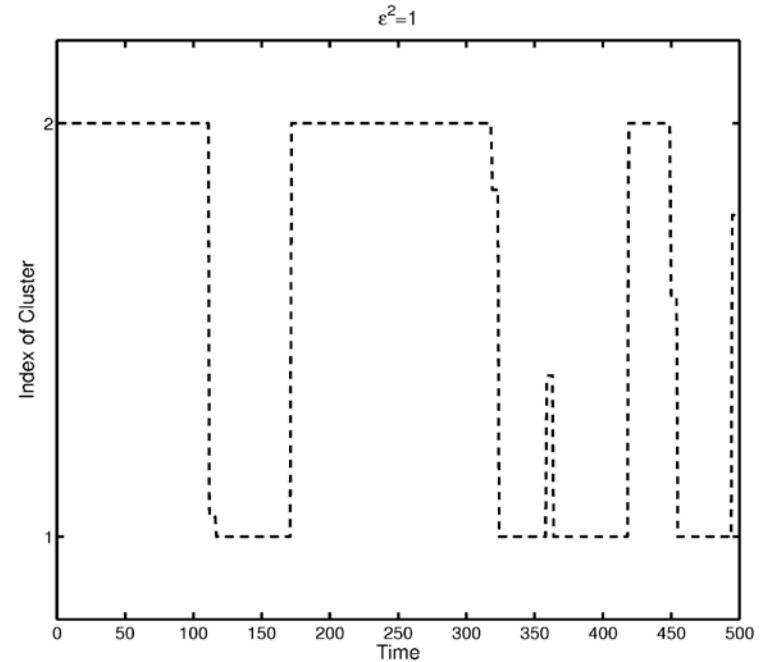
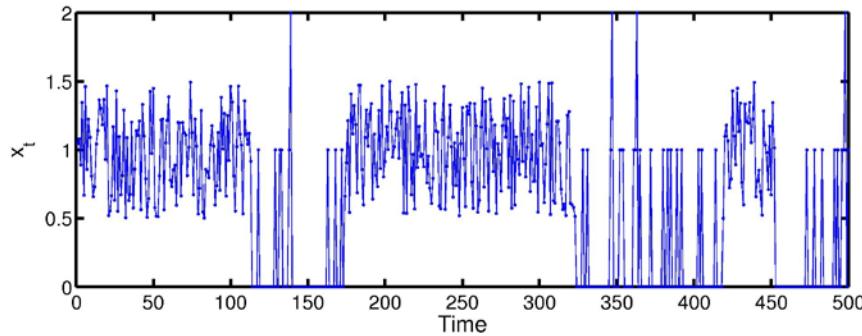
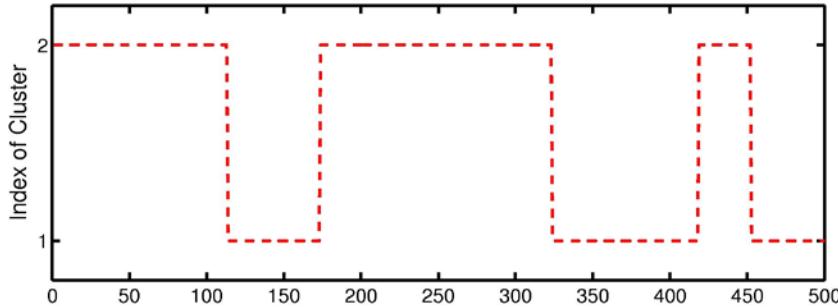
$$\begin{aligned} \mathbf{L}(\gamma_i(t), \mathbf{T}_i, \mu_i) &\rightarrow \min \\ g(x, \theta_i) &= \|x - \theta_i\|^2, \end{aligned}$$





Toy Example I

$$\begin{aligned} \mathbf{L}(\gamma_i(t), \mathbf{T}_i, \mu_i) &\rightarrow \min \\ g(x, \theta_i) &= \|x - \theta_i\|^2, \end{aligned}$$

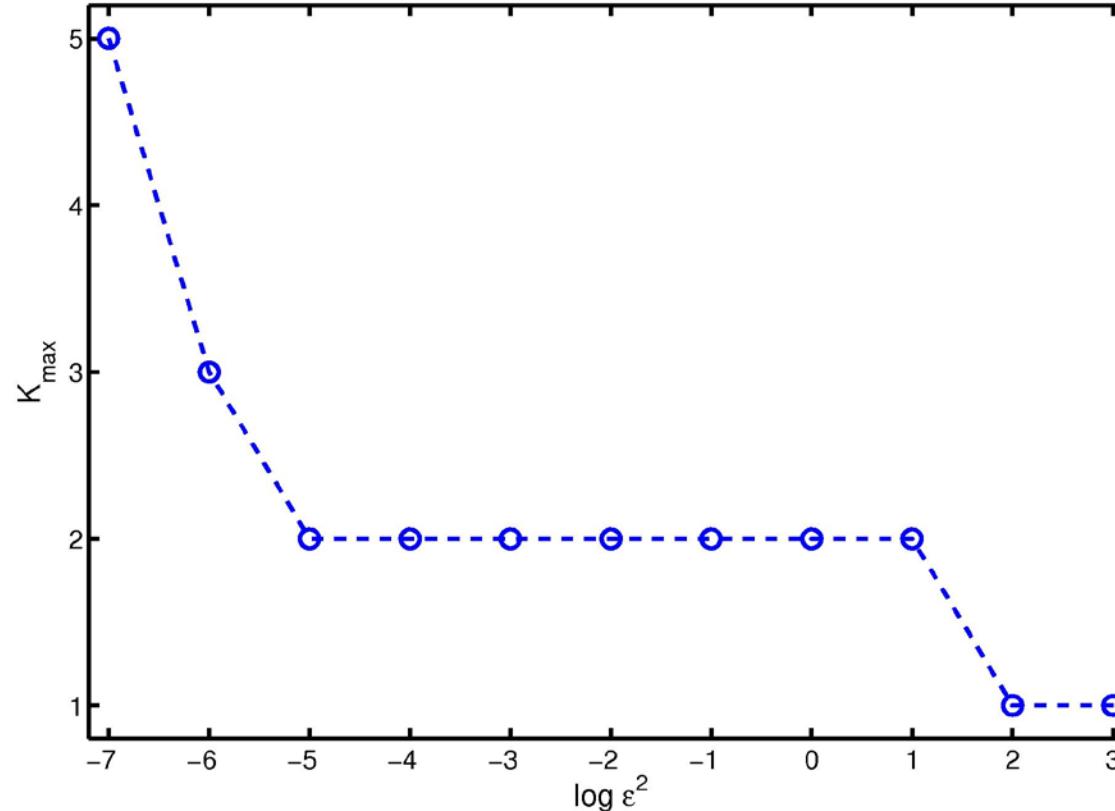




Toy Example I

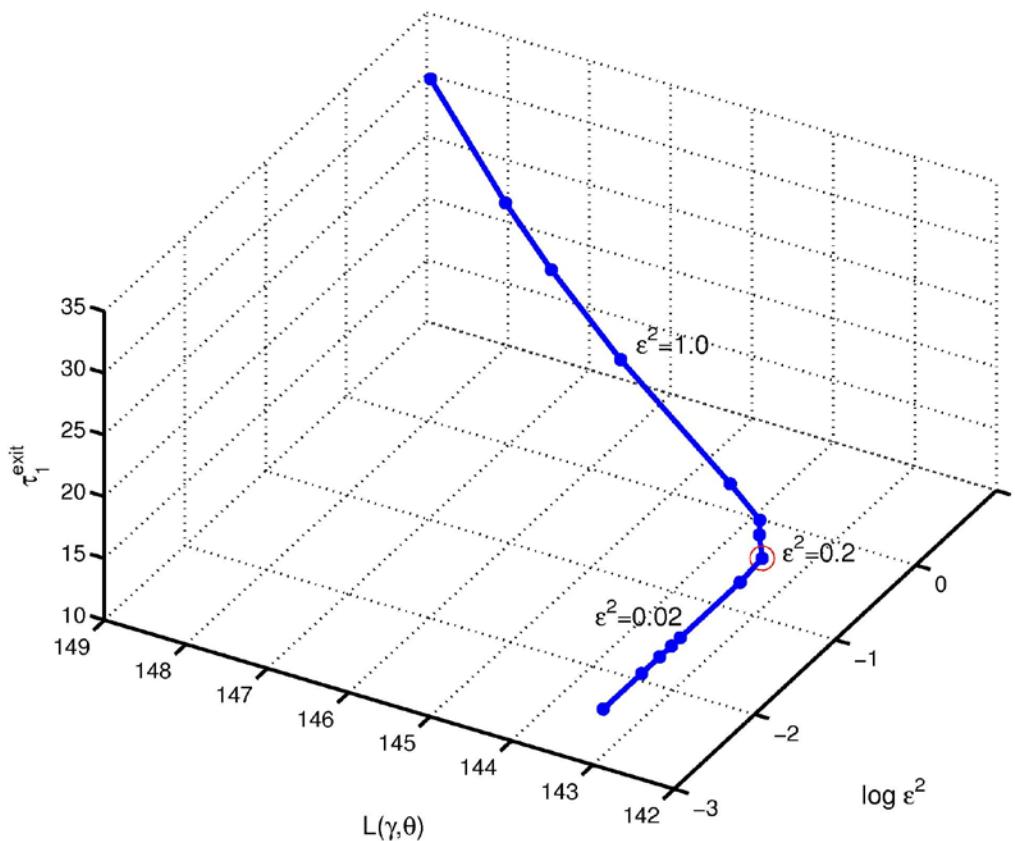
How to determine the optimal K: probabilistic model assumptions
a posteriori

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



Toy Example I

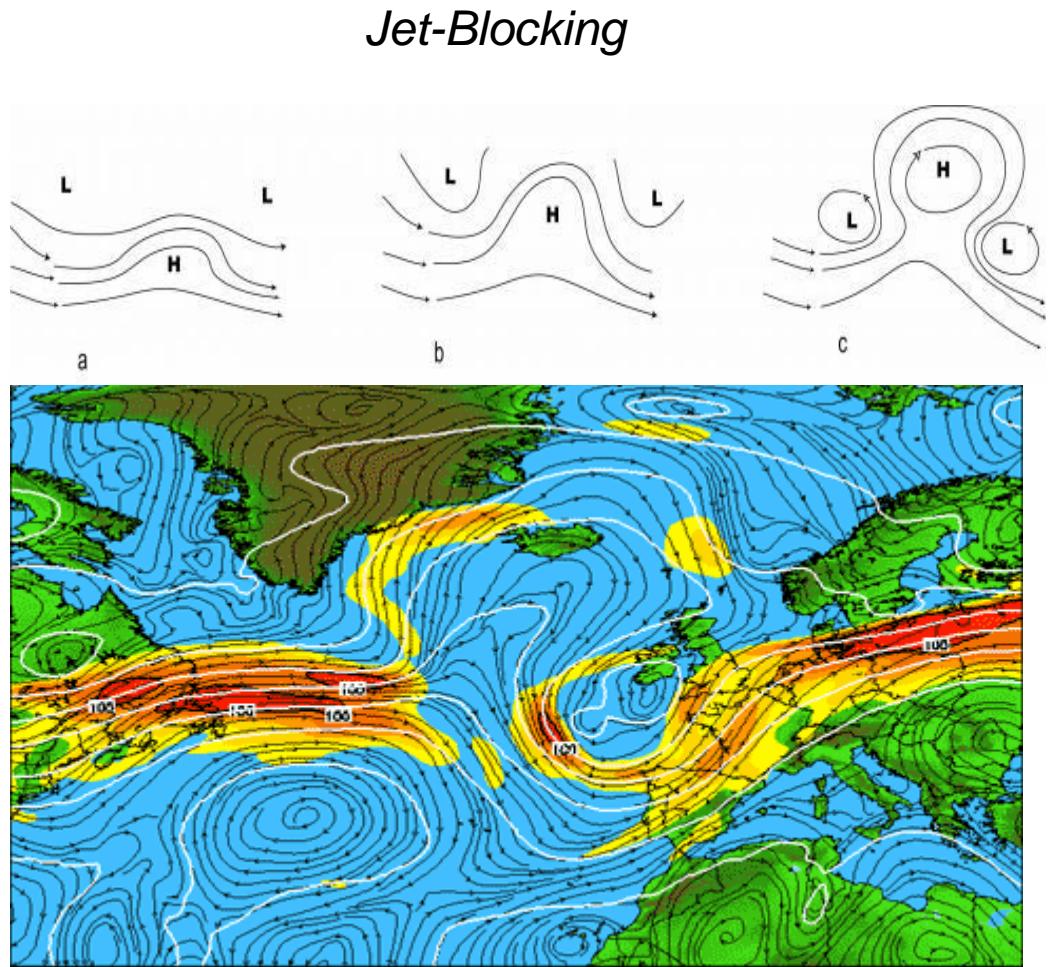
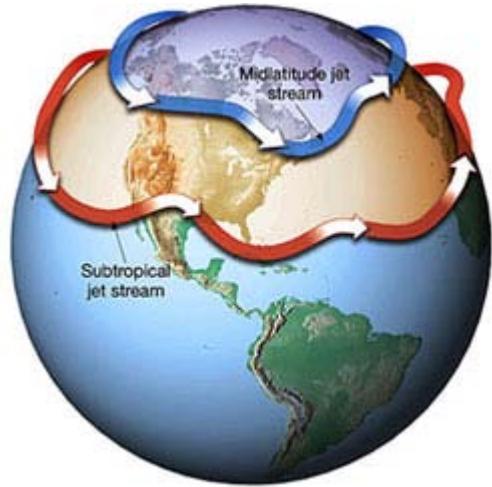
How to determine the optimal ϵ : standard L-Curve approach from Tikhonov-regularized linear least-squares problems
(Cullum(79), Hansen(99))



Application: meteorology
(cooperation with R. Klein)

“Hidden“ Weather Phases: motivation

Wind Jets transport moisture from US to Europe



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



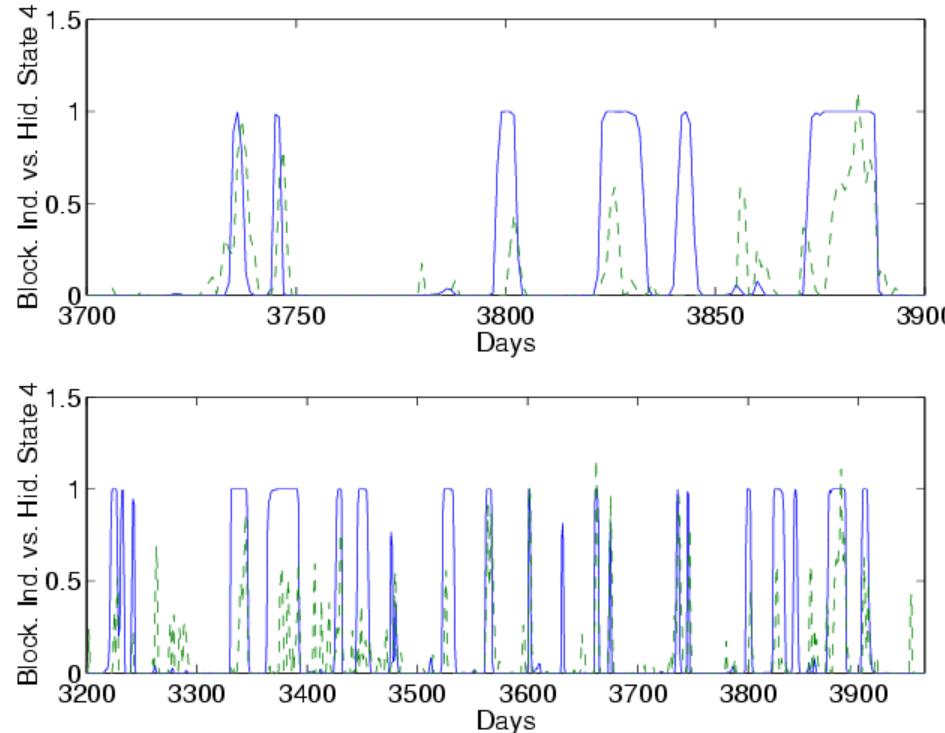
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$$\mathbf{L}(\gamma_i(t), \mathbf{T}_i, \mu_i) \rightarrow \min : K=4$$

Hidden State 4: Jet Blocking Situation

Up to 4 hidden states are statistically separable



$$\mathbf{L}(\gamma_i(t), \mathbf{T}_i, \mu_i) \rightarrow \min$$

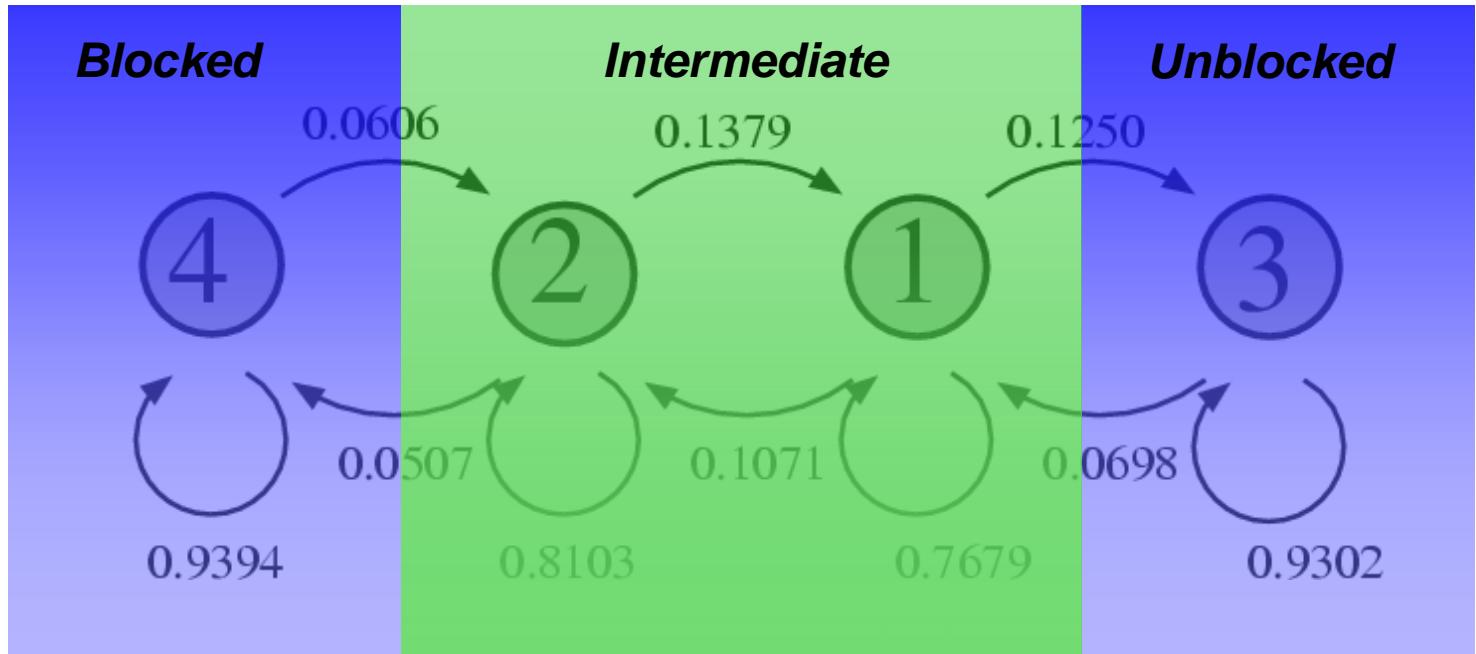
$$g(x, \theta_i) = \|x - \mathcal{T}_i \mathcal{T}_i^T x\|^2$$

*Comparison with
Lejenas-Okland
blocking index*

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



SPP 1276 "MetStröm" Project



Looking through Markovian  : predictions

$$\mathbf{L}(\gamma_i(t), \mathbf{T}_i, \mu_i) \rightarrow \min$$

$$g(x, \theta_i) = \| x - \mathcal{T}_i \mathcal{T}_i^T x \|^2$$

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Example: *climatic trends in circulation dynamics*
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Circulation Patterns for UK(1945-2007)

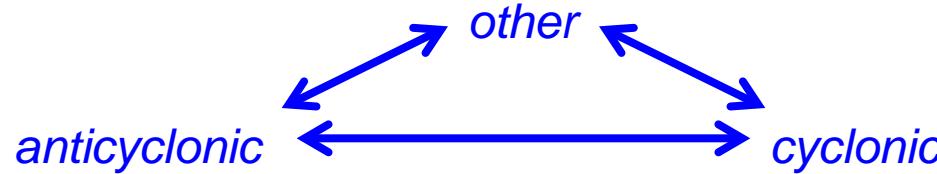
Historical Circulation Data: weather regimes

(Data from the Univ. of East Anglia)

3 atmospheric states considered

Lamb, Geophys. Mem. (1972),

Jones/Hulme/Briffa, Int.J.of Climat. (1977),



$$\mathbf{L}(\gamma_i(t), \mathbf{T}_i, \mu_i) \rightarrow \min$$

$$x_t : X_t \rightarrow X_{t+1}$$

$$g(x_t, P^i) = -\log P_{X_t X_{t+1}}^i$$

Clustering of Markovian Transitions with FEM-Clustering



Memo II: Markov Chain Log-Likelihood

Observed Time Series: $\{X_1, \dots, X_T\}$, $X_t \in s_1, \dots, s_m$

Markov-Property:

$$\text{P}[X_t = s_j | X_1, X_2, \dots, X_{t-1} = s_i] = \text{P}[X_t = s_j | X_{t-1} = s_i] = P_{ij}(t)$$

Log-Likelihood:

$$\text{L}(P(t)) = \log \text{P}[X_1, \dots, X_T]$$

$$\begin{aligned}\sum_{j=1}^m P_{ij}(t) &= 1, \quad \text{for all } t, i \\ P_{ij}(t) &\geq 0, \quad \text{for all } t, i, j\end{aligned}$$

$$\begin{aligned}&= \log \text{P}[X_1] + \sum_i^m \sum_{j=1}^m \sum_{t \in \{t_{ij}\}} \log P_{ij}(t) \rightarrow \max_{P(t)}\end{aligned}$$

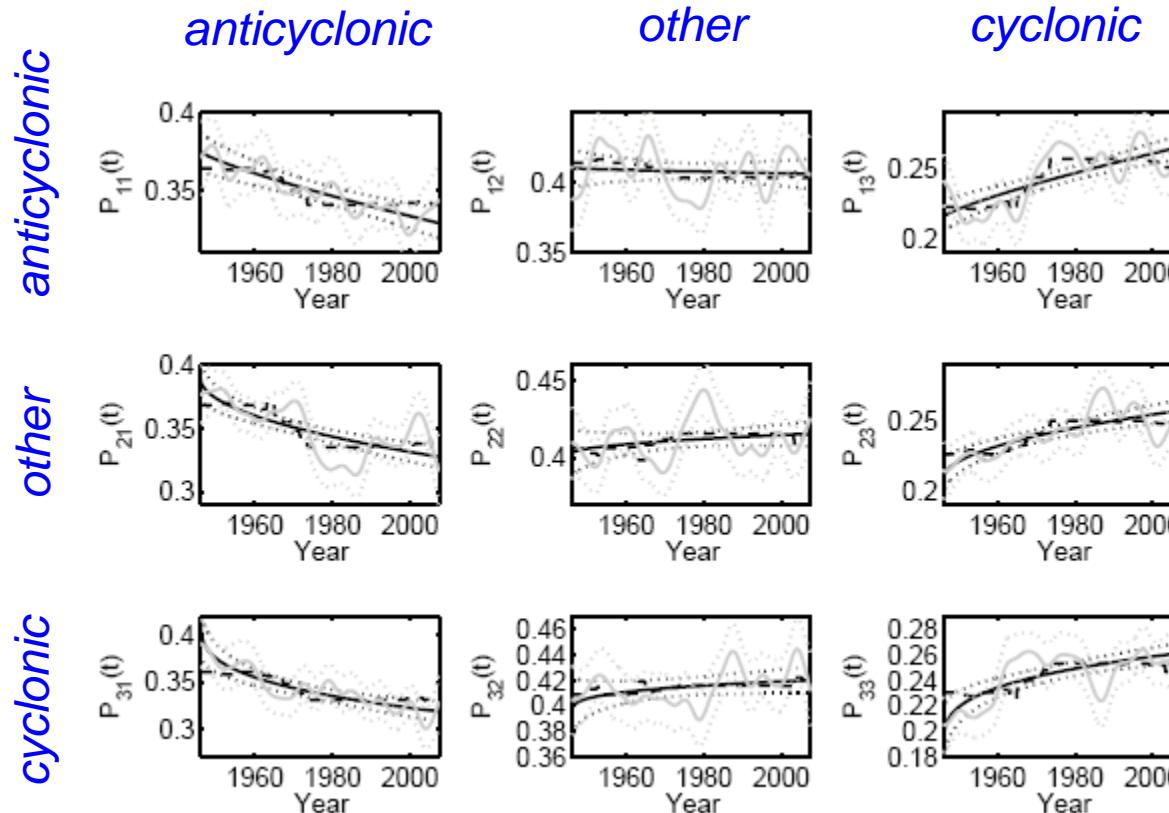
Maximization problem is ill-posed => regularization necessary



Circulation Patterns for UK(1945-2007)

*Historical Circulation Data: weather regimes
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3 atmospheric states considered*

H., submitted to Journal of Atmos. Sci. (2008)



$$L(\gamma_i(t), T_i, \mu_i) \rightarrow \min$$
$$g(x_t, P^i) = -\log P_{X_t X_{t+1}}^i$$

$$x_t : X_t \rightarrow X_{t+1}$$

$$\Gamma(\gamma_i(t), T_i, \mu_i) \rightarrow \min$$



FEM: Regularized Clustering Functional

Regularized clustering functional:

(H. 08, to appear in J. of Atmos. Sci.)

$$\mathbf{L}^\epsilon(\Theta, \Gamma(t), \epsilon^2) = \mathbf{L}(\Theta, \Gamma(t)) + \epsilon^2 \sum_{i=1}^{\mathbf{K}} \int_0^T (\partial_t \gamma_i(t))^2 dt \rightarrow \min_{\Gamma(t), \Theta},$$

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

$$x_t : X_t \rightarrow X_{t+1}$$

$$g(x_t, P^i) = -\log P_{X_t X_{t+1}}^i$$

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

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



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$$x_t : X_t \rightarrow X_{t+1}$$

$$g(x_t, P^i) = -\log P_{X_t X_{t+1}}^i$$

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

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

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

**Iterative Subspace Minimization:
sparse QP can be used**

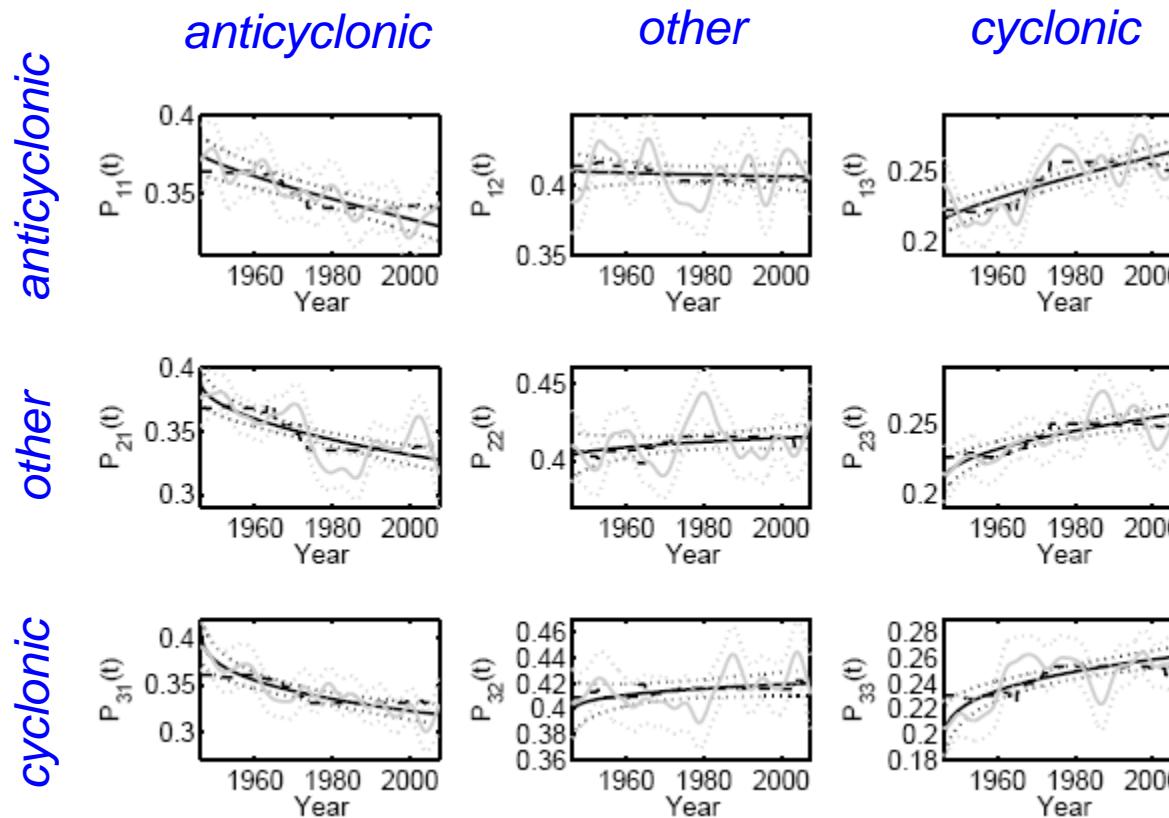


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Circulation Patterns for UK(1945-2007)

*Historical Circulation Data: 28 Lamb regimes
(Data from the Univ. of East Anglia)
3 atmospherical states considered*



$$L(\gamma_i(t), T_i, \mu_i) \rightarrow \min$$
$$g(x_t, P^i) = -\log P_{X_t, X_{t+1}}^i$$

$$x_t : X_t \rightarrow X_{t+1}$$

$$\Gamma(\gamma_i(t), T_i, \mu_i) \rightarrow \min$$

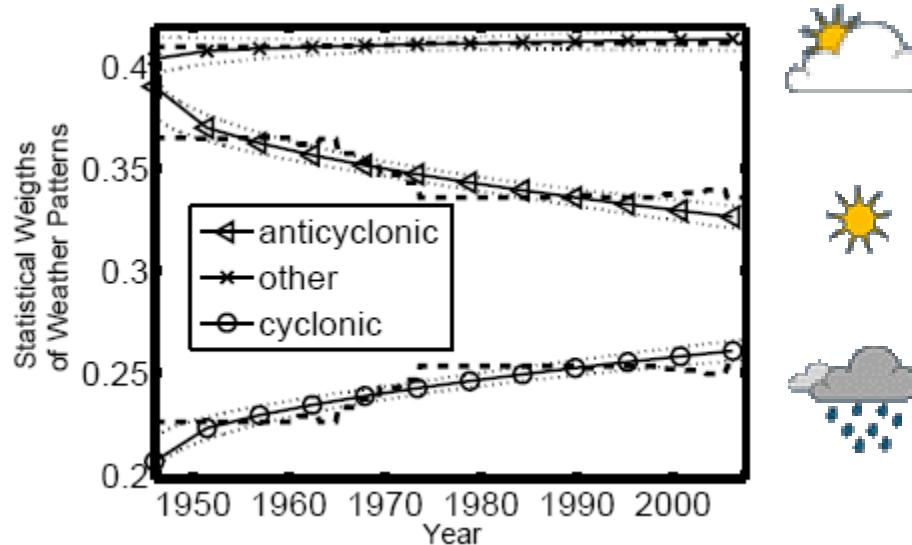


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Historical Circulation Data: weather regimes
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H., submitted to *Journal of Atmos. Sci.* (2008)

$$\pi(t) P(t) = \pi(t)$$



$$\begin{aligned} \mathbf{L}(\gamma_i(t), \mathbf{T}_i, \mu_i) &\rightarrow \min \\ x_t : X_t \rightarrow X_{t+1} \\ g(x_t, P^i) &= -\log P_{X_t X_{t+1}}^i \end{aligned}$$



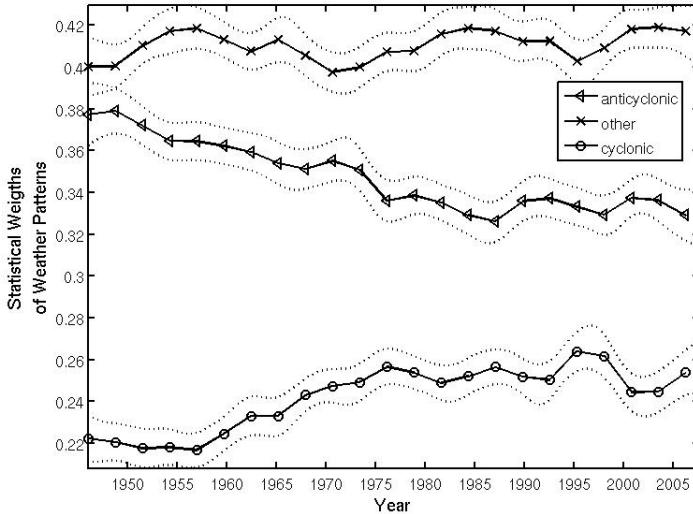
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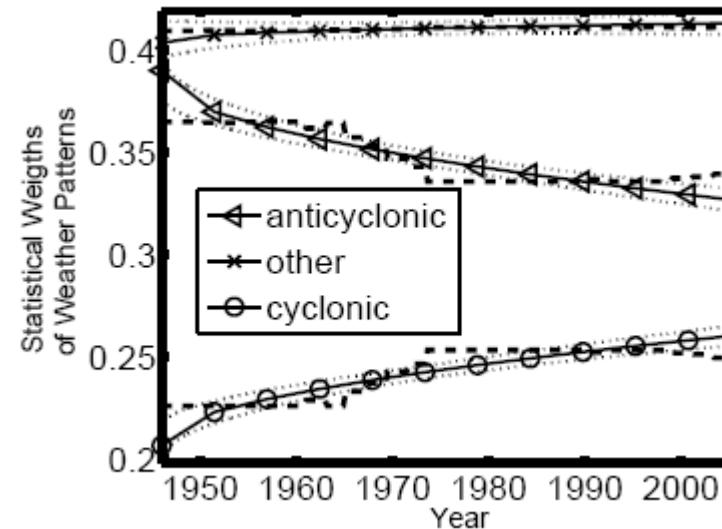
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Gaussian Kernel Estimator



FEM-Clustering vs. Single Trend



$$L(\gamma_i(t), \mathbf{T}_i, \mu_i) \rightarrow \min$$
$$g(x_t, P^i) = -\log P_{X_t, X_{t+1}}^i$$

$$x_t : X_t \rightarrow X_{t+1}$$

$$\mathbf{L}(\gamma_i(t), \mathbf{T}_i, \mu_i) \rightarrow \min$$

Example: *climatic trends* in temperatures

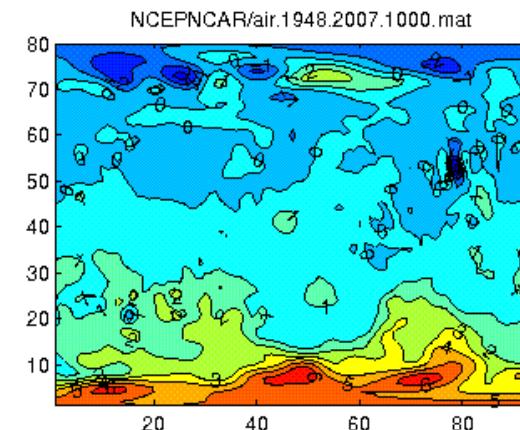
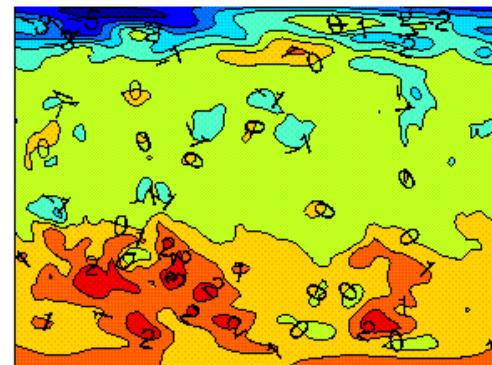
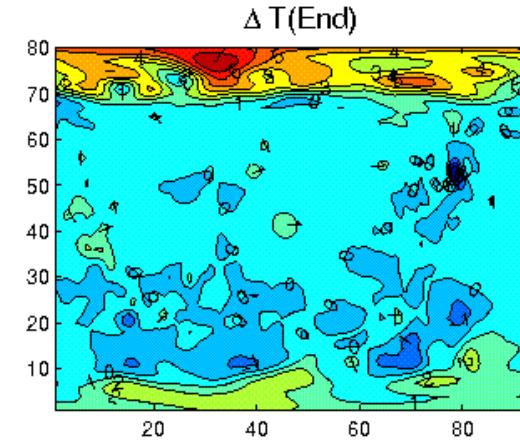
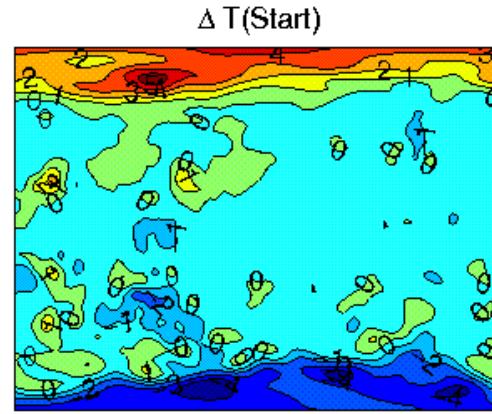


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Global Data Analysis

*Global Historical Temperature Data
(80x120 grid, daily values 1947-2007)
(Data from the NCAR, Boulder, US)*





Global Data Analysis

*Global Historical Temperature Data
(80x120 grid, daily values 1947-2007)
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