A new solution to the label switching problem of MCMC outputs

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Outline

- Independence mixture model

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- Label Switching Phenomenon

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- A mixture representation of the posterior distribution

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- Extension: Hidden Markov models and applications

Independence mixture model

- Observed data: $\boldsymbol{y} = (y_1, \ldots, y_n)$, where $y_i \in \mathbb{R}^p$
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- Component specific parameters: $\boldsymbol{\theta} = (\theta_1, \ldots, \theta_k) \in \Theta^k$
- Problem: Given k and $\boldsymbol{y}$, estimate $(\boldsymbol{\pi}, \boldsymbol{\theta})$.

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- However:

$$P(Z_i = z_i | y_i, \boldsymbol{\pi}, \boldsymbol{\theta}) = \frac{\pi_{z_i} f(y_i; \theta_{z_i})}{\sum_{j=1}^{k} \pi_j f(y_i; \theta_j)}.$$

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- Posterior distribution:

$$
\begin{aligned}
f(\boldsymbol{\pi}, \boldsymbol{\theta}|\boldsymbol{y}) &\propto L(\boldsymbol{\pi}, \boldsymbol{\theta}|\boldsymbol{y}) f(\boldsymbol{\pi}, \boldsymbol{\theta}) \Rightarrow \\
f(\boldsymbol{\pi}, \boldsymbol{\theta}|\boldsymbol{y}) &= f(\tau(\boldsymbol{\pi}, \boldsymbol{\theta})|\boldsymbol{y}), \; \forall \tau \in \mathcal{T}_k.
\end{aligned}
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Consequences: Label Switching Problem

- Marginal posterior distribution for label $j = 1, \ldots, k$:
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- "A-marginallia", i.e: $\forall i, j = 1, 2, \ldots, k$,
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  4. Label invariant loss functions (Celeux et al., 2000)

Toy Example

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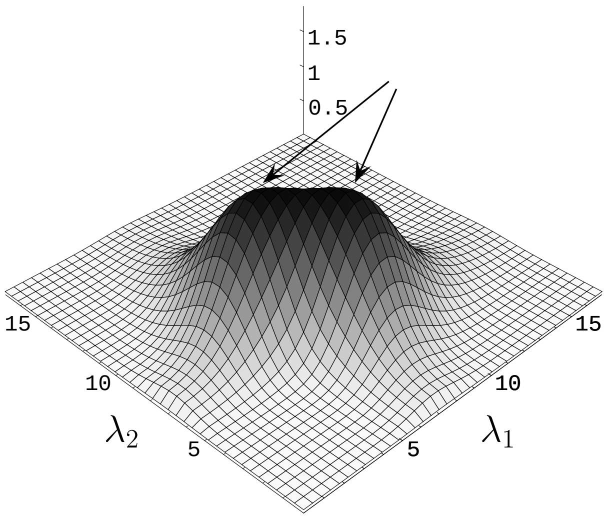
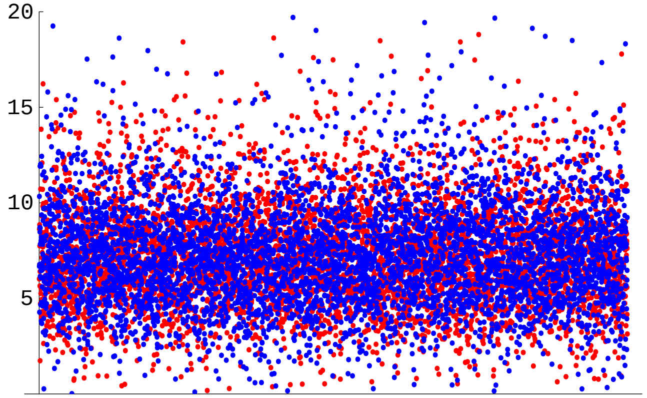


exact evaluation



Gibbs Sampler

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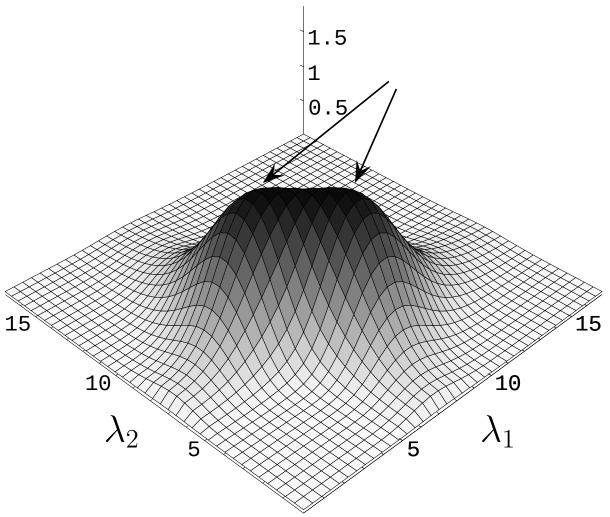

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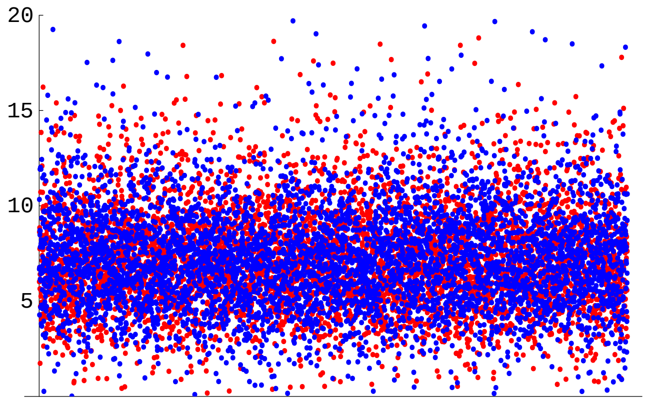

Gibbs Sampler

- How we will separate the symmetric areas?

A mixture representation of the posterior distribution

Definition 1: Let $\tau = (t_1, \ldots, t_k) \in \mathcal{T}_k$, be a permutation of the index set. The corresponding relabelling $\tau \boldsymbol{z}$ of the allocation vector $\boldsymbol{z} = (z_1, \ldots, z_n) \in \mathcal{Z} := \{1, \ldots, k\}^n$ is given by $\tau \boldsymbol{z} = (t_{z_1}, \ldots, t_{z_n}) \in \mathcal{Z}$.

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Example: Let $n = 10, k = 3, \boldsymbol{z} = \{2, 1, 2, 2, 3, 1, 2, 3, 3, 3\}$ and $\tau = \{2, 3, 1\}$. Then, $\tau \boldsymbol{z} = \{3, 2, 3, 3, 1, 2, 3, 1, 1, 1\}$.

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- Let $\Xi_{\boldsymbol{z}} = \{\tau\boldsymbol{z} : \tau \in \mathcal{T}_k\}$ be the equivalence class of $\boldsymbol{z}$ implied by the equivalence relation.

A mixture representation of the posterior distribution

- Consider now an arbitrary set $\mathcal{Z}_0$, consisting of exactly one representative from each equivalence class and let

$$f_{\mathcal{Z}_0}(\boldsymbol{\pi}, \boldsymbol{\theta}|\boldsymbol{y}) := \sum_{\boldsymbol{z} \in \mathcal{Z}_0} \frac{k!\, w(\boldsymbol{z}|\boldsymbol{y})}{(k - k_0(\boldsymbol{z}))!} f(\boldsymbol{\pi}, \boldsymbol{\theta}|\boldsymbol{y}, \boldsymbol{z}),$$

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- $f_{\mathcal{Z}_0}$ is a distribution for $(\boldsymbol{\pi}, \boldsymbol{\theta})$ with the same support as the posterior.
- $f_{\mathcal{Z}_0}$ non-symmetric.

A mixture representation of the posterior distribution

Theorem: The posterior distribution of $(\boldsymbol{\pi}, \boldsymbol{\theta})$ can be expressed as

$$f(\boldsymbol{\pi}, \boldsymbol{\theta}|\boldsymbol{y}) = \frac{1}{k!} \sum_{\tau \in \mathcal{T}_k} f_{\mathcal{Z}_0}\left(\tau(\boldsymbol{\pi}, \boldsymbol{\theta})|\boldsymbol{y}\right)$$

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Consequently: Work with the non symmetric components!

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- Let $(\boldsymbol{z}^{(i)}, (\boldsymbol{\pi}, \boldsymbol{\theta})^{(i)})$, $i = 1, 2, \ldots$ be a Markov chain with limit distribution $f(\boldsymbol{z}, \boldsymbol{\pi}, \boldsymbol{\theta} | \boldsymbol{y})$. For all i let τ_i be uniformly distributed on $\mathcal{T}_{\boldsymbol{z}^{(i)}}$. Then the limit distribution of the sequence $\tau_i^{-1}(\boldsymbol{\pi}, \boldsymbol{\theta})^{(i)}$ is $f_{\mathcal{Z}_0}(\boldsymbol{\pi}, \boldsymbol{\theta} | \boldsymbol{y})$.

The Equivalence Classes Representatives (ECR) Algorithm

- Determine $\mathcal{Z}_0$ and obtain a simulated output $(\boldsymbol{z}, \boldsymbol{\pi}, \boldsymbol{\theta})^{(i)}$, $i = 1, \ldots, M$, with target distribution $f(\boldsymbol{z}, \boldsymbol{\pi}, \boldsymbol{\theta} | \boldsymbol{y})$.

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- Use the reordered values $(\boldsymbol{\pi}', \boldsymbol{\theta}')^{(i)}$, $i = 1, \ldots, M$, in order to approximate the posterior distributions of the weights and of the component specific parameters.

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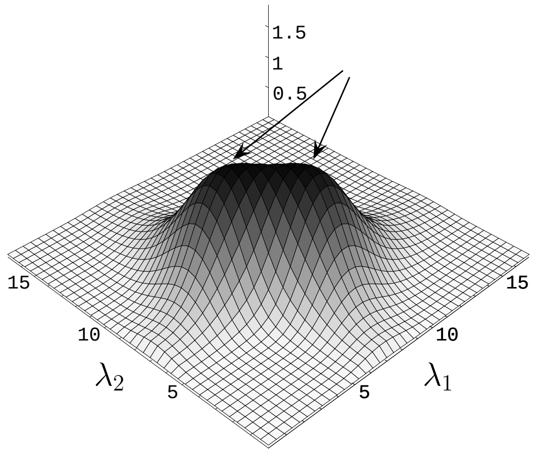
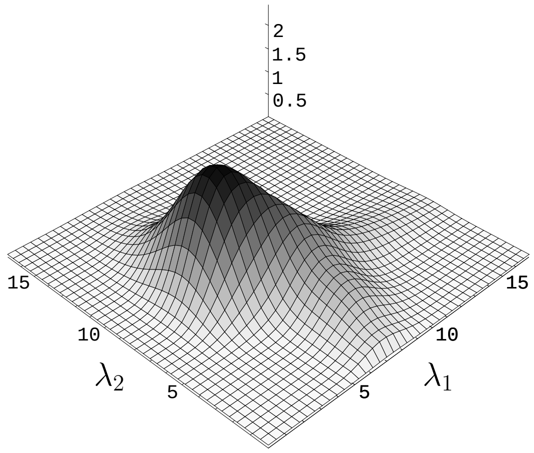
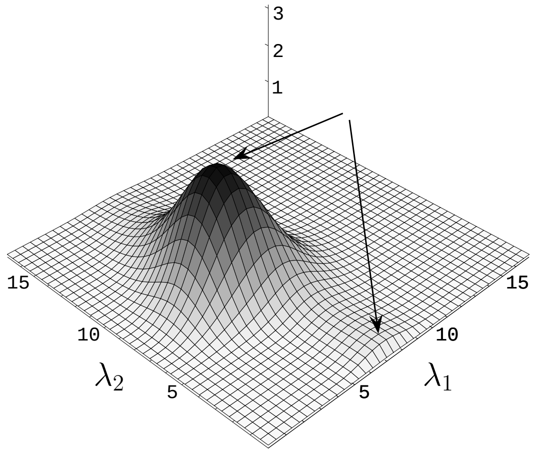


$f(\lambda_1, \lambda_2 | \boldsymbol{y})$



$f_{\mathcal{Z}_0'}(\lambda_1, \lambda_2 | \boldsymbol{y})$



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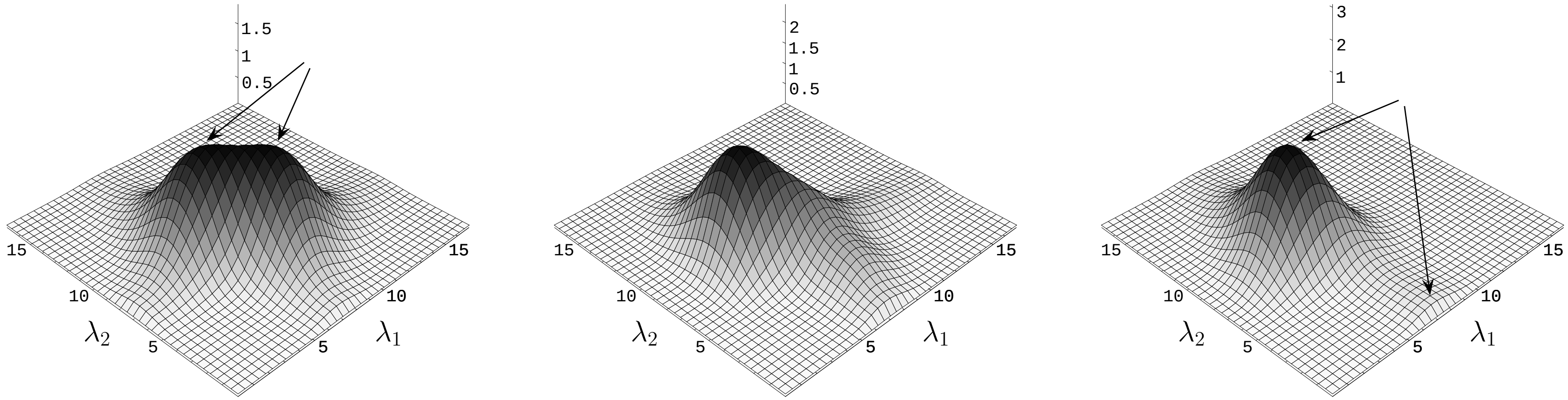
Toy Example revisited

- $\boldsymbol{y} = (6, 12, 9, 4, 6) \overset{\text{iid}}{\sim} 0.5\mathcal{P}(\lambda_1) + 0.5\mathcal{P}(\lambda_2)$.
- (Symmetric) posterior distribution of $\lambda_1, \lambda_2 | \boldsymbol{y}$:



$f(\lambda_1, \lambda_2|\boldsymbol{y})$ $\qquad f_{\mathcal{Z}'_0}(\lambda_1, \lambda_2|\boldsymbol{y})$ $\qquad f_{\mathcal{Z}_0}(\lambda_1, \lambda_2|\boldsymbol{y})$

- In $\mathcal{Z}'_0$: random selection of representatives.

Toy Example revisited

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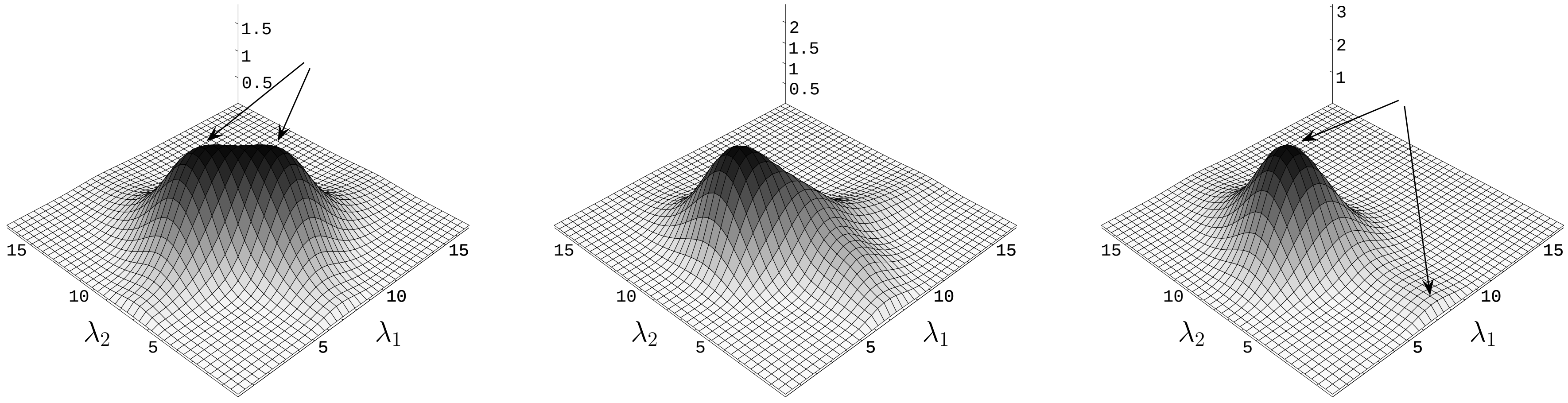

$f(\lambda_1, \lambda_2 | \boldsymbol{y})$ $\quad$ $f_{\mathcal{Z}_0'}(\lambda_1, \lambda_2 | \boldsymbol{y})$ $\quad$ $f_{\mathcal{Z}_0}(\lambda_1, \lambda_2 | \boldsymbol{y})$

- In $\mathcal{Z}_0'$: random selection of representatives.
- In $\mathcal{Z}_0$: ?

Selecting the representatives

Definition: The S similarity measure of two allocation vectors $\boldsymbol{z}_1 = (z_{11}, \ldots, z_{1n})$ and $\boldsymbol{z}_2 = (z_{21}, \ldots, z_{2n})$ is defined by $S(\boldsymbol{z}_1, \boldsymbol{z}_2) := \sum_{i=1}^{n} I(z_{1i} = z_{2i})$, where $I(A)$ is the indicator function of A.

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- $\mathcal{Z}_0 = \cup \{\tau(\Xi_{\boldsymbol{z}})\boldsymbol{z};\ \boldsymbol{z} \in \mathcal{Z}\}$.

Example: Reordering a single iteration

- Let $n = 10$, $k = 3$, $\boldsymbol{z}^{(i)} = (1, 2, 3, 3, 1, 2, 1, 3, 3, 2)$, $\boldsymbol{\pi}^{(i)} = (\pi_1^{(i)}, \pi_2^{(i)}, \pi_3^{(i)})$ and $\boldsymbol{\theta}^{(i)} = (\theta_1^{(i)}, \theta_2^{(i)}, \theta_3^{(i)})$.

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  3. $\tau = \{2, 1, 3\} \Rightarrow \tau\boldsymbol{z}^{(i)} = (2, 1, 3, 3, 2, 1, 2, 3, 3, 1)$ and $S(\tau\boldsymbol{z}^{(i)}, \hat{\boldsymbol{z}}^{\mathrm{MAP}}) = 2$.

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  6. $\tau = \{3, 2, 1\} \Rightarrow \tau\boldsymbol{z}^{(i)} = (3, 2, 1, 1, 3, 2, 3, 1, 1, 2)$ and $S(\tau\boldsymbol{z}^{(i)}, \hat{\boldsymbol{z}}^{\mathrm{MAP}}) = 3$.

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- $\tau = \{2,3,1\} \Rightarrow \tau^{-1} = \{3,1,2\}$, hence $(\boldsymbol{\pi}', \boldsymbol{\theta}')^{(i)} = \big((\pi_3^{(i)}, \pi_1^{(i)}, \pi_2^{(i)}), (\theta_3^{(i)}, \theta_1^{(i)}, \theta_2^{(i)})\big)$.

Example: Reordering a single iteration

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- In order to save computational cost, the optimal permutation can be find applying efficient integer programming algorithms (the assignment problem).

Examples: ECR vs simple methods

- $n = 160$ simulated observations from $0.10\mathcal{N}(-20, 1) + 0.65\mathcal{N}(20, 3) + 0.25\mathcal{N}(21, 0.5)$

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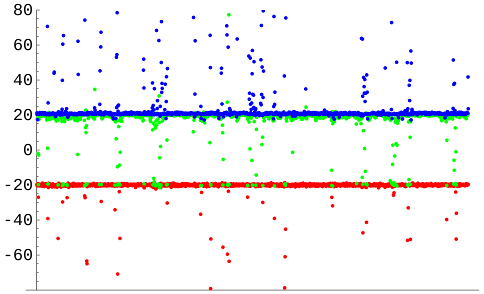
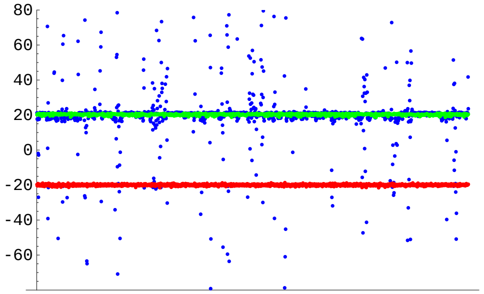
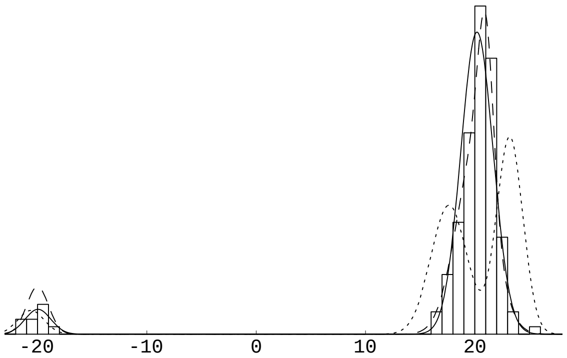


PR (Marin, et al., 2005)



ECR



Plug-in density estimate

- - - true pdf

· · · PR

— ECR

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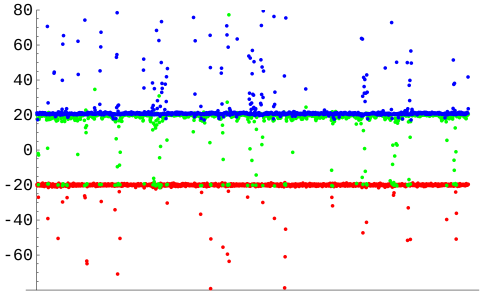
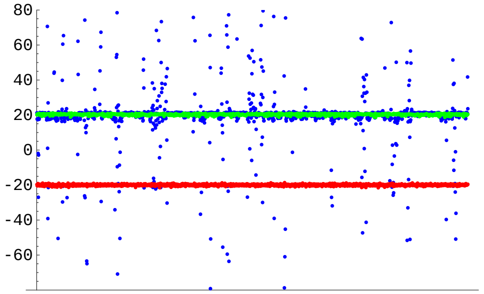
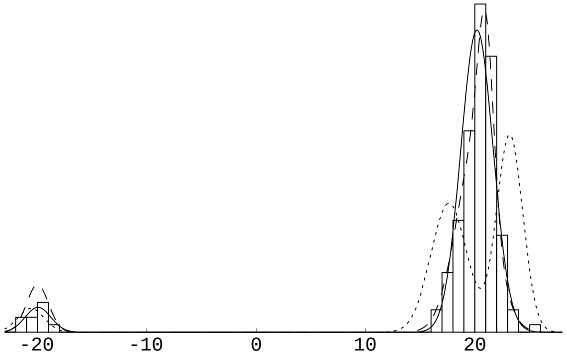
- 





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· · · PR

— ECR

	PR (Marin, et al., 2005)	ECR
$\widehat{\mathbf{E}}(\boldsymbol{\mu}\|\boldsymbol{y})$	$(23.08, 17.62, -20.59)$	$(20.46, 19.61, -19.96)$

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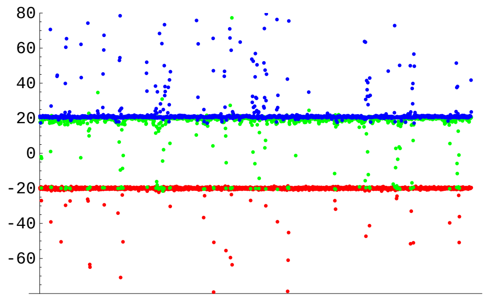
- 

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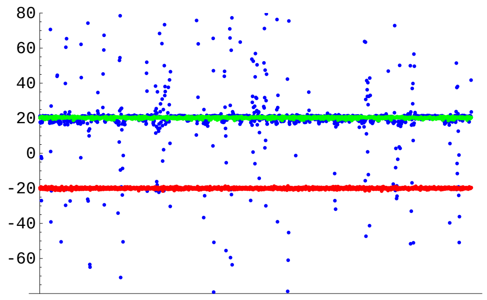
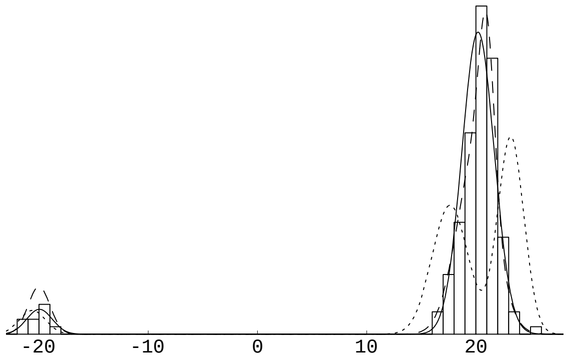
  

  ECR

  Plug-in density estimate

  - - - true pdf

  · · · PR

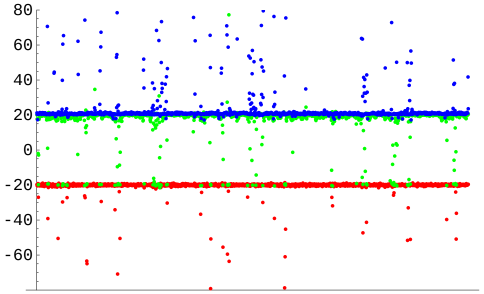
  — ECR

	PR	ECR
$\widehat{\mathbf{E}}(\boldsymbol{\mu}\vert\boldsymbol{y})$	$(23.08, 17.62, -20.59)$	$(20.46, 19.61, -19.96)$
$\widehat{\mathbf{E}}(\boldsymbol{\sigma}^2\vert\boldsymbol{y})$	$(1.83, 2.27, 1.42)$	$(2.01, 2.15, 1.36)$

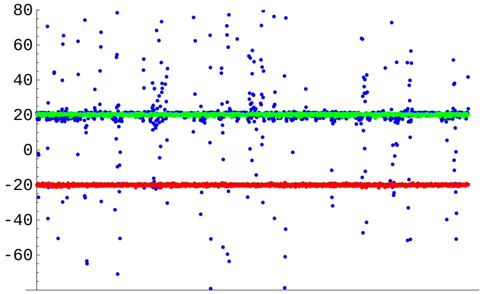
Examples: ECR vs simple methods

- $n = 160$ simulated observations from $0.10\mathcal{N}(-20,1) + 0.65\mathcal{N}(20,3) + 0.25\mathcal{N}(21,0.5)$

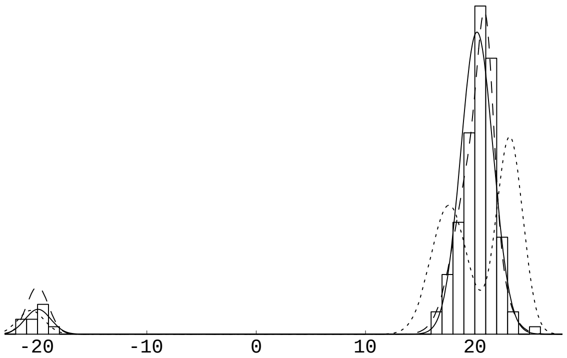
-



PR (Marin, et al., 2005)



ECR



Plug-in density estimate

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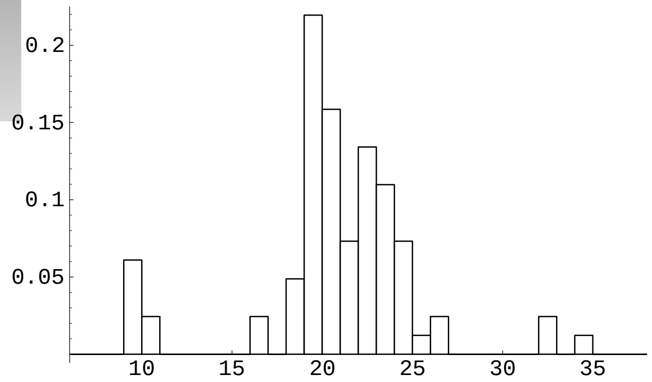
· · · PR

— ECR

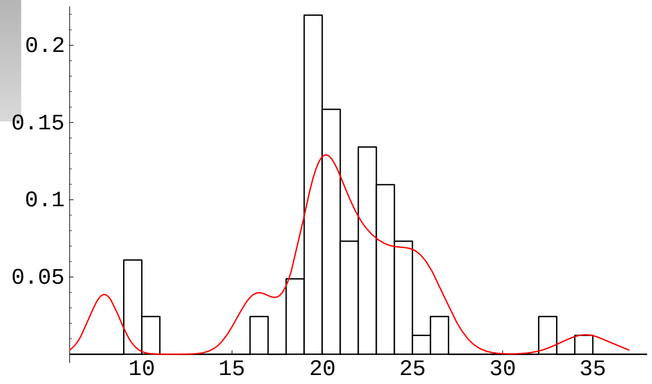
$\widehat{\mathbf{E}}(\boldsymbol{\mu}\vert\boldsymbol{y})$	$(23.08, 17.62, -20.59)$	$(20.46, 19.61, -19.96)$
$\widehat{\mathbf{E}}(\boldsymbol{\sigma}^2\vert\boldsymbol{y})$	$(1.83, 2.27, 1.42)$	$(2.01, 2.15, 1.36)$
$\widehat{\mathbf{E}}(\boldsymbol{\pi}\vert\boldsymbol{y})$	$(.522, .418, .060)$	$(.723, .216, .061)$

Univariate normal mixtures: Galaxy dataset



- $n = 82$, $k = 6$, $m = 50000$.

Univariate normal mixtures: Galaxy dataset



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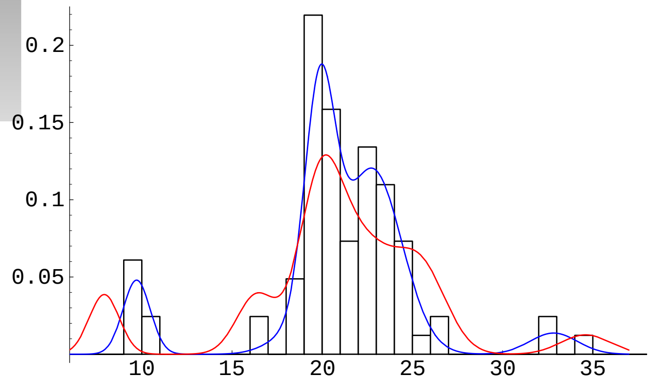
- Pivotal Reordering

Univariate normal mixtures: Galaxy dataset



- $n = 82$, $k = 6$, $m = 50000$.
- Pivotal Reordering
- Kullback - Leibler (256.68 sec)

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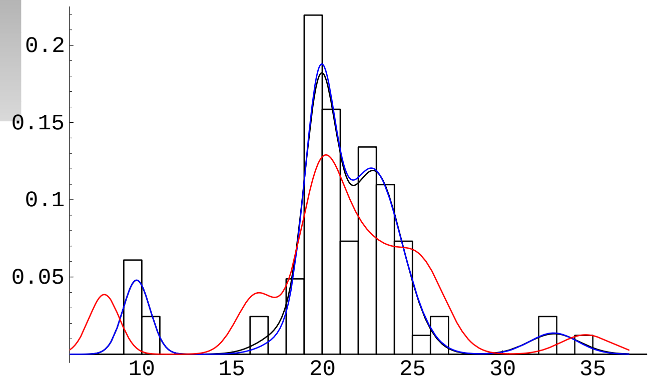


- $n = 82$, $k = 6$, $m = 50000$.
- Pivotal Reordering
- Kullback - Leibler (256.68 sec)
- ECR (1.56 sec)

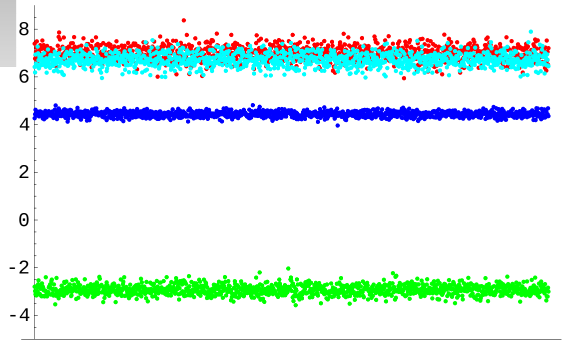
Examples: ECR vs sophisticated methods

$n = 200$ simulated observations from a $k = 4$ component mixture of bivariate normals, $m = 10000$ iterations of the multivariate random beta model (Papageorgiou and Dellaportas, 2005).

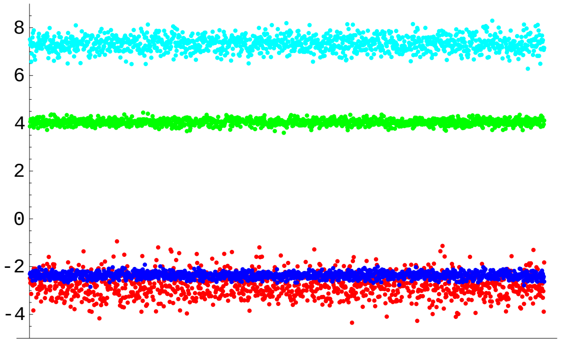
Examples: ECR vs sophisticated methods

parameter	real value	KL (Stephens, 1997)	ECR
$\boldsymbol{\pi}$	$(.25, .25, .25, .25)$	$(.30, .21, .24, .25)$	$(.30, .21, .24, .25)$
$\boldsymbol{\mu}$	$(4.5, -2.5)$	$(4.43, -2.36)$	$(4.43, -2.36)$
	$(-3.0, 4.0)$	$(-2.91, 4.04)$	$(-2.91, 4.04)$
	$(6.5, 7.0)$	$(6.73, 7.34)$	$(6.73, 7.34)$
	$(7.0, -3.0)$	$(6.99, -2.77)$	$(6.99, -2.77)$
$\boldsymbol{\Sigma}$	$\begin{pmatrix} 0.5 & -0.25 \\ -0.25 & 0.5 \end{pmatrix}$	$\begin{pmatrix} 0.54 & -0.20 \\ -0.20 & 0.81 \end{pmatrix}$	$\begin{pmatrix} 0.54 & -0.20 \\ -0.20 & 0.81 \end{pmatrix}$
	$\begin{pmatrix} 0.5 & -0.25 \\ -0.25 & 0.5 \end{pmatrix}$	$\begin{pmatrix} 1.74 & -0.77 \\ -0.77 & 0.69 \end{pmatrix}$	$\begin{pmatrix} 1.74 & -0.77 \\ -0.77 & 0.69 \end{pmatrix}$
	$\begin{pmatrix} 4 & 2.5 \\ 2.5 & 4 \end{pmatrix}$	$\begin{pmatrix} 3.30 & 2.14 \\ 2.14 & 4.09 \end{pmatrix}$	$\begin{pmatrix} 3.30 & 2.14 \\ 2.14 & 4.09 \end{pmatrix}$
	$\begin{pmatrix} 4 & 2.5 \\ 2.5 & 9 \end{pmatrix}$	$\begin{pmatrix} 3.55 & 2.27 \\ 2.27 & 10.13 \end{pmatrix}$	$\begin{pmatrix} 3.55 & 2.27 \\ 2.27 & 10.13 \end{pmatrix}$
CPU Time		16.31	0.45

Examples: ECR vs sophisticated methods



μ_{1j}



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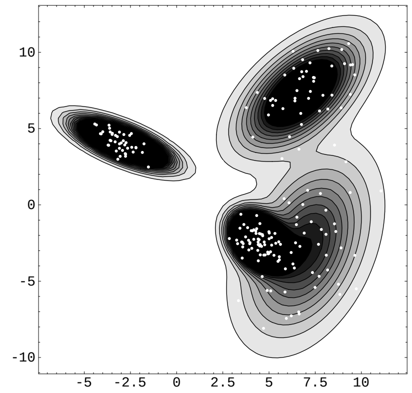

plug-in density estimate

Hidden Markov Model (HMM)

- $Z_1, \ldots, Z_n$: k-state stationary Markov chain with transition matrix $\boldsymbol{P} = (p_{ij})$, $i, j = 1, \ldots, k$, where: $P(z_t = j | z_{t-1} = i) := p_{ij}$.

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- Differences:

Independence Mixture:
For $i = 1, \ldots, n$ and $j = 1, \ldots, k$:

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$$f(\boldsymbol{\pi}, \boldsymbol{\theta} | \boldsymbol{y}) = \frac{1}{k!} \sum_{\tau \in \mathcal{T}_k} f_{\mathcal{Z}_0} \left(\tau(\boldsymbol{\pi}, \boldsymbol{\theta}) | \boldsymbol{y} \right)$$

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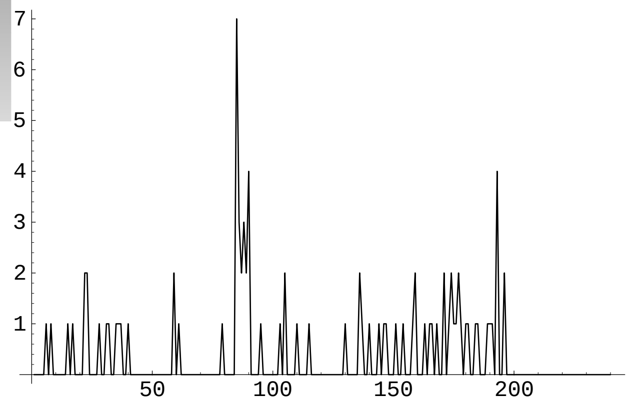
Corollary: ECR algorithm can be applied both to classic mixture models and HMM's as well!

Example: Discrete time inhomogeneus Poisson process



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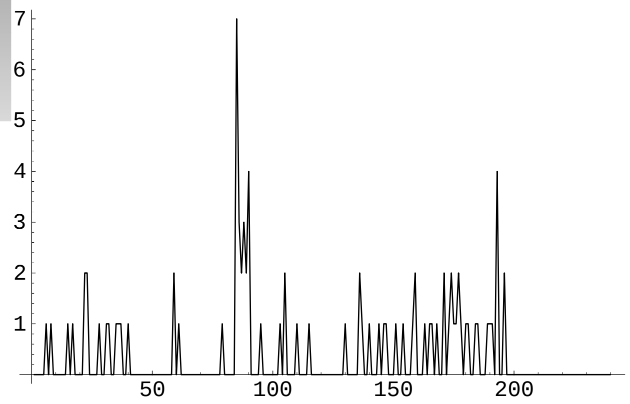

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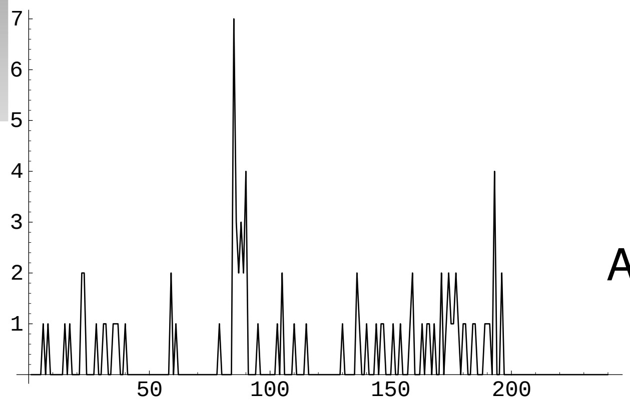

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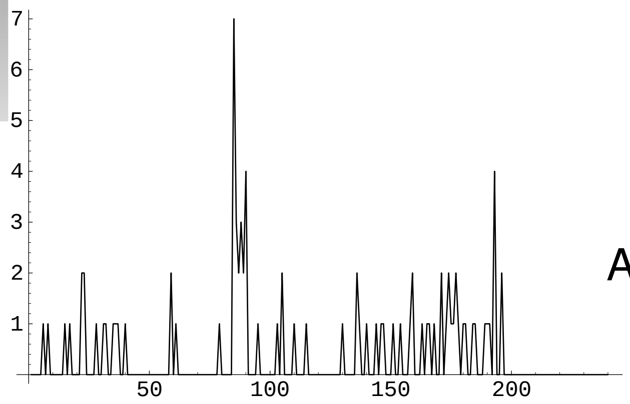

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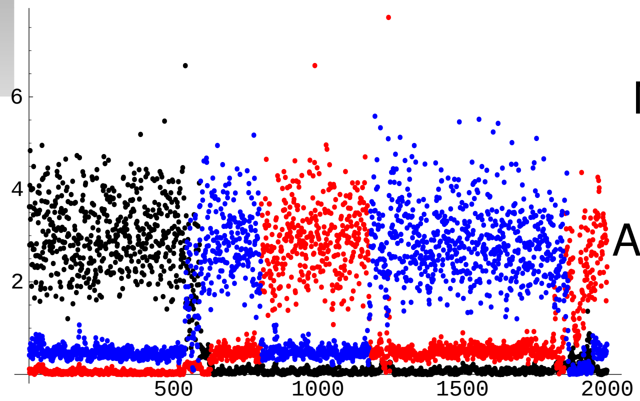
Raw output of $\lambda_1, \lambda_2, \lambda_3$



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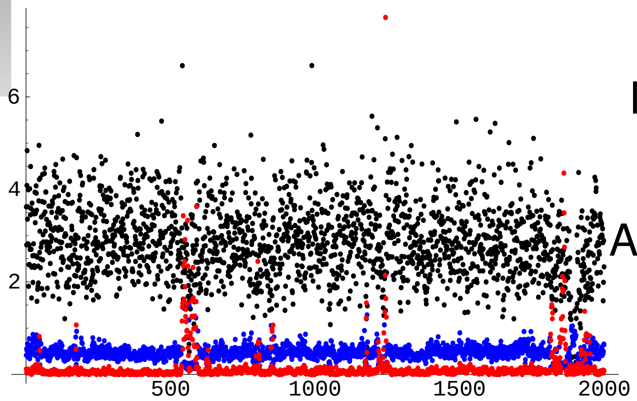

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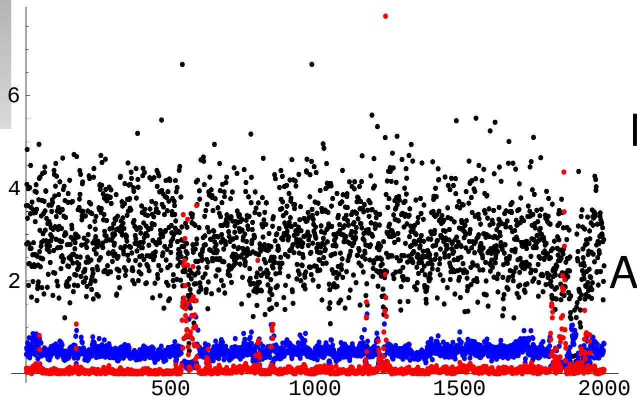

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Estimates:

$$\widehat{\mathbb{E}}(\boldsymbol{\lambda}|\boldsymbol{y}) = (0.14, 0.47, 2.85)$$

$$\widehat{\mathbb{E}}(\boldsymbol{P}|\boldsymbol{y}) = \begin{pmatrix} 0.846 & 0.113 & 0.041 \\ 0.090 & 0.883 & 0.027 \\ 0.237 & 0.199 & 0.563 \end{pmatrix}$$

Markovian Switching Autoregressive Model

Data: $y_t = 100(\log(\mathrm{GNP}_t) - \log(\mathrm{GNP}_{t-1}))$,
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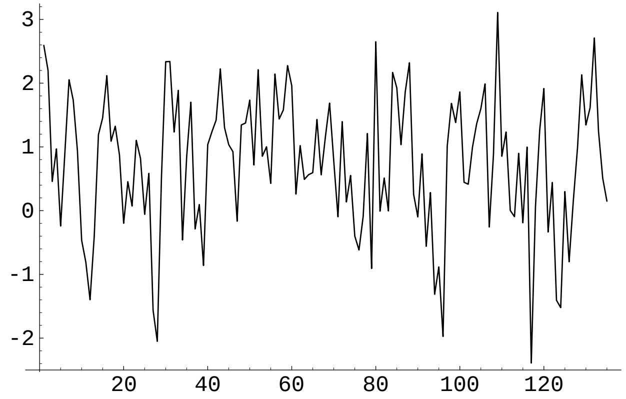

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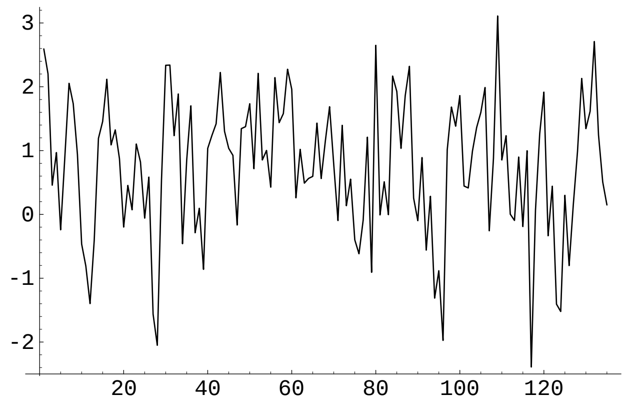

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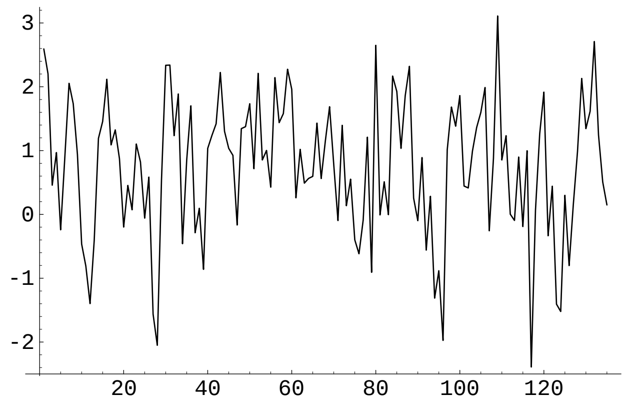

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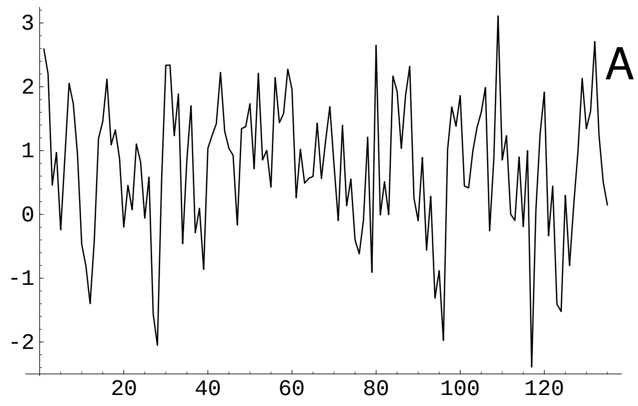
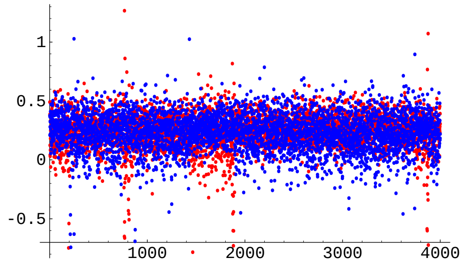


Markovian Switching Autoregressive Model

(β_{10}, β_{20})



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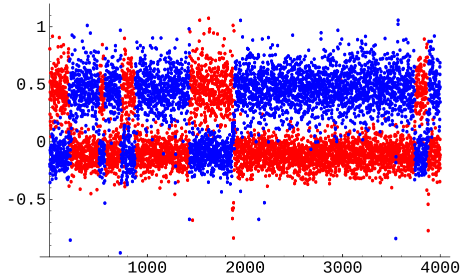

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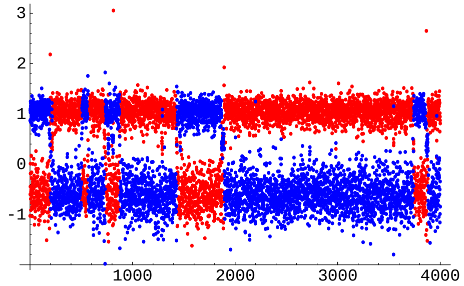

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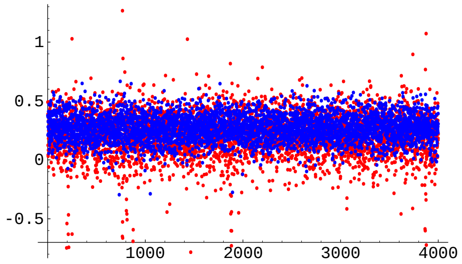

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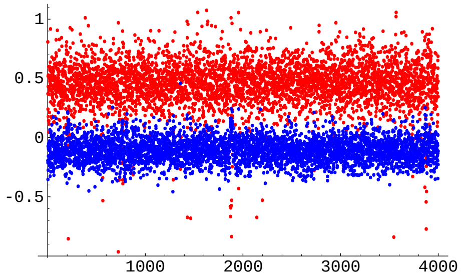

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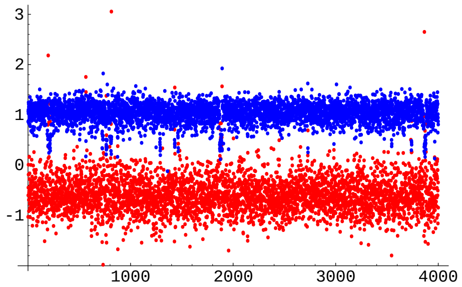

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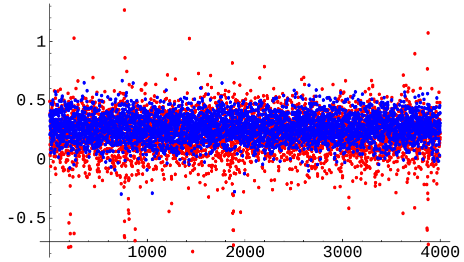

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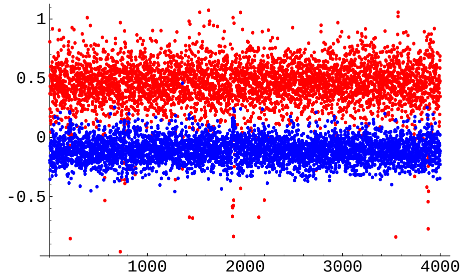

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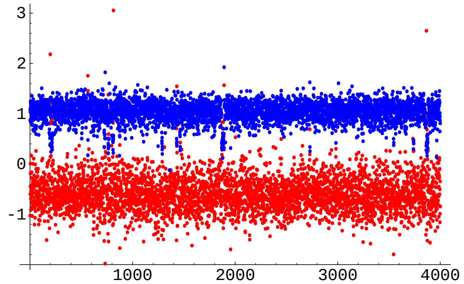

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Reordering: ECR algorithm

Estimates: $\widehat{\boldsymbol{\sigma}}^2 = (0.59, 0.53)$, $\quad \widehat{\boldsymbol{P}} = \begin{pmatrix} 0.538 & 0.462 \\ 0.277 & 0.723 \end{pmatrix}$

$$\widehat{\boldsymbol{\beta}} = \begin{pmatrix} 0.21 & 0.46 & -0.57 \\ 0.27 & -0.11 & 1.06 \end{pmatrix}$$

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  1. Theoretical background.
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