A not so short Introduction to Process Segmentation

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Outline

Introduction

- 2 The Piece-wise constant model
- 3 Computational issues for breaks positioning
- 4 Statistical properties of the estimators
- 5 Model selection for segmentation models
- 6 The Bayesian Strategy
- 7 Change points detection for dependent data

Segmentation models: definitions and notations

• We observe $\{y_1, \ldots, y_n\}$ a sequence of data modeled by a random process $\mathbf{Y} = \{Y_1, \ldots, Y_n\}$ with

$$Y_t \sim f(\theta_t).$$

- We suppose that there exists K + 1 change-points $t_0 = 1 < \ldots < t_K = n$ such that θ_t is constant between two changes and different from a change to another.
- *I_k* =]*t_{k-1}*, *t_k*]: interval of stationarity, *θ_k* the parameter between two changes:

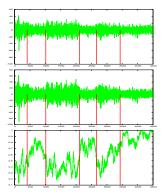
$$\forall t \in I_k, \ Y_t \sim f(\theta_k)$$

• θ can stand for the mean, variance, spectrum, etc...

Process Segmentation vs. Online Change point detection

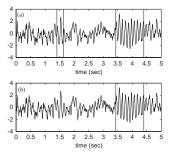
- Sequential observations: the detection of a change should be done with past observations only
- Example: quality control, earthquake detection, ...
- Main Reference: Basseville & Nikiforov (93) [3]
- Sequential analysis (mainly based on tests)

- Econometrics [17, 16]
- Medical Imagery [18]
- Climate series [22]
- Biology (sequence segmentation [6, 5], microarrays [25])



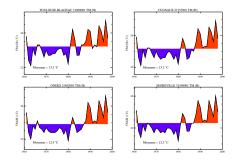
Market prices segmentation [19]

- Econometrics [17, 16]
- Medical Imagery [18]
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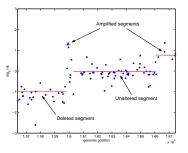
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- Econometrics [17, 16]
- Medical Imagery [18]
- Climate series [22]
- Biology (sequence segmentation [6, 5], microarrays [25])



Array CGH segmentation [25]

Main contributors (non exhaustive) !

- P. Perron (Boston University)
- T.L. Lai (Stanford University)
- D. Siegmund (Stanford University)
- P. Fearnhead (Lancaster University)
- P. Green (Bristol University)
- M. Lavielle (INRIA, Orsay)
- E. Lebarbier (AgroParisTech)

Outline of the presentation

- How to build the model ?
- How to estimate the parameters and the location of the breaks ?
- Properties of the breaks estimators ?
- How many breaks ?
- How to deal with dependent observations ?
- The Bayesian Perspective

Outline



2 The Piece-wise constant model

3 Computational issues for breaks positioning

- 4 Statistical properties of the estimators
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A piece-wise constant regression

• We observe a Gaussian process (iid) $\mathbf{Y} = \{Y_1, \dots, Y_n\}$ with

$$Y_t \sim \mathcal{N}(\mu_t, \sigma^2).$$

- We suppose that there exists K + 1 change-points $t_0 < \ldots < t_K$ such that the mean of the signal is constant between two changes and different from a change to another.
- *I_k* =]*t_{k-1}*, *t_k*]: interval of stationarity, μ_k the mean of the signal between two changes:

$$\forall t \in I_k, \ Y_t = \mu_k + E_t, \ E_t \sim \mathcal{N}(0, \sigma^2).$$

Generalization to piece-wise linear regressions

- The parameter subject to changes can be $\mathbb{E}(Y(t))$ and/or $\mathbb{V}(Y(t))$
- The model is extended to piece-wise linear regression
- *I_k* =]*t_{k-1}*, *t_k*]: interval of stationarity, *θ_k* the set of parameters between two changes:

$$orall t \in I_k, \ \ Y_t = \sum_{j_1}^{p} heta_j^k x_j(t) + E_t, \ \ E_t \sim \mathcal{N}(0, \sigma^2).$$

• Difference with splines: no continuity constraint at the breaks

Parameters and estimation strategy

- The parameters: $\mathbf{t} = \{t_0, \dots, t_K\}$, $\boldsymbol{\mu} = \{\mu_1, \dots, \mu_K\}$ and σ^2 .
- The estimation is done for a given K which is estimated afterwards.
- The log-likelihood of the model is:

$$\log \mathcal{L}_{\mathcal{K}}(\mathbf{Y}; \mathbf{t}, \boldsymbol{\mu}, \sigma^2) = \sum_{k=1}^{\mathcal{K}} \sum_{t=t_{k-1}+1}^{t_k} f(y_t; \mu_k, \sigma^2).$$

- When K and \mathbf{t} are known, how to estimate μ ?
- When K is known, how to estimate t?
- How to choose K ?

Penalized contrast estimators

• Penalized contrast estimators are of the form:

$$(\hat{\mathbf{t}}, \hat{\boldsymbol{ heta}}) = \arg\min_{\mathbf{t}, \boldsymbol{ heta}} \left\{ J_{\mathcal{K}}(\mathbf{Y}; \mathbf{t}, \boldsymbol{ heta}) - \beta \mathsf{pen}(\mathbf{t}) \right\}$$

- $J_{\mathcal{K}}(\mathbf{Y}; \mathbf{t}, \boldsymbol{\theta})$: to assess the quality of fit of the model
 - locate the changepoints as accurately as possible.
 - Can be broken down into local contrast (log-likelihoods)

$$J_{\mathcal{K}}(\mathbf{Y};\mathbf{t},\boldsymbol{ heta}) = \sum_{k} \log \ell(Y[t_{k-1}:t_k]; heta_k)$$

- pen(t) only depends on K (increases with K)
- β establishes a trade-off between the contrast and the penalty

Parameter estimation

• When K and t are known the estimation of μ is straightforward:

$$\widehat{\mu}_{k} = \frac{1}{\widehat{t}_{k} - \widehat{t}_{k-1}} \sum_{t=\widehat{t}_{k-1}+1}^{\widehat{t}_{k}} y_{t},$$

$$\widehat{\sigma}^{2} = \frac{1}{n} \sum_{k=1}^{K} \sum_{t=\widehat{t}_{k-1}+1}^{\widehat{t}_{k}} (y_{t} - \widehat{\mu}_{k})^{2}.$$

• Find \widehat{t} such that:

$$\widehat{\mathbf{t}} = \arg \max_{\mathbf{t}} \left\{ \log \mathcal{L}_{\mathcal{K}}(\mathbf{Y}; \mathbf{t}, \boldsymbol{\mu}, \sigma^2) \right\}.$$

Outline



2) The Piece-wise constant model

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Dynamic Programming to optimize the log-likelihood

- Partition *n* data points into *K* segments: complexity $\mathcal{O}(n^K)$.
- DP reduces the complexity to $\mathcal{O}(n^2)$ when K is fixed.
- Analogy with the shortest path problem:
 - "subpaths of optimal paths are themselves optimal"
- $RSS_k(i,j)$ cost of the path connecting *i* to *j* in *k* segments:

$$\begin{aligned} \forall 0 \le i < j \le n, \ \mathsf{RSS}_1(i,j) &= \sum_{t=i+1}^j (y_t - \bar{y}_{ij})^2, \\ \forall 1 \le k \le K - 1, \ \mathsf{RSS}_{k+1}(1,j) &= \min_{1 \le h \le j} \{\mathsf{RSS}_k(1,h) + \mathsf{RSS}_1(h+1,j)\}. \end{aligned}$$

Dynamic Programming on very large signals ?

- Even if DP reduces the computational burden to $\mathcal{O}(n^2)$ it may be problematic when $n\sim 10^6$
- Constraint the length of segments (Imin, Imax)
- Sequential strategies (Bayesian [13])
- Use the LARS framework [4]
- Find a trick to the trick to decrease the complexity of DP [26]

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Breaks estimator convergence

- Let $au = \{0 < \tau_0 < \ldots < \tau_K < 1\}$ and au^* the sequence of (true) normalized change points
- Let $\theta \in \mathbb{R}^d$ and θ^* be the (true) parameter subject to changes the true vector of parameters
- Let $\hat{\boldsymbol{\tau}}_n$ and $\hat{\theta}_n$ be minimum contrast estimators
- If K is known, then under very mild conditions [17]

$$(\hat{\boldsymbol{ au}}_n, \hat{ heta}_n) \stackrel{
ightarrow}{ op} (\boldsymbol{ au^{\star}}, heta^{\star})$$

- Note that the rate of convergence of $\hat{\tau}_n$ is n
- If K is unknown, convergence depends on $\beta_n \text{pen}(\mathbf{t})$ (Ex: $K \log(n)/2$)
- More generally β_n should tend to 0 at an appropriate rate
- Results include strongly mixing and strongly dependent processes [17]

Limit Distribution for the breaks-1

• Central Ingredient to get results ($\delta_k = \mu_{k+1} - \mu_k$)

$$orall \epsilon > 0, \ \exists \mathcal{C} < \infty, \ \mathbb{P}\left\{ n | \hat{t}_k - t_k^\star | < \mathcal{C} / \delta_k^2
ight\} < \epsilon$$

• For one break $t_1, \delta = \mu_2 - \mu_1$, and t_1 lies in a compact set

$$\{|t_1 - t_1^\star| < C\delta^{-2}\}$$

• Recall that $\hat{t}_1 = \arg\min\{RSS(t_1)\} = \arg\max\{RSS(t_1^*) - RSS(t_1)\}$

$$RSS(t_1^0) - RSS(t_1) = \begin{cases} -\delta^2(t_1^{\star} - t_1) + 2\delta \sum_{t_1+1}^{t_1^{\star}} \epsilon_t + o_p(1) \\ -\delta^2(t_1 - t_1^{\star}) - 2\delta \sum_{t_1^{\star}+1}^{t_1} \epsilon_t + o_p(1) \end{cases}$$

• The distribution of these sums depends on t₁

Limit Distribution for the breaks-2

• Let us define W such that W(0) = 0 and

$$W(m) = \begin{cases} -\delta^2 m + 2\delta \sum_{t=m+1}^{0} \epsilon_t, \text{ for } m > 0\\ -\delta^2 m + 2\delta \sum_{t=1}^{m} \epsilon_t, \text{ for } m < 0 \end{cases}$$

• Assuming a stricly stationary distribution for $\{\epsilon_t\}$ then

$$RSS(t_1^\star) - RSS(t_1) = W(t_1 - t_1^\star) + o_{
ho}(1)$$

• Using conditions (on ϵ_t) that ensure a unique max for W then

$$\hat{t}_1 - t_1^\star \mathop{
ightarrow}_d rg \max_m W(m)$$

• More general results can be found in the litterature [29, 23]

Confidence intervals for break dates

- Results use limit distributions, but may be difficult to handle in practice [30]
- Many techniques use likelihood ratios and sequential analysis [27, 28, 8]
- Resampling strategies are difficult to define in the case of multiple changes [15]
- Bayesian strategies are more suitable for confidence assessment in the case of multiple changes

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Penalized contrasts to estimate the number of segment

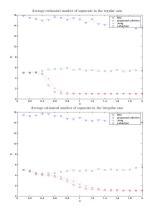
• The number of segments K should be estimated:

$$\widehat{\mathcal{K}} = rg\max_{\mathcal{K}} \left\{ \log \mathcal{L}_{\mathcal{K}}(\mathbf{Y}; \widehat{\mathbf{t}}, \widehat{\mu}, \widehat{\sigma}^2) - eta \mathsf{pen}(\mathcal{K})
ight\}.$$

- Main difficulty: breakpoints are discrete parameters
 - the likelihood is not differentiable wrt t
 - C_{n-1}^{K-1} possible segmentations for a model with K segments.
 - how to define the dimension of the model ?
- How to define pen(K) ?
- How to define β ?

Comparison of segmentation results

Criterion	pen(K)	β
AIC	2 <i>K</i>	1
BIC	2 <i>K</i>	$\log(n)/2$
Lavielle	2 <i>K</i>	adaptive
mBIC	$f(K, \sum_k \log n_k)$	$\log(n)/2$
Lebarbier	$c_1 + \overline{c_1 \log(n/K)}$	adaptive



Simulations [25] and $\hat{K} = f(\sigma)$ with $K^{\star} = 5$

Construction of a Bayesian Criterion mBIC [31]

• Define \mathcal{M}_K the segmentation model with K segments, then

$$\mathsf{mBIC}(\mathcal{K}) = \frac{\mathsf{log}\,\mathsf{Pr}\{\mathbf{Y}|\mathcal{M}_{\mathcal{K}}\}}{\mathsf{Pr}\{\mathbf{Y}|\mathcal{M}_0\}}$$

- Derive an asymptotic approximation of the Bayes factor
- Use asymptotic results $\lim_{n\to\infty} t_k/n = \tau_k$ and a prior for au of the form:

$$\pi(\boldsymbol{ au}) = g(\boldsymbol{ au})/n^{\mathcal{K}}, \ \mathcal{C}_1 < \max g(\boldsymbol{ au}) < \mathcal{C}_2$$

• In the case σ^2 known we get:

$$\mathsf{mBIC}(K) = SSB(\hat{\mathbf{t}}) - \sum_{k} \log(\hat{t}_{k+1} - \hat{t}_{k}) + (0.5 - K)\log(n) + O_p(1)$$

Penalty function in a non asymptotic framework-1

- Consider the regression: $Y(t) = s(t) + \epsilon(t)$
- Define S_m the set of piece-wise constant functions on partition m = {I_k}_{k=1,Km}:

$$\mathcal{S}_m = \left\{ u = \sum_{k=1}^{K_m} u_k \mathbb{I}\{I_k\}, (u_k)_k \in \mathbb{R}^{K_m} \right\}$$

• The approach of Birge-Massart is to consider that $s \notin S_m$ but that S_m is just an approximation set

Penalty function in a non asymptotic framework-2

- Define \bar{s}_m the projection of s on S_m : it is an approximation of s but is unknown
- Define \hat{s}_m the estimator of \bar{s}_m in \mathcal{S}_m whose quadratic risk is $\mathbb{E}\|s-\hat{s}_m\|^2$
- This risk can be broken down such that (bias/variance trade-off)

$$\mathbb{E}\|\boldsymbol{s} - \hat{\boldsymbol{s}}_m\|^2 = \mathbb{E}\|\boldsymbol{s} - \bar{\boldsymbol{s}}_m\|^2 + \mathbb{E}\|\bar{\boldsymbol{s}}_m - \hat{\boldsymbol{s}}_m\|^2$$

- Bias term: $\mathbb{E}||s \bar{s}_m||^2$ measures the distance of the unknown s to its approximator \bar{s}_m in S_m
- Variance term: $\mathbb{E} \| \bar{s}_m \hat{s}_m \|^2$ measures the quality of estimation
- The ideal estimator will achieve the best Bias/Variance trade-off

Penalty function in a non asymptotic framework-3

• In the case of process segmentation, this framework leads to a penalty of the form[21]

$$eta imes \mathsf{pen}(K) = rac{K}{n} \sigma^2 \left(c_1 + c_2 \log rac{n}{K}
ight)$$

- (c_1, c_2) to be calibrated and σ^2 to be estimated
- Emipirical behavior: minimization of the risk can lead to a lack of power in detection

Using the Slope heuristic-1

- General heuristic that is very effective and easy to implement in practice
- Idea: construct the sequence of β_i using {(pen(K_i), J_{K_i})} the convex hull of the set {(pen(K), J_K)}

$$eta_i = rac{J_{\mathcal{K}_i} - J_{\mathcal{K}_{i+1}}}{\mathsf{pen}(\mathcal{K}_{i+1}) - \mathsf{pen}(\mathcal{K}_i)}$$

- Look at the length *l_i* of intervals [*β_i*, *β_{i+1}*] and retain the value(s) of *K_i* such that *l_j* >> *l_i*: find the "biggest jump" of dimension
- Strategy close to L-curve strategies [18]

Using the Slope heuristic-2

Normalize J_K s.t. (average slope=-1)

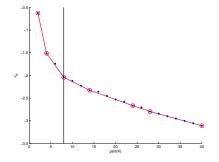
$$\widetilde{J}_{\mathcal{K}} = rac{J_{\mathsf{Kmax}} - J_{\mathcal{K}}}{J_{\mathsf{Kmax}} - J_1}(\mathsf{Kmax}\!-\!1)\!+\!1$$

• Use the empirical second derivative

$$D_{K}^{2} = \widetilde{J}_{K-1} - \widetilde{J}_{K} + \widetilde{J}_{K+1}$$

• Choose the best K(S) s.t.

$$\hat{K}(S) = \arg \max\{D_K^2 > S\}$$



blue line: contrast, red line: convex hull

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Change points detection for dependent data

Principle of the Bayesian view of process segmentation

• Model determination using hierarchical modelling:

$$\mathsf{Pr}\{\mathbf{Y}, \boldsymbol{\mu}, \boldsymbol{K}\} = \mathsf{Pr}\{\boldsymbol{K}\} \times \mathsf{Pr}\{\boldsymbol{\mu}|\boldsymbol{K}\} \times \mathsf{Pr}\{\mathbf{Y}|\boldsymbol{\mu}, \boldsymbol{K}\}$$

- Change-points {t_k}_k are considered as random variables with distribution π(t; λ, K)
- The objective : recover the *posterior* distribution: $\pi(\mathbf{t}|\mathbf{Y}, \boldsymbol{\mu}, \sigma^2, K)$
- Considering random variables makes some issues easier to assess: confidence intervals, dependent data, uncertainty about model choice
- Computationnaly intensive: MCMC, Hasting Metropolis, Reversible Jump, Forward-Backward Recursions

The multiple change point problem and the Reversible Jump algorithm-1 [14]

- Suppose that the number of segments is $K \sim \mathcal{P}(\lambda)$
- With K given, breaks positions are uniformely distributed on [0; n]:

$$t_1 < \ldots < t_K | K \sim \mathcal{U}[0; n]$$

• Then the mean of each segment $\{\mu_k\}_k$ are *iid* s.t.:

$$\boldsymbol{\mu} | \mathbf{t}, \boldsymbol{K} \sim \boldsymbol{\Gamma}(\alpha, \beta)$$

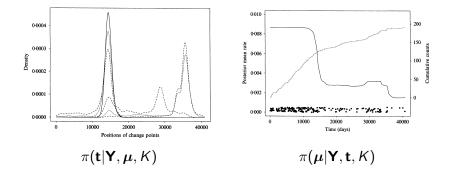
• RJ-MCMC is used to compute $\pi(K, \mathbf{t}, \boldsymbol{\mu} | \mathbf{Y})$

The multiple change point problem and the Reversible Jump algorithm-2 [14]

- The target distribution is $\pi(K, \mathbf{t}, \boldsymbol{\mu} | \mathbf{Y})$
- Dimension of the model change according to *K*: how to design appropriate moves ?
 - a change to the mean of a randomly chosen segment
 - b change of a position of a randomly chosen break
 - c 'birth' of a new segment at a randomly chosen location on [0, n]
 - d 'death' of a randomly chosen segment

The Bayesian Strategy

Posterior inference of change-points location



Limitations of the RJ-MCMC algorithm

- Jumps in dimension lead to very demanding algorithms
- The posterior of the mean is very smooth: not in accordance with the "abrupt-changes" model
- Reparametrization of the model with $\mathbf{r} = \{r_t\}$, a sequence of length n s.t.:

$$\{r_t = 1\}$$
 if $t = t_k$

• Use a temperature parameter during the Hastings-Metropolis algorithm to discriminate the local and global maxima of the posterior

A new formulation of the Bayesian change-point problem [20]

- $r_t \sim \mathcal{B}(\lambda)$, and $K = \sum_t r_t \sim \mathcal{B}(n-1,\lambda)$
- The sequence **r** is of fixed length: no need of jumps in dimension to assess $\pi(\mathbf{r}|\mathbf{Y})$
- The model on **Y** is unchanged:

$$\forall t \in I_k \ Y_t \sim \mathcal{N}(\mu_k, \sigma^2)$$

• The sequence of means μ_k is modelled s.t.

$$oldsymbol{\mu} \sim \mathcal{N}(\mathbf{m}; s^2)$$

Back to penalized constrast estimators

 For any configuration of change-points the posterior distribution of r is

$$\pi(\mathbf{r}|\mathbf{Y}; \boldsymbol{\theta}) \propto \exp\left\{-\phi RSS(\mathbf{r}, K_r) - \gamma K_r\right\}$$

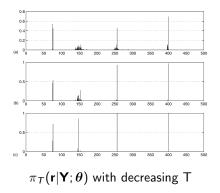
- This is the *joint* distribution of a vector of size n-1
- The MAP estimator of **r** is a penalized contrast estimator !
- This posterior distribution can be computed with a Hastings-Metropolis algorithm
- Use SAEM [9] to estimate heta the set of hyperparameters

Running the H-M algorithm at low temperature

- Strategy inspired from Simulated Annealing algorithms
- Introduce a temperature parameter T s.t. $\pi_T(\mathbf{r}|\mathbf{Y}; \boldsymbol{\theta})$ changes to

$$\exp\left\{-\frac{\phi}{T}RSS(\mathbf{r},K_r)-\frac{\gamma}{T}K_r\right\}$$

 When T → 0, π_T(r|Y; θ) CV to the uniform distribution of the seg of global maxima of π(r|Y; θ)



Running the H-M algorithm at low temperature

- Difficulties in using MCMC: how to design moves (between different models) which enable the MCMC algorithm to mix well, and being able to detect convergence of the chain.
- Idea: use recursions inspired from the Forward-Backward algorithm [12]
- Objective : perform direct simulation from the posterior distribution of **t** and *K*

Using point process to describe the sequence of changes

- Introduce some dependency among change-points $\pi(t_k|t_{k-1})$
- Introduce a point-process on integers with g(t) > 0 the time between two successive points (product-partition model)
- G(t) = ∑^t_{s=1} g(s) is the distribution function of the distance bewteend two successive points (g₀(t) the mass function of the first point after 0) then

$$\pi_{\mathcal{K}}(\mathbf{t}) = g_0(t_1) \left(\prod_{k=2}^{\mathcal{K}} g(t_k - t_{k-1})\right) (1 - G(t_{k+1} - t_k))$$

• Suppose a Negative Binomial distribution for g(t) (discrete version of Gamma distributions, k = 1 leads to Markov distrib.)

$$g(t) = \mathcal{C}_{t-k}^{k-1} p^k (1-p)^{t-k}$$

F. Picard (CNRS-LBBE)

Basic Recursions

- Define $\forall s \ge t \ P(t,s) = \Pr\{Y_{t:s} | t, s \text{ in the same segment}\}$
- Define $Q(t) = \Pr{Y_{t:n} | \text{changepoint at } t 1}$

$$Q(t) = \sum_{s=t}^{n-1} P(t,s)Q(s+1)g(s+1-t) + P(t,n)(1-G(n-t))$$

• Then the posterior distribution of the change points is:

 $\Pr\{t_k|t_{k-1}, Y_{1:n}\} = P(t_{k-1}+1, t_k)Q(t_k+1)g(t_k-t_{k-1})/Q(t_{k-1}+1)$

Model selection using posterior distributions

• Model selection can be performed using

$$\pi(K|Y_{1:n}) \propto \pi(K)\pi(Y_{1:n}|K)$$

- ${\ensuremath{\bullet}}$ Redefine the recursion conditioning by K
- Define $Q_j^K(t) = \Pr\{Y_{t:n}|t_j = t 1, K\}$

$$Q_j^K(t) = \sum_{s=t}^{n-K+j} P(t,s) Q_{j+1}^K(s+1) \pi_K(t_j = t-1|t_{j+1} = s)$$

Finally

$$\Pr\{Y_{1:n}|K\} = \sum_{s=1}^{n-K} P(1,s)Q_1^K(s+1)$$

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The piece-wise AutoRegressive Model [16]

• Piece-wise constant volatility and regression parameters $\theta_t = (\mu_t, \alpha_{\bullet,t})^T$:

$$Y_t = \mu_t + \sum_{s=1}^k \alpha_{s,t} Y_{t-s} + \sigma_t \epsilon_t \ t > k$$

- The jump process is modeled with r_t s.t. $r_t \sim \mathcal{B}(p)$
- Denoting by (Z_t^T, γ_t) the set of new parameters:

$$(\theta_t^T, \sigma_t) = (1 - r_t) \times (\theta_{t-1}^T, \sigma_{t-1}) + r_t \times (Z_t^T, \gamma_t),$$

• Forward-Backward recursions are used to calculate:

$$\mathbb{E}(\boldsymbol{\theta}_n^T, \sigma_n | Y_{1:n})$$

Conclusions & perspectives

- Very old/wide subject !!!
- Sequential analysis are taking some new importance due to the increase in the size of the datasets
- Other projects involve the segmentation of many series [10, 24, 1, 7]
- Towards semi parametric models and links with functional data [24, 2, 11]
- Slides @ http://pbil.univ-lyon1.fr/members/fpicard/



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