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On the Estimation of conditional quantiles.

Véronique Maume-Deschamps contains joint works with Kevin Elie-Dit-Cosaque, Didier Rullière and Antoine Usseglio-Carleve.

Mascotnum 2021 meeting





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- Quantile Oriented Sensitivity indices
- Computing / estimating conditional quantiles
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Why conditional qua	ntiles?			
Quantiles				

Quantile is widely used as a risk measure (VaR). Recall: for X a random variable (a risk) with distribution function F_X ,

- $q_{\alpha}(X) = \operatorname{VaR}_{\alpha}(X) = \inf\{t \ / \ F_X(t) \ge \alpha\} = F_X^{-1}(\alpha),$
- RiskMetrics popularized the use of VaR as a risk measure (1994).
- Basel Committee : Internal approach to capital management using VaR (1996),

Many natural examples where conditional quantiles are relevant: some variables are better known than others, you may estimate quantiles of the later knowing the first ones. Quantile Oriented Sensitivity Analysis (QOSA).

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Why conditional qua	ntiles?			
A financia	al example			

Consider four assets: iShares Core U.S. Aggregate Bond ETF, PowerShares DB Commodity Index Tracking Fund, WisdomTree Europe SmallCap Dividend Fund and SPDR Dow Jones Industrial Average ETF.



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Why conditional qua	ntiles?			
A financia	l example			

Consider four assets: iShares Core U.S. Aggregate Bond ETF, PowerShares DB Commodity Index Tracking Fund, WisdomTree Europe SmallCap Dividend Fund and SPDR Dow Jones Industrial Average ETF.

How to use the knowledge of the 4 variables in order to estimate risk measures for WisdomTree Japan Hedged Equity Fund.

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Why conditional quantiles?

A spatial example



Source: Geographic Information Technology Training Alliance. How to estimate risk measures related to X(s) knowing $X_{s_1,...,s_p}$?

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Quantile Oriented Sens	itivity indices			
Uncertainty	/			

Model

$$f: \begin{vmatrix} \mathbb{R}^d & \to & \mathbb{R} \\ \mathbf{x} = (x_1, \dots, x_d) & \mapsto & y = f(\mathbf{x}) \end{vmatrix}$$

with

- f: mathematical or numerical model,
- x: uncertain input parameters,
- y: model's output.

E.g. f is the Profit & Loss amount at time t = 1, the x_i 's are different lines of insurance portfolio (automobile claims, home insurance, asset management, ...).

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Uncertain	itv			

Model

The uncertainty on the input parameters is modelled by a probability distribution $\mathbb P$ on $\mathbb R^d$ and we get

$$Y = f(X_1, \ldots, X_d)$$

with the vector $\mathbf{X} = (X_1, \dots, X_d)$ distributed as \mathbb{P} .

Sensitivity Analysis (SA)

The study of how uncertainty in the output of a model (numerical or otherwise) can be apportioned to different sources of uncertainty in the model's inputs (Saltelli et al. (2004) e.g.).

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Sobol ind	ices			

Independent X_i 's. Defined by Sobol (1993)¹.

$$S_{i} = \frac{\operatorname{var}\left(\mathbb{E}[Y|X_{i}]\right)}{\operatorname{var}(Y)}$$

$$S_{i} = \frac{\operatorname{var}(Y) - \mathbb{E}\left(\operatorname{var}[Y|X_{i}]\right)}{\operatorname{var}(Y)}$$

$$S_{i} = \frac{\mathbb{E}\left[\left(Y - \mathbb{E}[Y]\right)^{2}\right] - \mathbb{E}\left(\mathbb{E}\left[\left(Y - \mathbb{E}[Y|X_{i}]\right)^{2} | X_{i}\right]\right)}{\mathbb{E}\left[\left(Y - \mathbb{E}[Y]\right)^{2}\right]}$$

$$S_{i} = \frac{\min_{\theta} \mathbb{E}\left[\left(Y - \theta\right)^{2}\right] - \mathbb{E}\left(\min_{\theta} \mathbb{E}\left[\left(Y - \theta\right)^{2} | X_{i}\right]\right)}{\min_{\theta} \mathbb{E}\left[\left(Y - \theta\right)^{2}\right]}$$

¹ Ilya M Sobol (1993). In: Mathematical Modelling and Computational Experiments

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Quantile Oriented Sensitivity indices

Quantile oriented sensitivity analysis

QOSA: Quantile Oriented Sensitivity Analysis index: (Fort *et al.* 2016)

$$S_{i}^{\alpha} = \frac{\min_{\theta \in \mathbb{R}} \mathbb{E}\left[\psi_{\alpha}(\boldsymbol{Y}, \theta)\right] - \mathbb{E}\left[\min_{\theta \in \mathbb{R}} \mathbb{E}\left[\psi_{\alpha}\left(\boldsymbol{Y}, \theta\right) | X_{i}\right]\right]}{\min_{\theta \in \mathbb{R}} \mathbb{E}\left[\psi_{\alpha}(\boldsymbol{Y}, \theta)\right]}$$

$$S_{i}^{\alpha} = \frac{\mathbb{E}\left[\psi_{\alpha}\left(Y, q_{\alpha}(Y)\right)\right] - \mathbb{E}\left[\psi_{\alpha}\left(Y, q_{\alpha}(Y|X_{i})\right)\right]}{\mathbb{E}\left[\psi_{\alpha}(Y, q_{\alpha}(Y))\right]}$$

with the contrast function $\psi_{\alpha} : (y, \theta) \mapsto (y - \theta)(\alpha - \mathbf{1}_{y \leq \theta}), \alpha \in [0, 1].$ Remark ψ is related to quantiles:

$$q_{lpha}(Y) = rgmin_{ heta \in \mathbb{R}} \mathbb{E}(\psi_{lpha}(Y, heta)).$$

Elliptic distributions

Quantile Oriented Sensitivity indices

Quantile oriented sensitivity analysis

QOSA: Quantile Oriented Sensitivity Analysis index: (Fort *et al.* 2016)

$$\mathcal{S}_{i}^{lpha} = rac{\mathbb{E}\left[\psi_{lpha}\left(Y, q_{lpha}(Y)
ight)
ight] - \mathbb{E}\left[\psi_{lpha}\left(Y, q_{lpha}(Y|X_{i})
ight)
ight]}{\mathbb{E}\left[\psi_{lpha}(Y, q_{lpha}(Y))
ight]}$$

Properties:

- $0 \leq S_i^{\alpha} \leq 1$
- $S_i^{\alpha} = 0 \iff Y$ and X_i are independent
- $S_i^{\alpha} = 1 \iff Y$ is X_i measurable

Application example: Y is the observed ozone concentration, **X** contains several variables such as: day type, deterministic prevision of ozone concentration, temperature, humidity ... Which of these variables have influence on the quantiles of Y?

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Estimatin	g QOSA			

Estimating Sobol' index may avoid the estimation of the conditional distribution by using var $(\mathbb{E}[Y|X_i]) = Cov(Y, Y')$ with

$$Y' = f(\mathbf{X}'), \ \mathbf{X}' = (X'_1, \dots, X'_{i-1}, \mathbf{X}'_i, X'_{i+1}, \dots, X'_n)$$

 X'_i independent copy of X_j .

The estimation of QOSA' index requires to estimate the conditional distribution $Y|X_i$.

- Kernel methods² optimal window width difficult to calibrate, requires a large number of calls to the costly function *f*.
- Random Forest method Less calls to *f*, time consuming nevertheless.

²Véronique Maume-Deschamps and Ibrahima Niang (2018). In: *Statistics & Probability Letters*

Thomas Browne et al. (2017). In: hal.archives-ouvertes.fr

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Computing / estima	ting conditional quantiles			
Gaussian	case			

Assume (Y, \mathbf{X}) is Gaussian with expectation $\mu = (\mu_Y, \mu_{\mathbf{X}})$ and covariance matrix

$$\boldsymbol{\Sigma} = \begin{pmatrix} \sigma_{\boldsymbol{Y}}^2 & \boldsymbol{\Sigma}_{\boldsymbol{Y}\boldsymbol{X}}^T \\ \boldsymbol{\Sigma}_{\boldsymbol{Y}\boldsymbol{X}} & \boldsymbol{\Sigma}_{\boldsymbol{X}} \end{pmatrix}$$

If $\Sigma_{\mathbf{X}}$ is invertible, then $Y|\mathbf{X}$ follows a normal law with expectation $\mu_{Y|\mathbf{X}} = \mu_Y + \Sigma_{Y\mathbf{X}}^T \Sigma_{\mathbf{X}}^{-1} (\mathbf{X} - \mu_{\mathbf{X}})$ and variance $\sigma_{Y|\mathbf{X}}^2 = \sigma_Y^2 - \Sigma Y \mathbf{X}^T \Sigma_{\mathbf{X}}^{-1} \Sigma_{Y\mathbf{X}}$. Then, the conditional quantiles are easily computable:

$$q_{Y|\mathbf{X}}^{\alpha} = \mu_{Y|\mathbf{X}} + \phi^{-1}(\alpha)\sigma_{Y|\mathbf{X}}.$$

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Quantile	regression			

Approximate the conditional quantile by³:

 $\hat{q}_{\alpha}(X_2|\mathbf{X}_1) = \beta^{*T}\mathbf{X}_1 + \beta_0^*$

where β^* and β^*_0 are the solutions of the following minimization problem:

$$(\beta^*, \beta_0^*) = \operatorname*{arg\,min}_{\beta \in \mathbb{R}^N, \beta_0 \in \mathbb{R}} \mathbb{E}[\psi_{\alpha}(X_2, \beta^T \mathbf{X}_1 + \beta_0)]$$

Recall:

$$\psi_{\alpha}(\mathbf{x},\theta) = (\mathbf{x}-\theta)(\alpha - \mathbf{1}_{\mathbf{x}\leq\theta})$$

and

$$q_{\alpha}(X_2|\mathbf{X}_1) = rgmin_{\theta \in \mathbb{R}} \mathbb{E}(\psi_{\alpha}(X_2, \theta)|\mathbf{X}_1).$$

³ R. Koenker and G. Jr. Bassett (1978). In: Econometrica

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Computing / estimating	g conditional quantiles			
Other meti	noas			

- Random Forest,
- Neural networks,
- Nearest neighbors.

A survey with various methods is proposed by Torosian et al.⁴

⁴ Léonard Torossian et al. (2020). In: *Reliability Engineering & System Safety*

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Consistent Elliptic distributions

Definition

A \mathbb{R}^d random vector **X** has a consistent elliptic distribution if it writes⁵:

$$\mathbf{X} \stackrel{d}{=} \mu + \epsilon \mathcal{N}(\mathbf{0}, \mathbf{\Sigma})$$

with ϵ a positive random variable, independent of the underlying normal vector. This means that, a consistent elliptical distribution is a normal distribution with random variance $\epsilon^2 \Sigma$.

⁵ Y. Kano (1994). In: Journal of Multivariate Analysis

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An equivalent definition

$$\mathbf{X} \stackrel{d}{=} \mu + \epsilon \mathcal{N}(\mathbf{0}, \mathbf{\Sigma})$$
 rewrites as⁶

$$\mathbf{X} \stackrel{d}{=} \mu + R \Lambda U^{(d)}$$

where $\Lambda\Lambda^{T} = \Sigma$, $U^{(d)}$ is a *d*-dimensional random vector uniformly distributed on \mathcal{S}^{d-1} , $R \stackrel{d}{=} \chi_{d}\epsilon$, R and $U^{(d)}$ are independent. *R* is called the radius of **X**, χ_{d}^{2} is a χ -squared distribution, independent of ϵ and of the underlying Gaussian process. **X** is said to be a consistent (R, d)-elliptical random vector with parameters μ and Σ .

⁶S. Cambanis, S. Huang, and G. Simons (1981). In: *Journal of Multivariate Analysis*

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Properties of elliptic distributions

 Sub-vectors of elliptical vectors are elliptical, more precisely, Let X = (X₁, X₂) be a consistent (R, d)-elliptical random vector with parameters μ and Σ. X₁ and X₂ are d₁ and d₂-dimensional subvectors of X. Let us write Σ :

$$\Sigma = egin{pmatrix} \Sigma_{11} & \Sigma_{12} \ \Sigma_{21} & \Sigma_{22} \end{pmatrix}$$

Then X_1 and X_2 are respectively (R, d_1) - and (R, d_2) -elliptical with parameters μ_1 , Σ_{11} and μ_2 , Σ_{22} , respectively.

- Conditional distributions of elliptical vectors are also elliptical.
- Linear combinations of coordinates / sub-vectors of elliptic distributions are also elliptic.

Definitions

Properties of elliptic distributions

- Sub-vectors of elliptical vectors are elliptical,
- Conditional distributions of elliptical vectors are also elliptical. More precisely,

 $\mathbf{X}_2|(\mathbf{X}_1 = x_1)$ is still elliptical, with radius R^* given by:

$$R^* \stackrel{d}{=} R\sqrt{1-\beta} | \left(R\sqrt{\beta} U^{(d)} = C_{11}^{-1}(x_1 - \mu_1)
ight),$$

where C_{11} is the root of Σ_{11} , and $\beta \sim Beta(\frac{d_1}{2}, \frac{d_2}{2})$.

• Linear combinations of coordinates / sub-vectors of elliptic distributions are also elliptic.

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• Normal distributions: $\epsilon = 1$.



Danialé comparence

- Student distributions: with ν degrees of freedom: $\epsilon \stackrel{d}{=} \sqrt{\frac{\nu}{\chi_{d}^{2}}}$.
- Slash distributions: $\epsilon \stackrel{d}{=} \mathcal{P}(1, a)$.
- Laplace distibution: $\epsilon \stackrel{d}{=} \sqrt{\mathcal{E}(\lambda)}$.
- Many other.

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- Normal distributions: $\epsilon = 1$.
- Student distributions: with ν degrees of freedom: $\epsilon \stackrel{d}{=} \sqrt{\frac{\nu}{\chi^2_{-}}}$.

Derarie Student



- Slash distributions: $\epsilon \stackrel{d}{=} \mathcal{P}(1, a)$.
- Laplace distibution: $\epsilon \stackrel{d}{=} \sqrt{\mathcal{E}(\lambda)}$.
- Many other.

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- Normal distributions: $\epsilon = 1$.
- Student distributions: with ν degrees of freedom: $\epsilon \stackrel{d}{=} \sqrt{\frac{\nu}{\chi^2_{-}}}$.
- Slash distributions: $\epsilon \stackrel{d}{=} \mathcal{P}(1, a)$.



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- Laplace distibution: $\epsilon \stackrel{d}{=} \sqrt{\mathcal{E}(\lambda)}$.
- Many other.

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- Normal distributions: $\epsilon = 1$.
- Student distributions: with ν degrees of freedom: $\epsilon \stackrel{d}{=} \sqrt{\frac{\nu}{\chi_d^2}}$.
- Slash distributions: $\epsilon \stackrel{d}{=} \mathcal{P}(1, a)$.
- Laplace distibution: $\epsilon \stackrel{d}{=} \sqrt{\mathcal{E}(\lambda)}$.

Densili Laplace



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Condition	al quantiles			

We are interested in conditional quantiles for elliptical distributions. We have seen that conditional elliptical distribution are still elliptical. Assume a X is a (R, 1) elliptical random vector with parameters μ and $\sigma^2 \in \mathbb{R}^+$, then

$$X = \mu + \sigma R U^{(1)}$$

where $U^{(1)} = -1$ or 1 with probability $\frac{1}{2}$. Thus, for $\alpha > \frac{1}{2}$,

$$q_{\alpha}(X) = \mu + \sigma \Phi_R^{-1}(2\alpha - 1)$$

where Φ_R is the distribution function of *R*.

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Definitions				

Conditional quantiles

Proposition

Let $X = (X_1, X_2)$ a (R, N + 1)-elliptical random vector with parameters μ and Σ . Write

$$\Sigma = egin{pmatrix} \Sigma_{11} & \Sigma_{12} \ \Sigma_{12}^T & \Sigma_{22} \end{pmatrix}$$

Then for $\alpha \geq \frac{1}{2}$,

$$q_{\alpha} \left(X_{2} | \mathbf{X}_{1} = \mathbf{x}_{1} \right) = \mu_{2|1} + \sqrt{\Sigma_{2|1}} \Phi_{R^{*}}^{-1} (2\alpha - 1)$$
with
$$\begin{cases}
\mu_{2|1} = \mu_{2} + \Sigma_{12}^{T} \Sigma_{11}^{-1} (\mathbf{x}_{1} - \mu_{1}) \\
\Sigma_{2|1} = \Sigma_{22} - \Sigma_{12}^{T} \Sigma_{11}^{-1} \Sigma_{12}
\end{cases}$$

Problem: the distribution of R^* is hardly accessible.

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Quantile regression

Quantile Regression for elliptic distributions

Write α' for $2\alpha - 1$.

Theorem

Let $X = (\mathbf{X}_1, X_2)$ be an elliptical distribution, the optimal quantile regression β^* is given by :

$$\beta^* = \boldsymbol{\Sigma}_{11}^{-1} \boldsymbol{\Sigma}_{12}$$

The Quantile Regression Predictor with level $\alpha \in [\frac{1}{2}, 1]$ is given by:

$$\hat{q}_lpha(X_2|\mathbf{X}_1=\mathbf{x}_1)=\mu_{2|1}+\sqrt{\Sigma_{2|1}}\Phi_R^{-1}(lpha')$$

It satisfies

$$\hat{q}_{\alpha}(X_2|X_1) \sim \mathcal{E}_1\left(\mu_2 + \Sigma_{2|1}\Phi_R^{-1}(lpha'), \Sigma_{12}^T\Sigma_{11}^{-1}\Sigma_{12}, R\right)$$

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Quantile regression

How good is the quantile regression?

Gaussian case

$$\begin{cases} q_{\alpha}(X_{2}|\mathbf{X}_{1} = \mathbf{x}_{1}) = \mu_{2|1} + \sigma_{2|1}\Phi^{-1}(\alpha') \\ \hat{q}_{\alpha}(X_{2}|\mathbf{X}_{1} = \mathbf{x}_{1}) = \mu_{2|1} + \sigma_{2|1}\Phi^{-1}(\alpha') \end{cases}$$

The Quantile Regression Predictor is exactly the conditional quantile.

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Quantile regression

How good is the quantile regression?

Student case

$$\begin{cases} q_{\alpha}(X_{2}|\mathbf{X}_{1}=\mathbf{x}_{1}) = & \mu_{2|1} + \sigma_{2|1}\sqrt{\frac{\nu}{\nu+N}}\sqrt{1+\frac{1}{\nu}d_{1}}\Phi_{\nu+N}^{-1}(\alpha') \\ \hat{q}_{\alpha}(X_{2}|\mathbf{X}_{1}=\mathbf{x}_{1}) = & \mu_{2|1} + \sigma_{2|1}\Phi_{\nu}^{-1}(\alpha') \end{cases}$$

where Φ_{ν} is the distribution function of a Student law with ν degrees of freedom.

The error may be huge, especially if the Mahalanobis distance $d_1 = (\mathbf{x}_1 - \mu_1)^T \sum_{11}^{-1} (\mathbf{x}_1 - \mu_1)$ is high. The picture is for N = 5.



Student Quantile Regression

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In case $\alpha \sim 1$, alternative methods have to be proposed. More precisely, we found an equivalent of $\Phi_{R^*}^{-1}(\alpha')$.

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Some asymptotic relationships

Theorem

Under some technical assumptions, their exist $0<\ell<+\infty$ and $\eta\in\mathbb{R}$ such that :

$$\left[\Phi_R^{-1}\left(1-\frac{1}{\frac{\ell}{1-\alpha}+2(1-\ell)}\right)\right]^{\frac{1}{\eta}} \underset{\alpha \to 1}{\sim} \Phi_{R^*}^{-1}(\alpha)$$

This allows to approximate the conditional quantiles.

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Property

The Gaussian, Student and Slash distributions satisfy the previous assumptions, with coefficients η and ℓ given in the table below.

Distribution	η	l		
Gaussian	1	1		
Student, $\nu > 0$	$rac{N}{ u}+1$	$rac{\Gamma\left(rac{ u+N+1}{2} ight)\Gamma\left(rac{ u}{2} ight)}{\Gamma\left(rac{ u+N}{2} ight)\Gamma\left(rac{ u+1}{2} ight)}\left(1+rac{q_1}{ u} ight)^{rac{N+ u}{2}}rac{ u^{rac{N}{2}+1}}{ u+N}$		
Slash, <i>a</i> > 0	$\frac{N}{a} + 1$	$\frac{\Gamma\left(\frac{N+1+\vartheta}{2}\right)\eta_1^{\frac{N+\vartheta}{2}}}{\Gamma\left(\frac{N+2}{2}\right)(N+\vartheta)\chi_{N+\vartheta}^2(q_1)2^{\frac{\vartheta}{2}-1}\Gamma\left(\frac{1+\vartheta}{2}\right)}$		

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Extremal correction in the Student case

Student Extremal Predictor



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Estimations						

Under additional assumptions (heavy tail + order two condition), estimations of the parameters ℓ , η , γ + asymptotic normality of the estimators are given⁷.

⁷ Antoine Usseglio-Carleve (2018). In: Electronic Journal of Statistics

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Financial example



These four values are the first available every day \Rightarrow anticipate the behaviour of the return of WisdomTree Japan Hedged Equity Fund X_2 .
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Financial (example			

The sample size is 2520. The first 2519 days (from January 3, 2007 to December 5, 2016) = learning sample, and we focus on the 2520th day: $\mathbf{x}_1 = (-0.0185\%, -0.4464\%, 0.9614\%, 0.1405\%)$. Estimate quantiles of $X_2 | \mathbf{X}_1 = \mathbf{x}_1$.

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The sample size is 2520. The first 2519 days (from January 3, 2007 to December 5, 2016) = learning sample, and we focus on the 2520th day: $\mathbf{x}_1 = (-0.0185\%, -0.4464\%, 0.9614\%, 0.1405\%)$. Estimate quantiles of $X_2 | \mathbf{X}_1 = \mathbf{x}_1$. Data exploration:

- the daily returns can be considered as independent.
- the marginals seem symmetrical.
- the measured tail index is approximately the same for the marginals.

Could be assumed to be elliptical.

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E.g., for $\alpha = 0.999$, the estimated VaR is 3.1%.

High level quantiles

Conclusion / perspectives for part I.

- Regression methods are not satisfactory for non gaussian distributions.
- Framework adapted to a large class of risk measures (TVaR, *L^p* quantile, Haezendonck-Goovaerts risk measures).
- New technics needed in the high dimension case (N large).
- More details in references below⁸.
- Mixed approaches for non central but non extreme risk levels?
- Non symetric distributions?

V. Maume-Deschamps, D. Rullière, and A. Usseglio-Carleve (2017b). In: Methodology and Computing in Applied Probability Antoine Usseglio-Carleve (2018). In: Electronic Journal of Statistics

 $^{^{8}}$ V. Maume-Deschamps, D. Rullière, and A. Usseglio-Carleve (2017a). In: Journal of Multivariate Analysis

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Methods for conditional quantiles estimation

- Quantile regression is bad if you are far from gaussian,
- Kernel methods to estimate the conditional distribution function $F_{Y|X}(t) = \mathbb{P}(Y \le t|X)$, difficulty to adapt the window.
- Random forest methods,
- Neural networks methods.

In this part, we focus on random forest methods, having in mind that we aim at estimating QOSA indices:

Methods for conditional quantiles estimation

In this part, we focus on random forest methods, having in mind that we aim at estimating QOSA indices:

$$S_{i}^{\alpha} = \frac{\min_{\theta \in \mathbb{R}} \mathbb{E}\left[\psi_{\alpha}(Y, \theta)\right] - \mathbb{E}\left[\min_{\theta \in \mathbb{R}} \mathbb{E}\left[\psi_{\alpha}(Y, \theta) | X_{i}\right]\right]}{\min_{\theta \in \mathbb{R}} \mathbb{E}\left[\psi_{\alpha}(Y, \theta)\right]}$$

$$S_{i}^{\alpha} = \frac{\mathbb{E}\left[\psi_{\alpha}\left(Y, q_{\alpha}(Y)\right)\right] - \mathbb{E}\left[\psi_{\alpha}\left(Y, q_{\alpha}(Y|X_{i})\right)\right]}{\mathbb{E}\left[\psi_{\alpha}(Y, q_{\alpha}(Y))\right]},$$

with $\psi_{\alpha}(x,\theta) = (x-\theta)(\alpha - \mathbf{1}_{x \leq \theta}).$

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A remark on the definition of QOSA

 $\psi_{\alpha}(\mathbf{x}, \theta)$: a non symetric distance.

 $\mathbb{E} [\psi_{\alpha} (Y, \theta)]$ is a mean dispersion measure of Y which is minimized for $\theta = q^{\alpha}(Y)$. So that QOSA indices compare the dispersion of Y around its quantile with its conditional counterpart.



pintball function, theta=2, alpha=0.8

Other indices have been proposed by Kucherenko *et al.* in order to assess the impact of Y over quantiles, but their interpretation is questionnable:

$$\bar{k}_{i,1}^{\alpha} = \mathbb{E}\left[\left|q^{\alpha}\left(Y\right) - q^{\alpha}\left(Y|X_{i}\right)\right|\right] \ \bar{k}_{i,2}^{\alpha} = \mathbb{E}\left[\left(q^{\alpha}\left(Y\right) - q^{\alpha}\left(Y|X_{i}\right)\right)^{2}\right].$$

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A remark on the definition of QOSA

Comparison on the toy model: $Y = X_1 - X_2$ with $X_i \rightsquigarrow \mathcal{E}(1)$.



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Normalized versions





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Recall CA	PT			

Classification And Regression Tree⁹. Input variables: $\mathbf{X} = (X_1, \dots, X_d)$, Output variable: Y.

- Tree: constant piecewise predictor, obtained by binary recursive partitioning.
- Separate the data from the current node, by looking for the split reducing the most the heterogeneity of Y at the two child nodes.



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Agregate several CART's to reduce the estimation variance

- Training sample: $\mathcal{D}_n = (\mathbf{X}^i, Y^i), i = 1, \dots, n$
- Θ_ℓ, ℓ = 1,..., k are independent random variables which determine how a tree is constructed (bootstrap on D_n and which variables are considered for the splits of each node), Θ_ℓ is assumed to be independent of D_n.
- A_n(x; Θ_ℓ, D_n): the leaf that is obtained when dropping x down the tree.
- $N_n(\mathbf{x}, \Theta_{\ell}, \mathcal{D}_n)$: the number of points which are in $A_n(\mathbf{x}; \Theta_{\ell}, \mathcal{D}_n)$.
- *N*^b_n(**x**, Θ_ℓ, D_n): the number of points of the bootstrapped sample, which are in *A*_n(**x**; Θ_ℓ, D_n).

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Random forest conditional distributions functions estimation

Methods with random forest are often using the bootstrap sample, consider the random variable $B_j(\Theta_\ell, \mathcal{D}_n)$ as the number of times that the observation (\mathbf{X}^j, Y^j) has been drawn from the original dataset for the ℓ -th tree construction. Consider the weights:

$$\omega_{n,i}(\mathbf{x},\Theta) = \frac{1}{k} \sum_{j=1}^{k} \frac{\mathbf{1}_{\mathbf{X}^{i} \in A_{n}(\mathbf{x},\Theta_{j},\mathcal{D}_{n})}}{N_{n}(\mathbf{x},\Theta_{j},\mathcal{D}_{n})},$$
$$\omega_{n,i}^{b}(\mathbf{x},\Theta) = \frac{1}{k} \sum_{\ell=1}^{k} \frac{B_{i}(\Theta_{\ell},\mathcal{D}_{n}) \mathbf{1}_{\mathbf{X}^{i} \in A_{n}(\mathbf{x};\Theta_{\ell},\mathcal{D}_{n})}}{N_{n}^{b}(\mathbf{x};\Theta_{\ell},\mathcal{D}_{n})},$$

and the corresponding estimations of $F(y|\mathbf{X} = \mathbf{x})$:

$$\hat{F}_{n}^{b}(\mathbf{y}|\mathbf{X}=\mathbf{x}) = \sum_{i=1}^{n} \omega_{n,i}^{b}(\mathbf{x}) \mathbf{1}_{\{\mathbf{Y}^{i} \leq \mathbf{y}\}}.$$

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Random forest conditional quantiles estimation

Once the conditional distribution function is estimated, the conditional quantiles are estimated straightforwardly:

$$\hat{q}_{\alpha}(Y|\mathbf{X}) = \inf\{t \in \mathbb{R}, \hat{F}_n(t|\mathbf{X}) \geq \alpha\}.$$

With standard arguments, the consistency of $\hat{F}_n(t|\mathbf{X})$ leads to the consistency of $\hat{q}_{\alpha}(Y|\mathbf{X})$, provided that for all \mathbf{x} , the conditional $y \mapsto F(y|\mathbf{X} = \mathbf{x})$ is continuous and increasing.

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Consistency of random forests

Results by Scornet, Biau, Vert (2015) in a linear model context:

$$Y = m(X) + \varepsilon$$
 with $\varepsilon \rightsquigarrow \mathcal{N}(0, \sigma^2)$ and $m(X) = \sum_{i=1}^d m_i(X_i)$.

$$m_n(\mathbf{x},\Theta) = \sum_{i=1}^n \omega_{n,i}(\mathbf{x},\Theta) Y^i,$$

 $\omega_{n,i}$ as before. Under various assumptions including tree size wrt n and a forest correlation control, for $\mathbf{X} \rightsquigarrow \mathcal{U}[0,1]^d$,

$$\mathbb{E}[(m_n(\mathbf{X}) - m(\mathbf{X}))^2] \longrightarrow 0, \text{ with } m_n = \mathbb{E}_{\Theta}(m_{n,k}).$$

- No results for $m(\mathbf{x})$
- Results for fully grown trees and for limited grown trees.

Random forests estimations

Consistency of conditional distribution

Assume $Y = f(\mathbf{X}) + \varepsilon$, with ε a centred random variable, independent on \mathbf{X} . In Meinshausen $(2006)^{10}$, convergence results for $\widehat{F}(y|\mathbf{X} = \mathbf{x})$ for a simplified random forest model. The $\omega_{n,i}(\mathbf{x})$'s are considered as constant (while they are random variables - depending on Θ , \mathbf{X}^{i} , Y^{i} , i = 1, ..., n)

+ various assumptions including tree growth and some regularity on $F(y|\mathbf{X} = \mathbf{x})$.

¹⁰ Nicolai Meinshausen (2006). In: Journal of Machine Learning Research

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Consistency: assumptions

Conditions

Relations between k (number of trees) and $N_n^b(\mathbf{x}; \Theta, \mathcal{D}_n)$ (number of bootstrap observations in a leaf node):

$$\mathbf{0} \ \mathbf{k} = \mathcal{O}\left(\mathbf{n}^{\alpha}\right), \text{ with } \alpha > \mathbf{0}.$$

 $^{a}f\left(n
ight)=\Omega\left(g\left(n
ight)
ight)\iff \exists k>0, \exists n_{0}>0\mid orall n\geqslant n_{0}\quad \left|f\left(n
ight)
ight|\geqslant k\cdot\left|g\left(n
ight)
ight|$

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Consistency: assumptions

Conditions

Relations between k (number of trees) and $N_n^b(\mathbf{x}; \Theta, \mathcal{D}_n)$ (number of bootstrap observations in a leaf node):

$$\begin{array}{l} \bullet \quad k = \mathcal{O}\left(n^{\alpha}\right), \text{ with } \alpha > 0. \\ \hline \bullet \quad & \forall \mathbf{x}, \quad \mathbb{E}\left[N_{n}^{b}\left(\mathbf{x}; \Theta, \mathcal{D}_{n}\right)\right] = \Omega\left(\sqrt{n}\left(\ln\left(n\right)\right)^{\beta}\right), \text{ with } \beta > 1, \text{ and} \\ \quad & \forall \mathbf{x}, \quad CV\left(N_{n}^{b}(\mathbf{x}; \Theta, \mathcal{D}_{n})\right) = \mathcal{O}\left(\frac{1}{n^{(1+\alpha)/2}\left(\ln\left(n\right)\right)^{\gamma/2}}\right), \text{ with } \gamma > 1.^{a} \end{array}$$

 $^{a}\mathrm{CV}\left(X\right) = \sigma_{X}/\mathbb{E}(X)$

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Conditions

Relations between k (number of trees) and $N_n^b(\mathbf{x}; \Theta, \mathcal{D}_n)$ (number of bootstrap observations in a leaf node):

$$\mathbf{0} \ \mathbf{k} = \mathcal{O}(\mathbf{n}^{\alpha}), \text{ with } \alpha > \mathbf{0}.$$

2
$$\forall \mathbf{x}, \quad \mathbb{E}\left[N_n^b(\mathbf{x}; \Theta, \mathcal{D}_n)\right] = \Omega\left(\sqrt{n}\left(\ln(n)\right)^{\beta}\right), \text{ with } \beta > 1, \text{ and}$$

$$\forall \mathbf{x}, \quad CV(N_n^b(\mathbf{x}; \Theta, \mathcal{D}_n)) = \mathcal{O}\left(\frac{1}{n^{(1+\alpha)/2} \left(\ln{(n)}\right)^{\gamma/2}}\right), \text{ with } \gamma > 1.^{\epsilon}$$

The variations of function $F(y|\mathbf{X} = \cdot)$ is small on the trees' leaves: $\forall \mathbf{x}, \forall y,$

$$\sup_{\mathbf{z},\mathbf{z}'\in A_n(\mathbf{x},\Theta_j)}\left|F\left(y\,|\,\mathbf{z}\right)-F\left(y\,|\,\mathbf{z}'\right)\right|\underset{n\to\infty}{\overset{a.s.}{\longrightarrow}}0.$$

 $^{a}\mathrm{CV}\left(X
ight)=\sigma_{X}/\mathbb{E}(X)$

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Consistency: result¹¹

Theorem

Assume the 3 conditions above are verified and $F(\cdot | \mathbf{X} = \mathbf{x})$ is continuous and increasing, $\forall \mathbf{x} \in \mathbb{R}^d$. Let F_n be either \hat{F}_n^b or \hat{F}_n ,

$$\sup_{y \in \mathbb{R}} |F_n(y|\mathbf{X} = \mathbf{x}) - F(y|\mathbf{X} = \mathbf{x})| \xrightarrow[n \to \infty]{a.s.} 0$$

Idea of the proof: The main idea is to use an auxiliary sample: let $(\mathbf{X}^{i\diamond}, Y^{i\diamond}, i = 1, ..., n)$ be a second sample, independent from $(\mathbf{X}^i, Y^i, i = 1, ..., n)$ and consider the weights and the corresponding estimation of $F(y|\mathbf{X} = \mathbf{x})$:

$$\omega_{n,i}^{\diamond}(\mathbf{x},\Theta) = \frac{1}{k} \sum_{j=1}^{k} \frac{\mathbf{1}_{\mathbf{X}^{i\diamond} \in \mathcal{A}_{n}(\mathbf{x},\Theta_{j},\mathcal{D}_{n})}}{N_{n}(\mathbf{x},\Theta_{j},\mathcal{D}_{n})}, \ F_{n}^{\diamond}(y|\mathbf{X}=\mathbf{x}) = \sum_{i=1}^{n} \omega_{i}^{\diamond}(\mathbf{x}) \mathbf{1}_{\{Y^{i\diamond} \leqslant y\}}.$$

¹¹ Kevin Elie-Dit-Cosaque and Véronique Maume-Deschamps (2020). In: *hal.archives-ouvertes.fr*

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The two samples method.

We prove:

- $|F_n(y|\mathbf{X} = \mathbf{x}) F_n^{\diamond}(y|\mathbf{X} = \mathbf{x})| \xrightarrow[n \to \infty]{a.s.} 0$, uses a Hoeffding like inequality + Vapnik-Chervonenkis classes¹² (proximity of N^{\diamond} and N^b),
- **2** $|F_n^{\diamond}(y|\mathbf{X} = \mathbf{x}) F(y|\mathbf{X} = \mathbf{x})| \xrightarrow[n \to \infty]{a.s.} 0$, uses Vapnik-Chervonenkis classes again.
- **3** use a Dini argument to conclude with the $\sup_{y \in \mathbb{R}}$.

¹² V. N. Vapnik and A. Ya. Chervonenkis (1971). In: Theory of Probability and its Applications

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QOSA estimation

Estimation strategies for the QOSA indices

Recall:

$$S_{i}^{lpha} = 1 - rac{\mathbb{E}\left[\psi_{lpha}\left(Y, q^{lpha}(Y|X_{i})
ight)
ight]}{\mathbb{E}\left[\psi_{lpha}(Y, q^{lpha}(Y))
ight]} = 1 - rac{\mathbb{E}\left[\min_{ heta \in \mathbb{R}} \mathbb{E}\left[\psi_{lpha}\left(Y, heta
ight)|X_{i}
ight]
ight]}{\mathbb{E}\left[\psi_{lpha}(Y, q^{lpha}(Y))
ight]}$$

Training sample: $\mathcal{D}_n = (\mathbf{X}^j, Y^j)_{j=1,...,n}$, the denominator is easily estimated with $\widehat{P}_1 = \frac{1}{n} \sum_{j=1}^n \psi_\alpha \left(Y^j, \widehat{q}^\alpha(Y) \right).$

Two strategies to estimate the numerator:

- Quantile based estimators $\mathbb{E}\left[\psi_{\alpha}\left(Y, q^{\alpha}(Y|X_{i})\right)\right]$,
- Minimum based estimators $\mathbb{E}\left[\min_{\theta \in \mathbb{R}} \mathbb{E}\left[\psi_{\alpha}\left(Y,\theta\right) | X_{i}\right]\right]$.

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Methods based on **two** training samples:

 $\begin{aligned} \mathcal{D}_{n}^{\star} &= \left(\mathbf{X}^{\star j}, Y^{\star j}\right)_{j=1,...,n} \text{ for computing the index,} \\ \mathcal{D}_{n} &= \left(\mathbf{X}^{j}, Y^{j}\right)_{j=1,...,n} \text{ for estimating the conditional quantile.} \\ \widehat{R}_{i} &= \frac{1}{n} \sum_{i=1}^{n} \psi_{\alpha} \left(Y^{\star j}, \widehat{q}^{\alpha} \left(Y | X_{i} = X_{i}^{\star j}\right)\right) \end{aligned}$

Construct the forest with $\mathcal{D}_n^i = (X_i^j, Y^j)_{i=1,...,n}$ from \mathcal{D}_n .

Quantile estimation with a weighted approach: $\widehat{R}_{i}^{1,b}$ or $\widehat{R}_{i}^{1,o}$

$$F_{k,n}^{b}(y|X_{i} = x_{i}) = \sum_{j=1}^{n} w_{n,j}^{b}(x_{i}) \mathbf{1}_{\{Y^{j} \leq y\}}$$
$$\hat{q}^{\alpha}(Y|X_{i} = x_{i}) = \inf \{Y^{p}, \ p = 1, \dots, n : F_{k,n}^{b}(Y^{p}|X_{i} = x_{i}) \geq \alpha \}$$

2 Quantile estimation within a leaf: $\hat{R}_i^{2,b}$ or $\hat{R}_i^{2,o}$.

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Methods based on two training samples:

 $\mathcal{D}_{n}^{\star} = (\mathbf{X}^{\star j}, Y^{\star j})_{j=1,...,n} \text{ for computing the index,}$ $\mathcal{D}_{n} = (\mathbf{X}^{j}, Y^{j})_{j=1,...,n} \text{ for estimating the conditional quantile.}$ $\widehat{R}_{i} = \frac{1}{n} \sum_{i=1}^{n} \psi_{\alpha} \left(Y^{\star j}, \widehat{q}^{\alpha} \left(Y | X_{i} = X_{i}^{\star j} \right) \right)$

Construct the forest with $\mathcal{D}_n^i = (X_i^j, Y^j)_{i=1,...,n}$ from \mathcal{D}_n .

- **Quantile estimation with a weighted approach**: $\widehat{R}_{i}^{1,b}$ or $\widehat{R}_{i}^{1,o}$
- **2** Quantile estimation within a leaf: $\widehat{R}_i^{2,b}$ or $\widehat{R}_i^{2,o}$. For one tree, $\widehat{q}_{\ell}^{b,\alpha}$ ($Y | X_i = x_i$) on the leaf containing x_i . On the forest:

$$\widehat{q}^{\alpha}\left(\left.Y\right|X_{i}=x_{i}\right)=\frac{1}{k}\sum_{\ell=1}^{k}\widehat{q}_{\ell}^{b,\alpha}\left(\left.Y\right|X_{i}=x_{i}\right).$$

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Minimum based estimators

Minimum estimation with a weighted approach:

 $\begin{aligned} \mathcal{D}_{n} &= (\mathbf{X}^{j}, Y^{j})_{j=1,...,n} \text{ and } (\mathbf{X}^{\star j})_{j=1,...,n} \text{ i.e. requires 1.5 training samples.} \\ \text{Estimate } \mathbb{E} \left[\min_{\theta \in \mathbb{R}} \mathbb{E} \left[\psi_{\alpha} \left(Y, \theta \right) | X_{i} \right] \right] \text{ with } \end{aligned}$

$$\frac{1}{n}\sum_{m=1}^{n}\min_{p=1,\dots,n}\sum_{j=1}^{n}w_{n,j}^{b}\left(X_{i}^{\star m}\right)\psi_{\alpha}\left(Y^{j},Y^{p}\right)$$

 $\implies \widehat{Q}_i^{1,b} \text{ or } \widehat{Q}_i^{1,o}.$

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Minimum based estimators

Minimum estimation within a leaf: $\mathcal{D}_n = (\mathbf{X}^j, Y^j)_{j=1,...,n}$. Estimate $\mathbb{E}[\min_{\theta \in \mathbb{R}} \mathbb{E}[\psi_{\alpha}(Y, \theta) | X_i]]$ with

$$\frac{1}{k}\sum_{\ell=1}^{k}\left[\frac{1}{N_{\textit{leaves}}^{\ell}}\sum_{m=1}^{N_{\textit{leaves}}^{\ell}}\left(\min_{\boldsymbol{p}\in\mathcal{L}_{\ell,m}^{b}}\sum_{j\in\mathcal{L}_{\ell,m}^{b}}\frac{\psi_{\alpha}\left(\boldsymbol{Y}^{j},\boldsymbol{Y}^{\boldsymbol{p}}\right)}{|\mathcal{L}_{\ell,m}^{b}|}\right)\right]$$

 $\implies \widehat{Q}_i^{2,b} \text{ or } \widehat{Q}_i^{2,o}.$

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QOSA estimation

Principles of the Cross-Validation

Preliminary studies have showned that size's leaves is crutial in the estimation \implies cross-validation strategy in order to choose the number of elements in the leaves.

- Shuffle the dataset randomly and split the dataset in k folds
- Por each unique group: Take the group as a test dataset; Take the remaining groups as a training dataset; Fit a model on the training set and evaluate it on the test set; Retain the evaluation score and discard the model
- Summarize the skill of the model using the sample of model evaluation scores



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Leaf size issue

We use
$$\widehat{R}_{i}^{1} = \frac{1}{n} \sum_{j=1}^{n} \psi_{\alpha} \left(Y^{j}, \widehat{q}^{\alpha} \left(Y | X_{i} = X_{i}^{j} \right) \right)$$
 as score.

- In the cross validation process, among a grid of possible sizes, construct a forest with leaf size realizing the minimal score.
- Using the Out of Bag (OoB) sample.
 - For a given observation (X^j_i, Y^j) from Dⁱ_n, consider the set of trees built with the bootstrap samples not containing this observation (it is *Out of Bag*).
 - **2** Aggregate the estimations from these trees to make the OoB estimation: $\hat{q}_{oob}^{b,\alpha} \left(Y | X_i = X_i^j \right)$ of $q^{\alpha} \left(Y | X_i = X_i^j \right)$.
 - O Calculate the OoB score:

$$\widehat{OOB}_{i}^{b} = \frac{1}{n} \sum_{j=1}^{n} \psi_{\alpha} \left(Y^{j}, \widehat{q}_{oob}^{b,\alpha} \left(Y | X_{i} = X_{i}^{j} \right) \right) .$$

Among a grid of possible sizes, construct a forest with leaf size realizing the minimal OoB score.

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l eaf size i	ssue			

We use
$$\widehat{R}_{i}^{1} = \frac{1}{n} \sum_{j=1}^{n} \psi_{\alpha} \left(Y^{j}, \widehat{q}^{\alpha} \left(Y | X_{i} = X_{i}^{j} \right) \right)$$
 as score.

- In the cross validation process, among a grid of possible sizes, construct a forest with leaf size realizing the minimal score.
- Using the Out of Bag (OoB) sample. Among a grid of possible sizes, construct a forest with leaf size realizing the minimal OoB score.

Using the OoB sample is much less time consuming since, it does not require cutting out the training sample and it takes place during the forest construction process.

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Simulation studies				

Sum of exponential laws

case $X_i \rightsquigarrow \mathcal{E}(\lambda_i), \lambda_i \in \mathbb{R}^+$ distinct; $Y = \sum_{i=1}^n X_i$ a semi-closed form formula may be obtained by using calculations from Marceau (2014).

Simulation study for $\lambda_1 = 0.5$, $\lambda_2 = 1$, $\lambda_3 = 1.5$, $\lambda_4 = 2$.

```
sample size = 10^4,
nb trees = 100,
boxplots on 100 repetitions.
```

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Sum of exponential laws

Quantile based methods



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Minimum based methods



Simulation studies

Comparison with kernel methods

Consider a toy model: $Y = X_1 - X_2$ with $X_i \rightsquigarrow \mathcal{E}(1)$ independent. RMSE and run time of the random forest based estimators: with $\widehat{Q}_i^{1,o}$ and $\widehat{Q}_i^{2,o}$ as well as those based on kernel: $\widetilde{S}_i^{\alpha 13}$ and $\check{S}_i^{\alpha 14}$, sample size is 10^4 .

	RF with $\widehat{Q}_{i}^{1,o}$	RF with $\widehat{Q}_i^{2,o}$	$\widetilde{S}_{i}^{\alpha}$	\check{S}^{lpha}_i
$\alpha = 0.1$	0.007	0.009	0.061	0.020
$\alpha = 0.25$	0.008	0.009	0.042	0.013
$\alpha = 0.5$	0.008	0.008	0.027	0.019
$\alpha = 0.75$	0.008	0.008	0.014	0.035
$\alpha = 0.99$	0.006	0.006	0.013	0.084
run time	1 hr	18 min 24 sec	1 min 51 sec	1 hr 55 min

¹³Véronique Maume-Deschamps and Ibrahima Niang (2018). In: *Statistics & Probability Letters*

¹⁴ Thomas Browne et al. (2017). In: *hal.archives-ouvertes.fr*

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Simulation studies				
A real dat	aset			

Bias between the predictions from MOCAGE (Modèle de Chimie Atmosphérique à Grande Echelle) and the observed ozone concentration. This dataset¹⁵ contains 10 variables with 1041 observations. O3obs: observed ozone concentration will be explained by the 9 other variables

JOUR: type of day (holiday vs no holi-	STATION: site of observations (5 differ-
day)	ent sites)
MOCAGE: ozone concentration pre-	TEMPE: officially predicted tempera-
dicted by a fluid mechanics model	tures
RMH2O: humidity ratio	NO2: nitrogen dioxide concentration
VentMOD: wind force	VentANG: wind direction
NO: nitric oxide concentration	

¹⁵ Philippe Besse et al. (2007). In: Pollution atmosphérique

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Application on a real dataset: results



Evolution of the ranking of the QOSA indices (brut indices on the left, in %ages on the right)in function of the levels α .

Considering the central effects $leads^{16}$ to consider MOCAGE and TEMPE as the most influencial variables, then STATION and

<u>NO2. We see that for quantile levels ≥ 0.6 wind is also important.</u>

¹⁶ Philippe Besse et al. (2007). In: Pollution atmosphérique

Baptiste Broto, Francois Bachoc, and Marine Depecker (2020). In: SIAM/ASA Journal on Uncertainty Quantification

Simulation studies

Conclusion / perspectives for part II.

- Random forest methods usefull for conditional quantile and QOSA estimations, but costly.
- Methods implemented in Python¹⁷ (QOSA) and Julia¹⁸ (conditional distributions).
- Asymptotic distributions to get confidence intervals?
- To be compared with Generalized Random Forest¹⁹.

¹⁷ Kévin Elie-Dit-Cosaque (2020).

¹⁸ Benoit Fabrège and Véronique Maume-Deschamps (2020).

¹⁹Susan Athey, Julie Tibshirani, Stefan Wager, et al. (2019). In: *The Annals of Statistics*
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Plan



- 2 Elliptic distributions
- 3 Random forest estimation



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Conclusions

- Importance of conditional quantile estimations
 - Various methods exists, we have seen only few.
 - Specific methods available for some classes of distributions such as elliptical distributions.
 - Specific attention for high level quantiles (uses extreme value theory).
- Interest of QOSA indicies
 - Give different informations than Sobol indices, pertinent if you are interested in different quantile levels.
 - Interpretation not so easy, especially if inputs are dependent \rightarrow go the qosa-Shapley (mixture of Shapley effect²⁰ and QOSA indices (work in progress).

²⁰ Art B Owen and Clémentine Prieur (2016). In: *arXiv preprint arXiv:1610.02080*

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Thanks for your attention. Merci pour votre attention.

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