Robust regression via Maximum Mean Discrepancy

Pierre Alquier

RIKEN

AIP
Center for
Advanced Intelligence Project

New Trends in Statistical Learning II
Porquerolles, June 2022

Contents

Contents

The Maximum Likelihood Estimator (MLE)

Let $X_1, \dots, X_n$ be i.i.d in $\mathcal{X}$ from a probability distribution P_0.

Statistical inference :

- propose a model $(P_\theta, \theta \in \Theta)$, assume $P_0 = P_{\theta_0}$.
- compute $\hat{\theta}_n = \hat{\theta}_n(X_1, \dots, X_n)$.

Letting p_θ denote the density of P_θ, then

$$\hat{\theta}_n^{MLE} = \arg\max_{\theta\in\Theta} L_n(\theta), \text{ where } L_n(\theta) = \prod_{i=1}^{n} p_\theta(X_i).$$

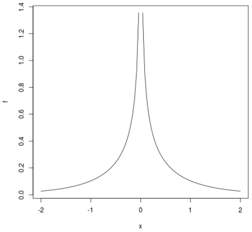
Example : $P_{(m,\sigma)} = \mathcal{N}(m, \sigma^2)$ then

$$\hat{m} = \frac{1}{n}\sum_{i=1}^{n} X_i \text{ and } \hat{\sigma}^2 = \frac{1}{n}\sum_{i=1}^{n}(X_i - \hat{m})^2.$$

MLE not unique / not consistent

Example :

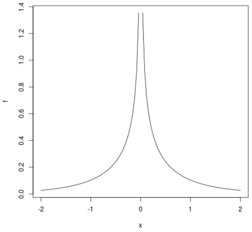
$$p_\theta(x) = \frac{\exp(-|x-\theta|)}{2\sqrt{\pi|x-\theta|}},$$



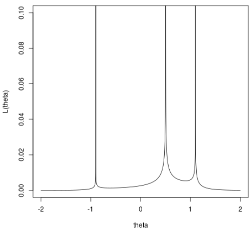
MLE not unique / not consistent

Example :

$$p_\theta(x) = \frac{\exp(-|x-\theta|)}{2\sqrt{\pi|x-\theta|}},$$



$$L_n(\theta) = \frac{\exp\left(-\sum_{i=1}^n |X_i-\theta|\right)}{(2\sqrt{\pi})^n \prod_{i=1}^n \sqrt{|X_i-\theta|}}.$$



MLE fails in the presence of outliers

What is an outlier ?

Huber proposed the contamination model : with probability ε, X_i is not drawn from P_{θ_0} but from Q that can be anything :

$$P_0 = (1-\varepsilon)P_{\theta_0} + \varepsilon Q.$$

Example : $P_\theta = \mathcal{U}nif[0,\theta]$, then

$$L_n(\theta) = \frac{1}{\theta^n}\prod_{i=1}^{n} \mathbb{1}_{\{0\leq X_i \leq \theta\}} \Rightarrow \hat{\theta} = \max_{1\leq i\leq n} X_i.$$

In the case of the following contamination, the MLE is extremely far from the truth :

$$P_0 = (1-\varepsilon).\mathcal{U}nif[0,1] + \varepsilon.\mathcal{N}(10^{10},1)...$$

Minimum Distance Estimation

$$\text{Empirical distribution : } \hat{P}_n := \frac{1}{n}\sum_{i=1}^{n} \delta_{X_i}.$$

Minimum Distance Estimation (MDE)

Let $d(\cdot,\cdot)$ be a metric on probability distributions.

$$\hat{\theta}_d := \arg\min_{\theta\in\Theta} d\left(P_\theta, \hat{P}_n\right).$$

Wolfowitz, J. (1957). The minimum distance method. *The Annals of Mathematical Statistics*.

Idea : MDE with an adequate d leads to robust estimation.

Bickel, P. J. (1976). Another look at robustness : a review of reviews and some new developments. *Scandinavian Journal of Statistics*. Discussion by Sture Holm.

Parr, W. C. & Schucany, W. R. (1980). Minimum distance and robust estimation. *JASA*.

Yatracos, Y. G. (1985). Rates of convergence of minimum distance estimators and Kolmogorov's entropy. *Annals of Statistics*.

Integral Probability Semimetrics

Integral Probability Semimetrics (IPS)

Let $\mathcal{F}$ be a set of real-valued, measurable functions and put

$$d_{\mathcal{F}}(P, Q) = \sup_{f \in \mathcal{F}} \left| \mathbb{E}_{X \sim P}[f(X)] - \mathbb{E}_{X \sim Q}[f(X)] \right|.$$

Müller, A. (1997). Integral probability metrics and their generating classes of functions. *Applied Probability*.

- assumptions required in order to ensure that $d_{\mathcal{F}}(P, Q) = 0 \Rightarrow P = Q$ (that is, $d_{\mathcal{F}}$ is a metric).
- assumptions required in order to ensure that $d_{\mathcal{F}} < +\infty$.

Non-asymptotic bound for MDE

Theorem 1

- $X_1, \dots, X_n$ i.i.d from P_0,
- for any $f \in \mathcal{F}$, $\sup_{x\in\mathcal{X}} |f(x)| \leq 1$.

Then

$$\mathbb{E}\left[d_{\mathcal{F}}(P_{\hat{\theta}_{d_{\mathcal{F}}}}, P_0)\right] \leq \inf_{\theta\in\Theta} d_{\mathcal{F}}(P_\theta, P_0) + 4.\mathrm{Rad}_n(\mathcal{F}).$$

Rademacher complexity

$$\mathrm{Rad}_n(\mathcal{F}) := \sup_P \mathbb{E}_{Y_1,\dots,Y_n\sim P}\,\mathbb{E}_{\epsilon_1,\dots,\epsilon_n}\left[\sup_{f\in\mathcal{F}} \frac{1}{n}\sum_{i=1}^n \epsilon_i f(Y_i)\right].$$

where $\epsilon_1, \dots, \epsilon_n$ are i.i.d Rademacher variables :

$$\mathbb{P}(\epsilon_1 = 1) = \mathbb{P}(\epsilon_1 = -1) = 1/2.$$

Example 1 : set of indicators

$$\mathbb{1}_A(x) = \begin{cases} 1 \text{ if } x \in A, \\ 0 \text{ if } x \notin A. \end{cases}$$

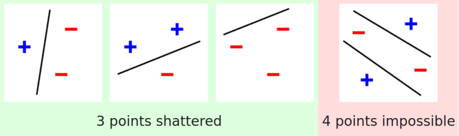


Image from Wikipedia.

Reminder - Vapnik-Chervonenkis dimension

Assume that $\mathcal{F} = \{\mathbb{1}_A, A \in \mathcal{A}\}$ for some $\mathcal{A} \subseteq \mathcal{P}(\mathcal{X})$,

- $S_{\mathcal{F}}(x_1, \dots, x_n) := \{(f(x_1), \dots, f(x_n)), f \in \mathcal{F}\}$,
- $\mathrm{VC}(\mathcal{F}) := \max\{n : \exists x_1, \dots, x_n, |S_{\mathcal{F}}(x_1, \dots, x_n)| = 2^n\}$.

Theorem (Bartlett and Mendelson)

$$\mathrm{Rad}_n(\mathcal{F}) \leq \sqrt{\frac{2.\mathrm{VC}(\mathcal{F}) \log(n+1)}{n}}.$$

Bartlett, P. L. & Mendelson, S. (2002). Rademacher and Gaussian complexities : Risk bounds and structural results. *JMLR*.

Example 1 : KS and TV distances

Two classical examples :

- $\mathcal{A} = \{$all measurable sets in $\mathcal{X}\}$, then $d_{\mathcal{F}}(\cdot,\cdot)$ is the total variation distance $\mathrm{TV}(\cdot,\cdot)$.
  - $\mathrm{VC}(\mathcal{F}) = +\infty$ when $|\mathcal{X}| = +\infty$,
  - in general, $\mathrm{Rad}_n(\mathcal{F}) \nrightarrow 0$.
- $\mathcal{X} = \mathbb{R}$, $\mathcal{A} = \{(-\infty, x], x \in \mathbb{R}\}$, then $d_{\mathcal{F}}(\cdot,\cdot)$ is the Kolmogorov-Smirnov distance $\mathrm{KS}(\cdot,\cdot)$.
  - KS distance was actually proposed by S. Holm for robust estimation,
  - $\mathrm{VC}(\mathcal{F}) = 1$.

$$\mathbb{E}\left[\mathrm{KS}(P_{\hat{\theta}_{\mathrm{KS}}}, P_0)\right] \leq \inf_{\theta\in\Theta} \mathrm{KS}(P_\theta, P_0) + 4.\sqrt{\frac{2\log(n+1)}{n}}.$$

Example 2 : Maximum Mean Discrepancy (MMD)

- Let $(\mathcal{H}, \langle \cdot, \cdot \rangle_{\mathcal{H}})$ be a RKHS with kernel
$$k(x, y) = \langle \phi(x), \phi(y) \rangle_{\mathcal{H}} .$$
- If $\|\phi(x)\|_{\mathcal{H}} = k(x, x) \leq 1$ then $\mathbb{E}_{X \sim P}[\phi(X)]$ is well-defined .
- The map $P \mapsto \mathbb{E}_{X \sim P}[\phi(X)]$ is one-to-one if k is *characteristic*.
- For example, $k(x, y) = \exp(-\|x - y\|^2/\gamma^2)$ works.

Definition - MMD

$$\mathrm{MMD}_k(P, Q) = \sup_{\substack{f \in \mathcal{H} \\ \|f\|_{\mathcal{H}} \leq 1}} \left| \mathbb{E}_{X \sim P}[f(X)] - \mathbb{E}_{X \sim Q}[f(X)] \right|$$
$$= \left\| \mathbb{E}_{X \sim P}[\phi(X)] - \mathbb{E}_{X \sim Q}[\phi(X)] \right\|_{\mathcal{H}} .$$

Example 2 : MMD

$$\mathcal{F} = \{f \in \mathcal{H} : \|f\|_{\mathcal{H}} \leq 1\} \Rightarrow \mathrm{Rad}_n(\mathcal{F}) \leq \sqrt{\frac{\sup_x k(x,x)}{n}}.$$

Theorem 2

For k bounded by 1 and characteristic,

$$\mathbb{E}\left[\mathrm{MMD}_k(P_{\hat{\theta}_{\mathrm{MMD}_k}}, P_0)\right] \leq \inf_{\theta\in\Theta} \mathrm{MMD}_k(P_\theta, P_0) + \frac{2}{\sqrt{n}}.$$

Joint work with Badr-Eddine Chérief-Abdellatif (Oxford).

Chérief-Abdellatif, B.-E. and Alquier, P. Finite Sample Properties of Parametric MMD Estimation : Robustness to Misspecification and Dependence. **Bernoulli**, 2022.

Example 2 : MMD

We actually have

$$\mathrm{MMD}_k^2(P_\theta, \hat{P}_n) = \mathbb{E}_{X,X'\sim P_\theta}[k(X,X')] - \frac{2}{n}\sum_{i=1}^{n}\mathbb{E}_{X\sim P_\theta}[k(X_i,X)] + \frac{1}{n^2}\sum_{1\leq i,j\leq n} k(X_i,X_j)$$

and so

$$\nabla_\theta \mathrm{MMD}_k^2(P_\theta, \hat{P}_n) = 2\mathbb{E}_{X,X'\sim P_\theta}\left\{\left[k(X,X') - \frac{1}{n}\sum_{i=1}^{n} k(X_i,X)\right]\nabla_\theta[\log p_\theta(X)]\right\}$$

that can be approximated by sampling from P_θ.

Example 2 : MMD

Dziugaite, G. K., Roy, D. M., & Ghahramani, Z. (2015). Training generative neural networks via maximum mean discrepancy optimization. *UAI 2015*.

define the estimator and used it to train GANs.

Briol, F. X., Barp, A., Duncan, A. B., & Girolami, M. (2019). Statistical Inference for Generative Models with Maximum Mean Discrepancy. *Preprint arXiv :1906.05944*.

$$\text{assumptions} \Rightarrow \quad \sqrt{n}(\hat{\theta}_{\mathrm{MMD}_k} - \theta_0) \rightsquigarrow \mathcal{N}(0, V_0(k)).$$

Example 3 : Wasserstein

Another classical metric belongs to the IPS family :

$$\mathrm{W}_\delta(P,Q) = \sup_{\substack{f:\mathcal{X}\to\mathbb{R} \\ \mathrm{Lip}(f)\leq 1}} \left| \mathbb{E}_{X\sim P}[f(X)] - \mathbb{E}_{X\sim Q}[f(X)] \right|$$

where $\mathrm{Lip}(f) := \sup_{x\neq y} |f(x) - f(y)|/\delta(x,y)$.

- In general, $\mathrm{Rad}_n(\mathcal{F}) \nrightarrow 0$, so will not converge in full generality as with MMD and KS.
- However, nice results can be proven under additional assumptions :

Bernton, E., Jacob, P. E., Gerber, M. & Robert, C. P. (2019). On parameter estimation with the Wasserstein distance. *Information and Inference : A Journal of the IMA*.

MDE and robustness

Reminder

$$\mathbb{E}\left[d_{\mathcal{F}}(P_{\hat{\theta}_{d_{\mathcal{F}}}}, P_0)\right] \leq \inf_{\theta \in \Theta} d_{\mathcal{F}}(P_\theta, P_0) + 4.\mathrm{Rad}_n(\mathcal{F}).$$

Huber's contamination model : $P_0 = (1-\varepsilon)P_{\theta_0} + \varepsilon Q$.

$$\begin{aligned} d_{\mathcal{F}}(P_{\theta_0}, P_0) &= \sup_{f \in \mathcal{F}} \left| \mathbb{E}_{X \sim P_{\theta_0}} f(X) - (1-\varepsilon)\mathbb{E}_{X \sim P_{\theta_0}} f(X) - \varepsilon \mathbb{E}_{X \sim Q} f(X) \right| \\ &= \sup_{f \in \mathcal{F}} \left| \varepsilon \mathbb{E}_{X \sim P_{\theta_0}} f(X) - \varepsilon \mathbb{E}_{X \sim Q} f(X) \right| \\ &= \varepsilon . d_{\mathcal{F}}(P_{\theta_0}, Q) \leq 2\varepsilon \quad \text{if for any } f \in \mathcal{F}, \sup_x |f(x)| \leq 1 \end{aligned}$$

Corollary - in Huber's contamination model

$$\mathbb{E}\left[d_{\mathcal{F}}(P_{\hat{\theta}_{d_{\mathcal{F}}}}, P_{\theta_0})\right] \leq 4\varepsilon + 4.\mathrm{Rad}_n(\mathcal{F}).$$

MDE and robustness : toy experiment

Model : $\mathcal{N}(\theta, 1)$, $X_1, \dots, X_n$ i.i.d $\mathcal{N}(\theta_0, 1)$, $n = 100$ and we repeat the exp. 200 times. Kernel $k(x, y) = \exp(-|x - y|)$.

	$\hat{\theta}_{MLE}$	$\hat{\theta}_{\mathrm{MMD}_k}$	$\hat{\theta}_{\mathrm{KS}}$
mean abs. error	0.081	0.094	0.088

Now, $\varepsilon = 2\%$ of the observations drawn from a Cauchy.

mean abs. error	0.276	0.095	0.088

Now, $\varepsilon = 1\%$ are replaced by $1,000$.

mean abs. error	10.008	0.088	0.082

Contents

Regression with MMD

What follows is based on a joint paper with Mathieu Gerber (Bristol).

Alquier, P. and Gerber, M. (2020). *Universal Robust Regression via Maximum Mean Discrepancy*. Preprint arXiv, submitted.

Examples

We observe independent pairs $(X_1, Y_1), \dots, (X_n, Y_n)$.

1. Gaussian linear regression model :
   - $Y_i = \theta^T X_i + \varepsilon_i$, $\varepsilon_i \sim \mathcal{N}(0, \sigma^2)$.
   - can we rewritten as $Y_i \sim \mathcal{N}(\theta^T X_i, \sigma^2)$.
2. Gaussian nonlinear regression model (heteroskedastic) :
   - $Y_i = G(\theta_1^T X_i) + \varepsilon_i$, $\varepsilon_i \sim \mathcal{N}(0, (\theta_2^T X_t)^2)$.
   - can we rewritten as $Y_i \sim \mathcal{N}(G(\theta^T X_i), (\theta_2^T X_t)^2)$.
3. Poisson regression : $Y_i = \mathcal{P}(\exp(\theta^T X_i))$.
4. logistic, gamma, binomial, whateveryouwant regression...

Problem in these examples

Regression model

In general, we will consider a parametric model $(P_\theta)_{\theta\in\Theta}$, a function $g : (\Lambda \times \mathcal{X}) \to \Theta$ and

$$Y_i | X_i = x \sim P_{g(\lambda,x)}.$$

Until now, MMD estimation allows us to model the distributions, not conditional distributions.

	truth	model	empirical
X	P_X^0	Q_μ	$\hat{P}_X^0 = \frac{1}{n}\sum_{i=1}^n \delta_{X_i}$
$Y\|X$	$P_{Y\|X}^0$	$P_{g(\lambda,X)}$	NA
(X,Y)	$P^0 = P_X^0 P_{Y\|X}^0$	$R_{(\mu,\lambda)} = Q_\mu P_{g(\lambda,X)}$	$\hat{P}^0 = \frac{1}{n}\sum_{i=1}^n \delta_{(X_i,Y_i)}$

Various approaches

	truth	model	empirical
X	P_X^0	Q_μ	$\hat{P}_X^0 = \frac{1}{n}\sum_{i=1}^n \delta_{X_i}$
$Y\|X$	$P_{Y\|X}^0$	$P_{g(\lambda,X)}$	NA
(X,Y)	$P^0 = P_X^0 P_{Y\|X}^0$	$R_{(\mu,\lambda)} = Q_\mu P_{g(\lambda,X)}$	$\hat{P}^0 = \frac{1}{n}\sum_{i=1}^n \delta_{(X_i,Y_i)}$

Fix a kernel $k((x,y),(x',y'))$. 3 approaches :

1. completely parametric : $\widehat{(\mu,\lambda)} = \arg\min_{(\mu,\lambda)} \mathrm{MMD}_k(Q_\mu P_{g(\lambda,X)}, \hat{P}^0)$.

   $\to$ what is the effect of a misspecification in Q_μ?

2. semi-parametric 1 : $\widehat{(Q,\lambda)} = \arg\min_{(Q,\lambda)} \mathrm{MMD}_k(QP_{g(\lambda,X)}, \hat{P}^0)$.

   $\to$ we dont know how to minimize this.

3. semi-parametric 2 : $\widehat{\lambda} = \arg\min_{\lambda} \mathrm{MMD}_k(\hat{P}_X^0 P_{g(\lambda,X)}, \hat{P}^0)$.

   $\to$ our approach.

Explicit minimization problem

$$\widehat{\lambda} = \arg\min_{\lambda} C(\lambda) := \mathrm{MMD}_k(\hat{P}^0_X P_{g(\lambda,X)}, \hat{P}^0).$$

$$\begin{aligned} C(\lambda) = \frac{1}{n} \sum_{i,j=1}^{n} & \mathbb{E}_{Y\sim P_{g(\lambda,X_i)}, Y'\sim P_{g(\lambda,X_j)}} k((X_i, Y), (X_j, Y')) \\ & - \frac{2}{n} \sum_{i,j=1}^{n} \mathbb{E}_{Y\sim P_{g(\lambda,X_i)}} k((X_i, Y), (X_j, Y_j)) \\ & \qquad + \frac{1}{n} \sum_{i,j=1}^{n} k((X_i, Y_i), (X_j, Y_j)) \end{aligned}$$

We also proposed an approximation $\tilde{\lambda}$ of this estimator by removing the non-diagonal terms. We have an asymptotic theory for $\tilde{\lambda}$.

Theoretical results : fixed design

$$\widehat{\lambda} = \arg\min_{\lambda} C(\lambda) := \mathrm{MMD}_k(\hat{P}^0_X P_{g(\lambda,X)}, \hat{P}^0).$$

Theorem

Assume $|k| \leq 1$. Then

$$\mathbb{E}_{Y_1,\dots,Y_n}\left[\mathrm{MMD}_k(\hat{P}^0_X P_{g(\hat{\lambda},X)}, \hat{P}^0_X P^0_{Y|X})\right] \leq \min_{\lambda} \mathrm{MMD}_k(\hat{P}^0_X P_{g(\lambda,X)}, \hat{P}^0_X P^0_{Y|X}) + \frac{2}{\sqrt{n}}.$$

The result is a relatively easy adaptation of the general theory of MMD.

Theoretical results : fixed design

Theorem

Assume :

1. $|k| \leq 1$,
2. $k((x,y),(x',y')) = k_1(x,x')k_2(y,y')$, with associated RKHS $\mathcal{H}_1$ and $\mathcal{H}_2$.
3. for any $f_2 \in \mathcal{H}_2$, for any $\lambda \in \Lambda$, $f_1(x) := \mathbb{E}_{Y\sim P_{g(\lambda,x)}}[f_2(Y)]$ satisfies $f_1 \in \mathcal{H}_1$.

There is a constant $C(k_1)$ that depends only on k_1 such that

$$\mathbb{E}\left[\mathrm{MMD}_k(P_X^0 P_{g(\hat{\lambda},X)}, P^0)\right] \leq \min_{\lambda} \mathrm{MMD}_k(P_X^0 P_{g(\lambda,X)}, P^0) + \frac{C(k_1)\sqrt{2}+3}{\sqrt{n}}.$$

Kernels satisfying our conditions

For any $f_2 \in \mathcal{H}_2$, for any $\lambda \in \Lambda$, $f_1(x) := \mathbb{E}_{Y \sim P_{g(\lambda,x)}}[f_2(Y)]$ satisfies $f_1 \in \mathcal{H}_1$.

- not easy.
- famous paper claiming that it is true regardless of $P_{g(\lambda,x)}$, + erratum.
- derivations in our paper to provide examples : 10 pages. Take home message : Matérn kernels + a transformation of the inputs work for all the classical regression models.

Numerical examples : linear regression

τ	type	n	$\beta_{\mathrm{ols},n}$	$\beta_{\mathrm{lad},n}$	$\beta_{\mathrm{rob},n}$	$\hat{\beta}_n$	$\tilde{\beta}_n$
0		100	0.372	0.353	0.350	0.355	0.334
		1 000	0.116	0.092	0.104	0.108	0.107
		5 000	0.053	0.039	0.046	0.049	0.047
1	Y	100	0.464	0.339	0.385	0.350	0.342
		1 000	0.181	0.094	0.106	0.105	0.097
		5 000	0.103	0.043	0.049	0.054	0.051
2	Y	100	0.647	0.351	0.359	0.337	0.333
		1 000	0.241	0.097	0.110	0.114	0.115
		5 000	0.175	0.039	0.047	0.051	0.052
3	Y	100	0.724	0.331	0.343	0.329	0.320
		1 000	0.309	0.100	0.108	0.113	0.110
		5 000	0.250	0.043	0.048	0.053	0.055
1	X	100	0.870	0.356	0.374	0.342	0.338
		1 000	0.836	0.111	0.105	0.104	0.096
		5 000	0.818	0.065	0.049	0.054	0.052
2	X	100	1.575	0.400	0.347	0.337	0.331
		1 000	1.467	0.160	0.110	0.112	0.115
		5 000	1.401	0.119	0.046	0.051	0.052
3	X	100	1.838	0.442	0.344	0.331	0.323
		1 000	1.805	0.216	0.108	0.113	0.109
		5 000	1.771	0.183	0.048	0.054	0.056

Table 1: Results for the Gaussian linear regression model. For each experimental setting we report the RMSE over 25 replications.

Numerical examples : gamma regression

ϵ	n	θ_{mle}	θ_{rob}	$\hat{\theta}_n$	$\tilde{\theta}_n$
0%	100	0.478	0.425	0.501	0.498
	1 000	0.123	0.120	0.142	0.144
	5 000	0.055	0.053	0.067	0.069
1%	100	0.394	0.398	0.521	0.521
	1 000	0.250	0.108	0.149	0.148
	5 000	0.350	0.049	0.071	0.070
2%	100	0.395	0.381	0.539	0.545
	1 000	0.353	0.113	0.146	0.145
	5 000	0.551	0.056	0.073	0.073
3%	100	0.441	0.407	0.471	0.475
	1 000	0.349	0.119	0.157	0.158
	5 000	0.631	0.069	0.076	0.078

ϵ	n	β_{mle}	β_{rob}	$\hat{\beta}_n$	$\tilde{\beta}_n$
0%	100	0.308	0.306	0.444	0.443
	1 000	0.087	0.093	0.132	0.133
	5 000	0.041	0.043	0.061	0.063
1%	100	0.297	0.313	0.473	0.475
	1 000	0.114	0.098	0.132	0.133
	5 000	0.070	0.042	0.061	0.059
2%	100	0.302	0.301	0.490	0.493
	1 000	0.120	0.094	0.127	0.127
	5 000	0.105	0.046	0.066	0.067
3%	100	0.296	0.296	0.403	0.406
	1 000	0.119	0.091	0.138	0.136
	5 000	0.129	0.044	0.067	0.069

Figure 1: Results for the Gamma regression model. For each experimental setting, we report the mean square error over 25 replications.

La fin

終わり

ありがとう ございます。