Superefficient estimation of the intensity of a stationary Poisson point process via the Stein method

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Considered as the father of different problems related to optimal estimation, stochastic calculus, ...
Back to the initial ideas of Charles Stein

Considered as the father of different problems related to optimal estimation, stochastic calculus, . . . Everything started in the following context

- Let $X \sim \mathcal{N}(\theta, \sigma^2 I_d)$
  where $I_d$ is the $d$-dimensional identity matrix.
- Objective: estimate $\theta$ based on a **single** (for simplicity) observation $X$. 

Stein (1956) 

$$
\hat{\theta}_{S} = \left(1 - \frac{b(a + X^2_i)}{\|X\|_2} - 1\right) X_i \quad i = 1, \ldots, d \Rightarrow \text{MSE}(\hat{\theta}_{S}) \leq \text{MSE}(\hat{\theta}_{mle}) \text{ when } d \geq 3
$$

James-Stein (1961) 

$$
\hat{\theta}_{JS} = X \left(1 - \frac{(d - 2)}{\|X\|_2^2}\right) \Rightarrow \text{MSE}(\hat{\theta}_{JS}) \leq \text{MSE}(\hat{\theta}_{mle}) \text{ when } d \geq 3
$$

Stein (1981) key-ingredients for the class: 

$$
\hat{\theta} = X + g(X),
g: \mathbb{R}^d \to \mathbb{R}^d.
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- $\hat{\theta}^{mle} = X$ minimizes $\operatorname{MSE}(\hat{\theta}) = \mathbb{E}\left(\|\hat{\theta} - \theta\|^2\right)$ among unbiased estimators.
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- Stein (1956)
  
  $\widehat{\theta}_S = \left( (1 - b(a + X_i^2)^{-1})X_i \right)_{i=1, \ldots, d} \Rightarrow \text{MSE}(\widehat{\theta}_S) \leq \text{MSE}(\widehat{\theta}_{mle}) \text{ when } d \geq 3$

- James-Stein (1961)
  
  $\widehat{\theta}_{JS} = X(1 - (d - 2)/\|X\|^2) \Rightarrow \text{MSE}(\widehat{\theta}_{JS}) \leq \text{MSE}(\widehat{\theta}_{mle}) \text{ when } d \geq 3$

- Stein (1981) key-ingredients for the class: $\widehat{\theta} = X + g(X), \quad g : \mathbb{R}^d \rightarrow \mathbb{R}^d$. 
MSE of $\hat{\theta} = X + g(X)$ ($X \sim \mathcal{N}(\theta, \sigma^2 I_d, \sigma^2 \text{ known})$

\[
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$$\text{MSE}(\hat{\theta}) = \mathbb{E}\|X - \theta\|^2 + \mathbb{E}\|g(X)\|^2 + 2 \sum_{i=1}^{d} \mathbb{E}((X_i - \theta_i) g_i(X))$$
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1. Using an IbP for Gaussian r.v. $\mathbb{E}[Zh(Z)] = \mathbb{E}[h'(Z)]$, $Z \sim \mathcal{N}(0, 1)$

$$\text{MSE}(\hat{\theta}) = \text{MSE}(\hat{\theta}_{mle}) + \mathbb{E}\|g(X)\|^2 + 2\sigma^2 \sum_{i=1}^{d} \mathbb{E}\nabla g_i(X)$$
MSE of \( \hat{\theta} = X + g(X) \) \( (X \sim \mathcal{N}(\theta, \sigma^2 I_d, \sigma^2 \text{ known}) \)

\[
\text{MSE}(\hat{\theta}) = \text{E}[\|X - \theta\|^2] + \text{E}[\|g(X)\|^2] + 2 \sum_{i=1}^{d} \text{E}((X_i - \theta_i)g_i(X))
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2. Now choose \( g = \sigma^2 \nabla \log f \). Use the well-known fact [based on product and chain–rules] that for \( h : \mathbb{R} \rightarrow \mathbb{R} \),

\[
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$$(\log(h)')^2 + 2(\log h)'' = 4 \frac{\sqrt{h}''}{\sqrt{h}}. \text{ Get }$$

$$\text{MSE}(\hat{\theta}) = \text{MSE}(\hat{\theta}_{mle}) + 4\sigma^2 \mathbb{E}\left(\nabla \nabla \frac{\sqrt{f(X)}}{\sqrt{f(X)}}\right) \leq \text{MSE}(\hat{\theta}_{mle}) \text{ if } \nabla \nabla \sqrt{f} \leq 0.$$
MSE of $\hat{\theta} = X + g(X)$ ($X \sim \mathcal{N}(\theta, \sigma^2 I_d, \sigma^2 \text{ known})$)

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**Goal**: mimic both steps, derive a Stein estimator for the intensity of a Poisson point process [extension Privault-Réveillac (2009), $d = 1$]
Point processes

- $S$: Polish state space of the point process (equipped with the $\sigma$-algebra of Borel sets $\mathcal{B}$).
- A configuration of points is denoted $x = \{x_1, \cdots, x_n, \cdots\}$. For $B \subset S: x_B = x \cap B$.
- $N_{lf}$: space of locally finite configurations, i.e.
  \[ \{x, n(x_B) = |x_B| < \infty\}, \forall B \text{ bounded} \in S \]
  equipped with
  \[ N_{lf} = \sigma(\{x \in N_{lf}, n(x_B) = m\}; B \in \mathcal{B}, B \text{ bounded}, m \geq 1). \]

**Definition**

A point process $X$ defined on $S$ is a measurable application defined on some probability space $(\Omega, \mathcal{F}, \mathbb{P})$ with values on $N_{lf}$.

Measurability of $X \iff N(B) = |X_B|$ is a r.v. for any bounded $B \in \mathcal{B}$. 
Definition of a Poisson point process with intensity $\rho(\cdot)$.

- $\forall m \geq 1$, $\forall$ bounded and disjoint $B_1, \cdots, B_m \subset S$, the r.v. $X_{B_1}, \cdots, X_{B_m}$ are independent.
- $N(B) \sim \mathcal{P}(\int_B \rho(u)du)$
- $\forall B \subset S$, $\forall F \in \mathcal{N}_f$

$$\mathbb{P}(X_B \in F) = \sum_{n \geq 0} \frac{e^{-\int_B \rho(u)du}}{n!} \int_B \cdots \int_B 1(\{(x_1, \cdots, x_n) \in F\}) \prod_{i=1}^n \rho(x_i)dx_i$$

Notation : $X \sim \text{Poisson}(S, \rho)$. 
Case considered here $\rho(u) \equiv \theta$.

- $X$ homogeneous Poisson point process with intensity $\theta$.
- We assume observing $X$ on $W \subset \mathbb{R}^d$.
- Given $N(W) = n$, we denote $X_1, \ldots, X_n$ the $n$ points in $W$.
- The MLE estimate of the intensity $\theta$ is $\hat{\theta} = N(W)/|W|$.
- Construction of a Stein estimator of $\theta$?
\( S \): space of Poisson functionals \( F \) defined on \( \Omega \) by

\[
F = f_0 1(N(W) = 0) + \sum_{n \geq 1} 1(N(W) = n)f_n(X_1, \ldots, X_n),
\]

\( f_0 \in \mathbb{R}, f_n : W^n \rightarrow \mathbb{R}^d \) measurable symmetric functions called form functions of \( F \).
Towards a Stein estimator (1)

- MLE is defined by $\hat{\theta}^{mle} = N(W)/|W|$.
- Aim: define $\hat{\theta}$ of the form $\hat{\theta} = \hat{\theta}^{mle} + \frac{1}{|W|}\zeta$ where $\zeta = \nabla \log(F)$.
- Relation $\text{MSE}(\hat{\theta}) < \text{MSE}(\hat{\theta}^{mle})$ satisfied?

$$\text{MSE}(\hat{\theta}) = \mathbb{E}\left[\left(\hat{\theta}^{mle} + \frac{1}{|W|}\nabla \log F - \theta\right)^2\right]$$

$$= \text{MSE}(\hat{\theta}^{mle}) + \frac{1}{|W|^2} \left(\mathbb{E}[\nabla \log F]^2 + 2\mathbb{E}[\nabla \log F(N(W) - \theta|W|)]\right)$$

$\implies$ Need to transform $2\mathbb{E}[G(N(W) - \theta|W|)]$ with $G = \nabla \log F$ using a IbP formula.

- Notion of derivative?
Differential operator: let $\pi : W^2 \to \mathbb{R}^d$

$$D_x^\pi F = - \sum_{n \geq 1} 1(N(W) = n) \sum_{i=1}^n (\nabla_{x_i} f_n)(X_1, \ldots, X_n)\pi(X_i, x) ,$$

where $S' = \{ F \in S : 'the f_n are cont. diff. in any variable x_i' \}$ and where $\nabla_{x_i} f_n$ gradient of $x_i \mapsto f_n(\ldots, x_i, \ldots)$.
Lemma [product and chain rules]

For any $x \in W$, for all $F, G \in S'$, $g \in C^1_b(\mathbb{R})$ we have

$$D^\pi_x(FG) = (D^\pi_x F)G + F(D^\pi_x G) \quad \text{and} \quad D^\pi_x g(F) = g'(F)D^\pi_x F.$$
Lemma [product and chain rules]

For any $x \in W$, for all $F, G \in S'$, $g \in C^1_b(\mathbb{R})$ we have

$$D_x^\pi (FG) = (D_x^\pi F)G + F(D_x^\pi G) \quad \text{and} \quad D_x^\pi g(F) = g'(F)D_x^\pi F.$$ 

To get an IbP type formula, we need to introduce $\text{Dom}(D^\pi)$ of $S'$ as

$$\text{Dom}(D^\pi) = \left\{ F \in S' : \forall n \geq 1 \text{ and } z_1, \ldots, z_n \in \mathbb{R}^d \right\}$$

$$f_{n+1}\big|_{z_{n+1} \in \partial W}(z_1, \ldots, z_{n+1}) = f_n(z_1, \ldots, z_n), \quad f_1|_{z \in \partial W}(z) = 0 \right\}, \quad (1)$$

Remark: compatibility conditions important to derive a correct Stein estimator.
Integration by parts formula

Theorem

Let \( G \in \text{Dom}(\overrightarrow{D}^\pi) \), \( V : \mathbb{R}^d \to \mathbb{R} \), \( V \in C^1(W, \mathbb{R}^d) \)

\[
E \left[ \int_W D^\pi_x G \cdot V(x) dx \right] = E \left[ F \left( \sum_{u \in X_W} \nabla \cdot V(u) - \theta \int_W \nabla \cdot V(u) du \right) \right]
\]

where \( V : W \to \mathbb{R}^d \) is defined by \( V(u) = \int_W V(x) \pi(u, x) dx \).
Integration by parts formula

**Theorem**

Let $G \in \text{Dom}(\overline{D}^\pi)$, $V : \mathbb{R}^d \to \mathbb{R}$, $V \in C^1(W, \mathbb{R}^d)$

$$
\mathbb{E} \left[ \int_W D_x^\pi G \cdot V(x) dx \right] = \mathbb{E} \left[ F \left( \sum_{u \in X_W} \nabla \cdot \mathcal{V}(u) - \theta \int_W \nabla \cdot \mathcal{V}(u) du \right) \right]
$$

where $\mathcal{V} : W \to \mathbb{R}^d$ is defined by $\mathcal{V}(u) = \int_W V(x)\pi(u, x)dx$.

Main application: let $\pi(u, x) = u^\top V(x)$, we can find some $V$ (omit details) such that $\mathcal{V}(u) = u/d$ and $\nabla \cdot \mathcal{V}(u) = 1$. Then

$$
\nabla G = \nabla^{\pi, V} G = -\frac{1}{d} \sum_{n \geq 1} 1(N(W) = n) \sum_{i=1}^n \nabla_{x_i} g_n(X_1, \ldots, X_n) \cdot X_i
$$

$$
\Rightarrow \quad \mathbb{E}[\nabla G] = \mathbb{E} [G(N(W) - \theta|W|)] .
$$
Towards a Stein estimator (2) : end of the proof

**Theorem**

Let \( \hat{\theta} = \hat{\theta}^{mle} + \frac{1}{|W|} \zeta \) where \( \zeta = \nabla \log(F) \) is such that \( \zeta \in \text{Dom}(D^\pi) \) then

\[
\text{MSE}(\hat{\theta}) = \text{MSE}(\hat{\theta}^{mle}) + \frac{4}{|W|^2} E\left( \nabla \nabla \frac{\sqrt{F}}{\sqrt{F}} \right).
\]

**Proof:**

\[
\text{MSE}(\hat{\theta}) = E\left[ \left( \hat{\theta}^{mle} + \frac{1}{|W|} \nabla \log F - \theta \right)^2 \right]
\]

\[
= \text{MSE}(\hat{\theta}^{mle}) + \frac{1}{|W|^2} \left( E[(\nabla \log F)^2] + 2E[(\nabla \log F)(N(W) - \theta|W|)] \right)
\]

\[
= \text{MSE}(\hat{\theta}^{mle}) + \frac{1}{|W|^2} \left( E[(\nabla \log F)^2] + 2E[\nabla \nabla \log F] \right)
\]

\[
= \ldots
\]
Non-uniqueness of the integration by parts formula

- Natural and easier to define an isotropic Stein estimator. With

\[ \nabla \log F = -\frac{1}{d} \sum_{n \geq 1} \mathbf{1}(N(W) = n) \sum_{i=1}^{n} \nabla x_i (\log f_n)(X_1, \ldots, X_n) \cdot X_i \]

\( \log F \) is isotropic \( \Rightarrow \nabla \log F \) is isotropic (and so will be \( \hat{\theta} \)).
- Other possible choices to get \( \text{div} \mathcal{V}(y) = 1 \):
  \[ V(x) = (d|W|)^{-1/2} \mathbf{1}(x \in W)1^\top, \pi(y, x) = y^\top V(x) \]. New gradient operator:

\[ \nabla \log F = -\sum_{n \geq 1} \mathbf{1}(N(W) = n) \sum_{i=1}^{n} \left( \text{div} x_i \log f_n \right)(X_1, \ldots, X_n) \times \bar{X}_i \]

- Formula \( E[\nabla \log F] = E[\log F(N(W) - \theta|W|)] \) still holds. But...

1. non isotropic.
2. can induce some discontinuity problems when computing \( \nabla \log F \) and \( \nabla \nabla \log F \) . . .
Example in the $d$-dimensional euclidean ball $W = B_d(0, 1)$

- For $1 \leq k \leq n$, $x_{(k),n}$ $k$th closest (wrt $\| \cdot \|$) point of $\{x_1, \ldots, x_n\}$ to zero.
- $X_k$ $k$th closest point to 0 of the PPP $X$ (defined on $\mathbb{R}^d$)
- We define

  \[ \varphi(t) = e^{\gamma(1-t)^\kappa} \mathbf{1}(t \leq 1), \quad \gamma \in \mathbb{R}, \; \kappa > 2 \]

  \[ F_k = \mathbf{1}(N(W) < k) + \sum_{n \geq k} \mathbf{1}(N(W) = n) \varphi(\|X_{(k),n}\|^2) \]

  \[ Gain(\hat{\theta}_k) = 1 - \frac{\text{MSE}(\hat{\theta}_k)}{\text{MSE}(\hat{\theta}_{mle})} \]
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$$F_k = \mathbf{1}(N(W) < k) + \sum_{n \geq k} \mathbf{1}(N(W) = n) \varphi(\|X_{(k),n}\|^2)^2.$$ 

$$\text{Gain}(\hat{\theta}_k) = 1 - \frac{\text{MSE}(\hat{\theta}_k)}{\text{MSE}(\hat{\theta}_{mle})}$$

**Theorem**

$$\zeta_k = \nabla \log(F_k) \in \text{Dom}(\overrightarrow{D}) \quad \varphi > 0, \quad \varphi'(1) = 0$$

and

$$\hat{\theta}_k = \hat{\theta}_{mle} - \frac{4d}{|W|} \frac{\varphi'(\|X_{(k)}\|^2)}{\varphi(\|X_{(k)}\|^2)} = \hat{\theta}_{mle} - \frac{4d}{|W|} \left\{ \gamma \kappa \left(1 - \|X_{(k)}\|^2\right)^{\kappa-1} \right\}$$

$$\text{Gain}(\hat{\theta}_k) = E[ G(\|X_{(k)}\|^2) ] \quad \text{where} \quad G(t) = -\frac{16}{d^2 \theta |W|} \frac{t (\varphi'(t) + t \varphi''(t))}{\varphi(t)}$$
Theoretical gains with $\varphi(t) = e^{\gamma(1-t)^\kappa}; \kappa = 3; \gamma = -3$

- $m = 50000$ replications of $PPP_\theta(B(0, 1), \theta), d = 2$.

- Empirical and Monte-Carlo approximations of theoretical gains, for different parameters $k, \kappa, \gamma$.

- General comments:
  1. The IbP formula is empirically checked.
  2. The parameters $k, \kappa, \gamma$ and $\theta$ are strongly connected. A bad choice can lead to **negative** gains [$\varphi'(t) + t\varphi''(t)$ may be negative for some values of $t$].
• $m = 50000$ replications of $PPP(\mathcal{B}(0, 1), \theta)$, $d = 2$.

• Monte-Carlo approximations of theoretical gains for different values of $k$. The parameters $\kappa$ and $\gamma$ optimize $\text{Gain}(\hat{\theta}_k)$ for each value of $\theta$.

• **General comments:**
  1. For any $k$, if we optimize in terms of $\kappa$ and $\gamma$, the gain becomes always positive.
  2. Still, if we want interesting values of gains, $k$ needs to be optimized.
Simulation based on \( m = 50000 \) replications.

For each value of \( \theta, d \)

\[
(k^*, \gamma^*, \kappa^*) = \text{argmax}_{(k, \gamma, \kappa)} \text{Gain}(\hat{\theta}_k) = \text{argmax}_{(k, \gamma, \kappa)} \mathbb{E}[\mathcal{G}(\|X(k)\|^2)].
\]

<table>
<thead>
<tr>
<th>( \theta = 5, d = 1 )</th>
<th>MLE</th>
<th>STEIN</th>
<th>Gain (%)</th>
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<td>sd</td>
<td>mse</td>
<td>mean</td>
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<td>sd</td>
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<td>mse</td>
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<tr>
<td>40</td>
<td>3.1</td>
<td>9.58</td>
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</table>
Data-driven estimator: replace $\theta$ by $\hat{\theta}_{mle}$ in the optimization

- Simulation based on $m = 5000$ replications.
- For each value of $\theta$, $d$, let $\Theta(\theta, \rho) = [\theta - \rho \sqrt{\theta/|W|}, \theta + \rho \sqrt{\theta/|W|}]$. Then, we suggest define $\kappa^*$, $\gamma^*$ as the maximum of

$$
\int_{\Theta(\hat{\theta}_{MLE}, \rho)} \text{Gain}(\hat{\theta}_k) d\theta = \frac{16}{d^2|W|} \mathbb{E} \int_{\Theta(\hat{\theta}_{MLE}, \rho)} \frac{G(Y_{(k)})}{\theta} d\theta.
$$

(2)

<table>
<thead>
<tr>
<th>$\theta$, $d$</th>
<th>$\rho$ = 0</th>
<th>$\rho$ = 1</th>
<th>$\rho$ = 1.6449</th>
<th>$\rho$ = 1.96</th>
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<td>48.8</td>
<td>47.9</td>
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<td>32.0</td>
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<td>$\theta = 20$, $d = 1$</td>
<td>37.3</td>
<td>38.6</td>
<td>34.5</td>
<td>28.0</td>
</tr>
<tr>
<td>$d = 2$</td>
<td>27.3</td>
<td>33.1</td>
<td>31.0</td>
<td>26.5</td>
</tr>
<tr>
<td>$d = 3$</td>
<td>20.8</td>
<td>28.6</td>
<td>28.1</td>
<td>23.8</td>
</tr>
<tr>
<td>$\theta = 40$, $d = 1$</td>
<td>22.3</td>
<td>30.8</td>
<td>29.2</td>
<td>23.9</td>
</tr>
<tr>
<td>$d = 2$</td>
<td>16.3</td>
<td>24.0</td>
<td>28.2</td>
<td>24.4</td>
</tr>
<tr>
<td>$d = 3$</td>
<td>12.7</td>
<td>19.0</td>
<td>24.5</td>
<td>22.0</td>
</tr>
</tbody>
</table>
A few more comments

- Even if the results are done under the Poisson assumption, if the simulated model
  - is clustered (e.g. Thomas, LGCP) the empirical gains (compared to $N(W)/|W|$) are significant.
  - is regular the empirical gains seems to be close to zero (not really worse than $N(W)/|W|$)

Perspectives

1. Deriving a general IbP formula for inhomogeneous Poisson point processes or Cox point processes seems reasonable.
2. Exploit the IbP for other statistical methodologies.


\[
\varphi(t) = e^{\gamma(1-r)^k}; \quad k = 3; \quad \gamma = -3
\]

\[\Rightarrow \quad G(t) \text{ is not positive everywhere but when } t \text{ is large (i.e. when } \|X(\cdot)\| \text{ is large, i.e. when } k \text{ is large), then } G(\cdot) \text{ is positive and can reach high values.}\]
Comparison with Privault-Réveillac’s estimator when $d = 1$

- Assume $X$ is observed on $\tilde{W} = [0, 2]$.
- Let $X_1$ be the closest point of $X$ to 0, then $\hat{\theta}_{pr}$ is defined for some $\kappa > 0$ by

$$\hat{\theta}_{pr} = \hat{\theta}_{mle} + \frac{2}{\kappa} \mathbf{1}(N(\tilde{W}) = 0) + \frac{2X_1}{2(1 + \kappa) - X_1} \mathbf{1}(0 < X_1 \leq 2).$$

Note that $X_1 \sim \mathcal{E}(\theta)$.
- The gain writes

$$\text{Gain}(\hat{\theta}_{pr}) = \frac{2}{\theta \kappa^2} \exp(-2\theta) - \frac{2}{\theta} \mathbb{E}\left(\frac{X_1}{2(1 + \kappa) - X_1} \mathbf{1}(X_1 \leq 2)\right).$$

---

Gain optimized in $\kappa$ in terms of $\theta$. 

![Graph showing gain optimized in $\kappa$ in terms of $\theta$.]