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Statistical estimation of the division rate of a size-structured population

M. Doumic, M. Hoffmann, P. Reynaud-Bouret, V. Rivoirard

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Main results







2 Goldenshluger and Lepski's method





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The informal problem and the PDE translation

- A cell grows.
- Depending on its size x, the cell has a certain chance to divide itself in 2 offsprings, ie 2 cells of size x/2.
- We are interesting by the evolution of the whole population of cells, each of them having this behavior.

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Size-Structured Population Equation (finite time)

$$\begin{cases} \frac{\partial}{\partial t}(n(t,x)) + \kappa \frac{\partial}{\partial x}(g(x)n(t,x)) + B(x)n(t,x) = 4B(2x)n(t,2x),\\ n(t,x=0) = 0, \quad t > 0\\ n(0,x) = n_0(x), \quad x \ge 0. \end{cases}$$

- n(t,x) the "amount" of cells with size $x \neq density$),
- g the "qualitative" growth rate of one cell: linear is $g = 1 \dots$
- *B* is the division rate, which depends on the size

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Asymptotics of the PDE

It can be shown (Perthame Ryzhik 2005 for instance) that

- n(t, .) grows exponentially fast ie I_t = ∫ n(t, x)dx asymptotically proportional to e^{λt},
- the renormalized $n(t, x)/I_t$ tends to a density N, which satisfies

Size-Structured Population Equation (asymptotics)

$$\begin{cases} \kappa \frac{\partial}{\partial x} (g(x)N(x)) + \lambda N(x) = \mathcal{L}(BN)(x) \\ B(0)N(0) = 0, \qquad \int N(x) dx = 1, \end{cases}$$

where

The inverse problem

Under the previous differential equation, we consider the inverse problem of finding B given a "noisy" version of N.

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- Analytical point of view: N_{ϵ} is a noisy version of N, less regular than N (it is likely that no derivative exists) and $||N N_{\epsilon}||_2 \le \epsilon$. (see Perthame, Zubelli, etc)

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- Statistical point of view: we observe a *n*-sample $X_1, ..., X_n$ of iid variables with density *N*.

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Analytical point of view

Pro: taking into account maybe more approximations (but not all), results true for any N_{ϵ} .

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Con: N_{ϵ} is probably differentiable. If there are numerical methods which adapt to the regularity of N (discrepancy principle), they need to know ϵ .

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Pro: Framework close to what biologists do, true inverse problem. We can adapt to the regularity, noise is given by the sample size.

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Estimation of N

Let $K : \mathbb{R} \to \mathbb{R}_+$ continuous function $/ \int K = 1$ and $\int K^2 < \infty$.

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$$\hat{N}_h(x) := \frac{1}{n} \sum_{i=1}^n K_h(x - X_i),$$

 $K_h = \frac{1}{h} K(./h).$

Bias-Variance decomposition

$$\mathbb{E}\left(\left\|\boldsymbol{N}-\hat{\boldsymbol{N}}_{h}\right\|_{2}\right)\leq\left\|\boldsymbol{N}-\boldsymbol{K}_{h}\star\boldsymbol{N}\right\|_{2}+\frac{1}{\sqrt{nh}}\|\boldsymbol{K}\|_{2},$$

where $K_h \star N = \mathbb{E}(\hat{N}_h)$

How to adaptively select h?

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How to adaptively select h? Recent work of Goldenshluger and Lepski (2009, 2010) Here just a "toy" version, but that's exactly what we needed.

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Main results

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Selection of bandwidth

Set for any x and any h, h' > 0, $\hat{N}_{h,h'}(x) := \frac{1}{n} \sum_{i=1}^{n} (K_h \star K_{h'})(x - X_i) = (K_h \star \hat{N}_{h'})(x),$

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"estimator" of the bias term

$$A(h) := \sup_{h' \in \mathcal{H}} \left\{ \|\hat{N}_{h,h'} - \hat{N}_{h'}\|_2 - \frac{\chi}{\sqrt{nh'}} \|K\|_2 \right\}_+$$

where, given $\varepsilon > 0$, $\chi := (1 + \varepsilon)(1 + ||K||_1)$.

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$$\hat{h} := \arg\min_{h \in \mathcal{H}} \left\{ A(h) + rac{\chi}{\sqrt{nh}} \|K\|_2
ight\} \quad ext{and} \quad \hat{N} := \hat{N}_{\hat{h}}.$$

First result

Oracle inequality If $\mathcal{H} = \{1/\ell \ / \ \ell = 1, ..., \ell_{max}\}$ and if $\ell_{max} = \delta n$, if moreover $\|N\|_{\infty} < \infty$, then for any $q \ge 1$,

$$\mathbb{E}\left(\|\hat{N}-N\|_{2}^{2q}\right) \leq \Box_{q}\chi^{2q}\inf_{h\in\mathcal{H}}\left\{\|K_{h}\star N-N\|_{2}^{2q}+\frac{\|K\|_{2}^{2q}}{(hn)^{q}}\right\}+$$
$$\Box_{q,\varepsilon,\delta,\|K\|_{2},\|K\|_{1},\|N\|_{\infty}}\frac{1}{n^{q}}.$$

Estimation of $D = \frac{\partial}{\partial x} (g(x)N(x))$

If K is differentiable, $\int K = 1$ and $\int |K'|^2 < \infty$.

$$\hat{D}_h(x) := \frac{1}{n} \sum_{i=1}^n g(X_i) \mathcal{K}'_h(x - X_i)$$

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Bias-Variance de composition:

$$\mathbb{E}(\left\|D - \hat{D}_h\right\|_2) \le \|D - K_h \star D\|_2 + \frac{1}{\sqrt{nh^3}} \|g\|_{\infty} \|K'\|_2.$$

GL's trick $\hat{D}_{h,h'}(x) := \frac{1}{n} \sum_{i=1}^{n} g(X_i) (K_h \star K_{h'})' (x - X_i),$ $\tilde{A}(h) := \sup_{h' \in \tilde{\mathcal{H}}} \left\{ \| \hat{D}_{h,h'} - \hat{D}_{h'} \|_2 - \frac{\tilde{\chi}}{\sqrt{nh'^3}} \| g \|_{\infty} \| K' \|_2 \right\}_+,$

where, given $\tilde{\varepsilon} > 0$, $\tilde{\chi} := (1 + \tilde{\varepsilon})(1 + \|K\|_1)$.

Estimation of
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GL's trick

$$\hat{D}_{h,h'}(x) := \frac{1}{n} \sum_{i=1}^{n} g(X_i) (K_h \star K_{h'})'(x - X_i),$$

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where, given $\tilde{\varepsilon} > 0$, $\tilde{\chi} := (1 + \tilde{\varepsilon})(1 + \|K\|_1)$.

Finally, we estimate D by using $\hat{D}:=\hat{D}_{\tilde{h}}$ with

$$\tilde{h} := \operatorname{argmin}_{h \in \tilde{\mathcal{H}}} \left\{ \tilde{A}(h) + \frac{\tilde{\chi}}{\sqrt{nh^3}} \|g\|_{\infty} \|K'\|_2 \right\}.$$

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Result for the derivative D

Oracle inequality for DIf $\tilde{\mathcal{H}} = \{1/\ell \ / \ \ell = 1, ..., \ell_{max}\}$ and if $\ell_{max} = \sqrt{\delta' n}$, if moreover $\|N\|_{\infty}$ and $\|g\|_{\infty} < \infty$, then for any $q \ge 1$, $\mathbb{E}\left(\|\hat{D} - D\|_{2}^{2q}\right) \le \Box_{q} \tilde{\chi}^{2q} \inf_{h \in \tilde{\mathcal{H}}} \left\{\|K_{h} \star D - D\|_{2}^{2q} + \left[\frac{\|g\|_{\infty} \|K'\|_{2}}{\sqrt{nh^{3}}}\right]^{2q}\right\}$ $+\Box_{q,\tilde{\epsilon},\delta',\|K'\|_{2},\|K\|_{1},\|K'\|_{1},\|N\|_{\infty},\|g\|_{\infty}\frac{1}{n^{q}}.$

Main results

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Estimation of λ and κ

 λ is estimated via another (or simultaneous experiment).

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 λ is estimated via another (or simultaneous experiment).

Assumption on $\hat{\lambda}$

There exist some q > 1 such that

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$$arepsilon_\lambda = \mathbb{E}(|\hat{\lambda}-\lambda|^q) < \infty$$
 ,

•
$$R_{\lambda} = \mathbb{E}(\hat{\lambda}^{2q}) < \infty.$$

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Let c > 0,

$$\hat{\kappa} = \hat{\lambda} \frac{\sum_{i=1}^{n} X_i}{\sum_{i=1}^{n} g(X_i) + c}.$$

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The inversion of \mathcal{L}

It remains to (approximately) invert \mathcal{L} . (see Perthame, Zubelli, Doumic (2009))

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Define T > 0, an integer $k \ge 1$ and the regular grid on [0, T] with mesh $k^{-1}T$ defined by

 $0 = x_{0,k} < x_{1,k} < \cdots < x_{i,k} := \frac{i}{k}T < \cdots < x_{k,k} = T.$ Set $\varphi_{i,k} =: \frac{k}{T} \int_{x_{i,k}}^{x_{i+1,k}} \varphi(x) dx$ for $i = 0, \dots, k-1$, and define by induction the sequence

$$H_{i,k}(\varphi) := \frac{1}{4} (H_{i/2,k}(\varphi) + \varphi_{i/2,k}) \text{ with } \begin{cases} H_0(\varphi) := \frac{1}{3} \varphi_{1,k}, \\ H_1(\varphi) := \frac{4}{21} \varphi_{0,k} + \frac{1}{7} \varphi_{1,k} \end{cases}$$

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for any sequence $u_i, i = 1, 2, \ldots$,

$$u_{i/2} := \begin{cases} u_{i/2} & \text{if } i \text{ is even} \\ \frac{1}{2}(u_{(i-1)/2} + u_{(i+1)/2}) & \text{otherwise.} \end{cases}$$

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Finally, we define

$$\mathcal{L}_{k}^{-1}(\varphi)(x) := \sum_{i=0}^{k-1} H_{i,k}(\varphi) \mathbb{1}_{[x_{i,k},x_{i+1,k})}(x).$$

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Hence we are able to estimate H = BN by

$$\hat{H} = \mathcal{L}_k^{-1}(\hat{\kappa}\hat{D} + \hat{\lambda}\hat{N}).$$

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Oracle inequality for the estimation of H = BN

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Theorem

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• $+ \inf_{h \in \mathcal{H}} \left[\|K_h \star N - N\|_2^q + \left(\frac{\|K\|_2}{\sqrt{nh}} \right)^q \right] +$
• $+ \varepsilon_{\lambda} +$

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•
$$+\varepsilon_{\lambda}+$$

• $+\left(\Box_{\alpha}|\mathcal{L}(BN)|_{\mathcal{C}^{\alpha}(T)}T^{\alpha+1/2}k^{-\alpha}\right)^{q}$ +

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•
$$+ \inf_{h \in \mathcal{H}} \left[\|K_h \star N - N\|_2^q + \left(\frac{\|K\|_2}{\sqrt{nh}} \right)^q \right] + \frac{1}{2} + \varepsilon_{\lambda} + \varepsilon_{\lambda}$$

• +
$$\left(\Box_{\alpha}|\mathcal{L}(BN)|_{\mathcal{C}^{\alpha}(T)}T^{\alpha+1/2}k^{-\alpha}\right)^{q}$$
 +

•
$$\Box_{\dots} \frac{1}{n^{q/2}}$$
.

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Rate of convergence for the estimation of B

We finally set $\hat{B} = \hat{H}/\hat{N}$ and $\tilde{B} = \max(\min(\hat{B}, \sqrt{n}), -\sqrt{n})$.

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Theorem

If one knows a bound $\alpha \geq s$, one can choose a kernel K and a family of \mathcal{H} and \mathcal{H}' independent of s such that for any compact [a, b] of [0, T] (under technical assumptions),

$$\mathbb{E}\left[\left\| (\tilde{B}-B)\mathbf{1}_{[a,b]} \right\|_{2}^{q}\right] = O\left(n^{-\frac{qs}{2s+3}}\right).$$

Main results

Simulations



Simulations



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Concluding remarks

 work still in progress: simulations and comparison to analytical methods

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- Probabilistic interpretation not used: evolution of one cell look like TCP window size, but the whole population (?) → chaos and not necessarily independence (work in progress of Hoffmann, Krell, Lepoutre ...)
- Calibration of GL's method not done, comparison with the L-curve method in analysis (χ Νstep?)