Nonparametric estimation of the division kernel based on a PDE stationary distribution approximation

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en collaboration avec
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Introduction

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Introduction

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- Size-structured population: Individuals are characterized by their sizes, i.e. variables that grow deterministically with time. Here we have in mind that each cell contains some toxicities which play the role of the size.
  - Population with age and size structure modelled by branching process: Harris (1963), Jagers (1969), Athreya and Ney (1970), Tran (2008), Bansaye et al. (2011), Cloez (2011), Hoffmann and Olivier (2014), Bansaye and Méléard (2015) and Doumic et al. (2015).
  - PDE models for size-structured population: Diekmann et al. (1998), Michel (2006), Perthame (2007), Doumic et al. (2009) and Doumic and Gabriel (2010).

Motivation

Our model is motivated by the detection of the cellular aging in biology such as the one put into light by Stewart et al. (2005).

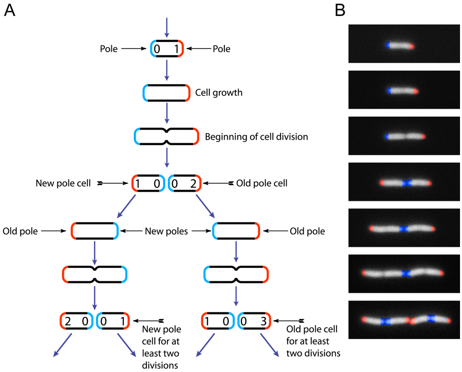

Figure : Cell division of E. Coli *.

*Figure and video are produced by Stewart el al. (2005)

Microscopic model

- Genealogical tree:
  - A cell divides at a rate $R > 0$ and the toxicity grows with rate $\alpha > 0$.
  - Along branches: the toxicity $(X_t, t \geq 0)$ satisfies

$$\mathrm{d}X_t = \alpha \, \mathrm{d}t.$$

  - When a cell divides, a random fraction Γ of the toxicity goes in the first daughter cell and a fraction $1 - \Gamma$ in the second one. We assume that Γ has a symmetric distribution on $[0, 1]$ with a density h.

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- We describe the population of cells at time t by a random point measure in $\mathcal{M}_F(\mathbb{R}_+)^\dagger$:

$$Z_t(\mathrm{d}x) = \sum_{i=1}^{N_t} \delta_{X_t^i}(\mathrm{d}x),$$

where $N_t = \langle Z_t, 1 \rangle = \int_{\mathbb{R}_+} Z_t(\mathrm{d}x)$ is the number of cells living at time t.

$^\dagger \mathcal{M}_F(\mathbb{R}_+)$: the space of finite measures on $\mathbb{R}_+$ embedded with the topology of weak convergence.

Stochastic differential equation

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- For all test function $f_t(x) = f(x,t) \in \mathcal{C}_b^{1,1}(\mathbb{R}_+ \times \mathbb{R}_+, \mathbb{R})^{\ddagger}$, the population of cells is described by:

$$\begin{aligned}\langle Z_t, f_t\rangle =& \langle Z_0, f_0\rangle + \int_0^t \int_{\mathbb{R}_+} \Big(\partial_s f_s(x) + \alpha \partial_x f_s(x)\Big) Z_s(dx)ds \\ &+ \int_0^t \int_0^1 \Big(f_s\left(\gamma x\right) + f_s\left((1-\gamma)x\right) - f_s\left(x\right)\Big) R\, h(\gamma)\, \mathrm{d}\gamma\, \mathrm{d}s + M_t^f,\end{aligned}$$

where M_t^f is a square integrable martingale.

‡ $\mathcal{C}_b^{1,1}(\mathbb{R}_+ \times \mathbb{R}_+, \mathbb{R})$: the set of bounded functions of class $\mathcal{C}^1$ in t and x with bounded derivatives.

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1 Stochastic individual-based model of size-structured populations

2 Estimation of the division kernel

Estimation of the division kernel: case of incomplete data

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The evolution of cells is observed at a fixed time T $\rightarrow$ the whole division tree is not completely observed.

- When the whole division tree is observed (*e.g.* observation of the cell population up to a fixed time T): Hoang, V. H. (2015). Estimating the division kernel of a size-structured population. preprint arXiv:1509.02872.

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- To estimate h, the idea is to approximate the evolution of the population of cells when the initial population size is large by a growth-fragmentation equation.

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- Assume $N_0 = K$, consider the following renormalized stochastic process:

$$Z_t^K(dx) = \frac{1}{K} \sum_{i=1}^{N_t^K} \delta_{X_t^i}(dx),$$

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  where N_t^K is the number of cells alive at time t.
- The parameter K is related to the large population limit which corresponds to $K \to +\infty$.

Growth-fragmentation equation

- Following the works of Fournier and Méléard (2004) and Tran (2008), we prove that $(Z^K)_{K\in\mathbb{N}^*}$ converges to the (weak) solution of the following PDE:

$$\partial_t n(t,x)+\alpha\partial_x n(t,x)+Rn(t,x) = 2R\int_0^1 n\Big(t,\frac{x}{\gamma}\Big)\frac{1}{\gamma}h(\gamma)d\gamma, \quad n(0,x)=n_0(x).$$

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- By the *general relative entropy* (GRE) (see Perthame and Ryzhik (2005)), the division kernel h satisfies the assumptions for the existence (λ, N) of the following eigenvalue problem

$$\begin{cases} \alpha\partial_x N(x) + (\lambda+R)N(x) = 2R\int_0^{+\infty} N(y)h\Big(\frac{x}{y}\Big)\frac{dy}{y}, x\geq 0, \\ N(0)=0, \quad \int N(x)dx = 1, \quad N(x)\geq 0, \quad \lambda > 0, \end{cases}$$

where λ is the first eigenvalue and N is the first eigenvector.

Asymptotic of the PDE

- By the use of the GRE, we have

$$\int_0^{+\infty} \left| n(t,x)e^{-\lambda t} - \langle n_0, \phi \rangle N(x) \right| \phi(x) dx \stackrel{t \to +\infty}{\longrightarrow} 0,$$

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- Since $e^{-\lambda t} n(t,x) \approx N(x)$ as t is large, we assume that we have n i.i.d observations $X_1, \ldots, X_n$ where X_i's have probability distribution $N(x)dx$.
- We estimate h from the data $X_1, \ldots, X_n$ and the eigenvalue problem:

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Estimation procedure: change of variable

- Setting $x = e^u$ and $y = e^v$, $u, v \in \mathbb{R}$ and introduce the functions

$$g(u) = e^u h(e^u),$$

and

$$M(u) = e^u N(e^u), \quad D(u) = \partial_u\big(u \mapsto N(e^u)\big).$$

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- Then the growth-fragmentation equation (asymptotic form)

$$\alpha \partial_x N(x) + (\lambda + R)N(x) = 2R \int_0^{+\infty} N(y) h\Big(\frac{x}{y}\Big) \frac{dy}{y}$$

becomes

$$\alpha D(u) + (\lambda + R)M(u) = 2R\big(M \star g\big)(u).$$

Estimation procedure: assumptions

Assumptions

(A1) The density h is continuous on $[0, 1]$.

(A2) There exists a positive constant C such that for any $t \in (0, 1)$,

$$\int_0^t h(x)dx \leq \min\left(1, Ct^4\right).$$

(A3) For all $\xi \in \mathbb{R}$, $M^*(\xi) \neq 0$.

Estimation procedure

Proposition

Under Assumption (A1)-(A3), the Fourier transform of g is given by

$$g^*(\xi) = \frac{\alpha D^*(\xi)}{2RM^*(\xi)} + \frac{\lambda + R}{2R}, \quad \xi \in \mathbb{R}.$$

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- A natural estimator of g^* is based on unbiased estimates of $D^*(\xi)$ and $M^*(\xi)$:

$$\widehat{M^*(\xi)} = \frac{1}{n}\sum_{j=1}^{n} e^{\mathbf{i}\xi U_j}, \quad \widehat{D^*(\xi)} = (-\mathbf{i}\xi)\frac{1}{n}\sum_{j=1}^{n} e^{(\mathbf{i}\xi - 1)U_j}.$$

Due to the change of variables, we consider the i.i.d random variables $U_1, \dots, U_n$ where $U_i = \log(X_i)$ having density $M(u) = e^u N(e^u)$.

Estimation procedure

- Let K a kernel function in $\mathbb{L}^2(\mathbb{R})$ such that its Fourier transform K^* exists and is compactly supported. Define $K_\ell(\cdot) := \ell^{-1}K(\cdot/\ell)$ for $\ell > 0$, we set

$$g_\ell = K_\ell \star g.$$

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Following Neumann (1997), Comte, Samson and Stirnemann (2009) and Comte and Lacour (2011), we propose an estimator $\hat{g}_\ell$ of g is such that its Fourier transform takes the following form:

$$\widehat{g_\ell}^*(\xi) = K_\ell^*(\xi) \times \left(\frac{\alpha \widehat{D^*(\xi)}}{2R} \frac{\mathbb{1}_{\left\{|\widehat{M^*(\xi)}| \geq n^{-1/2}\right\}}}{\widehat{M^*(\xi)}} + \frac{\lambda + R}{2R} \right).$$

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Estimators of g and h

Taking the inverse Fourier transform of $\hat{g}_\ell^*$ to obtain the estimator $\hat{g}_\ell$ of g, then the estimator of the division kernel h as follows:

$$\hat{g}_\ell(u) = \frac{1}{2\pi}\int_{\mathbb{R}} \hat{g}_\ell^*(\xi)e^{-\mathbf{i}u\xi}d\xi, \quad \hat{h}_\ell(\gamma) = \gamma^{-1}\hat{g}_\ell\big(\log(\gamma)\big), \quad \gamma \in (0,1).$$

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Theorem

Suppose Assumptions (A1), (A2) and (A3) are satisfied and the kernel bandwidth ℓ which depends on n satisfies $\lim_{n\to+\infty} \ell = 0$. Provided that

$$\lim_{n\to+\infty} \frac{1}{n}\left(\left\| \frac{K_\ell^*(\xi)\xi}{M^*(\xi)} \right\|_2^2 + \left\| \frac{K_\ell^*(\xi)}{M^*(\xi)} \right\|_2^2 \right) = 0,$$

we have

$$\lim_{n\to+\infty} \mathbb{E}\left[\|\hat{g}_\ell - g\|_2^2 \right] = 0, \quad \lim_{n\to+\infty} \mathbb{E}\left[\|\hat{h}_\ell - h\|_2^2 \right] = 0$$

Numerical simulations

Bandwidth selection rule:

We apply resampling techniques inspired from the principle of cross-validation: we divide the observations $X_1, \dots, X_n$ into two sub-samples $\mathbf{X}^E := (X_i)_{i \in E}$ and $\mathbf{X}^{E^C} := (X_i)_{i \in E^C}$ where $E \subset \{1, \dots, n\}$ such that such that $|E| = n/2$ and $E^C = \{1, \dots, n\} \setminus E$.

Let $(E_j, E_j^C)_{1 \leq j \leq V}$, $V \leq V_{\max} = C_n^{n/2}$ be the sequence of subsets selected from $\{1, \dots, n\}$. Let $\mathcal{L}$ be a family of bandwidths possible, define

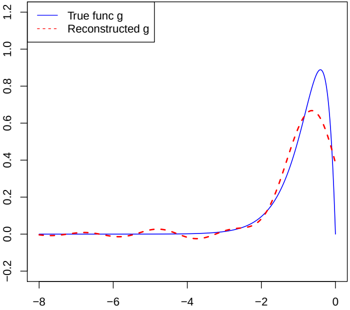
$$\hat{J}(\ell, \ell') := \frac{1}{V} \sum_{i=1}^{V} \left[\|\hat{g}_\ell^{*(E_j)}\|_2^2 - 2 \left\langle \hat{g}_\ell^{*(E_j)}, \hat{g}_{\ell'}^{*(E_j^C)} \right\rangle \right]$$

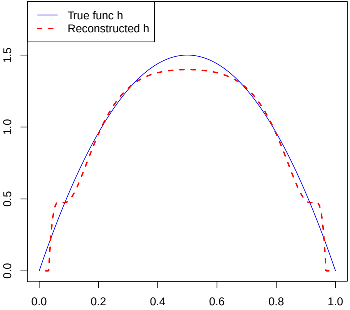
The the final estimator of g is obtained by putting $\hat{g} := \hat{g}_{\hat{\ell}}$ where

$$\hat{\ell}_{CV} := \underset{\ell \in \mathcal{L}}{\operatorname{argmin}} \left\{ \min_{\ell' \in \mathcal{L}} \hat{J}(\ell, \ell') \right\}.$$

Numerical simulations

Reconstruction of the density of Beta(2, 2): $h(x) = Cx(1-x)\mathbb{1}_{[0,1]}(x)$.





Left: Reconstruction of $g(x) = e^x h(e^x)$. *Right: Reconstruction of* $\tilde{h} = \frac{1}{2}\big(h(x) + h(1-x)\big)$.

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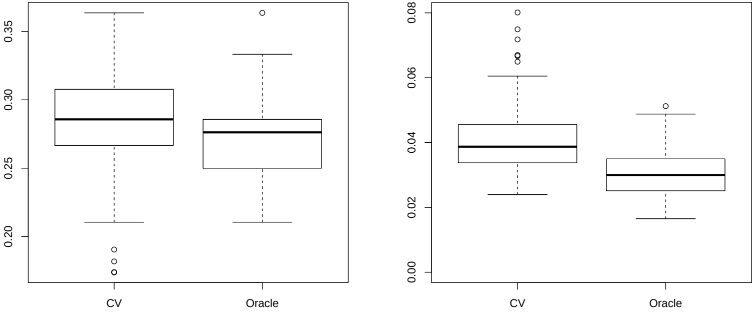

Left: CV bandwidths vs Oracle bandwidths. Right: $\mathbb{L}^2$*-risk of* $\hat{g}$ *over* $M = 100$ *samples of size* $n = 30000$.

References

- PhD manuscript: V. H. Hoang. *Adaptive estimation for inverse problems with applications to celle divisions.*
- V. H. Hoang. *Estimating the Division Kernel of a Size-Structured Population. 2015.* Submitted.
- V. H. Hoang, T. M. Pham Ngoc, V. Rivoirard and V. C. Tran. *Nonparametric estimation of the fragmentation kernel based on a stationary distribution approximation.* Work in progress

Merci de votre attention