On the Mathematical Foundation of ABC

A Robust Set for Estimating Mechanistic Network Models

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Presentation plan

The four sections and the main references

1. A mathematical frame for ABC
2. A convergence result for $\varepsilon \downarrow 0$
3. Optimal transport theory in ABC
4. Some lower bounds for $n \to \infty$

- E. Bernton, P.E. Jacob, M. Gerber, C.P. Robert. *Approximate Bayesian computation with the Wasserstein distance*. J. R. Statist. Soc. B (2019). Vol. 81, Issue 2, pp. 235–269.
- S.A. Sisson, Y. Fan, M.A. Beaumont. *Handbook of Approximate Bayesian Computation*. Chapman & Hall/CRC, Handbooks of Modern Statistical Methods, 2019.
- C. Villani. *Optimal Transport. Old and New*. Springer, 2009.

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The model $\{\mu^n_\vartheta\}_{\vartheta \in \mathcal{H}}$ is *generative* meaning that, $\widetilde{\forall}\, \vartheta \in \mathcal{H}$, it's possible to generate how many $z^{1:n} = (z^1, \dots, z^n) \in \mathcal{Y}^n$ with $z^{1:n} \sim \mu^n_\vartheta$ we desire.

Pseudo-observations: $z^{1:n} \sim \mu^n_\vartheta$ in $\mathcal{Y}^n$, $\widetilde{\forall}\, \vartheta \in \mathcal{H}$. *Deviation measure:* $\mathcal{D}$, pseudo-metric on $\mathcal{Y}^n$.

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1. The function $\vartheta \mapsto \mu^n_\vartheta[D^n_\varepsilon]$, to be seen as defined π-a.s., belongs to $\mathscr{M}(\mathcal{H}, [0,1])$.
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For any $Y \in \mathcal{B}(\mathcal{Y}^n)$, $\mu^n_{(\cdot)}[Y] \in \mathscr{B}(\mathcal{H}, [0,1])$ (coherently w.r.t. A0 - b).

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There exist $\delta, \bar{\varepsilon} \in]0, \infty[$ and $g \in L^1(\pi)$ with $g \geq \delta\ [\pi]$ all such that, $\widetilde{\forall}\, \vartheta \in \mathcal{H}$,

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There exist $\delta, \bar{\varepsilon} \in\,]0, \infty[$ and $g \in L^1(\pi)$ with $g \geq \delta\ [\pi]$ all such that, $\widetilde{\forall}\, \vartheta \in \mathcal{H}$,

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- A2 would imply 2 of A0 - b employing any $\varepsilon_0 \in\,]0, \bar{\varepsilon}]$.
- A2 implies $f^n_{(\,\cdot\,)}(y^{1:n}) \in L^1(\pi)$ with $L^1(\pi)$-norm lower or equal than $\|g\|_1 := \|g\|_{L^1(\pi)}$.
- Even the following generalization of A2 would work.

Axiom [A2] (under A1) There exist $g \in L^1(\pi)$ with $g > 0\ [\pi]$ and $\tilde{\varepsilon} \in\,]0, \infty[$ such that, for any $\varepsilon \in\,]0, \tilde{\varepsilon}[$, there exists $\delta_\varepsilon \in\,]0, \infty[$ such that, $\widetilde{\forall}\, \vartheta \in \mathcal{H}$,

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costnet

We denote by $\mathrm{m} := \mathrm{m}^{d_{\mathcal{Y}} \cdot n}$ the Lebesgue measure on $\mathcal{B}(\mathbb{R}^{d_{\mathcal{Y}} \cdot n})$.

Axiom [A1]

$\widetilde{\forall}\, \vartheta \in \mathcal{H}$, the two following conditions hold.

1. $\mu^n_\vartheta \ll \mathrm{m}$ with $f^n_\vartheta := \mathrm{d}\mu^n_\vartheta / \mathrm{dm}$ such that, $\widetilde{\forall}\, z^{1:n} \in \mathcal{Y}^n\,[\mathrm{m}]$, $f^n_{(\cdot)}(z^{1:n}) \in \mathscr{B}(\mathcal{H}, \mathbb{R}_+)$.
2. $f^n_\vartheta(\cdot)$ is continuous and $f^n_{(\cdot)}(y^{1:n})$ is not π-a.s. identically zero.

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In particular, if $\mathcal{D}$ is an actual metric, then A3 trivially holds.

Proposition

Under assumptions A1, A2 and A3, the three following conditions hold.

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1. *The ABC rejection algorithm and the ABC posterior are well defined for any $\varepsilon \in]0, \varepsilon_0 \vee \bar{\varepsilon}[$.*
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3. *The ABC posterior strongly converges to the true posterior as $\varepsilon \downarrow 0$: $\forall\, B \in \mathcal{B}(\mathcal{H})$,*

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costnet

Let's visualize $(\mathcal{Y}, \varrho_{\mathcal{Y}})$ as a separable and complete metric space, thus also a Radon space, i.e. any element in $\mathscr{P}(\mathcal{Y})$ is a Radon probability measure (outer regular on Borel subsets and inner regular on open subsets); and let's choose an unit cost function $c \colon \mathcal{Y} \times \mathcal{Y} \to [0, \infty]$ which is lower semicontinuous (so Borel measurable) and a parameter $p \in [1, \infty[$ of summability.

We denote by $\mathscr{P}_p(\mathcal{Y})$ the subclass of $\mathscr{P}(\mathcal{Y})$ whose elements have finite p-th moment.

Kantorovich's formulation. For $\mu, \nu \in \mathscr{P}_p(\mathcal{Y})$, consider the subclass $\Gamma(\mu, \nu)$ of $\mathscr{P}(\mathcal{Y} \times \mathcal{Y})$ whose elements γ are the couplings with marginals μ and ν. Then the Kantorovich's formulation of the optimal transport problem related to $(\mathcal{Y}, \varrho_{\mathcal{Y}})$, c and p is

$$\mathcal{K}(\mu, \nu) \doteq \inf_{\gamma \in \Gamma(\mu, \nu)} \int_{\mathcal{Y} \times \mathcal{Y}} c(y, y') \, d\gamma(y, y').$$

It can be shown that there exists a minimizer $\gamma^* \in \Gamma(\mu, \nu)$ for such a problem which could be determined by means of gradient descent algorithms.

Example

For $c = (\varrho_{\mathcal{Y}})^p$, $\mathcal{K}$ coincides with the p-power of the Wasserstein distance: $\mathcal{K} = \mathcal{W}_p^p$.

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For $c = (\varrho_{\mathcal{Y}})^p$, $\mathcal{K}$ coincides with the p-power of the Wasserstein distance: $\mathcal{K} = \mathcal{W}_p^p$.

Monge's formulation. For $\mu, \nu \in \mathscr{P}_p(\mathcal{Y})$, consider the subclass $\mathrm{T}(\mu,\nu)$ of $\mathscr{B}(\mathcal{Y}) := \mathscr{B}(\mathcal{Y},\mathcal{Y})$ whose elements T satisfy $T_{\#}\mu = \nu$ (push-forward or image measure of μ through T). Then, at least when μ and ν are both atomic (not diffuse) or otherwise when μ is not atomic (diffuse), the Monge's formulation of the optimal transport problem related to $(\mathcal{Y}, \varrho_{\mathcal{Y}})$, c and p is

$$\mathcal{M}(\mu,\nu) \doteq \inf_{T \in \mathrm{T}(\mu,\nu)} \int_{\mathcal{Y}} c(y, T(y))\, \mu(\mathrm{d}y).$$

Example

Assume $d_{\mathcal{Y}} = 1$ and $\mathcal{Y} = \mathbb{R}$ with $\varrho_{\mathcal{Y}}$ equal to the Euclidean metric. If there exists a function $\varphi\colon \mathbb{R} \to \mathbb{R}$ which is convex and such that $c(y,y') = \varphi(y-y')$, $y, y' \in \mathbb{R}$, then, for $\mu,\nu \in \mathscr{P}_p(\mathbb{R})$ with μ not atomic, the function $T^* := F_\nu^{-1} \circ F_\mu \in \mathrm{T}(\mu,\nu)$ is an optimal transport map w.r.t. the Monge's formulation (the unique if φ is strictly convex) and the following identity holds:

$$\mathcal{M}(\mu,\nu) = \int_{\mathbb{R}} \varphi(y - T^*(y))\, \mu(\mathrm{d}y) = \int_0^1 \varphi(F_\mu^{-1}(t) - F_\nu^{-1}(t))\, \mathrm{d}t.$$

Radon's metric. For any $\mu,\nu \in \mathscr{P}_p(\mathcal{Y})$, $\varrho_{\mathcal{R}}(\mu,\nu) \doteq \sup_{h \in C^0(\mathcal{Y},[-1,1])} \int_{\mathcal{Y}} h(y)\, (\mu-\nu)(\mathrm{d}y)$ defines a metric on $\mathscr{P}_p(\mathcal{Y})$ whose notion of convergence corresponds with the total variation one.

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Assume $d_{\mathcal{Y}} = 1$ and $\mathcal{Y} = \mathbb{R}$ with $\varrho_{\mathcal{Y}}$ equal to the Euclidean metric. If there exists a function $\varphi\colon \mathbb{R} \to \mathbb{R}$ which is convex and such that $c(y,y') = \varphi(y-y')$, $y, y' \in \mathbb{R}$, then, for $\mu,\nu \in \mathscr{P}_p(\mathbb{R})$ with μ not atomic, the function $T^* := F_\nu^{-1} \circ F_\mu \in \mathrm{T}(\mu,\nu)$ is an optimal transport map w.r.t. the Monge's formulation (the unique if φ is strictly convex) and the following identity holds:

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Radon's metric. For any $\mu,\nu \in \mathscr{P}_p(\mathcal{Y})$, $\varrho_{\mathcal{R}}(\mu,\nu) \doteq \sup_{h \in C^0(\mathcal{Y},[-1,1])} \int_{\mathcal{Y}} h(y)\,(\mu-\nu)(\mathrm{d}y)$ defines a metric on $\mathscr{P}_p(\mathcal{Y})$ whose notion of convergence corresponds with the total variation one.

Monge's formulation. For $\mu, \nu \in \mathscr{P}_p(\mathcal{Y})$, consider the subclass $\mathrm{T}(\mu, \nu)$ of $\mathscr{B}(\mathcal{Y}) := \mathscr{B}(\mathcal{Y}, \mathcal{Y})$ whose elements T satisfy $T_{\#}\mu = \nu$ (push-forward or image measure of μ through T). Then, at least when μ and ν are both atomic (not diffuse) or otherwise when μ is not atomic (diffuse), the Monge's formulation of the optimal transport problem related to $(\mathcal{Y}, \varrho_{\mathcal{Y}})$, c and p is

$$\mathcal{M}(\mu, \nu) \doteq \inf_{T \in \mathrm{T}(\mu, \nu)} \int_{\mathcal{Y}} c(y, T(y))\, \mu(\mathrm{d}y).$$

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$\mu_n = \widehat{\mu}_n := n^{-1} \sum_{k=1}^n \delta_{y^k}$ and $\mu_{\vartheta,n} = \widehat{\mu}_{\vartheta,n} := n^{-1} \sum_{k=1}^n \delta_{z^k}$ (empirical distributions).

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Axiom [B1] (under B0)

There exists unique $\mu_\star \in \mathscr{P}(\mathcal{Y})$, possibly in $\mathscr{P}_p(\mathcal{Y})$, such that the following occurs.

1. For any $n \in \mathbb{N}^*$, $\omega \mapsto \mathcal{T}(\mu_n, \mu_\star)$ is $\mathcal{A}$-measurable as a function from Ω to $\mathbb{R}_+$.
2. $\mathcal{T}(\mu_n, \mu_\star) \to 0$, $\mathbb{P}$-a.s., as $n \to \infty$.

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$\widetilde{\forall}\, \vartheta \in \mathcal{H}$, there exists unique $\mu_\vartheta \in \mathscr{P}(\mathcal{Y})$, possibly in $\mathscr{P}_p(\mathcal{Y})$, such that the following occurs.

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4. There exist $\sigma \in [0, \tau]$ and $\varepsilon_1 > 0$ such that, $\widetilde{\forall}\, \vartheta \in \mathcal{H}$ and $\forall\, \varepsilon \in]0, \varepsilon_1[$,

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3 of B2 is equivalent to any version of that in which an upper bound for ε is imposed. Furthermore if, $\widetilde{\forall}\, \vartheta \in \mathcal{H}$ and $\forall\, \varepsilon > 0$, $\mu_\vartheta^n[\mathcal{T}(\mu_{\vartheta,n}, \mu_\vartheta) > \varepsilon] \to 0$ as $n \to \infty$ (shortly put), then any $\tau \in [0, 1[$ satisfies 3 of B2 while only $\sigma = 0$ but any $\varepsilon_1 > 0$ fulfill 4 of B2.

Axiom [B3] (under 1 and 2 of B2)

There exists $\vartheta_\star \in \mathcal{H}$ which minimizes $\vartheta \mapsto \mathcal{T}(\mu_\vartheta, \mu_\star)$ over $\mathcal{H}$: simbolically,

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Axiom [B4] (under B3)

There exist a neighborhood $U_\star \subset \mathcal{H}$ of $\vartheta_\star$, a connected neighborhood $I_0 \subset \mathbb{R}_+$ of zero and a strictly increasing function $\psi \colon I_0 \to \mathbb{R}_+$ all such that, $\widetilde{\forall}\, \vartheta \in U_\star$,

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We write "for any $(y^{1:n})_n$" meaning to vary of $(y^{1:n}(\omega))_n \equiv (y^{1:n})_n$, with $y^{1:n}(\omega) \equiv y^{1:n}$ in $\mathcal{Y}^n$ for any $n \in \mathbb{N}^*$, w.r.t. a $\omega \in \Omega$. Lastly, for $\varepsilon > 0$, we denote by ε^{-} any element of $]0, \varepsilon]$.

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costnet

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Under assumptions B0, B1, 1, 2 *and* 3 *of* B2 *and* B3, *the following occurs so far as* $\varepsilon_\star < \varepsilon_0$, *for* $\varepsilon \in]0, \varepsilon_0 - \varepsilon_\star[$, $(y^{1:n})_n$ *with* $n \equiv n_\varepsilon$ *large enough and with probability* **P** *going to* 1 *as* $n \to \infty$.

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1. $\pi^{\varepsilon_\star+\varepsilon}_{y^{\mathbf{1}:n}}\left[\mathcal{T}_{(\,.\,)} \geq \varepsilon_\star + \varepsilon^-/3\right] \geq (1-\tau)\,\pi\left[\varepsilon_\star + \varepsilon^-/3 \leq \mathcal{T}_{(\,.\,)} \leq \varepsilon_\star + \varepsilon/3\right]$.
2. $\pi^{\varepsilon_\star+\varepsilon}_{y^{\mathbf{1}:n}}\left[\mathcal{H} \setminus \arg\min_{\mathcal{H}} \mathcal{T}_{(\,.\,)}\right] \geq (1-\tau)\,\pi\left[\varepsilon_\star < \mathcal{T}_{(\,.\,)} \leq \varepsilon_\star + \varepsilon/3\right]$.
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$$\lambda_\varepsilon := (1-\sigma)\,\pi\left[\mathcal{T}_{(\,.\,)} \leq \varepsilon_\star + 5\varepsilon/3\right] + \tau\pi\left[\mathcal{T}_{(\,.\,)} > \varepsilon_\star + 5\varepsilon/3\right] > 0$$

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Let's discuss how a condition consistent with A2 as the following could interact.

Axiom [A2′] (under A1)

There exist $\delta, \varepsilon' \in]0, \infty[$ and $g \in L^1(\pi)$ with $g \geq \delta\ [\pi]$ all such that, $\widetilde{\forall}\, \vartheta \in \mathcal{H}$ and $\forall\, (z^{1:n})_n$ with $z^{1:n} \in D^n_{\varepsilon'}$, for any $n \in \mathbb{N}^*$,

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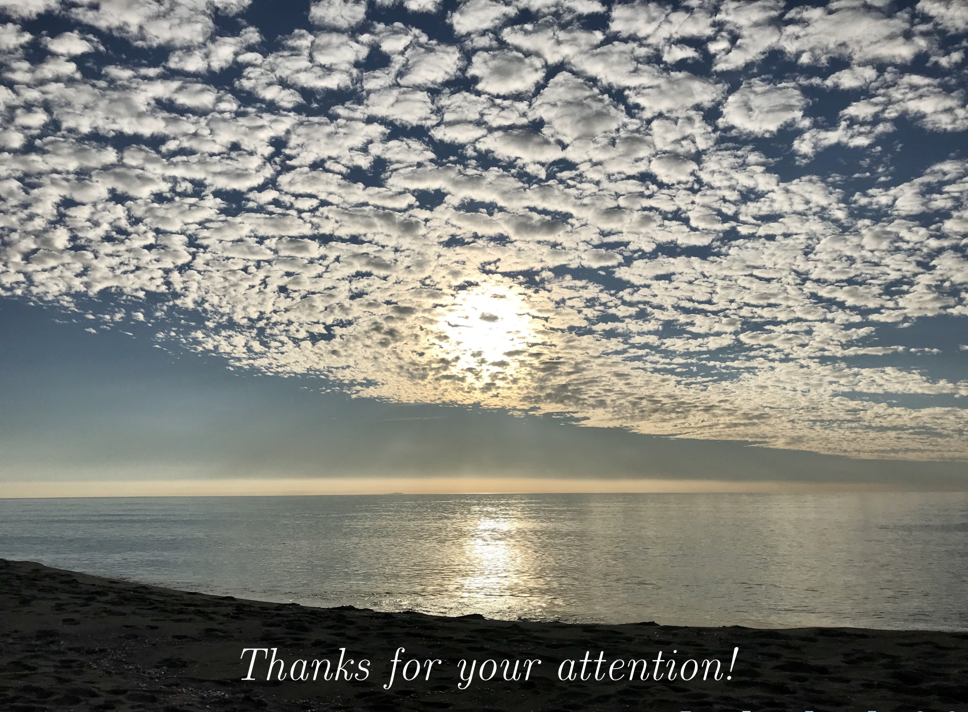
Thanks for your attention!