Differential equations and empirical likelihood

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June 23, 2016

Workshop on New Applications of Empirical Likelihood

Institute for Mathematical Sciences, National University of Singapore

General formulation

- Observed data:

$$\mathbf{Y}_i = \mathbf{X}(t_i) + \varepsilon_i, \qquad i = 1, \ldots, n; \tag{1}$$

  where $t_i \in [T_0, T_1]$.

- Parametric ODE model:

$$\frac{d}{dt}\mathbf{X}(t) = G(\mathbf{X}(t), t; \theta) \tag{2}$$

  subject to an initial condition $\mathbf{X}(T_0) = \mathbf{X}_0$.

- If $G(\mathbf{x}, t; \theta) \equiv G(\mathbf{x}, \theta)$, then the system is *autonomous*.

Estimating θ by regression

- Treat $\mathbf{X}(t)$ as a function of (θ, X_0).
- If X_0 is known, the trajectory for $\mathbf{X}(t) = \mathbf{X}(t, \theta)$ can be determined for all $t \in [T_0, T_1]$, *up to a given level of precision* by numerically solving (2), for example by Runge-Kutta method.
- One obvious approach is to estimate θ by solving the least squares problem:

$$\widehat{\theta}^{LS} = \arg\min_{\theta \in \Theta} \sum_{i=1}^{n} w_i \|\mathbf{Y}_i - \mathbf{X}(t_i; \theta)\|^2 \tag{3}$$

based on some *known weights* $\{w_i\}_{i=1}^{n}$.

Computational bottleneck

- Typically, (3) is solved by iteratively solving a sequence of linearized regression problem (e.g., Levenberg-Marquardt method). This involves, at each step of the iterations,
  1. Solve for $\mathbf{X}(t;\theta)$ on $[T_0, T_1]$ given the current value of θ.
  2. Solve for $\frac{d}{dt}\mathbf{X}(t;\theta)$ on the same interval, by solving the corresponding ODE.
- Both these steps need knowledge of X_0, and evaluation of the trajectory on a fine grid.

Alternative approaches : Two-stage estimation

- The first stage involves estimating $X(t)$ and $X'(t)$ separately using local polynomial method.
- The second stage involves nonlinear regression based on the following description:

$$\widehat{\mathbf{X}}'(t_i) = G(\widehat{\mathbf{X}}(t_i), t_i; \theta) + \mathbf{e}_i, \qquad i = 1, \ldots, n.$$

- The method has been analyzed in detail by Chen and Wu (2008a, 2008b).
- Choice of weights in the nonlinear regression can impact the quality of estimation. Brunel (2008) (who used splines rather than local polynomial regression for smoothing $\mathbf{X}(t)$), established $\sqrt{n}$-consistency of $\widehat{\theta}$ under a careful choice of weights that vanish at the boundaries.

Alternative approaches : Parameter cascading

- A penalized least squares method whereby the trajectory X is represented in terms of splines and the ODE itself acts as a penalty on the trajectory. The parameters of the ODE are fitted using a parameter cascading method (Ramsay, Hooker, Campbell and Cao, 2007).
- Specifically, after expressing $\widehat{X}(t) = \sum_{j=1}^{M} \beta_j \Phi_j(t)$, they minimize

$$\sum_{i=1}^{n} w_i \|\mathbf{Y}_i - \widehat{\mathbf{X}}(t_i)\|^2 + \lambda \int \|\widehat{\mathbf{X}}'(t) - G(\widehat{\mathbf{X}}(t), t; \theta)\|^2 dt$$

  for some $\lambda > 0$.
- Qi and Zhao (2010) provided theoretical analysis of the parameter cascading method.

Alternative approaches : Linear functionals

- Hall and Ma (2014) proposed another smoothing-based estimator by making use of a class of linear *test functionals*.
- Specifically, if ψ_j, $j = 1, \ldots, J$ are C^1 functions supported on $[c, 1-c]$ for some $c \in (0, 1/2)$, and satisfying $\psi_j(c) = \psi_j(1-c) = 0$, then estimate θ by minimizing

$$\sum_{j=1}^{J} W_j \| \int_c^{1-c} \left(\psi_j(t)\widehat{\mathbf{X}}(t) + \psi_j(t) G(\widehat{\mathbf{X}}(t), t; \theta) \right) dt \|^2$$

  where $\widehat{\mathbf{X}}(t)$ is obtained by local polynomial regression.
- They show that the estimator is $\sqrt{n}$-consistent under appropriate range of the bandwidth and appropriately chosen $\{\psi_j\}_{j=1}^{J}$.

Empirical likelihood framework

- The main idea is to combine the nonparametric smoothing with the parametric regression of $\widehat{\mathbf{X}}'_{\mathbf{h}}(t)$ on $\widehat{\mathbf{X}}_{\mathbf{h}}(t)$, so that the bandwidths of smoothers can be chosen simultaneously.
- *EL step:* Use the following normal equations as the "core estimating equations":

$$\sum_{i=1}^{n} w_i \frac{\partial}{\partial\theta} \|\widehat{\mathbf{X}}'_{\mathbf{h}}(t_i) - G(\widehat{\mathbf{X}}_{\mathbf{h}}(t_i), t_i; \theta)\|^2 = 0 \qquad (4)$$

  where $\mathbf{w} := (w_i)_{i=1}^{n} \in \mathcal{S}_n$ (n-dimensional simplex).
- Need additional estimating equations to control the bandwidths $\mathbf{h}$ and improve stability.

Parametric integral constraint

- We impose the restriction

$$\sum_{i=1}^{n} w_i \left(\widehat{\mathbf{X}}''(t_i) - \frac{\partial}{\partial t} G(\widehat{\mathbf{X}}(t), t; \theta) \,|_{t=t_i} \right) = 0. \qquad (5)$$

- Maximize $\prod_{i=1}^{n} w_i$ subject to (4) and (5), given θ and $\mathbf{h}$, to obtain

$$\ell_P(\theta, \mathbf{h}) := \sum_{i=1}^{n} \log \hat{w}_i(\theta, \mathbf{h}).$$

Nonparametric integral constraints

- Given a set of weights $\boldsymbol{\nu} := (\nu_i)_{i=1}^n \in \mathcal{S}_n$, we require:

$$\sum_{i=1}^{n} \nu_i(\mathbf{Y}_i - \widehat{\mathbf{X}}(t_i)) = 0. \tag{6}$$

- Based on bias-variance trade-off used to select the optimal global bandwidth, we also impose:

$$\sum_{i=1}^{n} \nu_i \left((Y_{j,i} - \widehat{X}_{j,h_j}(t_i))^2 - c(K_j) n h_j^5 (\widehat{X}''_{j,h_j}(t_i))^2 \right) = 0, \tag{7}$$

for $j = 1, ldots, d$, where $c(K_j)$ is a constant determined by the kernel K_j used in obtaining the smoother $\widehat{X}_{j,h_j}$.

- Maximize $\prod_{i=1}^n \nu_i$ subject to (4) and (5), given $\mathbf{h}$, to obtain

$$\ell_{NP}(\mathbf{h}) := \sum_{i=1}^{n} \log \hat{\nu}_i(\mathbf{h}).$$

Final penalized loss function

- We minimize the following loss function to obtain the final estimates of θ and $\mathbf{h}$.

$$L(\theta, \mathbf{h}) = -\ell_P(\theta, \mathbf{h}) - \ell_{NP}(\mathbf{h}) + \eta \sum_{j=1}^{d} \mathrm{trace}(\mathbf{S}_{j,h_j}^{(1)}) \qquad (8)$$

  where $\eta \geq 0$ is a specified constant, and $\mathbf{S}_{j,h_j}^{(k)}$ denotes the smoother matrix used to obtain $\widehat{X}_{j,h_j}^{(k)}(t)$ for $k = 0, 1, 2$.
- We choose either $\eta = 0$ (no trace-based penalty), or $\eta = 2$ (motivated by AIC).

Simulation study

We use the following *Lotka-Volterra* system as a testbed for our procedure. The same system has been studied by Brunel (2008) and Ramsay et al. (2007).
$\mathbf{X}(t) = (x(t), y(t))^T$, where

$$\begin{aligned} x'(t) &= \theta_1 x(t) - \theta_3 x(t) y(t) \\ y'(t) &= -\theta_2 y(t) + \theta_4 x(t) y(t). \end{aligned}$$

Observational errors:

$$\boldsymbol{\varepsilon}_i = (\varepsilon_i^x, \varepsilon_i^y)^T \overset{i.i.d.}{\sim} N(0, \sigma^2 I_2).$$

Detailed settings

- We compare with the results obtained by Brunel (2008). So, we choose an interval $[T_0, T_1]$ such that $T_1 - T_0 = 20$. Also, we choose $(x(T_0), y(T_0)) = (1, 3)$, $(\theta_1, \theta_2, \theta_3, \theta_4) = (1, 1.5, 1.5, 2)$ and $\sigma = 0.2$.
- We report the results when we have $n = 200$ equally spaced time points in the interval.
- The proposed procedure requires a decent initial estimator for fast convergence. We use a two-step procedure where the first step involves estimation of $(x(t), y(t))$ and their derivatives by local quadratic regression. However, we use cross-validated bandwidths (h_1^{opt}, h_2^{opt}) for obtaining $(\widehat{x}(t), \widehat{y}(t))$, and $(h_1^{opt}/2, h_2^{opt}/2)$ for obtaining $(\widehat{x}'(t), \widehat{y}'(t))$.

Parameter	Criterion	Brunel	Initial	Proposed $(\eta = 0)$	Proposed$(\eta = 2)$
θ_1	Bias	-.08	-.0550	-.0693	-.0345
	(SD)	(.07)	(.0677)	(.0806)	(.0709)
θ_2	Bias	-0.10	-.1422	-.0950	-.0716
	(SD)	(.10)	(.1358)	(.1266)	(.1110)
θ_3	Bias	-.13	-.1047	-.1117	-.0475
	(SD)	(.09)	(.0718)	(.1040)	(.0813)
θ_4	Bias	-.17	-.1845	-.1410	-.0831
	(SD)	(.12)	(.1130)	(.1524)	(.1073)
σ_x^2	Bias		-.0135	-.0204	-.0185
	(SD)		(.0035)	(.0028)	(.0051)
σ_y^2	Bias		-.0132	-0.0215	-.0193
	(SD)		(.0036)	(.0028)	(.0048)
$\hat{h}_x$	Mean		.0106	.0071	.0079
$\hat{h}_y$	Mean		.0106	.0068	.0076

Summary and future work

- Empirical likelihood method provides a flexible approach for estimating ODEs without having to evaluate the trajectories explicitly.
- Appropriate penalization scheme is needed to adjust for bandwidth, which can also be incorporated by combining the parametric and nonparametric aspects.
- The method enjoys a certain robustness to noise characteristics.
- Asymptotic theory needs to developed.

References

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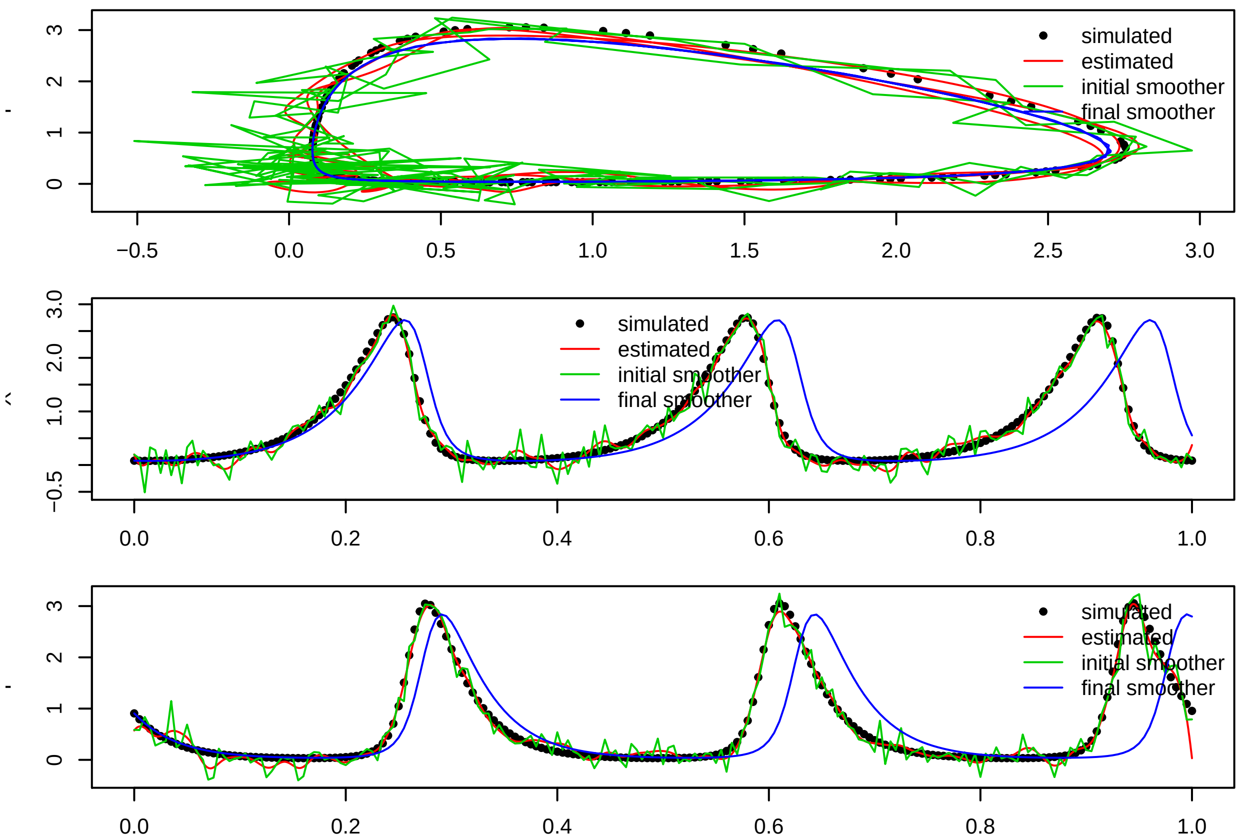

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initial smoother
final smoother
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0.2
0.4
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1.0
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simulated
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initial smoother
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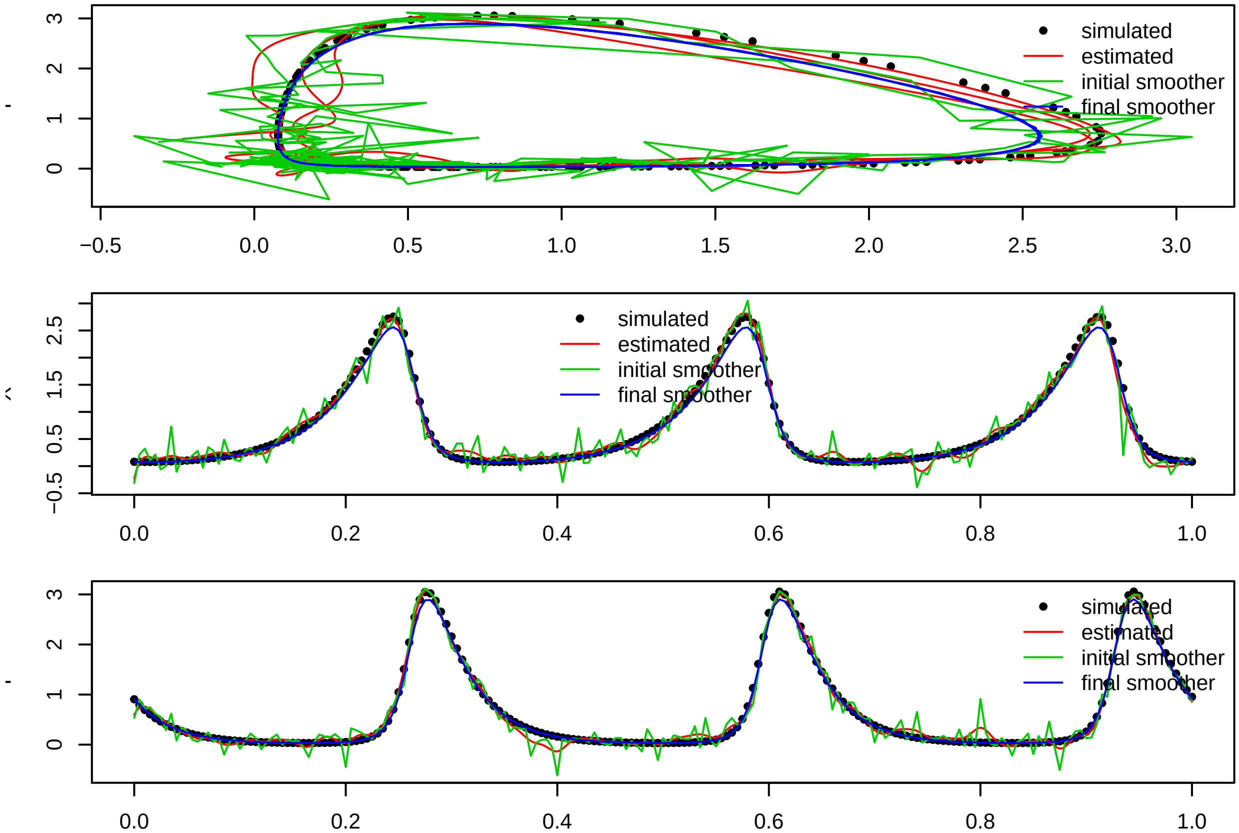
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