A Response Surface Approach for Sensitivity Analysis in Differential Equations.

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Abstract

We show the advantages of using a response surface approach to evaluate the impact of different factors to the problem of estimating the solution and structural parameters of a system of differential equations. The factors considered are: distance of initial point to the true value, noise in the data and amount of smoothing in the estimation method. The method of estimation is based on the statistical analysis of functional data known as profiled estimation. We considered simulating from the predator - prey system of differential equations. As responses of the experiment we used bias and variation of the estimation procedure.

Differential Equations and Functional Data

System of Differential equations

$$\dot{\mathbf{x}}(t) = \mathbf{f}(\mathbf{x}, t \mid \boldsymbol{\theta}) \quad t \in [0, T]$$

Functional data

$$y_{ij} = x_i(t_{ij}) + \varepsilon_{ij} \quad i = 1,\dots,n;\ j = 1,\dots,m_i$$

Predator-Prey system

$$\dot{R}(t) = aR(t) - bR(t)F(t)$$

$$\dot{F}(t) = -cF(t) + dR(t)F(t)$$

Profiled Estimation of Differential Equations

Expansion of solution

$$\hat{x}_i = \sum_k^{K_i} c_{ik}\phi_{ik}(t) = \mathbf{c}_i^T \boldsymbol{\varphi}_i(t) \quad i = 1,\dots,n$$

ϕ_{ik} a basis for $F_i[0,T]$

Inner optimization

$$\min_{\mathbf{c}} J(c \mid \theta, \sigma, \lambda) = \sum_{i=1}^n w_i \left\| y_i - \hat{x}_i(\mathbf{t}_i) \right\|^2 + \sum_{i=1}^n \lambda_i \int_0^T \left[L_{i,\theta}(\hat{x}_i(t)) \right]^2 dt$$

$$L_{i,\theta}(\hat{x}_i(t)) = \frac{d\hat{x}_i(t)}{dt} - f_i(x, t \mid \theta)$$

Outer optimization

$$\hat{\boldsymbol{\theta}} = \arg\min_{\theta} H(\theta) = \sum_{i=1}^n w_i \left\| y_i - \hat{x}_i(\mathbf{t}_i) \right\|^2$$

Variance-covariance Matrix of the estimator

$$V(\hat{\boldsymbol{\theta}}) \approx \left[\left(\frac{d^2 H(\hat{\boldsymbol{\theta}})}{d\theta d\theta^T} \right)^{-1} \frac{d^2 H(\hat{\boldsymbol{\theta}})}{d\theta dy^T} \right] \Sigma \left[\left(\frac{d^2 H(\hat{\boldsymbol{\theta}})}{d\theta d\theta^T} \right)^{-1} \frac{d^2 H(\hat{\boldsymbol{\theta}})}{d\theta dy^T} \right]^T$$

Simulation Scenarios

Structural values: ***a=2, b=1.2, c=1, d=0.9***

Initial conditions: ***F(0)=0.5, R(0) = 1***

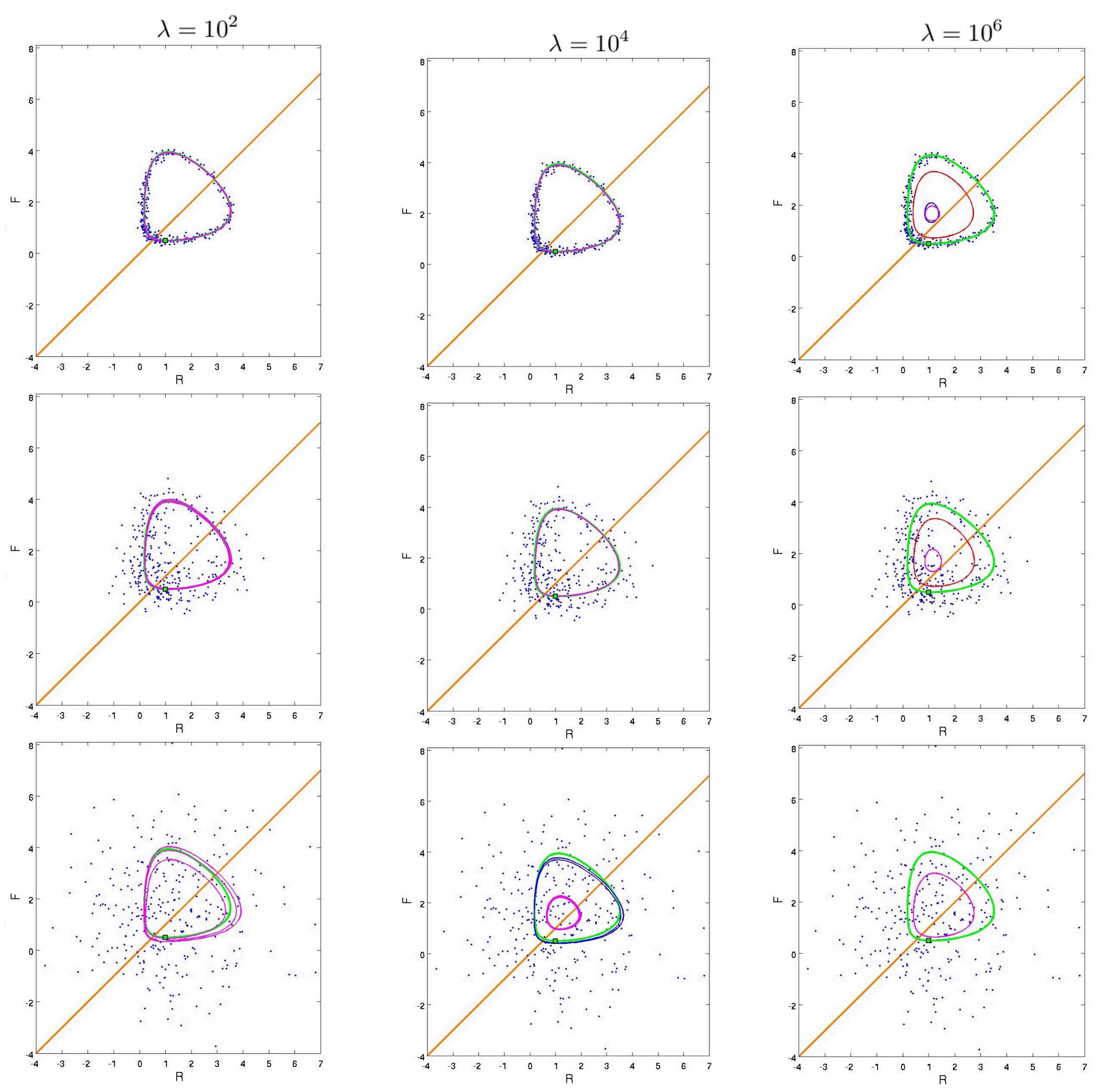
Replicated 3^3 factorial design

Simulation Scenarios

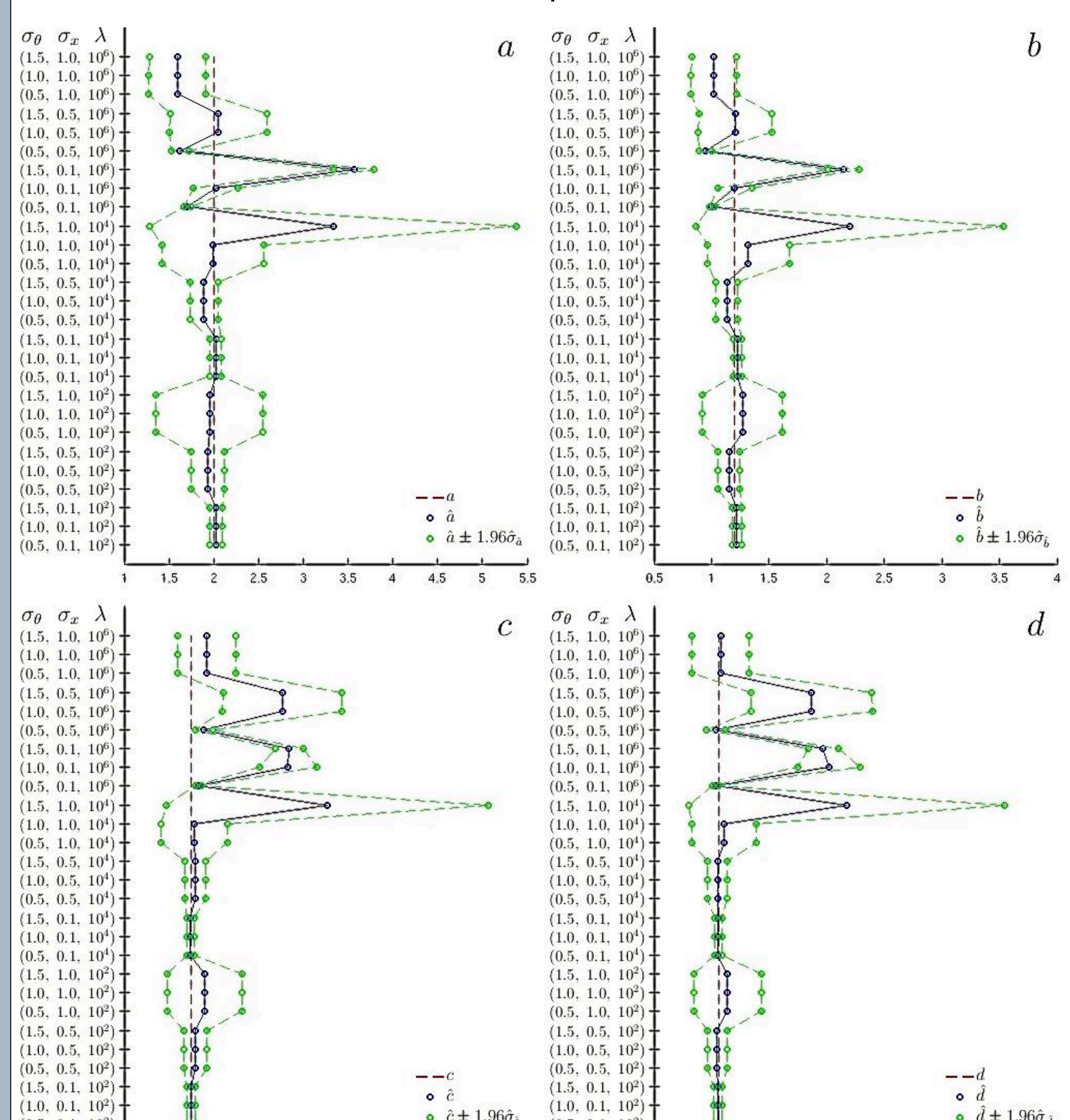
Factors	Levels		
Parameter Noise	0.5	1	1.5
Data Noise	0.1	0.5	1
Lambda (smoothing)	10^2	10^4	10^6

Graphical Results

Green = true solution



Confidence Intervals for parameters
First replicate



Response Surface Analysis

Experimental variables

Parameter noise : $I = \|\theta - \theta_0\|$

Data noise : σ_x

Smoothing : $L = \log(\lambda)$

Responses

$$Y_{bias} = \sqrt{\sum_{i=1}^4 \left(\frac{\sum_{r=1}^2 \hat{\theta}_i^r}{2} - \theta_i \right)^2}$$

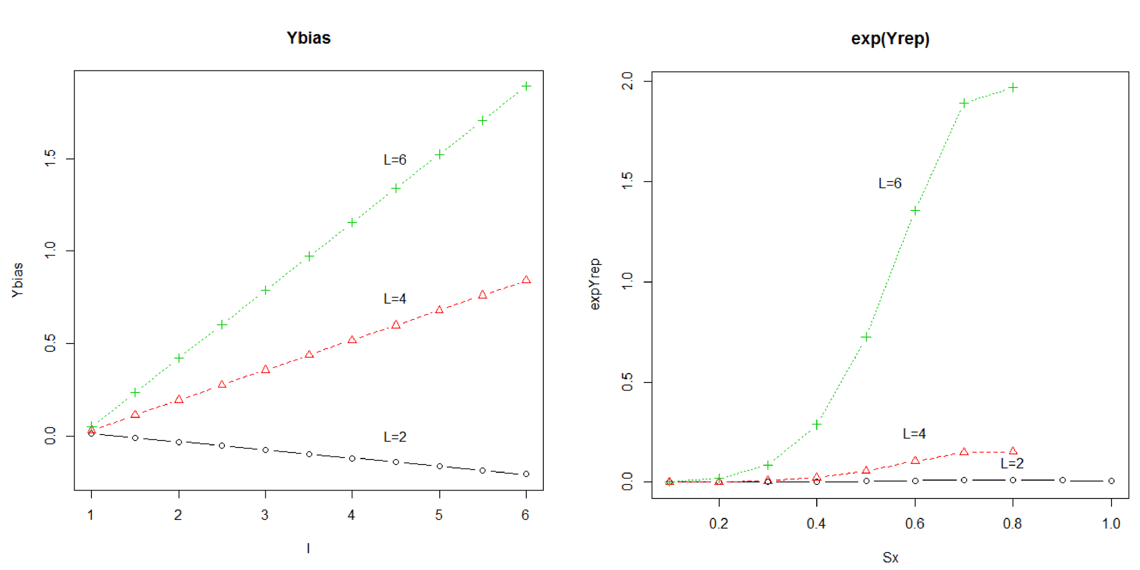
$$Y_{rep} = \ln\left(\sqrt{\sum_{i=1}^4 \left(\hat{\theta}_i^1 - \hat{\theta}_i^2 \right)^2} \right)$$

Statistical Analysis

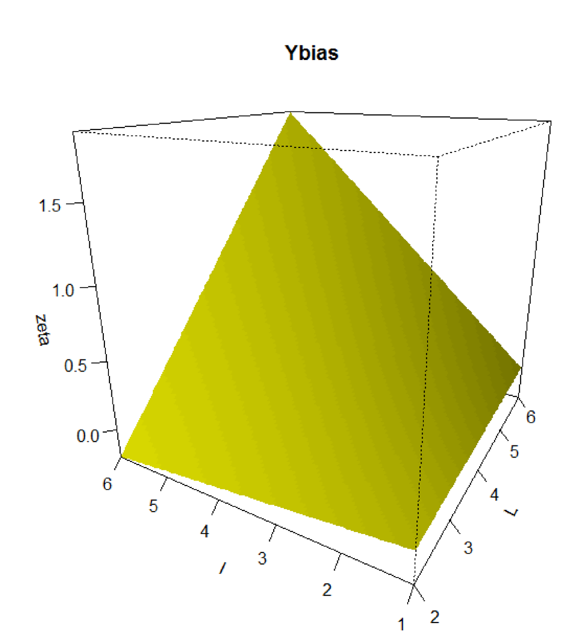
Y_bias		
Variables	Estimate	P-value
Intercept	-0.71	0.027
Sx	-0.02	0.91
L	0.14	0.01
I	0.16	0.06
(Sx-0.53)^2	0.17	0.84
(Sx-0.53)(L-4)	0.09	0.53
(L-4)^2	0.01	0.83
(Sx-0.53)(I-2.3)	-0.26	0.16
(L-4)(I-2.3)	0.1	0.07
(I-2.3)^2	0.021	0.64
(Sx-0.53)(L-4)(I-2.3)	-0.18	0.14

Y_rep		
Variables	Estimate	P-value
Intercept	-11.34	0.0001
Sx	6.77	0.0002
L	1.28	0.002
I	-0.004	0.99
(Sx-0.53)^2	-14.72	0.02
(Sx-0.53)(L-4)	-0.8	0.4
(L-4)^2	-0.28	0.36
(Sx-0.53)(I-2.3)	1.11	0.36
(L-4)(I-2.3)	0.47	0.21
(I-2.3)^2	0.62	0.06
(Sx-0.53)(L-4)(I-2.3)	0.44	0.56

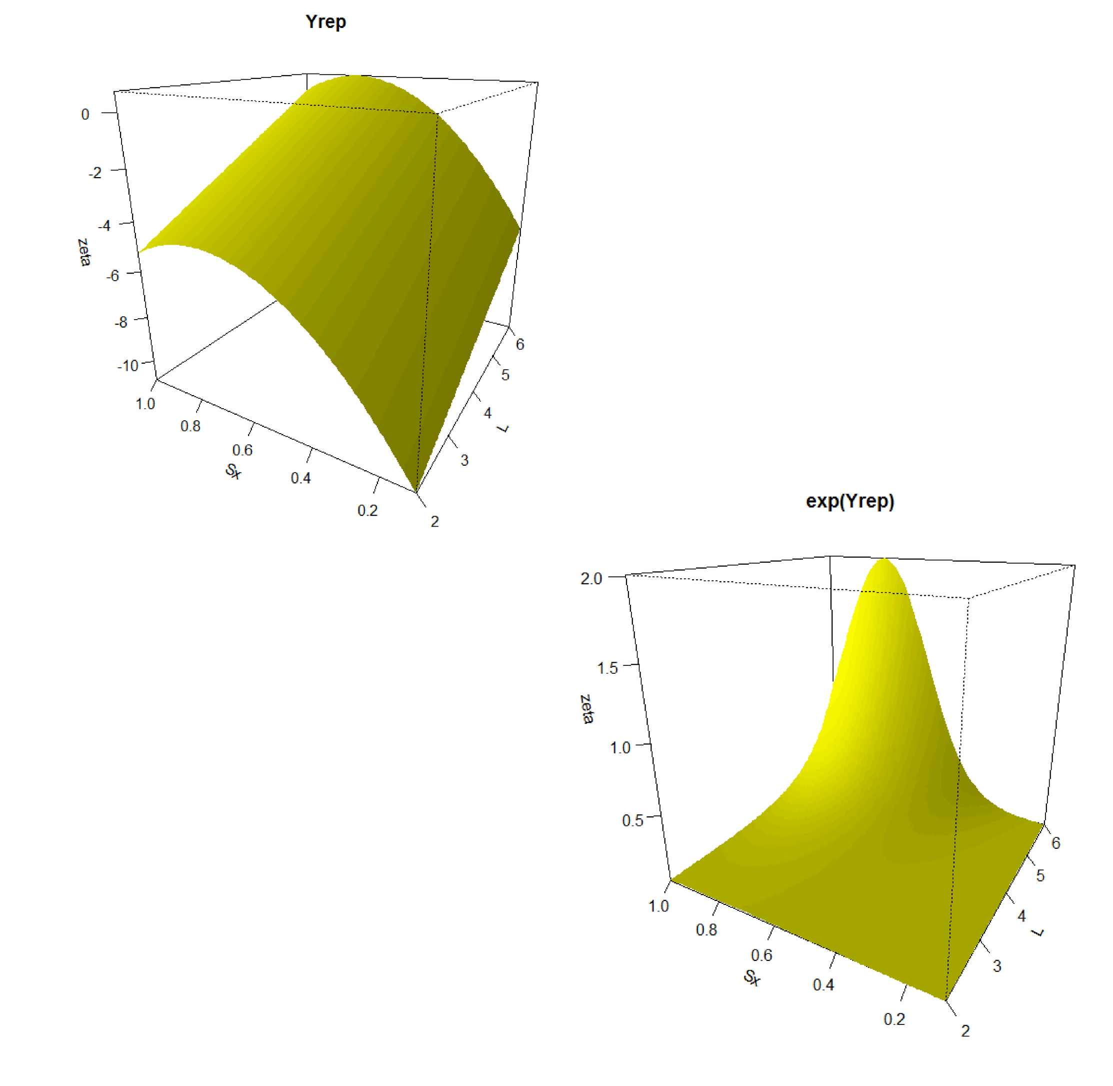
Interaction Plots



Response Surface Plots



Response Surface Plots



Discussion

- The approach can be applied to a wide variety of systems for sensitivity analysis
- It provides a concise model for sensitivity
- Linear, quadratic and interaction effects supplied
- In this example:
  - Large values of the smoothing constant worsen significantly all aspects of estimation procedure
  - There are also interaction effects of smoothing and bias
  - There are no interaction effects between smoothing and variance of the estimation procedure
  - There is no significant effect of remoteness of the starting value on variation.

References

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3. E. Castaño, A. Villeda, V. Aguirre, A Sensitivity Analysis of Profiled Estimation in an Inverse Problem. Technical Report DE-C12.4, ITAM, (2012), 16 pages.

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Acknowledgements

Víctor Aguirre acknowledges financial support from Asociación Mexicana de la Cultura A.C.