Local Sensitivity Analysis

Ian Price

20 Jan, 2010

Why Sensitivity?

For given data and a model to that data, the likelihood estimator is essentially a function of the model parameters. There are several methodologies based on gradient methods or least squares that function more accurately and efficiently when derivative information of that function with respect to its parameters are available. This motivates us to find these derivatives, which are dependent on the solutions to our sensitivity equations.

Why Sensitivity? CTD

When there is limited or no data for a conceptual model, one venue for model validation is to test the sensitivity of a given parameter fit. Thus, a model that is touted for its qualitative behaviour without quantitative behaviour can show that these properties are conserved when there is perturbation to the presented model.

Why Sensitivity? CTD

In the presence of a small data set and many parameters, responses will not change equally to similar changes in parameters: some are sensitive and some are not. The parameter space we wish to fit can be reduced by examining which parameters are sensitive and which are not.

Example

$$MLE(\underline{p}) = \sum_{k=0}^{m} \sum_{i=1}^{n} \frac{(X_i(t_k, \underline{p}) - data_i(t_k))^2}{2\sigma^2}$$

Where X is the solution to a differential equation $X' = f(t, X, p)$, $X(0) = X^0$.

Then, for each component of the parameter set, a value for the change in response when the value of the j^{th} component is given by:

$$\frac{\partial}{\partial p_j}\left(MLE(\underline{p}) \right) = \sum_{k=0}^{m} \sum_{i=1}^{n} \frac{(X_i(t_k, \underline{p}) - data_i(t_k))}{\sigma^2} \cdot \frac{\partial X_i(t_k)}{\partial p_j}$$

Forward/Adjoint Sensitivity

Two types of Local Sensitivity Procedures are commonly used, Forward and Adjoint

Forward Sensitivity Analysis (FSA):

- Computationally expensive
- Works for any system

Adjoinit Sensitivity Analysis (ASA):

- Easy computation
- Need an explicit formula for the adjoint

We'll typically use FSA algorithms.

What do we expect as output from our sensitivity analysis?

For an n variable IVP with m parameters, the forward sensitivity is simultaneously solving m+1 IVPs, each of dimension n, to produce your solution, as well as a n x m matrix of time dependent functions that are your sensitivities.

Forward Sensitivity Analysis

Let's define a system of n variables, X, with m parameters p. Then we differentiate the equations of X with each respective component parameter of p, to solve for the columns of our sensitivity matrix S. The differential equation for X is solved with function f dependent on X and p. f has Jacobian J with respect to state variables X.

$$\dot{\underline{X}} = f(\underline{X}, \underline{p}), \quad \underline{X} \in \mathbb{R}^n, \quad \underline{p} \in \mathbb{R}^m,$$

$$\underline{X}(0) = X_0; \; f : \mathbb{R}^n x \mathbb{R}^m \mapsto \mathbb{R}^n$$

Notation:

$$S^{n \times m}(t) = \begin{bmatrix} s_{11}(t) & s_{12}(t) & \ldots & s_{1m}(t) \\ s_{21}(t) & s_{22}(t) & \ldots & s_{2m}(t) \\ \ldots & \ldots & \ldots & \ldots \\ s_{n1}(t) & s_{n2}(t) & \ldots & s_{nm}(t) \end{bmatrix}$$

$$s_{ij} = \frac{\partial x_i}{\partial p_j}$$

Computing Sensitivity

The IVP for the first column of the sensitivity matrix is written out explicitly. The initial conditions are typically assumed to be zero.

$$\frac{\partial}{\partial t}\begin{bmatrix} s_{11}(t) \\ s_{21}(t) \\ \dots \\ \dots \\ \dots \\ \dots \\ s_{n1}(t) \end{bmatrix} = J^{n \times n}\begin{bmatrix} s_{11}(t) \\ s_{21}(t) \\ \dots \\ \dots \\ \dots \\ \dots \\ s_{n1}(t) \end{bmatrix} + \begin{bmatrix} \dfrac{\partial f_1(\underline{X}, \underline{p})}{\partial p_1} \\ \dfrac{\partial f_2(\underline{X}, \underline{p})}{\partial p_1} \\ \dots \\ \dfrac{\partial f_n(\underline{X}, \underline{p})}{\partial p_1} \end{bmatrix}$$

We use vector notation to simplify the presentation of material for the computation.

$$\underline{s}_j = [\, s_{1j}, s_{2j}, \ldots, s_{nj} \,]^T$$

$$\dot{\underline{s}}_1 = J^{n\ x\ n}\, \underline{s}_1 + \left[\frac{\partial f(\underline{X}, \underline{p})}{\partial p_1} \right]^{n\ x\ 1}$$

$$\dot{\underline{s}}_2 = J^{n\ x\ n}\, \underline{s}_2 + \left[\frac{\partial f(\underline{X}, \underline{p})}{\partial p_2} \right]^{n\ x\ 1}$$

$$\ldots$$

$$\dot{\underline{s}}_m = J^{n\ x\ n}\, \underline{s}_m + \left[\frac{\partial f(\underline{X}, \underline{p})}{\partial p_m} \right]^{n\ x\ 1}$$

Example: IVP

$$\dot{y}_1 = -p_1 y_1 + p_2 y_2 y_3$$

$$\dot{y}_2 = p_1 y_1 - p_2 y_2 y_3 - p_3 y_2^2$$

$$\dot{y}_3 = p_3 y_2^2$$

$$\overline{y}^0 = [1, 0, 0]$$

Example: Sensitivity Equations

$$\dot{\underline{s}}_1 = J\,\underline{s}_1 + \begin{bmatrix} -y_1 \\ y_1 \\ 0 \end{bmatrix}$$

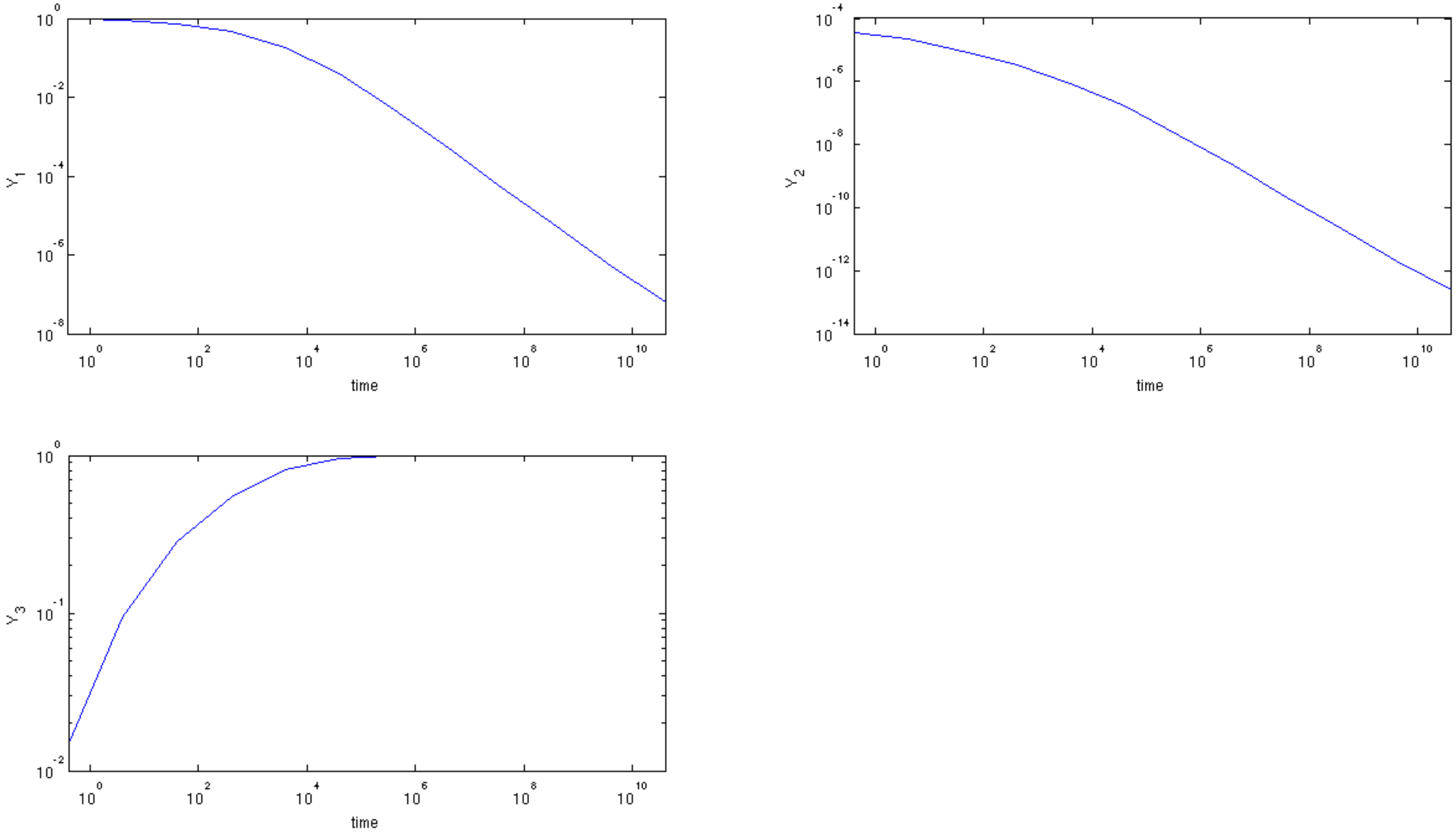
$$J^{3x3} = \begin{bmatrix} -p_1 & p_2 y_3 & p_2 y_2 \\ p_1 & -p_2 y_3 - 2 p_3 y_2 & -p_2 y_2 \\ 0 & 2 p_3 y_2 & 0 \end{bmatrix}$$

$$\dot{\underline{s}}_2 = J\,\underline{s}_2 + \begin{bmatrix} y_2 y_3 \\ -y_2 y_3 \\ 0 \end{bmatrix}$$

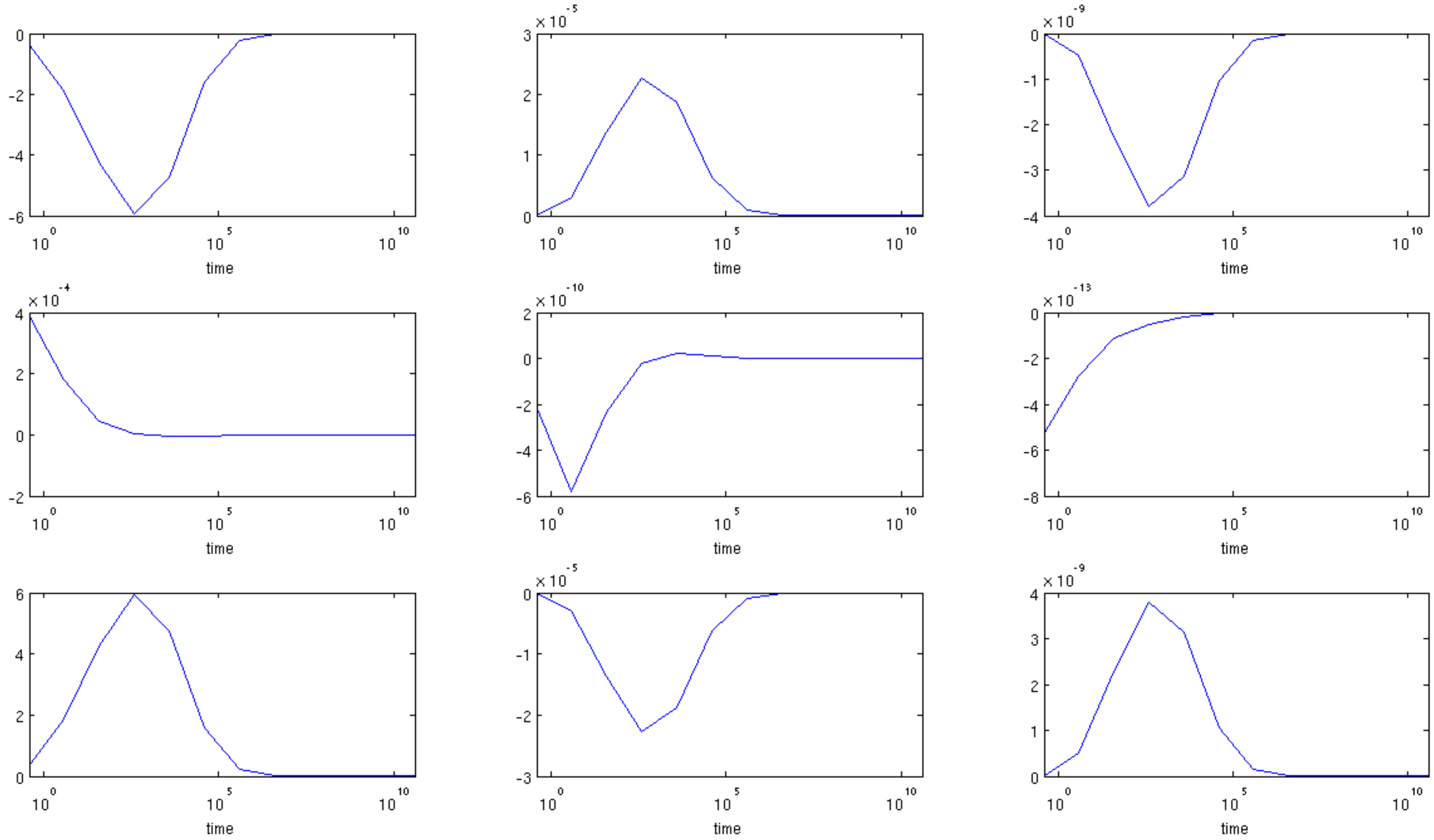
$$S(t_0) = 0^{3x3}$$

$$\dot{\underline{s}}_3 = J\,\underline{s}_3 + \begin{bmatrix} 0 \\ -y_2^2 \\ y_2^2 \end{bmatrix}$$

Trajectories



Local Sensitivities



Local / Global Sensitivity

- Local sensitivity refers to the sensitivity of parameters with respect to a given parameter set. This is in lines with FSA procedure as we have shown in this presentation.
- Global sensitivity refers to the various outcomes the structure of the model is capable of outputting, exploring all reasonable parameter ranges. This is typically done in a more ad hoc manner, such as using genetic algorithms or metropolis-hastings methods.

References

- Cacuci, Dan. Sensitivity and Uncertainty Analysis Theory. 2003
- Hindman & Marsh. User Documentation for CVODES v2.5. 2006
- Saltelli. Sensitivity Analysis. 2001.