Extending eigenvalue analysis to nonlinear models via incorporating higher order terms of Taylor series expansion

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Abstract

This paper is a concept paper about a suggestion proposed by Nathan Forrester, in the last year conference to extend eigenvalue analysis to nonlinear models. His idea was to consider higher order terms of the Taylor series expansion when approximating nonlinear models. In this paper, we demonstrate the feasibility of Nathan's idea. The main contribution of this paper is to devise a pragmatic approach to solve the resulting equations of Taylor series expansion. This pragmatic approach is based on our novel concept of 'smoothed Jacobian' matrix, which is computed from both the ordinary Jacobian matrix and the set of Hessian matrices. Recall that the elements of the ordinary Jacobian matrix represent slopes of relationships, while the elements of the Hessian matrices represent curvatures of relationships. So by integrating the elements the ordinary Jacobian with the elements of the Hessian matrices, we are actually smoothing the slopes given the knowledge about curvatures. Consequently we are smoothing the time trajectories of eigenvalues and eigenvectors in nonlinear models.

Keywords: *system dynamics, nonlinear model analysis, eigenvalue analysis, Taylor series expansion, behavior modes.*

1. Mathematical Background

Any nonlinear system dynamics model consists of a set of nonlinear functions between state variables and net rates. In approximating any single nonlinear function in the model: If we only use the first order term of Taylor series expansion – which is the current practice – we have to compute the gradient vector associated with this function. However, if we also used the second order term of Taylor series, we have to compute the Hessian matrix associated with this function. In general, in a model with 'n' state variables, one has to compute 'n' Hessian matrices – in addition to computing the Jacobian matrix (where each row of the Jacobian is, in fact, a gradient vector).

Note that in many nonlinear functions, the higher order terms (i.e. the third and higher) will equal zero. This assumption is based on the following two reasons:

1. Many table functions can be approximated by a second order polynomial (so differentiating twice is enough).

2. A major source of nonlinearity is the multiplication of two state variables in a rate equation (so also in this case differentiating twice is enough).

So, based on the above assumption, one may conclude that in a certain category of nonlinear system dynamics models, all structural information of the model can be captured in the Jacobian and the 'n' Hessian matrices.

The following equation demonstrates Taylor series expansion associated with the i^{th} net rate.

$$\dot{\mathbf{x}}(\mathrm{i}) = \dot{\mathbf{x}}_{\mathbf{o}}(\mathrm{i}) + \mathrm{grad}_{\mathrm{i}}^{\mathrm{T}}(\mathbf{x} - \mathbf{x}_{\mathbf{o}}) + 0.5(\mathbf{x} - \mathbf{x}_{\mathbf{o}})^{\mathrm{T}}\ \mathbf{H}_{\mathrm{i}}(\mathbf{x} - \mathbf{x}_{\mathbf{o}})$$

where

$\dot{\mathbf{x}}(\mathrm{i})$ is the value of net rate 'i' at time t (t represents any point of time during the simulation)

$\mathbf{x}$ is the state variables vector at time t.

$\mathbf{x}_{\mathrm{o}}$ is the state variables vector at a specified anchor point, in the n-dimensional space.

$\dot{\mathbf{x}}_{\mathbf{o}}(\mathrm{i})$ is the value of net rate 'i' computed at $\mathbf{x}_{\mathrm{o}}$

$\mathrm{grad}_{\mathrm{i}}^{\mathrm{T}}$ is the transpose of the gradient associated with net rate 'i' computed at $\mathbf{x}_{\mathrm{o}}$

$\mathbf{H}_{\mathrm{i}}$ is the Hessian matrix associated with net rate 'i' computed at $\mathbf{x}_{\mathrm{o}}$

Note that in this paper, we denote matrices by bold and capital letters, vectors by bold and small letters, and scalar values by small letters.

In the above equation, taking $\mathbf{x}_o$ as the equilibrium point, and denoting $\mathbf{x}$-$\mathbf{x}_o$ by vector $\mathbf{y}$ yields:

$$\dot{\mathbf{y}}(i) = \text{grad}_i^T \mathbf{y} + 0.5 \mathbf{y}^T \mathbf{H}_i \mathbf{y}$$

Note that net rates equal zero at the equilibrium point, and also note that $\dot{\mathbf{y}}(i) = \dot{\mathbf{x}}(i)$

Basically, vector $\mathbf{y}$ represents the deviation vector from the equilibrium point. It is important here to stress that the above equation is valid at any point in the n-dimensional space – i.e. not only in the neighborhood of the equilibrium point. Moreover, it does not matter if the model actually reaches equilibrium, or never reaches it.

The main contribution of the paper is to devise a pragmatic approach to solve the above equation. This is done via putting the above equation in the following compact form:

$$\dot{\mathbf{y}} = \mathbf{J}^s \mathbf{y} \qquad (1)$$

where

$\dot{\mathbf{y}}$ is the net rate vector at any point of time

$\mathbf{y}$ is the deviation vector at any point of time

$\mathbf{J}^s$ is a nxn matrix. The i^{th} row of this matrix, $\mathbf{J}^s(i,:)$, is defined as follows

$$\mathbf{J}^s(i,:) = \text{grad}_i^T + 0.5 \mathbf{y}^T \mathbf{H}_i$$

The beauty of equation 1 is that it is not an approximation, but rather an exact equation at any point. Consequently, it is valid at any point in time.

Each element of matrix $\mathbf{J}^s$ is either a zero, or a constant, or a linear function of the state variables. In this paper, we call matrix $\mathbf{J}^s$ the *'smoothed Jacobian'*.

Using a Symbolic Toolbox (e.g. Matlab Symbolic Toolbox) one can *symbolically* compute the *smoothed* eigenvalues[1] and *smoothed* eigenvectors associated with matrix $\mathbf{J}^s$. Based on the eigenvalues and eigenvectors, one can solve the time trajectory of vector $\mathbf{y}$, as demonstrated below:

$$\mathbf{y} = \mathbf{w}_1 \exp(\lambda_1 t) + \mathbf{w}_2 \exp(\lambda_2 t) + \ldots + \mathbf{w}_n \exp(\lambda_n t)$$

where:

$\mathbf{w}_1, \mathbf{w}_2, \ldots \mathbf{w}_n$ are the weights vectors

$\lambda_1, \lambda_2, \ldots, \lambda_n$ are the *smoothed* eigenvalues

[1] The eigenvalues are called smoothed as they are derived from the smoothed Jacobian.

For more information about how to compute the weight vectors, the reader may refer to Saleh et al. 2006.

Based on the above equation, the state variables vector trajectory can be expressed as:

$$\mathbf{x} = \mathbf{w}_1 \exp(\lambda_1 t) + \mathbf{w}_2 \exp(\lambda_2 t) + \ldots + \mathbf{w}_n \exp(\lambda_n t) + \mathbf{x}_o \qquad (2)$$

Recall that $\mathbf{x}_o$ is the state variables vector at the equilibrium point.

Equation 2 enables us to decompose the behavior of state variables into several modes of behavior. By plotting the *smoothed* eigenvalues across time, it is possible to detect bifurcation points in behavior modes, and hence to chop the simulation time into distinct phases. This process will be demonstrated on a simple model in the next section.

2. Case Study

In this paper, we will apply the above concept on a simple epidemic model described in chapter 9, in Sterman 's book (Sterman, 2000). The model is called the "SIR" model as it consists of the following three stocks: Susceptible Population (S), Infectious Population (I) and Recovered Population (R). The following figure shows the stock and flow diagram of the model, and the model itself is attached as a supplementary material.

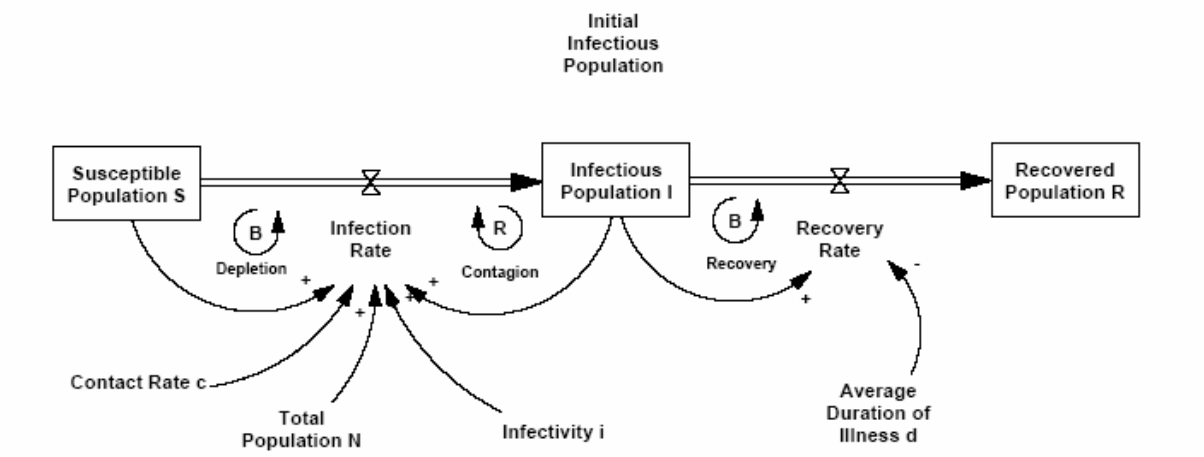

Figure 1: Stock and flow diagram of the SIR model

As shown, in the above figure, there are the following 3 loops in the model:

1. The Balancing "Depletion" Loop
2. The Balancing "Recovery" Loop
3. The Reinforcing "Contagion" Loop.

By removing auxiliary variables, the model can be put in the following condensed form (the reader may check attached model):

dS/dt = -0.00015*I*S;

dI/dt = (0.00015*I*S)-(0.5*I);

dR/dt = 0.5*I;

From the above equation, it is clear that the source of nonlinearity in rate equations is the multiplication of two state variables; hence as stated before, all structural information in the model can be captured by the Jacobian matrix and the '3' Hessian matrices, which are as follows:

$$\mathbf{J} = \begin{bmatrix} -0.00015*I & -0.00015*S & 0 \\ 0.00015*I & 0.00015*S - 0.5 & 0 \\ 0 & 0.5 & 0 \end{bmatrix}$$

$$\mathbf{H_S} = \begin{bmatrix} 0 & -0.00015 & 0 \\ -0.00015 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

$$\mathbf{H_I} = \begin{bmatrix} 0 & 0.00015 & 0 \\ 0.00015 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

$$\mathbf{H_R} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

Note that all elements of the '3' Hessian matrices are either constants or zeros. This is another proof that higher order terms in Taylor series expansion (i.e. third order and above) are zeros.

In our analysis, we selected the point S=0, I=0 and R =0 as our equilibrium point $\mathbf{x}_o$. Note that it does not matter that the model will never reach this equilibrium point. In fact, the model never approaches the neighborhood around the origin point; this is because the summation of the '3' stocks is always constant, and equals the total population. In general, one can select any other equilibrium point and carry out the same process.

In this case vector **x** equals vector **y**; and equation 1 can take the following form:

$$\dot{\mathbf{x}} = \mathbf{J}^s \mathbf{x}$$

To compute matrix $\mathbf{J}^s$ one has to first compute matrix **J** at $\mathbf{x}_o$. Recall that the gradient vectors correspond to rows in the **J** matrix computed at $\mathbf{x}_o$. Matrix **J** computed at $\mathbf{x}_o$ is as follows:

$$\mathbf{J}\big|_{\mathbf{xo}} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & -0.5 & 0 \\ 0 & 0.5 & 0 \end{bmatrix}$$

And hence matrix $\mathbf{J^s}$ matrix is as follows (see equation 1):

$$\mathbf{J^s} = \begin{bmatrix} -0.000075 * I & -0.000075 * S & 0 \\ 0.000075 * I & 0.000075 * S - 0.5 & 0 \\ 0 & 0.5 & 0 \end{bmatrix}$$

The first row of $\mathbf{J^s}$ is computed from the following formula: $grad_S{}^T + 0.5\ \mathbf{x^T}\ \mathbf{H}_S$

The second row of $\mathbf{J^s}$ is computed from the following formula: $grad_I{}^T + 0.5\ \mathbf{x^T}\ \mathbf{H}_I$

And the third row of $\mathbf{J^s}$ is computed from the following formula: $grad_R{}^T + 0.5\ \mathbf{x^T}\ \mathbf{H}_R$

Note that the "smoothed Jacobian" matrix $\mathbf{J^s}$ is different than the "ordinary Jacobian" matrix **J**. For example, the first element of the first row in matrix $\mathbf{J^s}$ is equal -0.000075*I; while the corresponding element in matrix **J** is equal -0.00015*I. This is an important issue. Recall that the normal practice is to focus only on the ordinary matrix, and to ignore the 2nd order term of the Taylor series expansion. This can be considered an error term. And as the width of the analysis interval increases, this error term can be significant. For this reason, we postulate that in nonlinear models, it is preferred to use the smoothed Jacobian instead of the ordinary Jacobian.

Now, there are '3' *smoothed* eigenvalues associated with matrix $\mathbf{J^s}$. By using the Matlab symbolic toolbox we derived the following formulas:

λ_1 = -1/4+3/80000*S-3/80000*I+1/80000*(4e+008-120000*S-120000*I+9*S^2-
18*I*S+9*I^2)^(1/2)

λ_2 = -1/4+3/80000*S-3/80000*I-1/80000*(4e+008-120000*S-120000*I+9*S^2-
18*I*S+9*I^2)^(1/2)

$\lambda_3 = 0$

Matlab computations showed that the third *smoothed* eigenvalue is always zero. Now, by substituting the values of S, I, and R at ay time instant (obtained via simulation) in the above formulas, we can obtain the corresponding values for the *smoothed* eigenvalues. . The figures below plot the real and imaginary parts of the first and second *smoothed* eigenvalues across time.

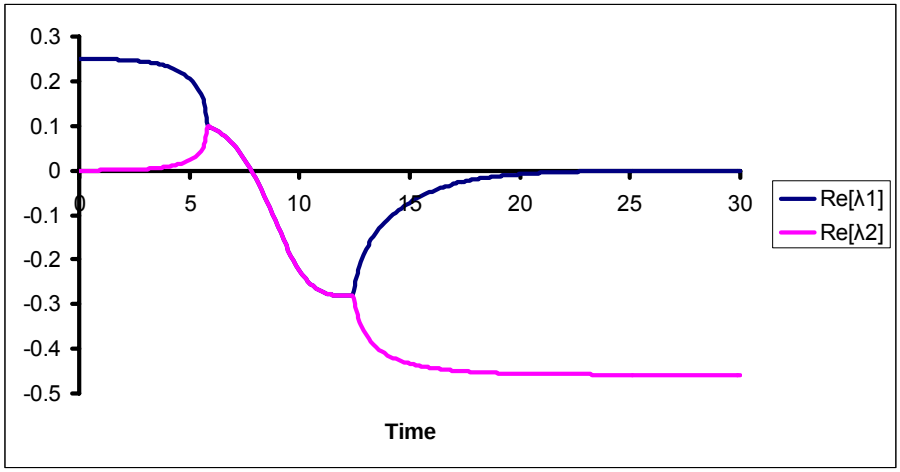

Figure 3: Real parts of the *smoothed* eigenvalues across time

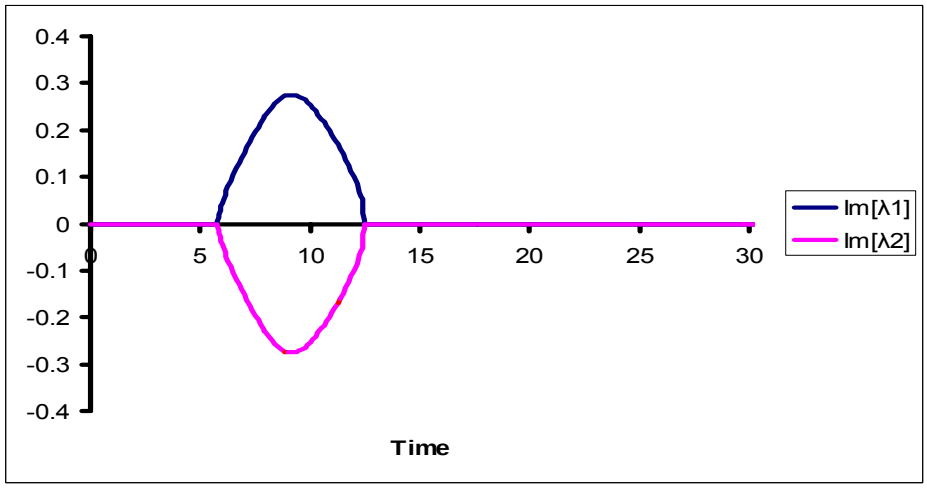

Figure 4: Imaginary parts of the *smoothed* eigenvalues across time

The above figures show that there are two bifurcations points.

- Time 6: 2 real positive modes merge to one complex mode
- Time 12.5: 1 complex mode split to 2 real negative modes

So basically one can chop time into the following 3 phases:

1. Exponential growth [0,6]
2. Part of oscillation cycle [6,12.5]
3. Exponential decay [12.5, ∞]

3. Conclusion and Future Work

In this paper, we adopted the idea of Nathan Forrester to consider the second order term of Taylor series expansion, when approximating nonlinear models. Moreover, we invented a new concept, which is the smoothed Jacobian matrix. This matrix is valid in any point in the n-dimensional space -- in contrast to the ordinary Jacobian which is valid only in the neighborhood of the current operating point; as in dealing with the ordinary matrix, we ignore the 2^{nd} order term of the Taylor series expansion. This can be considered an error term, and as the width of the analysis interval increases, this error term can be significant. In this paper we postulate that in nonlinear models, it is preferred to use the smoothed Jacobian instead of the ordinary Jacobian. Recall that the elements of the smoothed matrix can be considered smoothed slopes of relationships. The smoothing process is actualized via incorporating the curvatures specified by the Hessian matrices. Finally, by tracking the values of this smoothed matrix across time; and symbolically computing the corresponding smoothed eigenvalues and eigenvectors, one can identify the modes of behavior at any time instant.

In our future work, we will pursuit the following 4 directions:

1. Apply the approach to larger and more complex models.

2. Assess the impacts of changing the gains of loops on the smoothed eigenvalues. In this point, we will follow the procedure outlined by Kampmann & Oliva 2006.

3. Assess the impacts of changing the values of parameters on the smoothed eigenvalues and weights. In this point, we will follow the procedure outlined by Saleh et al. 2006.

4. Extend the analysis to include higher orders terms of Taylor expansion (third and above) which will be relevant in highly nonlinear models.

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