Sensitivity Analysis of Coupled Chaotic Dynamical Systems with the Pseudo-Orbit Tracing Property

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Abstract
This paper focuses on the sensitivity analysis of coupled nonlinear dynamical systems, which under certain conditions exhibit the chaotic behavior. Sensitivity functions calculated via conventional methods of sensitivity analysis are inherently uninformative and inconclusive. The use of the pseudo-orbit shadowing property in dynamical systems allows calculating sensitivity functions correctly and accurately for chaotic dynamics. The "pseudo-orbit" algorithm is illustrated on the coupled multiscale nonlinear chaotic dynamical system, which is obtained by coupling the fast and slow versions of the original well-known Lorenz model.

Keywords: sensitivity analysis, dynamical system, shadowing lemma, chaos

1 Introduction
Mathematical modeling represents a very powerful and effective instrument to study complex processes occurring in technical, economic, social and natural systems. State of the art mathematical models used in various branches of natural science are defined as a set of (partial) differential equations that contain a large number of parameters some of which can be inaccurate. Parameter errors and their time and space variability generate parametric uncertainty in mathematical models. It is therefore important to estimate the influence of parameter variations on the
model output results. Sensitivity analysis, which is an essential element of model building and quality assurance, addresses this very important issue [1, 2, 9]. Usually the forward and adjoint algorithms are used in sensitivity analysis. However, these conventional methods of sensitivity analysis are failed to compute sensitivity functions or sensitivity coefficients for chaotic dynamical systems [3, 11, 13]. The reason is that the conventional methods used to calculate the sensitivity functions are based on the numerical solution of the linearized Cauchy problem with respect to variations in the state vector \( \delta \mathbf{x}(t) \), where \( \mathbf{x} \in \mathbb{R}^n \) is the state vector of the system under consideration, \( t \) is the time and \( n \) is the dimension of the phase space. Variations \( \delta \mathbf{x}(t) \) characterize the separation in time of two trajectories that are initialized infinitely close to each other. The rate of separation of these trajectories in the phase space can be estimated by the following formula: \( \| \delta \mathbf{x}(t) \| = \| \delta \mathbf{x}(0) \| e^{\lambda t} \), where \( \lambda \) is the largest Lyapunov exponent and \( \delta \mathbf{x}(0) \) is the initial separation. For the chaotic dynamics, the largest Lyapunov exponent \( \lambda > 0 \) and, therefore, two trajectories diverge exponentially in time. As a result, calculated sensitivity functions (coefficients) grow exponentially in time and they are extremely inaccurate and inherently uninformative. As a result, it is very difficult to draw a clear conclusion on the system sensitivity with respect to variations in the parameters. The use of sensitivity analysis method, developed on the basis of the theory of shadowing pseudo-orbits in dynamical systems, allows calculating sensitivity functions (derivatives of a certain cost function with respect to model parameters) correctly and accurately [13]. In this paper, we consider the application of this approach to sensitivity analysis of a coupled nonlinear chaotic dynamical system obtained by coupling of fast and slow versions of the well-known Lorenz system [4].

2 Forward and adjoint sensitivity analysis

Let us consider a generic autonomous dynamical system

\[
\frac{d\mathbf{x}(t)}{dt} = f \left( \mathbf{x}(t), \mathbf{\alpha}(t) \right), \quad t \in [0, \tau] = T, \quad \mathbf{x}(0) = \mathbf{x}_0, \tag{1}
\]

where \( \mathbf{x} \in X \subseteq \mathbb{R}^n \) is the state vector the components of which belong to the class of continuously differentiable functions \( C^1(T) \), \( \mathbf{\alpha} \in \mathcal{P} \subseteq \mathbb{R}^m \) is a parameter vector the components of which belong to the class of piecewise continuous functions \( \tilde{C}^1(T) \), and \( f \in \mathbb{R}^n \) is a nonlinear vector-valued function defined in the domain \( X \times \mathcal{P} \times T \), that is continuous with respect to both \( \mathbf{x} \) and \( \mathbf{\alpha} \), continuously differentiable with respect to \( \mathbf{x} \), as well as piecewise continuous with respect to \( t \), such that \( f : X \times \mathcal{P} \times T \rightarrow X \), and \( \mathbf{x}_0 \) is a given vector-function. To estimate the influence of model parameter variations on the state variables a sensitivity coefficient can be used, which is the derivative of a certain component of
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a model state vector with respect to some model parameter. For the $i$-th state vector component $x_i$ with respect to $j$-th parameter vector component $\alpha_j$ the sensitivity coefficient is defined as [9]

$$
S_{ij} = \lim_{\delta \alpha_j \to 0} \left[ \frac{x_i(\alpha_j^0 + \delta \alpha_j) - x_i(\alpha_j^0)}{\delta \alpha_j} \right],
$$

where $\delta \alpha_j$ is the infinitesimal perturbation of parameter $\alpha_j$ around some fixed point $\alpha_j^0$. Approximating the state vector $x(\alpha + \delta \alpha)$ around $x(\alpha)$ by a Taylor expansion one can obtain the following linear equation:

$$
x(\alpha + \delta \alpha) = x(\alpha) + \left[ \frac{\partial x(t)}{\partial \alpha} \right]_{\alpha^0} \delta \alpha + O \left( \| \delta \alpha \|^2 \right),
$$

where $\left[ \frac{\partial x(t)}{\partial \alpha} \right]_{\alpha^0} \in \mathbb{R}^{n \times m}$ is a sensitivity matrix. Differentiating (1) with respect to $\alpha$ we obtain the set of non-homogeneous sensitivity equations:

$$
\frac{dS_j}{dt} = M \cdot S_j + D_j, \quad j = 1, \ldots, m,
$$

where $S_j = (\partial x/\partial \alpha_j) = (S_{1,j}, S_{2,j}, \ldots, S_{n,j})^T$ is the sensitivity vector with respect to parameter $\alpha_j$, $D_j = (\partial f_1/\partial \alpha_j, \ldots, \partial f_n/\partial \alpha_j)^T$, and $M$ is a Jacobian matrix. Once we have solved equations (1) and (4), it is possible to analyze the sensitivity of the system (1) with respect to the parameter $\alpha_j$. Let us introduce a generic function, which characterizes the dynamical system:

$$
J (x, \alpha) = \int_0^T \Phi(t;x,\alpha)dt,
$$

where $\Phi$ is a nonlinear function. The gradient of $J$ with respect to the vector of parameters $\alpha$ around the unperturbed state vector $x^0$

$$
\nabla \alpha J (x^0, \alpha^0) = \left[ \frac{dJ}{d\alpha_i}, \ldots, \frac{dJ}{d\alpha_m} \right]^T_{x^0, \alpha^0},
$$

quantifies the influence of parameters on the model output results. In particular, the effect of the $j$-th parameter can be estimated as follows:
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\[
\frac{dJ}{d\alpha_j} \approx J \left( x^0 + \delta x^0; \alpha_j^0, \ldots, \alpha_j^0 + \delta \alpha_j, \ldots, \alpha_m^0 \right) - J \left( x^0, \alpha^0 \right),
\]

(6)

where \( \delta \alpha_j \) is the variation in parameter \( \alpha_j^0 \). Note that

\[
\frac{dJ}{d\alpha_j} = \sum_{i=1}^{m} S_j \frac{\partial J}{\partial x_i} + \frac{\partial J}{\partial \alpha_j},
\]

where \( S_j \) are sensitivity coefficients (2) used, for example, in the theory of automatic control [9]. However, the accuracy of sensitivity estimates (6) strongly depends on the choice of perturbation \( \delta \alpha_j \). The use of the Gâteaux differential as a measure of the sensitivity eliminates the need to set the value \( \delta \alpha \) [1]:

\[
\delta J \left( x^0, \alpha^0 \right) = \int_0^\tau \left( \frac{\partial \Phi}{\partial x} \right) \cdot \delta x + \left( \frac{\partial \Phi}{\partial \alpha} \right) \cdot \delta \alpha \, dt,
\]

(7)

where \( \delta x \) is the state vector variation due to the variation in the parameter vector in the direction \( \delta \alpha \). Linearizing (1) around an unperturbed orbit \( x^0(t) \), we obtain the variational equations for calculating \( \delta x \):

\[
\frac{\partial \delta x}{\partial t} = \left[ \frac{\partial f}{\partial x} \right] \cdot \delta x + \left[ \frac{\partial f}{\partial \alpha} \right] \cdot \delta \alpha, \quad t \in [0, \tau], \quad \delta x(0) = 0.
\]

(8)

Then the variation \( \delta J \) can be calculated using the equation (8). Since

\[
\delta J \left( x^0, \alpha^0 \right) = \left( \nabla_{\alpha} J, \delta \alpha \right),
\]

where \( \langle \cdot \rangle \) is a scalar product, the model sensitivity with respect to parameter variations can be estimated by calculating the components of the gradient \( \nabla_{\alpha} J \). However, this method is computationally ineffective if the number of model parameters \( m \) is large. The use of adjoint equations allows obtaining the required sensitivity estimates within a single computational experiment [1, 2, 5] since the gradient \( \nabla_{\alpha} J \) can be calculated as:

\[
\nabla_{\alpha} J \left( x^0, \alpha^0 \right) = \int_0^\tau \left[ \left[ \frac{\partial \Phi}{\partial \alpha} \right] \cdot \delta \alpha \right]^T \cdot x^* \, dt,
\]

(9)

where the vector function \( x^* \) is the solution of the adjoint model

\[
-\frac{\partial \delta x^*}{\partial t} - \left[ \frac{\partial f}{\partial x} \right] \cdot x^* = -\left[ \frac{\partial \Phi}{\partial x} \right], \quad t \in [0, \tau], \quad x^*(\tau) = 0.
\]

(10)

The equation (1) is numerically integrated in the inverse time direction.
3 Coupled multiscale nonlinear dynamical system

A multiscale nonlinear dynamical system used in this study is obtained by coupling the fast and slow versions of the original Lorenz model (L63) [4] and can be written as follows [6, 10, 11]:

\[
\begin{align*}
\dot{x} &= \sigma(y-x) - c(aX + k), \\
\dot{y} &= r x - y - xz + c(aY + k), \\
\dot{z} &= xy - bz + cz, \\
\dot{X} &= \varepsilon \sigma(Y - X) - c(x + k), \\
\dot{Y} &= \varepsilon (rX - Y - aXZ) + c(y + k), \\
\dot{Z} &= \varepsilon (aXY - bZ) - cz,
\end{align*}
\]

where lower case letters represent the fast subsystem and capital letters – the slow subsystem, \(\sigma, r, b\) are the parameters of L63 model, \(c\) is a coupling strength parameter for the \(x\) and \(y\) variables, \(c_z\) is a coupling strength parameter for \(z\), \(k\) is an “uncentering” parameter, \(\varepsilon\) is the time scale factor, and \(a\) is a parameter representing the amplitude scale factor. The value \(a = 1\) indicates that two systems have the same amplitude scale. Thus, the state vector of the system is \(\mathbf{x} = (x, y, z, X, Y, Z)^T\) and the parameter vector is \(\mathbf{a} = (\sigma, r, b, a, c, c_z, k, \varepsilon)^T\).

Without loss of generality, we can assume that \(a = 1\), \(k = 0\) and \(c = c_z\), then \(\mathbf{a} = (\sigma, r, b, c, \varepsilon)^T\). The unperturbed parameter values are taken as

\[
\sigma^0 = 10, \quad r^0 = 28, \quad b^0 = 8/3, \quad \varepsilon^0 = 0.1, \quad c^0 \in [0.1; 1.0].
\]

Chosen values of \(\sigma, r\) and \(b\) correspond to chaotic behaviour of the L63 model. The parameter \(\varepsilon = 0.1\) indicates that the slow system is 10 times slower than the fast system. Essential dynamical, correlation and spectral properties of the system (12) were considered in [12]. The system behaviour strongly depends on the value of parameter \(c\) since this parameter controls the synchronization between fast and slow subsystems. Qualitative changes in the dynamical properties of a system can be detected by determining and analyzing the corresponding spectrum of Lyapunov exponents. The system (12) has six distinct exponents. If the parameter \(c\) tends to zero, then the system (12) has two positive, two zero and two negative Lyapunov exponents. Numerical experiments showed that initially positive two largest conditional Lyapunov exponents decrease monotonically with an increase in the parameter \(c\). At about \(c \approx 0.8\) they approach the \(x\)-axis and at about \(c \approx 0.95\) negative values. Thus, for \(c > 0.95\) the dynamics of both fast and slow subsystems become phase synchronous [8, 13]. When \(c > 1.0\), a limit circle dynamical regime is observed since all six exponents become negative.
4 Sensitivity analysis of the system

Let us consider the influence of variations in the parameter $r$ on the system dynamics using the forward approach. The parameter $r$ plays an important role in the formation of system’s dynamical structure and transition to chaotic behavior. Let us define the following sensitivity coefficients:

$$
S_{1r} = \frac{\partial x}{\partial r}, \quad S_{2r} = \frac{\partial y}{\partial r}, \quad S_{3r} = \frac{\partial z}{\partial r}, \\
S_{4r} = \frac{\partial X}{\partial r}, \quad S_{5r} = \frac{\partial Y}{\partial r}, \quad S_{6r} = \frac{\partial Z}{\partial r}.
$$

The associated system of sensitivity equations can be written as:

$$
\begin{align*}
\dot{S}_{1r} &= \sigma (S_{2r} - S_{1r}) - cS_{4r}, \\
\dot{S}_{2r} &= x + rS_{1r} - S_{2r} - (xS_{3r} + zS_{1r}) + cS_{5r}, \\
\dot{S}_{3r} &= (xS_{2r} + yS_{1r}) - bS_{3r} + cS_{6r}, \\
\dot{S}_{4r} &= \varepsilon \sigma (S_{5r} - S_{4r}) - cS_{1r}, \\
\dot{S}_{5r} &= \varepsilon [x + rS_{4r} - S_{5r} - (XS_{6r} + ZS_{4r})] + cS_{2r}, \\
\dot{S}_{6r} &= \varepsilon [(XS_{5r} + YS_{4r}) - bS_{6r}] - cS_{3r}.
\end{align*}
$$

Fig 1 Time dynamics of sensitivity coefficients with respect to parameter $r$
Envelopes of calculated sensitivity coefficients grow in time and the coefficients themselves demonstrate the oscillating behavior (Fig. 1). Similar dynamics of sensitivity coefficients were observed for the original L63 model [3, 13]. However, calculated coefficients are inherently uninformative since it is very difficult to draw a clear conclusion from them about system sensitivity to variations in the parameter $r$. Similarly, obtained sensitivity coefficients with respect to other parameters are also uninformative and inconclusive. This is because the average values of sensitivity coefficients (the components of $\nabla_{\alpha} \langle J(\alpha) \rangle$) over a certain period of time cannot be correctly estimated within the framework of conventional methods of sensitivity analysis, since for chaotic systems it is observed [3, 11, 13] that $\nabla_{\alpha} \langle J(\alpha) \rangle \neq \langle \nabla_{\alpha} J(\alpha) \rangle$ since the integral

$$I = \lim_{t \to \infty} \lim_{\delta \alpha \to 0} \left[ \frac{J(\alpha + \delta \alpha) - J(\alpha)}{\delta \alpha} \right] dt$$

(14)

does not possess uniform convergence and two limits ($\tau \to \infty$ и $\delta \alpha \to 0$) would not commute. The problem can be resolved based on the theory of shadowing of pseudo-orbits (approximate trajectories) in dynamical systems [7]. The term "shadowing" refers to the situation when a true trajectory of a dynamical system lies uniformly close to a pseudo-trajectory. The shadowing lemma [7] states that for the vector field generating the flow $\Phi'$, the shadowing property is performed in a small neighborhood of a compact hyperbolic set for dynamical system $\Phi'$.

Let $x$ be a trajectory of the dynamical system obtained with the perturbed parameter vector (“pseudo-orbit”), which stays uniformly close to the “true” orbit obtained with unperturbed parameter vector. Then the integral (14) is convergent and the average sensitivities $\langle \nabla_{\alpha} J(\alpha) \rangle$ can be easily estimated. Thus, the problem now is to calculate the pseudo-orbit. There are several methods for solving this problem. One of these approaches is based on the inversion of the so-called “shadow” operator [13]. For simplicity, let us consider an autonomous dynamical system with one independent variable and one parameter $\nabla_{\alpha} f(x,\alpha)$. The sensitivity analysis aims to estimate the sensitivity coefficient $S_{\alpha} = \partial x/\partial \alpha$. Let us introduce the following transform: $x'(x) = x + \delta x (x)$, where $x$ and $x'$ are true trajectory and pseudo-orbit respectively. The orbit $x'$ is generated due to the variation in parameter $\alpha$. It can be shown that $\delta f (x) = A \delta x (x)$, where $A = \left[ - (\partial f / \partial x) + (d/dt) \right]$ is a “shadow” operator. Thus, to find a pseudo-orbit we need to solve the equation $\delta x = A^{-1} \delta f$, i.e. we must numerically invert the operator $A$ for a given $\delta f$. To solve this problem, functions $\delta x$ и $\delta f$ are decomposed into their constituent Lyapunov covariant vectors and then expansion coefficients are calculated numerically. Finally, the desired sensitivity coefficient is calculated as $S_{\alpha} = \langle \delta x \rangle / \delta \alpha$. 

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To illustrate the applicability of the “pseudo-orbit” algorithm described shortly above for sensitivity analysis of the system (11), the response function (5) is defined as \( J = \dot{x} \). For \( c = 1.0 \), the sensitivity function \( S_r = \langle \partial J / \partial r \rangle \) is estimated to be \( S_r \approx 2.38 \). To obtain this result only a single phase trajectory \( x(t) \) for \( t \in [0, \tau] \) was used. Here \( \tau = 2 \cdot 10^3 \Delta t \), where \( \Delta t = 10^{-2} \) is the integration time step.

Direct integration of the equations (11) over the time interval \([0, 10^6 \Delta t]\), followed by application of formula (6) provides the sensitivity function estimate \( S_r \approx 19.38 \). Use of the ensemble approach provides sensitivity function estimates similar to those obtained by the “pseudo-orbit” algorithm. However, to obtain statistically significant results, the number of ensemble members should be large enough (on the order of several hundreds). Thus, the computation time required for sensitivity analysis of the system (11) by the “pseudo-orbit” algorithm is reduced by orders of magnitude compared with the computational cost required to implement the ensemble approach.

4 Conclusion

In this paper, we considered some aspects of sensitivity analysis of nonlinear dynamical systems, which under certain conditions exhibit the chaotic behavior. For chaotic dynamics, sensitivity functions (coefficients) calculated using conventional methods of sensitivity analysis are inherently uninformative and inconclusive. The approach developed on the basis of pseudo-orbit shadowing property in dynamical systems [7, 13] provides estimating the sensitivity functions (coefficients) correctly, accurately and effectively in terms of the computation time. We demonstrated the applicability of the “pseudo-orbit” algorithm for sensitivity analysis of the coupled multiscale nonlinear dynamical system. The results obtained can be very useful in a variety of disciplines, including the study of climate change.

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References


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