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Transformation invariant stochastic catastrophe theory☆

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Abstract

Catastrophe theory is a mathematical formalism for modeling nonlinear systems whose discontinuous behavior is determined by smooth changes in a small number of driving parameters. Fitting a catastrophe model to noisy data constitutes a serious challenge, however, because catastrophe theory was formulated specifically for deterministic systems. Loren Cobb addressed this challenge by developing a stochastic counterpart of catastrophe theory (SCT) based on Itô stochastic differential equations. In SCT, the stable and unstable equilibrium states of the system correspond to the modes and the antimodes of the empirical probability density function, respectively. Unfortunately, SCT is not invariant under smooth and invertible transformations of variables—this is an important limitation, since invariance to diffeomorphic transformations is essential in deterministic catastrophe theory. From the Itô transformation rules we derive a generalized version of SCT that does remain invariant under transformation and can include Cobb's SCT as a special case. We show that an invariant function is obtained by multiplying the probability density function with the diffusion function of the stochastic process. This invariant function can be estimated by a straightforward time series analysis based on level crossings. We illustrate the invariance problem and its solution with two applications.

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1. Introduction

Ever since its creation by Thom [1] and its subsequent popularization by Zeeman [2,3], catastrophe theory (CT) has been applied to a wide range of different systems from physics, engineering, biology, psychology, and sociology. A small subset of specific phenomena that were analyzed and modeled using CT includes quantum morphogenesis, the formation of

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caustics in ray optics, the stability of ships, the stability of black holes, the surface changes in interatomic potential, Euler struts, the size of bee societies, morphogenesis or cell differentiation in embryology, bistability of perception, binocular vision, motor learning, sudden transitions in attitudes, and the cognitive development of children (for details see [4–15]). In all these applications, the behavior of the system under study shows sudden, discontinuous changes or phase transitions as a result of small, continuous changes in variables that influence the system (cf. the freezing of water when temperature is gradually decreased, or the collapse of a bridge under slowly mounting pressure).

In general, CT applies to systems that may respond to continuous changes in control variables by a discontinuous change from one equilibrium state to another. For clarity of exposition we first discuss the case of a single state variable x (see [5] for higher-order catastrophes that can have more than one state variable). CT implies that the behavior of the system under study follows

$$\mathrm{d}x = \frac{-\mathrm{d}V(x)}{\mathrm{d}x}\mathrm{d}t, \tag{1}$$

meaning that the state of the system will change as a result of a change in $V(x)$. $V(x)$ is a potential function, and incorporates the control variables $c_1, c_2, \ldots, c_n$. The system is in equilibrium when $\mathrm{d}V(x; c_1, c_2, \ldots, c_n)/\mathrm{d}x = 0$. Thus, CT is concerned with systems that move toward an equilibrium state of minimum "energy" (i.e., gradient dynamical systems; for a detailed treatment see [5,6,16,17]).

CT offers a mathematical basis for the classification of gradient dynamical systems with respect to the number and type of critical points. This configuration of critical points is invariant under diffeomorphic coordinate transformations, that is, transformations that are smooth (i.e., differentiable up to arbitrary order) and invertible (i.e., one-to-one). This means that two systems are equivalent when their potential functions can be transformed into one another. Specifically, assume two equivalent potential functions $V_1(x; c)$ and $V_2(y; d)$, consisting here of one state variable and one control variable. Equivalence means that there exist diffeomorphic transformations $y = \varphi(x; c)$ and $d = \eta(c)$, and a smooth, real function $\gamma(c)$ such that the potential functions can be locally transformed into one another (p. 59 in [5]):

$$V_1(x; c) = V_2(\varphi(x; c); \eta(c)) + \gamma(c). \tag{2}$$

Geometrically, (2) entails that a transformation that smoothly bends or stretches an object preserves its topological features (cf. pp. 90–92 in [5]).

The invariance property is inherent to CT and allows it to classify systems as belonging to a small set of qualitatively different models, the so-called elementary catastrophes (under the constraint that there be at most two state variables and four control variables; see [5] for details). The major theme of this article is to develop a stochastic variant of deterministic catastrophe theory that is consistent with the invariance property.

As CT was developed as an abstract topological theory for deterministic systems, it may not be immediately obvious how to extend the theory to stochastic systems. Loren Cobb was the first to address this problem and propose a stochastic version of catastrophe theory (SCT; [18–21]). In Cobb's method of maximum likelihood estimation (MLE), stable and unstable equilibria are associated with the modes and antimodes, respectively, of the system's stationary probability density function (pdf). In contrast to deterministic catastrophes, however, Cobb's stochastic catastrophes are not invariant under nonlinear diffeomorphic transformations. This highlights an important discrepancy between deterministic CT and its stochastic counterpart, as Cobb duly acknowledged: "However, MLE's are not invariant under general diffeomorphisms of the measured variables. Therefore, much of the topological generality of catastrophe theory may have been lost in the statistical portion of our theory" (p. 317 in [22]; see also [23]).

In this article we generalize the method of Cobb by taking into account the Itô transformation rule, thereby arriving at the non-normalized stationary density function of a Stratonovich stochastic differential equation. In contrast to the method of Cobb, this generalized SCT is unaffected by smooth and invertible transformations.[1] We show that an invariant function

[1] These transformations may involve the control variables as well as the behavioral variables (i.e., the measurement scales). Although our conceptual focus is on transformations of measurement scales, the results reported here hold regardless of what type of variable is transformed.

may be obtained by multiplying the probability density function by the diffusion function of the stochastic process. This invariant function preserves the configuration of critical points under diffeomorphic transformation. Thus, the generalized SCT outlined here offers a methodology to test transition hypotheses in stochastic systems that is fully consistent with deterministic catastrophe theory.

The outline of this paper is as follows. Section 2 outlines stochastic catastrophe theory. We describe the pioneering work by Cobb, and point out the invariance problem. Next, we extend Cobb's work to derive a generalized SCT that is invariant under diffeomorphic transformations. This is the core of the paper. Section 3 outlines a time series method based on level crossings to estimate the invariant function. Section 4 illustrates the use of the invariant function with two applications. Section 5 concludes.

2. Stochastic catastrophe theory

Most practical scientific investigations are subject to some sort of noise, originating either from imperfect measurement or from the inherent stochastic nature of the system under study. What happens to catastrophe models when the underlying dynamics is contaminated by a non-negligible amount of noise? Is it still possible to apply CT to such cases? And how should this be accomplished?[2]

2.1. Cobb's stochastic catastrophe theory

In an effort to address the questions mentioned above, Cobb combined deterministic CT with stochastic systems theory (e.g., [18,19,22,20,21]). The use of Itô stochastic differential equations (e.g., [26]) allowed Cobb to establish a link between the potential function of a deterministic catastrophe system and the stationary probability density function (pdf) of the corresponding stochastic process. This leads to definitions of a stochastic equilibrium state and stochastic bifurcation that are compatible with their deterministic counterparts.

[2] In this article we study stochastic bifurcations in terms of the behavior of distributions. An alternative approach is to focus on sample path behavior (i.e., Random Dynamical Systems [24,25]).

The method of Cobb will be discussed by considering a system of one state variable and several control variables, whose dynamics obey (1). For ease of presentation the explicit dependence of the potential function on the control variables is omitted. The deterministic behavior of the system described by (1) can be made stochastic and put in the form of a stochastic differential equation (SDE) by simply adding a stochastic Gaussian white noise driving term $\mathrm{d}W(t)$:

$$\mathrm{d}x = \frac{-\mathrm{d}V(x)}{\mathrm{d}x}\mathrm{d}t + \sigma(x)\mathrm{d}W(t). \tag{3}$$

The deterministic term on the right-hand side, $-\mathrm{d}V(x)/\mathrm{d}x$, is the *drift function* $\mu(x)$, while $\sigma(x)$ is the *diffusion function*, and $W(t)$ is a Wiener process (i.e., idealized Brownian motion). The diffusion function $\sigma(x)$ is the square root of the infinitesimal variance function and determines the relative influence of the noise process. The reader is referred to the extensive literature on SDEs (e.g., [26–29]) for details.

Before proceeding, it is important to mention that when the diffusion function $\sigma(x)$ depends on x, (3) can be interpreted in various ways. Mathematically most convenient is the Itô interpretation [30], in which the value of x during an infinitesimal timestep $\mathrm{d}t$ is taken to be the value at the beginning of the timestep, that is, $x = x(t)$. Another interpretation is due to Stratonovich [31], who used the value of x at the middle of the timestep, that is, $x = x(t + (1/2)\mathrm{d}t) = x(t) + (1/2)\mathrm{d}x(t)$ (cf. [32]). We will later see that this difference in interpretation is in fact crucial for a transformation invariant stochastic catastrophe theory.

Cobb interpreted (3) in the Itô sense, and calculated the stationary pdf $f(x)$ by solving the corresponding Fokker–Planck equation, yielding

$$f(x) = N_a \exp[-V_{\mathrm{sto}}(x)], \tag{4}$$

where N_a is a normalizing constant (cf. p. 270 in [27]) and the stochastic potential function $V_{\mathrm{sto}}(x)$ is given by

$$V_{\mathrm{sto}}(x) = -2\int_a^x \frac{\mathrm{d}z\{\mu(z) - (1/2)[\sigma^2(z)]'\}}{[\sigma^2(z)]}, \tag{5}$$

where $\mu(z)$ is the drift function, $\sigma(z)$ is the diffusion function (cf. (3)), a is an arbitrary interior point of the state space, and the prime denotes differentiation with respect to z. When the diffusion function is constant, $\sigma(x) = c$, the stochastic potential function is proportional to the deterministic potential func-

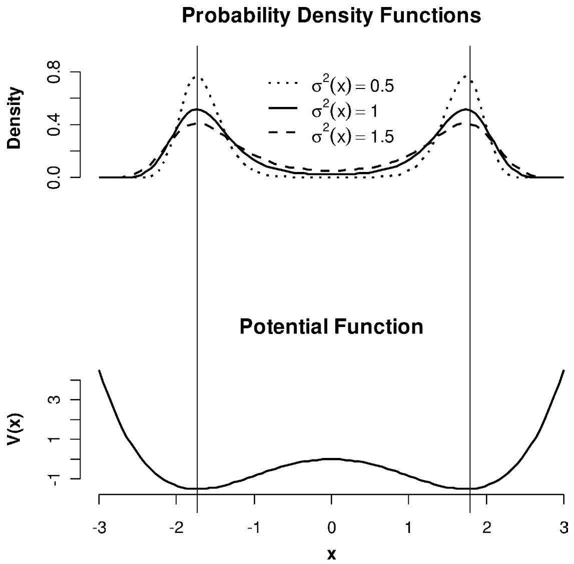

Fig. 1. Correspondence between the deterministic potential function $V(x)$ and the probability density function $f(x)$ for constant diffusion function $\sigma(x)$. Stable states correspond to minima of the potential function and modes of the pdf, whereas unstable states correspond to maxima of the potential function and antimodes of the pdf.

tion: $V_{\mathrm{sto}}(x) = 2V(x)/c^2$. From (4), it then follows that $f'(x) = 0$ whenever $V'(x) = 0$. To illustrate, Fig. 1 shows the cusp potential function $V(x) = (1/6)x^4 - x^2$ and the pdfs for the corresponding Itô SDE with $\sigma^2(x) = 1/2$, 1, and 3/2. The stable and unstable equilibria of the potential function are associated with the modes and antimodes, respectively, of the stationary pdfs (cf. p. 273 in [27]). A decrease in the diffusion variance is associated with a pdf that is more sharply peaked in the neighborhood of the minima of the potential function.

Cobb's catastrophe fitting procedure (e.g., [18,21]) inserts a specific catastrophe potential function in (4), *sets* $\sigma(x)$ *to a constant* and then determines parameter values using maximum likelihood estimation. To illustrate, consider the cusp catastrophe model that is characterized by the potential function $V(x) = (1/4)x^4 - (1/2)cx^2 - \mathrm{d}x$. The method of Cobb proceeds by fitting the pdf:

$$p(y|\alpha, \beta) = N \exp\left[-\frac{1}{4}y^4 + \frac{1}{2}\beta y^2 + \alpha y\right], \qquad (6)$$

where N is a normalizing constant. In (6), the observed dependent variable x has been rescaled by $y = (x - \lambda)/\sigma$, and α and β are linear functions of the two control variables c and d as follows: $\alpha = k_0 + k_1 c + k_2 d$ and $\beta = l_0 + l_1 c + l_2 d$. The parameters $\lambda, \sigma, k_0, k_1, k_2, l_0, l_1$, and l_2 can be estimated using maximum likelihood procedures [22].[3]

The procedure introduced by Cobb clearly hinges on the fact that the deterministic potential function $V(x)$ and the stationary pdf $f(x)$ convey the same information about the configuration of critical points (i.e., equilibrium points, for which the first derivative of the potential function is zero). Under the assumptions that the diffusion function $\sigma(x)$ is constant, and that the current measurement scale is not to be nonlinearly transformed, Cobb's definition of a stochastic stable equilibrium state as a mode of the pdf is perfectly reasonable. A qualitative change in the potential function, as a result of parameter variation, corresponds to a similar qualitative change in the stationary pdf. In this way, stochastic bifurcations are characterized by a change in the number of stochastic stable equilibrium states, that is, a change in the number of modes of the stationary pdf.

2.2. *The invariance problem*

As mentioned in the introduction, deterministic CT features a classification scheme that allows even an ill-defined system to be categorized as one of several elementary catastrophes. The only requirement is that the system's underlying dynamics is described by (1) with no more than two state variables and four control variables. To apply the classification scheme, however, the system under consideration must be transformed to its canonical form using diffeomorphic transformations. For this reason, the invariance under diffeomorphic transformation [cf. (2)] is a crucial property of deterministic CT. The main limitation of SCT as developed by Cobb is that it is *not* invariant under nonlinear diffeomorphic transformation of the measurement scale. As noted earlier, Cobb himself was well aware of the discrepancy between deterministic CT and his SCT that uses maximum likelihood estimation.

To see why Cobb's method is not invariant under nonlinear diffeomorphic transformations, recall

[3] Hartelman [33,34] developed a robust and flexible computer program, *Cuspfit*, that implements the method of Cobb. *Cuspfit* is freely available at http://users.fmg.uva.nl/hvandermaas/.

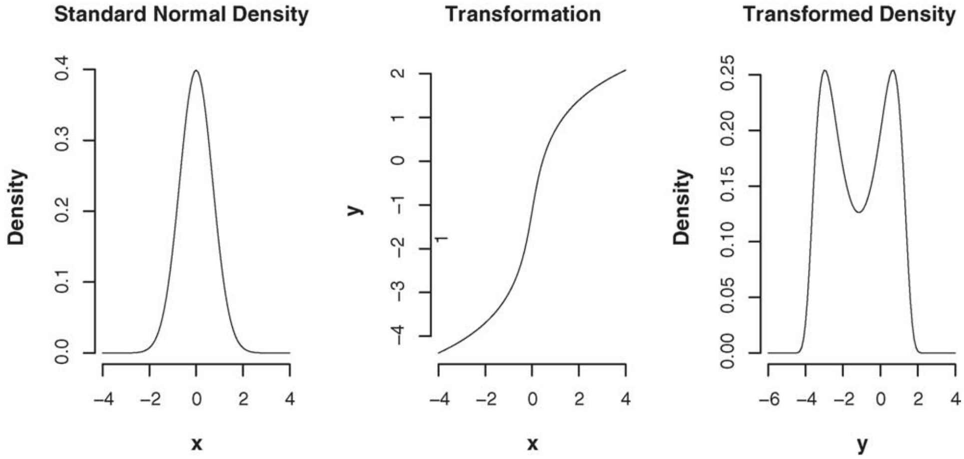

Fig. 2. Probability density functions are not invariant under transformations I. The left panel shows a variable x that has a standard normal pdf. The middle panel shows the transformation to a new variable y according to $y = \ln[x + \sqrt{x^2 + 0.1}]$. The right panel shows the pdf for y. The transformation changes the configuration of critical points, as the left panel is unimodal and the right panel is bimodal.

that the method is based entirely on the shape of the pdf, and note that a change of variables will invoke the chain rule that leads to an additional Jacobian term. Specifically, if the pdf of a continuous random variable x is $f(x)$, then the pdf of the transformed variable $y = \varphi(x)$ is $\{f[\varphi^{-1}(y)]\}/\varphi'[\varphi^{-1}(y)]$, where φ^{-1} is the inverse of φ (e.g., pp. 28–30 in [35]). For instance, a variable x having a standard normal density, $x \sim N(0, 1)$, $f(x) = (1/\sqrt{2\pi}) \exp(-(1/2)x^2)$, may be transformed to a new variable y by means of $y = \varphi(x) = \exp(x)$. Then $\varphi'(\cdot) = \exp(\cdot)$, $\varphi^{-1}(\cdot) = \ln(\cdot)$, and consequently $\varphi'[\varphi^{-1}(y)] = y$. Hence, the density of y is given by $(1/y\sqrt{2\pi}) \exp[-(1/2)(\ln y)^2]$. The additional Jacobian term $1/\varphi'[\varphi^{-1}(y)]$ that is involved in the transformation may dramatically alter the shape of the density, changing the configuration of critical points. Therefore, no invariant characteristics can be extracted from the pdf alone.

Fig. 2 illustrates the above point. The left panel shows a *unimodal*, standard normal density for a variable x. The middle panel shows the diffeomorphic transformation $y = \varphi(x) = \ln[x + \sqrt{x^2 + a}]$ for $a = 0.1$. Note that when $a = 1$, $y = \operatorname{arcsinh}(x)$. The slope at $x = 0$ for $\varphi(x)$ is given by $1/\sqrt{a}$. The right panel shows the density for y, which is given by $(\exp(y) + a\exp(-y)/\sqrt{8\pi}) \exp\{-(1/2)[(1/2)(\exp(y) - a\exp(-y))]^2\}$. For $0 < a < 1$, the density for the transformed variable y is now *bimodal*, having maxima at $\ln(1 + \sqrt{1-a})$ and $\ln(1 - \sqrt{1-a})$, and a minimum at $\ln(\sqrt{a})$.

For processes that obey a stochastic differential equation, the correspondence between the potential function and the pdf in terms of the configuration of critical points only holds when the diffusion function $\sigma(x)$ is constant, meaning that the noise is additive rather than multiplicative. Nonlinear diffeomorphic transformations of the measurements generally result in a diffusion function that is no longer constant. In such a case, the pdf no longer provides reliable information with respect to the existence of stable and unstable states. We underscore this important observation by considering two concrete examples.

As a first example, Fig. 3A plots a representative simulated time series obtained from the cusp catastrophe SDE $\mathrm{d}x = (2x - x^3)\mathrm{d}t + \sigma(x)\,\mathrm{d}W(t)$ with $\sigma(x)=1$ [cf. (3)], for which the deterministic potential function has two stable equilibrium states.[4] Fig. 3C shows that the corresponding pdf is indeed clearly bimodal, correctly indicating the presence of the two stable states. Fig. 3B plots the very same data transformed according to $y = (1/2)[\exp(3x) - (1/2)\exp(-3x)]$.

[4] To avoid clutter, we show results for only a single simulated time series. The results for other randomly generated time series are qualitatively similar, as the reader may ascertain by using the R program freely available at http://users.fmg.uva.nl/ewagenmakers/SCT.

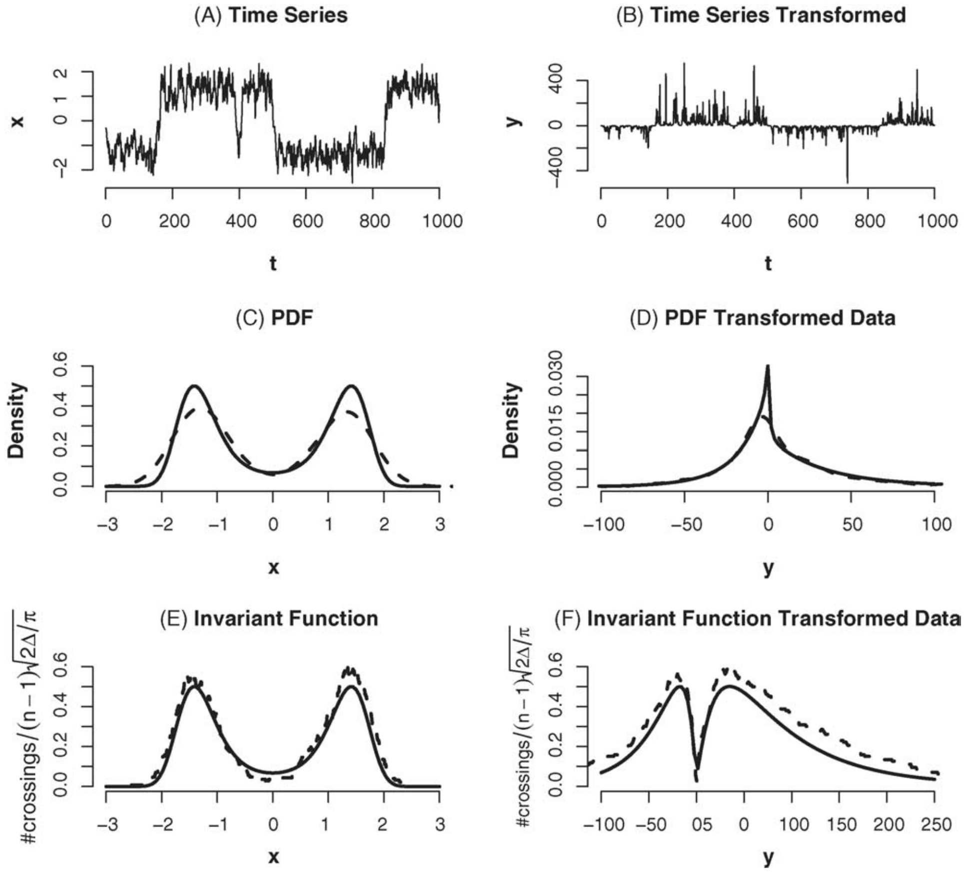

Fig. 3. Probability density functions are not invariant under transformations II. Panel (A): A sample times series of 1000 observations from the cusp catastrophe system $\mathrm{d}x = (2x - x^3)\mathrm{d}t + \mathrm{d}W(t)$, simulated with discrete time steps of length 0.1. Panel (B): The same times series as in panel (A), transformed according to $y = (1/2)[\exp(3x) - (1/2)\exp(-3x)]$. Panel (C): The solid black line gives the analytical pdf, and the dashed black line gives a kernel density estimate for the sample data from panel (A). Panel (D): The solid black line gives the analytical pdf, and the dashed black line gives a kernel density estimate for the transformed data from panel (B). Panel (E): The solid black line gives the analytical invariant function, and the dashed black line gives the level crossing function for the sample data from panel (A). Panel (F): The solid black line gives the analytical invariant function, and the dashed black line gives the level crossing function for the transformed data from panel (B).

Fig. 3D shows that the associated pdf is now unimodal, falsely suggesting that there is only one stable state. In Fig. 3C and D, the solid line is the analytical (‘true’) pdf calculated from the data-generating SDE (using (3), (4), and the pdf transformation rule mentioned above), and the dashed line is a standard kernel density estimate based on the simulated data sets shown in Fig. 3A and B.[5] Fig. 3E and F will be discussed later.

Fig. 4A illustrates the second example. In this case, transformation of the measurement scale makes a single-state system masquerade as a two-state system. A representative simulated time series was obtained from the Ornstein–Uhlenbeck SDE $\mathrm{d}x = -x\mathrm{d}t + \mathrm{d}W(t)$, for which the deterministic potential function has a single stable equilibrium state. Fig. 4C shows that the corresponding pdf is indeed unimodal.

[5] For all kernel density estimation reported here, we used a Gaussian kernel and determined the window width h using Silverman's rule of thumb $h = 0.9An^{-1/5}$ (Eq. 3.31 in [36]), where $A = \min$ (*standard deviation, interquartile range*/1.34), and n is the number of observations.

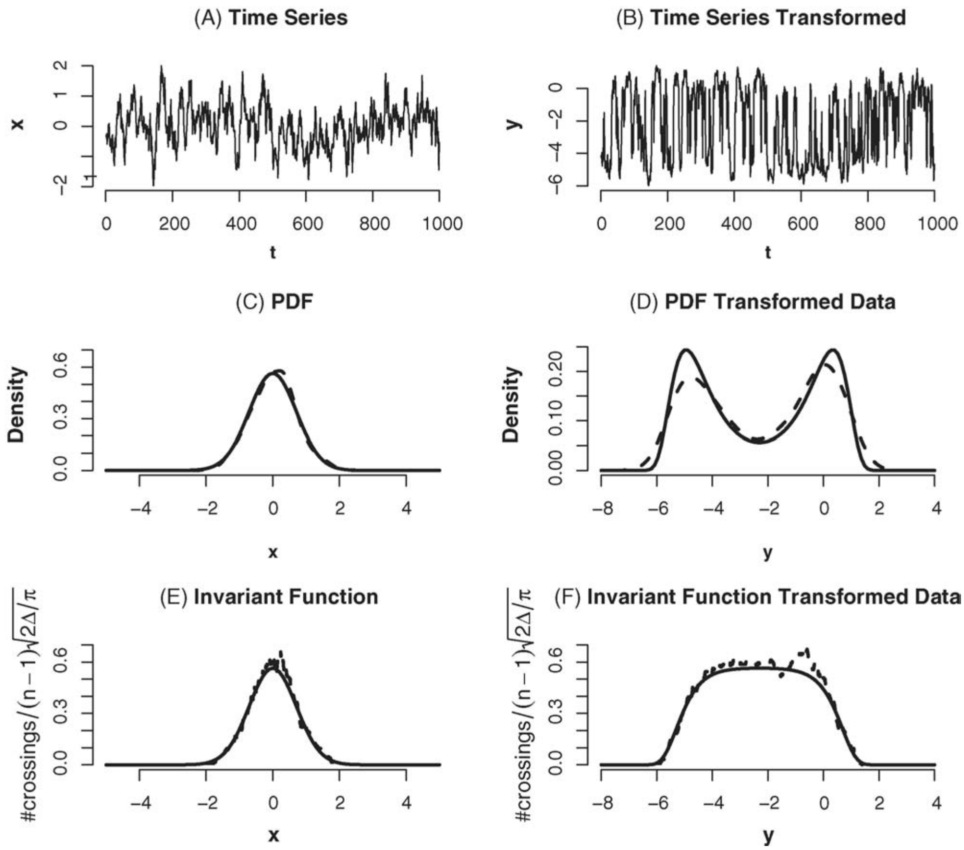

Fig. 4. Probability density functions are not invariant under transformations III. Panel (A): A sample times series of 1000 observations from the SDE $\mathrm{d}x = -x\,\mathrm{d}t + \mathrm{d}W(t)$, simulated with discrete time steps of length 0.1. Panel (B): The same times series as in panel (A), transformed according to $y = \ln[x + \sqrt{x^2 + 0.01}]$. Panel (C): The solid black line gives the analytical pdf, and the dashed black line gives a kernel density estimate for the sample data from panel (A). Panel (D): The solid black line gives the analytical pdf, and the dashed black line gives a kernel density estimate for the transformed data from panel (B). Panel (E): The solid black line gives the analytical invariant function, and the dashed black line gives the level crossing function for the sample data from panel (A). Panel (F): The solid black line gives the analytical invariant function, and the dashed black line gives the level crossing function for the transformed data from panel (B).

Fig. 4B plots the same data transformed according to $y = \ln[x + \sqrt{x^2 + a}]$ with $a = 0.01$. Fig. 4D shows that the associated pdf is now bimodal, incorrectly suggesting the existence of two stable states. As in Fig. 3, the solid line in Fig. 4C and D corresponds to the analytical pdf calculated from the data-generating SDE, and the dashed line is a standard kernel density estimate based on the simulated data sets shown in Fig. 4A and B. Fig. 4E and F will be discussed later.

In sum, the shape of the pdf does not convey transformation-invariant information as regards the configuration of equilibrium points of the stochastic system under study. The following section presents a straightforward theoretical solution to the problem of invariance under nonlinear diffeomorphic transformations of the measurement scale.

2.3. *Toward an invariant stochastic catastrophe theory*

The invariance problem outlined above can be solved once we consider the Itô transformation rule for stochastic differential equations (SDEs) more carefully (see also [33]). Assume a general Itô SDE of the form $\mathrm{d}x = \mu(x)\,\mathrm{d}t + \sigma(x)\,\mathrm{d}W(t)$ [cf. (3)], and a diffeomorphic transformation $y = \varphi(x)$. According to the

Itô transformation rule (p. 95 in [29]; [27]), the transformed SDE is given by

$$\mathrm{d}y = \tilde{\mu}(y)\,\mathrm{d}t + \tilde{\sigma}(y)\,\mathrm{d}W(t), \tag{7}$$

where a tilde indicates "transformed". The transformed drift function is given by

$$\tilde{\mu}(y) = \mu(\varphi^{-1}(y))\varphi'(\varphi^{-1}(y)) + \sigma(\varphi^{-1}(y))^2 \tfrac{1}{2}\varphi''(\varphi^{-1}(y)), \tag{8}$$

and the transformed diffusion function is given by

$$\tilde{\sigma}(y) = \sigma(\varphi^{-1}(y))\varphi'(\varphi^{-1}(y)). \tag{9}$$

As an example, consider the SDE $\mathrm{d}x = ax\,\mathrm{d}t + bx\,\mathrm{d}W(t)$, and the transformation $y = \varphi(x) = \ln x$. The diffusion function $\tilde{\sigma}(y)$ of the transformed SDE is then given by $\tilde{\sigma}(y) = b\exp(y)\varphi'(\exp(y)) = b$. Note that the original SDE has multiplicative noise, whereas the transformed system has additive noise.

Now recall that the pdf, or the stationary density function f is not invariant under transformation because it is given by

$$\left.\begin{array}{l} x \sim f(x) \\ y = \varphi(x) \end{array}\right\} \tilde{f}(y) = \frac{f(\varphi^{-1}(y))}{\varphi'(\varphi^{-1}(y))}, \tag{10}$$

which introduces the extra Jacobian term $1/\varphi'[\varphi^{-1}(y)]$. Combining (9) and (10) yields

$$\tilde{f}(y)\tilde{\sigma}(y) = f(\varphi^{-1}(y))\sigma(\varphi^{-1}(y)), \tag{11}$$

showing that the pdf $f(x)$ is not invariant under transformation, but $f(x)\sigma(x)$ is. The diffusion function $\sigma(x)$ needs to be included because it cancels the Jacobian term that is problematic for transformation-invariant inference when the pdf is considered in isolation. We will call $f(x)\sigma(x)$ the *transformation invariant function* $I(x)$, and we believe statistical inference for stochastic catastrophe models should be performed on this function.

From (11), (4), and (5), some calculation leads to

$$\begin{aligned} I(x) &= f(x)\sigma(x) \\ &= N_a \exp[-V_{\mathrm{sto}}(x)]\sigma(x) \\ &\propto \exp\left[2\int_a^x \mathrm{d}z \left\{\mu(z) - \frac{1}{4}[\sigma^2(z)]'\right\} / [\sigma^2(z)]\right]. \end{aligned} \tag{12}$$

Note that the multiplicative diffusion function makes the invariant function differ from the pdf given in (4) and (5) only in a seemingly minute detail: the numerator in the integral contains the factor 1/4 instead of 1/2. This minute difference is quite fundamental, however, since the factor 1/2 corresponds to the stationary pdf from an Itô SDE, whereas the factor 1/4 results from a Stratonovich SDE. This can be seen more easily by rewriting $f(x)$ as

$$f(x) = N[\sigma^2(x)]^{v} \exp\left[2\int_a^x \frac{\mu(z)}{\sigma^2(z)}\mathrm{d}z\right], \tag{13}$$

where $v = -1$ for the Itô interpretation, and $v = -(1/2)$ for the Stratonovich interpretation (cf. pp. 269–272 in [27]). Multiplication of an Itô pdf by $\sigma(x)$ will effectively transform it to a Stratonovich pdf, save for the value of the normalizing constant. Thus, another way to state the above result is to say that the invariance property of deterministic catastrophe theory is preserved under the Stratonovich interpretation of a stochastic differential equation, but is destroyed under the Itô interpretation. This result is quite consistent with other studies that also favor the Stratonovich interpretation over the Itô interpretation for the description of dynamical systems in physics [37–40]. Of particular relevance for the present discussion is the work by van Kampen [41], who showed that the "Langevin approach" of adding external noise[6] to a deterministic system in the manner of (3) is only physically meaningful under the Stratonovich interpretation.

When the noise term $\sigma(x)$ is constant, the pdf is a proper measure of the equilibrium points of a stochastic catastrophe system, as the pdf is then proportional to the invariant function $I(x)$. The invariant function may thus be considered a generalization of Cobb's method, because for additive noise Cobb's method is identical to the method proposed here. When the noise term is not constant but rather depends on the state of the system, differences between the pdf and the invariance function arise. The invariant function $I(x)$ takes account of the "metric" of the measurement scale by an adjustment in terms of the diffusion function $\sigma(x)$.

[6] "External" indicates that the source of the noise is unaffected by the system itself, and that this noise could in principle be turned off by manipulating a parameter.

2.4. Invariant stochastic catastrophe theory for multivariate SDEs

This section generalizes the result of the previous section to the case of multi-dimensional SDEs. Consider the time homogeneous system

$$\mathrm{d}\vec{x} = \vec{\mu}(\vec{x})\,\mathrm{d}t + \underline{\sigma}(\vec{x})\,\mathrm{d}\vec{W}(t), \tag{14}$$

(matrices are underlined) and assume that $\underline{\sigma}(\vec{x})$ is nonsingular for all $\vec{x}$. Also assume that the stationary pdf associated with (14) has a vanishing probability current. Let $\underline{\sigma}^t$ denote the transpose of $\underline{\sigma}$. Define the function $\vec{Z}[\vec{\mu}, \underline{\sigma}, \vec{x}]$ componentwise by

$$Z_i[\vec{A}, \underline{B}, \vec{x}] = 2\sum_j [\underline{\sigma}\,\underline{\sigma}^t]^{-1}_{ij}(\vec{x}) \times \left[\vec{\mu}(\vec{x}) - \frac{1}{2}\sum_k \frac{\partial[\underline{\sigma}\,\underline{\sigma}^t]_{jk}(\vec{x})}{x_k}\right],$$

and assume that $\vec{Z}$ can be written $\vec{Z}[\vec{\mu}, \underline{\sigma}, \vec{x}] = -\nabla\Phi_{\mathrm{sto}}(\vec{x})$, that is, $\vec{Z}$ is the gradient of some stochastic potential function Φ_{sto}. Then the stationary pdf of (14) for which probability current vanishes for all $\vec{x}$ is given by (p. 147 in [29])

$$f(\vec{x}) = \exp[\Phi_{\mathrm{sto}}(\vec{x})],$$

where

$$\Phi_{\mathrm{sto}}(\vec{x}) = -\int^{\vec{x}} \vec{Z}[\vec{\mu}, \underline{\sigma}, \vec{z}]\,\mathrm{d}\vec{z}.$$

The multivariate Itô transformation rules for the system under consideration are given by (p. 96 in [29])

$$\tilde{\mu}_i(\vec{\varphi}(\vec{x})) = \sum_k J_{ik}(\vec{x})\mu_k(\vec{x}) + \frac{1}{2}\sum_{k,m}[\underline{\sigma\sigma^t}]_{km}(\vec{x})\frac{\partial J_{ik}}{\partial x_m} \tag{15}$$

$$\underline{\tilde{\sigma}}(\vec{\varphi}(\vec{x})) = \underline{J}(\vec{x})\underline{\sigma}(\vec{x}) \tag{16}$$

Here $\underline{J}(\vec{x}) = \partial\vec{\varphi}/\partial\vec{x}^t$ is the Jacobian matrix of $\vec{\varphi}$. The general transformation rule for the probability density functions of $Y = \varphi(X)$, $X \sim f(x)$, reads $Y \sim \tilde{f}(y) = f(\vec{\varphi}^{-1}(y))/|J(\vec{\varphi}^{-1}(\vec{y}))|_+$ (e.g., [35]), where $|\cdot|_+$ denotes the absolute value of the determinant. From this, and from (16), it follows that $f(\vec{\varphi}(\vec{x}))|\underline{\tilde{\sigma}}(\varphi(\vec{x}))| = f(\vec{x})|\underline{\sigma}(\vec{x})| = K(\vec{x})$ is a multivariate analogue of the invariant function $I(x)$ of the univariate case.

3. Implementation: estimating the invariant function via level crossings

The previous sections presented a theoretical analysis as to why statistical procedures for stochastic catastrophe models should ultimately be based on the transformation invariant function $I(x) = f(x)\sigma(x)$. This section discusses how the invariant function can be estimated from actual data. Obviously, in order to estimate $\sigma(x)$ as defined in (3), the data has to be available in the form of a time series, that is, the data must have been obtained through successive measurements. The method proposed here is to estimate $I(x)$ in a single computation via the so-called *level crossing function*.

A different approach to the one advocated here would be to separately estimate $f(x)$ and $\sigma^2(x)$, and then multiply $\hat{f}(x)$ by $\sqrt{\hat{\sigma}^2(x)}$. The estimate for $f(x)$ could be based on a standard kernel density estimation routine (e.g., [42,36]), and the estimate for $\sigma^2(x)$ could be based on any of the available nonparametric diffusion variance estimators. We considered this approach and implemented the nonparametric diffusion variance estimators developed by Florens (cf. [43–45]), and Jiang and Knight [46,47]. For the SDEs under consideration in this article, we found that these two estimators behaved very similarly. Both estimators were systematically biased in their estimation of a nonconstant diffusion variance. As a result of this bias, the simple level crossing function provided a much more accurate estimate of the invariant function than did either of the composite methods. For this reason, we will disregard the composite methods, and instead focus entirely on the simple level crossing function.

Consider the level crossing probability $p_\Delta(x)$, that is, the probability that two successive observations, X_t and $X_{t+\Delta}$, lie on opposite sides of a level x (i.e., one value being higher than x, one value being lower than x):

$$p_\Delta(x) = p[(X_t - x)(X_{t+\Delta} - x) < 0]. \tag{17}$$

To clarify the concept of level crossings, Fig. 5 shows an example time series for which level "$x = 6$" is crossed four times, and level "$x = 2$" is crossed two times. Note that the occurrence of a level crossing, and hence (17),

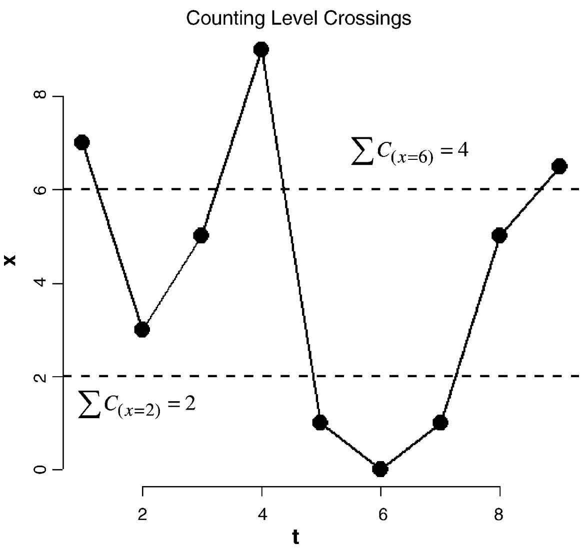

Fig. 5. Illustration of the level crossing function. Level "$x = 6$" is crossed four times, and level "$x = 2$" is crossed two times. A level x is crossed when two successive observations, say X_t and $X_{t+\Delta}$, lie on opposite sides of x. This means that a crossing of x occurs when $(X_t - x)(X_{t+\Delta} - x)$ is negative.

depends solely on the rank order of the observations. This is important because a diffeomorphic transformation, which is by definition monotonically increasing or decreasing, does not affect the rank order of the observations. Hence, $p_\Delta(x)$ is invariant under diffeomorphic transformations. In other words, under the diffeomorphic transformation $y = \varphi(x)$ the event $X_t > x$ is equivalent to the event $Y_t > y$.

Florens (lemma 1 in [43]) proved that under mild regularity conditions for a stochastic system described by (3) with constant diffusion function $\sigma(x) = 1$, the probability of crossing a level x in the next time step Δ is given by

$$p_\Delta(x) = f(x)\sqrt{2\Delta/\pi} + O(\Delta), \tag{18}$$

where O is Landau's symbol.

The invariance of (18) in combination with the Itô transformation rule allow a generalization of Florens' result to non-constant diffusion functions. To see this, consider an SDE with constant diffusion function $\sigma(x) = 1$ (i.e., an SDE to which Florens' lemma may be applied), and a diffeomorphic transformation $y = \varphi(x)$. The transformed SDE has a non-constant diffusion function $\tilde{\sigma}(y)$. From (9) and (10), it follows that $f(\varphi^{-1}(y)) = \tilde{f}(y)\tilde{\sigma}(y)$. The invariance of the level crossing function implies that $p_\Delta(y) = p_\Delta(\varphi^{-1}(y))$. With (18), it follows that for SDEs with constant and non-constant diffusion functions the probability of crossing a level x in the next time step Δ is given by

$$p_\Delta(x) = f(x)\sigma(x)\sqrt{2\Delta/\pi} + O(\Delta). \tag{19}$$

Thus, the *level crossing function* $\ell(x) = p_\Delta(x)/\sqrt{2\Delta/\pi}$ approximates the invariant function $I(x) = f(x)\sigma(x)$ up to order $\sqrt{\Delta}$. For empirical data, an estimate of the level crossing probability $p_\Delta(x)$ is easily obtained by averaging the number of actual crossings. Let $C_x(X_k, X_{k+1})$ denote whether or not level x was crossed by successive observations X_k and X_{k+1}, as follows:

$$C_x(X_k, X_{k+1}) = \begin{cases} 1 & (X_k - x)(X_{k+1} - x) < 0, \\ 0 & \text{otherwise.} \end{cases} \tag{20}$$

An estimate of the level crossing function, $\hat{\ell}(x)$, is then given by

$$\hat{\ell}(x) = \frac{1}{\sqrt{2\Delta/\pi}} \frac{1}{n-1} \sum_{i=1}^{n-1} C_x(X_k, X_{k+1}), \tag{21}$$

where n is the total number of observations. Hartelman [33] showed that $\hat{\ell}(x)$ converges almost surely, and converges in distribution, to $\ell(x)$. Furthermore, when $n\sqrt{\Delta} \to \infty$ as $\Delta \to 0$ and $n \to \infty$, $\hat{\ell}(x)$ is asymptotically unbiased and pointwise consistent (pp. 151–153 in [33]).

We now return to our earlier examples (i.e., Figs. 3 and 4) and consider the theoretical invariant function and the estimated level crossing function. Fig. 3E and F show the invariant functions for the example cusp SDE time series shown in Fig. 3A and B, respectively. The 'true' analytical invariant functions for the original SDE and the transformed SDE are shown as solid black lines. The invariant functions for the simulated time series, as estimated by the level crossing function $\hat{\ell}(x)$, are shown as dashed black lines. The original and transformed invariant functions are identical except for a stretching along the x-axis, and hence the invariant functions are the same with respect to the configuration of critical points. In this particular case, both functions show clear bimodality. This is consistent with the fact that the data-generating cusp SDE has two equilibrium states.

Fig. 4E and F show the invariant functions for the exemplary data from the Ornstein–Uhlenbeck SDE $\mathrm{d}x = -x\,\mathrm{d}t + \mathrm{d}W(t)$. The Ornstein–Uhlenbeck SDE has a single equilibrium state. The invariant functions for the original time series and for the transformed time series convey the same information with respect to the number of stable states: both functions are unimodal, correctly indicating a single equilibrium state. Figs. 3 and 4 both illustrate how consideration of the invariant function (panels E and F) may lead to conclusions that differ dramatically from those reached based on a consideration of the pdf (panels C and D). In addition, there is good agreement between the estimated level crossing function $\hat{\ell}(x)$ and the theoretical invariant function.

4. Application

The applications discussed in this section concern the duration of eruptions from the Old Faithful geyser in Yellowstone National Park, USA [48], and the X-ray flux measured from the galactic black hole Cygnus X–1 [49,50]. It is not our aim to discuss the data-generating mechanisms from the Old Faithful geyser or the Cygnus X–1 black hole. Rather, we have included these applications in order to show that the inconsistency between the pdf and the invariant function with respect to the number of stable states is more than just a theoretical possibility. In addition, the applications may be helpful to better understand the situations in which inconsistencies arise.

4.1. Eruption durations from the Old Faithful geyser

The first application concerns the eruption durations of the famous Old Faithful geyser, recorded continuously from August 1 to August 15, 1985 ([48], see also [36] for the analysis of a similar

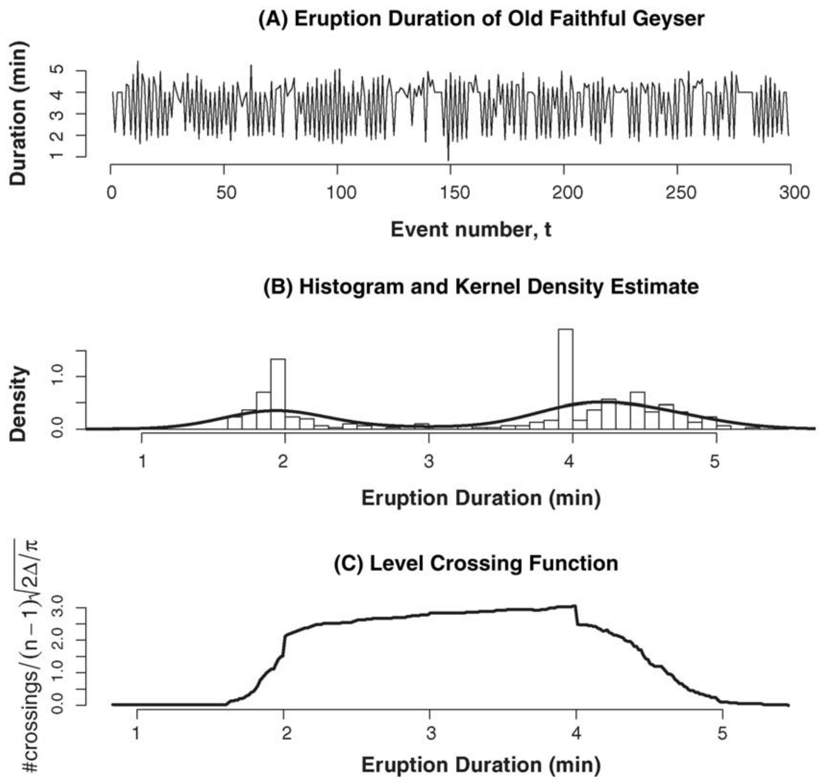

Fig. 6. Analysis of eruption durations from the Old Faithful geyser. Panel (A): Time series of eruption durations. Panel (B): Histogram and kernel density estimate of the data from panel (A). Panel (C): Estimated level crossing function of the data from panel (A).

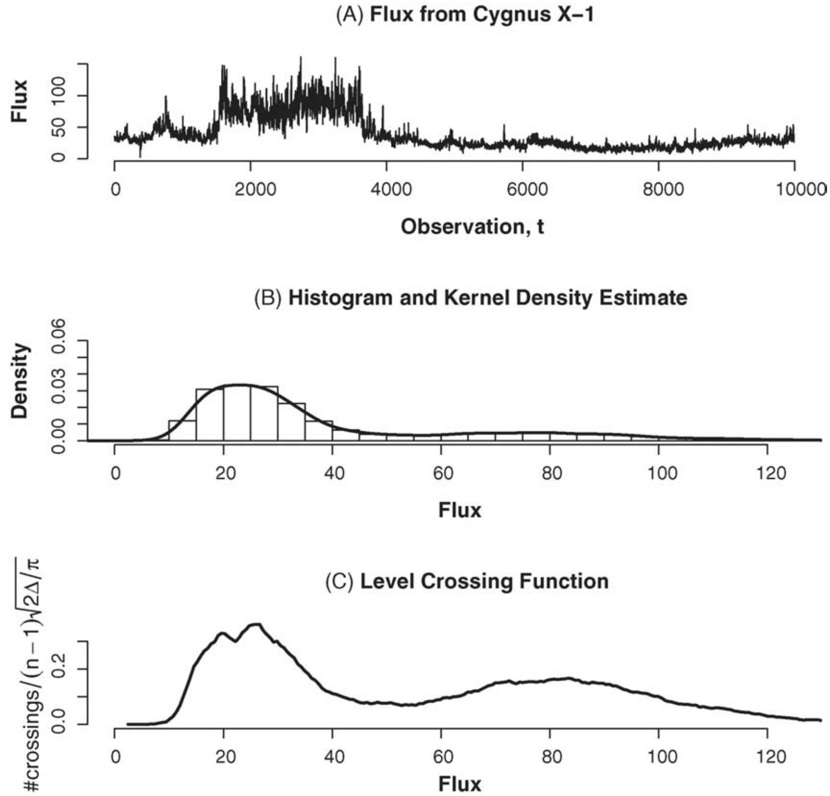

Fig. 7. Analysis of X-ray flux from the Cygnus X–1 galactic black hole. Panel (A): Time series of X-ray flux. Panel (B): Histogram and kernel density estimate of the data from panel (A). Panel (C): Estimated level crossing function of the data from panel (A).

data set).[7] Fig. 6A shows the duration of 299 eruptions.

As can be seen from Fig. 6B, the frequency histogram and the associated kernel density estimate are bimodal. According to the method of Cobb, this bimodality suggests the existence of two stable states. However, Fig. 6C shows that the estimated invariant level crossing function has only a single mode, albeit a very flat one. Thus, for this particular time series the invariant function does not provide any evidence for two stable states.

The reason for the discrepancy between the pdf and the level crossing function lies in the oscillating nature of the time series. An oscillating time series such as a single frequency sine wave will yield a bimodal pdf. Nevertheless, such a system does not have two stable states, and the level crossing function will be flat.

4.2. *X-ray flux from the Cygnus X–1 galactic black hole*

The second application concerns the flux from the Cygnus X–1 black hole, monitored from 1996 to 2003 with the Rossi X-ray Timing Explorer [49,50]. Fig. 7A shows the first $n = 10{,}000$ observations.[8]

A visual inspection of Fig. 7A suggest that in the interval between $t = 1700$ and $t = 3700$, the flux of Cygnus X–1 is both higher and more variable than at

[7] This time series comes with the statistical software package R [51]. In this data set, some nocturnal measurements of duration were coded as 2, 3 or 4 min, having originally been described as “short”, “medium”, or “long” [48].

[8] The complete time series ($n = 34{,}256$) shows a similar pattern of results, albeit much less pronounced. By focusing on the first 10,000 observations, the relative contribution of the data component with high flux and high variability is increased. This more clearly brings out the difference between the pdf and the invariance function.

the other measurement occasions. The pdf, plotted in Fig. 7B, does not reflect the intuition that Cygnus X–1 has more than one mode of operation, although the right tail of the pdf is admittedly pronounced. Fig. 7C shows that the invariant level crossing function does provides clear evidence for bimodality.

The discrepancy between the pdf and the level crossing function can be understood by noting that the level crossing function provides an estimate of the invariant quantity $f(x)\sigma(x)$. The diffusion function $\sigma(x)$ is relatively high for the observations in the interval between $t = 1700$ and $t = 3700$, thereby intensifying the contribution of this component.

In sum, the applications to the eruptions from the Old Faithful geyser and the flux from the Cygnus X–1 galactic black hole highlight the practical ramifications of our theoretical analysis. The invariant function $I(x) = f(x)\sigma(x)$ is a reliable indicator of the number of equilibrium states. The probability density function, however, can be misleading in this respect.

5. Concluding remarks

Deterministic catastrophe theory is concerned with the configuration of a system's equilibrium points. The qualitative pattern of equilibrium points is robust against diffeomorphic transformations of the measurement scale. The stochastic counterpart of catastrophe theory, developed by Loren Cobb (e.g., [21]) is not invariant under nonlinear diffeomorphic transformations of the measurement scale, as it is based on the probability density function $f(x)$. This undermines the generality of catastrophe theory, and points to an important discrepancy between deterministic and stochastic catastrophe theory.

Our results show that in contrast to $f(x)$, the function $I(x) = f(x)\sigma(x)$ remains invariant under nonlinear diffeomorphic transformations. $I(x)$ may be interpreted as the non-normalized stationary density of a Stratonovich stochastic differential equation. It is this function that incorporates noise while retaining a close connection to its deterministic counterpart. In practical applications $I(x)$ can be estimated via a simple method based on level crossings. The methodology outlined here offers the possibility to test transition hypotheses for stochastic systems that is fully consistent with deterministic catastrophe theory.

We have stressed throughout this article that consideration of $I(x)$ may lead to quite different conclusions than does consideration of $f(x)$ alone. We have presented this work in the context of catastrophe theory. However, the issue of multimodality is also of interest for several applications outside the realm of bifurcation theory. Whenever data are available in the form of a time series such as stock market fluctuations or fluctuations in the weather, we strongly recommend the use of $I(x)$ over the use of $f(x)$. When data are not available in the form of a time series, the researcher should realize that nonlinear diffeomorphic transformations change the shape of $f(x)$ at will. This is not a concern when there are strong reasons to believe that the underlying mechanism is linearly related to the behavioral variable. In many fields of research, however, the choice of a measurement scale is to some extent arbitrary [52]. In such cases, the shape of the pdf is not informative with respect to the nature of the underlying mechanism.

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