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## Generalized Fokker–Planck equation with generalized interval probability

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### ABSTRACT

The Fokker–Planck equation is widely used to describe the time evolution of stochastic systems in drift-diffusion processes. Yet, it does not differentiate two types of uncertainties: aleatory uncertainty that is inherent randomness and epistemic uncertainty due to lack of perfect knowledge. In this paper, a generalized differential Chapman–Kolmogorov equation based on a new generalized interval probability theory is derived, where epistemic uncertainty is modeled by the generalized interval while the aleatory one is by the probability measure. A generalized Fokker–Planck equation is proposed to describe drift-diffusion processes under both uncertainties. A path integral approach is developed to numerically solve the generalized Fokker–Planck equation. The resulted interval-valued probability density functions rigorously bound the real-valued ones computed from the classical path integral method. The method is demonstrated by numerical examples.

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### 1. Introduction

The Fokker–Planck equation is a general probabilistic approach to describe the dynamics of various stochastic systems, such as physical, chemical, biological and economical ones. It models the time evolution of the probability distribution in a system under uncertainty, which describes generic drift-diffusion processes. However, it does not differentiate the two types of uncertainties. Variability is the inherent randomness in the system because of fluctuation and perturbation. Variability is also referred to as aleatory uncertainty, stochastic uncertainty, simulation uncertainty, and irreducible uncertainty. In contrast, incertitude is due to lack of perfect knowledge or enough information about the system. It is also known as epistemic uncertainty, reducible uncertainty, and model form uncertainty. The classical Fokker–Planck equation models the two types of uncertainties together with one single probability distribution, which only captures the accumulative effect.

The need to separately quantify the two types of uncertainties has been well-recognized (e.g. [1–4]). They need to be represented explicitly if we want to increase the confidence of modeling or simulation results. Neglecting epistemic uncertainty may lead to decisions that are not robust. Sensitivity analysis is a typical way to assess robustness, which is to check how much deviation the analysis result may have if input distribution parameters or distribution types deviate away from the ones used in the analysis. Second-order Monte Carlo sampling can also be applied where samples of model parameters are drawn to assess different models and the effect of epistemic uncertainty can be revealed. Obviously, considerable workload is required for both approaches. Mixing epistemic and aleatory uncertainties may increase costs of risk management. If extra knowledge or information of the collected data is available, they can be further clustered into

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smaller groups or intrinsic mathematical relationships can be identified so that variance can be reduced, which reflects pure randomness more accurately for risk analysis.

In studying the dynamics of stochastic systems, it is desirable that aleatory and epistemic uncertainties are separately quantified so that their respective effects can be easily computed, distinguished, and analyzed. In this paper, we propose an efficient approach to quantify aleatory and epistemic uncertainties by interval probability in modeling drift-diffusion processes. Instead of a precise value of probability  $P(E)=p$  associated with an event  $E$ , a pair of lower and upper probabilities  $P(E)=[\underline{p},\bar{p}]$  are used to represent a set of possible values. The range of the interval  $[\underline{p},\bar{p}]$  captures the epistemic uncertainty component. Interval probability thus differentiates incertitude from variability both qualitatively and quantitatively in a concise form.

The general purpose of using interval probability or imprecise probability in analyzing system dynamics is to improve the robustness of prediction in a generic and efficient way. In this paper, a generalized differential Chapman–Kolmogorov equation under both uncertainty components based on a generalized interval probability is first derived. The generalized interval probability provides a convenient calculus structure to estimate lower and upper bounds. Then a path integral approach is developed to numerically solve the generalized Fokker–Planck equation, which is a special case of the generalized differential Chapman–Kolmogorov equation. It is also demonstrated that the interval-valued probability density function as the solution of the generalized Fokker–Planck equation by the proposed path integral method rigorously bounds the real-valued one computed from the classical path integral method. Therefore, the generalized Fokker–Planck equation can effectively quantify the epistemic uncertainty associated with parameters and model forms.

In the remainder of the paper, an overview of relevant work in imprecise probability and path integral methods to solve the classical Fokker–Planck equation are given in Section 2. In Section 3, the generalized differential Chapman–Kolmogorov equation is derived. Section 4 describes the proposed path integral approach to solve the generalized Fokker–Planck equation. In Section 5, two numerical examples are used to demonstrate the new approach, which is able to analyze system dynamics under both uncertainty components.

## 2. Background

### 2.1. Imprecise probability

Probability theory provides common ground to quantify uncertainty and so far is the most popular approach. It is based on precise values of probability measures or moments. However, precise probability has limitations in representing epistemic uncertainty. The most significant one is that it does not differentiate *total ignorance* from other probability distributions. Total ignorance means that the analyst has zero knowledge about the system under study. Based on the principle of maximum entropy, uniform distributions are usually applied in this case. A problem arises because introducing a uniform or any particular form of a distribution has itself introduced extra information that is not justifiable by the zero knowledge. Different possible values are equally likely in a uniform distribution, which is not guaranteed to be true when we are totally ignorant. The principle of maximum entropy leads to the Bertrand-style paradoxes such as the Van Fraassen’s cube factory [5]. Therefore, “Knowing the unknown” as modeled in precise probability does not represent the total ignorance. In contrast, the interval probability  $P=[0,1]$  does.

Another limitation of precise probability is representing *indeterminacy* and *inconsistency* in the context of subjective probability. When people have limited ability to determine the precise values of their own subjective probabilities, precise probability does not capture indeterminacy. Therefore Bayesians who insist on subjective probability still do sensitivity analysis. Furthermore, when subjective probabilities from different people are inconsistent, a precise value does not capture a range of opinions or estimations adequately without assuming some consensus on the precise values for a collection of opinions. “Agreeing to disagree” is not the best way to indicate inconsistency.

Imprecise probability  $[\underline{p},\bar{p}]$  combines epistemic uncertainty (as an interval) with aleatory uncertainty (as probability measure), which is regarded as a generalization of traditional probability. Gaining more knowledge can reduce the level of imprecision and indeterminacy, i.e. the interval width. When  $\underline{p}=\bar{p}$ , the degenerated interval probability becomes a traditional precise one. Our proposed approach uses imprecise probabilities to quantify aleatory and epistemic uncertainties separately. Many forms of imprecise probabilities have been developed. For example, the Dempster–Shafer theory [6,7] characterizes evidence with discrete probability masses associated with a power set of values. The theory of coherent lower previsions [1] models uncertainties with the lower and upper previsions with behavioral interpretations. The possibility theory [8] represents uncertainties with Necessity–Possibility pairs. Probability bound analysis [9] captures uncertain information with pairs of lower and upper distribution functions or p-boxes. F-probability [10] incorporates intervals and represents an interval probability as a set of probabilities which maintain the Kolmogorov properties. A random set [11] is a multi-valued mapping from the probability space to the value space. Fuzzy probability [12] considers probability distributions with fuzzy parameters. A cloud [13] is a combination of fuzzy sets, intervals, and probability distributions.

In the applications of interval probability, the interval bounds  $\underline{p}$  and  $\bar{p}$  can be solicited as the lowest and highest subjective probabilities about a particular event from a domain expert, where probability represents the degree of belief. One expert may hesitate to offer just a precise value of probability. Different experts could have different beliefs. In both cases, the range of probabilities gives the interval bounds. When used in data analysis with frequency interpretation, the

interval bounds can be confidence intervals that are calculated from data. For instance, the Kolmogorov–Smirnov confidence band to enclose a cumulative distribution function can be used, where the width of the band captures the epistemic component. If extra data are collected, the interval width can be reduced, and the confidence band converges towards a precise distribution function.

One common problem of the above set-based imprecise probability theories is that the calculation is cumbersome. Linear and nonlinear optimization methods are usually dependent upon to search lower and upper bounds of probabilities during reasoning. Different from them, we recently proposed an imprecise probability with a generalized interval form [14,15]. The probability values are generalized intervals. Generalized interval [16,17] is an extension of the set-based classical interval [18] with better algebraic and semantic properties based on the Kaucher arithmetic [19]. A generalized interval  $\mathbf{x} := [\underline{x}, \bar{x}] (\underline{x}, \bar{x} \in \mathbb{R})$  is a pair of numbers instead of a set. Therefore it is not constrained by  $\underline{x} \leq \bar{x}$  any more. [0.2,0.1] is also a valid interval and called *improper*, while the traditional interval [0.1,0.2] is called *proper*. With such extension, the probabilistic calculus structure defined in generalized interval probability is greatly simplified based on the algebraic properties. At the same, it supports logic interpretation of numerical results, which also helps verify computation. See more details of generalized interval and generalized interval probability in Appendix A.

## 2.2. Path integral methods to solve the classical Fokker–Planck equation

Various numerical methods to solve the classical Fokker–Planck equation have been developed, including Monte Carlo [20], finite difference [21], spectral approximation [22,23], and path integral [24]. In particular, the path integral method has been shown as a simple yet numerically efficient and accurate approach. Wehner and Wolfer [25] used a short-time transition probability density matrix to approximate the evolution of drift-diffusion processes. Boundary condition [26] and time-dependent parameters [27] were also demonstrated. To improve numerical efficiency and accuracy, Naess and Johnsen [28] developed a B-spline interpolation approach where continuous probability density functions are approximated based upon limited discrete evaluations such that the error reduction speed is increased to  $O(\tau)$  with time step size  $\tau$ . Di Paola and Santoro [29] extended the path integral approach for systems under Gaussian white noise perturbation as in the classical Fokker–Planck equation to the Kolmogorov–Feller equation under Poisson white noise. Kougioumtzoglou and Spanos [30] developed a variational formulation to improve the efficiency of path integral without the need of short-time steps in nonlinear oscillation problems where diffusion coefficients are constants.

In this paper, a path integral method to solve the generalized Fokker–Planck equation under both aleatory and epistemic uncertainties is proposed, where generalized interval probability density functions are estimated. A generalized differential Chapman–Kolmogorov equation, which is more generic than the generalized Fokker–Planck equation, is first derived in the next section.

## 3. Generalized differential Chapman–Kolmogorov equation with generalized interval probability

The differential Chapman–Kolmogorov equation is universally used to describe time evolution of probability distributions. In this section, a generalized differential Chapman–Kolmogorov equation based on generalized interval is derived such that the dynamics of generalized interval probability can be described.

Following the definition of interval derivative by Markov [47], the derivative of a generalized interval function  $\mathbf{f}(t) = [\underline{f}(t), \bar{f}(t)]$  is defined as

$$d\mathbf{f}(t)/dt := \lim_{\Delta t \rightarrow 0} (\mathbf{f}(t + \Delta t) - \text{dual}\mathbf{f}(t))/\Delta t = [\lim_{\Delta t \rightarrow 0} (\underline{f}(t + \Delta t) - \underline{f}(t))/\Delta t, \lim_{\Delta t \rightarrow 0} (\bar{f}(t + \Delta t) - \bar{f}(t))/\Delta t]$$

where dual is defined as in Eq. (1.1) in Appendix A1. Note that all boldface symbols in this paper are generalized intervals. We define the derivative of generalized interval probability  $\mathbf{p}(x, t | y, t')$  with respect to time  $t$  as follows. With state variables  $x, y \in \mathbb{R}^n$ ,

$$\frac{\partial}{\partial t} \mathbf{p}(x, t | y, t') := \lim_{\Delta t \rightarrow 0} \frac{1}{\Delta t} \{ \mathbf{p}(x, t + \Delta t | y, t') - \text{dual}\mathbf{p}(x, t | y, t') \} \quad (1)$$

Because of the logic coherent constraint in generalized interval probability (see Appendix A2), we have

$$\int dz \mathbf{p}(z, t + \Delta t | x, t) = 1 \quad (2)$$

where state variable  $z \in \mathbb{R}^n$ . With the Markovian property, this leads to

$$\mathbf{p}(x, t + \Delta t | y, t') = \int dz \mathbf{p}(x, t + \Delta t | z, t) \mathbf{p}(z, t | y, t') \quad (3)$$

Replace the first term in Eq. (1) with Eq. (3) and multiply the second term by Eq. (2). Eq. (1) now becomes

$$\frac{\partial}{\partial t} \mathbf{p}(x, t | y, t') = \lim_{\Delta t \rightarrow 0} \frac{1}{\Delta t} \left\{ \int dz [\mathbf{p}(x, t + \Delta t | z, t) \mathbf{p}(z, t | y, t') - \text{dual}\mathbf{p}(z, t + \Delta t | x, t) \mathbf{p}(x, t | y, t')] \right\} \quad (4)$$

Consider two subdomains  $\|x-z\| \leq \varepsilon$  and  $\|x-z\| > \varepsilon$  separately where  $\varepsilon$  is small enough. Eq. (4) can be regarded as

$$\frac{\partial}{\partial t} \mathbf{p}(x,t|y,t') = \mathbf{I}_{\|x-z\| \leq \varepsilon} + \mathbf{I}_{\|x-z\| > \varepsilon}$$

where  $\mathbf{I}_{\|x-z\| \leq \varepsilon}$  is the right-side integral in Eq. (4) within the small neighborhood that captures continuous diffusion processes, whereas  $\mathbf{I}_{\|x-z\| > \varepsilon}$  is the one outside the neighborhood that represents jump processes.

Within the small neighborhood  $\|x-z\| \leq \varepsilon$ , let  $x-z=h$  and define  $\mathbf{f}(x,h) := \mathbf{p}(x+h,t+\Delta t|x,t)\mathbf{p}(x,t|y,t')$ . Then  $\mathbf{p}(z,t+\Delta t|x,t)\mathbf{p}(x,t|y,t') = \mathbf{f}(x,-h)$  and  $\mathbf{p}(x,t+\Delta t|z,t)\mathbf{p}(z,t|y,t') = \mathbf{p}(x,t+\Delta t|x-h,t)\mathbf{p}(x-h,t|y,t') = \mathbf{f}(x-h,h)$ . Apply the Taylor alike expansion  $\mathbf{f}(x-h,h) = \mathbf{f}(x,h) - \text{dual} \sum_{i=1}^n \frac{\partial \mathbf{f}}{\partial x_i} h_i + \frac{1}{2} \sum_{i,j=1}^n \frac{\partial^2 \mathbf{f}}{\partial x_i \partial x_j} h_i h_j + O(\varepsilon^3)$ , where  $\frac{\partial \mathbf{f}}{\partial x_i} := \lim_{\Delta x_i \rightarrow 0} \{\mathbf{f}(x+\Delta x_i, h) - \text{dual} \mathbf{f}(x, h)\} / \Delta x_i$  and similarly

$$\frac{\partial^2 \mathbf{f}(x,h)}{\partial x_i \partial x_j} := \lim_{\substack{\Delta x_i \rightarrow 0 \\ \Delta x_j \rightarrow 0}} \{\mathbf{f}(x+\Delta x_i+\Delta x_j, h) - \text{dual} \mathbf{f}(x+\Delta x_i, h) - \text{dual} \mathbf{f}(x+\Delta x_j, h) + \mathbf{f}(x, h)\} / \Delta x_i \Delta x_j.$$

Then

$$\begin{aligned} \mathbf{I}_{\|x-z\| \leq \varepsilon} &= \lim_{\Delta t \rightarrow 0} \frac{1}{\Delta t} \left\{ \int_{\|x-z\| \leq \varepsilon} dz [\mathbf{p}(x,t+\Delta t|z,t)\mathbf{p}(z,t|y,t') - \text{dual} \mathbf{p}(z,t+\Delta t|x,t)\mathbf{p}(x,t|y,t')] \right\} \\ &= \lim_{\Delta t \rightarrow 0} \frac{1}{\Delta t} \left\{ \int_{\|h\| \leq \varepsilon} dh [\mathbf{f}(x-h,h) - \text{dual} \mathbf{f}(x,-h)] \right\} \\ &= \lim_{\Delta t \rightarrow 0} \frac{1}{\Delta t} \left\{ \int_{\|h\| \leq \varepsilon} dh \left[ \mathbf{f}(x,h) - \text{dual} \sum_{i=1}^n \frac{\partial \mathbf{f}}{\partial x_i} h_i + \frac{1}{2} \sum_{i,j=1}^n \frac{\partial^2 \mathbf{f}}{\partial x_i \partial x_j} h_i h_j - \text{dual} \mathbf{f}(x,-h) + O(\varepsilon^3) \right] \right\} \\ &= \lim_{\Delta t \rightarrow 0} \frac{1}{\Delta t} \left[ \int_{\|h\| \leq \varepsilon} dh \mathbf{f}(x,h) - \text{dual} \int_{\|h\| \leq \varepsilon} dh \mathbf{f}(x,-h) \right] - \text{dual} \lim_{\Delta t \rightarrow 0} \frac{1}{\Delta t} \int_{\|h\| \leq \varepsilon} dh \sum_{i=1}^n \frac{\partial \mathbf{f}}{\partial x_i} h_i \\ &\quad + \frac{1}{2} \lim_{\Delta t \rightarrow 0} \frac{1}{\Delta t} \int_{\|h\| \leq \varepsilon} dh \sum_{i,j=1}^n \frac{\partial^2 \mathbf{f}}{\partial x_i \partial x_j} h_i h_j + \lim_{\Delta t \rightarrow 0} \frac{1}{\Delta t} O(\varepsilon^4) \\ &= -\text{dual} \sum_{i=1}^n \left[ \lim_{\Delta t \rightarrow 0} \frac{1}{\Delta t} \int_{\|h\| \leq \varepsilon} dh \frac{\partial \mathbf{f}}{\partial x_i} h_i \right] + \frac{1}{2} \sum_{i,j=1}^n \left[ \lim_{\Delta t \rightarrow 0} \frac{1}{\Delta t} \int_{\|h\| \leq \varepsilon} dh \frac{\partial^2 \mathbf{f}}{\partial x_i \partial x_j} h_i h_j \right] + \lim_{\Delta t \rightarrow 0} \frac{1}{\Delta t} O(\varepsilon^4) \end{aligned}$$

since  $\int_{\|h\| \leq \varepsilon} dx \mathbf{f}(x,h) = \int_{\|h\| \leq \varepsilon} dx \mathbf{f}(x,-h)$ . Furthermore,

$$\frac{1}{\Delta t} \int_{\|h\| \leq \varepsilon} dh \frac{\partial \mathbf{f}}{\partial x_i} h_i = \frac{\partial}{\partial x_i} \left[ \frac{1}{\Delta t} \int_{\|h\| \leq \varepsilon} h_i \mathbf{f} dh \right] = \frac{\partial}{\partial x_i} \left[ \mathbf{p}(x,t|y,t') \frac{1}{\Delta t} \int_{\|h\| \leq \varepsilon} h_i dh \mathbf{p}(x+h,t+\Delta t|x,t) \right],$$

and similarly

$$\frac{1}{\Delta t} \int_{\|h\| \leq \varepsilon} dh \frac{\partial^2 \mathbf{f}}{\partial x_i \partial x_j} h_i h_j = \frac{\partial^2}{\partial x_i \partial x_j} \left[ \mathbf{p}(x,t|y,t') \frac{1}{\Delta t} \int_{\|h\| \leq \varepsilon} h_i h_j dh \mathbf{p}(x+h,t+\Delta t|x,t) \right].$$

In addition,  $\lim_{\Delta t \rightarrow 0} O(\varepsilon^4) / \Delta t = \lim_{\Delta t \rightarrow 0} O(\varepsilon^3) / 1 = O(\varepsilon^3)$

We define

$$\mathbf{A}_i(x,t) := \lim_{\Delta t \rightarrow 0} \frac{1}{\Delta t} \int_{\|h\| \leq \varepsilon} h_i dh \mathbf{p}(x+h,t+\Delta t|x,t) \tag{5}$$

$$\mathbf{B}_{ij}(x,t) := \lim_{\Delta t \rightarrow 0} \frac{1}{\Delta t} \int_{\|h\| \leq \varepsilon} h_i h_j dh \mathbf{p}(x+h,t+\Delta t|x,t) \tag{6}$$

If  $X(t) = (x_1(t), \dots, x_n(t))$  represents the state of the system at time  $t$ , then  $\int_{\|h\| \leq \varepsilon} h_i dh \mathbf{p}(x+h,t+\Delta t|x,t) = \mathbb{E}[x_i(t+\Delta t) - x_i(t)|X(t)]$  is the expected state value change in the  $i$ th direction. Therefore, Eq. (5) is interpreted as the state value change rate along one direction, known as the *drift* vector. Similarly,  $\int_{\|h\| \leq \varepsilon} h_i h_j dh \mathbf{p}(x+h,t+\Delta t|x,t) = \mathbb{E}[(x_i(t+\Delta t) - x_i(t))(x_j(t+\Delta t) - x_j(t))|X(t)]$ . Eq. (6) is the combined area change rate in two directions, known as the *diffusion* matrix.

We now have

$$\mathbf{I}_{\|x-z\| \leq \varepsilon} = -\text{dual} \sum_{i=1}^n \frac{\partial}{\partial x_i} [\mathbf{A}_i(x,t)\mathbf{p}(x,t|y,t')] + \frac{1}{2} \sum_{i,j=1}^n \frac{\partial}{\partial x_i \partial x_j} [\mathbf{B}_{ij}(x,t)\mathbf{p}(x,t|y,t')] + O(\varepsilon^3)$$

for the diffusion process.

For the jump process

$$\begin{aligned} \mathbf{I}_{\|x-z\|>\varepsilon} &= \lim_{\Delta t \rightarrow 0} \frac{1}{\Delta t} \left\{ \int_{\|x-z\|>\varepsilon} dz [\mathbf{p}(x, t + \Delta t | z, t) \mathbf{p}(z, t | y, t') - \text{dual} \mathbf{p}(z, t + \Delta t | x, t) \mathbf{p}(x, t | y, t')] \right\} \\ &= \int_{\|x-z\|>\varepsilon} dz \left[ \lim_{\Delta t \rightarrow 0} \frac{1}{\Delta t} \{ \mathbf{p}(x, t + \Delta t | z, t) \} \mathbf{p}(z, t | y, t') \right] - \text{dual} \int_{\|x-z\|>\varepsilon} dz \left[ \lim_{\Delta t \rightarrow 0} \frac{1}{\Delta t} \{ \mathbf{p}(z, t + \Delta t | x, t) \} \mathbf{p}(x, t | y, t') \right] \end{aligned}$$

We define

$$\mathbf{W}(y|x, t) := \lim_{\Delta t \rightarrow 0} \frac{1}{\Delta t} \{ \mathbf{p}(y, t + \Delta t | x, t) \} \quad (7)$$

as the *rate of transition* from  $x$  to  $y$ . Then

$$\mathbf{I}_{\|x-z\|>\varepsilon} = \int_{\|x-z\|>\varepsilon} dz [\mathbf{W}(x|z, t) \mathbf{p}(z, t | y, t')] - \text{dual} \int_{\|x-z\|>\varepsilon} dz [\mathbf{W}(z|x, t) \mathbf{p}(x, t | y, t')]$$

As  $\varepsilon \rightarrow 0$ , the subdomain  $\|x-z\|>\varepsilon$  becomes the complete domain.

Therefore, with the consideration of both  $\|x-z\| \leq \varepsilon$  and  $\|x-z\| > \varepsilon$ , the *generalized differential Chapman–Kolmogorov equation* is

$$\begin{aligned} \frac{\partial}{\partial t} \mathbf{p}(x, t | y, t') &= -\text{dual} \sum_{i=1}^n \frac{\partial}{\partial x_i} [\mathbf{A}_i(x, t) \mathbf{p}(x, t | y, t')] + \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n \frac{\partial^2}{\partial x_i \partial x_j} [\mathbf{B}_{ij}(x, t) \mathbf{p}(x, t | y, t')] \\ &\quad + \int dz \mathbf{W}(x|z, t) \mathbf{p}(z, t | y, t') - \text{dual} \int dz \mathbf{W}(z|x, t) \mathbf{p}(x, t | y, t') \end{aligned} \quad (8)$$

When the drift vector and diffusion matrix in Eq. (8) are zeros, it is called *interval master equation* that models jump processes. When the rates of transition  $\mathbf{W}(x|z, t)$  and  $\mathbf{W}(z|x, t)$  in Eq. (8) are zeros, it is called *generalized Fokker–Planck equation* that models drift-diffusion processes. Again, all equations have been generalized to differentiate epistemic and aleatory uncertainties, where interval-valued probabilities and coefficients replace those corresponding real-valued ones.

#### 4. Path integral to solve generalized Fokker–Planck equation

Here a path integral approach is proposed to solve the generalized Fokker–Planck equation. The algorithm is described in Section 4.1. In Section 4.2, the bounds computed by the algorithm are analyzed based on the principles of interpretability [16] in generalized interval. Generalized interval provides more semantic power to help verify completeness and soundness of range estimations by logic interpretations. A *complete* range estimation of possible values includes all possible occurrences without underestimation. A *sound* range estimation does not include impossible occurrences without overestimation.

##### 4.1. The proposed path integral method

The generalized Fokker–Planck equation based on generalized interval probability is

$$\frac{\partial}{\partial t} \mathbf{p}(x, t | y, t') = -\text{dual} \sum_{i=1}^n \frac{\partial}{\partial x_i} [\mathbf{A}_i(x, t) \mathbf{p}(x, t | y, t')] + \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n \frac{\partial^2}{\partial x_i \partial x_j} [\mathbf{B}_{ij}(x, t) \mathbf{p}(x, t | y, t')] \quad (9)$$

where  $\mathbf{A}$  is a vector of interval-valued drift rates and  $\mathbf{B}$  is a matrix of interval-valued diffusion coefficients. The interval values represent the epistemic uncertainty associated with the parameters. Following the derivation of Risken [31], we can have the *short-time transition probability density* as

$$\mathbf{p}(x', t + \tau | x, t) \propto \exp \left( -\frac{1}{2\tau} [x' - x - \mathbf{A}(x, t)\tau]^T \mathbf{B}^{-1}(x, t) [x' - x - \mathbf{A}(x, t)\tau] \right) \quad (10)$$

where  $\mathbf{B}^{-1}$  is the inverse matrix of  $\mathbf{B}$ . Eq. (10) is used in the path integral approach to numerically solve Eq. (9). Let the initial probability distribution at time  $t_0$  be  $\mathbf{q}(x, t_0)$  and the discrete time intervals  $t_k = t_0 + k\tau$  for  $k = 1, 2, \dots$ . The distributions at time  $t = t_k$  is calculated by

$$\mathbf{q}(x, t_k) = \int_{\mathbb{R}^n} dy_{k-1} \mathbf{p}(x, t_k | y_{k-1}, t_{k-1}) \int_{\mathbb{R}^n} dy_{k-2} \mathbf{p}(y_{k-1}, t_{k-1} | y_{k-2}, t_{k-2}) \cdots \int_{\mathbb{R}^n} dy_0 \mathbf{p}(y_1, t_1 | y_0, t_0) \mathbf{q}(y_0, t_0) \quad (11)$$

The numerical implementation is based on matrices. Suppose that the number of states  $N$  is finite. The initial probability distribution is an  $N \times 1$  interval vector  $\mathbf{Q}(t_0)$ . The short-time transition probability density is an  $N \times N$  interval matrix  $\mathbf{P}(t)$  calculated by Eq. (10). Its element  $\mathbf{P}_{ij}(t)$  represents the probability of transition from state  $j$  to state  $i$  at time  $t$ . Then the distribution at time  $t = t_k$  is

$$\mathbf{Q}(t_k) = \mathbf{P}(t_{k-1}) \mathbf{P}(t_{k-2}) \cdots \mathbf{P}(t_0) \mathbf{Q}(t_0) \quad (12)$$

Notice that each column of  $\mathbf{P}(t)$  should sum up to 1, which is required by the logic coherence constraint. That is, if the transition rate is calculated by Eq. (10) as

$$\mathbf{P}'_{ij}(t) = \exp\left(-\frac{1}{2\tau}[x_i - x_j - \mathbf{A}(x_j, t)\tau]^T \mathbf{B}^{-1}(x_j, t)[x_i - x_j - \mathbf{A}(x_j, t)\tau]\right) \quad (13)$$

then the normalized transition probability density is

$$\mathbf{P}_{ij}(t) = \mathbf{P}'_{ij}(t) / \text{dual} \sum_{l=1}^N \mathbf{P}'_{lj}(t) \quad (14)$$

Notice that Eq. (12) holds because the multiplication distributivity of three probability intervals  $\mathbf{p}_1$ ,  $\mathbf{p}_2$ , and  $\mathbf{p}_3$  ( $0 \leq \mathbf{p}_1, \mathbf{p}_2, \mathbf{p}_3 \leq 1$ ) exists [32–34]. That is,

$$(\mathbf{p}_1 + \mathbf{p}_2)\mathbf{p}_3 = \mathbf{p}_1\mathbf{p}_3 + \mathbf{p}_2\mathbf{p}_3 \quad (15)$$

#### 4.2. Interpretation and verification

Suppose that all elements in interval drift vectors  $\mathbf{A}(x, t) \in \mathbb{I}\mathbb{R}^n$  and diffusion matrices  $\mathbf{B}(x, t) \in \mathbb{I}\mathbb{R}^{n \times n}$  are proper. We may find inverse matrices  $\mathbf{B}^{-1}(x, t) \in \mathbb{I}\mathbb{R}^{n \times n}$  with all elements in  $\mathbf{B}^{-1}(x, t)$  are also proper such that  $\mathbf{B} \cdot \text{dual} \mathbf{B}^{-1} = I$ . This can be achieved by solving interval linear equations  $\mathbf{B} \cdot \mathbf{X} = I$  where  $I$  is the identity matrix. Various numerical methods have been developed (e.g. [35–38]). Based on the principles of interpretation [16],  $\mathbf{B} \cdot \text{dual} \mathbf{B}^{-1} = I$  can be interpreted as

$$\forall B \in [\underline{B}, \overline{B}]^\Delta, \exists C \in [\underline{B}^{-1}, \overline{B}^{-1}]^\Delta, B \cdot C = I \quad (16)$$

where  $[\underline{B}, \overline{B}]^\Delta$  and  $[\underline{B}^{-1}, \overline{B}^{-1}]^\Delta$  represent the respective sets of matrices corresponding to  $\mathbf{B}$  and  $\mathbf{B}^{-1}$ . The operator  $\Delta$  converts a generalized interval to the classical set-based interval as defined in Eq. (1.4) in Appendix A1. Similarly, Eq. (13) is interpreted as

$$\forall A \in [\underline{A}, \overline{A}]^\Delta, \forall C \in [\underline{B}^{-1}, \overline{B}^{-1}]^\Delta, \exists p'_{ij} \in [\underline{P}'_{ij}, \overline{P}'_{ij}]^\Delta, p'_{ij} = \exp\left(-\frac{1}{2\tau}[x_i - x_j - A\tau]^T C[x_i - x_j - A\tau]\right) \quad (17)$$

Because of the monotonicity of the exponential function,  $\mathbf{P}'_{ij}$  in Eq. (13) is proper given that  $\mathbf{A}$  and  $\mathbf{B}^{-1}$  are proper. Nevertheless,  $\mathbf{P}_{ij}$  calculated by Eq. (14) can be either proper or improper. If  $\underline{P}'_{ij} / \sum_l \underline{P}'_{lj} < \overline{P}'_{ij} / \sum_l \overline{P}'_{lj}$ ,  $\mathbf{P}_{ij}$  is proper. Otherwise, it is improper. Within column  $j$ , improper  $\mathbf{P}_{ij}$ 's occur where their values are relatively large.

When  $\mathbf{P}_{ij} \in \mathbb{I}\mathbb{R}$ , Eq. (14) is interpreted as

$$\forall p'_{ij} \in [\underline{P}'_{ij}, \overline{P}'_{ij}]^\Delta, \exists p_{ij} \in [\underline{P}_{ij}, \overline{P}_{ij}]^\Delta, \exists s_j \in \left[ \sum_{l=1}^N \underline{P}'_{lj}, \sum_{l=1}^N \overline{P}'_{lj} \right]^\Delta, p_{ij} = p'_{ij} / s_j \quad (18)$$

Combining Eqs. (16)–(18), we have the overall interpretation

$$\forall A \in [\underline{A}, \overline{A}]^\Delta, \forall B \in [\underline{B}, \overline{B}]^\Delta, \exists p_{ij} \in [\underline{P}_{ij}, \overline{P}_{ij}]^\Delta, \exists C \in [\underline{B}^{-1}, \overline{B}^{-1}]^\Delta, \exists p'_{ij} \in [\underline{P}'_{ij}, \overline{P}'_{ij}]^\Delta, \exists s_j \in \left[ \sum_{l=1}^N \underline{P}'_{lj}, \sum_{l=1}^N \overline{P}'_{lj} \right]^\Delta, \\ p_{ij} = \exp\left(-\frac{1}{2\tau}[x_i - x_j - A\tau]^T C[x_i - x_j - A\tau]\right) / s_j \quad (19)$$

where the existential quantifier ( $\exists$ ) associated with  $[\underline{P}_{ij}, \overline{P}_{ij}]^\Delta$  indicates the completeness of the estimation of  $\mathbf{P}_{ij}$ 's in Eq. (14), which are usually associated with small probability values.

When  $\mathbf{P}_{ij} \in \mathbb{I}\mathbb{R}$ , Eq. (14) is interpreted as

$$\forall p'_{ij} \in [\underline{P}'_{ij}, \overline{P}'_{ij}]^\Delta, \forall p_{ij} \in [\underline{P}_{ij}, \overline{P}_{ij}]^\Delta, \exists s_j \in \left[ \sum_{l=1}^N \underline{P}'_{lj}, \sum_{l=1}^N \overline{P}'_{lj} \right]^\Delta, p_{ij} = p'_{ij} / s_j \quad (20)$$

Combining Eqs. (16), (17) and (20), we have

$$\forall A \in [\underline{A}, \overline{A}]^\Delta, \forall B \in [\underline{B}, \overline{B}]^\Delta, \forall p_{ij} \in [\underline{P}_{ij}, \overline{P}_{ij}]^\Delta, \exists C \in [\underline{B}^{-1}, \overline{B}^{-1}]^\Delta, \exists p'_{ij} \in [\underline{P}'_{ij}, \overline{P}'_{ij}]^\Delta, \exists s_j \in \left[ \sum_{l=1}^N \underline{P}'_{lj}, \sum_{l=1}^N \overline{P}'_{lj} \right]^\Delta, \\ p_{ij} = \exp\left(-\frac{1}{2\tau}[x_i - x_j - A\tau]^T C[x_i - x_j - A\tau]\right) / s_j \quad (21)$$

where the universal quantifier ( $\forall$ ) associated with  $[\underline{P}_{ij}, \overline{P}_{ij}]^\Delta$  indicates the soundness of the estimation of  $\mathbf{P}_{ij}$ 's in Eq. (14), which are typically associated with large probability values. Eqs. (19) and (21) provide the interpretations of the short-time transition probability density during computation in each iteration.

**Theorem 1.** (Markov Logic Coherence Constraint). Given an interval matrix  $\mathbf{P} \in \mathbb{K}\mathbb{R}^{n \times n}$  and an interval vector  $\mathbf{Q} \in \mathbb{K}\mathbb{R}^n$  with their respective elements  $\mathbf{p}_{ij}$  ( $i=1, \dots, n; j=1, \dots, n$ ) and  $\mathbf{q}_i$  ( $i=1, \dots, n$ ) as generalized intervals, if  $\sum_{i=1}^n \mathbf{p}_{ij} = 1$  ( $\forall j=1, \dots, n$ ) and  $\sum_{i=1}^n \mathbf{q}_i = 1$ , then the elements of  $\mathbf{T} = \mathbf{P} \cdot \mathbf{Q}$  denoted as  $\mathbf{t}_i$  ( $i=1, \dots, n$ ) also satisfy  $\sum_{i=1}^n \mathbf{t}_i = 1$ .

**Proof.**

$$\sum_{i=1}^n \mathbf{t}_i = \sum_{i=1}^n \left[ \sum_{j=1}^n \mathbf{p}_{ij} \cdot \mathbf{q}_j \right] = \sum_{j=1}^n \left[ \sum_{i=1}^n \mathbf{p}_{ij} \cdot \mathbf{q}_j \right] = \sum_{j=1}^n \left[ \mathbf{q}_j \sum_{i=1}^n \mathbf{p}_{ij} \right] = \sum_{j=1}^n [\mathbf{q}_j \cdot 1] = 1$$

**Remark.** Theorem 1 shows that the logic coherence constraint is automatically satisfied during the state transition based on generalized interval probability.

If the system reaches the steady state, there is an equilibrium distribution  $\Pi$  of the possible states satisfying

$$\Pi = \mathbf{P} \cdot \Pi \quad (22)$$

The elements  $\pi_i$  ( $i=1, \dots, n$ ) of  $\Pi$  and  $\mathbf{p}_{ij}$  ( $i=1, \dots, n; j=1, \dots, n$ ) of  $\mathbf{P}$  are divided into two categories, proper and improper. Let  $\mathcal{P}$  denote the set of indices for those proper interval elements, i.e.  $\pi_i \in \mathbb{I}\mathbb{R}$  ( $i \in \mathcal{P}$ ) and  $\mathbf{p}_{ij} \in \mathbb{I}\mathbb{R}$  ( $ij \in \mathcal{P}$ ), and  $\mathcal{I}$  the set of indices for those improper interval elements, i.e.  $\pi_i \in \mathbb{I}\mathbb{R}$  ( $i \in \mathcal{I}$ ) and  $\mathbf{p}_{ij} \in \mathbb{I}\mathbb{R}$  ( $ij \in \mathcal{I}$ ). Eq. (22) can then be re-arranged as

$$\begin{bmatrix} \Pi_{\mathcal{P}} \\ \Pi_{\mathcal{I}} \end{bmatrix} = \begin{bmatrix} \mathbf{P}^{(1)} & \mathbf{P}^{(2)} \\ \mathbf{P}^{(3)} & \mathbf{P}^{(4)} \end{bmatrix} \cdot \begin{bmatrix} \Pi_{\mathcal{P}} \\ \Pi_{\mathcal{I}} \end{bmatrix} \quad (23)$$

Let  $\mathbf{P}_{\mathcal{P}}^{(i)}$  and  $\mathbf{P}_{\mathcal{I}}^{(i)}$  be the respective proper and improper components of  $\mathbf{P}^{(i)}$  ( $i=1$  to 4). The first set of equations  $\Pi_{\mathcal{P}} = \mathbf{P}^{(1)} \cdot \Pi_{\mathcal{P}} + \mathbf{P}^{(2)} \cdot \Pi_{\mathcal{I}}$  can be interpreted as

$$\forall \mathbf{P}_{\mathcal{I}}^{(1)} \in \mathbf{P}_{\mathcal{I}}^{(1)\Delta}, \forall \mathbf{P}_{\mathcal{I}}^{(2)} \in \mathbf{P}_{\mathcal{I}}^{(2)\Delta}, \forall \pi_{\mathcal{I}} \in \Pi_{\mathcal{I}}^{\Delta}, \exists \mathbf{P}_{\mathcal{P}}^{(1)} \in \mathbf{P}_{\mathcal{P}}^{(1)\Delta}, \exists \mathbf{P}_{\mathcal{P}}^{(2)} \in \mathbf{P}_{\mathcal{P}}^{(2)\Delta}, \exists \pi_{\mathcal{P}} \in \Pi_{\mathcal{P}}^{\Delta}, \mathbf{P}^{(1)} \cdot \pi_{\mathcal{P}} + \mathbf{P}^{(2)} \cdot \pi_{\mathcal{I}} = \pi_{\mathcal{P}} \quad (24)$$

The second set of equations  $\mathbf{P}^{(3)} \cdot \Pi_{\mathcal{P}} + \mathbf{P}^{(4)} \cdot \Pi_{\mathcal{I}} = \Pi_{\mathcal{I}}$  can be interpreted as

$$\forall \mathbf{P}_{\mathcal{P}}^{(3)} \in \mathbf{P}_{\mathcal{P}}^{(3)\Delta}, \forall \mathbf{P}_{\mathcal{P}}^{(4)} \in \mathbf{P}_{\mathcal{P}}^{(4)\Delta}, \forall \pi_{\mathcal{P}} \in \Pi_{\mathcal{P}}^{\Delta}, \exists \mathbf{P}_{\mathcal{I}}^{(3)} \in \mathbf{P}_{\mathcal{I}}^{(3)\Delta}, \exists \mathbf{P}_{\mathcal{I}}^{(4)} \in \mathbf{P}_{\mathcal{I}}^{(4)\Delta}, \exists \pi_{\mathcal{I}} \in \Pi_{\mathcal{I}}^{\Delta}, \mathbf{P}^{(3)} \cdot \pi_{\mathcal{P}} + \mathbf{P}^{(4)} \cdot \pi_{\mathcal{I}} = \pi_{\mathcal{I}} \quad (25)$$

The combination of Eqs. (24) and (25) leads to the interpretation of Eq. (23) or Eq. (22) as

$$\forall \mathbf{P}_{\mathcal{I}}^{(1)} \in \mathbf{P}_{\mathcal{I}}^{(1)\Delta}, \forall \mathbf{P}_{\mathcal{I}}^{(2)} \in \mathbf{P}_{\mathcal{I}}^{(2)\Delta}, \forall \mathbf{P}_{\mathcal{P}}^{(3)} \in \mathbf{P}_{\mathcal{P}}^{(3)\Delta}, \forall \mathbf{P}_{\mathcal{P}}^{(4)} \in \mathbf{P}_{\mathcal{P}}^{(4)\Delta}, \exists \mathbf{P}_{\mathcal{P}}^{(1)} \in \mathbf{P}_{\mathcal{P}}^{(1)\Delta}, \exists \mathbf{P}_{\mathcal{P}}^{(2)} \in \mathbf{P}_{\mathcal{P}}^{(2)\Delta}, \exists \mathbf{P}_{\mathcal{I}}^{(3)} \in \mathbf{P}_{\mathcal{I}}^{(3)\Delta}, \exists \mathbf{P}_{\mathcal{I}}^{(4)} \in \mathbf{P}_{\mathcal{I}}^{(4)\Delta}, \exists \pi \in \Pi^{\Delta} \\ \mathbf{P} \cdot \pi = \pi \quad (26)$$

The existential quantifiers associated with the elements of  $\Pi$  in Eq. (26) indicate the controllable stability of the equilibrium distribution in the steady state. If there are uncontrollable deviations associated with transition probabilities  $\mathbf{P}_{\mathcal{I}}^{(1)}$ ,  $\mathbf{P}_{\mathcal{I}}^{(2)}$ ,  $\mathbf{P}_{\mathcal{P}}^{(3)}$ , and  $\mathbf{P}_{\mathcal{P}}^{(4)}$ , we should be able to choose  $\mathbf{P}_{\mathcal{P}}^{(1)}$ ,  $\mathbf{P}_{\mathcal{P}}^{(2)}$ ,  $\mathbf{P}_{\mathcal{I}}^{(3)}$ , and  $\mathbf{P}_{\mathcal{I}}^{(4)}$  such that the steady state is maintained. Therefore, Eq. (26) provides the logic basis to maintain the stability of the system subject to incomplete knowledge of states and state transitions, which can improve the robustness of the dynamic control in stochastic systems.

## 5. Demonstrative examples

The generalized interval with Kaucher arithmetic and the proposed path integral algorithm to solve the generalized Fokker–Planck equation in Section 4 are implemented in INTLAB [39], which is a MATLAB package for the classical set-based interval analysis. Here, it is demonstrated by two examples. The first example is a bi-stable stochastic resonance system. The second one is a Van der Pol oscillator.

### 5.1. Bi-stable stochastic resonance

The bi-stable stochastic resonance phenomenon is a nonlinear response of a system with sinusoidal inputs simultaneously subject to noises, where the system oscillates between two states. The phenomenon has been observed in systems such as neural tissue and rotational machinery. It can be described by stochastic differential equations, such as the following one [40,41]:

$$dx/dt = c_1 x - c_2 x^3 + a_0 \sin(2\pi f_0 t) + N(t) \quad (27)$$

where state  $x$  changes along time  $t$ ,  $c_1$  and  $c_2$  are coefficients,  $a_0$  and  $f_0$  are the amplitude and modulation frequency of the periodic input respectively, and the noise  $N(t) = \sqrt{2B}\xi(t)$  has the intensity of  $B$  with  $\mathbb{E}(N(t), N(t+s)) = 2B\delta(s)$ ,  $\delta(\cdot)$  is the Dirac delta function, and  $\xi(t)$  is a zero-mean, unit variance Gaussian white noise. Instead of directly solving Eq. (27) to find the point-wise paths in system evolution, we solve the equivalent Fokker–Planck equation

$$\frac{\partial}{\partial t} p(x, t) = -\frac{\partial}{\partial x} (Ap(x, t)) + \frac{\partial^2}{\partial x^2} (Bp(x, t)) \quad (28)$$

where  $A = c_1x - c_2x^3 + a_0 \sin(2\pi f_0 t)$ , to find the complete distribution evolution of the system. In this example, we use the parameter values  $c_1 = c_2 = 1$ ,  $a_0 = 1$ ,  $f_0 = 0.01$ , and  $B = 0.31$  [41]. First we solved the real-valued case of Eq. (28) with the classical path-integral method [31]. Then by choosing the interval drift coefficient  $\mathbf{A} = [A - 0.1, A + 0.1]$  and interval diffusion coefficient  $\mathbf{B} = [B - 0.031, B + 0.031]$ , we solved the generalized version of Eq. (28) using the proposed path integral method. The results are plotted in Fig. 1, with the initial distribution at  $t=0$  as  $\exp(-(x-\mu)^2/2\sigma^2)/(\sqrt{2\pi}\sigma)$  where  $\mu = 1.0$  and  $\sigma = 0.02$  in both cases. The figure shows that the distribution of states evolves along time. The system oscillates between two distinctive states where it has the highest probabilities to stay. The time step used in computation is  $\tau = 0.2$ .

A zoom-in view of the result as shown in Fig. 2 provides a closer look. It can be seen that the lower (solid line) and upper (dotted line) bounds of probability densities as the solution of the generalized Fokker-Planck equation accurately enclose the solution in the real-valued case (dots) solved by the classical path integral method. Therefore, it serves our purpose of reliable simulation where the interval-valued solution rigorously bounds the real-valued solution.

Notice that the widths of the interval probability densities at the most probable states (the peaks) are generally larger than those at other states. They are also improper intervals. However, they do not overestimate the ranges, according to the interpretation in Eq. (21). For the less probable states, the probability densities are proper intervals and they are narrower. They do not underestimate the ranges either, according to the interpretation in Eq. (19). Therefore, the interval probability densities provide rigorous bounds.

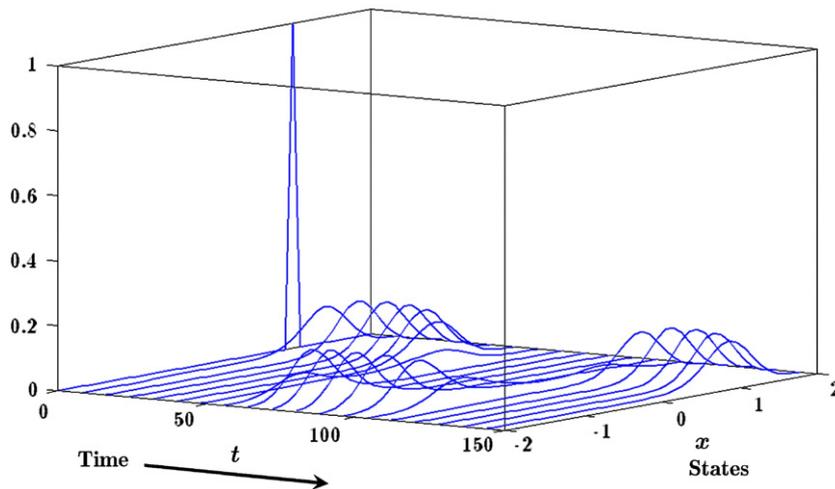


Fig. 1. The solution of the Fokker-Planck equation for the bi-stable stochastic resonance system by the path integral method.

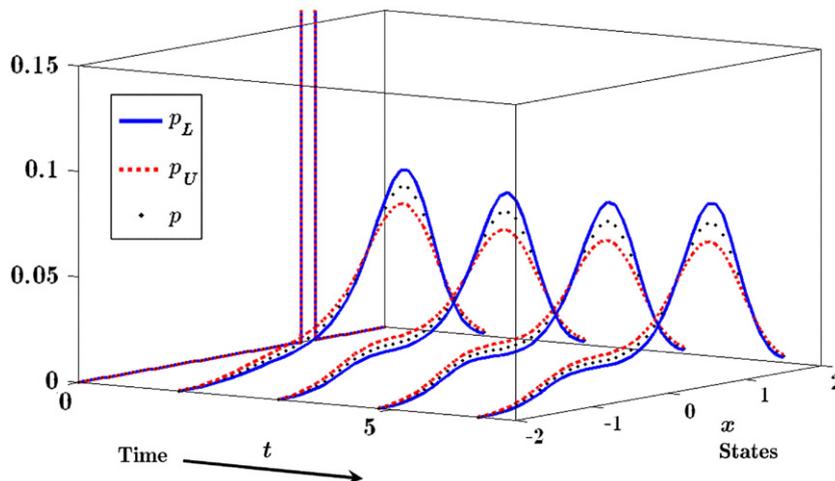


Fig. 2. A zoom-in view of the solution in Fig. 1 where interval-valued solution rigorously bounds the real-valued solution.

## 5.2. Van der Pol oscillator

The Van der Pol oscillator is a non-conservative oscillator with nonlinear damping. The system dynamics with the white noise excitation can be described by [42]

$$\frac{\partial}{\partial t} p(x_1, x_2, t) = -\frac{\partial}{\partial x_1} (g_1(x_1, x_2) p(x_1, x_2, t)) - \frac{\partial}{\partial x_2} (g_2(x_1, x_2) p(x_1, x_2, t)) + D \frac{\partial^2}{\partial x_2^2} p(x_1, x_2, t) \quad (29)$$

where the position  $x_1$  and velocity  $x_2$  represent the system's state that evolves along the time  $t$ . Functions  $g_1(x_1, x_2) = x_2$  and  $g_2(x_1, x_2) = 2\zeta\omega_0(1 - \varepsilon x_1^2)x_2 - \omega_0^2 x_1$  define the drifting coefficients, where the damping is determined by the scalar parameters  $\zeta$ ,  $\omega_0$ , and  $\varepsilon$ .  $D$  is an excitation constant.

Here we demonstrate the proposed path integral method to solve the two-dimensional Van der Pol oscillator problem. In this example, the oscillator parameters are given by  $\zeta = 0.05$ ,  $\omega_0 = 1$ ,  $\varepsilon = 1$ , and  $D = 0.1$ . The drift vector is  $A = [g_1(x_1, x_2) \quad g_2(x_1, x_2)]^T$  and the diffusion matrix used here is

$$B = \begin{bmatrix} D & 0 \\ 0 & Dx_2^2 \end{bmatrix}$$

Fig. 3 shows the path integral solution of the Van der Pol oscillator problem. The initial distribution is Gaussian as  $\exp(-(x_1 - \mu_1)^2 / 2\sigma_1^2) \exp(-(x_2 - \mu_2)^2 / 2\sigma_2^2) / (2\pi\sigma_1\sigma_2)$  with precise parameters  $\mu_1 = 2$ ,  $\mu_2 = 5$ ,  $\sigma_1 = 1/3$ , and  $\sigma_2 = 1/3$ . During the path integral computation, the drift and diffusion coefficients were set to be  $\pm 10\%$  of the nominal ones. Fig. 3 plots the probability density functions of the nominal, lower-bound, and upper-bound cases with iso-contour lines in the discrete state space with  $9 \times 11$  states. The nominal density functions computed from the classical path integral method are bounded by the lower- and upper-bound density functions computed from the new path integral of the generalized Fokker–Planck equation. By  $t = 1.0$ , the system reaches the steady state.

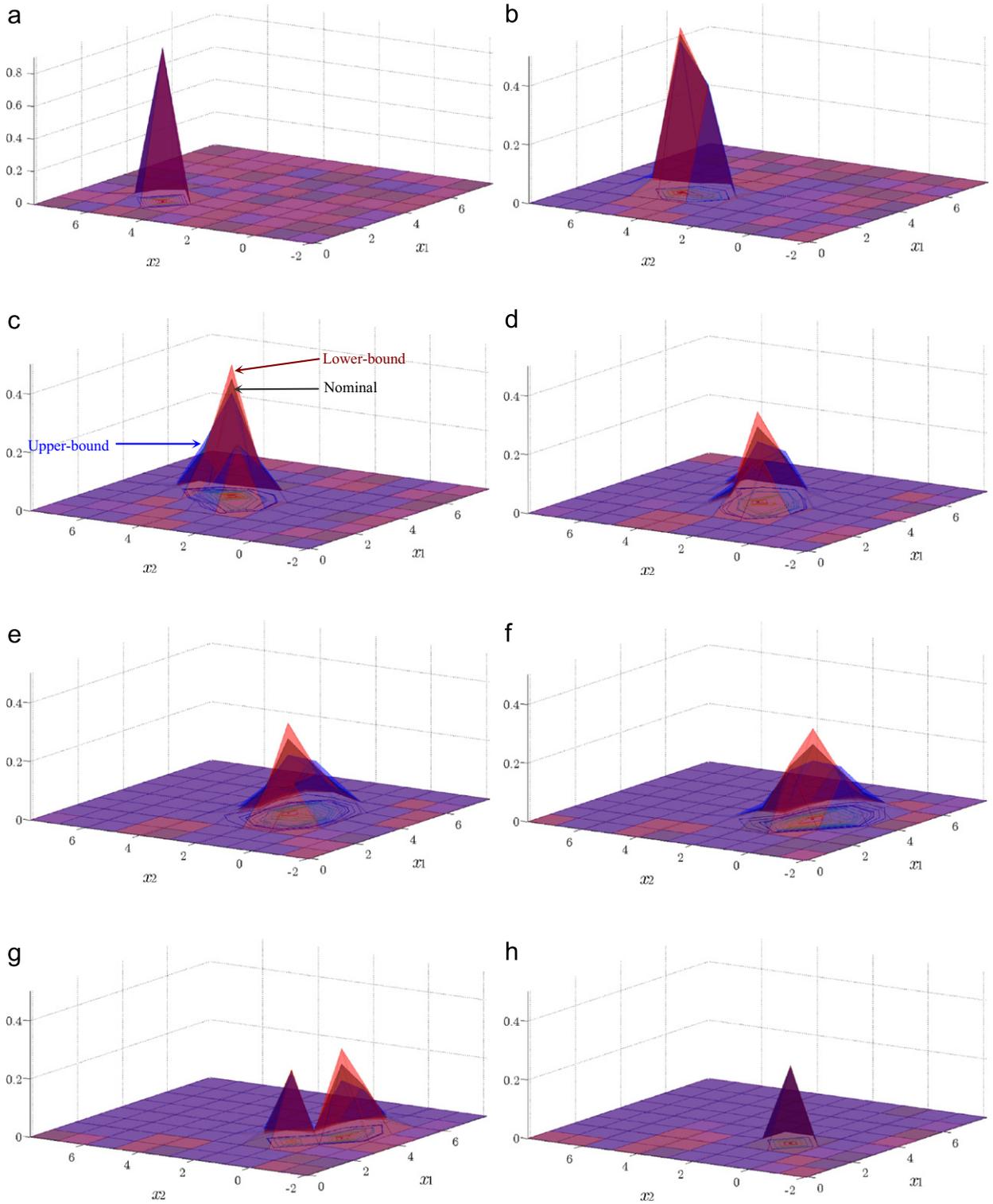
Again, because of the interpretability advantage provided by Eqs. (21) and (19) respectively, the interval probability densities at the most probable states for each iteration do not overestimate the extent of epistemic uncertainty, nor do those at the less probable states underestimate the ranges. After the system reaches the steady state, the interval densities are complete prediction of the epistemic uncertainty effect without under estimation because of the interpretation in Eq. (26).

In both of the numerical examples, epistemic uncertain is captured by the interval-valued drift and diffusion coefficients. During the computation of distribution evolution, the effects of two uncertainty types are quantified separately. The envelope defined by the lower and upper density functions provides a range of possibilities simultaneously for uncertain model forms and parameters without introducing heavy computational overhead as in sensitivity analysis or second-order Monte Carlo sampling. The resulted bounds computed from the generalized Fokker–Planck equation also inherently provide the confidence of completeness or soundness of the range estimation for epistemic uncertainty. This confidence is not available from the other two approaches in assessing the classical Fokker–Planck equation without extensive and time-consuming samplings of possible model parameter combinations.

## 6. Concluding remarks

In this paper, we derived a generalized differential Chapman–Kolmogorov equation that describes the time evolution of generalized interval probability under aleatory and epistemic uncertainties, where probability values are generalized intervals. A generalized Fokker–Planck equation is proposed to describe the system dynamics where drift and diffusion coefficients as well as probability densities are generalized intervals. A path integral approach is developed to numerically solve the equation. The Kaucher interval arithmetic provides a convenient calculus structure and significantly simplifies the computation. The logic interpretation of generalized interval helps verify the completeness and soundness of interval probabilities for each step of simulation. This offers a rigorous approach to represent and estimate epistemic uncertainty during its propagation in computation, where both input uncertainty because of measurement errors and model uncertainty because of approximation and numerical treatment can be quantified. The resulted interval probability densities rigorously bound the real-valued nominal ones computed from the classical path integral method. The interval probabilities thus provide the extra information of how sensitive the estimated distributions are with respect to the uncertain input parameters.

The result of the path integral computation and the associated computational cost are dependent on both the number of states and the time step. Different choices of the two can lead to different results of interval probability densities and steady states. In the future work, we need to study the effects of time step size and the number of states in order to find the conditions such that the numerical solutions with intervals converge to analytical solutions of real values as the interval widths reduce towards zeros. This will assist both the sensitivity analysis of drift-diffusion coefficients with respect to output distributions and the numerical stability assessment. In addition, the computational efficiency of the path integral method needs improvement. Most of the time for computing the short-time transition probability density matrix is spent on the inverse of the diffusion coefficient matrix. More efficient numerical algorithms to compute the inverse of interval matrices are desirable.



**Fig. 3.** The path integral solution of the Van der Pol oscillator problem. (a)  $t=0$ , (b)  $t=0.125$ , (c)  $t=0.25$ , (d)  $t=0.375$ , (e)  $t=0.5$ , (f)  $t=0.625$ , (g)  $t=0.75$  and (h)  $t=1.0$ .

Appendix

A1. Generalized interval

Here, only the most relevant concepts and notations of generalized interval are introduced. More background information can be found in [43–46]. Compared to the *semi-group* formed by the classical set-based intervals, generalized intervals form a *group*. This property significantly simplifies the computational structure. The set of generalized intervals is denoted by  $\mathbb{K}\mathbb{R} = \{[\underline{x}, \bar{x}] | \underline{x}, \bar{x} \in \mathbb{R}\}$ . The set of proper intervals is  $\mathbb{I}\mathbb{R} = \{[\underline{x}, \bar{x}] | \underline{x} < \bar{x}\}$ , and the set of improper intervals is  $\mathbb{I}\mathbb{R} = \{[\underline{x}, \bar{x}] | \underline{x} \geq \bar{x}\}$ . The relationship between proper and improper intervals is established with the operator dual as

$$\text{dual}[\underline{x}, \bar{x}] := [\bar{x}, \underline{x}] \tag{1.1}$$

The *less than or equal to* partial order relationship between two generalized intervals is defined as

$$[\underline{x}, \bar{x}] \leq [\underline{y}, \bar{y}] \Leftrightarrow \underline{x} \leq \underline{y} \wedge \bar{x} \leq \bar{y} \tag{1.2}$$

The *inclusion* relationship is defined as

$$[\underline{x}, \bar{x}] \subseteq [\underline{y}, \bar{y}] \Leftrightarrow \underline{y} \leq \underline{x} \wedge \bar{x} \leq \bar{y} \tag{1.3}$$

In this paper, we denote the classical set-based interval as  $[\underline{x}, \bar{x}] := \{x \in \mathbb{R} | \underline{x} \leq x \leq \bar{x}\}$ . The relationship between generalized interval and classical interval is established with the operator  $\Delta$  defined as

$$[\underline{x}, \bar{x}]^\Delta := [\min(\underline{x}, \bar{x}), \max(\underline{x}, \bar{x})] \tag{1.4}$$

Generalized interval provides more semantic power to help verify completeness and soundness of range estimations by logic interpretations. The four examples in Table 1 illustrate the interpretations for operator “+”, where the range estimation  $[z, \bar{z}] = [4, 7]$  in the 1st row is *complete*. The estimation  $[z, \bar{z}] = [7, 4]$  in the 4th row is *sound*.  $-$ ,  $\times$ ,  $/$  have the similar semantic properties.

Based on the generalized interval, the new form of imprecise probability resembles the classical precise probability, as introduced next.

A2. Generalized interval probability

**Definition 1.** Given a sample space  $\Omega$  and a  $\sigma$ -algebra  $\mathbf{A}$  of random events over  $\Omega$ , the *generalized interval probability*  $\mathbf{p} \in \mathbb{K}\mathbb{R}$  is defined as  $\mathbf{p} : \mathcal{A} \rightarrow [0, 1] \times [0, 1]$  which obeys the axioms of Kolmogorov: (1)  $\mathbf{p}(\Omega) = [1, 1]$ ; (2)  $[0, 0] \leq \mathbf{p}(E) \leq [1, 1]$  ( $\forall E \in \mathcal{A}$ ); and (3) for any countable mutually disjoint events  $E_i \cap E_j = \emptyset$  ( $i \neq j$ ),  $\mathbf{p}(\cup_{i=1}^n E_i) = \sum_{i=1}^n \mathbf{p}(E_i)$ . Here “ $\leq$ ” is defined as in Eq. (1.2).

**Definition 2.** The probability of *union* is defined as  $\mathbf{p}(A) := \sum_{S \subseteq A} (-\text{dual})^{|A|-|S|} \mathbf{p}(S)$  for  $A \subseteq \Omega$ .

Two examples of union are

$$\mathbf{p}(E_1 \cup E_2) = \mathbf{p}(E_1) + \mathbf{p}(E_2) - \text{dual} \mathbf{p}(E_1 \cap E_2)$$

and

$$\mathbf{p}(E_1 \cup E_2 \cup E_3) = \mathbf{p}(E_1) + \mathbf{p}(E_2) + \mathbf{p}(E_3) - \text{dual} \mathbf{p}(E_1 \cap E_2) - \text{dual} \mathbf{p}(E_2 \cap E_3) - \text{dual} \mathbf{p}(E_1 \cap E_3) + \mathbf{p}(E_1 \cap E_2 \cap E_3)$$

The most important property of the generalized interval probability is the *logic coherence constraint* (LCC): That is, for a mutually disjoint event partition  $\cup_{i=1}^n E_i = \Omega$ ,  $\sum_{i=1}^n \mathbf{p}(E_i) = 1$ . If the sample space is continuous and the integral of a continuous interval function  $\mathbf{f}(x) = [\underline{f}(x), \bar{f}(x)]$  is defined as  $\int \mathbf{f}(x) dx := [\int \underline{f}(x) dx, \int \bar{f}(x) dx]$  [47], the LCC is  $\int dx \mathbf{p}(x) = 1$ . The LCC ensures that generalized interval probability is logically coherent with precise probability. For instance, given that  $\mathbf{p}(\text{down}) = [0.2, 0.3]$ ,  $\mathbf{p}(\text{idle}) = [0.3, 0.5]$ ,  $\mathbf{p}(\text{working}) = [0.5, 0.2]$  for a system’s working status, we can interpret it as

$$(\forall p_1 \in [0.2, 0.3])(\forall p_2 \in [0.3, 0.5])(\exists p_3 \in [0.2, 0.5])(p_1 + p_2 + p_3 = 1)$$

Accordingly, we differentiate non-focal events (“*working*” in this example) from focal events (“*down*”, “*idle*”) based on the respective logic quantifiers in the interpretation. An event  $E$  is *focal* if the associated semantics for  $\mathbf{p}(E)$  is universal.

**Table 1**  
Illustrations of the semantic extension of generalized interval.

| Algebraic relation: $[\underline{x}, \bar{x}] + [\underline{y}, \bar{y}] = [\underline{z}, \bar{z}]$ | Corresponding logic interpretation  | Quantifier of $[z, \bar{z}]$ | Range estimation of $[z, \bar{z}]$ |
|--|---|------------------------------|------------------------------------|
| $[2, 3] + [2, 4] = [4, 7]$   | $(\forall x \in [2, 3])(\forall y \in [2, 4])(\exists z \in [4, 7])(x + y = z)$ | $\exists$                    | $[4, 7]$ is complete               |
| $[2, 3] + [4, 2] = [6, 5]$   | $(\forall x \in [2, 3])(\forall z \in [5, 6])(\exists y \in [2, 4])(x + y = z)$ | $\forall$                    | $[5, 6]$ is sound                  |
| $[3, 2] + [2, 4] = [5, 6]$   | $(\forall y \in [2, 4])(\exists x \in [2, 3])(\exists z \in [5, 6])(x + y = z)$ | $\exists$                    | $[5, 6]$ is complete               |
| $[3, 2] + [4, 2] = [7, 4]$   | $(\forall z \in [4, 7])(\exists x \in [2, 3])(\exists y \in [2, 4])(x + y = z)$ | $\forall$                    | $[4, 7]$ is sound                  |

Otherwise, it is *non-focal* if the associated semantics is existential. While the epistemic uncertainty associated with focal events is critical to the analyst, the one associated with non-focal events is not.

The concepts of conditional probability and independence are essential for the classical probability theory. With them, we can decompose a complex problem into simpler and manageable components. Similarly, they are critical for imprecise probabilities. Different from all other forms of imprecise probabilities, which are based on convex probability sets, our conditional probability is defined directly from marginal probability.

**Definition 3.** If  $\mathbf{p}(C) > 0$ , the *conditional probability*  $\mathbf{p}(E|C)$  for all  $E, C \in \mathcal{A}$  is defined as

$$\mathbf{p}(E|C) := \frac{\mathbf{p}(E \cap C)}{\text{dual}\mathbf{p}(C)} = \left[ \frac{\underline{\mathbf{p}}(E \cap C)}{\underline{\mathbf{p}}(C)}, \frac{\overline{\mathbf{p}}(E \cap C)}{\overline{\mathbf{p}}(C)} \right] \quad (2.1)$$

Thanks to the unique algebraic properties of generalized intervals, this definition can greatly simplify computation in applications. Only algebraic computation is necessary.

**Definition 4.** For  $A, B, C \in \mathcal{A}$ ,  $A$  is said to be *conditionally independent* with  $B$  on  $C$  if and only if

$$\mathbf{p}(A \cap B|C) = \mathbf{p}(A|C)\mathbf{p}(B|C) \quad (2.2)$$

**Definition 5.** For  $A, B \in \mathcal{A}$ ,  $A$  is said to be *independent* with  $B$  if and only if

$$\mathbf{p}(A \cap B) = \mathbf{p}(A)\mathbf{p}(B) \quad (2.3)$$

The independence in Definition 5 is a special case of conditional independence in Definition 4, where  $C$  is the complete sample space  $\Omega$ . The conditional independence in Definition 4 also has a second form, as shown in Theorem A.1.

**Theorem A.1.** For  $A, B, C \in \mathcal{A}$ ,  $\mathbf{p}(A \cap B|C) = \mathbf{p}(A|C)\mathbf{p}(B|C) \Leftrightarrow \mathbf{p}(A|B \cap C) = \mathbf{p}(A|C)$ .

**Proof.**

$$\begin{aligned} \mathbf{p}(A \cap B|C) = \mathbf{p}(A|C)\mathbf{p}(B|C) &\Leftrightarrow \mathbf{p}(A \cap B \cap C) / \text{dual}\mathbf{p}(C) = \mathbf{p}(A|C) \cdot \mathbf{p}(B \cap C) / \text{dual}\mathbf{p}(C) \\ &\Leftrightarrow \mathbf{p}(A \cap B \cap C) / \text{dual}\mathbf{p}(B \cap C) = \mathbf{p}(A|C) \Leftrightarrow \mathbf{p}(A|B \cap C) = \mathbf{p}(A|C). \quad \square \end{aligned}$$

**Corollary A.2.** For  $A, B, C, D \in \mathcal{A}$  and  $A \cap D = \emptyset$ , the conditional independence between  $A$  and  $B$  given  $C$  and between  $A$  and  $D$  given  $C$  infers the independence between  $A \cup D$  and  $B$  given  $C$ .

**Proof.**

$$\begin{aligned} \mathbf{p}(A \cup D|B \cap C) &= \mathbf{p}((A \cup D) \cap B \cap C) / \text{dual}\mathbf{p}(B \cap C) = [\mathbf{p}(A \cap B \cap C) + \mathbf{p}(D \cap B \cap C)] / \text{dual}\mathbf{p}(B \cap C) \\ &= \mathbf{p}(A \cap B \cap C) / \text{dual}\mathbf{p}(B \cap C) + \mathbf{p}(D \cap B \cap C) / \text{dual}\mathbf{p}(B \cap C) \\ &= \mathbf{p}(A|B \cap C) + \mathbf{p}(D|B \cap C) = \mathbf{p}(A|C) + \mathbf{p}(D|C) = \mathbf{p}(A \cup D|C) \quad \square \end{aligned}$$

The most intuitive meaning of “independence” is that an independence relationship satisfies several *graphoid* properties. It has been shown that generalized interval probability with the defined independence is graphoid [48]. With  $X, Y, Z, W$  as sets of disjoint random variables and “ $\perp$ ” denoting independence, the conditional independence in Definition 3 satisfies all of the following graphoid properties:

- (G1) Symmetry:  $X \perp Y|Z \Rightarrow Y \perp X|Z$
- (G2) Decomposition:  $X \perp (W, Y)|Z \Rightarrow X \perp Y|Z$
- (G3) Composition:  $(X \perp Y|Z) \wedge (X \perp W|Z) \Rightarrow X \perp (W, Y)|Z$
- (G4) Contraction:  $(X \perp Y|Z) \wedge (X \perp W|(Y, Z)) \Rightarrow X \perp (W, Y)|Z$
- (G5) Reduction:  $(X \perp Y|Z) \wedge (X \perp (W, Y)|Z) \Rightarrow X \perp W|(Y, Z)$
- (G6) Weak union:  $X \perp (W, Y)|Z \Rightarrow X \perp W|(Y, Z)$
- (G7) Redundancy:  $X \perp Y|X$
- (G8) Intersection:  $(X \perp W|(Y, Z)) \wedge (X \perp Y|(W, Z)) \Rightarrow X \perp (W, Y)|Z$

The stochastic independence in precise probability is semi-graphoid satisfying symmetry, decomposition, weak union, and contraction. When the probability distributions are strictly positive, intersection is also satisfied. Then, it becomes graphoid.

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