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Continuous Stochastic Cellular Automata That Have a Stationary Distribution and No Detailed Balance

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Abstract

Marroquin and Ramirez (1990) have recently discovered a class of discrete stochastic cellular automata with Gibbsian invariant measure that have a non-reversible dynamic behavior. Practical applications include more powerful algorithms than the Metropolis algorithm to compute MRF models. In this paper we describe a large class of stochastic dynamical systems that has a Gibbs asymptotic distribution but does not satisfy reversibility. We characterize sufficient properties of a sub-class of stochastic differential equations in terms of the associated Fokker-Planck equation for the existence of an asymptotic probability distribution in the system of coordinates which is given. Practical implications include VLSI analog circuits to compute coupled MRF models.

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It is well known (see Stratonovitch, 1963, for instance) that one can associate, under some conditions, to a stochastic continuous automata (i.e., a stochastic differential equation) a so-called Fokker-Planck (F-P) equation in the probability distribution of the state variables. In this note, we wish to characterize conditions under which the F-P equation admits a stationary solution of the Gibbs type.

Let $\mathbf{x}$ a n-dimensional vector of state variables, and $W(\mathbf{x},t)$ the probability distribution of the state variables described by $\mathbf{x}$ at time t. The F-P equation is:

$$\frac{\partial}{\partial t}W(\mathbf{x},t) = \left(-\sum_{\alpha=1}^{n} \frac{\partial}{\partial x_\alpha} d_\alpha(\mathbf{x}) + \frac{1}{2} \sum_{\alpha,\beta=1}^{n} \frac{\partial^2}{\partial x_\alpha \partial x_\beta} K_{\alpha\beta}(\mathbf{x}) \right) W(\mathbf{x},t)$$

where $d_\alpha(\mathbf{x})$ is the *drift vector* and $K_{\alpha\beta}(\mathbf{x})$ is the *diffusion matrix* (see Stratonovitch, 1963, p. 76).

The stationary solution $w(\mathbf{x})$ of the F-P satisfies the equation:

$$\sum_{\alpha=1}^{n} \frac{\partial}{\partial x_\alpha} G_\alpha(\mathbf{x}) = 0 \ , \tag{1}$$

where we have defined the *probability current* $G_\alpha(\mathbf{x})$:

$$G_\alpha(\mathbf{x}) = d_\alpha(\mathbf{x})w(\mathbf{x}) - \frac{1}{2}\frac{\partial}{\partial x_\beta} K_{\alpha\beta}(\mathbf{x})w(\mathbf{x}) \ . \tag{2}$$

In order to find the stationary solution, we do *not* assume, as Stratonovitch and everybody else does, that $G_\alpha(\mathbf{x}) = 0$ and set $w(\mathbf{x}) = e^{-U(\mathbf{x})}$ in equation (1), obtaining:

$$\sum_{\alpha=1}^{n} \frac{\partial}{\partial x_\alpha} \left(d_\alpha(\mathbf{x}) e^{-U(\mathbf{x})} - \frac{1}{2}\frac{\partial}{\partial x_\beta} e^{-U(\mathbf{x})} K_{\alpha\beta}(\mathbf{x}) \right) =$$

$$= \sum_{\alpha=1}^{n} \frac{\partial}{\partial x_\alpha} e^{-U(\mathbf{x})} \left(d_\alpha(\mathbf{x}) + \frac{1}{2} K_{\alpha\beta}(\mathbf{x}) \frac{\partial}{\partial x_\beta} U(\mathbf{x}) - \frac{1}{2}\frac{\partial}{\partial x_\beta} K_{\alpha\beta}(\mathbf{x}) \right) = 0$$

Assuming that the diffusion matrix is constant, that is $K_{\alpha\beta}(\mathbf{x}) = K_{\alpha\beta}$, we obtain:

$$e^{-U(\mathbf{x})}\sum_{\alpha=1}^{n}\left[-\frac{\partial}{\partial x_\alpha}U(\mathbf{x})\left(d_\alpha(\mathbf{x})+\frac{1}{2}K_{\alpha\beta}\frac{\partial}{\partial x_\beta}U(\mathbf{x})\right)+\frac{\partial}{\partial x_\alpha}d_\alpha(\mathbf{x})+\frac{1}{2}K_{\alpha\beta}\frac{\partial^2}{\partial x_\beta\partial x_\alpha}U(\mathbf{x})\right]=0$$

Provided that the diffusion matrix K is invertible we can effectuate the coordinate transformation

$$x_\alpha \rightarrow \frac{1}{2}K_{\beta\alpha}x_\beta$$

and defining the vector $(\mathbf{d})_\alpha = d_\alpha(\mathbf{x})$ we rewrite the previous equation as

$$-\nabla U\cdot\mathbf{d}-\nabla U\cdot\nabla U+\nabla\cdot\mathbf{d}+\nabla^2 U=$$

$$=-\nabla U(\mathbf{d}+\nabla U)+\nabla(\mathbf{d}+\nabla U)=0\ .$$

We finally obtain

$$(\nabla-\nabla U)\cdot(\nabla U+\mathbf{d})=0, \tag{3}$$

which is the condition for stationary distribution.

Thus, one solution is:

$$\nabla U+\mathbf{d}=0\Leftarrow\mathbf{d}=-\nabla U, \tag{4}$$

which is equivalent to the so called *potential conditions*, that amount to say that $\mathbf{d}$ is the gradient of a potential. If the potential conditions are satisfied the probability current $G_\alpha(\mathbf{x})$ is identically zero, and thus *detailed balance* holds. Therefore we recover the well known result that detailed balance implies the existence of a stationary Gibbs distribution $w(\mathbf{x})=e^{-U(\mathbf{x})}$. However condition (3) shows that the converse is not true. In fact equation (3) has also the solution

$$(\nabla-\nabla U)\cdot\mathbf{f}=0, \tag{5}$$

with $\mathbf{f}=\nabla U+\mathbf{d}$ and this solution is *not trivial only if* $\mathbf{f}\neq 0$, that is if $\mathbf{d}$ is not the gradient of a function. Equation (3) has therefore a "larger" space of solutions than the one represented by the potential conditions. Of course in both cases the solution U must be such that $w(\mathbf{x}) = e^{-U(\mathbf{x})}$ is a probability distribution, and therefore the following additional condition must hold:

$$\int d\mathbf{x}\; e^{-U(\mathbf{x})} < \infty$$

A simple and interesting example that proves the existence of non-trivial solutions U such that $w(\mathbf{x}) = e^{-U(\mathbf{x})}$ is the following.

Example of existence

Consider the stochastic differential equation in $\mathcal{R}^2$

$$\begin{cases} \dot{x} = -2x + y + \xi_x(t) \\ \dot{y} = -x - 2y + \xi_y(t) \end{cases} \tag{6}$$

where $\xi_x(t)$ and $\xi_y(t)$ are Gaussian noise terms, that is

$$< \xi_x(t)\xi_x(t') > = < \xi_y(t)\xi_y(t') > = 2\delta(t - t') \ .$$

The F-P equation associated to (6) is

$$\frac{\partial}{\partial t} W(\mathbf{x}, t) = -\nabla \cdot (W(\mathbf{x}, t)\mathbf{d}(\mathbf{x})) + 2\nabla^2 W(\mathbf{x}, t)$$

where the drift vector is $\mathbf{d}(\mathbf{x}) = (-2x + y, -x - 2y)$. It is easy to verify that $\mathbf{d}(\mathbf{x})$ is not a conservative field, so that detailed balance does not hold. However a stationary solution of the F-P exists, with $w(\mathbf{x}) = e^{-U(\mathbf{x})}$ and

$$U(\mathbf{x}) = x^2 + y^2 \ .$$

In fact, defining $\mathbf{f} = \nabla U + \mathbf{d}$ we have

$$\mathbf{f} = (2x - (2x - y), 2y - (x + 2y)) = (y, -x)$$

and therefore equation (5) is satisfied, since

$$(\nabla - \nabla U) \cdot \mathbf{f} = \nabla \cdot \mathbf{f} - \nabla U \cdot \mathbf{f} = 2(x, y) \cdot (y, -x) = 0 \ .$$

Notice that in absence of noise the differential equation (6) is linear, with characteristic eigenvalues $\lambda = -2 \pm i$, and the associated trajectories are inward spirals. This makes perfectly plausible the fact that, in presence of noise, the probability distribution of the variables is a Gaussian centered in the origin.

Remarks:

- In the linear case, that is when $\mathbf{d}(\mathbf{x}) = A\mathbf{x}$ and A is a symmetric matrix, detailed balance always holds, because $\mathbf{d} = -\nabla U$ with $U(\mathbf{x}) = -\frac{1}{2}\mathbf{x}A\mathbf{x}$. However the stationary solution $w(\mathbf{x}) = e^{-U(\mathbf{x})}$ exists only if the matrix A is negative definite, that is if $w(\mathbf{x})$ is integrable.

- Stratonovitch (1963, p. 79) says that even when potential conditions are not met but $\mathbf{d}$ is a linear function of x and $K_{\alpha\beta}(x)$ are independent of x, the F-P equations can be solved. In fact it is easy to see that if $\mathbf{d}(\mathbf{x}) = A\mathbf{x}$ and A *is not* symmetric the potential conditions do not hold but the function $U(\mathbf{x}) = -\frac{1}{2}\mathbf{x}A\mathbf{x}$ is a solution of equation (5).

- *If* the forces d_α in the Langevin equation are conservative, i.e., $\mathbf{d} = -\nabla U$, *then, if* the fluctuations are thermic-like, detailed balance is satisfied and a Gibbs stationary distribution exists (Equation 4 is satisfied).

- It appears that our results may be derivable from the formulation of Graham (1980) and the more general case considered by Jauslin (1984) and Zeeman (1988). An in-depth analysis of many properties of the Fokker-Planck equation relevant for this note can be found in Tan and Wyatt (1985).

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