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Conditions for Gibbs-type solutions of stationary Fokker–Planck equations

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Abstract. Solutions depending on the noise scale ε in the same way as the Gibbs distribution are typical for systems with detailed balance (uniform in ε), but apply also more geneally. We give criteria for their existence as well as conditions for an elementary evaluation.

1. Introduction

To find an explicit solution of time-independent Fokker-Planck equations is a problem of considerable practical interest. Clearly, for systems at thermal equilibrium it is solved by the Gibbs distribution; more generally, detailed balance (Graham and Haken 1971, Graham 1973) provides a systematic solution method. Here we shall specify some quite different criteria, which do not rely upon physical notions or upon symmetry transformations, but can be checked from the Fokker-Planck equation in a straightforward way. We shall focus on distributions that involve the scale ε of the noise intensity in the same way as the temperature occurs in the Gibbs distribution:

$$p(\boldsymbol{x}, \varepsilon) = \exp[-\phi(\boldsymbol{x})/\varepsilon]. \tag{1.1}$$

This form applies when detailed balance holds uniformly in ε, but also in quite different cases. The necessary conditions for (1.1) are thus also necessary for uniform detailed balance (which may sometimes be 'hidden' by an inadequate choice of the system variables), and the sufficient (but not necessary) conditions ensure an elementary construction of ϕ and may hold with or without detailed balance.

For simplicity we shall first treat the cases with a state-independent diffusion; the subsequent extension will require an extra assumption as far as the necessary condition is concerned. A critical discussion will be given at the end of the paper.

2. Equations with constant diffusion

We consider the stationary Fokker-Planck equation

$$[-K^i(\boldsymbol{x})p(\boldsymbol{x}) + \varepsilon D^{ij}p_{,j}(\boldsymbol{x})]_{,i} = 0 \tag{2.1}$$

with the symmetric and non-negative diffusion matrix $\boldsymbol{D}$, supposed here to be constant. The symbol '$_{,i}$' denotes the derivative with respect to x^i, and summation over equal indices is always understood.

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2.1. Uniform detailed balance

In order to clarify both the common and the different features, we briefly outline the implications of uniform detailed balance. Here (and only here) we suppose that time reversal results in the decomposition of the drift $\boldsymbol{K}$ into an irreversible part $\boldsymbol{d}$ and a reversible one $\boldsymbol{r}$:

$$K^i = d^i + r^i. \tag{2.2}$$

Detailed balance implies

$$d^i p = \varepsilon D^{ij} p_{,j},$$

so that with a regular $\boldsymbol{D}$

$$\varepsilon(\ln p)_{,i} = (D^{-1})_{ij} d^j.$$

If the right-hand side is indeed a gradient, i.e. if

$$(D^{-1})_{ij} d^j_{,k} \qquad \text{is symmetric in } i, k \tag{2.3}$$

(the 'potential condition'), then (1.1) follows, with ϕ given by $D^{ij}\phi_{,j} = d^i$. The further condition is

$$(r^i p)_{,i} = 0 = r^i_{,i} - \varepsilon^{-1} r^i \phi_{,i}.$$

Here the uniformity in ε becomes important: it implies both

$$r^i \phi_{,i} = 0 \tag{2.4}$$

and

$$r^i_{,i} = 0. \tag{2.5}$$

2.2. Consequences of the Gibbs-type form (1.1)

We now disregard time reversal and simply insert (1.1) into (2.1). This yields

$$\varepsilon^{-1}[(K^i + D^{ij}\phi_{,j})\phi_{,i}] + \varepsilon^0[K^i_{,i} + D^{ij}\phi_{,ij}] = 0.$$

Uniformity in ε forces both brackets to zero. With the definition

$$r^i \triangleq K^i + D^{ij}\phi_{,j} \tag{2.6}$$

the properties (2.4), (2.5) are recovered; this also motivates the use of the same symbol $\boldsymbol{r}$. However, the situation differs from before inasmuch as ϕ must now be calculated from

$$(K^i + D^{ij}\phi_{,j})\phi_{,i} = 0, \tag{2.7}$$

before $\boldsymbol{r}$ is known. Solving (2.7) is not quite simple, and since we shall nowhere assume that ϕ is known globally from (2.7) alone, we only give a few comments (and refer to Ludwig 1975, Ryter and Jordan 1984): at a stationary point of $\boldsymbol{K}$ ($\boldsymbol{K} = \boldsymbol{0}$; denoted by $\hat{}$ in what follows) the gradient of ϕ vanishes, and the matrix $C_{ij} \triangleq \partial^2\phi/\partial x^i\,\partial x^j$ of its second derivatives is determined by

$$\hat{\boldsymbol{C}}\hat{\boldsymbol{B}} + \hat{\boldsymbol{B}}^{\mathrm{T}}\hat{\boldsymbol{C}} + 2\hat{\boldsymbol{C}}\boldsymbol{D}\hat{\boldsymbol{C}} = \boldsymbol{0}, \tag{2.8}$$

where $B^i_j(\boldsymbol{x}) \triangleq K^i_{,j}(\boldsymbol{x})$ and where $\boldsymbol{B}^{\mathrm{T}}$ denotes the transpose of $\boldsymbol{B}$. If $\hat{\boldsymbol{C}}^{-1}$ exists, it can be obtained from

$$\hat{\boldsymbol{B}}\hat{\boldsymbol{C}}^{-1}+\hat{\boldsymbol{C}}^{-1}\hat{\boldsymbol{B}}^{\mathrm{T}}+2\boldsymbol{D}=\boldsymbol{0} \tag{2.9}$$

by standard methods (Gantmacher 1970).

The characteristics of (2.7) emerge from the attractors of $\boldsymbol{K}$. They can be used for the construction of $\phi(\boldsymbol{x})$, when the starting values near the attractors are known, as for example by $\phi=\hat{\phi}+\hat{C}_{ij}\,\delta x^i\,\delta x^j/2$ near a point attractor. Similar expansions hold near attractive cycles or tori. Unfortunately, the resulting $\phi(\boldsymbol{x})$ need not be single-valued globally (Graham and Tel 1984).

We just mention that if ϕ were available from (2.7), one could easily check (2.5) to verify if (1.1) holds.

Instead of considering (2.7) further, we now use (2.4) to rewrite $\boldsymbol{r}$ as

$$r^i(\boldsymbol{x})=A^{ij}(\boldsymbol{x})\phi_{,j}(\boldsymbol{x}) \qquad \text{with } A^{ji}=-A^{ij} \tag{2.10}$$

and note that (2.5) implies that $\boldsymbol{A}$ only depends on ϕ:

$$r^i=A^{ij}(\phi)\phi_{,j}. \tag{2.11}$$

With (2.6) this leads to

$$K^i=[A^{ij}(\phi)-D^{ij}]\phi_{,j}. \tag{2.12}$$

The matrix $\boldsymbol{A}$ can be evaluated at a stationary point of $\boldsymbol{K}$: since grad $\phi=\boldsymbol{0}$ there, (2.12) leads to

$$\hat{\boldsymbol{B}}=(\hat{\boldsymbol{A}}-\boldsymbol{D})\hat{\boldsymbol{C}}, \tag{2.13}$$

so that by (2.8), (2.9), $\hat{\boldsymbol{A}}=\boldsymbol{A}(\hat{\phi})$ is known.

2.3. *A sufficient condition*

An interesting consequence can now be derived with the further assumption that

$$\boldsymbol{A}(\phi)=\text{constant}. \tag{2.14}$$

By (2.12) and (2.13) this results in

$$\text{grad}\ \phi=\hat{\boldsymbol{C}}\hat{\boldsymbol{B}}^{-1}\boldsymbol{K}(\boldsymbol{x}), \tag{2.15}$$

and the corresponding integrability condition states that

$$\hat{\boldsymbol{C}}\hat{\boldsymbol{B}}^{-1}\boldsymbol{B}(\boldsymbol{x}) \qquad \text{must be symmetric for all } \boldsymbol{x}. \tag{2.16}$$

Clearly, when (2.16) holds, $\phi(\boldsymbol{x})$ is obtained from (2.15) by integration along any paths.

An example without detailed balance, that satisfies (2.16), is the optical bistability model of Graham and Schenzle (1981) with $\gamma=\delta$.

2.4. *A necessary condition*

The more general question is whether an antisymmetric $A(\phi)$ (fulfilling (2.13)) can be found such that (2.12) becomes a total system. Here we give a necessary condition, which results from the further expansion around the stationary point and which is essentially based on the fact that

$$\hat{\boldsymbol{A}}_{,i}=\boldsymbol{A}'(\hat{\phi})\hat{\phi}_{,i}=\boldsymbol{0} \qquad \text{since } \hat{\phi}_{,i}=0. \tag{2.17}$$

Differentiating (2.12) with respect to x^k gives

$$B^i_k = (A')^{ij}\phi_{,j}\phi_{,k} + (A^{ij} - D^{ij})C_{jk},$$

and the next derivative with respect to x^n, evaluated now at the stationary point, results in

$$\hat{\boldsymbol{B}}_{,n} = (\hat{\boldsymbol{A}} - \boldsymbol{D})\hat{\boldsymbol{C}}_{,n}.$$

As $\boldsymbol{C}_{,n}$ must be symmetric for every n, this means, in view of (2.13), that

$$\hat{\boldsymbol{C}}\hat{\boldsymbol{B}}^{-1}\hat{\boldsymbol{B}}_{,n} \qquad \text{must be symmetric for every } n. \tag{2.18}$$

In N dimensions (i.e. with N $\boldsymbol{x}$-variables) this represents $N^2(N-1)/2$ conditions.

2.5. *A further condition for singular diffusion*

When $\boldsymbol{D}$ is singular, then its product with the matrix $\boldsymbol{T}$ of its algebraic complements vanishes, so that (2.12) leads to the somewhat simpler form

$$\boldsymbol{TK}(\boldsymbol{x}) = \boldsymbol{TA}(\phi)\,\mathrm{grad}\,\phi. \tag{2.19}$$

This relation is particularly useful in two dimensions, where

$$\boldsymbol{A}(\phi) = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} f(\phi). \tag{2.20}$$

In a rotated coordinate system (u, v) with the u axis pointing into the direction of the diffusion and the v axis perpendicular to it, (2.19) can be rewritten as

$$K^v = f(\phi)\phi_{,u} = \{F[\phi(u, v)]\}_{,u} \qquad (F' \triangleq f)$$

with the solution

$$F[\phi(u, v)] = \int^u K^v(u', v)\,\mathrm{d}u' + V(v), \tag{2.21}$$

and $\phi(u, v)$ is the inverse of F. The two functions F and V are specified, when (2.21) and (2.20) are inserted into (2.12). If this insertion fails, then clearly (1.1) does not hold. We note that for this consideration the existence of a stationary point of the drift is not required.

3. State-dependent diffusion

When the diffusion matrix $\boldsymbol{D}$ depends on $\boldsymbol{x}$, it is natural to include a noise-induced drift $\varepsilon\boldsymbol{a}(\boldsymbol{x})$ (see Ryter and Deker (1980) for a discussion of $\boldsymbol{a}$):

$$\{-[K^i(\boldsymbol{x}) + \varepsilon a^i(\boldsymbol{x})]p(\boldsymbol{x}) + \varepsilon[D^{ij}(\boldsymbol{x})p(\boldsymbol{x})]_{,j}\}_{,i} = 0. \tag{3.1}$$

3.1. *Consequences of the Gibbs-type form (1.1)*

Inserting (1.1) into (3.1) gives

$$\varepsilon^{-1}[(K^i + D^{ij}\phi_{,j})\phi_{,i}] - [K^i_{,i} - (a^i - D^{ij}_{,j})\phi_{,i} + D^{ij}_{,i}\phi_{,j} + D^{ij}\phi_{,ij}] - \varepsilon[a^i_{,i} - D^{ij}_{,ij}] = 0,$$

where the three square brackets have to vanish separately. The first one restates (2.7) and the third one shows that

$$a^i = D^{ij}_{,j} + b^i, \qquad \text{where } b^i_{,i} = 0. \tag{3.2}$$

With (2.6) the second one reduces thus to

$$r^i_{,i} = b^i \phi_{,i}. \tag{3.3}$$

Clearly, (2.10) remains valid, but (3.3) now only implies that

$$r^i_{,i} = A^{ij}_{,i}\phi_{,j} = b^j \phi_{,j},$$

such that

$$b^i = A^{ki}_{,k} + c^i \qquad \text{where } c^i\phi_{,i} = 0 \qquad \text{and} \qquad c^i_{,i} = 0. \tag{3.4}$$

In view of (3.2) a slightly simpler form results for (3.1):

$$\{-(K^i + \varepsilon b^i)p + \varepsilon D^{ij} p_{,j}\}_{,i} = 0 \tag{3.5}$$

where $b^i_{,i} = 0$. We note that the part $\boldsymbol{b}$ of the noise-induced drift does not originate from the $\boldsymbol{x}$ dependence of $\boldsymbol{D}$ and that it could already have been included in § 2. We further mention that when (3.4) is inserted for $\boldsymbol{b}$ in (3.5), then $\boldsymbol{c}$ does not contribute.

3.2. *The sufficient condition*

We may again consider the special case $\boldsymbol{A}$ = constant. By (3.4) this entails $\boldsymbol{b} = \boldsymbol{c}$, which, in the sense of the above remark, is equivalent to $\boldsymbol{b} = \boldsymbol{0}$. Furthermore, (2.12) (with $\boldsymbol{A} = \hat{\boldsymbol{A}}$) and (2.13) are still valid, so that

$$\text{grad } \phi = \{\hat{\boldsymbol{B}}\hat{\boldsymbol{C}}^{-1} - [\boldsymbol{D}(\boldsymbol{x}) - \hat{\boldsymbol{D}}]\}^{-1}\boldsymbol{K}(\boldsymbol{x}). \tag{3.6}$$

It is easy to check whether the right-hand side is actually a gradient. If so, $\phi(\boldsymbol{x})$ is readily evaluated, otherwise $\boldsymbol{A}$ is not constant or (1.1) fails.

3.3. *A further assumption*

Returning to the general case, we observe that the presence of $\boldsymbol{b}$ modifies the situation of § 2 considerably. To illustrate this, we point out that one could in principle solve (2.7) for ϕ, determine $\boldsymbol{A}$ from (2.6) and (2.11), and then check whether (3.4) holds; in other words, $\boldsymbol{b}$ alone may decide whether (1.1) applies.

In order to stay within the frame of § 2 we now assume

$$\boldsymbol{b} = \boldsymbol{0} \tag{3.7}$$

or, less restrictively, $\boldsymbol{b}^i\phi_{,i} = 0$, so that we have again

$$r^i_{,i} = 0 \qquad \text{and thus} \qquad \boldsymbol{A} = \boldsymbol{A}(\phi).$$

3.4. *The necessary condition*

The argument of § 2.4 takes now a slightly more complicated form. With the abbreviation $\boldsymbol{G} \triangleq (\boldsymbol{A} - \boldsymbol{D})^{-1}$, (2.12) becomes

$$\phi_{,i} = G_{ij}K^j,$$

whence

$$\phi_{,ik} = (G_{,k})_{ij}K^j + G_{ij}B^j_k.$$

At the stationary point this is equivalent to (2.13). At a small displacement $\boldsymbol{\delta x}$ the first-order variation is

$$\delta\phi_{,ik} = (\hat{G}_{,k})_{ij}\delta K^j + \delta G_{ij}\hat{B}^j_k + \hat{G}_{ij}\delta B^j_k$$

with $\hat{\boldsymbol{G}}_{,k} = \hat{\boldsymbol{G}}\hat{\boldsymbol{D}}_{,k}\hat{\boldsymbol{G}}$, $\boldsymbol{\delta G} = \hat{\boldsymbol{G}}\boldsymbol{\delta D}\hat{\boldsymbol{G}}$ in view of (2.17) and with $\hat{\boldsymbol{G}} = \hat{\boldsymbol{C}}\hat{\boldsymbol{B}}^{-1}$.

This must be symmetric in i, k. A more compact form follows for $\boldsymbol{\delta x} \hat{=} \delta x^n$: then

$$(\hat{C}\hat{B}^{-1})_{ij}[(\hat{D}_{,k}\hat{C})^j_n + (\hat{D}_{,n}\hat{C} + \hat{B}_{,n})^j_k] \qquad \text{must be symmetric in } i, k \text{ for every } n. \tag{3.8}$$

4. Summary and discussion

Based on the expansion around a stationary point of the drift, we established the necessary conditions (2.18) and (3.8) for a distribution of the Gibbs type (1.1) to exist; they hold if a noise-induced drift is only admitted in the minimum form which is imposed by a possible state-dependence of the diffusion.

A more restrictive assumption ($\boldsymbol{A}$ constant) made it possible to establish the explicit expressions (2.15) and (3.6) for the gradient of the exponent ϕ: the corresponding integrability condition takes the compact form (2.16) when the diffusion is constant.

Since ϕ is a proper scalar (which follows from (2.7) and from the fact that both $\boldsymbol{K}$ and $\boldsymbol{D}$ transform like contravariant tensors, see Ryter and Deker (1980)) and since p is a scalar density, it follows that (1.1) is invariant under any changes of the $\boldsymbol{x}$-variables with a constant Jacobian. It is not difficult to verify that this invariance holds throughout this paper, with the important exception of § 2.1: detailed balance is typically not preserved even under linear transformations. Thus, if (2.18) or (3.8) is not met, a time reversal symmetry cannot hold in any admissibly transformed variables.

We have to add two remarks about the extension to state-dependent diffusion. The first one concerns § 2.1, more precisely the splitting of the noise-induced drift $\boldsymbol{a}$ analogous to (2.2): from the general notion of detailed balance (Graham and Haken 1971, Graham 1973) it can easily be inferred that $D^{ij}_{,j}$ is irreversible, but for (1.1) to hold, it is also necessary that the remaining part, which is not induced by the $\boldsymbol{x}$ dependence of $\boldsymbol{D}$, be purely reversible. This latter requirement is of course fulfilled by (3.7), but it need not hold in general, see Ryter and Deker (1980). The second remark concerns § 2.5: while (2.19) also holds with an $\boldsymbol{x}$-dependent $\boldsymbol{T}$, the following calculation becomes more involved and is not reproduced here.

To close, we mention that the present theory immediately exhibits the well known facts that one-dimensional equations (see (3.6), which reduces by (2.9) to $\phi'(x) = -K(x)/D(x)$), as well as systems with a linear drift and constant diffusion (see (2.16) and (2.15)), are trivially integrable.

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Note added in proof. As will be shown in a forthcoming paper, the form (1.1) also has an impact on dynamical properties: a basic relation between the eigenfunctions of the forward operator and those of the backward operator becomes independent of ε.

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