TIME SAMPLING OF DIFFUSION SYSTEMS USING SEMIGROUP DECOMPOSITION METHODS

J. M. Lemos * **J. M. F. Moura** **

* *INESC-ID/IST, R. Alves Redol 9, 1000-029 Lisboa, Portugal,*
jlml@inesc.pt
** *Carnegie Mellon University, Pittsburgh PA 15213-3890, U. S. A.,*
moura@ece.cmu.edu

Abstract: The paper considers the time sampling of the *a priori* probability distribution function of the state of a diffusion process by semigroup decomposition methods. We approximate the semigroup generated by the evolution equation associated to the diffusion by Trotter's formula. We benchmark the approximation against an exact method, *viz.* the Wei-Norman decomposition). We illustrate both methods through the discretization of the Fokker-Planck equation associated with the PLL estimation error probability distribution function.

Keywords: Sampling, diffusions, Fokker-Planck equation, semigroups, Trotter's formula, Wei-Norman method, distributed parameter.

1. INTRODUCTION

Diffusion models (Jazwinski, 1970; Lipster and Shiryayev, 1984) find many important applications in diversified fields of science and technology. In Biology examples range from cell (*e.g.* ion currents) (Smith, 2002) to population models (population dispersal) (Britton, 2003). Industrial processes with large spatial dimensions provide also examples. In the class of transport/reaction-diffusion processes (Grindrod, 1996), one or more variables with a space dependency are described by a diffusion model or a degenerate diffusion model as in the case of distributed collector solar fields (Silva *et al.*, 2003). The classical problem of course is heat diffusion in a bar heated at a central point, whose temperature satisfies the well known heat equation. Diffusion models in dynamic congestion control protocols for communication networks allow to address traffic variability (Mukherjee *et al.*, 1991). Analysis of tracking properties of adaptive algorithms for time varying systems, both for signal processing (Benveniste, 1987) and control (Coito *et al.*, 1995) relies on diffusion models. As a final example, dif-

fusion models are a basic starting point for signal processing and communication problems. The phase lock loop (PLL) estimation error verifies a diffusion model (Viterbi, 1963) and will hereafter be taken as a case study.

The time evolution of the state of a diffusion process satisfies a stochastic ordinary differential equation, and its probability density function (p.d.f.) is the solution of the Fokker-Planck partial differential equation (Jazwinski, 1970). Computer based design and implementation of estimation and control algorithms require discrete time models that adequately represent the system dynamics. When a probability distribution (or other space functions such as temperature) is used as a "state," this becomes the problem of time sampling an infinite dimensional system.

The sampling problem consists of, given the state distribution at time t_k, compute (eventually approximate) the state distribution at the next sampling time t_{k+1}. Once the "discrete time model" relating both space functions is available, for the sake of illustration, it may be applied to a control problem by selecting the value of the manipulated value to apply to the plant such that the state distribution attains some prescribed value. This, together with a time varying sampling

interval, is the path followed in (Silva, 2003; Silva *et al.*, 2003a) to design predictive controllers for distributed collector solar systems. In relation to estimation problems, the Fokker-Planck equation corresponds to the prediction step in optimal nonlinear filtering problems where the message is continuous and the observations are discrete. As such, addressing the discretization of the Fokker-Planck equation sheds light on the relation between continuous and discrete optimal nonlinear filters.

To solve the sampling problem for infinite dimension systems, we resort here to semigroup decomposition methods. For the class of problems considered, a semigroup is (McBride, 1987) a family of bounded (continuous) linear operators, indexed by time, which describe the time response of dynamic systems evolving from an initial condition state.

Semigroups may be decomposed by expressing them in simpler semigroups that can be exactly computed. This paper considers two decomposition methods. The Wei-Norman method (Wei *et al.*, 1964; Ocone, 1980) is an exact method (which may not always be applied), relying on a change of time scale, given by the solution of the so called Wei-Norman equations. The second is an approximate method known as Trotter's formula (Trotter, 1959). Actually, Trotter's formula can be obtained as a first order Taylor's expansion of the solution of the Wei-Norman equations, whenever these represent the underlying semigroup.

The Wei-Norman method was originally developed for finite dimensional operators and applied to express the solution of ordinary differential equations as a product of exponentials (Wei, 1964). In Numerical Analysis, this set of ideas was the subject of recent interest within the context of geometric integration and discretization methods for differential equations on manifolds, based on the use of Lie group methods (Celledoni *et al.*, 2001). The method was extended to infinite dimensional operators and applied to the discretization of optimal non-linear filters (Ocone, 1980; Brockett, 1981; Cohen de Lara, 1997). Trotter's formula has been used in Quantum physics to solve Schröedinger's equation (Weinholtz, 1982) and is sometimes rediscovered to solve engineering problems in a somewhat empirical way without any reference to Trotter (Dresnack, 1968; Camacho *et al.*, 1988). In (Silva, 2003), a controller for a distributed collector solar field is designed on the basis of a discrete time model obtained by the application of Trotter's formula. In (Neidhart *et al.*, 1998) error bounds for Trottter's formula approximation are derived (see also the references therein).

The contribution of this paper consists in showing how semigroup decomposition methods may be applied for sampling the Fokker-Planck equation associated to diffusion processes and in relating the time propagation in this way and by sampling the original diffusion model.

The paper is organized as follows: After stating the paper's purpose and placing its contribution in perspective in this introduction, basic concepts on semigroups including the Wei-Norman method and Trotter's formula are reviewed in section 2. The application to diffusion systems is presented in section 3, where the Fokker-Planck equation is sampled using Trotter's formula. In the case of linear diffusions, the Fokker-Planck equation is solved by the Wei-Norman approach and this is explored in order to shed light on the type of approximation yielded by Trotter's formula. Furthermore, it is shown that Trotter's formula yields a probabilistic interpretation of the discretization of the Fokker-Planck equation. Conclusions are drawn in section 4.

2. SEMIGROUP CONCEPTS

This section presents basic concepts and results concerning semigroups that will be used subsequently.

Consider the Banach space X of continuous functions equipped with the supremum norm.

Definition 1 (McBride, 1987)

A semigroup of operators of class C_0 is a family of operators T_t defined in X and indexed by the parameter $t \in \mathbb{R}$ (time) such that:

(1) T_t is defined $\forall t \geq 0$;
(2) T_t satisfyies the *semigroup condition*: $\forall s,\, t \in \mathbb{R}$

$$T_{t+s} = T_t T_s \qquad (1)$$

(3) T_t satisfyies the continuity condition

$$\lim_{t \to \infty} T_t x = x \ \forall x \in \mathrm{X}$$

(4) T_t is bounded $\forall t \geq 0$:

$$\exists c \in \mathbb{R} : \forall x \in \mathrm{X} \ \|Tx\| \leq c\|x\|$$

Definition 2 (McBride, 1987)

The *infinitesimal generator* of the semigroup T_t is the operator defined by

$$A = \lim_{t \to 0} t^{-1}(T_t - I)$$

where I is the identity operator.

Remark 1

The set $B(\mathrm{X})$ of bounded linear operators in a Banach space X is itself a Banach space with respect to the norm induced by the norm defined in X:

$$\|T_t\| \triangleq \sup \left\{ \frac{\|T_t x\|}{\|x\|} \ : \ x \in \mathrm{X} \setminus \{0\} \right\}$$

Under this norm, definition 2 states that the semigroup T_t satisfies the following differential equation, known as an evolution equation:

$$\frac{d}{dt} T_t = A T_t = T_t A \qquad (2)$$

with the initial condition $T_0 = I$. The solution T_t of (2) is referred to as the integral operator corresponding

to A or, by abuse of notation, as the "exponential of A."

2.1 Trotter's formula

Consider the situation in which A is the sum of two operators A_1 and A_2. Let T_t^1 and T_t^2 be the corresponding operators (semigroups), *i. e.* assume that

$$\frac{d}{dt}T_t^i = A_i T_t^i \quad i = 1, 2 \qquad (3)$$

while T_t satisfies

$$\frac{d}{dt}T_t = (A_1 + A_2) T_t \qquad (4)$$

In general, it it is not true that T_t results from the composition of T_t^1 and T_t^2. However, this is approximately true for small t, meaning that T_t can be approximated by the iterated composition of T_Δ^1 and T_Δ^2 over small intervals of time Δ. This is stated in the following theorem:

Theorem 1 (Trotter, 1959)

Let T_t^1 and T_t^2 satisfy the *norm condition*:

$$\exists \omega \in \mathbb{R} : \forall t > 0 \ \|T_t^i\| \le e^{\omega_i t} \quad i = 1, 2$$

and that $D(A_1 + A_2) = D(A_1) \cap D(A_2)$ is dense in X, where $D(A)$ denotes the domain of A. Then, (the closure of) $A_1 + A_2$ generates a semigroup of class C_0 iff (the closure of) $R(\lambda I - A_1 - A_2)$ is dense in X for some $\lambda > \omega_1 + \omega_2$, where $R(A)$ denotes the range of A. If $A_1 + A_2$ (or its closure) generates a semigroup of class C_0, this is given by

$$T_t = \lim_{\Delta \to 0} \left(T_\Delta^1 T_\Delta^2\right)^{\lceil t/\Delta \rceil} \qquad (5)$$

where $\lceil t/\Delta \rceil$ represents the greatest integer that does not exceed t/Δ.

Expression (5) is commonly known as Trotter's formula. The approximation embodied by Trotter's formula may be extended to a finite sum of operators.

Remark 2

Trotter's formula is one of a family characterized by the equality of the first derivative at $t = 0$ of the semigroup generated with its approximation. Another approximation formula is the semi-sum formula (Weinholtz, 1981), given by

$$T_{n\Delta} \approx \left[\frac{1}{2}(T_{2\Delta}^1 + T_{2\Delta}^2)\right]^n \qquad (6)$$

2.2 The Wei-Norman method

Since, in (4), T_t is in general not given by the composition of T_t^1 and T_t^2, one can ask whether there is a change of time variable such that the composition results in an exact equality. This is the approach of the Wei-Norman method (Wei, 1964; Ocone, 1980). The Baker-Campbell-Hausdorf (BCH) formula plays

here a key role. Let $\mathcal{L}$ be the Lie Algebra generated by the linear operators $A_1, \ldots, A_m$. This is the vector space generated by all the operators, together with the operators generated, in all possible combinations, by the Lie product defined by

$$[A_i, A_j] \stackrel{\triangle}{=} A_i A_j - A_j A_i \quad \forall A_i, A_j \in \mathcal{L} \qquad (7)$$

Theorem 2 (Ocone, 1980; Lara, 1997)

Assume that $\mathcal{L}$ is of finite dimension and denote by $e^{A_i t}$ the integral operator corresponding to the infinitesimal generator A_i. The following equality, known as the BCH formula, holds for $A, B \in \mathcal{L}$:

$$e^A B e^{-A} = B + [A, B] + \frac{1}{2!}[A, [A, B]] +$$

$$+ \frac{1}{3!}[A, [A, [A, B]]] + \ldots \qquad (8)$$

Remark 3

Remark that for commuting operators, *i.e.* when $AB = BA$, the formula reduces to

$$e^A B e^{-A} = B \qquad (9)$$

In order to explain the Wei-Norman method, consider the evolution equation (4) in the situation in which A_1 and A_2 form a basis of the Lie algebra that they generate, with the commuting rule

$$[A_1, A_2] = \gamma A_2 \qquad (10)$$

where $\gamma \in \mathbb{R}$ is a known parameter.

An example is provided by the PDE

$$\frac{\partial}{\partial t}p(x, t) = -u(t)\frac{\partial}{\partial x}p(x, t) + R(t) \qquad (11)$$

which provides a simple model for a distributed collector solar field (Silva, 2003). Here $p(x, t)$ is the temperature of a moving fluid (oil) at position x and time t, u is the oil flow and R is a continuous function modelling incident sun radiation. Defining the infinitesimal generators

$$A_1 p(x, t) \stackrel{\triangle}{=} -u(t)\frac{\partial}{\partial x}p(x, t) \qquad (12)$$

$$A_2 p(x, t) \stackrel{\triangle}{=} R(t) \qquad (13)$$

equation (11) is associated to the evolution equation (4), where T_t is the integral operator transferring the temperature spatial distribution at time $t = 0$ to the temperature spatial distribution at time $t > 0$. An abuse of notation is made because the operators depend on t.

Assume that the exact solution of (4) can be written as

$$T_t = e^{A_1 g_1(t)} e^{A_2 g_2(t)} \qquad (14)$$

and look for conditions satisfied by the real valued functions g_1 and g_2. To find these, differentiate (14) and use (3) and the special case (9) of the BCH formula to get

$$\frac{d}{dt}T_t = \dot{g_1}e^{A_1 g_1}A_1 e^{A_2 g_2} + \dot{g_2}e^{A_2 g_2}A_2 =$$

$$= \left[\dot{g}_1 e^{A_1 g_1} A_1 e^{-A_1 g_1} + \right.$$
$$\left. + \dot{g}_2 e^{A_1 g_1} e^{A_2 g_2} A_2 e - A_2 g_2 e^{-A_1 g_1} \right] e^{A_1 g_1} e^{A_2 g_2} =$$
$$= \left[\dot{g}_1 A_1 + \dot{g}_2 e^{A_1 g_1} A_2 e^{-A_1 g_1} \right] T_t \qquad (15)$$

From (8) and (10), it follows that

$$e^{A_1 g_1} A_2 e^{-A_1 g_1} = e^{\gamma g_1(t)} A_2 \qquad (16)$$

and hence, combining (15, 16) and equating to (4))

$$A_1 + A_2 = \dot{g}_1 A_1 + \dot{g}_2(t) e^{\gamma g_1(t)} A_2 \qquad (17)$$

Since A_1 and A_2 form a basis, the corresponding co-efficients should be equal and the Wei-Norman equations for the case at hand follow:

$$\dot{g}_1(t) = 1 \qquad (18)$$

$$\dot{g}_2(t) = e^{\gamma g_1(t)} \qquad (19)$$

Since $T_0 = I$, the initial conditions must be

$$g_1(0) = 0 \qquad g_2(0) = 0 \qquad (20)$$

This ODE initial problem has the solution

$$g_1(t) = t \qquad (21)$$

$$g_2(t) = \frac{1}{\gamma} \left(e^{\gamma t} - 1 \right) \qquad (22)$$

Hence, the Wei-Norman decomposition of the semi-group that represents the exact solution of (4) is

$$T_t = e^{A_1 t} e^{A_2 \left(\frac{1}{\gamma} (e^{-\gamma t}) - 1 \right)} \qquad (23)$$

The integral operators corresponding to A_1 and A_2 are

$$\exp(tA_1) p(x, 0) = p(x - \int_0^t u(\sigma) d\sigma, 0) \qquad (24)$$

$$\exp(tA_2) p(x, 0) = p(x, 0) + \int_0^t R(\sigma) d\sigma \qquad (25)$$

Their composition according to (23) yields the solution of (11) as

$$p(x, t) = p(x - \int_0^t u(\sigma) d\sigma, 0) + \int_0^t R(\sigma) d\sigma \quad (26)$$

THis is the formula used in (Silva, 2003) as a basis for control design. Although (26) can be obtained using the standard Laplace's method, it is derived here as a simple application of the Wei-Norman method.

In general, the Wei-Norman equations always have a solution, although it may not be global. It should also be remarked (Brockett, 1981) that the functions g_i only depend on the constants γ that define the commuting rules of the infinitesimal operators A_i and not on the actual form of the operators. Thus, by solving the Wei-Norman equations, a whole family of linear evolution equations is solved.

2.3 *Error bounds*

Whenever the Lie algebra generated by the partial operators is finite, the Wei-Norman method can be used to establish error bounds on approximate semi-group decomposition methods such as Trotter's formula. Consider again the example of section 2.2, in which the Wei-Norman decomposition is given by (14), while Trotter's formula approximation, denoted T_t^T is given by

$$T_t^T = e^{A_1 t} e^{A_2 t} \qquad (27)$$

The norm of the error over a small interval Δ is given by

$$\|T_\Delta - T_\Delta^T\| = \|e^{A_1 g_1(\Delta)} e^{A_2 g_2(\Delta)} - e^{A_1 \Delta} e^{A_2 \Delta}\| \qquad (28)$$

where $\| \cdot \|$ denotes the operator norm defined in Remark 1. Expand $g_1(\Delta)$ and $g_2(\Delta)$ in Taylor series around $\Delta = 0$ and assume that (as for bounded operators) the following series expansions converge

$$e^{A_i \Delta} = I + A_i \Delta + \frac{1}{2!} A_i^2 \Delta^2 + \dots \qquad (29)$$

By expanding the error operator in (28), it is possible to obtain the following bound:

$$\|T_\Delta - T_\Delta^T\| \le \frac{1}{2} \| [A_1, A_2] \| \Delta^2 + O(\Delta^3) \qquad (30)$$

Remark 4

Trotter's formula equates terms up to first order and, if the operators commute, it is exact. This is a consequence of the fact that the first order expansion of the solution of the Wei-Norman equations is

$$g_i(\Delta) \approx \Delta \qquad (31)$$

Actually, Trotter's formula corresponds to the highest order Taylor's approximation of the solution of the Wei-Norman equations that does not imply the computation of the Lie brackets of the infinitesimal operators. For error bounds for unbounded operators see (Neidhardt, 1998).

3. THE FOKKER-PLANK EQUATION

The semigroup decomposition methods reviewed in the previous section are now applied to sample the PDE that propagates in time the p. d. f. of the state of a diffusion model.

3.1 *Diffusion models*

Consider the diffusion process with state x given by the solution of the stochastic differential equation

$$dx_t = f(x_t) dt + \sigma dw_t \qquad (32)$$

where σ is a constant parameter, the initial condition $x(0) = x_0$ is a random variable with p.d.f. p_{x_0} and w_t is a standard Wiener process. For $t > 0$ the probability density function $p(x, t)$ of the state x of the diffusion process satisfies the Fokker-Planck equation (Jazwinski, 1970), given by

$$\frac{\partial p}{\partial t} = -f_x(x) p - f(x) \frac{\partial p}{\partial x} + \frac{\sigma^2}{2} \frac{\partial^2 p}{\partial x^2} \qquad (33)$$

with the initial condition

$$p(x,\, 0) = p_{x_0}(x) \qquad (34)$$

and the boundary conditions

$$p(\pm\infty,\, t) = 0, \quad \forall t > 0 \qquad (35)$$

Two particular cases of interest to be considered hereafter are the linear case, in which

$$f(x) = ax \qquad (36)$$

and the PLL error dynamics (Viterbi, 1963), in which

$$f(x) = ax - K_{PLL}sin(x) \qquad (37)$$

Here, $a \leq 0$, and K_{PLL} are constant parameters.

3.2 *Applying Trotter's formula*

To apply Trotter's formula to the Fokker-Planck equation (33), define the infinitesimal generators L_1, L_2, and L_3 by

$$L_1 p(x,\, t) = -f_x(x) \cdot p(x,\, t) \qquad (38)$$

$$L_2 p(x,\, t) = -f(x)\frac{\partial}{\partial x} p(x,\, t) \qquad (39)$$

$$L_3 p(x,\, t) = \frac{1}{2}\sigma^2 \frac{\partial^2}{\partial x^2} p(x,\, t) \qquad (40)$$

The Fokker-Planck equation (33) is written

$$\frac{\partial}{\partial t} p(x,\, t) = (L_1 + L_2 + L_3)\, p(x,\, t) \qquad (41)$$

The following proposition summarizes a number of facts needed for applying Trotter's formula. The proof is readily done using standard techniques.

Proposition 1

A) The semigroups T_t^i generated by the infinitesimal generators L_i, $i = 1,\, 2,\, 3$, are given by

$$T_\Delta^1 p(x,\, t) = p(x,\, t) \cdot \exp\left(-f_x(x)\Delta\right) \qquad (42)$$

$$T_\Delta^2 p(x,\, t) = p(\alpha^{-1}(\alpha(x) + \Delta),\, t) \qquad (43)$$

with

$$\alpha(x) = -\int^x \frac{d\xi}{f(\xi)} \qquad (44)$$

α^{-1} denoting the inverse of α, and

$$T_\Delta^3 p(x,\, t) = p(x,\, t) * G(x,\, \Delta) \qquad (45)$$

where $*$ stands for convolution and G is a Gaussian kernel given by

$$G(x,\, \Delta) = \frac{1}{(2\pi\sigma^2\Delta)^{1/2}} \exp\left(-\frac{x^2}{2\sigma^2\Delta}\right) \qquad (46)$$

B) By using a Taylor series development, the following approximations are seen to hold for small Δ:

$$T_\Delta^1 p(x,\, t) \approx \frac{1}{1 + f_x(x)\Delta} p(x,\, t) \qquad (47)$$

and

$$T_\Delta^2 p(x,\, t) \approx p(x - f(x)\Delta,\, t) \qquad (48)$$

C) The operators T^i, $i = 1,\, 2,\, 3$ satisfy the conditions of Definition 1 as well as the norm condition of Theorem 1.
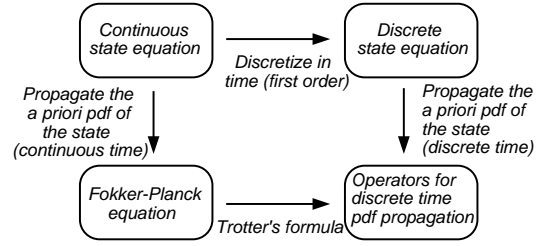

Fig. 1. Probabilistic interpretation of sampling the Fokker-Planck equation using Trotter's formula.

Remark 5

Instead of using the expressions (42-45) or the approximations (47, 48), the semigroups T^i, $i = 1,\, 2,\, 3$ may be approximated by applying finite differences to each of the equations

$$\frac{\partial p}{\partial t} = L_i p \qquad (49)$$

The semi-sum formula (6) reduces then to the explicit method for the discretization of the PDE and Trotter's formula to the scheme proposed heuristically in (Bella *et al.*, 1968).

Proposition 2

Given the operators defined in Proposition 1, Trotter's formula yields the following approximation of the semigroup generated by the Fokker-Planck equation (33):

$$p(x,\, t + \Delta) \approx T_\Delta^1 T_\Delta^2 T_\Delta^3 p(x,\, t) \qquad (50)$$

3.3 *Probabilistic interpretation*

The following proposition states a probabilistic interpretation of the application of Trotter's formula to the Fokker-Planck equation.

Sample the diffusion model (32) to obtain the stochastic difference equation:

$$x_{k+1} = x_k + f(x_k)\Delta + \sigma(w_{k+1} - w_k) \qquad (51)$$

where $x_k := x(k\Delta)$, $w_k := w(k\Delta)$ and $\Delta \in \mathbb{R}$ is the discretization step. As $\Delta \to 0$ the solution of (51) converges to the solution of (32) in mean square (Jazwinski, 1970).

Proposition 3

For Δ small the diagram of fig. 1 is valid, *i. e.*, the operators which propagate in discrete time the p.d.f. of the state of the discrete model are the same as the ones obtained by applying Trotter's formula to the Fokker-Planck equation.

Proof of proposition 3

Since the random variable

$$\zeta = \theta(x_k) = x_k + f(x_k)\Delta \qquad (52)$$

is independent of the increment $w_{k+1} - w_k$ of the Wiener process it follows that

$$p_{x(k+1)} = p_\zeta * \mathcal{N}(0, \sigma^2 \Delta) \qquad (53)$$

where $\mathcal{N}$ denotes a Gaussian kernel and p_z denotes the p. d. f. of the random variable z. Furthermore

$$p_\zeta(\zeta) = p_{x(k)} \cdot \frac{1}{\left| \frac{d\theta(x_k)}{dx_k} \right|} \bigg|_{x(k)=\theta^{-1}(\zeta)} \qquad (54)$$

From (52)

$$\frac{1}{\left| \frac{d\theta(x_k)}{dx_k} \right|} = \frac{1}{1 + f_x(x_k)\Delta} \qquad (55)$$

and the action of the operator T_Δ^1 is recovered (compare with (47)). Furthermore, again from (52)

$$x_k = \zeta - f(x_k)\Delta \qquad (56)$$

When Δ is small, $x_k \approx \zeta$ and

$$x_k \approx \zeta - f(\zeta)\Delta \qquad (57)$$

i.e. by (48) the change of variable in (54) is seen to be approximately the same as the one defined by the operator T_Δ^2.

In conclusion, computing the p.d.f. of x_{k+1} from the p.d.f. of x_k involves the operations defined by Trotter's formula approximated up to first order in Δ.

Remark 6

For (54) to be valid, the function $\theta(x_k)$ must be monotonous, *i.e.*, its total derivative must be either strictly positive or strictly negative in all its domain. This is true in the linear case (36). For the PLL error dynamics (37)

$$\frac{d\theta}{dx_k} = 1 + \Delta a - K_{PLL}\Delta \cos x_k \qquad (58)$$

Since $K_{PLL} > 0$ (Viterbi, 1963) and $a \leq 0$, the monotonicity conditions are then either

$$\frac{1}{K_{PLL} - a} > \Delta \qquad (59)$$

for positive derivative or, for negative derivative

$$\frac{1}{-K_{PLL} - a} > \Delta \quad \text{and} \quad K_{PLL} > -a \qquad (60)$$

or

$$\frac{1}{-K_{PLL} - a} < \Delta \quad \text{and} \quad K_{PLL} < -a \qquad (61)$$

3.4 *The linear case*

Although in the linear case the Fokker-Planck equation may be solved exactly by standard methods, it is interesting to apply the Wei-Norman method and compare the exact decomposition thereby obtained with the approximation resulting from Trotter's formula.

Assuming therefore that (36) holds, the infinitesimal operators L_i, $i = 1, 2, 3$ defined in (38-40) are a basis for a Lie Algebra with the commuting rules

$$[L_1, L_2] = 0 \qquad (62)$$

$$[L_1, L_3] = 0 \qquad (63)$$

$$[L_2, L_3] = 2aL3 \qquad (64)$$

Let T_t be the integral operator expressing the solution of the Fokker-Planck equation. According to the Wei-Normal method, assume a decomposition of the form

$$T_t = e^{L_1 g_1(t)} e^{L_2 g_2(t)} e^{L_3 g_3(t)} \qquad (65)$$

By following the procedure described in section 2.2, the functions $g_i(t)$, $i = 1, 2, 3$ are seen to satisfy the set of ODE's with zero initial conditions:

$$\frac{dg_1(t)}{dt} = 1 \qquad (66)$$

$$\frac{dg_2(t)}{dt} = 1 \qquad (67)$$

$$\frac{dg_3(t)}{dt} = e^{-2ag_2(t)} \qquad (68)$$

$$\qquad (69)$$

Therefore

$$T_t = \exp(L_1 t) \exp(L_2 t) \exp\left(L_3 \frac{1 - e^{-2at}}{2at}t\right) \qquad (70)$$

Observe now that the integral operator defined by

$$U_t = \exp(L_3 g_3(t)) \qquad (71)$$

is to be interpreted as the solution of the evolution equation

$$\frac{d}{dt}U_t = L_3 \dot{g}_3(t)U_t \qquad (72)$$

Therefore, the integral operator

$$\exp\left(L_3 \frac{1 - e^{-2at}}{2at}t\right)$$

is to be obtained by solving the PDE

$$\frac{\partial}{\partial t}p(x, t) = \frac{\sigma^2}{2} e^{-2at} \frac{\partial^2}{\partial x^2} p(x, t) \qquad (73)$$

with the initial condition

$$p(x, 0) = p_0(x) \quad -\infty < x < +\infty \qquad (74)$$

This problem can be solved by applying the Fourier transform in x to both sides of (73). The resulting integral operator is a convolution of the initial condition with the Gaussian kernel

$$Q(x, t) = \frac{\exp\left[-\frac{x^2}{\frac{\sigma^2}{a}(1-e^{-2at})}\right]}{\left[\pi \frac{\sigma^2}{a}\left(1 - e^{-2at}\right)\right]^{1/2}} \qquad (75)$$

Assume that the initial condition is $p(x, 0) = \delta(x)$ where δ is the Dirac impulse function. Eq. (70) expresses therefore the solution of the Fokker-Planck equation in the linear case by the following operations:

1.A convolution with the Gaussian kernel (75). Since the initial condition is an impulse, the Gaussian kernel is left unchanged.
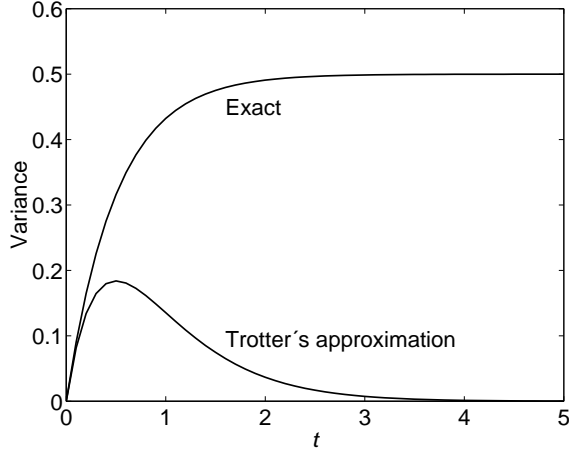
Fig. 2. Time evolution of the variance of the solution of the Fokker-Planck equation for the linear case.

Fig. 3. Time evolution of the solution of the Fokker-Planck equation for the PLL, as computed by Trotter's formula.

2.A replacement of x by xe^{-at} (corresponding to operator T^2).

3.Multiplication by e^{-at}.

The resulting solution is the Gaussian function

$$p(x,\,t) = \frac{1}{\sqrt{2\pi\sigma_x^2(t)}} \exp\left\{-\frac{x^2}{2\sigma_x^2(t)}\right\} \qquad (76)$$

with the variance

$$\sigma_x^2(t) = -\frac{\sigma^2}{2a}\left(1 - e^{2at}\right) \qquad (77)$$

Remark 7

The approximation yielded by Trotter's formula is obtained by replacing $g_3 = (1 - e^{-2at})/2a$ in (70) by its first order Taylor series development and hence must be only a local approximation. This may be evidenced by observing that the approximation given by Trotter's formula is a Gaussian as in (76) but with the variance replaced by

$$\sigma_T^2(t) = \sigma^2 t e^{2at} \qquad (78)$$

Fig. 2 compares the exact variance $\sigma_x^2(t)$ with $\sigma_T^2(t)$. As it is apparent they are close only for small values of t. Hence, Trotter's formula must be used iteratively, over a small time interval each time. The reason for this is apparent from (49). Trotter's formula implicitly assumes that the r.h.s. of the third equation in (66) is 1, neglecting the influence of operator T^2. In general, Trotter's formula neglects the interaction between the operators along the intervals during which it is applied.

3.5 *Numerical example – The PLL error dynamics*

In the cases in which the Lie algebra associated to the infinitesimal generators is not of finite dimension, the Wei-Norman decomposition cannot be computed and one has to resort to numerical methods. Trotter's formula is then a possibility, being particularly useful if a control application of the sampled model is planned.
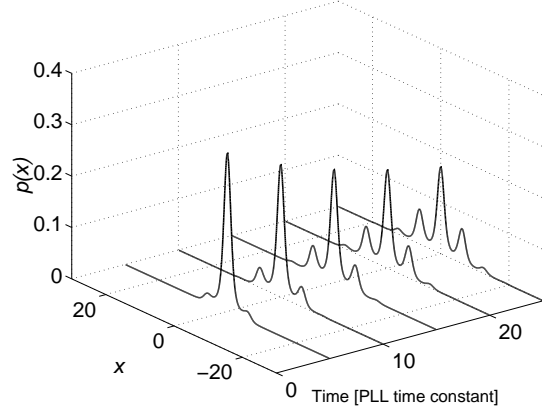
The numerical implementation of the sampling algorithm defined by (50) raises a number of issues concerned with space discretization. The first difficulty relies on the computation of $T_\Delta^2 p(x,\,t)$ since this requires $p(x - f(x)\Delta,\,t)$, whose value is usually not available in the computer memory (because it does not exactly correspond to one of the points of the spatial grid). Although a time varying sampling interval can be used such as to match the space and time grids (Silva, 2003), interpolation is needed if the time increment Δ is required to be constant. Linear or cubic interpolation may be used. Cubic interpolation provides a better approximation but has the drawback of not ensuring the positivity of the solution. Furthermore, the use of interpolation induces an undesirable effect referred in (Dresnack, 1968) as "pseudo-diffusion" and which amounts to not preserving space impulse functions, but instead spreading them over different grid points.

Another important issue are the stability conditions to be respected when approximating the different operators with a discrete grid. For T^3 (convolution with a Gaussian kernel) this amounts to

$$h^2 < C \cdot \Delta \qquad (79)$$

where C is a constant and h is the spatial step (length of the interval between two grid points). This means that, for a given spatial resolution, the time step cannot be lower than a certain interval.

Fig. 2 shows the time evolution of the solution of the Fokker-Planck equation for the PLL, as computed by Trotter's formula when $a = 0$ and $K_{PLL} = 1$. In this case, the error will diffuse along the real line, spreading over wider and wider intervals. In order to reduce the computational burden, the space grid is gradually increased by adding more and more intervals of length 2π.

4. CONCLUSIONS

The paper considers semigroup decomposition based methods for time sampling of diffusion models. When the associated Lie algebra is finite, it is possible to use the Wei-Norman method, which yields an exact decomposition. Otherwise, one can resort to Trotter's formula, which yields a first order approximation, that can be iterated over small time intervals. The relation between both methods is discussed. The methods considered are illustrated through application to the Fokker-Planck equation.

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