Cubature on C^1 space

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Abstract. We explore in this paper cubature formulas over the space of functions having a first continuous derivative, i.e., C^1. We show that the classical Lyons-Victoir formulas are not optimal in this case and explain what is the origin of the loss of optimality and how to construct optimal ones; to illustrate we give cubature formulas up to (including) order 4.

Mathematics Subject Classification (2010). Primary 60H35, 65D32, 91G60; Secondary: 65C30, 65C05.

Keywords. Cubature Formulae; Stochastic Analysis; Chen Series; cubature on infinite dimensional space; Cubature Wiener.

1. Introduction

We consider the following controlled ordinary differential equation (ODE)

$$dx(t) = f(t, x(t), u(t))dt, \quad x(0) = x_0. \tag{1.1}$$

where f is supposed as smooth as required with respect to all variables and $u(t)$ a C^1 control that acts on $x(t)$ with $u(0) = u'(0) = 0$. Let T be some final time (which will be set to 1 in all that follows) and denote by $C_0^1([0,T];\mathbb{R})$ the space of u. In order to explicitly mark the dependence of x on u we will also write $x_u(t)$ for the solution of (1.1).

We place ourselves in a situation where many $u(t)$ can be chosen and the average (or any aggregate quantity such as higher order moments, etc.) of some functional of $x(T)$ over all such $u(t)$ is to be computed. Typical frameworks where this is relevant is in inverse problems where one can chose several controls u, measure the output on the system depending on $x(T)$ and want to identify some parts of the function f by doing this (see [2, 6, 7] for examples).

We need to make precise what average means. Since our primary space for $u(t)$ is $C_0^1([0,T];\mathbb{R})$ a possible way to formalize this average is to consider a one dimensional brownian motion W_t (we write sometimes, as is usual, the

This work was funded by ANR project C-QUID, EMAQS.

time as index instead of $W(t)$ but this means the same thing) and write the following 3-dimensional SDE:

$$dx(t) = f(t, x(t), u(t))dt, \quad x(0) = x_0 \tag{1.2}$$
$$du(t) = w(t)dt, \quad u(0) = 0 \tag{1.3}$$
$$dw(t) = dW_t, \quad w(0) = W_0 = 0. \tag{1.4}$$

where the last equality means of course $w(t) = W_t$; the third equality is there only in order to give a formal 3D SDE.

We can now make precise the quantity of interest which is

$$\mathbb{E}F(x(T)) \tag{1.5}$$

where F is some (smooth enough) real function.

The justification of this formal writing is the following: the Brownian motion selects paths on the (Wiener) space of continuous functions null at the origin on $[0,T]$ denoted $C_0^0([0,T];\mathbb{R})$. Any $C_0^1([0,T];\mathbb{R})$ is the definite primitive of a function in the Wiener space. Thus as realizations of W span the Wiener space, $u(t)$ will span the required space.

Following works on infinite dimensional cubature formulas on Wiener space by [8, 4, 5] (see also [9, 11] for an application of cubature to finance and [1] to SPDE; many other works appeared in the literature on these subjects) we want to approximate the mean in (1.5) by a finite sum

$$\mathbb{E}F(x(T)) \simeq \sum_{k=1}^{n} \lambda_k F(x_{u_k}(T)). \tag{1.6}$$

where each u_k corresponds to a given realization ω_k of the Brownian motion W and the corresponding $u_k(t)$ is given as above

$$u_k(t) = \int_0^t \omega_k(s)ds. \tag{1.7}$$

Such an approximation is called a cubature formula. The question is what weights λ_k and paths ω_k are best for some given n and how good are the approximation properties of such a cubature formula.

A first thought is to use cubature formulas that work on the Wiener space $C_0^0([0,T];\mathbb{R})$ (cf. cited references for the details). As it will be seen in the following this is not necessary the most efficient choice because of the specific structure of the problem. The purpose of this work is to find optimal cubature formulas for the space $C_0^1([0,T];\mathbb{R})$ up to (including) fourth order.

The plan of the paper is the following: further motivating remarks are the object of Section 2 while a quick introduction to cubature formulas on Wiener space is presented in Section 3. Preliminary computations are given in Section 4 while the actual cubature formulas are given in Section 5.

2. Further remarks and motivation

Denote $Y = \begin{pmatrix} x \\ u \\ w \end{pmatrix}$ and note that our equation can be written as

$$dY = \begin{pmatrix} f \\ w \\ 0 \end{pmatrix} dt + \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \circ dW_t \tag{2.1}$$

where $\circ dW_t$ signals a Stratonovich formulation (which is the one well adapted to cubature framework because of the Wong-Zakai theorem [12]).

We realize that a different circumstance where the term $\mathbb{E}F(x(T))$ appears is in the forward Kolmogorov (or Fokker-Planck) PDE associated to the time evolution of the density of the SDE (2.1). If we denote by $\rho(t,x,u,w)$ the 3D density it satisfies the following degenerate 3-dimensional, time-dependent PDE:

$$\frac{\partial}{\partial_t}\rho(t,x,u,w) + \frac{\partial}{\partial_x}(f\rho) + \frac{\partial}{\partial_u}\rho - \frac{1\partial^2}{2\partial_w^2}\rho = 0, \tag{2.2}$$

$$\rho(0) = \delta_{x=x_0}. \tag{2.3}$$

Then since

$$\mathbb{E}F(x(T)) = \int_{\mathbb{R}^3_+} F(x)\rho(T,x,u,w)dxdudw \tag{2.4}$$

the method presented here also applies to the evaluation of the right hand side of the equation above. An equivalent formulation involving a degenerate backward (in time) PDE can also be invoked:

$$\mathbb{E}F(x(T)) = \mathcal{F}(0,x_0,0,0) \tag{2.5}$$

where

$$\frac{\partial}{\partial_t}\mathcal{F}(t,x,u,w) + f(t,x,u)\frac{\partial}{\partial_x}\mathcal{F} + \frac{\partial}{\partial_u}\mathcal{F} + \frac{1\partial^2}{2\partial_w^2}\mathcal{F} = 0 \tag{2.6}$$

$$\mathcal{F}(T,x,u,w) = F(x). \tag{2.7}$$

Thus the method presented here can be used to solve degenerate PDEs of type (2.6).

3. Background on cubature formulas

We follow [8, 4] and introduce below the principle of computing cubature formulas on the Wiener space. Suppose we want to compute $\mathbb{E}g(Z(T))$ with g a regular function where $Z(t) = (Z_0(t), ..., Z_d(t))^T \in \mathbb{R}^{d+1}$ solves the SDE

$$dZ = \sum_{\ell=0}^{d+1} \zeta_\ell(Z(t))dB_\ell(t), \tag{3.1}$$

where $B_1(t)$,...$B_d(t)$ are components of a d-dimensional Brownian motion and we denote $B_0(t) = t$ and set $\zeta_0(\cdot) = 1$ (which ensures $Z_0(t) = t$).

If a path $\omega(t) = (\omega_0(t), ..., \omega_d(t)) \in \mathbb{R}^{d+1}$ with $\omega_0(t) = t$ is given and has some regularity one can define $\xi_\omega(t)$ as the solution of the following ODE

$$d\xi_\omega(t) = \sum_{\ell=0}^{d+1} \zeta_\ell(\xi_\omega(t)) d\omega_\ell(t). \tag{3.2}$$

Use now stochastic Taylor formulas [10, 3] to write

$$\mathbb{E}g(Z(T)) = g(Z(0)) + \sum_j a_j(g, \zeta_0, ..., \zeta_d)\mathbb{E}(P_j) + R \tag{3.3}$$

where R is a remainder of order higher than a predefined order N, $a_j(g, \zeta_0, ..., \zeta_d)$ is a real (known) functional depending on $g, \zeta_0, ..., \zeta_d$ and P_j are stochastic polynomials, i.e. integrals of the type

$$\int_0^T \int_0^{s_1} \int_0^{s_2} ... \int_0^{s_{m-1}} \circ dB_{\alpha_m}(t) ... \circ dB_{\alpha_1}(t) \tag{3.4}$$

with $\alpha_p \in \{0, 1, ..., d\}$ for each p. The order of a stochastic polynomial is computed adding 1/2 for each integral involving $\alpha_j > 0$ and 1 for each $\alpha_j = 0$.

If the function g is smooth enough and the remainder R does not contain terms of order $\leq N$ a cubature formula of order N

$$\mathbb{E}g(X(T)) \simeq \sum_{k=1}^{n} \lambda_k \xi_{\omega^k}(T) \tag{3.5}$$

is obtained by requiring that cubature paths ω^k and weights λ_k satisfy for each polynomial P_j as in (3.4):

$$\sum_{k=1}^{n} \lambda_k \left(\int_0^T \int_0^{s_1} \int_0^{s_2} ... \int_0^{s_{m-1}} d\omega^k_{\alpha_m}(t) ... d\omega^k_{\alpha_1}(t) \right) \tag{3.6}$$

$$= \mathbb{E}\left(\int_0^T \int_0^{s_1} \int_0^{s_2} ... \int_0^{s_{m-1}} \circ dB_{\alpha_m}(t) ... \circ dB_{\alpha_1}(t) \right). \tag{3.7}$$

4. Stochastic Taylor expansion for averages of deterministic functionals over the class $C^1_0([0,T];\mathbb{R})$

We will use the following convention: for any function $G(\cdot)$ we denote by $\partial_k G$ the partial derivative of function G with respect to its k-th argument. We write the stochatic Taylor formula [10] and iterate:

$$\mathbb{E}F(x(T)) = \mathbb{E}F(x(0)) + \mathbb{E}\int_0^T \partial_1 F(x(s_1)) f(s_1, x(s_1), u(s_1)) ds_1 \tag{4.1}$$

$$= F(x(0)) + \mathbb{E}\int_0^T \partial_1 F(x(s_1)) f(s_1, x(s_1), u(s_1)) ds_1. \tag{4.2}$$

To simplify the notations from now on we will only write in formula above $(\partial_1 Ff)(s_1)$ instead of $\partial_1 F(x(s_1))f(s_1, x(s_1), u(s_1))$. We obtain by iterating :

$$\tag{4.3}$$

$$\mathbb{E}F(x(T)) = F(x(0)) + (\partial_1 Ff)(0) \cdot \mathbb{E}\left(\int_0^T ds_1\right) \tag{4.4}$$

$$+\mathbb{E}\int_0^T \int_0^{s_1} (\partial_1 F(\partial_1 f + \partial_2 ff + \partial_3 fW))(s_2) ds_2 ds_1 \tag{4.5}$$

The first conclusion that can be drawn from this initial computation is that the only first order term in T is $\mathbb{E}\left(\int_0^T ds_1\right)$; thus a first order cubature formula (in the sense of [8] for instance) has only to satisfy the requirement:

$$\sum_{k=1}^{n} \lambda_k \int_0^T ds_1 = \mathbb{E}\left(\int_0^T ds_1\right) = 1, \tag{4.6}$$

i.e.

$$\sum_{k=1}^{n} \lambda_k = 1. \tag{4.7}$$

The important remark here is that many terms are missing among which (we only write terms up to order 3/2 because the others are more cumbersome to write):

$$\mathbb{E}\left(\int_0^T dW_{s_1}\right), \tag{4.8}$$

$$\mathbb{E}\left(\int_0^T \int_0^{s_1} \circ dW_{s_2} \circ dW_{s_1}\right), \tag{4.9}$$

$$\mathbb{E}\left(\int_0^T \int_0^{s_1} ds_2 \circ dW_{s_1}\right), \tag{4.10}$$

$$\mathbb{E}\left(\int_0^T \int_0^{s_1} \circ dW_{s_2} ds_1\right), \tag{4.11}$$

$$\mathbb{E}\left(\int_0^T \int_0^{s_1} \int_0^{s_2} \circ dW_{s_3} \circ dW_{s_2} \circ dW_{s_1}\right), \tag{4.12}$$

terms of order 4 involving Stratonovich integrals (4.13)

... (4.14)

It follows that classical cubature formulas derived for fully general equations on Wiener space lose optimality here. The purpose of this work is to explain what are the constraints that optimal cubature formulas satisfy and give examples of optimal weights and paths up to (including) fourth order.

Continuing in the same way the enumeration of orders as they appear iterating the integral form of the stochastic Taylor formula we obtain that the following integrals appear

1. order 1: term $\mathbb{E}\left(\int_0^T ds_1\right)$. The constraint is, as seen above,

$$\sum_{k=1}^{n} \lambda_k = 1. \tag{4.15}$$

2. (unique) term of order 2: $\mathbb{E}\left(\int_0^T \int_0^{s_1} ds_2 ds_1\right)$. There is no new requirement brought by this term.
3. (unique) term of order 5/2: $\mathbb{E}\left(\int_0^T \int_0^{s_1} \int_0^{s_2} \circ dW_{s_3} ds_2 ds_1\right)$. The requirement is

$$\sum_{k=1}^{n} \lambda_k \left(\int_0^T \int_0^{s_1} \int_0^{s_2} d\omega_k(s_3) ds_2 ds_1 \right) = \mathbb{E}\left(\int_0^T \int_0^{s_1} \int_0^{s_2} \circ dW_{s_3} ds_2 ds_1 \right) = 0. \tag{4.16}$$

   We recall that the integral $\int_0^{s_2} d\omega_k(s_3)$ is a Riemann-Stiltjes integral.
4. (unique) term of order 3: $\mathbb{E}\left(\int_0^T \int_0^{s_1} \int_0^{s_2} ds_3 ds_2 ds_1\right)$. There is no new requirement brought by this term.
5. only two terms of order 7/2:

$$\mathbb{E}\left(\int_0^T \int_0^{s_1} \int_0^{s_2} \int_0^{s_3} \circ dW_{s_4} ds_3 ds_2 ds_1 \right) = 0 \tag{4.17}$$

$$\mathbb{E}\left(\int_0^T \int_0^{s_1} \int_0^{s_2} \int_0^{s_3} ds_4 \circ dW_{s_3} ds_2 ds_1 \right) = 0. \tag{4.18}$$

6. order 4 and higher: all the terms beginning by the terms of order 3.5 and higher.

5. Cubature formulas

5.1. Cubature formulas or order 3

As seen above cubature formulas up to order 2 (included) are somehow trivial. We thus start our list of cubature formulas from order 5/2. Note that a formula of order 5/2 is automatically of order 3 too since terms of order 3 do not bring any new requirement (other that the one implied already by the term at order 1).

There are two equations: (4.15) and (4.16). We will thus need at least two paths and thus two weights (except if one wants to use the null function, but we will not consider this here). A natural choice is to use some path ω_1 and $\omega_2 = -\omega_1$ and $\lambda_1 = \lambda_2 = 1/2$. Then the constraints are both satisfied. We obtain for instance a second order formula:

$$\lambda_1 = \lambda_2 = 1/2, \ \omega_1(t) = t, \omega_2(t) = -t. \tag{5.1}$$

5.2. Cubature formulas or order $7/2$

There are two new constraints of order 7/2. But there constraints are again satisfied if one uses $n = 2$ $\lambda_1 = \lambda_2 = 1/2$ and $\omega_2 = -\omega_1$. Thus e.g. formula (5.1) is also of order 7/2.

5.3. Cubature formulas or order 4

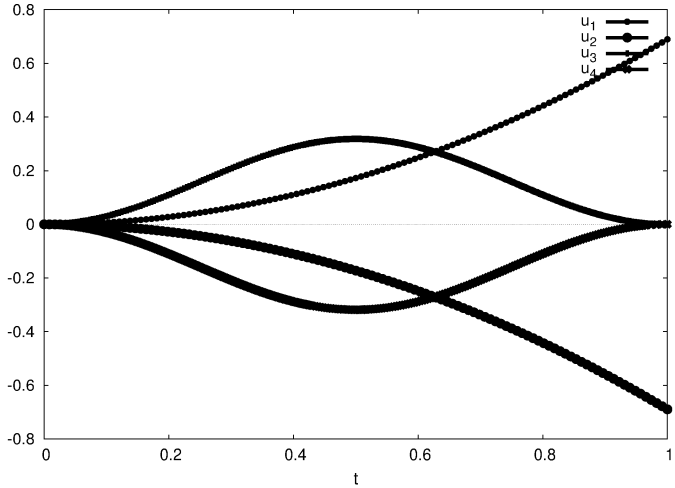

FIGURE 1. The four functions u_k for a 4-order quadrature formula.

Two new terms appear that bring new constraints:

$$\mathbb{E}\left(\int_0^T \int_0^{s_1} \int_0^{s_2} \int_0^{s_3} \int_0^{s_4} \circ dW_{s_5} \circ dW_{s_4} ds_3 ds_2 ds_1\right) = \frac{1}{48} \quad (5.2)$$

$$\mathbb{E}\left(\int_0^T \int_0^{s_1} \int_0^{s_2} \int_0^{s_3} \int_0^{s_4} \circ dW_{s_5} ds_4 \circ dW_{s_3} ds_2 ds_1\right) = 0. \quad (5.3)$$

We do not enter here into the specifics of the calculation above(see cited references for some hints). In terms of the cubature paths and weights the two new constraints read:

$$\sum_{k=1}^n \lambda_k \left(\int_0^T \int_0^{s_1} \int_0^{s_2} \int_0^{s_3} \int_0^{s_4} d\omega_k(s_5) d\omega_k(s_4) ds_3 ds_2 ds_1\right) = \frac{1}{48} (5.4)$$

$$\sum_{k=1}^n \lambda_k \left(\int_0^T \int_0^{s_1} \int_0^{s_2} \int_0^{s_3} \int_0^{s_4} d\omega_k(s_5) ds_4 d\omega_k(s_3) ds_2 ds_1\right) = 0.(5.5)$$

Note that the choice $n = 2$, $\lambda_1 = \lambda_2 = 1/2$ and $\omega_2 = -\omega_1$ will certainly **not** satisfy these constraints. We chose to add two more functions and look for a $n = 4$ fourth order cubature formula. In order to build on conclusions from lower order we further choose to set

$$\lambda_2 = \lambda_1,\ \lambda_3 = \lambda_4, \omega_2 = -\omega_1,\ \omega_3 = -\omega_4. \tag{5.6}$$

Denoting

$$\alpha_k = \int_0^T \int_0^{s_1} \int_0^{s_2} \int_0^{s_3} \int_0^{s_4} d\omega_k(s_5) d\omega_k(s_4) ds_3 ds_2 ds_1 \tag{5.7}$$

$$= \int_0^T \int_0^{s_1} \int_0^{s_2} \int_0^{s_3} \omega_k(s_4) d\omega_k(s_4) ds_3 ds_2 ds_1 \tag{5.8}$$

$$= \int_0^T \int_0^{s_1} \int_0^{s_2} \frac{\omega_k^2(s_3)}{2} ds_3 ds_2 ds_1 \tag{5.9}$$

and

$$\beta_k = \int_0^T \int_0^{s_1} \int_0^{s_2} \int_0^{s_3} \int_0^{s_4} d\omega_k(s_5) ds_4 d\omega_k(s_3) ds_2 ds_1 \tag{5.10}$$

$$= \int_0^T \int_0^{s_1} \int_0^{s_2} \int_0^{s_3} \omega_k(s_4) ds_4 d\omega_k(s_3) ds_2 ds_1 \tag{5.11}$$

we obtain that the following requirements are to be satisfied:

$$\lambda_1 \alpha_1 + \left(\frac{1}{2} - \lambda_1\right) \alpha_3 = \frac{1}{96} \tag{5.12}$$

$$\lambda_1 \beta_1 + \left(\frac{1}{2} - \lambda_1\right) \beta_3 = 0. \tag{5.13}$$

Let us introduce the parameter $\theta \in \mathbb{R}$ and choose $\omega_1 = \theta t = -\omega_2$; we compute and obtain $\alpha_1 = \frac{\theta^2}{5!} = \beta_1$. It suffices now to choose a family of functions where to look for ω_3 and its opposite ω_4. Instead of piecewise linear functions as in [8] we propose here oscillatory functions $\omega_3(t) = \sin(\frac{2\pi t}{T}) = -\omega_4$. The unknowns are now θ and λ_1. Note that ω_3 is such $\int_0^1 \omega_3(t) dt = 0$.

For this choice of ω_3 we obtain (for $T = 1$)

$$\alpha_3 = \frac{8\,\pi^2 - 3}{192\,\pi^2},\ \beta_3 = -\frac{8\,\pi^2 - 21}{96\,\pi^2}. \tag{5.14}$$

Replacing and solving for θ and λ_1 one obtains:

$$\lambda_1 = \frac{5(2\pi^2 - 21)}{6(2\pi^2 - 15)} \simeq 0.39712223492734, \tag{5.15}$$

$$\theta = \frac{\sqrt{8\,\pi^2 - 21}}{\sqrt{4\,\pi^2 - 9}} \simeq 1.378974145172718. \tag{5.16}$$

Note that the natural constraints $\theta^2 > 0$ and $\lambda_1 \in [0, 1/2]$ are satisfied. This is not necessarily the case for other (arbitrary chosen) pairs of functions.

We obtain thus the following integration formula for C_0^1 functions (see also Figure 1):

$$\lambda_2 = \lambda_1 = \frac{5(2\pi^2 - 21)}{6(2\pi^2 - 15)},\ \lambda_3 = \lambda_4 = \frac{1}{2} - \lambda_1, \theta = \frac{\sqrt{8\,\pi^2 - 21}}{\sqrt{4\,\pi^2 - 9}}, \tag{5.17}$$

$$u_1(t) = \theta\frac{t^2}{2} = -u_2(t),\ u_3(t) = \frac{1 - \cos(2\pi t)}{2\pi} = -u_4(t). \tag{5.18}$$

Remark 5.1. Of course, the methodology presented here can be extended easily to the situation of a multi-dimensional control $u(t)$ of $x(t)$.

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