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Taylor Moment Expansion for Continuous-Discrete Gaussian Filtering

Zheng Zhao, Toni Karvonen, Roland Hostettler, *Member, IEEE*, and Simo Särkkä, *Senior Member, IEEE*

Abstract—The note is concerned with Gaussian filtering in non-linear continuous-discrete state-space models. We propose a novel Taylor moment expansion (TME) Gaussian filter which approximates the moments of the stochastic differential equation with a temporal Taylor expansion. Differently from classical linearisation or Itô–Taylor approaches, the Taylor expansion is formed for the moment functions directly and in time variable, not by using a Taylor expansion on the non-linear functions in the model. We analyse the theoretical properties, including the positive definiteness of the covariance estimate and stability of the TME filter. By numerical experiments, we demonstrate that the proposed TME Gaussian filter significantly outperforms the state-of-the-art methods in terms of estimation accuracy and numerical stability.

Index Terms—continuous-discrete state-space model, Gaussian filtering, Kalman filtering, stochastic differential equation, Taylor moment expansion

I. INTRODUCTION

In this note, we study Gaussian filtering of a continuous-discrete state-space model

$$d\mathbf{x}_t = \mathbf{f}(\mathbf{x}_t, t) dt + \mathbf{L}(\mathbf{x}_t, t) d\mathbf{W}_t, \quad (1a)$$

$$\mathbf{y}_k = \mathbf{h}(\mathbf{x}_k) + \mathbf{v}_k, \quad (1b)$$

where $\mathbf{x}_t \in \mathbb{R}^D$ is a D -dimensional Itô process, $\mathbf{y}_k \in \mathbb{R}^S$ is the measurement at time t_k , and \mathbf{W}_t denotes an S -dimensional Wiener process with diffusion matrix \mathbf{Q} . We also assume the non-linear drift and dispersion functions $\mathbf{f}(\mathbf{x}_t, t)$ and $\mathbf{L}(\mathbf{x}_t, t)$ are sufficiently regular so that (1a) has a weakly unique solution [1], [2]. As we are mostly concerned with the continuous-time part (1a), for simplicity, we model the measurement \mathbf{y}_k in (1b) with a non-linear function $\mathbf{h}(\mathbf{x}_k)$ and an additive noise $\mathbf{v}_k \sim \mathcal{N}(\mathbf{0}, \mathbf{V}_k)$, where \mathcal{N} denotes a Gaussian distribution. Furthermore, we denote $\mathbf{\Gamma}(\mathbf{x}_t, t) = \mathbf{L}(\mathbf{x}_t, t) \mathbf{Q} \mathbf{L}^\top(\mathbf{x}_t, t)$, and Γ_{ij} denotes the i -th row and j -th column entry of $\mathbf{\Gamma}(\mathbf{x}_t, t)$. When $D = 1$ and $S = 1$, we use scalar notations x_t , $f(x_t, t)$ and $\Gamma(x_t, t)$.

The aim is to form Gaussian approximations to the filtering density for any t_k , $k = 1, \dots, T$ as follows:

$$p(\mathbf{x}_k | \mathbf{y}_{1:k}) \approx \mathcal{N}(\mathbf{x}_k | \mathbf{m}_k, \mathbf{P}_k). \quad (2)$$

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Zheng Zhao, Toni Karvonen, and Simo Särkkä were with Department of Electrical Engineering and Automation, Aalto University, Finland.

Toni Karvonen was also with Alan Turing Institute, United Kingdom.

Roland Hostettler was with Department of Engineering Sciences, Uppsala University.

Above, we have used the notation $\mathbf{x}_k \triangleq \mathbf{x}_{t_k}$ at time t_k , and $\mathbf{y}_{1:k} = \{\mathbf{y}_1, \mathbf{y}_2, \dots, \mathbf{y}_k\}$. Additionally, $\mathbf{m}_k, \mathbf{P}_k$ are the mean and covariance of (2), respectively.

In order to obtain the exact posteriors on the left hand side of (2), it would be necessary to compute the transition densities $p(\mathbf{x}_k | \mathbf{x}_{k-1})$ for the continuous model (1a) (see, e.g., [3], [4]). It turns out that the transition density is only analytically tractable in limited cases, such as for linear stochastic differential equations (SDEs). In the Gaussian filtering framework, we are interested in constructing a Gaussian approximation to the transition density:

$$p(\mathbf{x}_k | \mathbf{x}_{k-1}) \approx \mathcal{N}(\mathbf{x}_k | \mathbb{E}[\mathbf{x}_k | \mathbf{x}_{k-1}], \text{Cov}[\mathbf{x}_k | \mathbf{x}_{k-1}]), \quad (3)$$

which is also the approach that we employ here. Above, $\mathbb{E}[\mathbf{x}_k | \mathbf{x}_{k-1}]$ and $\text{Cov}[\mathbf{x}_k | \mathbf{x}_{k-1}]$ denote the conditional expectation and covariance of \mathbf{x}_k given \mathbf{x}_{k-1} , respectively.

One classical way to approximate the transition density (3) is the Itô–Taylor expansion [5]–[7] which can be used to form a discretised solution to the SDE by expanding Itô integrals iteratively using Itô’s lemma. The Euler–Maruyama scheme is the simplest instance of this kind of methods, and the mean and covariance in (3) are computed as

$$\begin{aligned} \mathbb{E}[\mathbf{x}_k | \mathbf{x}_{k-1}] &\approx \mathbf{x}_{k-1} + \mathbf{f}(\mathbf{x}_{k-1}, t_{k-1}) \Delta t, \\ \text{Cov}[\mathbf{x}_k | \mathbf{x}_{k-1}] &\approx \mathbf{\Gamma}(\mathbf{x}_{k-1}, t_{k-1}) \Delta t. \end{aligned} \quad (4)$$

However, the Euler–Maruyama scheme only works well when the time interval Δt is small enough. Other commonly used choices are, for example, Milstein’s method and the strong order 1.5 Itô–Taylor (Itô-1.5) method [4], [5]. However, because of the difficulty of the involved iterated Itô integrals, it is not easy to construct higher order Itô–Taylor expansions [5] and hence this approach is inherently low order in Δt . This motivates us to develop higher order weak approximations by using the proposed Taylor moment expansion.

Another widely used approach is to approximate ODEs for the first two moments of the Itô process [8]–[10]. The mean and covariance of the Itô process (1a) for any $t \in (t_{k-1}, t_k]$ are characterised by

$$\begin{aligned} \frac{d\mathbf{m}_t}{dt} &= \mathbb{E}[\mathbf{f}(\mathbf{x}_t, t)], \\ \frac{d\mathbf{P}_t}{dt} &= \mathbb{E}[\mathbf{f}(\mathbf{x}_t, t) (\mathbf{x}_t - \mathbf{m}_t)^\top] \\ &\quad + \mathbb{E}[(\mathbf{x}_t - \mathbf{m}_t) \mathbf{f}^\top(\mathbf{x}_t, t)] + \mathbb{E}[\mathbf{\Gamma}(\mathbf{x}_t, t)], \end{aligned} \quad (5)$$

where $\mathbf{m}_t = \mathbb{E}[\mathbf{x}_t]$ and $\mathbf{P}_t = \mathbb{E}[(\mathbf{x}_t - \mathbf{m}_t) (\mathbf{x}_t - \mathbf{m}_t)^\top]$ [4]. The initial values of \mathbf{m}_t and \mathbf{P}_t are given at time t_{k-1} .

Notice that when using this scheme in Gaussian filtering, it is not necessary to directly approximate the transition density (3). By solving the ODEs, they directly give the prediction step of filtering when the initial conditions are given by the previous filtering posterior. Unfortunately, the ODEs are only tractable for linear SDEs along with certain other isolated special cases, because of the expectations in (5). To disentangle the intractability problem of these ODEs, one practical solution is to linearise $\mathbf{f}(\mathbf{x}_t, t)$ and $\mathbf{L}(\mathbf{x}_t, t)$ around \mathbf{m}_t , which leads to the continuous-discrete extended Kalman filter (CD-EKF) [8]. Another solution is to assume that the densities are Gaussian, in which case the expectations in the ODEs can be calculated with Gaussian quadrature or sigma-point methods [11]–[13]. Finally, the ODEs are solved with numerical solvers, such as Runge–Kutta (RK) methods. For simplicity of later discussion, we use *Linear-ODE* and *Gauss-ODE* to refer to the methods solving (5) using linearisation and Gaussian assumptions, respectively.

The contributions of this note are as follows. (1) We develop a novel Taylor moment expansion based Gaussian filter for continuous-discrete state-space models. (2) We analyse the positive definiteness of TME covariance estimate and the stability of TME Gaussian filter. (3) We show by numerical experiments that the proposed TME Gaussian filter outperforms the state-of-the-art methods in terms of both estimation accuracy and numerical stability.

II. TAYLOR MOMENT EXPANSION FOR GAUSSIAN FILTERING

As a Gaussian distribution is entirely characterised by its mean and covariance, a reasonable approach to Gaussian filtering is to use moment matching to form a Gaussian approximation to the transition density. The previously presented Itô–Taylor and ODE methods are useful tools for this purpose. In this note, we present another *Taylor moment expansion* (TME) based approach, which allows us to derive higher order approximations to the transition density [4], [14]–[16].

A. Taylor Moment Expansion

Let $\phi(\mathbf{x}_t)$ be an arbitrary twice-differentiable scalar function of the process \mathbf{x}_t . By Itô’s lemma and taking the expectation yields

$$\begin{aligned} d\mathbb{E}[\phi(\mathbf{x}_t)] &= \mathbb{E}[\nabla\phi(\mathbf{x}_t)\mathbf{f}(\mathbf{x}_t, t)] dt \\ &\quad + \frac{1}{2}\mathbb{E}[\text{tr}(\nabla\nabla^T\phi(\mathbf{x}_t)\mathbf{\Gamma}(\mathbf{x}_t, t))] dt, \end{aligned} \quad (6)$$

where ∇ and $\nabla\nabla^T$ give the Jacobian and Hessian of $\phi(\mathbf{x}_t)$, respectively. With a proper choice of ϕ , this will lead to the moment ODEs as shown in (5) [4]. The aim now is to form a Taylor expansion of the function $\mathbb{E}[\phi(\mathbf{x}_t)]$. We notice that the right-hand side of (6) can be reformulated with the (generalized) infinitesimal generator

$$\begin{aligned} \mathcal{A}g &= \frac{\partial g}{\partial t} + \nabla g\mathbf{f}(\mathbf{x}_t, t) + \frac{1}{2}\text{tr}(\nabla\nabla^T g\mathbf{\Gamma}(\mathbf{x}_t, t)), \\ &= \frac{\partial g}{\partial t} + \sum_i \frac{\partial g}{\partial x_i} f_i(\mathbf{x}_t, t) + \frac{1}{2} \sum_{i,j} \frac{\partial^2 g}{\partial x_i \partial x_j} \Gamma_{ij}, \end{aligned} \quad (7)$$

for any regular smooth function g , where x_i is the i -th component of \mathbf{x}_t (see, e.g., [1, Ch. 7] or [4, Ch. 9]). Thus (6) becomes

$$\frac{d\mathbb{E}[\phi(\mathbf{x}_t)]}{dt} = \mathbb{E}[\mathcal{A}\phi(\mathbf{x}_t)], \quad (8)$$

which requires that $\phi \in C^2$ is twice differentiable. We also denote by \mathcal{A}^r the r -th iteration of the generator. By taking derivatives of (8) to M times, we have

$$\frac{d^M \mathbb{E}[\phi(\mathbf{x}_t)]}{dt^M} = \mathbb{E}[\mathcal{A}^M \phi(\mathbf{x}_t)], \quad (9)$$

which requires that $\phi \in C^{2M}$ [4]. Notice that (9) above also requires sufficient smoothness of $\mathbf{f}(\mathbf{x}, t)$ and $\mathbf{\Gamma}(\mathbf{x}, t)$. We can now form an M -th order Taylor expansion of the function $\mathbb{E}[\phi(\mathbf{x}_k)]$ at time t_k and centred at time t_{k-1} as follows:

$$\begin{aligned} \mathbb{E}[\phi(\mathbf{x}_k)] &\approx \sum_{r=0}^M \frac{1}{r!} \frac{d^r \mathbb{E}[\phi(\mathbf{x}_{k-1})]}{dt^r} \Delta t^r \\ &= \sum_{r=0}^M \frac{1}{r!} \mathbb{E}[\mathcal{A}^r \phi(\mathbf{x}_{k-1})] \Delta t^r, \end{aligned} \quad (10)$$

where $\Delta t = t_k - t_{k-1}$. Conditioning (10) on \mathbf{x}_{k-1} gives

$$\mathbb{E}[\phi(\mathbf{x}_k) | \mathbf{x}_{k-1}] \approx \sum_{r=0}^M \frac{1}{r!} \mathcal{A}^r \phi(\mathbf{x}_{k-1}) \Delta t^r. \quad (11)$$

In Gaussian filtering, we are only interested in functions ϕ having certain polynomial forms. For the mean and covariance, we introduce two sets of functions: $\{\phi_i = x_i : i = 1, \dots, D\}$ and $\{\phi_{ij} = x_i x_j : i, j = 1, \dots, D\}$, where x_i is the i -th component of \mathbf{x}_k . Then, we have the mean $\mathbb{E}[\mathbf{x}_k | \mathbf{x}_{k-1}] = [\mathbb{E}[\phi_1 | \mathbf{x}_{k-1}], \dots, \mathbb{E}[\phi_D | \mathbf{x}_{k-1}]]^T$ and the covariance $\text{Cov}[x_i x_j | \mathbf{x}_{k-1}] = \mathbb{E}[\phi_{ij} | \mathbf{x}_{k-1}] - \mathbb{E}[\phi_i | \mathbf{x}_{k-1}] \mathbb{E}[\phi_j | \mathbf{x}_{k-1}]$. Using the approximation (11), we can now form the Taylor moment expansion (TME) estimator for the transition density as shown in Definition 1.

Definition 1 (Taylor Moment Expansion (TME) of Transition Density). *The M -th order Taylor expansion based estimates of the mean \mathbf{a}_M , the second moment \mathbf{B}_M , and the covariance $\mathbf{\Sigma}_M$ of the transition density (3) are given by*

$$\begin{aligned} \mathbf{a}_M &\triangleq \mathbf{a}_M(\mathbf{x}_{k-1}, \Delta t) \\ &= \sum_{r=0}^M \frac{1}{r!} \mathcal{A}^r \mathbf{x}_{k-1} \Delta t^r \approx \mathbb{E}[\mathbf{x}_k | \mathbf{x}_{k-1}], \\ \mathbf{B}_M &\triangleq \mathbf{B}_M(\mathbf{x}_{k-1}, \Delta t) \\ &= \sum_{r=0}^M \frac{1}{r!} \mathcal{A}^r (\mathbf{x}_{k-1} \mathbf{x}_{k-1}^T) \Delta t^r \approx \mathbb{E}[\mathbf{x}_k \mathbf{x}_k^T | \mathbf{x}_{k-1}], \\ \mathbf{\Sigma}_M &\triangleq \mathbf{\Sigma}_M(\mathbf{x}_{k-1}, \Delta t) \\ &= \mathbf{B}_M - \mathbf{a}_M \mathbf{a}_M^T \approx \text{Cov}[\mathbf{x}_k | \mathbf{x}_{k-1}], \end{aligned} \quad (12)$$

respectively. Here the application of the generator \mathcal{A} on vector or matrix input means that we apply the operator elementwise.

Remark 2. Note that if an M -th order TME approximation is used, the covariance estimator $\mathbf{\Sigma}_M$ in Definition 1 is a

polynomial of degree $2M$ in Δt , which comes from the product $\mathbf{a}_M \mathbf{a}_M^\top$. To keep the order of Δt consistent in mean and covariance, Σ_M needs to be truncated to degree M .

In addition, it is also important to recover the remainder $R(\mathbf{x}_{k-1}, \Delta t)$ of TME, such that (10) becomes

$$\mathbb{E}[\phi(\mathbf{x}_k)] = \sum_{r=0}^M \frac{1}{r!} \mathbb{E}[\mathcal{A}^r \phi(\mathbf{x}_{k-1})] \Delta t^r + R(\mathbf{x}_{k-1}, \Delta t).$$

By Taylor's theorem, the remainder admits the form

$$R(\mathbf{x}_{k-1}, \Delta t) = \int_{t_{k-1}}^{t_k} \int_{t_{k-1}}^{u_M} \cdots \int_{t_{k-1}}^{u_1} \mathbb{E}[\mathcal{A}^{M+1} \phi(\mathbf{x}_s)] ds du_1 \cdots du_M, \quad (13)$$

provided that ϕ and the SDE coefficients are sufficiently smooth [14], [16]. The convergence properties of TME can be analysed in the same way as any other Taylor expansion.

The difference between the TME and the aforementioned ODE and Itô-Taylor schemes is mainly how the Gaussian approximation to the continuous model is done. The Itô-Taylor approach first discretises the SDE solution which gives the discretised approximation $\hat{\mathbf{x}}_k$, and then obtains the moment $\mathbb{E}[\phi(\hat{\mathbf{x}}_k)]$ using the approximation. In ODE approach we need to postulate certain hypothesis, such as Gaussian assumptions or linearisation before solving the ODEs (5). In contrast, TME gives the estimate of $\mathbb{E}[\phi(\mathbf{x}_k)]$ directly, without forming the discretised approximation $\hat{\mathbf{x}}_k$ or approximation to the ODEs.

B. TME Gaussian Filtering

Using Definition 1, we now formulate the proposed TME Gaussian filter by utilising an M -th order TME estimate of the transition density $p(\mathbf{x}_k | \mathbf{x}_{k-1}) \approx \mathcal{N}(\mathbf{x}_k | \mathbf{a}_M, \Sigma_M)$. Notice that although we are using simplified notations \mathbf{a}_M , \mathbf{B}_M , and Σ_M , those terms are functions of \mathbf{x}_{k-1} and Δt .

Let us assume the filtering posterior from previous time step t_{k-1} is $p(\mathbf{x}_{k-1} | \mathbf{y}_{1:k-1}) = \mathcal{N}(\mathbf{x}_{k-1} | \mathbf{m}_{k-1}, \mathbf{P}_{k-1})$. We first perform prediction with respect to the continuous model (1a), and thus the prediction density $p(\mathbf{x}_k | \mathbf{y}_{1:k-1}) = \mathcal{N}(\mathbf{x}_k | \mathbf{m}_k^-, \mathbf{P}_k^-)$ is characterised by

$$\begin{aligned} \mathbb{E}[\mathbf{x}_k | \mathbf{y}_{1:k-1}] &= \int \mathbf{x}_k \int p(\mathbf{x}_k | \mathbf{x}_{k-1}) p(\mathbf{x}_{k-1} | \mathbf{y}_{1:k-1}) d\mathbf{x}_{k-1} d\mathbf{x}_k \\ &\approx \mathbb{E}[\mathbf{a}_M] = \mathbf{m}_k^-, \end{aligned} \quad (14)$$

and also

$$\begin{aligned} \text{Cov}[\mathbf{x}_k | \mathbf{y}_{1:k-1}] &\approx \mathbb{E}[\Sigma_M + \mathbf{a}_M \mathbf{a}_M^\top] - \mathbf{m}_k^- (\mathbf{m}_k^-)^\top = \mathbf{P}_k^-. \end{aligned} \quad (15)$$

Note that we are using $\mathbf{P}_k^- = \mathbb{E}[\Sigma_M + \mathbf{a}_M \mathbf{a}_M^\top] - \mathbf{m}_k^- (\mathbf{m}_k^-)^\top$ instead of directly $\mathbf{P}_k^- = \mathbb{E}[\mathbf{B}_M] - \mathbf{m}_k^- (\mathbf{m}_k^-)^\top$. Recall from Remark 2 that they are not equal, as we truncate Σ_M to keep the power of Δt consistent. By using $\mathbf{P}_k^- = \mathbb{E}[\mathbf{B}_M] - \mathbf{m}_k^- (\mathbf{m}_k^-)^\top$, it is difficult to perform such truncation. Furthermore, the prediction covariance \mathbf{P}_k^- is not always positive definite, which is an issue that is discussed in Section III-A.

The resulting filtering algorithm is the following, where we also use the general discrete Gaussian filter update step [3].

Algorithm 3 (TME Gaussian Filter). *Starting from initial filtering condition $\mathbf{x}_0 \sim \mathcal{N}(\mathbf{x}_0 | \mathbf{m}_0, \mathbf{P}_0)$, the equations of TME Gaussian filter for $k = 1, 2, \dots, T$ are as follows:*

• *Prediction:*

$$\begin{aligned} \mathbf{m}_k^- &= \int \mathbf{a}_M \mathcal{N}(\mathbf{x}_{k-1} | \mathbf{m}_{k-1}, \mathbf{P}_{k-1}) d\mathbf{x}_{k-1}, \\ \mathbf{P}_k^- &= \int (\Sigma_M + \mathbf{a}_M \mathbf{a}_M^\top) \mathcal{N}(\mathbf{x}_{k-1} | \mathbf{m}_{k-1}, \mathbf{P}_{k-1}) d\mathbf{x}_{k-1} \\ &\quad - \mathbf{m}_k^- (\mathbf{m}_k^-)^\top. \end{aligned} \quad (16)$$

• *Update:*

$$\begin{aligned} \mathbf{m}_k &= \mathbf{m}_k^- + \mathbf{K}_k (\mathbf{y}_k - \boldsymbol{\mu}_k), \\ \mathbf{P}_k &= \mathbf{P}_k^- - \mathbf{K}_k \mathbf{S}_k \mathbf{K}_k^\top, \end{aligned} \quad (17)$$

where $\boldsymbol{\mu}_k = \mathbb{E}[\mathbf{h}(\mathbf{x}_k)]$, $\mathbf{S}_k = \mathbb{E}[(\mathbf{h}(\mathbf{x}_k) - \boldsymbol{\mu}_k)(\mathbf{h}(\mathbf{x}_k) - \boldsymbol{\mu}_k)^\top]$, and $\mathbf{K}_k = \mathbb{E}[(\mathbf{x}_k - \mathbf{m}_k^-)(\mathbf{h}(\mathbf{x}_k) - \boldsymbol{\mu}_k)^\top] \mathbf{S}_k^{-1}$. In this update step, the expectations are taken with respect to the predicted $\mathbf{x}_k \sim \mathcal{N}(\mathbf{m}_k^-, \mathbf{P}_k^-)$.

The calculation of Gaussian integrals in Algorithm 3 is intractable for many non-linear integrands (i.e., \mathbf{a}_M , \mathbf{B}_M , and Σ_M). Herein, we consider numerically approximating them by using quadrature and sigma-point methods, such as Gauss-Hermite [11], unscented transform [17], and spherical cubature method [18]. It is also worth mentioning that as the sigma-point approximation is an operation of linearly weighted summation, the positive definiteness of \mathbf{P}_k^- is preserved from Σ_M provided that the quadrature weights are positive. This is true for Gauss-Hermite quadrature, spherical cubature, and unscented transformation with suitable parameter selection. In this note we assume that such a positive-weight integration rule is used.

III. THEORETICAL ANALYSIS OF TAYLOR MOMENT EXPANSION GAUSSIAN FILTER

In this section, we first study the positive definiteness of the covariance estimates produced by the Taylor moment expansion (TME) and then prove the stability of the TME Gaussian filter for a class of non-linear state-space models.

A. Positive Definiteness of Taylor Moment Expansion

In the Gaussian filtering context, it is essential for the covariance estimate to stay positive definite (p.d.). Unfortunately, this is not always true when using TME, as we truncate the full Taylor expansion [19]. We now formulate the following theorem to show conditions for the positive definiteness of the TME covariance estimate.

Theorem 4. *The M -th order TME covariance estimate Σ_M is positive definite for Δt on an interval $U \subseteq \mathbb{R}^+$, if*

$$P_M(\Delta t) = \sum_{r=1}^M w_r \Delta t^r > 0, \quad (18)$$

for all $\Delta t \in U$, where $w_r = \frac{1}{r!} \lambda_{\min}(\Phi_{\mathbf{x}_t, r})$, and $\lambda_{\min}(\cdot)$ denotes the minimum eigenvalue of a square matrix. The coefficients are

$$\Phi_{\mathbf{x}_t, r} = \mathcal{A}^r (\mathbf{x}_t \mathbf{x}_t^\top) - \sum_{s=0}^r \binom{r}{s} \mathcal{A}^s \mathbf{x}_t (\mathcal{A}^{r-s} \mathbf{x}_t)^\top, \quad (19)$$

where $\binom{r}{s}$ denotes the binomial coefficient.

Proof. By Cauchy product and Definition 1, we can formulate the (u, v) -th entry of Σ_M as

$$[\Sigma_M]_{uv} = \sum_{r=0}^M \frac{1}{r!} \left[\mathcal{A}^r (x_u x_v) - \sum_{s=0}^r \binom{r}{s} \mathcal{A}^s x_u \mathcal{A}^{r-s} x_v \right] \Delta t^r$$

and further rearrange it into matrix form

$$\Sigma_M = \sum_{r=1}^M \frac{1}{r!} \Phi_{\mathbf{x}_t, r} \Delta t^r. \quad (20)$$

Using Weyl's inequality [20], we have $\lambda_{\min}(\Sigma_M) \geq \sum_{r=1}^M \frac{1}{r!} \lambda_{\min}(\Phi_{\mathbf{x}_t, r}) \Delta t^r$. Thus the positive definiteness of Σ_M is implied by the polynomial on the right in (20). \square

Equation (20) reveals that the covariance estimate Σ_M is a polynomial function of Δt with coefficients formed by $\{\Phi_{\mathbf{x}_t, r} : r = 1, \dots, M\}$. The idea behind Theorem 4 is to construct a lower bound for the minimum eigenvalue of Σ_M in terms of the eigenvalues of the coefficients matrices $\Phi_{\mathbf{x}_t, r}$. The following Proposition 5 gives applications of using Theorem 4 for the positive definiteness of the second and third order of TME estimates.

Proposition 5. Let Σ_2 and Σ_3 be the TME estimates of the covariance with expansion order 2 and 3, respectively. Also let us denote by $\mathbf{f} \triangleq \mathbf{f}(\mathbf{x}_t, t)$ and $\Gamma \triangleq \Gamma(\mathbf{x}_t, t)$. Then

- 1) Σ_2 is p.d. for $\Delta t > 0$ if $(\Gamma \nabla \mathbf{f})^\top + \Gamma \nabla \mathbf{f}$ and Γ are positive semi-definite (p.s.d.), and one of Γ and $(\Gamma \nabla \mathbf{f})^\top + \Gamma \nabla \mathbf{f}$ is p.d.
- 2) Σ_3 is p.d. for $\Delta t > 0$ if $\Phi_{\mathbf{x}_t, 3}$ is p.s.d. and $\lambda_{\min}(\Phi_{\mathbf{x}_t, 2}) > \frac{-2\sqrt{6}}{3} \sqrt{\lambda_{\min}(\Phi_{\mathbf{x}_t, 1}) \lambda_{\min}(\Phi_{\mathbf{x}_t, 3})}$.

Proof. By Definition 1,

$$\begin{aligned} \Sigma_2 &= \Phi_{\mathbf{x}_t, 1} \Delta t + \frac{1}{2} \Phi_{\mathbf{x}_t, 2} \Delta t^2 \\ &= \Gamma \Delta t + \frac{1}{2} ((\Gamma \nabla \mathbf{f})^\top + \Gamma \nabla \mathbf{f}) \Delta t^2. \end{aligned} \quad (21)$$

Thus $\boldsymbol{\eta}^\top \Sigma_2 \boldsymbol{\eta} > 0$ for any real non-zero vector $\boldsymbol{\eta}$ and $\Delta t > 0$, if $\lambda_{\min}(\Gamma) > 0$ and $\lambda_{\min}((\Gamma \nabla \mathbf{f})^\top + \Gamma \nabla \mathbf{f}) \geq 0$ or $\lambda_{\min}(\Gamma) = 0$ and $\lambda_{\min}((\Gamma \nabla \mathbf{f})^\top + \Gamma \nabla \mathbf{f}) > 0$.

For Σ_3 , by Theorem 4, we have the polynomial

$$P_3(\Delta t) = w_1 \Delta t + w_2 \Delta t^2 + w_3 \Delta t^3. \quad (22)$$

The polynomial $P_3(\Delta t)$ is positive and has no real roots for $\Delta t > 0$, if and only if $w_2 > -2\sqrt{w_1 w_3}$ and $w_3 \geq 0$, which is equivalent to $\lambda_{\min}(\Phi_{\mathbf{x}_t, 2}) > \frac{-2\sqrt{6}}{3} \sqrt{\lambda_{\min}(\Phi_{\mathbf{x}_t, 1}) \lambda_{\min}(\Phi_{\mathbf{x}_t, 3})}$ and $\lambda_{\min}(\Phi_{\mathbf{x}_t, 3}) \geq 0$. It follows that Σ_3 is p.d. \square

Remark 6. In the limit $\Delta t \rightarrow 0$, the TME covariance estimate will always be p.d., provided Γ is p.d.

Example 7. The TME variance estimate of SDE

$$dx_t = \tanh x_t dt + dW_t, \quad (23)$$

where W_t is a standard Wiener process, is always p.d. This follows from Theorem 4 and observing that $\Phi_{x, 1} = 1 > 0$, $\Phi_{x, 2} = 1 - \tanh^2 x_t \geq 0$, and $\{\Phi_{x, r} = 0 : r \geq 3\}$.

The coefficients $\Phi_{\mathbf{x}_t, r}$, the expansion order M , and the time interval Δt jointly determine the positive definiteness of TME covariance estimate. The properties of $\Phi_{\mathbf{x}_t, r}$ are more of interest, as we usually have M and Δt fixed. Next, we show that $\Phi_{\mathbf{x}_t, r}$ is only concerned with the SDE coefficients.

Lemma 8. Consider the SDE (1a) with time-homogeneous $\mathbf{f}(\mathbf{x}_t)$ and constant \mathbf{L} . Let $\Phi_{\mathbf{x}, r}^{u, v} \triangleq [\Phi_{\mathbf{x}, r}]_{uv}$ be the u -th column and v -th row entry of $\Phi_{\mathbf{x}, r}$. We denote $\alpha_r^u \triangleq \alpha_r(x_u) = \mathcal{A}^r(x_u)$, and partial derivative $\partial_i \alpha_r^u \triangleq \partial \alpha_r^u / \partial x_i$. Then a general expression of $\Phi_{\mathbf{x}, r}^{u, v}$ is

$$\begin{aligned} \Phi_{\mathbf{x}, r}^{u, v} &= \sum_{i, j} \sum_{s=0}^{r-1} \binom{r-1}{s} (\partial_i \alpha_s^u \partial_j \alpha_{r-s-1}^v) \Gamma_{ij} + \mathcal{A} \Phi_{\mathbf{x}, r-1}^{u, v} \\ &= \sum_{s=0}^{r-1} \mathcal{A}^s \sum_{l=0}^{r-s-1} \binom{r-s-1}{l} \text{tr}((\nabla \alpha_s^u)^\top \nabla \alpha_{r-s-1-l}^v \Gamma) \end{aligned} \quad (24)$$

starting from $\Phi_{\mathbf{x}, 0}^{u, v} = 0$.

Proof. See Appendix I. \square

Lemma 8 gives an explicit form of $\Phi_{\mathbf{x}_t, r}$, which is shown to be the function of \mathbf{f} , Γ , and their partial derivatives. It implies that once M and Δt are given, the positive definiteness of Σ_M fully depends on the SDE coefficients. The functions \mathbf{f} and Γ have to satisfy certain properties for Σ_M to be positive definite.

Example 9. Let us consider a one-dimensional Itô process

$$dx_t = f(x_t) dt + L dW_t, \quad (25)$$

then by Lemma 8,

$$\begin{aligned} \Phi_{x, 0} &= 0, \\ \Phi_{x, 1} &= \Gamma, \\ \Phi_{x, 2} &= 2f' \Gamma, \\ \Phi_{x, 3} &= 2(2(f')^2 + 2ff'' + f''') \Gamma, \\ \Phi_{x, 4} &= ((9(f'')^2 + 6ff'''' + 16f''' f') \Gamma + 8(f')^3 \\ &\quad + 6f^2 f''' + 26ff'' f' + \frac{24}{16} f'''' \Gamma^2) \Gamma, \\ &\vdots \end{aligned} \quad (26)$$

where $f', f'', \dots, f''''', \dots$ are the derivatives of $f(x)$ of orders 1, 2, \dots , 5, \dots . Also, $\Gamma = L^2 Q$, and Q is the diffusion constant of the Wiener process W_t .

B. Stability of TME Gaussian Filter

It is important and useful that the filter is in some sense stable. Some classical stability results for linear Kalman filters can be found in [8], [21] while more recent results on the

stability of different approximate Gaussian (Kalman) filters for non-linear systems have been analysed in [22]–[24]. In this section, we follow [24] and prove that the TME Gaussian filter is stable in the mean-square sense if a number of assumptions on the system and the sigma-point approximation, verifiable before the filter is run, are satisfied. This means that we show that

$$\sup_{k \geq 1} \mathbb{E}[\|\mathbf{x}_k - \mathbf{m}_k\|_2^2] < \infty,$$

where the expectation is taken over all state and measurement trajectories, and $\|\cdot\|_2$ denotes the Euclidean norm.

For simplicity, in (1) we assume $\mathbf{f}(\mathbf{x}_t)$ is time-homogeneous (not explicitly depending on time), Γ is a positive definite constant, $\mathbf{V}_k = \mathbf{V}$ for all $k \geq 1$, and that the measurement model is linear: $\mathbf{h}(\mathbf{x}_k) = \mathbf{H}\mathbf{x}_k$ for some matrix \mathbf{H} . Then the generic continuous-discrete SDE (1) then has the discretised form

$$\begin{aligned} \mathbf{x}_k &= \mathbf{a}(\mathbf{x}_{k-1}, \Delta t) + \boldsymbol{\tau}(\mathbf{x}_{k-1}, \Delta t), \\ \mathbf{y}_k &= \mathbf{H}\mathbf{x}_k + \mathbf{v}_k, \end{aligned} \quad (27)$$

where $\boldsymbol{\tau}(\mathbf{x}_{k-1}) \triangleq \boldsymbol{\tau}(\mathbf{x}_{k-1}, \Delta t)$ is a zero-mean random variable whose covariance $\text{Cov}[\boldsymbol{\tau}(\mathbf{x}_{k-1})] = \boldsymbol{\Sigma}(\mathbf{x}_{k-1}, \Delta t)$. Notice that we denote by $\mathbf{a}(\mathbf{x}_{k-1}) \triangleq \mathbf{a}(\mathbf{x}_{k-1}, \Delta t)$ and $\boldsymbol{\Sigma}(\mathbf{x}_{k-1}) \triangleq \boldsymbol{\Sigma}(\mathbf{x}_{k-1}, \Delta t)$ the *exact* mean and covariance functions of \mathbf{x}_t , respectively. It follows that $\mathbf{a} = \mathbf{a}_M + \mathbf{R}_M$, where $\mathbf{R}_M(\mathbf{x}_{k-1}) \triangleq \mathbf{R}_M(\mathbf{x}_{k-1}, \Delta t)$ is the Taylor remainder (13). The assumptions needed for the stability analysis of the system (27) are collected below in Assumption 10. If \mathbf{A} is a matrix, $\|\mathbf{A}\|$ stands for the spectral norm.

Assumption 10. *The following properties hold:*

- 1) *There are non-negative constants C_M , λ_τ , and λ_P such that $\sup_{k \geq 1} \|\mathbf{R}_M(\mathbf{x}_{k-1})\| \leq C_M$ almost surely, $\sup_{k \geq 1} \mathbb{E}[\text{tr}(\boldsymbol{\Sigma}(\mathbf{x}_{k-1}))] \leq \lambda_\tau$, and $\sup_{k \geq 1} \mathbb{E}[\text{tr}(\mathbf{P}_k)] \leq \lambda_P$.*
- 2) *There is $C \geq 0$ such that*

$$\|\mathbf{a}_M(\mathbf{x}) - \mathcal{S}_{\mathbf{m}, \mathbf{P}}(\mathbf{a}_M)\|_2 \leq \|\nabla \mathbf{a}_M(\mathbf{x})\|^2 \|\mathbf{x} - \mathbf{m}\|_2^2 + C \text{tr}(\mathbf{P})$$

for any vectors \mathbf{x} and \mathbf{m} and any positive semi-definite matrix \mathbf{P} , where $\mathcal{S}_{\mathbf{m}, \mathbf{P}}(\mathbf{g})$ stands for the sigma-point approximation of the Gaussian integral

$$\int \mathbf{g}(\mathbf{x}) \mathcal{N}(\mathbf{x} \mid \mathbf{m}, \mathbf{P}) d\mathbf{x}.$$

- 3) *There is $\lambda \geq 0$ such that $\sup_{k \geq 1} \|\mathbf{I} - \mathbf{K}_k \mathbf{H}\| \leq \lambda$ almost surely and*

$$\lambda_f^2 \triangleq \sup_{k \geq 1} \lambda^2 \sup_{\mathbf{x}} \|\nabla \mathbf{a}_M(\mathbf{x})\|^2 < 1/4.$$

The Assumption 10 postulates conditions on the sigma-point approximations and systems. An example to satisfy the assumptions is that the drift function \mathbf{f} is smooth enough and all of its partial derivatives up to certain orders are uniformly bounded. More practical examples that satisfy Assumption 10 can be found in [24]. It is typically necessary that the measurement model matrix \mathbf{H} is a scaled identity matrix and the discretised dynamics \mathbf{a} in (27) defines an exponentially stable system. Although these assumptions are quite restrictive,

stability results with more general assumptions are currently not yet available in literature [24].

Theorem 11. *Suppose that Assumption 10 is satisfied. Then the TME Gaussian filter for system (27) has*

$$\mathbb{E}[\|\mathbf{x}_k - \mathbf{m}_k\|_2^2] \leq (4\lambda_f^2)^k \text{tr}(\mathbf{P}_0) + \frac{C_e}{1 - 4\lambda_f^2}$$

for all $k \geq 1$, where C_e is defined in (29).

Proof. It is easy to see that [24, Proof of Theorem IV.3]

$$\kappa \triangleq \sup_{k \geq 1} \|\mathbf{K}_k\| \leq \lambda_P \|\mathbf{H}\| \|\mathbf{V}^{-1}\|.$$

Denote $\mathbf{A}_k = \mathbf{I} - \mathbf{K}_k \mathbf{H}$. Using the discretised system (27), the filtering error can be written as

$$\begin{aligned} \mathbf{e}_k &\triangleq \mathbf{x}_k - \mathbf{m}_k \\ &= \mathbf{a}(\mathbf{x}_{k-1}) + \boldsymbol{\tau}(\mathbf{x}_{k-1}) - \mathbf{m}_k - \mathbf{K}_k(\mathbf{y}_k - \mathbf{H}\mathbf{m}_k) \\ &= \mathbf{A}_k [\mathbf{a}(\mathbf{x}_{k-1}) - \mathcal{S}_{\mathbf{m}_{k-1}, \mathbf{P}_{k-1}}(\mathbf{a}_M)] \\ &\quad + (\mathbf{I} - \mathbf{K}_k \mathbf{H}) \boldsymbol{\tau}(\mathbf{x}_{k-1}) - \mathbf{K}_k \mathbf{v}_k \\ &= \mathbf{A}_k [\mathbf{a}_M(\mathbf{x}_{k-1}) - \mathcal{S}_{\mathbf{m}_{k-1}, \mathbf{P}_{k-1}}(\mathbf{a}_M)] \\ &\quad + \mathbf{A}_k \mathbf{R}_M(\mathbf{x}_{k-1}) + \mathbf{A}_k \boldsymbol{\tau}(\mathbf{x}_{k-1}) - \mathbf{K}_k \mathbf{v}_k. \end{aligned}$$

The inequality $(a_1 + \dots + a_n)^2 \leq n(a_1^2 + \dots + a_n^2)$ gives

$$\begin{aligned} \mathbb{E}[\|\mathbf{e}_k\|_2^2] &\leq 4\mathbb{E}[\|\mathbf{A}_k [\mathbf{a}_M(\mathbf{x}_{k-1}) - \mathcal{S}_{\mathbf{m}_{k-1}, \mathbf{P}_{k-1}}(\mathbf{a}_M)]\|_2^2] \\ &\quad + 4\mathbb{E}[\|\mathbf{A}_k \mathbf{R}_M(\mathbf{x}_{k-1})\|_2^2] \\ &\quad + 4\mathbb{E}[\|\mathbf{A}_k \boldsymbol{\tau}(\mathbf{x}_{k-1})\|_2^2] + 4\mathbb{E}[\|\mathbf{K}_k \mathbf{v}_k\|_2^2]. \end{aligned} \quad (28)$$

Assumption 10 yields the following bounds:

$$\begin{aligned} \mathbb{E}[\|\mathbf{A}_k [\mathbf{a}_M(\mathbf{x}_{k-1}) - \mathcal{S}_{\mathbf{m}_{k-1}, \mathbf{P}_{k-1}}(\mathbf{a}_M)]\|_2^2] &\leq \lambda_f^2 \mathbb{E}[\|\mathbf{e}_{k-1}\|_2^2] + C\lambda^2 \lambda_P, \\ \mathbb{E}[\|\mathbf{A}_k \mathbf{R}_M(\mathbf{x}_{k-1})\|_2^2] &\leq C_M^2 \lambda^2, \\ \mathbb{E}[\|\mathbf{A}_k \boldsymbol{\tau}(\mathbf{x}_{k-1})\|_2^2] &\leq \lambda^2 \lambda_\tau, \\ \mathbb{E}[\|\mathbf{K}_k \mathbf{v}_k\|_2^2] &\leq \text{tr}(\mathbf{V}) \kappa^2. \end{aligned}$$

Upon insertion of these estimates into (28) we get the recursive mean-square error inequality

$$\mathbb{E}[\|\mathbf{e}_k\|_2^2] \leq 4\lambda_f^2 \mathbb{E}[\|\mathbf{e}_{k-1}\|_2^2] + C_e,$$

where

$$C_e = 4(\lambda^2[C\lambda_P + C_M^2 + \lambda_\tau] + \text{tr}(\mathbf{V})\kappa^2). \quad (29)$$

Because we have assumed that $4\lambda_f^2 < 1$, the claim then follows from the discrete Grönwall's inequality (e.g., [24, Theorem IV.2]). \square

IV. NUMERICAL EXPERIMENTS

To examine the effectiveness of the TME estimator in Definition 1, we first conduct experiments on the moment estimation of SDEs. After that, we examine and compare the accuracy and numerical stability of the proposed TME Gaussian filter against state-of-the-art methods.

A. Moment Estimation of SDEs

We consider a non-linear SDE:

$$dx_t = \tanh x_t dt + dW_t, \quad (30)$$

where W_t is a standard Wiener process, with known initial condition $x_0 = 0.5$. The aim is to compare the estimates of the moments of the transition densities. The true mean and covariance are estimated using Monte Carlo (MC) sampling with 10^6 independent trajectories. We simulated the samples from the models using Euler–Maruyama with sufficiently small time interval (10^{-5} s). The estimates were examined in the time interval $T = 0$ s to $T = 5$ s.

We chose the following methods as described in Section I to compare with the TME method:

- the ODE approach by solving (5) using Gaussian assumption, 4th order Runge–Kutta solver, and 3rd order Gauss–Hermite integration (Gauss-RK4);
- the ODE approach by solving (5) using linearisation, and 4th order Runge–Kutta solver (Linear-RK4);
- the Itô–Taylor strong order 1.5 based approach from [5], [6] (Itô-1.5).

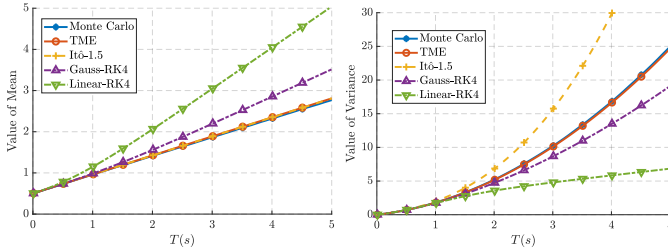


Fig. 1: The mean and variance estimates of model (30).

In Figure 1, we show the mean and variance estimates as functions of time. We observe that the Itô-1.5 and (the second order) TME methods coincide for the estimation of mean function, and are closest to the Monte Carlo result. This is because their formulations for this model are identical, and exact to the true mean of (30). The Gauss-RK4 and Linear-RK4 can only estimate the mean accurately within short time intervals, while Gauss-RK4 is slightly better than Linear-RK4.

When estimating the variance of (30), only the TME method succeeds to follow the Monte Carlo result closely. The variance estimate yield by TME is $\Delta t + (1 - \tanh^2 x_0)\Delta t^2$, which is exact to this model (see, Example 7). The Gauss-RK4, Linear-RK4, and Itô-1.5 all deviate from Monte Carlo for long time intervals.

B. 3D Coordinated Turn Tracking

In this part, we conduct Gaussian filtering on a 3D coordinated turn model. Performing filtering on this model is considered challenging due to its non-linearities and high dimensionality [6], [25]. The model is given by

$$d\mathbf{x}_t = \mathbf{f}(\mathbf{x}_t) dt + \mathbf{L} d\mathbf{W}_t, \quad (31a)$$

$$\mathbf{y}_k = \begin{bmatrix} \sqrt{p_x^2 + p_y^2 + p_z^2} \\ \tan^{-1}(p_y/p_x) \\ \tan^{-1}(p_z/\sqrt{p_x^2 + p_y^2}) \end{bmatrix} + \epsilon_k, \quad (31b)$$

where the state $\mathbf{x}_t = [p_x \ p_y \ p_z \ v_x \ v_y \ v_z \ \theta]^T$ and

$$\mathbf{f}(\mathbf{x}_t) = [v_x \ -\theta v_y \ v_y \ \theta v_x \ v_z \ 0 \ 0]^T, \quad (32)$$

$$\mathbf{L} = \text{diag}[0 \ \sigma_1 \ 0 \ \sigma_1 \ 0 \ \sigma_1 \ \sigma_2].$$

In this model, we denote by p_x , p_y , and p_z the position of the target in Cartesian coordinates, and v_x , v_y , and v_z are the corresponding velocities. State θ governs the turning rate of the target which controls the non-linearity of this model. In addition, \mathbf{W}_t is a standard Wiener process. The measurement noise $\epsilon_k \sim \mathcal{N}(0, \mathbf{V})$ and $\mathbf{V} = \text{diag}[\sigma_r^2 \ \sigma_\theta^2 \ \sigma_\phi^2]$.

Name	Description	Method	Integration
EKF-RK	ODE type of Gaussian filter with 4th order Runge–Kutta solver [4], [13]	Solving (5) with linearisation (Linear-ODE)	Not needed
CKF-RK			Spherical cubature
UKF-RK		Solving (5) with Gaussian assumption (Gauss-ODE)	Unscented transform
GHKF-RK			3rd order Gauss–Hermite
CKF-1.5	Itô-1.5 Gaussian filter [6]	Itô–Taylor discretisation with strong order 1.5 [6]	Spherical cubature
UKF-1.5			Unscented transform
GHKF-1.5			3rd order Gauss–Hermite
CKF-T*	TME Gaussian filter (Alg. 3)	*-th order TME (Def. 1)	Spherical cubature
UKF-T*			Unscented transform
GHKF-T*			3rd order Gauss–Hermite

TABLE I: The list of the state-of-the-art methods compared in 3D coordinate turn tracking.

The parameters σ_1 , σ_2 , σ_r^2 , σ_θ^2 , and σ_ϕ^2 are the same as in [6]. However, we choose the initial turning rate $\theta_0 = 30^\circ/\text{s}$ which is significantly higher than the $\theta_0 = 3$ to $6^\circ/\text{s}$ used in [6]. These two θ_0 settings are illustrated in Figure 2.

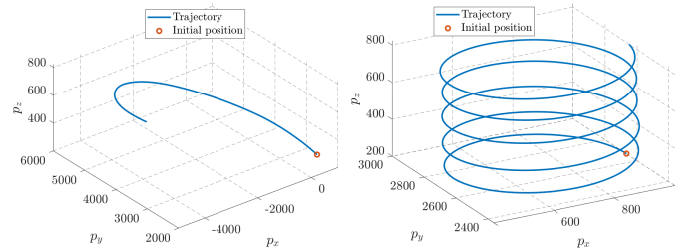


Fig. 2: Examples of trajectory simulation ($t = 0$ s to 60 s). The left figure shows the setting of initial turning rate $\theta_0 = 3^\circ/\text{s}$ [6], while on the right figure, we use $\theta_0 = 30^\circ/\text{s}$.

The other parameters are the same as in [6]. The initial condition is drawn from a normal distribution with mean $\mathbf{m}_0 = [1000 \text{ m} \ 0 \text{ m/s} \ 2650 \text{ m} \ 150 \text{ m/s} \ 200 \text{ m} \ 10 \text{ m/s} \ 30^\circ/\text{s}]^T$ and covariance $\mathbf{P}_0 = \text{diag}[100^2 \ 100^2 \ 100^2 \ 100^2 \ 100^2 \ 100^2 \ 10^2]$. We simulate the ground-truth trajectories using Euler–Maruyama with small enough time step $\Delta t \times 10^{-5}$ s, where Δt is the time interval between two measurements. The total time length of the trajectory is fixed to $T = 210$ s. To test the effectiveness of filters, we select the time interval Δt range from 0.5 s to

mation to the transition density of the SDE by using a Taylor moment expansion (TME). We derived the corresponding TME Gaussian filter, and analysed the positive definiteness of the TME covariance estimates and stability of the TME Gaussian filter. The numerical experiments indicate that even a second order TME Gaussian filter is in line with the state-of-the-art. With higher expansion order, the proposed TME filter substantially outperform the state-of-the-art methods, in terms of both estimation accuracy and numerical stability.

APPENDIX I PROOF OF LEMMA 8

Let $\beta_r^{u,v} \triangleq \beta_r(x_u x_v) = \mathcal{A}^r(x_u x_v)$ denote the r -th iteration of operator \mathcal{A} on $x_u x_v$, and $\partial_i \beta_r^{u,v} = \partial \beta_r^{u,v} / \partial x_i$. For $r = 0$ and 1, we readily find $\alpha_0^u = x_u$, $\alpha_1^u = f_u$, $\alpha_0^v = x_v$, $\alpha_1^v = f_v$, $\beta_0^{u,v} = x_u x_v = \alpha_0^u \alpha_0^v$, and $\beta_1^{u,v} = \alpha_0^u \alpha_1^v + \alpha_0^v \alpha_1^u + \Gamma_{uv}$.

We can calculate $\Phi_{x,r}^{u,v}$ by (19) and initially reveal $\Phi_{x,0}^{u,v} = 0$, $\Phi_{x,1}^{u,v} = \Gamma_{uv}$. From this pattern above, we will first show $\beta_r^{u,v}$ has a general expression

$$\beta_r = \sum_{s=0}^r \binom{r}{s} \alpha_s^u \alpha_{r-s}^v + \Phi_{x,r}^{u,v}, \quad (34)$$

where $\Phi_{x,r}^{u,v}$ is

$$\Phi_{x,r}^{u,v} = \sum_{i,j} \sum_{s=0}^{r-1} \binom{r-1}{s} (\partial_i \alpha_s^u \partial_j \alpha_{r-s}^v) \Gamma_{ij} + \mathcal{A} \Phi_{x,r-1}^{u,v}, \quad (35)$$

It is apparent that (34) and (35) hold for $r = 1$. By Algorithm 1, the iteration of $\beta_r^{u,v}$ is

$$\beta_{r+1}^{u,v} = \mathcal{A}(\beta_r^{u,v}) = \sum_i \frac{\partial \beta_r^{u,v}}{\partial x_i} f_i + \frac{1}{2} \sum_{i,j} \frac{\partial^2 \beta_r^{u,v}}{\partial x_i \partial x_j} \Gamma_{ij}. \quad (36)$$

With Equation (34), we continue Equation (36) to yield

$$\begin{aligned} \beta_{r+1}^{u,v} &= \sum_{s=0}^r \binom{r}{s} (\alpha_{s+1}^u \alpha_{r-s}^v + \alpha_s^u \alpha_{r-s+1}^v) \\ &\quad + \sum_{i,j} \left(\sum_{s=0}^r \binom{r}{s} \partial_i \alpha_s^u \partial_j \alpha_{r-s}^v \right) \Gamma_{ij} + \mathcal{A} \Phi_{x,r}^{u,v} \\ &= \sum_{s=0}^{r+1} \binom{r+1}{s} \alpha_s^u \alpha_{r-s+1}^v + \Phi_{x,r+1}^{u,v} = \beta_{r+1}. \end{aligned} \quad (37)$$

Thus expressions (34) and (35) are proved by induction for $r \geq 1$. From Lemma 4, we now derive an iterated form of $\Phi_{x,r}$ as

$$\begin{aligned} \Phi_{x,r}^{u,v} &= \beta_r^{u,v} - \sum_{s=0}^r \binom{r}{s} \alpha_s^u \alpha_{r-s}^v \\ &= \sum_{i,j} \sum_{s=0}^{r-1} \binom{r-1}{s} (\partial_i \alpha_s^u \partial_j \alpha_{r-s-1}^v) \Gamma_{ij} + \mathcal{A} \Phi_{x,r-1}^{u,v} \\ &= \sum_{s=0}^{r-1} \binom{r-1}{s} \text{tr}((\nabla \alpha_s^u)^\top \nabla \alpha_{r-s-1}^v \Gamma) + \mathcal{A} \Phi_{x,r-1}^{u,v} \\ &= \sum_{s=0}^{r-1} \mathcal{A}^s \sum_{l=0}^{r-s-1} \binom{r-s-1}{l} \text{tr}((\nabla \alpha_s^u)^\top \nabla \alpha_{r-s-1-l}^v \Gamma) \end{aligned}$$

starting from $\Phi_{x,0} = 0$.

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