GAUSS-QUADRATURE METHOD FOR ONE-DIMENSIONAL MEAN-FIELD SDEs*

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Abstract. Mean-field SDEs, also known as McKean–Vlasov equations, are stochastic differential equations where the drift and diffusion depend on the current distribution in addition to the current position. We describe an efficient numerical method for approximating the distribution at time t of the solution to the initial-value problem for one-dimensional mean-field SDEs. The idea is to time march (e.g., using the Euler–Maruyama time-stepping method) an m-point Gauss-quadrature rule. With suitable regularity conditions, convergence with first order is proved for Euler–Maruyama time stepping. We also estimate the work needed to achieve a given accuracy in terms of the smoothness of the underlying problem. Numerical experiments are given, which show the effectiveness of this method as well as two second-order time-stepping methods. The methods are also effective for ordinary SDEs in one dimension, as we demonstrate by comparison with the multilevel Monte Carlo method.

 ${\bf Key \ words.} \ {\rm Gauss \ quadrature, \ McKean-Vlasov \ equations, \ mean-field \ SDEs, \ numerical \ approximation$

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1. Introduction. McKean–Vlasov or mean-field SDEs are a class of stochastic differential equations where the drift and diffusion depend on the current position along the path and on the current distribution. They were derived to describe propagation of chaos in a system of particles that interact only by their empirical mean in the limit of large number of particles [20]. We study mean-field SDEs in one dimension and are interested in the following initial-value problem: determine the real-valued process $X^{\mu}(t), t > 0$, such that

$$(1) \ X^{\mu}(t) - X^{\mu}(0) = \int_{0}^{t} \int_{\mathbb{R}} a(X^{\mu}(s), y) P_{s}^{\mu}(dy) \, ds + \int_{0}^{t} \int_{\mathbb{R}} b(X^{\mu}(s), y) P_{s}^{\mu}(dy) \, dW(s),$$

where P_s^{μ} denotes the distribution of $X^{\mu}(s)$ and the initial distribution $X^{\mu}(0) \sim \mu$ for some prescribed probability measure μ . Here, $a: \mathbb{R}^2 \to \mathbb{R}$ is the drift, $b: \mathbb{R}^2 \to \mathbb{R}$ is the diffusion, W(t) is a one-dimensional Brownian motion (independent of $X^{\mu}(0)$), and we interpret the stochastic integral as an Ito integral. We also write this as

$$dX^{\mu}(t) = P_t^{\mu}(a(X^{\mu}(t), \cdot)) dt + P_t^{\mu}(b(X^{\mu}(t), \cdot)) dW(t), \qquad X^{\mu}(0) \sim \mu_t$$

where $\nu(\phi) \coloneqq \int_{\mathbb{R}} \phi(x) \nu(dx)$ for an integrable function $\phi \colon \mathbb{R} \to \mathbb{R}$ and a measure ν on \mathbb{R} . Under the following condition, (1) has a unique strong solution with a smooth density [2, Theorem 2.1]. (Though (1) is well-posed more generally [9, 25, 16], Assumption 1.1 is close to the ones in our error analysis.)

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ASSUMPTION 1.1. Suppose that pth moments of the initial distribution μ are finite for all $p \ge 1$ and that the coefficients a and b are smooth with all derivatives uniformly bounded.

Several numerical methods have been proposed for (1) and their convergence behavior analyzed. Early work includes [6, 5], which show convergence of a method based on Monte Carlo evaluation of the averages and Euler-Maruyama time stepping. The same method was studied using Malliavin calculus in [2] and more refined convergence results proved. More recently, [23] has developed the multilevel Monte Carlo method in cases where the drift and diffusion depend on the distribution via the mean of a function of $X^{\mu}(t)$. Cubature methods have also been developed in [21].

We are interested in numerical approximation of the distribution of $X^{\mu}(t_n)$ by a probability measure Q_n , where $t_n = n\Delta t$ for a time step $\Delta t > 0$. Consider a one-step numerical method that pushes forward the measure Q_n to Q_{n+1} . For an example, let

(2)
$$\Psi(x, \Delta t, Q) \coloneqq x + \Delta t Q(a(x, \cdot)) + \sqrt{\Delta t} Q(b(x, \cdot)) \xi$$

for $\xi \sim N(0, 1)$ or a random variable with a nearby distribution, such as the two-point random variable with $\mathbb{P}(\xi = \pm 1) = 1/2$. For the Euler–Maruyama method, Q_{n+1} is the distribution of $X_{n+1} = \Psi(X_n, \Delta t, Q_n)$, assuming ξ is independent of X_n and $X_0 \sim \mu$. In the case that a, b are independent of their second argument,

$$X_{n+1} = X_n + \Delta t \, a(X_n) + \sqrt{\Delta t} \, b(X_n) \, \xi_n$$

where ξ_n are *iid* copies of ξ , which is the standard Euler–Maruyama method. For ordinary SDEs, it is well-known that first-order weak convergence results if a, b and the test function $\phi \colon \mathbb{R} \to \mathbb{R}$ are sufficiently smooth [17]:

$$\mathbb{E}[\phi(X^{\mu}(1))] - \mathbb{E}[\phi(X_N)] = P_1^{\mu}(\phi) - Q_N(\phi) = \mathcal{O}(\Delta t), \qquad t_N = 1.$$

This method is of limited practical value for approximating $P_t^{\mu}(\phi)$. The support of Q_N is uncountable if Gaussian random variables ξ are used or otherwise countable but very large in number, and the expectation $Q_N(\phi)$ is usually approximated via a Monte Carlo method that samples from Q_N . For the mean-field SDE, this is more problematic, as all the particles must be tracked at the same time as $Q_n(a(X_n, \cdot))$ and $Q_n(b(X_n, \cdot))$ must be evaluated at each time step.

In this paper, we explore an alternative to Monte Carlo integration and employ instead Gauss quadrature, which provides accurate quadrature rules that converge rapidly in the number of quadrature points, under smoothness criterion on the integrand. The idea then is to replace Q_n by an m_n -point Gauss quadrature and thereby reduce the number of points that we follow with the time stepping. That is, we propagate weights w_n^i and quadrature points x_n^i of an m_n -point rule Q_n , and approximate

$$P_1^{\mu}(\phi) \approx Q_N(\phi) \coloneqq \sum_{i=1}^{m_N} w_N^i \phi(x_N^i), \qquad t_N = 1$$

We derive a choice of m_n in section 4 that gives first-order convergence for smooth problems. The computation of the Gauss-quadrature rules is very efficient using standard algorithms [12, 10, 4]. This leads to numerical methods for mean-field SDEs that are very efficient and we find methods that require $\mathcal{O}(|\log \epsilon|^3/\epsilon)$ work to achieve accuracy ϵ for mean-field SDEs with smooth coefficients and initial distributions (see Theorem 5.3). This compares favorably with the $\mathcal{O}(1/\epsilon^2)$ work required for multilevel Monte Carlo methods, as we see in section 6.1.

Mean-field SDEs arise as reduced-order models for systems of interacting particles. The drift and diffusion are defined in terms of the distribution of X(t), so that moments of X(t) can be included in their definition. In other words, the interaction with the ensemble of particles is approximated by moments and mean-field SDEs, including one-dimensional mean-field SDEs, are of interest in studying high-dimensional systems. The techniques in this paper apply to mean-field SDEs in one spatial dimension, as Gauss quadrature is most natural for integrals over the real line, where algorithms are readily available to compute the quadrature rule. In principle, the methods and theory extend to higher dimensions, though it would be difficult to compute a suitable cubature rule. It would require a cubature rule that can be easily computed and satisfies Gauss-quadrature-type error estimates (see Theorem 2.2). These are currently unavailable (see [27] for a recent discussion of Gaussian cubature).

This paper is organized as follows: section 2 reviews key facts about Gauss quadrature and develops preliminary lemmas. Section 3 describes the method for Gauss quadrature with Euler–Maruyama time stepping, which we call the GQ1 method. The error analysis for stochastic ODEs is developed in section 4, where we show how to choose the number m_n of Gauss points. In section 5, we extend the error analysis to mean-field SDEs and modify the choice of m_n for this case. We also discuss a straightforward generalization of the methodology to the initial-value problem for

(3)
$$X^{\mu}(t) - X^{\mu}(0) = \int_{0}^{t} A\left(\int_{\mathbb{R}} a(X^{\mu}(s), y) P_{s}^{\mu}(dy)\right) ds + \int_{0}^{t} B\left(\int_{\mathbb{R}} b(X^{\mu}(s), y) P_{s}^{\mu}(dy)\right) dW(s),$$

for smooth functions $A, B: \mathbb{R} \to \mathbb{R}$, which allows a nonlinear dependence on the time-*t* distribution. In section 6, we describe two extensions of GQ1: namely, GQ1e, which uses GQ1 with extrapolation, and GQ2, which use Gauss quadrature with a second-order time-stepping method. The remainder of the section gives a number of numerical experiments, including a comparison with the multilevel Monte Carlo method for ordinary SDEs.

1.1. Notation. For a measure μ on \mathbb{R} and an integrable function $\phi \colon \mathbb{R} \to \mathbb{R}$, denote $\mu(\phi) \coloneqq \int_{\mathbb{R}} \phi(x) \, \mu(dx)$. Let $C^k(\mathbb{R}^d)$ denote the space of k-times continuously differentiable real-valued functions on \mathbb{R}^d and $F^{k,\beta} \coloneqq \{\phi \in C^k(\mathbb{R}^d) \colon \|\phi\|_{k,\beta} < \infty\}$, where

$$\left\|\phi\right\|_{k,\beta} \coloneqq \max_{0 \le |\alpha| \le k} \sup_{x \in \mathbb{R}^d} \frac{\left|\phi^{(\alpha)}(x)\right|}{1 + \left|x\right|^{\beta}}$$

using the multi-index notation. Let $C_K^k(\mathbb{R}^d) \coloneqq \{\phi \in C^k(\mathbb{R}^d) \colon \|\phi^{(\alpha)}\|_{\infty} \leq K, 0 \leq |\alpha| \leq k\}$, where $\|\cdot\|_{\infty}$ denotes the supremum norm. Throughout the paper, we use c as a generic constant that varies from place to place.

2. Gauss quadrature and error estimates. Before describing the algorithm, we review Gauss quadrature and associated error estimates. Let \mathcal{P}_n denote the polynomials up to degree n.

DEFINITION 2.1 (Gauss quadrature). We say weights $w^i > 0$ and points $x^i \in \mathbb{R}$ for i = 1, ..., m define an m-point Gauss-quadrature rule with respect to a measure μ

on \mathbb{R} if

$$\int_{\mathbb{R}} p(x) \,\mu(dx) = \sum_{i=1}^{m} w^i \, p(x^i) \qquad \forall \, p \in \mathcal{P}_{2m-1}.$$

The m-point Gauss-quadrature rule for a discrete measure

$$\mu = \sum_{i=1}^{N} v^i \,\delta_{y^i},$$

with weights $v^i > 0$ and points y^i , can be found via the three-term recurrence relation for the orthogonal polynomials corresponding to the inner product $\langle f, g \rangle_{\mu} := \int_{\mathbb{R}} f(x) g(x) \mu(dx)$. First, form the matrix A with diagonal $[1, y^1, \ldots, y^N]$ and first row and column given by $[1, \sqrt{v^1}, \ldots, \sqrt{v^N}]$ (all other entries zero). By applying orthogonal transformations, reduce A to a symmetric tridiagonal matrix with diagonal $[\alpha^0, \alpha^1, \ldots, \alpha^N]$ and off-diagonal $[\beta^0, \beta^1, \ldots, \beta^N]$. The α^i and β^i define the three-term recurrence relation. Next, define the Jacobi matrix, which is the symmetric tridiagonal matrix with diagonal $[\alpha^0, \alpha^1, \ldots]$ and off-diagonals $[\sqrt{\beta^0}, \sqrt{\beta^1}, \ldots]$. To find the mpoint Gauss-quadrature rule, the leading $m \times m$ submatrix of the Jacobi matrix should be chosen. Its eigenvalues determine the quadrature points and the first component of the normalized eigenvectors determines the weights, as given by the well-known Golub–Welsch algorithm. See [4, 12, 10].

Thus, to compute the *m*-point Gauss-quadrature rule for an *N*-point discrete measure, we reduce the original matrix $(N + 1) \times (N + 1)$ matrix *A* to tridiagonal form using a Lanczos procedure and solve a symmetric eigenvalue problem for an $m \times m$ matrix. The complexity is $\mathcal{O}(N^2 + m^3)$, which becomes burdensome when either *m* or *N* is large. It is the rapid convergence properties of Gauss quadrature that enable us to control the problem size.

Let us describe the errors for Gauss quadrature. For an integrable function $\phi \colon \mathbb{R} \to \mathbb{R}$, denote the approximation error

$$E(\phi) = \int_{\mathbb{R}} \phi(x) \,\mu(dx) - \sum_{i=1}^{m} w^i \,\phi(x^i).$$

THEOREM 2.2. Let $\phi \in C^{2m}(\mathbb{R})$. The error for m-point Gauss quadrature is

$$E(\phi) = \frac{\phi^{(2m)}(\xi)}{(2m)!} \langle p_m, p_m \rangle_{\mu} \qquad \forall \phi \in C^{2m}(\mathbb{R}),$$

for some $\xi \in \mathbb{R}$, where $\langle p_m, p_m \rangle_{\mu} = \int_{\mathbb{R}} p_m(x)^2 \mu(dx)$, $p_m(x) = (x - x^1) \cdots (x - x^m)$, and x^i are the Gauss-quadrature points.

Proof. See [24, Theorem 3.6.24] for the proof.

This theorem shows that Gauss quadrature converges rapidly as the number of points $m \to \infty$ for smooth integrands ϕ . We require the following alternative characterization of the error in terms of a minimax polynomial. A similar result is available for continuous measures in [3, Theorem 5.4].

THEOREM 2.3. Consider a discrete probability measure $\mu = \sum_{i=1}^{N} v^i \, \delta_{y^i}$ and approximation by the m-point Gauss-quadrature rule $\sum_{i=1}^{m} w^i \, \delta_{x^i}$. The absolute error

$$|E(\phi)| \le \min_{p \in \mathcal{P}_{2m-1}} \left| \max_{i=1,\dots,N} |p(y^i) - \phi(y^i)| + \max_{i=1,\dots,m} |p(x^i) - \phi(x^i)| \right|.$$

Proof. Let $p \in \mathcal{P}_{2m-1}$. As *m*-point Gauss quadrature is exact for $p \in \mathcal{P}_{2m-1}$,

$$E(\phi) = E(\phi - p) = \sum_{i=1}^{N} v^{i} (\phi - p)(y^{i}) - \sum_{i=1}^{m} w^{i} (\phi - p)(x^{i})$$

so that

$$|E(\phi)| \le \sum_{i=1}^{N} v^{i} \max_{i=1,\dots,N} |\phi(y^{i}) - p(y^{i})| + \sum_{i=1}^{m} w^{i} \max_{i=1,\dots,m} |\phi(x^{i}) - p(x^{i})|.$$

Since $\sum_{j=1}^{N} v^{i} = \sum_{j=1}^{m} w^{i} = 1$, this completes the proof.

For the numerical solution of SDEs, we are interested in the discrete measure generated by applying Euler–Maruyama with a two-point approximation to the Gaussian increment, which increases the number of points in the support by a factor of two on each step. Using the resulting tree structure, the support can be grouped into points that stem from a smaller set of points. We write down a special error estimate in this setting.

COROLLARY 2.4. Let μ be a discrete measure with support $\{y^1, \ldots, y^{Nm}\}$ and consider approximation by m-point Gauss quadrature. Suppose that there exists z^i such that

$$\max_{j=(i-1)N+1,...,iN} |z^{i} - y^{j}| \le \delta \quad for \ i = 1,...,m.$$

Then,

$$|E(\phi)| \le \delta (2R)^{2m-1} \frac{1}{(2m)!} \sup_{x \in (-R,R)} |\phi^{(2m)}(x)| \qquad \forall \phi \in C^{2m}(\mathbb{R}),$$

where $R = \max\{|z^i|, |y^j|: i = 1, \dots, m, j = 1, \dots, Nm\}.$

Proof. Consider interpolation of ϕ by $p \in \mathcal{P}_{2m-1}$ based on the 2m interpolation points $z^1, \ldots, z^m, x^1, \ldots, x^m$, where x^i denote the Gauss-quadrature points. The error at y^j satisfies

$$p(y^{j}) - \phi(y^{j}) = \left[(y^{j} - z^{1}) \cdots (y^{j} - z^{m}) (y^{j} - x^{1}) \cdots (y^{j} - x^{m}) \right] \frac{1}{(2m)!} \phi^{(2m)}(\xi),$$

for some $\xi \in (-R, R)$ (by standard error analysis for Lagrange interpolation). In the product, for each j, one term is bounded by δ . Each $|y^j - z^i| \leq 2R$ by definition of R. Hence,

$$\max_{j} \left| p(y^{j}) - \phi(y^{j}) \right| \le \delta \left(2R \right)^{2m-1} \frac{1}{(2m)!} \sup_{x \in (-R,R)} \left| \phi^{(2m)}(x) \right|.$$

The polynomial p is exact at x^i and Theorem 2.3 completes the proof.

3. GQ1: Gauss quadrature with Euler–Maruyama. We now explain our method in detail: initialize Q_0 with a discrete approximation,

$$Q_0 = \sum_{i=1}^{m_0} w_0^i \,\delta_{x_0^i},$$

to the initial distribution μ . In the case that $\mu = \delta_x$ or $X^{\mu}(0) = x$ for some known $x \in \mathbb{R}$, take the one-point quadrature rule with $x_0^1 = x$, weight $w_0^1 = 1$, and $m_0 = 1$.

Suppose that the weights w_n^i and points x_n^i of Q_n are known at step n. To determine Q_{n+1} , generate the Euler-Maruyama points $X_{n+1}^{i\pm}$ defined by

(4)
$$X_{n+1}^{i\pm} = x_n^i + Q_n(a(x_n^i, \cdot)) \Delta t \pm Q_n(b(x_n^i, \cdot)) \Delta t^{1/2}, \quad i = 1, \dots, m_n$$

and define the corresponding weights $W_{n+1}^{i\pm} = w_n^i/2$. Together the points $X_{n+1}^{i\pm}$ and weights $W_{n+1}^{i\pm}$ define a $2m_n$ -point quadrature rule, which we denote Q_{n+1}^{\pm} . If left unchecked, this leads to a 2^n -factor increase in the size of the quadrature rule, which becomes costly.

At each step, we may continue with $Q_{n+1} = Q_{n+1}^{\pm}$ (if the number of points is acceptable or the final time is reached) or approximate and reduce the number of points using Gauss quadrature. To approximate, we use the following algorithm.

Algorithm 1

- 1. Choose a support [-R, R].
- 2. For $|X_{n+1}| \ge R$, generate two points at $\pm R$ with weights $\sum_{\pm X_{n+1}^j \ge R} W_{n+1}^j$.
- 3. For $|X_{n+1}| < R$, generate the m_{n+1} -point Gauss-quadrature rule for the measure Q_{n+1}^{\pm} restricted to (-R, R) (i.e., for the measure $Q_R(\cdot) = Q_{n+1}^{\pm}(\cdot \cap (-R, R)))$.
- 4. Combine the points and weights, to define an $(m_{n+1}+2)$ -point quadrature rule Q_{n+1} .

The iteration is repeated until the final time is reached.

Following an error analysis in the next sections, we give formulas for the number of points m_n and support radius R in terms of Δt and t_n . First, we establish conditions for boundedness of moments for Q_n .

LEMMA 3.1. Suppose that $a, b \in C_K^0(\mathbb{R}^2)$ and that $Q_0(e^{\alpha x^2}) < \infty$ for some $\alpha > 0$. Then, for some $c, \lambda > 0$ independent of Δt ,

$$Q_n(e^{\lambda x^2}) \le c \qquad \forall t_n \le 1$$

Proof. Consider Ψ defined in (2) where ξ is the two-point random variable given by $\mathbb{P}(\xi = \pm 1) = 1/2$. Let $X_{n+1} = \Psi(X, \Delta t, Q_n)$ for a fixed value X. Then

$$\begin{split} X_{n+1}^2 &\leq X^2 + 2\,\Delta t\,Q_n(a(X,\cdot))\,X + \Delta t^2\,Q_n(a(X,\cdot))^2 + \Delta t\,Q_n(b(X,\cdot))^2 \\ &\quad + 2(X + \Delta t\,Q_n(a(X),\cdot))\,Q_n(b(X,\cdot))\sqrt{\Delta t}\,\xi \\ &\leq X^2 + \Delta t\,Q_n(a(X,\cdot))\,(X^2 + 1) + \Delta t^2\,Q_n(a(X,\cdot))^2 + \Delta t\,Q_n(b(X,\cdot))^2 \\ &\quad + 2\,(X + \Delta t\,Q_n(a(X,\cdot)))\,Q_n(b(X,\cdot))\,\sqrt{\Delta t}\,\xi. \end{split}$$

Hence, as a, b are bounded by K,

$$\begin{split} X_{n+1}^2 &\leq X^2 \left(1 + \Delta t \, K \right) + \Delta t \, K + \Delta t^2 \, K^2 + \Delta t \, K^2 \\ &\quad + 2 \left(X + \Delta t \, Q_n(a(X, \cdot)) \right) Q_n(b(X, \cdot)) \sqrt{\Delta t} \, \xi \\ &\leq X^2 \left(1 + K \, \Delta t \right) + c \, \alpha \, \Delta t + 2 \left(X + \Delta t \, Q_n(a(X, \cdot)) \right) Q_n(b(X, \cdot)) \sqrt{\Delta t} \, \xi \end{split}$$

Note that $(e^x + e^{-x})/2 \le e^{x^2}$ for $x \in \mathbb{R}$ and

$$\mathbb{E}\left[e^{\alpha X_{n+1}^2}\right] \le e^{\alpha X^2 (1+\Delta t K) + c \alpha \Delta t} e^{4 \alpha^2 (X+\Delta t Q_n(a(X,\cdot)))^2 \Delta t Q_n(b(X,\cdot))^2}$$

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Now
$$|(X + \Delta t Q_n(a(X, \cdot)))^2 Q_n(b(X, \cdot))^2| \le 2K^2 X^2 + 2\Delta t^2 K^4$$
. Consequently,
(5) $\mathbb{E}\left[e^{\alpha X_{n+1}^2}\right] \le e^{\alpha X^2 (1+c\Delta t+c\Delta t\alpha)+c\alpha \Delta t+c\Delta t^3\alpha^2}.$

Algorithm 1 is used in the iteration, so that the support is reduced and Gauss quadrature is applied. Note that

$$Q(e^{\alpha x^2}) \leq \int_{\mathbb{R}} e^{\alpha x^2} \, \mu(dx), \qquad \alpha > 0,$$

where Q is a Gauss-quadrature rule for μ (by applying Theorem 2.2 and noting that even derivatives of $e^{\alpha x^2}$ are nonnegative). Similarly, the support reduction moves mass inwards and the resulting integral of $e^{\alpha x^2}$ is reduced. Consequently, if $X \sim Q_n$ in (5), we have

$$Q_{n+1}(e^{\alpha x^2}) \le Q_n(e^{\alpha (1+c\,\Delta t+c\,\Delta t\,\alpha)x^2}) e^{c\,\alpha\,\Delta t(1+\Delta t^2\,\alpha)}.$$

We can iterate this to find a bound on $Q_n(e^{\alpha x^2})$ in terms of $Q_0(e^{\alpha x^2})$. The value of α changes at each step of the iteration, and

$$Q_{n+1}(e^{\alpha_0 x^2}) \le Q_n(e^{\alpha_1 x^2}) e^{c \alpha_0 \Delta t (1 + \Delta t^2 \alpha_0)},$$

where $\alpha_1 = \alpha_0 (1 + c \Delta t) + c \Delta t \alpha_0^2$.

Let $\alpha_{n+1} = \alpha_n (1 + c \Delta t) + c \Delta t \alpha_n^2$. If $\alpha_n \leq 1$, then $\alpha_{n+1} \leq \alpha_n (1 + 2c \Delta t) \leq \alpha_0 (1 + 2c \Delta t)^n \leq \alpha_0 e^{2ct_n}$. We see that if $\alpha_0 \leq e^{-2c}$, then $\alpha_n \leq e^{2ct_n} \alpha_0 \leq 1$ for $t_n \leq 1$. It is now easy to show that

$$Q_n(e^{\alpha_0 x^2}) \le Q_{n-m}(e^{\alpha_m x^2}) e^{2c},$$

for $t_n \leq 1$ and any $\alpha_0 \leq e^{-2c}$. In particular, $Q_n(e^{\lambda x^2}) \leq Q_0(e^{\alpha x^2})e^{2c}$ for $\lambda \leq e^{-2c} \min\{\alpha, 1\}$.

We examine the error incurred reducing the support to [-R, R].

LEMMA 3.2. Let μ be a probability measure on \mathbb{R} and suppose that $\mu(e^{\lambda x^2}) < K$, for some $\lambda > 0$. For $\Delta t > 0$, define the measure $\mu_{\Delta t}$ by

$$\mu_{\Delta t}(A) := \mu(A \cap 1_{(-R,R)}) + \mu((-\infty, -R])\,\delta_{-R}(A) + \mu([R,\infty))\,\delta_{R}(A),$$

for $R = \sqrt{(4/\lambda) |\log \Delta t|}$ and Borel sets $A \subset \mathbb{R}$. There exists c > 0, independent of Δt , such that

$$\left|\mu(\phi) - \mu_{\Delta t}(\phi)\right| \le c \left\|\phi\right\|_{0,\beta} \Delta t^2 \qquad \forall \phi \in F^{0,\beta}$$

Proof. It suffices to consider the two measures μ and $\mu_{\Delta t}$ on the tail $(-R, R)^c$, as they are equal on (-R, R). First, note that

$$\left| \mu(1_{(-R,R)^{c}} \phi) \right| \le e^{-\lambda R^{2}/2} \, \mu(\Phi), \qquad \Phi(x) \coloneqq e^{\lambda x^{2}} \, e^{-\lambda x^{2}/2} \, 1_{(-R,R)^{c}}(x) \, \left| \phi(x) \right|,$$

where 1_S denotes the indicator function on the set S. As $\phi \in F^{0,\beta}$, $|\phi(x)| \leq ||\phi||_{0,\beta} (1 + |x|^{\beta})$ and $|e^{-\lambda x^2/2} \phi(x)|$ is uniformly bounded by $c ||\phi||_{0,\beta}$ for a constant c independent of R and ϕ , but dependent on β and λ . Hence,

$$\left| \mu(1_{(-R,R)^{c}} \phi) \right| \le c \left\| \phi \right\|_{0,\beta} e^{-\lambda R^{2}/2} \, \mu(e^{\lambda x^{2}}) \le c \left\| \phi \right\|_{0,\beta} e^{-\lambda R^{2}/2}$$

For $R = \sqrt{(4/\lambda) |\log \Delta t|}$, we see that $e^{-\lambda R^2/2} \leq \Delta t^2$. Hence, $|\mu(1_{(-R,R)^c}\phi)|$ is bounded by $c \|\phi\|_{0,\beta} \Delta t^2$. The same applies to $|\mu_{\Delta t}(1_{(-R,R)^c}\phi)|$ by a similar argument and the proof is complete.

Thus, the support reduction with $R = \sqrt{(4/\lambda) |\log \Delta t|}$ maintains accuracy if $\mu(e^{\lambda x^2})$ is finite and the test function grows polynomially. Next, we estimate the error for the Gauss quadrature at step n.

LEMMA 3.3. Suppose that $a, b \in C_K^0(\mathbb{R}^2)$. Let $Q_R(\cdot) = Q_{n+1}^{\pm}(\cdot \cap (-R, R))$ and let Q be the m_{n+1} -point Gauss-quadrature rule approximating Q_R . If $m_{n+1} \ge m_n$, for all $\phi \in C^{2m_n}(\mathbb{R})$,

$$\left|Q_{R}(\phi) - Q(\phi)\right| \le K \left(2R\right)^{2m_{n}-1} \Delta t^{1/2} \frac{1}{(2m_{n})!} \sup_{x \in (-R,R)} \left|\phi^{(2m_{n})}(x)\right|.$$

Proof. If both $X_{n+1}^{j\pm}$ belong to (-R, R), let $z^j = x^j + Q_n(a(x^j, \cdot)) \Delta t$. Then

(6)
$$\left|X_{n+1}^{j\pm} - z^{j}\right| \le \left|Q_{n}(b(x^{j}, \cdot))\right| \Delta t^{1/2} \le K \Delta t^{1/2}$$

and $|z^j| \leq R$ (every z^j lies half way between $X_{n+1}^{j\pm}$). If only one $X_{n+1}^{j\pm} \in (-R, R)$, let z^j be that point. The measure Q_R has at most $2m_n$ points and we apply Corollary 2.4 with N = 2 and $\delta = K \Delta t^{1/2}$. In general, Q_R may have less than $2m_n$ points and we should trivially extend Q_R to apply Corollary 2.4 (i.e., extend Q_R to a $2m_{n+1}$ -point rule by adding zero-weighted points in (-R, R) consistent with (6)).

COROLLARY 3.4. Let $a, b \in C_K^0(\mathbb{R})$. Let Q be the m_{n+k} -point Gauss-quadrature rule for $Q_R(\cdot) = Q_{n+k}^{\pm}(\cdot \cap (-R, R))$ (i.e., after not performing Algorithm 1 (k-1)times). Suppose that $m_{n+k} \ge m_n$. For each k, there exists c > 0 such that, for all $\phi \in C^{2m_n}(\mathbb{R})$,

$$\left|Q_{R}(\phi) - Q(\phi)\right| \le c \left(2R\right)^{2m_{n}-1} \Delta t^{1/2} \frac{1}{(2m_{n})!} \sup_{x \in (-R,R)} \left|\phi^{(2m_{n})}(x)\right|.$$

Proof. This is a simple extension of Lemma 3.3 using Corollary 2.4.

4. Error analysis for ordinary SDEs. The proposed algorithm has much in common with those introduced by [22]. In that paper, Ito–Taylor methods for a general class of multidimensional SDEs are developed that use support-reduction strategies to improve efficiency. They reduce the support of the measure by reducing its diameter and eliminating points whilst maintaining moment conditions. Along with a nonuniform time-stepping regime, the authors provide detailed error and complexity analyses. The present situation is similar and effectively we are transplanting Algorithm 1 for their reduction strategies. Using appropriate Gauss-quadrature error estimates, much of their analysis applies in the present case.

The estimate in Corollary 3.4 depends on the radius R of the support. We now choose $R = \sqrt{(4/\lambda) |\log \Delta t|}$, for λ given by Lemma 3.1. Fix k (the number of steps between applying Algorithm 1) and β (to choose test functions $\phi \in F^{0,\beta}$).

PROPOSITION 4.1. Let $R = \sqrt{(4/\lambda) |\log \Delta t|}$ in Algorithm 1. Then, for all $\phi \in F^{0,\beta} \cap C^{2m_n}(\mathbb{R})$,

$$\begin{aligned} \left| Q_{n+k}^{\pm}(\phi) - Q_{n+k}(\phi) \right| &\leq c \,\Delta t^{1/2} \left| \frac{16}{\lambda} \log \Delta t \right|^{\frac{2m_n - 1}{2}} \frac{1}{(2m_n)!} \\ &\times \sup_{x \in (-R,R)} \left| \phi^{(2m_n)}(x) \right| + c \left\| \phi \right\|_{0,\beta} \Delta t^2. \end{aligned}$$

Proof. The error due to the Gauss quadrature on (-R, R) is described by Corollary 3.4. Applying Lemma 3.1 with Lemma 3.2, the error due to the support reduction is bounded by $c \|\phi\|_{0,\beta} \Delta t^2$. Summing the two gives the desired upper bound.

Given $\Delta t > 0$ and a $k \in \mathbb{N}$, we choose the number of points m_n as the smallest nonnegative integer such that

(7)
$$\log \Gamma(2m_n + 1) \ge M_1(m_n, \Delta t, n+k) \quad \forall t_{n+k} < 1,$$

where $\Gamma(x)$ denotes the gamma function and (8)

$$M_p(m,\Delta t,n) \coloneqq \left(p + \frac{1}{2}\right) \left|\log \Delta t\right| + \frac{2m - 1}{2} \log \left|\frac{16}{\lambda} \log \Delta t\right| + (m - 2) \left|\log(1 - t_n)\right|.$$

We now describe how fast m_n increases as Δt decreases. Assuming the Golub–Welsch algorithm takes $\mathcal{O}(m^3)$ operations, $\sum_n m_n^3$ gives the amount of work needed to apply Algorithm 1 at every time step and we describe its growth.

THEOREM 4.2. The number of Gauss-quadrature points m_n is a nondecreasing function of n. As the time step decreases, m_n is nondecreasing. The number of points m_n for Q_n satisfies

$$m_n \le 1 + \max\left\{\frac{3}{4} \left|\log \Delta t\right|, \frac{e^2}{2} \sqrt{\frac{16 \left|\log \Delta t\right|}{\lambda \left(1 - t_n\right)}}\right\}.$$

In particular, $\sum_{t_n < 1} m_n^3 = \mathcal{O}((|\log \Delta t| / \Delta t)^{3/2}).$

Proof. The function M_1 is increasing in n (via $t_n \in (0, 1)$) for $m \ge 2$. Hence, m_n is nondecreasing in n (m_n is discrete and may not change as t_n is varied by small amounts). Also, for fixed t_n , M_1 is a decreasing function of Δt , and hence m_n is nondecreasing as Δt decreases. From (8),

$$M_1(m, \Delta t, n) \le \frac{3}{2} \left| \log \Delta t \right| + m \log \frac{16 \left| \log \Delta t \right|}{\lambda \left(1 - t_n \right)}$$

Stirling's formula [1, eq. 6.1.37] tells us that

$$x! = \Gamma(x+1) = \sqrt{2\pi} x^{x+1/2} \exp\left(-x + \frac{\theta}{12x}\right), \quad \text{for some } \theta \in (0,1),$$

and hence $\log|(2m)!| = \log \Gamma(2m+1) \ge \frac{1}{2} \log(4\pi m) + 2m (\log(2m) - 1)$. Then,

$$\log \Gamma(2m+1) \ge 2m + 2m \left(\log(2m) - 2 \right) = 2m + m \log \frac{4m^2}{e^4}.$$

If $m \ge (3/4) |\log \Delta t|$ and $m \ge (e^2/2) \sqrt{16 |\log \Delta t|/(\lambda (1-t_n))}$, then $\log \Gamma(2m+1) \ge M_1(m, \Delta t, n)$. Hence, as $\sum_{k=1}^{\infty} k^{-3/2}$ is finite,

$$\sum_{t_n < 1} m_n^3 \le c \left(\frac{16 \left| \log \Delta t \right|}{\lambda \Delta t} \right)^{3/2}.$$

We now give the main convergence theorem for ordinary SDEs. In this case, the coefficients a(x, y) and b(x, y) are independent of the mean-field y. We choose the single-point initial distribution $\mu = \delta_x$ and write X(t) for $X^{\mu}(t)$ and P_t^x for $P_t^{\delta_x}$.

Assumption 4.3. Suppose that $K \ge 1 \ge \lambda > 0$ and assume that $x_0 \in [-K, K]$ and $a, b \in C_K^4(\mathbb{R})$ and $b^2(x) \ge \lambda$ for all $x \in \mathbb{R}$.

THEOREM 4.4. Let Assumption 4.3 hold. Consider the m_n -point Gauss-quadrature rule Q_n defined in Algorithm 1 with m_n given by (7) and $R = \sqrt{(4/\lambda)|\log \Delta t|}$. The total error satisfies

$$\left|P_{1}^{x}(\phi) - Q_{N}(\phi)\right| \leq \begin{cases} c \left\|\phi\right\|_{2,\beta} \left(1 + |x|^{c}\right) \Delta t \left|\log \Delta t\right| & \forall \phi \in F^{2,\beta}, \\ c \left\|\phi\right\|_{3,\beta} \left(1 + |x|^{c}\right) \Delta t & \forall \phi \in F^{3,\beta}, \end{cases}$$

for a constant c independent of K.

Proof. Let $g_n(x) \coloneqq P_{1-t_n}^x(\phi) \equiv \mathbb{E}[\phi(X(1-t_n)) | X(0) = x]$ for $x \in \mathbb{R}$. Notice that $g_N = \phi$ and $g_0(x) = P_1^x(\phi)$. Let $T_{\Delta t}(\phi)(x) = \mathbb{E}[\phi(\Psi(x, \Delta t, \cdot))]$ for Ψ defined in (2). The total error

$$P_1^x(\phi) - Q_N(\phi) = \sum_{n=1}^N E_n^T + \sum_{n=1}^N E_n^G,$$

where $E_n^G = Q_n^{\pm}(g_n) - Q_n(g_n)$ (the error due to Algorithm 1) and $E_n^T = Q_{n-1}(g_{n-1}) - Q_n^{\pm}(g_n) = Q_{n-1}(P_{\Delta t}^x(g_n)) - Q_{n-1}(T_{\Delta t}(g_n))$ (the bias error due to Euler–Maruyama over time step Δt). We estimate the two sources of error, focusing on the case where $\phi \in F^{2,\beta}$.

Local truncation error: Under Assumption 4.3, [22, eq. (35) with $\gamma = 1$] shows that E_n^T satisfies

$$\left| E_{n}^{T} \right| \leq \begin{cases} c \left\| \phi \right\|_{4,\beta} \left(1 + \left| x \right|^{c} \right) \frac{\Delta t^{2}}{1 - t_{n}}, & n = 1, \dots, N - 1, \\ c \left\| \phi \right\|_{2,\beta} \left(1 + \left| x \right|^{c} \right) \Delta t, & n = N. \end{cases}$$

Algorithm 1 error: We do not apply Algorithm 1 on the final step and so $E_N^G = 0$. For n = 1, ..., N - 1, Proposition 4.1 gives that

$$|E_n^G| = |Q_n^{\pm}(g_n) - Q_n(g_n)| \le c \left\| g_n^{(2m_{n-k})} \right\|_{\infty} \frac{1}{(2m_{n-k})!} \Delta t^{1/2} \left| \frac{16}{\lambda} \log \Delta t \right|^{\frac{2m_{n-k}-1}{2}} + c \left\| \phi \right\|_{0,\beta} \Delta t^2.$$

In [22, Lemma 8] it is provided that

$$\|g_n\|_{k,\beta} \le \|\phi\|_{2,\beta} \frac{1}{(1-t_n)^{(k-2)/2}} \qquad \forall k \ge 4.$$

Consequently,

$$\left| E_n^G \right| \le c \left\| \phi \right\|_{2,\beta} \frac{1}{(1-t_n)^{m_{n-k}-1}} \frac{1}{(2m_{n-k})!} \Delta t^{1/2} \left| \frac{16}{\lambda} \log \Delta t \right|^{\frac{2m_{n-k}-1}{2}} + c \left\| \phi \right\|_{0,\beta} \Delta t^2.$$

Notice that

$$\frac{1}{(1-t_n)^{m_{n-k}-1}} \frac{1}{(2m_{n-k})!} \Delta t^{1/2} \left| \frac{16}{\lambda} \log \Delta t \right|^{\frac{2m_{n-k}-1}{2}} \le \frac{1}{(1-t_n)} \Delta t^2$$

if

$$\Gamma(2m_{n-k}+1) \ge \Delta t^{-3/2} \left| \frac{16}{\lambda} \log \Delta t \right|^{\frac{2m_{n-k}-1}{2}} \frac{1}{(1-t_n)^{m_{n-k}-2}}.$$

This holds as we have chosen m_{n-k} satisfies $\log \Gamma(2m_{n-k}+1) \ge M_1(m_{n-k}, \Delta t, n)$, for

 M_1 defined in (8). Then, $|E_n^G| \leq c (\|\phi\|_{2,\beta} + 1) \Delta t^2 / (1 - t_n)$. Summing all the errors and using $\sum_{n=1}^{N-1} \Delta t / (1 - t_n) \leq \log(N) = |\log \Delta t|$, we complete the proof. For $\phi \in F^{3,\beta}$, the argument is similar except the $(1 - t_n)$ factors do not arise and so the $|\log \Delta t|$ term does not appear. П

5. Error analysis for mean-field SDEs. We now generalize our error analysis to mean-field SDEs. We wish to show that Q_n approximates $P_{t_n}^{\mu}$, starting from a good approximation of the initial distribution, $Q_0 \approx \mu$. To express the closeness of Q_0 to μ , we use the Wasserstein distance. For any probability measures μ, ν on \mathbb{R} , define the Wasserstein distance

$$W_{k,\beta}(\mu,\nu) \coloneqq \sup \left\{ \left| \mu(\phi) - \nu(\phi) \right| \colon \left\| \phi \right\|_{k,\beta} \le 1 \right\}.$$

ASSUMPTION 5.1. The initial measure Q_0 satisfies $Q_0(e^{\alpha x^2}) < \infty$ for some $\alpha > 0$ independent of Δt and approximates μ in the sense that $W_{2,\beta}(\mu, Q_0) \leq c \Delta t$.

Under this assumption, Lemma 3.1 applies and $Q_n(e^{\lambda x^2})$, for $t_n \leq 1$, is uniformly bounded for some $\lambda > 0$. We choose $R = \sqrt{(4/\lambda) |\log \Delta t|}$ in Algorithm 1.

We introduce a nonautonomous SDE corresponding to the mean-field SDE with $P_t^{\mu}(a(X,\cdot))$ and $P_t^{\mu}(b(X,\cdot))$ treated as known functions of (X,t). Let X(t;s,x) for $t \geq s$ denote the solution of

(9)
$$dX = \bar{a}(X,t) dt + \bar{b}(X,t) dW(t), \qquad X(s;s,x) = x$$

for $\bar{a}(X,t) \coloneqq P_t^{\mu}(a(X,\cdot))$ and $\bar{b}(X,t) \coloneqq P_t^{\mu}(b(X,\cdot))$. Here we fix the initial distribution as a delta measure at x and keep the same measure P_t^{μ} from (1) for the mean fields. Note that $\int_{\mathbb{R}} \mathbb{E}[\phi(X(t;0,x))] \mu(dx) = P_t^{\mu}(\phi)$, so that $P_t^{\mu}(\phi) = \mu(P_{0,t}(\phi))$ for $P_{s,t}(\phi)(x) \coloneqq \mathbb{E}[\phi(X(t;s,x))]$. In this notation, we drop the μ superscript, even though the nonautonomous SDE depends on μ via the drift and diffusion.

In the following assumption on the drift and diffusion, the mean-field diffusion bis used to set a nondegeneracy condition.

Assumption 5.2. Suppose that $a, b \in C_K^4(\mathbb{R}^2)$ and, for some $K \ge 1 \ge \lambda > 0$, that $\overline{b}^2(t,x) \ge \lambda$ for $x \in \mathbb{R}$ and $t \in [0,1]$.

The main theorem for the numerical approximation of mean-field SDEs by GQ1 is the following. The method of selecting the number of Gauss points m_n is modified to approximate the distribution uniformly on the time interval. In this case, $m_n \equiv m$ should be chosen independent of n. We choose m as the smallest integer greater than the initial number of points m_0 such that $\log \Gamma(2m+1) \geq M_1(m, \Delta t, n+k)$ where M_1 is given by

(10)
$$M_p^{\rm mf}(m,\Delta t,n) \coloneqq \left(p+m-\frac{3}{2}\right) \left|\log \Delta t\right| + \frac{2m-1}{2} \log \left|\frac{16}{\lambda} \log \Delta t\right|$$

or

(11)
$$M_p^{\text{smooth}}(m, \Delta t, n) \coloneqq \left(p + \frac{1}{2}\right) \left|\log \Delta t\right| + \frac{2m - 1}{2} \log \left|\frac{16}{\lambda} \log \Delta t\right|.$$

The choice of M_1 depends on the regularity of the underlying problem, as described in Theorem 5.4. The time t_n appears on the right-hand side in neither case and m is independent of n. In the following, the overall work for the time-stepping is dominated

by $\sum_{t_n \leq 1} m_n^3$ (the work to compute the Gauss-quadrature rule at each step). The work to compute the initial measure Q_0 is often negligible, for example, if the initial distribution is Gaussian or in other cases where accurate quadrature rules are easily computed.

THEOREM 5.3. Denote the initial number of points for the rule Q_0 by m_0 . For (10),

$$m \le \max\left\{m_0, 1 + \frac{e^2}{2}\sqrt{\frac{8\left|\log\Delta t\right|}{\lambda\,\Delta t}}\right\}$$

If the work to compute Q_0 is $\mathcal{O}(|\log \Delta t|^{3/2}/\Delta t^{5/2})$ and the initial number of points $m_0 = \mathcal{O}(|\log \Delta t|^{1/2}/\Delta t^{1/2})$, then the overall total work is $\mathcal{O}(|\log \Delta t|^{3/2}/\Delta t^{5/2})$. For (11),

$$m \le \max\left\{m_0, 1 + \frac{3}{4} \left|\log \Delta t\right|, 1 + \frac{e^2}{2} \sqrt{\frac{8 \left|\log \Delta t\right|}{\lambda}}\right\}$$

If the work to compute Q_0 is $\mathcal{O}(|\log \Delta t|^3/\Delta t)$ and the initial number of points $m_0 = \mathcal{O}(|\log \Delta t|)$, then the overall total work is $\mathcal{O}(|\log \Delta t|^3/\Delta t)$.

Proof. From (10),

$$M_1^{\mathrm{mf}}(m, \Delta t, n) \le m \log \frac{16 \left| \log \Delta t \right|}{\lambda \, \Delta t}$$

and

$$\log \Gamma(2m+1) \ge 2m + m \log \frac{4m^2}{e^4}$$

If $m \ge (e^2/2)\sqrt{16 |\log \Delta t|/(\lambda \Delta t)}$, then we have $\log \Gamma(2m+1) \ge M_1^{\text{mf}}(m, \Delta t, n)$. Similarly, from (11),

$$M_1^{\text{smooth}}(m, \Delta t, n) \leq \frac{3}{2} \left| \log \Delta t \right| + m \, \log \frac{16 \left| \log \Delta t \right|}{\lambda}$$

If $m \geq (3/4)|\log \Delta t|$ and $m \geq (e^2/2)\sqrt{16|\log \Delta t|/\lambda}$, then we see $\log \Gamma(2m+1) \geq M_1^{\text{smooth}}(m, \Delta t, n)$. The estimate for the total work follows as $\sum_{n=1}^N m^3 = m^3/\Delta t$.

In the following, we show upper bounds on the error for smooth and rough problems, and smooth in this case indicates infinite differentiability, which is much stronger than in Theorem 4.4. This is because infinite differentiability allows the reduction of the number of Gauss points m to $\mathcal{O}(|\log \Delta t|^{1/2})$ from $(|\log \Delta t|/\Delta t)^{1/2}$.

THEOREM 5.4. Let Assumptions 1.1, 5.1, and 5.2 hold and the number of Gauss points m be given by (10). For some c > 0

$$\max_{t_N \le 1} \left| P_{t_N}^{\mu}(\phi) - Q_N(\phi) \right| \le c \left\| \phi \right\|_{2,\beta} \Delta t \left| \log \Delta t \right| \qquad \forall \phi \in F^{2,\beta}.$$

If, in addition to Assumption 1.1, we have $W_{\infty,\beta}(\mu, Q_0) \leq c \Delta t$, and in addition to Assumption 5.2, we have $a, b \in C_K^{\infty}(\mathbb{R}^2)$, and the number of Gauss points m is given by (11), then

(12)
$$\max_{t_N \le 1} \left| P_{t_N}^{\mu}(\phi) - Q_N(\phi) \right| \le c \left\| \phi \right\|_{\infty,\beta} \Delta t \qquad \forall \phi \in F^{\infty,\beta}.$$

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For suitably smooth initial measures μ , the complexity bounds in Theorem 5.3 apply under these hypotheses by choosing Q_0 appropriately. For example, in the nonsmooth case, if μ is the uniform distribution on [a, b], the composite trapezoidal rule, where quadrature weights and points are available explicitly, requires $\mathcal{O}(1/\sqrt{\Delta t})$ points to achieve $\mathcal{O}(\Delta t)$ accuracy for twice-differentiable integrands and provides a suitable Q_0 . In the smooth case, for example, applying Gauss-Hermite quadrature to an initial Gaussian measure requires $m = \mathcal{O}(|\log \Delta t|)$ points to achieve $\mathcal{O}(\Delta t)$ accuracy for smooth integrands (see [13, eq. (8.7.13)] for the relevant error estimate). An *m*-point Gauss-Hermite rule can be used for Q_0 and computed in $\mathcal{O}(m)$ complexity [26], which means Theorem 5.3 implies $\mathcal{O}(|\log \Delta t|^3/\Delta t)$ total work for solving the mean-field SDE to $\mathcal{O}(\Delta t)$ accuracy in the sense of (12).

Before the proof, we develop a sequence of lemmas. First, we show that the Euler–Maruyama step depends continuously on the initial measure μ in terms of the Wasserstein distance.

LEMMA 5.5. Suppose that $a, b \in C_K^k(\mathbb{R}^2)$. There exists c > 0 such that, for any $x \in \mathbb{R}$,

(13)
$$\left| \delta(x) \right| \leq \begin{cases} c \,\Delta t \, \|g\|_{3,\beta} \,(1+|x|^{\beta}) \,W_{k,\beta}(\mu,\nu) & \forall g \in F^{3,\beta}, \\ c \,\Delta t \,\|g\|_{2,\beta} \,(1+|x|^{\beta}) \,(W_{k,\beta}(\mu,\nu)+1) & \forall g \in F^{2,\beta}, \end{cases}$$

where $\delta(x) := \mathbb{E}[g(\Psi(x, \Delta t, \mu))] - \mathbb{E}[g(\Psi(x, \Delta t, \nu))]$ and Ψ is defined by (2).

 $\textit{Proof. Let } x_{\lambda,\mu} = x + \lambda \, \mu(a(x,\cdot)) \, \Delta t + (\lambda \, \mu(b(x,\cdot))) \, \xi \, \sqrt{\Delta t} \text{ and }$

$$\phi(\lambda;g) = g(x_{\lambda,\mu}) - g(x_{\lambda,\nu}).$$

Then $\delta = \mathbb{E}[\phi(1;g)]$ and $\phi(0;g) = 0$ and

$$\phi'(\lambda;g) = g'(x_{\lambda,\mu}) \Big[\mu(a(x,\cdot)) \,\Delta t + \mu(b(x,\cdot)) \,\sqrt{\Delta t} \,\xi \Big] - g'(x_{\lambda,\nu}) \,\Big[\nu(a(x,\cdot)) \,\Delta t + \nu(b(x,\cdot)) \,\sqrt{\Delta t} \,\xi \Big].$$

Note that $\mathbb{E}[\phi'(0;g)] = g'(x)(\mu - \nu)(a(x, \cdot))\Delta t$ as $\mathbb{E}[\xi] = 0$. By Taylor's theorem,

$$\begin{split} \delta &= \mathbb{E} \bigg[\phi(0;g) + \phi'(0;g) + \int_0^1 \phi''(\lambda;g) \,\lambda \,d\lambda \bigg] \\ &= g'(x) \,\Delta t \,(\mu - \nu)(a(x,\cdot)) + \mathbb{E} \bigg[\int_0^1 \phi''(\lambda;g) \,\lambda \,d\lambda \bigg]. \end{split}$$

Now,

$$\begin{aligned} \left|\phi''(\lambda;g)\right| \\ &\leq \left|g''(x_{\lambda,\mu})\right| \left(\left[\mu(a(x,\cdot))\Delta t + \mu(b(x,\cdot))\sqrt{\Delta t}\xi\right]^2 - \left[\nu(a(x,\cdot))\Delta t + \nu(b(x,\cdot))\sqrt{\Delta t}\xi\right]^2\right) \\ &+ \left|g''(x_{\lambda,\mu}) - g''(x_{\lambda,\nu})\right| \cdot \left|\nu(a(x,\cdot))\Delta t + \nu(b(x,\cdot))\sqrt{\Delta t}\xi\right|^2. \end{aligned}$$

Hence, as a, b, ξ are all bounded,

$$|\delta| \le c (1 + |x|^{\beta}) W_{k,\beta}(\mu,\nu) \left(\|g\|_{0,\beta} \Delta t + \|g\|_{2,\beta} \Delta t + \|g\|_{3,\beta} \Delta t \right).$$

This now implies the first equation in (13). The second is similar.

LEMMA 5.6. Let Assumptions 1.1 and 5.2 hold. If $a, b \in C_K^k(\mathbb{R}^2)$, then \bar{a} and \bar{b} belong to $C_K^k(\mathbb{R}^2)$.

Proof. Under Assumption 1.1, P_t^{μ} has a smooth density and \bar{a}, \bar{b} inherit their smoothness from a, b, and the density. The argument is given in more detail in [2, p. 431].

LEMMA 5.7. Let Assumptions 1.1 and 5.2 hold and $g_{n,N} \coloneqq P_{t_n,t_N}\phi$. Then, for nonnegative integers r, k,

$$\|g_{n,N}\|_{k,\beta} \le c \|\phi\|_{r,\beta} \frac{1}{(t_N - t_n)^{(k-\min\{k,r\})/2}} \qquad \forall \phi \in F^{k,\beta}.$$

Proof. For the autonomous case, see [22, Lemma 8]. In this case, the drift and diffusion are nonautonomous. The argument generalizes as [8, Chapter 9, Theorem 7] applies also for time-dependent coefficients with the assumptions given.

The next lemma states a bound on the local truncation error.

LEMMA 5.8. Let Assumptions 1.1 and 5.2 hold. There exists c > 0 such that

$$|P_{t_{n-1},t_n}(\phi)(x) - \mathbb{E}\left[\Psi(x,\Delta t, P_{t_{n-1}}^{\mu})\right]| \le \begin{cases} c \|\phi\|_{4,\beta} \left(1 + |x|^c\right) \Delta t^2 & \forall \phi \in F^{4,\beta}, \\ c \|\phi\|_{2,\beta} \left(1 + |x|^c\right) \Delta t & \forall \phi \in F^{2,\beta}. \end{cases}$$

Proof. When a, b are independent of the second argument, this is implied by [22, Lemma 3 with $\gamma = 1$]. In our case, the drift is $\bar{a}(X, t)$ and diffusion $\bar{b}(X, t)$, which are smooth functions according to Lemma 5.6 and their lemma is easily extended.

Proof of Theorem 5.4. Define the measure $e_N = P_{t_N}^{\mu} - Q_N$ and consider $\phi \in F^{2,\beta}$. Let $g_{n,N} \coloneqq P_{t_n,t_N}(\phi)$, so that $g_{n,n} = \phi$. Decompose the error $e_N(\phi)$ for $N \ge 1$ as

(14)
$$e_N(\phi) = \sum_{n=1}^N E_n^{T_1} + E_n^{T_2} + E_n^G,$$

where $E_n^{T_1}$ represents the error from the Euler–Maruyama discretization of the nonautonomous system, $E_n^{T_2}$ represents the error from the mean-field, and E_n^G represents the error from Algorithm 1 applied to $g_{n,N}$. In detail, let

$$\begin{split} \mathbf{I} &\coloneqq Q_{n-1} \left(P_{t_{n-1},t_n}(P_{t_n,t_N}(\phi)) \right) = \int_{\mathbb{R}} P_{t_{n-1},t_N}(g_{n,N})(x) \, Q_{n-1}(dx), \\ \mathbf{II} &\coloneqq \int_{\mathbb{R}} \mathbb{E} \Big[g_{n,N}(\Psi(x,\Delta t,P_{t_{n-1}}^{\mu})) \Big] \, Q_{n-1}(dx), \\ \mathbf{III} &\coloneqq Q_n^{\pm}(P_{t_n,t_N}(\phi)) = \int_{\mathbb{R}} \mathbb{E} \Big[g_{n,N}(\Psi(x,\Delta t,Q_{n-1})) \Big] \, Q_{n-1}(dx), \\ \mathbf{IV} &\coloneqq Q_n(P_{t_n,t_N}(\phi)), \end{split}$$

where $\mathbb{E}[\cdot]$ denotes the expectation over ξ in the definition of Ψ (see (2)). Consider the telescoping sum

$$e_N(\phi) = \sum_{n=1}^N \Big(Q_{n-1}(P_{t_{n-1},t_N}(\phi)) - Q_n(P_{t_n,t_N}(\phi)) \Big).$$

We have (14) for $E_n^{T_1} = I - II$, $E_n^{T_2} = II - III$, $E_n^G = III - IV$. We estimate the three sources of error in turn. We focus on the rough case (i.e., $\phi \in F^{2,\beta}$) and briefly note the differences with the smooth case.

Local truncation error for nonautonomous SDE: From Lemma 5.8, with n < N,

$$\begin{aligned} \left| \mathbf{I} - \mathbf{II} \right| &= \left| Q_{n-1} \left(P_{t_{n-1}, t_n}(g_{n,N})(x) - \mathbb{E} \left[g_{n,N} (\Psi(x, \Delta t, P_{t_{n-1}}^{\mu})) \right] \right) \right| \\ &\leq c \left\| g_{n,N} \right\|_{4,\beta} \Big[1 + Q_{n-1}(|x|^c) \Big] \Delta t^2. \end{aligned}$$

By Lemma 3.1, $Q_n(|x|^c)$ is uniformly bounded and, by Lemma 5.7, $||g_{n,N}||_{4,\beta}$ is bounded by $c ||\phi||_{2,\beta}/(t_N - t_n)$. Similarly, for n = N, $||-|| \le c ||\phi||_{2,\beta}(1 + Q_{n-1}(|x|^c))$ Δt . Hence, $\sum_{n=1}^{N} ||-|| \le c ||\phi||_{2,\beta} \Delta t |\log \Delta t|$. In the smooth case, the estimate is the same, without the $(t_N - t_n)$ singularity and hence without the log term.

Mean-field error: From Lemma 5.5,

$$\begin{aligned} \left| \mathsf{II} - \mathsf{III} \right| &\leq \left| Q_{n-1} \left(\mathbb{E} \left[g_{n,N} (\Psi(x, \Delta t, P_{t_{n-1}}^{\mu})) \right] - \mathbb{E} \left[g_{n,N} (\Psi(x, \Delta t, Q_{n-1})) \right] \right) \right| \\ &\leq c \left(1 + Q_{n-1} (\left| x \right|^{\beta}) \right) \Delta t \left\| g_{n,N} \right\|_{3,\beta} W_{4,\beta} (P_{t_{n-1}}^{\mu}, Q_{n-1}). \end{aligned}$$

By Lemma 3.1, $Q_n(|x|^{\beta})$ is uniformly bounded and, by Lemma 5.7, $||g_{n,N}||_{3,\beta}$ is bounded by $c||\phi||_{2,\beta}/(t_N - t_n)^{1/2}$ for $n = 1, \ldots, N - 1$. Hence,

$$\left| |\mathsf{II} - \mathsf{III} \right| \le c \,\Delta t \, \left\| \phi \right\|_{2,\beta} W_{2,\beta}(P_{t_{n-1}}^{\mu}, Q_{n-1}) \frac{1}{(t_N - t_n)^{1/2}}.$$

For n = N,

$$\left| \mathsf{II} - \mathsf{III} \right| \le K \left(1 + Q_{N-1}(x^{\beta}) \right) \Delta t \left\| \phi \right\|_{2,\beta} W_{2,\beta}(P_{t_{N-1}}^{\mu}, Q_{N-1}) + \left\| \phi \right\|_{2,\beta} K \Delta t.$$

In the smooth case, $\phi \in F^{\infty,\beta}$ and $a, b \in C^{\infty}_{K}(\mathbb{R}^{2})$, so that $||g_{n,N}||_{3,\beta}$ is uniformly bounded and $||I - III| \leq c \Delta t ||\phi||_{\infty,\beta} W_{\infty,\beta}(P^{\mu}_{t_{n-1}}, Q_{n-1})$. Algorithm 1 error: We consider the case where Algorithm 1 is applied at every

Algorithm 1 error: We consider the case where Algorithm 1 is applied at every step n = 1, ..., N - 1. Then, for each n,

$$\mathsf{III} - \mathsf{IV} = Q_n^{\pm}(g_{n,N}) - Q_n(g_{n,N}).$$

Here Q_n is the measure given by approximating Q_n^{\pm} by Algorithm 1 and the associated error is described by Proposition 4.1. Thus, recalling that $R = \sqrt{(4/\lambda) |\log \Delta t|}$,

$$\left| \mathsf{III} - \mathsf{IV} \right| \le c \, (2R)^{2\,m_n - 1} \, \Delta t^{1/2} \, \frac{1}{(2\,m_n)!} \left\| g_{n,N}^{(2\,m_n)} \right\|_{\infty} + c \left\| \phi \right\|_{0,\beta} \Delta t^2.$$

Applying Lemma 5.7,

$$\begin{aligned} \left| \mathsf{III} - \mathsf{IV} \right| &\leq c \, (2R)^{2 \, m - 1} \, \Delta t^{1/2} \, \frac{1}{(2 \, m)!} \, \left\| \phi \right\|_{2,\beta} \frac{1}{(t_N - t_n)^{m - 1}} + c \left\| \phi \right\|_{0,\beta} \Delta t^2 \\ &\leq c \, (2R)^{2 \, m - 1} \, \frac{1}{(2 \, m)!} \, \left\| \phi \right\|_{2,\beta} \frac{1}{\Delta t^{m - 5/2}} \frac{1}{t_N - t_n} + c \left\| \phi \right\|_{0,\beta} \Delta t^2. \end{aligned}$$

This is bounded by $c \|\phi\|_{2,\beta} \Delta t^2 / (t_N - t_n)$ if $\log \Gamma(2m+1) \ge M_1^{\text{mf}}(m, \Delta t, n+k)$ for M_1^{mf} defined by (10).

In the smooth case, $|\mathsf{III} - \mathsf{IV}| \leq c\Delta t^2 \|\phi\|_{\infty,\beta}$ if $\log \Gamma(2m+1) \geq M_1^{\text{smooth}}(m, \Delta t, n+k)$ for M_1^{smooth} defined by (11). Sum the three upper bounds to show that

$$e_{N}(\phi) \leq c \left\|\phi\right\|_{2,\beta} \Delta t \left\|\log \Delta t\right\| + c \left\|\phi\right\|_{2,\beta} \sum_{n=1}^{N-1} \frac{\Delta t}{(t_{N} - t_{n})^{1/2}} W_{2,\beta}(P_{t_{n-1}}^{\mu}, Q_{n-1}) + c \left\|\phi\right\|_{2,\beta} \Delta t W_{2,\beta}(P_{t_{N-1}}^{\mu}, Q_{N-1}), \qquad t_{N} \leq 1.$$

Take the supremum over $\phi \in F^{2,\beta}$,

$$\begin{split} W_{2,\beta}(P_{t_N}^{\mu},Q_N) \\ &\leq c\,\Delta t \left|\log\Delta t\right| + \sum_{n=1}^{N-1} \frac{\Delta t}{(t_N-t_n)^{1/2}} \, W_{2,\beta}(P_{t_{n-1}}^{\mu},Q_{n-1}) + c\,\Delta t \, W_{2,\beta}(P_{t_{N-1}}^{\mu},Q_{N-1}). \end{split}$$

We assume that $W_{2,\beta}(P_0^{\mu}, Q_0) \leq c \Delta t$ in Assumption 5.1. Gronwall's inequality completes the proof of the rough case. In the smooth case, similar arguments show that

$$W_{\infty,\beta}(P_{t_N}^{\mu}, Q_N) \le c \,\Delta t + \sum_{n=1}^N \Delta t \, W_{\infty,\beta}(P_{t_{n-1}}^{\mu}, Q_{n-1})$$

and Gronwall's inequality again gives the result.

Consider (3), where a nonlinear dependence on the time-*t* distribution is allowed via functions $A, B: \mathbb{R} \to \mathbb{R}$. Our numerical method generalizes by replacing the definition of Ψ in (2) with

(15)
$$\Psi(x,\Delta t,Q) \coloneqq x + \Delta t A(Q(a(x,\cdot))) + \sqrt{\Delta t B(Q(b(x,\cdot)))} \xi.$$

Gauss quadrature can be used in the same way with the same choice of m_n and the same estimates apply as long as A, B have regularity consistent with Lemmas 5.5 and 5.8. This leads to the following convergence and complexity result.

COROLLARY 5.9. Let Assumptions 1.1, 5.1, and 5.2 hold and $A, B \in C_K^k(\mathbb{R}^d)$. Let the number of Gauss points m be given by (10) and let P_t^{μ} be the solution of (3) with initial distribution μ . Then, for some c > 0,

$$\max_{t_N \le 1} \left| P_{t_N}^{\mu}(\phi) - Q_N(\phi) \right| \le c \left\| \phi \right\|_{2,\beta} \Delta t \left| \log \Delta t \right| \qquad \forall \phi \in F^{2,\beta}.$$

If Q_0 is cheap to compute (see Theorem 5.4) and $m_0 = \mathcal{O}((|\log(\Delta t)|/\Delta t)^{1/2})$, the total work is $\mathcal{O}(|\log \Delta t|^{3/2}/\Delta t^{5/2})$. If, in addition to Assumption 1.1, we have $W_{\infty,\beta}(\mu, Q_0) \leq c \Delta t$, and in addition to Assumption 5.2, we have $a, b \in C_K^{\infty}(\mathbb{R}^2)$ and $A, B \in C_K^{\infty}(\mathbb{R})$, and the number of Gauss points m is given by (11), then

$$\max_{t_N \le 1} \left| P_{t_N}^{\mu}(\phi) - Q_N(\phi) \right| \le c \left\| \phi \right\|_{\infty,\beta} \Delta t \qquad \forall \phi \in F^{\infty,\beta}$$

If Q_0 is cheap to compute and $m_0 = \mathcal{O}(|\log \Delta t|)$, the total work is $\mathcal{O}(|\log \Delta t|^3 / \Delta t)$.

6. Numerical experiments. We now present a set of numerical experiments, exhibiting the behavior of GQ1 as described in section 3. We also try two methods that converge with second order.

GQ1e. The Richardson or Talay–Tubaro extrapolation involves taking two firstorder approximations $P(\Delta t)$ and $P(\Delta t/2)$ of a quantity P, and computing $\hat{P} := 2P(\Delta t/2) - P(\Delta t)$. If P has a second-order Taylor expansion, \hat{P} is a second-order accurate approximation to P. In the case that P is generated by GQ1, this is very simple to code and implement and is included in the experiments. Thus, we define GQ1e to be the quadrature rule Q defined by $2Q^{\Delta t/2} - Q^{\Delta t}$, where $Q^{\Delta t}$ is the result of applying GQ1 with time step Δt . The method results in a quadrature with some negative weights, which can lead to nonphysical results when used with highly oscillatory ϕ and the method should be used with caution.

GQ2. Suppose that the mean-field SDE has the following structure:

(16)
$$dX^{\mu}(t) = a(X^{\mu}(t), P_t^{\mu}(r)) dt + b(X^{\mu}(t), P_t^{\mu}(r)) dW(t)$$

for given functions $a, b: \mathbb{R} \times \mathbb{R}^d \to \mathbb{R}$ and $r: \mathbb{R} \to \mathbb{R}^d$. Mean-field SDEs of this type, involving moments of the solution in the coefficient functions or vectors of monomials $r(x) = [x, x^2, \ldots, x^d]$, were introduced in [16] for example. By working out the secondorder Ito–Taylor expansion, the following generalization, which we name GQ2, of the Euler–Maruyama-based method GQ1 can be derived: let $\Delta W = \Delta t \xi$ for ξ given by three-point distribution with $\mathbb{P}(\xi = 0) = 2/3$ and $\mathbb{P}(\xi = \pm\sqrt{3}) = 1/6$ (i.e., the three-point Gauss–Hermite rule for N(0,1)). For a given measure Q_n , define Q_{n+1} as the distribution of X_{n+1} given by

$$\begin{aligned} X_{n+1} &= X + a\,\Delta t + b\,\Delta W + \frac{1}{2}\partial_1 b\,b\left(\Delta W^2 - \Delta t\right) \\ &+ \frac{1}{2} \left(\partial_1 a\,b + \nabla b\cdot\mathcal{L}a + \frac{1}{2}\partial_{11}b\,b^2\right)\Delta W\,\Delta t \\ &+ \frac{1}{2} \left(\nabla a\cdot\mathcal{L}a + \frac{1}{2}\partial a_{11}\,b^2\right)\Delta t^2 \end{aligned}$$

for

$$\mathcal{L}a \coloneqq \left[a, Q_n\left(\partial_1 r \, a + \frac{1}{2}\partial_{11} r \, b^2\right), \dots, Q_n\left(\partial_d r \, a + \frac{1}{2}\partial_{dd} r \, b^2\right)\right],$$

where $X \sim Q_n$ (independent of ξ) and all functions a, b are evaluated at $(X, Q_n(r))$. Here, ∂_i and ∂_{ii} denotes the first- and second-derivatives with respect to the *i*th argument, ∇a denotes the usual gradient in \mathbb{R}^{d+1} , and \cdot the \mathbb{R}^{d+1} inner product.

Though we do not include it, GQ2 submits to similar techniques of error analysis to GQ1. We expect second-order convergence in the Wasserstein distance $W_{4,\beta}$, so that test functions require two extra derivatives compared to GQ1. The equation for the number of Gauss points m_n needs to be adjusted by taking p = 2 in (7), (10), or (11) as appropriate. The total work for a given accuracy ε is given by replacing Δt replaced by $\varepsilon^{1/2}$ in Theorems 4.2 and 5.3 (and increasing the regularity by two for all coefficients). For smooth mean-field equations, the work is $\mathcal{O}(|\log \varepsilon|^3 \varepsilon^{-1/2})$.

We expect second-order convergence for both of these methods and the initial distribution Q_0 should be chosen with $W_{4,\beta}(\mu, Q_0) \leq c\Delta t^2$.

The code for running these experiments is available for download [11].



FIG. 1. Geometric Brownian motion: The green line shows GQ1; the blue-dashed line shows GQ1e; the black-dash-dot line shows GQ2; the red-dotted line shows MLMC. The CPU time for MLMC is scaled to match GQ1 at the first data point. Errors are computed relative to the exact value. The yellows lines indicate reference slopes of -2, -1, and -1/2. (See online version for color.)

6.1. Geometric Brownian motion. We consider the ordinary SDE for geometric Brownian motion given by

$$dX(t) = \alpha X(t) dt + \sigma X(t) dW(t), \qquad X(0) = x,$$

for parameters α, σ and initial data x. For $\alpha = -1$, $\sigma = 0.5$, and x = 1, the exact value $\mathbb{E}[X(1)] = e^{-1}$. We use this as a test case to compare with the multilevel Monte Carlo (MLMC) method, as in [19, Example 8.49]. The CPU time is compared against error, averaging over ten runs of MLMC to reduce the variance. The CPU time for the MLMC MATLAB implementation (provided in [19]) is scaled to match GQ1 at the first data point. See Figure 1. The errors for the Gauss-quadrature methods are decaying at a much faster rate as the CPU time is increased. Theoretically, for a smooth problem like this, the work to achieve accuracy ε for GQ1 behaves like $\varepsilon^{-1}|\log \varepsilon|^3$, for GQ1e and GQ2 like $\varepsilon^{-1/2}|\log \varepsilon|^3$, and for MLMC like ε^{-2} . This is observed in the figure. Notice, however, that the linearly growing coefficients do not satisfy our assumptions.

6.2. Generalized Ornstein–Uhlenbeck process. Consider the following generalization of the Ornstein–Uhlenbeck SDE to a linear mean-field SDE:

$$dX(t) = \left[\alpha X(t) + \beta \mathbb{E}[X(t)]\right] dt + \sigma dW(t), \qquad X(0) = x,$$

for parameters $\alpha, \beta, \sigma \in \mathbb{R}$ and initial data $x \in \mathbb{R}$. By using Ito's formula, its first two moments can easily be calculated as

(17)
$$\mathbb{E}[X(t)] = x e^{(\alpha+\beta)t}, \quad \mathbb{E}[X(t)^2] = x^2 e^{2(\alpha+\beta)t} + \frac{\sigma^2}{2\alpha} [e^{2\alpha t} - 1].$$

It is used as a test case in [23], with $\alpha = -1/2$, $\beta = 4/5$, $\sigma^2 = 1/2$, and x = 1. We use these parameters and the results are shown in Figure 2. First-order convergence is observed for the first and second moments for GQ1, and second-order convergence is observed for both GQ1e and GQ2. The work is proportional to ε^{-1} and $\varepsilon^{-1/2}$, reflecting the estimates (up to log terms) for smooth problems in Theorem 5.3.



FIG. 2. Generalized Ornstein–Uhlenbeck SDE: The green line shows GQ1; the blue-dashed line GQ1e; the black-dash-dot line shows GQ2. The yellow lines show reference slopes of 1 and 2 (top) and -1/2 and -1 (bottom). The upper left- (resp., right-) hand plot shows the error in computing the mean (resp., second moment). The error is computed using reference values provided by (17). The bottom plots shows the CPU time in seconds. (See online version for color.)

6.3. Polynomial drift. The following mean-field Ito SDE

(18)
$$dX(t) = \left[\alpha X(t) + \mathbb{E}[X(t)] - X(t) \mathbb{E}[X(t)^2]\right] dt + X(t) dW(t), \qquad X(0) = x,$$

for a parameter $\alpha \in \mathbb{R}$, is considered in [7], where the first two moments of X(t) are shown to satisfy the system of ODEs

(19)
$$\frac{d\mathbb{E}[X]}{dt} = (\alpha+1)\mathbb{E}[X] - \mathbb{E}[X]\mathbb{E}[X^2],$$
$$\frac{d\mathbb{E}[X^2]}{dt} = (2\alpha+1)\mathbb{E}[X^2] + 2\left[\mathbb{E}[X]\right]^2 - 2\left[\mathbb{E}[X^2]\right]^2,$$

with initial conditions $\mathbb{E}[X] = x$ and $\mathbb{E}[X^2] = x^2$. We use this as a test with $\alpha = 2$ and x = 1 and results are shown in Figure 3. Again first-order (GQ1) and second-order (GQ1e and GQ2) convergence is observed for the first and second moments and the CPU times behave in line with Theorem 5.3.

6.4. Plane rotator. The following is a model for coupled oscillators [18] in the presence of noise:

(20)
$$dX^{\mu}(t) = \left[K \int_{\mathbb{R}} \sin(y - X^{\mu}(t)) P_{t}^{\mu}(dy) - \sin(X^{\mu}(t)) \right] dt + \sqrt{2k_{B}T} \, dW(t),$$

for coupling parameter K > 0, temperature $k_B T$, and initial condition $X^{\mu}(0) \sim \mu = N(\mu_0, \sigma_0^2)$. In this case, we have a Gaussian initial distribution μ , which can



FIG. 3. Polynomial drift: As for Figure 2 with the mean-field SDE (18). The error is computed by using an accurate numerical solution of (19) as a reference value.

be approximated by Gauss–Hermite quadrature. The associated points and weights can be found tabulated or computed via the three-term recursion for the Hermite polynomials. In the implementation, we take the latter strategy and start with Q_0 equal to the 40-point Gauss–Hermite rule.

The variable $X^{\mu}(t)$ represents an angle. In place of the diameter reduction step in Algorithm 1, we shift each point modulo 2π into $[0, 2\pi)$. Also, we partition $[0, 2\pi)$ into ten subintervals and apply Gauss quadrature on subintervals of width $L = \pi/5$. This significantly improves performance in experiments.

Following [23], we choose parameter values for K = 1, $k_BT = 1/8$, and initial mean $\mu_0 = \pi/4$ and variance $\sigma_0^2 = 3\pi/4$. Results are shown in Figure 4, which show errors for $P_1^{\mu}(\phi)$ for the test functions $\phi(x) = \sin^2(x)$ and $\phi(x) = \sin(x)$. Errors are computed by taking a reference solution given by GQ2. First-order convergence is observed for GQ1 and second-order convergence is observed for GQ2. The methods work rapidly and the finest solution has 434 quadrature points. In Figure 5, we show the pdf and cdf of the initial and final distributions.

6.5. Viscous Burgers equation. Consider the following mean-field SDE for a parameter $\sigma > 0$:

$$dX^{\mu}(t) = \int_{\mathbb{R}} \left(1 - H(X^{\mu}(t) - y) \right) P_t^{\mu}(dy) \, dt + \sigma \, dW(t),$$

where *H* is the Heaviside step function with H(x) = 0 for x < 0 and = 1 for $x \ge 0$, and an initial distribution $X^{\mu}(0)$ is prescribed. The drift term here can also be written as $\bar{a}(X,t) = \mathbb{P}(X^{\mu}(t) < X)$. Let $X^{\mu}(t)$ have cdf u(t,x); then V(t,x) = 1 - u(t,x)



FIG. 4. Plane rotator: error against time step and CPU time for computing $\mathbb{E}[\phi(X(1))]$ for $\phi(x) = \sin^2(x)$ (left) and $= \sin(x)$ (right), via GQ1 (green), QG1e (blue dashed), and GQ2 (black dash-dot) methods for (20). The yellow lines in the upper plots show slopes of 1 and 2, similar to the theoretical rate. The error is computed by taking a well-resolved GQ2 calculation for the reference value. (See online version for color.)



FIG. 5. Plane rotator: the pdf and cdf for initial distribution $N(\pi/4, 3\pi/4)$. The plots show initial (black) and final (blue) distributions. The pdf is computed by differentiating a spline approximation to the cdf. (See online version for color.)

satisfies the viscous Burgers equation

$$\frac{\partial V}{\partial t} = \frac{1}{2} \, \sigma^2 \, \frac{\partial^2 V}{\partial x^2} - V \, \frac{\partial V}{\partial x}, \qquad x \in \mathbb{R}.$$

In general, the solution of the initial-value problem for viscous Burgers equation can be written as the difference of two cdfs defined by initial-value problems for a mean-field SDE [6].



FIG. 6. Burgers equation for $\frac{1}{2}\sigma^2 = 0.1$: Comparison of the exact cdf at t = 1 given by (21) and the numerical approximation by GQ1e of (22) with for $\Delta t = 3 \times 10^{-4}$ and $\ell = 10^{-3}$ (using 74 quadrature points). (See online version for color.)

For $X^{\mu}(0)$ equal to delta measure at zero, the exact cdf is u(0, x) = H(x) and

(21)
$$u(t,x) = \frac{\operatorname{erfc}(-x/\sqrt{2\,\sigma^2\,t})}{\operatorname{erfc}(-x/\sqrt{2\,\sigma^2\,t}) + \exp((t-2\,x)/2\,\sigma^2)(2 - \operatorname{erfc}((t-x)/\sqrt{2\,\sigma^2\,t}))},$$

where erfc denotes the complementary error function [6]. We see in particular the solution represents a soliton travelling to the right with speed 1/2.

For the GQ methods, this problem presents two challenges. First, the mean-field term cannot be factored out as in (16) and $P_t^{\mu}(H(\cdot - X^{\mu}(t)))$ must be evaluated by quadrature for each particle representing $X^{\mu}(t)$. This increases computation time as m quadratures are needed at each step, instead of one. The lack of structure also means GQ2 cannot be used.

Second, the Heaviside function has a jump discontinuity at x = 0 and this lack of smoothness is evident in experiments. Introduce the regularized function

$$1 - H(x) \approx \frac{1}{2} \operatorname{erfc}(x/\ell), \qquad x \in \mathbb{R},$$

for a length scale $\ell > 0$. The equation

(22)
$$dX^{\mu}(t) = \int_{\mathbb{R}} \frac{1}{2} \operatorname{erfc}\left(\frac{X^{\mu}(t) - y}{\ell}\right) P_{t}^{\mu}(dy) \, dt + \sigma \, dW(t)$$

has smooth bounded coefficients and the behavior of the GQ algorithms is shown in Figure 7. The convergence behavior is broadly in line with the theory for $\phi(x) = x^2$, though GQ1e loses accuracy for small Δt when ℓ is reduced to $\ell = 0.001$ from $\ell = 0.1$ and the drift more closely resembles the Heaviside function. GQ1 and GQ1e accurately compute the first moment, which gives the center of the soliton at x = 1/2, to high accuracy (the error is 10^{-12} even for $\Delta t = 0.05$ and $\ell = 0.001$; not shown in the figures). Figure 6 shows a comparison of the cdf of GQ1e using $\ell = 0.001$ with the exact cdf for $\Delta t = 3 \times 10^{-4}$ with 74 quadrature points. The two agree with an $L^1(\mathbb{R})$ error of approximately 10^{-2} .

7. Conclusion. We have derived a time-stepping method based on Gauss quadrature for approximating the probability distribution of the solution of mean-field SDEs at a fixed time. The work per time step is dominated by the eigenvalue problem for



FIG. 7. Burgers equation for $\frac{1}{2}\sigma^2 = 0.1$: The error in approximating the second moment of (22) for $\ell = 0.1$ (left) and $\ell = 0.001$ (right). The green line marks GQ1 and the blue dashed-line marks GQ1e. (See online version for color.)

determining the Gauss quadrature. The total work required depends on the smoothness of the underlying problem and in the best case is $\mathcal{O}(\varepsilon^{-1/p} |\log \varepsilon|^3)$ operations when the underlying time-stepping method has *p*th order accuracy.

Though very effective for one-dimensional mean-field SDEs, their dependence on Gauss quadrature means the presented methods are difficult to extend to higher dimensions. The available methods for higher dimensions include [22, 23, 21] and are not as efficient. One-dimensional mean-field SDEs remain an interesting case due to their use in understanding high-dimensional interacting particle systems and the proposed methods are far more efficient than currently available methods.

The drift a and diffusion b in this paper are assumed to be bounded with bounded derivatives, which is unrealistic for many problems (including those in section 6 with polynomial a and b). Much work is currently being undertaken to extend the numerical analysis of SDEs to non-Lipschitz problems (for example, [14, 15]). Some of this will carry over to the Gauss-quadrature methods and mean-field SDEs, though nice properties such as Lemma 3.1 (boundedness of exponential moments for Euler-Maruyama) no longer hold in general. Some extensions are presented in [22], who also consider bounded coefficients but allow more general regularity conditions on the test functions than presented here. They also provide a nonuniform time-stepping scheme that allows more efficient approximation of less smooth problems.

REFERENCES

- M. ABRAMOWITZ AND I. A. STEGUN, Handbook of Mathematical Functions: With Formulas, Graphs, and Mathematical Tables, National Bureau of Standards Applied Mathematics Series 55, Dover Publications, New York, 1964.
- F. ANTONELLI AND A. KOHATSU-HIGA, Rate of convergence of a particle method to the solution of the McKean-Vlasov equation, Ann. Appl. Probab., 12 (2002), pp. 423–476, https: //doi.org/10.1214/aoap/1026915611.
- [3] K. ATKINSON, An Introduction to Numerical Analysis, 2nd ed., John Wiley & Sons, New York, 1989.
- [4] D. BOLEY AND G. H. GOLUB, A survey of matrix inverse eigenvalue problems, Inverse Probl., 3 (1987), pp. 595–622, https://doi.org/10.1088/0266-5611/3/4/010.
- [5] M. BOSSY AND D. TALAY, Convergence rate for the approximation of the limit law of weakly interacting particles: Application to the Burgers equation, Ann. Appl. Probab., 6 (1996), pp. 818–861, https://doi.org/10.1214/aoap/1034968229.
- [6] M. BOSSY AND D. TALAY, A stochastic particle method for the McKean-Vlasov and the Burgers equation, Math. Comp., 66 (1997), pp. 157–192, https://doi.org/10.1090/ s0025-5718-97-00776-x.

- [7] T. S. DOAN, M. RASMUSSEN, AND P. E. KLOEDEN, The mean-square dichotomy spectrum and a bifurcation to a mean-square attractor, Discrete Contin. Dyn. Syst. Ser. B, 20 (2015), pp. 875–887, https://doi.org/10.3934/dcdsb.2015.20.875.
- [8] A. FRIEDMAN, Partial Differential Equations of Parabolic Type, Dover Publications, New York, 2013.
- [9] J. GÄRTNER, On the McKean-Vlasov limit for interacting diffusions, Math. Nachr., 137 (1988), pp. 197–248, https://doi.org/10.1002/mana.19881370116.
- [10] W. GAUTSCHI, Orthogonal Polynomials: Computation and Approximation, Numerical Mathematics and Scientific Computation, Oxford University Press, Oxford, UK, 2004.
- H. GILSING AND T. SHARDLOW, SDELab: A package for solving stochastic differential equations, J. Comput. Appl. Math., 205 (2007), pp. 1002–1018, https://doi.org/10.1016/j.cam.2006.05. 037.
- [12] G. H. GOLUB AND J. H. WELSCH, Calculation of Gauss quadrature rules, Math. Comp., 23 (1969), pp. 221–230, https://doi.org/10.1090/S0025-5718-69-99647-1.
- [13] F. B. HILDEBRAND, Introduction to Numerical Analysis, 2nd ed., Dover Publications, New York, 1987.
- [14] M. HUTZENTHALER AND A. JENTZEN, On a Perturbation Theory and on Strong Convergence Rates for Stochastic Ordinary and Partial Differential Equations with Non-globally Monotone Coefficients, preprint, https://arxiv.org/abs/1401.0295, 2014.
- [15] M. HUTZENTHALER AND A. JENTZEN, Numerical Approximations of Stochastic Differential Equations with Non-globally Lipschitz Continuous Coefficients, Mem. Amer. Math. Soc. 236, American Mathematical Society, Providence, RI, 2015, https://doi.org/10.1090/memo/1112.
- [16] P. E. KLOEDEN AND T. LORENZ, Stochastic differential equations with nonlocal sample dependence, Stoch. Anal. Appl., 28 (2010), pp. 937–945, https://doi.org/10.1080/07362994.2010. 515194.
- [17] P. E. KLOEDEN AND E. PLATEN, Numerical Solution of Stochastic Differential Equations, Appl. Math. (N.Y.) 23, Springer-Verlag, Berlin, 1992, https://doi.org/10.1007/978-3-662-12616-5.
- [18] M. KOSTUR, J. LUCZKA, AND L. SCHIMANSKY-GEIER, Nonequilibrium coupled Brownian phase oscillators, Phys. Rev. E Stat. Nonlin. Soft Matter Phys., 65 (2002), 051115, https://doi. org/10.1103/PhysRevE.65.051115.
- [19] G. J. LORD, C. E. POWELL, AND T. SHARDLOW, An Introduction to Computational Stochastic PDEs, Cambridge University Press, New York, 2014, https://doi.org/10.1017/ cbo9781139017329.
- [20] H. P. MCKEAN, A class of Markov processes associated with nonlinear parabolic equations, Proc. Natl. Acad. Sci. U.S.A., 56 (1966), pp. 1907–1911.
- [21] E. F. V. MCMURRAY, Regularity of McKean-Vlasov Stochastic Differential Equations and Applications, Ph.D. thesis, Imperial College, London, UK, 2015.
- [22] T. MÜLLER-GRONBACH AND L. YAROSLAVTSEVA, Deterministic quadrature formulas for SDEs based on simplified weak Itô-Taylor steps, Found. Comput. Math., 16 (2016), pp. 1325–1366, https://doi.org/10.1007/s10208-015-9277-5.
- [23] L. F. RICKETSON, A Multilevel Monte Carlo Method for a Class of McKean-Vlasov Processes, preprint, https://arxiv.org/abs/arXiv:1508.02299, 2015.
- [24] J. STOER AND R. BULIRSCH, Introduction to Numerical Analysis, 3rd ed., Texts Appl. Math. 12, Springer-Verlag, New York, 2002, https://doi.org/10.1007/978-0-387-21738-3.
- [25] A.-S. SZNITMAN, Topics in propagation of chaos, in Ecole d'Eté de Probabilités de Saint-Flour XIX—1989, Lecture Notes in Math. 1464, Springer, Berlin, 1991, pp. 165–251, https://doi.org/10.1007/BFb0085169.
- [26] A. TOWNSEND, T. TROGDON, AND S. OLVER, Fast computation of Gauss quadrature nodes and weights on the whole real line, IMA J. Numer. Anal., 36 (2016), pp. 337–358, https: //doi.org/10.1093/imanum/drv002.
- [27] Y. XU, Generalized characteristic polynomials and Gaussian cubature rules, SIAM J. Matrix Anal. Appl., 36 (2015), pp. 1129–1142, https://doi.org/10.1137/140972810.