

Correction to “*Wasserstein distance estimates for the distributions of numerical approximations to ergodic stochastic differential equations*”

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Abstract

A method for analyzing non-asymptotic guarantees of numerical discretizations of ergodic SDEs in Wasserstein-2 distance is presented by Sanz-Serna and Zygalkakis in *Wasserstein distance estimates for the distributions of numerical approximations to ergodic stochastic differential equations*. They analyze the UBU integrator which is strong order two and only requires one gradient evaluation per step, resulting in desirable non-asymptotic guarantees, in particular $\mathcal{O}(d^{1/4}\epsilon^{-1/2})$ steps to reach a distance of $\epsilon > 0$ in Wasserstein-2 distance away from the target distribution. However, there is a mistake in the local error estimates in Sanz-Serna and Zygalkakis (2021), in particular, a stronger assumption is needed to achieve these complexity estimates. This note reconciles the theory with the dimension dependence observed in practice in many applications of interest.

Keywords: Markov Chain Monte Carlo; Langevin diffusion; Bayesian inference; numerical analysis of SDEs; strong convergence

1. Introduction

In Sanz-Serna and Zygalkakis (2021), the authors present a framework to analyze the convergence rate and asymptotic bias in Wasserstein-2 distance of numerical approximations to ergodic SDEs. In their framework, they consider underdamped Langevin dynamics on \mathbb{R}^{2d} which is given by

$$\begin{aligned} dv &= -\gamma v dt - c \nabla f(x) dt + \sqrt{2\gamma c} dW(t) \\ dx &= v dt, \end{aligned} \tag{1}$$

with $c, \gamma > 0$. It can be shown under mild assumptions that (1) is ergodic and has invariant measure π^* with density proportional to $\exp(-f(x) - \frac{1}{2c}\|v\|^2)$.

1.1 Assumptions

Let $\mathcal{H} : \mathbb{R}^d \rightarrow \mathbb{R}^{d \times d}$ be the Hessian of f .

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Assumption 1 $f : \mathbb{R}^d \rightarrow \mathbb{R}^d$ is twice differentiable, m -strongly convex and L -smooth, i.e.

$$\forall x \in \mathbb{R}^d, \quad mI_{d \times d} \prec \mathcal{H}(x) \prec LI_{d \times d},$$

where $I_{d \times d} \in \mathbb{R}^{d \times d}$ is the d -dimensional identity matrix.

Assumption 2 Let $\mathcal{H} : \mathbb{R}^d \rightarrow \mathbb{R}^{d \times d}$ be the Hessian of f , f be three times differentiable and there is a constant $L_1 \geq 0$ such that at each point $x \in \mathbb{R}^d$, for arbitrary $(w_1, w_2) \in \mathbb{R}^d \times \mathbb{R}^d$

$$\|\mathcal{H}'(x)[w_1, w_2]\| \leq L_1 \|w_1\| \|w_2\|.$$

Note that this assumption can be also reformulated in terms of the following norm.

Definition 3 For $A \in \mathbb{R}^{d \times d \times d}$

$$\|A\|_{\{1\}\{2\}\{3\}} = \sup \left\{ \sum_{i,j,k=1}^d A_{ijk} x_i y_j z_k \mid \sum_i x_i^2 \leq 1, \sum_j y_j^2 \leq 1, \sum_k z_k^2 \leq 1 \right\}$$

Then it is easy to check that Assumption 2 is equivalent to

$$\|\mathcal{H}'(x)\|_{\{1\}\{2\}\{3\}} \leq L_1 \quad \text{for every } x \in \mathbb{R}^d. \quad (2)$$

1.2 Wasserstein distance

Definition 4 Let π_1 and π_2 be two probability measures on \mathbb{R}^{2d} , the 2-Wasserstein distance between π_1 and π_2 with respect to the positive definite matrix $P \in \mathbb{R}^{2d \times 2d}$ is given by

$$\mathcal{W}_P(\pi_1, \pi_2) = \left(\inf_{\zeta \in Z} \int_{\mathbb{R}^{2d}} \|x - y\|_P^2 d\zeta(x, y) \right)^{1/2}, \quad (3)$$

where Z is the set of all couplings between π_1 and π_2 and $\|\xi\|_P = (\xi^T P \xi)^{1/2}$ for all $\xi \in \mathbb{R}^{2d}$.

2. UBU integrator and error in dimension dependence

In Sanz-Serna and Zygalkakis (2021) they considered the UBU integrator, a numerical integrator for (1), which is strong order 2 and only requires one gradient evaluation per iteration. It is defined by the following updated rule for a stepsize $h > 0$

$$v_{n+1} = \mathcal{E}(h)v_n - h\mathcal{E}(h/2)c\nabla f(y_n) + \sqrt{2\gamma c} \int_{t_n}^{t_{n+1}} \mathcal{E}(t_{n+1} - s)dW(s), \quad (4)$$

$$x_{n+1} = x_n + \mathcal{F}(h)v_n - h\mathcal{F}(h/2)c\nabla f(y_n) + \sqrt{2\gamma c} \int_{t_n}^{t_{n+1}} \mathcal{F}(t_{n+1} - s)dW(s), \quad (5)$$

$$y_n = x_n + \mathcal{F}(h/2)v_n + \sqrt{2\gamma c} \int_{t_n}^{t_{n+1/2}} \mathcal{F}(t_{n+1/2} - s)dW(s), \quad (6)$$

where $\mathcal{E}(t) = \exp(-\gamma t)$ and $\mathcal{F}(t) = \frac{1 - \exp(-\gamma t)}{\gamma}$. Due to the high strong order properties of the scheme, the UBU scheme shows improved dimension dependence in terms of non-asymptotic guarantees, $\mathcal{O}(d^{1/4})$. This is supported by numerics in some applications in

Zapatero (2017); Chada et al. (2023). In Sanz-Serna and Zygalkakis (2021) under Assumptions 1 and 2 they show in Theorem 25 this improved dimension dependence, however, there is a mistake in the local error estimates, in particular on page 31 they make use of the bound

$$\mathbb{E} (\|\mathcal{H}'(x)[\bar{v}, \bar{v}]\|^2) \leq L_1^2 \mathbb{E} (\|\bar{v}\|^4) \leq 3L_1^2 c^2 d \tag{7}$$

for $\bar{v} \sim \mathcal{N}(0, c)$. However, it is straightforward to show that

$$\mathbb{E} (\|\bar{v}\|^4) = c^2(d^2 + 2d)$$

and under Assumption 2 it is not possible to achieve non-asymptotic guarantees of order $\mathcal{O}(d^{1/4})$. The focus of this note is to reconcile the numerics with the theory by introducing a stronger assumption than Assumption 2, used in Chen and Gatmiry (2023) which achieves non-asymptotic guarantees of order $\mathcal{O}(d^{1/4})$ and is verifiable for many applications. This additional assumption is introduced in Section 2.1. We also correct an issue in the fifth step of the local error proof in Sanz-Serna and Zygalkakis (2021) and correct the constant C_0 in Theorem 25. This is done in Section 3.1 and in Section 3.2 a new version of Theorem 25 is stated with the new constants.

2.1 Strongly Hessian Lipschitz assumption

Chen and Gatmiry (2023) introduced the notion of strongly Hessian Lipschitz. We are going to use this new concept (Assumption 6) instead of Assumption 2, which was used in Sanz-Serna and Zygalkakis (2021), to correct dimension dependence in inequality (7).

The strongly Hessian Lipschitz property relies on the following tensor norm.

Definition 5 For $A \in \mathbb{R}^{d \times d \times d}$, let

$$\|A\|_{\{1,2\}\{3\}} = \sup_{x \in \mathbb{R}^{d \times d}, y \in \mathbb{R}^d} \left\{ \sum_{i,j,k=1}^d A_{ijk} x_{ij} y_k \mid \sum_{i,j=1}^d x_{ij}^2 \leq 1, \sum_{k=1}^d y_k^2 \leq 1 \right\}$$

Assumption 6 $f : \mathbb{R}^d \rightarrow \mathbb{R}$ is thrice differentiable and L_1^s -strongly Hessian Lipschitz if

$$\|\mathcal{H}'(x)\|_{\{1,2\}\{3\}} \leq L_1^s$$

for all $x \in \mathbb{R}^d$.

From the definition, it is clear that $\|A\|_{\{1,2\}\{3\}} \geq \|A\|_{\{1\}\{2\}\{3\}}$, and so by (2), the strong Hessian Lipschitz property (Assumption 6) implies the Hessian Lipschitz property (Assumption 2) with $L_1 = L_1^s$. We will show a result in the other direction in Lemma 8.

It is also easy to check that the strong Hessian Lipschitz property does not introduce dimension dependency for product target distributions, since $A \in \mathbb{R}^{d \times d \times d}$ with $A_{ijk} = 0$ unless $i = j = k$ (diagonal tensors), $\|A\|_{\{1,2\}\{3\}} = \max_i |A_{iii}|$, and so L_1^s equals the maximum of the supremum of the absolute value of third derivatives amongst the potentials of all components. Other examples of interest which do not introduce dimension dependency include the Bayesian multinomial regression (see (Chada et al., 2023, Lemma H.6)), ridge separable functions and 2-layer neural networks (see Chen and Gatmiry (2023)).

The following Lemma allows us to control the quantity

$$\mathbb{E}_{p \sim \mathcal{N}(0, I_d)} (\|A[p, p, \cdot]\|^2) = \mathbb{E}_{p \sim \mathcal{N}(0, I_d)} \left[\sum_{k \leq d} \left(\sum_{i, j \leq d} A_{ijk} p_i p_j \right) \left(\sum_{l, m \leq d} A_{lmk} p_l p_m \right) \right].$$

This is a special case of Lemma 13 of Chen and Gatmiry (2023), but with an explicit constant in the bound (their constant was not made explicit).

Lemma 7 *Let $p \sim \mathcal{N}(0, I_d)$, and*

$$g(p) = \sum_{k \leq d} \left(\sum_{i, j \leq d} A_{ijk} p_i p_j \right) \left(\sum_{l, m \leq d} A_{lmk} p_l p_m \right).$$

Then

$$\mathbb{E}g(p) \leq 3d \|A\|_{\{12\}\{3\}}^2.$$

Proof Due to the independence of the components, $\mathbb{E}(p_i p_j p_l p_m) = 0$ unless there are either two pairs of the same or four of the same amongst the indices. We know that $\mathbb{E}(p_i^4) = 3$. Hence, we have

$$\mathbb{E}(g(p)) = \sum_{i, j, k} (A_{iik} A_{jjk} + A_{ijk}^2 + A_{ijk} A_{jik}) \leq \sum_{i, j, k} (A_{iik} A_{jjk} + 2A_{ijk}^2).$$

We have that

$$\begin{aligned} \|A\|_{\{12\}\{3\}} &= \sup_{x, y} \left\{ \sum_{i_1, i_2, i_3} A_{i_1 i_2 i_3} x_{i_1} y_{i_2} y_{i_3} \left| \sum_{i_1, i_2} x_{i_1}^2 \leq 1, \sum_{i_3} y_{i_3}^2 \leq 1 \right. \right\} \\ &= \sup_y \left\{ \left(\sum_{i_1, i_2} \left(\sum_{i_3} A_{i_1 i_2 i_3} y_{i_3} \right)^2 \right)^{1/2} \left| \sum_{i_3} y_{i_3}^2 \leq 1 \right. \right\} \\ &= \sup_{y: \|y\| \leq 1} \left(\sum_{i_1, i_2} \langle A_{i_1, i_2, \cdot}, y \rangle^2 \right)^{1/2} = \left\| \sum_{i_1, i_2} A_{i_1, i_2, \cdot} \cdot A_{i_1, i_2, \cdot}^T \right\|^{1/2} \\ &= \left\| \sum_{i_1} A_{i_1, \cdot, \cdot}^T \cdot A_{i_1, \cdot, \cdot} \right\|^{1/2}. \end{aligned}$$

Now, it is easy to see that

$$2 \sum_{i, j, k} A_{ijk}^2 = 2 \text{Tr} \left(\sum_{i_1} A_{i_1, \cdot, \cdot}^T \cdot A_{i_1, \cdot, \cdot} \right) \leq 2d \|A\|_{\{12\}\{3\}}^2.$$

For the other term $\sum_{i, j, k} A_{iik} A_{jjk}$, we define a matrix $\bar{A} \in \mathbb{R}^{d \times d}$ as $\bar{A}_{ik} = A_{iik}$. Let $e \in \mathbb{R}^d$ be a vector of ones, i.e. $e_1 = 1, \dots, e_d = 1$. Using these, we have

$$\sum_{i, j, k} A_{iik} A_{jjk} = e^T \bar{A}^T \bar{A} e \leq d \|\bar{A}\|^2.$$

We have

$$\|A\|_{\{12\}\{3\}} = \sup_{x,y} \left\{ \sum_{i_1, i_2, i_3} A_{i_1 i_2 i_3} x_{i_1 i_2} y_{i_3} \left| \sum_{i_1, i_2} x_{i_1 i_2}^2 \leq 1, \sum_{i_3} y_{i_3}^2 \leq 1 \right. \right\}$$

by only considering x such that $x_{i_1 i_2} = 0$ for $i_1 \neq i_2$,

$$\geq \sup_{x,y} \left\{ \sum_{i_1, i_3} A_{i_1 i_1 i_3} x_{i_1 i_1} y_{i_3} \left| \sum_{i_1} x_{i_1 i_1}^2 \leq 1, \sum_{i_3} y_{i_3}^2 \leq 1 \right. \right\} = \|\bar{A}\|,$$

hence $\sum_{i,j,k} A_{iik} A_{jjk} \leq d \|A\|_{\{12\}\{3\}}^2$, and the claim of the lemma follows. \blacksquare

Using Lemma 7 and starting from the top of page 31 we have

$$\mathbb{E}(\|\mathcal{H}'(\bar{x})[\bar{v}, \bar{v}]\|^2) \leq 3(L_1^s)^2 c^2 d,$$

and we can simply replace L_1 by L_1^s in the estimates of Sanz-Serna and Zygalakis (2021).

Note that although the strongly Hessian Lipschitz assumption is stronger than the previous Hessian Lipschitz assumption (i.e. $L_1 \leq L_1^s$), it is possible to show that every Hessian Lipschitz function is also strongly Hessian Lipschitz, due to the following result.

Lemma 8 *For any $A \in \mathbb{R}^{d \times d \times d}$, $\|A\|_{\{12\}\{3\}} \leq \sqrt{d} \|A\|_{\{1\}\{2\}\{3\}}$. Hence every L_1 -Hessian Lipschitz function is $\sqrt{d}L_1$ -strongly Hessian Lipschitz.*

Proof In the proof of Lemma 7, we have shown that

$$\|A\|_{\{12\}\{3\}} = \left\| \sum_{i_1} A_{i_1, \cdot, \cdot}^T \cdot A_{i_1, \cdot, \cdot} \right\|^{1/2}.$$

Let $e_i = (0, \dots, 0, 1, 0, \dots, 0) \in \mathbb{R}^d$ be the unit vector with 1 in component i . Using Definition 3, we have for every $i \leq d$,

$$\begin{aligned} \|A\|_{\{1\}\{2\}\{3\}} &= \sup \left\{ \sum_{i,j,k=1}^d A_{ijk} x_i y_j z_k \left| \sum_i x_i^2 \leq 1, \sum_j y_j^2 \leq 1, \sum_k z_k^2 \leq 1 \right. \right\} \\ &\geq \sup \left\{ \sum_{i,j,k=1}^d A_{ijk} x_i y_j z_k \left| x_i = e_i, \sum_j y_j^2 \leq 1, \sum_k z_k^2 \leq 1 \right. \right\} = \|A_{i, \cdot, \cdot}^T \cdot A_{i, \cdot, \cdot}\|^{1/2}, \end{aligned}$$

and the claim follows by rearrangement. \blacksquare

3. Non-asymptotic guarantees for UBU

In Sanz-Serna and Zygalakis (2021) they consider contraction and discretization bias of the UBU scheme with $\gamma = 2$ and $h \leq 2$ in the 2-Wasserstein distance with respect to $P_h := \hat{P} \otimes I_d$, where

$$\hat{P} = \begin{pmatrix} 1 & 1 \\ 1 & 2 \end{pmatrix}. \quad (8)$$

They define the weighted Hilbert-space norm with respect to the matrix P_h , $\|\cdot\|_{L^2, P_h}$ and corresponding inner product $\langle \cdot, \cdot \rangle_{L^2, P_h}$. They then define the iterates of UBU, $(\xi_n)_{n \in \mathbb{N}}$ with $\xi_0 \sim \pi$, by the update rule $(v_{n+1}, x_{n+1}) = \xi_{n+1} = \psi_h(\xi_n, t_n)$, $t_n = nh$, $n = 0, 1, \dots$, $h > 0$ to be the one-step approximation governed by the UBU integrator with initial condition $\xi \in \mathbb{R}^{2d}$ and $\phi_h(\cdot, \cdot)$ to be the exact counterpart with shared Brownian increments. They introduce at each time level n , the random variable $\hat{\xi}_n \sim \pi^*$ to be the optimal coupling such that $\mathcal{W}_P(\pi^*, \Psi_{h,n}\pi) = \|\hat{\xi}_n - \xi_n\|_{L^2, P_h}$, where $\Psi_{h,n}\pi$ is the measure of ξ_n . They have shown in Sanz-Serna and Zygalakis (2021)[Theorem 18] that for $\gamma = 2$, $c = \bar{c}/(L + m)$, where $\bar{c} \in (0, 4)$, there is a h_0 , such that, for any $h \leq h_0$ and $n \in \mathbb{N}$

$$\|\xi_{n+1}^{(2)} - \xi_{n+1}^{(1)}\|_{P_h}^2 \leq \rho_h \|\xi_n^{(2)} - \xi_n^{(1)}\|_{P_h}^2, \quad (9)$$

where $\rho_h \in (0, 1)$ for realizations $(\xi_k^{(i)})_{k \in \mathbb{N}}$ for $i = 1, 2$ of the UBU discretization.

Assumption 9 (Assumption 22 of Sanz-Serna and Zygalakis (2021)) *There is a decomposition*

$$\phi_h(\hat{\xi}_n, t_n) - \psi_h(\hat{\xi}_n, t_n) = \alpha_h(\hat{\xi}_n, t_n) + \beta_h(\hat{\xi}_n, t_n),$$

and positive constants p, h_0, C_0, C_1, C_2 such that for $n \geq 0$ and $h \leq h_0$:

$$\left| \left\langle \Psi_h(\hat{\xi}_n, t_n) - \psi_h(\xi_n, t_n), \alpha_h(\hat{\xi}_n, t_n) \right\rangle \right| \leq C_0 h \|\hat{\xi}_n - \xi_n\|_{L^2, P_h} \|\alpha_h(\hat{\xi}_n, t_n)\|_{L^2, P_h} \quad (10)$$

and

$$\|\alpha_h(\hat{\xi}_n, t_n)\|_{L^2, P_h} \leq C_1 h^{p+1/2}, \quad \|\beta_h(\hat{\xi}_n, t_n)\|_{L^2, P_h} \leq C_2 h^{p+1}. \quad (11)$$

Theorem 10 (Theorem 23 of Sanz-Serna and Zygalakis (2021)) *Assume that the integrator satisfies Sanz-Serna and Zygalakis (2021)[Assumption 22] and in addition, there are constants $h_0 > 0, r > 0$ such that for $h \leq h_0$ the contractivity estimate (9) holds with $\rho_h \leq (1 - rh)^2$. Then, for any initial distribution π , stepsize $h \leq h_0$, and $n = 0, 1, \dots$,*

$$\mathcal{W}_{P_h}(\pi^*, \Psi_{h,n}\pi) \leq (1 - hR_h)^n \mathcal{W}_{P_h}(\pi^*, \pi) + \left(\frac{\sqrt{2}C_1}{\sqrt{R_h}} + \frac{C_2}{R_h} \right) h^p \quad (12)$$

with

$$R_h = \frac{1}{h} \left(1 - \sqrt{(1 - rh)^2 + C_0 h^2} \right) = r + o(1), \quad \text{as } h \downarrow 0.$$

The remaining subsections are devoted to correcting the constants in Assumption 22 for the UBU integrator and $p = 2$ and thereby the non-asymptotic guarantees by Theorem 23 of Sanz-Serna and Zygalakis (2021).

3.1 The local error of UBU: Error in the fifth step

Throughout this section we use the same notation as Sanz-Serna and Zygalkakis (2021)[Section 7.6], in particular, $(v_{n+1}, x_{n+1}) = \xi_{n+1}$ and $(\tilde{v}_{n+1}, \tilde{x}_{n+1})$ denotes the velocity component and position of a UBU step initialized at $\hat{\xi}_n = (\hat{v}_n, \hat{x}_n)$. In the fifth step of Sanz-Serna and Zygalkakis (2021)[Section 7.6] they use the equality

$$\left| \left\langle \psi_h(\hat{\xi}_n, t_n) - \psi_h(\xi_n, t_n), \alpha_h(\hat{\xi}_n, t_n) \right\rangle_{L^2, P_h} \right| = |\mathbb{E}(\langle \tilde{v}_{n+1} - v_{n+1}, \alpha_v \rangle)|.$$

Unfortunately, this is incorrect, due to the matrix inner product defined by P_h , we have

$$\left| \left\langle \psi_h(\hat{\xi}_n, t_n) - \psi_h(\xi_n, t_n), \alpha_h(\hat{\xi}_n, t_n) \right\rangle_{L^2, P_h} \right| = |\mathbb{E}(\langle \tilde{v}_{n+1} - v_{n+1}, \alpha_v \rangle + \langle \tilde{x}_{n+1} - x_{n+1}, \alpha_v \rangle)|.$$

The first term on the right-hand-side of this expression was bounded in Sanz-Serna and Zygalkakis (2021)[Eq. (43)] in terms of $\mathbb{E}(\|\hat{v}_n - v_n\|^2)$, $\mathbb{E}(\|\hat{x}_n - x_n\|^2)$ and $\mathbb{E}(\|\alpha_v\|^2)$. The additional term can be treated by the same argument as the fourth step of Sanz-Serna and Zygalkakis (2021)[Section 7.6] that is we estimate

$$\begin{aligned} |\mathbb{E}(\langle \tilde{x}_{n+1} - x_{n+1}, \alpha_v \rangle)| &= |\mathbb{E}(\langle \tilde{x}_{n+1} - \hat{x}_n - x_{n+1} + x_n, \alpha_v \rangle)| \\ &\leq (\mathbb{E}\|\tilde{x}_{n+1} - \hat{x}_n - x_{n+1} + x_n\|^2)^{1/2} (\mathbb{E}\|\alpha_v\|^2)^{1/2}. \end{aligned}$$

Now, from (5),

$$\tilde{x}_{n+1} - \hat{x}_n - x_{n+1} + x_n = \mathcal{F}(h)(\hat{v}_n - v_n) - h\mathcal{F}(h/2)c(\nabla f(\tilde{y}_n) - \nabla f(y_n))$$

with (6)

$$\tilde{y}_n = \hat{x}_n + \mathcal{F}(h/2)\hat{v}_n + \sqrt{2\gamma c} \int_{t_n}^{t_{n+1/2}} \mathcal{F}(t_{n+1/2} - s) dW(s),$$

and thus, since $\mathcal{F}(h) \leq h$

$$\mathbb{E}(\|\tilde{x}_{n+1} - \hat{x}_n - x_{n+1} + x_n\|^2)^{1/2} \leq h\mathbb{E}(\|\hat{v}_n - v_n\|^2)^{1/2} + \frac{h^2 cL}{2} (\mathbb{E}(\|\tilde{y}_n - y_n\|^2))^{1/2}.$$

Taking into account (6) and the definition of \tilde{y}_n

$$(\mathbb{E}\|\tilde{y}_n - y_n\|^2)^{1/2} \leq (\mathbb{E}(\|\hat{x}_n - x_n\|^2))^{1/2} + \frac{h}{2} (\mathbb{E}(\|\hat{v}_n - v_n\|^2))^{1/2}$$

and we conclude that $|\mathbb{E}(\langle \tilde{x}_{n+1} - x_{n+1}, \alpha_v \rangle)|$ is bounded above by

$$h \left(\frac{hcL}{2} (\mathbb{E}(\|\hat{x}_n - x_n\|^2))^{1/2} + \left(1 + \frac{h^2 cL}{4} \right) (\mathbb{E}(\|\hat{v}_n - v_n\|^2))^{1/2} \right) (\mathbb{E}\|\alpha_v\|^2)^{1/2}.$$

3.2 Theorem 25 of Sanz-Serna and Zygalkis (2021)

In this section we are stating the corrected version of Sanz-Serna and Zygalkis (2021)[Theorem 25].

Theorem 11 *Assume that f satisfies Assumptions 1 and 6. Set $\gamma = 2$ and $P_h = \hat{P} \otimes I_d$. Then, for $h \leq 2$, the UBU discretization satisfies Assumption 22 of Sanz-Serna and Zygalkis (2021) (Assumption 9) with $p = 2$,*

$$\begin{aligned} C_0 &= K_0 (3 + 2cL) \\ C_1 &= K_1 c^{3/2} L d^{1/2} \\ C_2 &= K_2 \left((1 + 4\sqrt{3})c^2 L^{3/2} + \left(3 + \frac{\sqrt{42}}{2}\right)c^{3/2} L + 6cL^{1/2} + \sqrt{3}c^2 L_1^s \right) d^{1/2}, \end{aligned}$$

where K_j , $j = 0, 1, 2$, are the following absolute constants

$$K_0 = \sqrt{\frac{4}{3 - \sqrt{5}}}, \quad K_1 = \frac{\sqrt{3}}{12}, \quad K_2 = \frac{1}{24} \sqrt{\frac{3 + \sqrt{5}}{2}}.$$

Proof Combining estimates of Section 3.1 in the norm $\|(v, x)\|_{P_h}^2 := \|v\|^2 + 2\langle v, x \rangle + 2\|x\|^2$ and using the fact that $\|(x, v)\| \leq \sqrt{\frac{2}{3 - \sqrt{5}}} \|(x, v)\|_{P_h}$ we have

$$\begin{aligned} & \left| \left\langle \psi_h(\hat{\xi}_n, t_n) - \psi_h(\xi_n, t_n), \alpha_h(\hat{\xi}_n, t_n) \right\rangle_{L^2, P_h} \right| \leq \\ & h \left(\left(\frac{hcL}{2} + cL \right) (\mathbb{E}(\|\hat{x}_n - x_n\|^2))^{1/2} + \left(3 + \frac{h^2 cL}{4} + \frac{hcL}{2} \right) (\mathbb{E}(\|\hat{v}_n - v_n\|^2))^{1/2} \right) (\mathbb{E}(\|\alpha_v\|^2))^{1/2} \\ & \leq h \sqrt{\frac{4}{3 - \sqrt{5}}} (3 + 2cL) \|\hat{\xi}_n - \xi_n\|_{L^2, P_h} \|\alpha_h\|_{L^2, P_h}, \end{aligned}$$

and the required C_0 constant, with C_2 given by following the argument of Sanz-Serna and Zygalkis (2021)[Section 7.6] using Lemma 7. ■

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