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MODIFIED EQUATIONS FOR STOCHASTIC DIFFERENTIAL EQUATIONS*

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Abstract.

We describe a backward error analysis for stochastic differential equations with respect to weak convergence. Modified equations are provided for forward and backward Euler approximations to Itô SDEs with additive noise, and extensions to other types of equation and approximation are discussed.

AMS subject classification (2000): 65C30.

Key words: stochastic differential equations, numerical approximation, backward error analysis.

1 Introduction.

This paper considers the backward error analysis of stochastic differential equations (SDEs), a technique that has been of great success in interpreting numerical methods for ODEs. It is possible to fit an ODE (the so called modified equation) to a numerical method to very high order accuracy. Backward error analysis has been particularly valuable for Hamiltonian systems, where symplectic numerical methods can be approximated by a modified ODE arising from a perturbed Hamiltonian system, giving an approximate statistical mechanics for symplectic methods. See the monograph [3] for a review and further references.

It is natural to ask whether such techniques extend to SDEs. The only prior work in this area that I am aware of, concerns linear Langevin equations [8]. We discuss modified equations for SDEs by perturbing the drift and diffusion functions by deterministic functions and looking for convergence in the weak sense of average with respect to smooth test functions. It is possible to determine a modified equation that approximates standard first order methods to second order accuracy for SDEs with additive noise. It is not possible to examine the case of SDEs with multiplicative noise, of convergence in the sense of mean square, nor is it possible to develop modified equations of higher order accuracy by working

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only with deterministic perturbations of the drift and diffusion coefficients. It remains to be seen whether a useful formulation of a modified equation can be introduced to describe numerical approximations of SDEs in greater generality.

The paper is divided into three, each section presents the main ideas without developing any proofs. Section 2 develops the modified equation for a one dimensional SDE, showing that the noise should be additive and the difficulty of dealing with higher order approximations. Modified equations are derived for the forward and backward Euler methods. In Section 3, the extension to higher dimensions is discussed in relation to a Langevin equation. In Section 4, we give conclusions and suggest a way of studying backward errors in the pathwise sense.

2 One dimension.

Consider Itô SDEs on the real line

$$dX = f(X)\,dt + \sigma(X)\,d\beta(t), \quad X(0) = Y, \tag{2.1}$$

where $f, \sigma\colon \mathbf{R} \to \mathbf{R}$ are smooth functions and $\beta(t)$ is a standard Brownian motion. Consider a numerical approximation $X_0, X_1, \ldots$ parameterised by a time step Δt that converges to the solution $X(t)$ in the weak sense: for $T > 0$,

$$|\mathbf{E}\phi(X_n) - \mathbf{E}\phi(X(n\Delta t))| = \mathcal{O}(\Delta t^p)\,, \quad 0 \le n\Delta t \le T,$$

for ϕ in a space of smooth test functions, where p is known as the weak order of the method. The simplest example is the forward Euler method (often called the Euler–Maruyama method), given by the iteration

$$X_{n+1} = X_n + f(X_n)\Delta t + \sigma(X_n)B_n(\Delta t), \quad X_0 = Y \tag{2.2}$$

where $B_n(\Delta t)$ are independent Gaussian random variables with mean zero and variance Δt. This method is first order, $p = 1$, in the weak sense. For a technical statement and proof with a review of other approximation methods, see [4, 5].

The goal is to modify the SDE (2.1) to define a process $\tilde{X}$ that better describes the numerical approximation X_n in the sense that

$$|\mathbf{E}\phi(X_n) - \mathbf{E}\phi(\tilde{X}(n\Delta t))| = \mathcal{O}(\Delta t^{p+q})\,, \quad 0 \le n\Delta t \le T,$$

where $q > 0$ is the increase in the order of accuracy. We define $\tilde{X}$ as the solution of the modified Itô SDE

$$d\tilde{X} = \left[f(\tilde{X}) + \tilde{f}(\tilde{X})\Delta t^p\right] dt + \left[\sigma(\tilde{X}) + \tilde{\sigma}(\tilde{X})\Delta t^p\right] d\beta(t), \quad \tilde{X}(0) = Y, \tag{2.3}$$

where $\tilde{f}$ and $\tilde{\sigma}$ are smooth functions to be determined, and look for convergence of one higher order

$$|\mathbf{E}\phi(X_n) - \mathbf{E}\phi(\tilde{X}(n\Delta t))| = \mathcal{O}(\Delta t^{p+1})\,, \quad 0 \le n\Delta t \le T. \tag{2.4}$$

The main technical fact we use in studying this problem is as follows. The pth order weak convergence of a numerical method can be reduced to studying the approximation of moments over one time step. See Theorem 14.5.2 of [4] or Theorem 9.1 of [5]. The key point is the following consistency condition: to achieve pth order weak convergence, we must have:

$$|\mathbf{E}\phi(X_1) - \mathbf{E}\phi(X(\Delta t))| = \mathcal{O}(\Delta t^{p+1}),$$

for all polynomials $\phi(x)$ up to degree $2p+1$. Thus to achieve (2.4), we impose

$$|\mathbf{E}\phi(X_1) - \mathbf{E}\phi(\tilde{X}(\Delta t))| = \mathcal{O}(\Delta t^{p+2}), \tag{2.5}$$

for the monomials $\phi(X) = X^k$, $k = 1, \dots, 2p+3$. This provides $2p+3$ conditions at each initial condition Y, though the modified equation only has two free variables $\tilde{f}(X)$ and $\tilde{\sigma}(X)$. We see already the difficulty in seeking such a modified equation.

DERIVATION. By applying Itô's formula, with (2.2) and (2.3),

$$\begin{aligned}\phi(\tilde{X}(\Delta t)) = \phi(X(\Delta t)) + \int_0^{\Delta t} & \phi'(\tilde{X}(s))\big[f(\tilde{X}(s)) + \Delta t^p \tilde{f}(\tilde{X}(s))\big] \\ & - \phi'(X(s))f(X(s))\; ds + mg + \tfrac{1}{2}\int_0^{\Delta t} \phi''(\tilde{X}(s))\big[\sigma(\tilde{X}(s))^2 \\ & + 2\Delta t^p \sigma(\tilde{X}(s))\tilde{\sigma}(\tilde{X}(s))\big] - \phi''(X(s))\,\sigma(X(s))^2\; ds,\end{aligned} \tag{2.6}$$

where mg denotes the martingale term. The drift and diffusion terms in (2.1) and (2.3) differ by $\mathcal{O}(\Delta t^p)$ terms. Hence,

$$\mathbf{E}\Big[\int_0^{\Delta t} \phi'(\tilde{X}(s))f(\tilde{X}(s))\; ds\Big] = \mathbf{E}\Big[\int_0^{\Delta t} \phi'(X(s))f(X(s))\; ds\Big] + \mathcal{O}(\Delta t^{p+2}),$$

$$\mathbf{E}\Big[\int_0^{\Delta t} \phi''(\tilde{X}(s))\sigma_i(\tilde{X}(s))^2\; ds\Big] = \mathbf{E}\Big[\int_0^{\Delta t} \phi''(X(s))\sigma(X(s))^2\; ds\Big] + \mathcal{O}(\Delta t^{p+2}).$$

Further,

$$\mathbf{E}\Big[\int_0^{\Delta t} \phi'(\tilde{X}(s))\tilde{f}(\tilde{X}(s))\; ds\Big] = \phi'(Y)\tilde{f}(Y)\Delta t + \mathcal{O}(\Delta t^2),$$

$$\mathbf{E}\Big[\int_0^{\Delta t} \phi''(\tilde{X}(s))\sigma(\tilde{X}(s))\tilde{\sigma}(\tilde{X}(s))\; ds\Big] = \phi''(Y)\sigma(Y)\tilde{\sigma}(Y)\Delta t + \mathcal{O}(\Delta t^2).$$

From (2.6)

$$\begin{aligned}\mathbf{E}\phi(\tilde{X}(\Delta t)) = \mathbf{E}\phi(X(\Delta t)) &+ \phi'(Y)\Delta t^{p+1}\tilde{f}(Y) \\ &+ \Delta t^{p+1}\phi''(Y)\sigma(Y)\tilde{\sigma}(Y) + \mathcal{O}(\Delta t^{p+2})\end{aligned}$$

and, if $\phi(X) = X^k$,

$$\begin{aligned}\mathbf{E}\tilde{X}(\Delta t)^k = \mathbf{E}X(\Delta t)^k &+ kY^{k-1}\Delta t^{p+1}\tilde{f}(Y) \\ &+ \Delta t^{p+1}k(k-1)Y^{k-2}\sigma(Y)\tilde{\sigma}(Y) + \mathcal{O}(\Delta t^{p+2}).\end{aligned} \tag{2.7}$$

Let $b_k(Y) := \mathbf{E}X_1^k - \mathbf{E}X(\Delta t)^k$. Then,

$$\begin{aligned} b_k(Y) &= \mathbf{E}X_1^k - \mathbf{E}\tilde{X}(\Delta t)^k + \mathbf{E}\tilde{X}(\Delta t)^k - \mathbf{E}X(\Delta t)^k \\ &= \mathbf{E}X_1^k - \mathbf{E}\tilde{X}(\Delta t)^k + kY^{k-1}\Delta t^{p+1}\tilde{f}(Y) \\ &\quad + \Delta t^{p+1}k(k-1)Y^{k-2}\sigma(Y)\tilde{\sigma}(Y) + \mathcal{O}(\Delta t^{p+2}). \end{aligned}$$

To achieve (2.5), we require that $\mathbf{E}X_1^k - \mathbf{E}\tilde{X}(\Delta t)^k = \mathcal{O}(\Delta t^{p+2})$ for $k = 1, \ldots, 2p+3$. Equivalently, we require that

$$b_k(Y) = kY^{k-1}\Delta t^{p+1}\tilde{f}(Y) + \Delta t^{p+1}k(k-1)Y^{k-2}\sigma(Y)\tilde{\sigma}(Y) + \mathcal{O}(\Delta t^{p+2}). \tag{2.8}$$

The conditions for $k = 1, 2$ yield equations for the terms $\tilde{f}$ and $\tilde{\sigma}$:

$$\Delta t^{p+1}\begin{pmatrix} 1 & 0 \\ 2Y & 2\sigma \end{pmatrix}\begin{pmatrix} \tilde{f}(Y) \\ \tilde{\sigma}(Y) \end{pmatrix} = \begin{pmatrix} b_1(Y) \\ b_2(Y) \end{pmatrix} + \mathcal{O}(\Delta t^{p+2}). \tag{2.9}$$

It is not clear how to provide for the conditions $k = 3, \ldots, 2p+3$.

To deal with the remaining k, first note that by row reductions, we can replace the conditions in (2.8) for $k = 3, \ldots, 2p+3$ with the following

$$b_k(Y) - kY^{k-1}b_1(Y) - k(k-1)Y^{k-2}b_2(Y) = \mathcal{O}(\Delta t^{p+2}). \tag{2.10}$$

Assume the following expression of b_k:

$$b_k(Y) = \Delta t^{p+1}\sum_{j=1}^{k}\frac{k!}{(k-j)!}Y^{k-j}\Gamma_j(Y) + \mathcal{O}(\Delta t^{p+2}).$$

The terms $\Gamma_j(Y)$ arise from the drift and diffusion function in a Taylor expansion on b_k. Examples where this holds are presented below. Then

$$b_k(Y) - k\,Y^{k-1}\,b_1(Y) = \Delta t^{p+1}\sum_{j=2}^{k}\frac{k!}{(k-j)!}Y^{k-j}\Gamma_j(Y) + \mathcal{O}(\Delta t^{p+2})$$

and

$$\begin{aligned} b_k(Y) &- kY^{k-1}b_1(Y) - k(k-1)Y^{k-2}b_2(Y) \\ &= \Delta t^{p+1}\sum_{j=3}^{k}\frac{k!}{(k-j)!}Y^{k-j}\Gamma_j(Y) + \mathcal{O}(\Delta t^{p+2}). \end{aligned}$$

Thus the condition (2.10) becomes

$$\sum_{j=3}^{k}\frac{k!}{(k-j)!}Y^{k-j}\Gamma_j(Y) = \mathcal{O}(\Delta t), \quad k = 3, \ldots, 2p+3.$$

We will achieve this condition in examples by showing $\Gamma_k(Y) = 0$ for $k = 3, \ldots, 2p+3$. In this case, the modified equation may be determined by solving the linear system (2.9) for $\tilde{f}, \tilde{\sigma}$. In terms of Γ_j, the modified terms are

$$\tilde{f}(Y) = \Gamma_1(Y), \quad \tilde{\sigma}(Y) = \Gamma_2(Y)/\sigma.$$

This provides a modified equation (2.3) that satisfies the one step consistency condition (2.5) subject to the conditions $\Gamma_k(Y) = 0$ for $k = 3, \ldots, 2p+3$. These conditions are very strong and the modified equation is only useful in special circumstances. This is best illustrated by looking at an example.

EXAMPLE: FORWARD EULER. To compute the modified equation for the forward Euler method, recall the following Itô–Taylor expansion (see Appendix A):

$$\begin{aligned}\mathbf{E}\phi(X(t)) = \phi(Y) &+ \phi'(Y)f(Y)\Delta t + \tfrac{1}{2}\phi''(Y)\sigma(Y)^2\Delta t \\ &+ \tfrac{1}{2}\Delta t^2\big[(\phi'(Y)f(Y))'f(Y) + \tfrac{1}{2}(\phi'(Y)f(Y))''\sigma(Y)^2\big] \\ &+ \tfrac{1}{4}\Delta t^2\big[(\phi''(Y)\sigma(Y)^2)'f(Y) + \tfrac{1}{2}(\phi''(Y)\sigma(Y)^2)''\sigma(Y)^2\big] + \mathcal{O}(\Delta t^3)\,.\end{aligned}$$

If $\phi(X) = X^k$ then

$$\mathbf{E}\phi(X(t)) = Y^k + \Delta t^2 \sum_{j=1}^{k} \frac{k!}{(k-j)!} Y^{k-j}\Gamma_j^1$$

where

$$\begin{aligned}\Gamma_1^1 &= \big(f(Y)\Delta t + \tfrac{1}{2}f'(Y)f(Y)\Delta t^2 + \tfrac{1}{4}f''(Y)\sigma(Y)^2\Delta t^2\big)/\Delta t^2, \\ \Gamma_2^1 &= \big(\tfrac{1}{2}\sigma(Y)^2\Delta t + \tfrac{1}{2}f(Y)\Delta t^2 + \tfrac{1}{2}f'(Y)\sigma(Y)^2\Delta t^2 + \tfrac{1}{4}(\sigma^2)'f(Y)\Delta t^2 \\ &\quad + \tfrac{1}{8}(\sigma(Y)^2)''\sigma(Y)^2\Delta t^2\big)/\Delta t^2, \\ \Gamma_3^1 &= \big(\tfrac{1}{4}(\sigma(Y)^2)'\Delta t^2 + \tfrac{1}{2}f(Y)\sigma(Y)^2\Delta t^2\big)/\Delta t^2, \\ \Gamma_4^1 &= \tfrac{1}{8}\sigma(Y)^4, \\ \Gamma_5^1 &= 0.\end{aligned}$$

For the forward Euler method (2.2),

$$\begin{aligned}\mathbf{E}\phi(X_1) &= \mathbf{E}(Y + f(Y)\Delta t + \sigma(Y)B_n(\Delta t))^k \\ &= Y^k + \Delta t^2 \sum_{j=1}^{k} \frac{k!}{(k-j)!} Y^{k-j}\Gamma_j^2 + \mathcal{O}(\Delta t^3)\,,\end{aligned}$$

where

$$\begin{aligned}&\Gamma_1^2 = f(Y)/\Delta t, \quad \Gamma_2^2 = \big(\tfrac{1}{2}f(Y)^2\Delta t^2 + \tfrac{1}{2}\sigma(Y)^2\Delta t\big)/\Delta t^2 \\ &\Gamma_3^2 = \big(\tfrac{1}{6}3f(Y)\Delta t^2\sigma(Y)^2\big), \quad \Gamma_4^2 = \big(\tfrac{3}{4!}\sigma(Y)^4\big), \quad \Gamma_5^2 = 0.\end{aligned}$$

Now $\Gamma_j = \Gamma_j^2 - \Gamma_j^1$. Forward Euler is a first order method in the weak sense and, for our modified equation, we must verify that $\Gamma_j = 0$ for $j = 3, \dots, 5$. It is clear that $\Gamma_4 = \Gamma_5 = 0$. The terms $\Gamma_3 = \frac{1}{4}(\sigma(Y)^2)'$ and to achieve $\Gamma_3 = 0$ we further require that σ be constant. In this case,

$$\tilde{f}(Y) = -\tfrac{1}{2} f'(Y) f(Y) - \tfrac{1}{4} f''(Y)\sigma^2, \quad \tilde{\sigma} = -\tfrac{1}{2} f'(Y)\sigma$$

and the modified equation for the forward Euler method is

$$d\tilde{X} = \big[f(\tilde{X}) - \Delta t\big(\tfrac{1}{2} f'(\tilde{X}) f(\tilde{X}) + \tfrac{1}{4} f''(\tilde{X})\sigma^2\big)\big]\, dt + \sigma(1 - \Delta t f'(\tilde{X})/2)\, d\beta(t). \tag{2.11}$$

Under suitable regularity conditions that we do not provide, it is possible to prove using Theorem 14.5.2 of [4] that the forward Euler method approximates the solution of (2.11) to weak second order accuracy:

$$|\mathbf{E}\phi(X_n) - \mathbf{E}\phi(\tilde{X}(n\Delta t))| = \mathcal{O}(\Delta t^2), \quad 0 \le n\Delta t \le T.$$

Even though the original equation is additive, the modified equation will in general feature multiplicative noise. In particular, we are unable to iterate to gain the next higher order modified equation. The exception is the linear equation $f(x) = \gamma x$, which has modified equation

$$d\tilde{X} = \big(\gamma - \tfrac{1}{2}\gamma^2 \Delta t\big)\tilde{X}\, dt + \sigma\big(1 - \tfrac{1}{2}\gamma\Delta t\big)\, d\beta(t).$$

Example: backward Euler. The backward Euler method or drift implicit scheme is

$$X_{n+1} = X_n + f(X_{n+1})\Delta t + \sigma(X_n) B_n(\Delta t), \quad X_0 = Y.$$

By similar techniques, the modified equation for the backward Euler method is

$$d\tilde{X} = \big[f(\tilde{X}) + \Delta t\big(\tfrac{1}{2} f'(\tilde{X}) f(\tilde{X}) + \tfrac{1}{4} f''(\tilde{X})\sigma^2\big)\big]\, dt + \sigma(1 + \Delta t f'(\tilde{X})/2)\, d\beta(t).$$

The modified equation for the linear case $f(X) = \gamma X$ is

$$d\tilde{X} = \big(\gamma + \tfrac{1}{2}\gamma^2 \Delta t\big)\tilde{X}\, dt + \sigma\big(1 + \tfrac{1}{2}\gamma\Delta t\big)\, d\beta(t).$$

3 Multiple dimensions.

We look at the following SDE in $\mathbf{R}^d$

$$d\boldsymbol{X} = \boldsymbol{f}(\boldsymbol{X})\, dt + \sum_{i=1}^{d} \sigma_i \boldsymbol{e}_i\, d\beta_i(t), \quad \boldsymbol{X}(0) = \boldsymbol{Y},$$

where $\boldsymbol{f}\colon \mathbf{R}^d \to \mathbf{R}^d$ is smooth, σ_i are constant scalars, $\boldsymbol{e}_i$ is the ith unit vector, and $\beta_i(t)$ are independent standard Brownian motions. We wish to develop the modified equation

$$d\tilde{\boldsymbol{X}} = [\boldsymbol{f}(\tilde{\boldsymbol{X}}) + \Delta t \tilde{\boldsymbol{f}}(\tilde{\boldsymbol{X}})]\, dt + \sum_{i=1}^{d} \sigma_i \boldsymbol{e}_i\, d\beta_i(t) + \sum_{i,j=1}^{d} \Delta t \tilde{\sigma}_{ij}(\tilde{\boldsymbol{X}}) \boldsymbol{e}_i\, d\beta_j(t). \tag{3.1}$$

We can perform similar calculations to Section 2 to compute modified drift $\tilde{\boldsymbol{f}}$ and diffusion $\tilde{\sigma}_{ij}$ terms, by looking at the consistency condition on moments $\mathbf{E}\phi(\tilde{\boldsymbol{X}}(\Delta t))$, where $\phi(\boldsymbol{X}) = X_i$ or $\phi(\boldsymbol{X}) = X_i X_j$ and $\boldsymbol{X} = [X_1, \dots, X_d]^T$. This leads to modified terms for the forward Euler method of the following form:

$$\tilde{\boldsymbol{f}}(\boldsymbol{Y}) = -\tfrac{1}{2} D\boldsymbol{f}(\boldsymbol{Y})\boldsymbol{f}(\boldsymbol{Y}) - \tfrac{1}{4}\sum_i \partial_i^2 \boldsymbol{f}(\boldsymbol{Y})\sigma_i^2, \quad \tilde{\sigma}_{ij}(\boldsymbol{Y}) = -\tfrac{1}{2}\partial_i f_j(\boldsymbol{Y})\sigma_i, \tag{3.2}$$

where $D\boldsymbol{f}$ is the Jacobian of $\boldsymbol{f}$ and $\partial_i = \partial/\partial X_i$ and $\partial_i^2 = \partial^2/\partial X_i^2$. Further it can be shown that all moments $\mathbf{E}\phi(\tilde{\boldsymbol{X}})$, where $\phi(\boldsymbol{X})$ is any polynomial in $X_1, \dots, X_d$ up to order five, equal the corresponding average for the numerical method to order Δt^2 terms (see Appendix B). Subject to regularity conditions, averages with respect to the forward Euler method and modified equation (3.1) converge with order Δt^2. This is particular to the Euler method and second order modified equations are not available for all first order weak methods, as we now present in an example.

EXAMPLE. Consider the following Langevin SDE describing the position q and momentum p of a mechanical system with internal energy $V(q)$, dissipation γ, and temperature $\sigma^2/2\gamma$

$$dq = p\, dt, \quad dp = [-\gamma p - V'(q)]\, dt + \sigma\, d\beta(t). \tag{3.3}$$

Rewrite in standard form, with $\boldsymbol{X} = [q, p]^T$,

$$f(\boldsymbol{X}) = \begin{pmatrix} p \\ -\gamma p - V'(q) \end{pmatrix}, \quad \sigma_1 = 0, \quad \sigma_2 = \sigma$$

and apply (3.2): The modified equation for the forward Euler equation is defined by

$$\tilde{f}(\boldsymbol{X}) = -\tfrac{1}{2}\begin{pmatrix} 0 & 1 \\ -V''(q) & -\gamma \end{pmatrix}\begin{pmatrix} p \\ -\gamma p - V'(q) \end{pmatrix} = \begin{pmatrix} -\gamma p - V'(q) \\ -V''(q)p + \gamma^2 p + \gamma V'(q) \end{pmatrix}$$

and

$$\tilde{\sigma}_{11} = 0, \quad \tilde{\sigma}_{22} = -\tfrac{1}{2}\gamma\sigma, \quad \tilde{\sigma}_{12} = 0, \quad \tilde{\sigma}_{21} = -\sigma.$$

Subject to regularity condition, this modified equation describes the behaviour of the forward Euler approximation weakly to second order.

Hamiltonian systems should be solved by symplectic integrators, because the discretised system inherits many dynamical qualities of the underlying differential equations. It is interesting to consider extending symplectic method to equations like (3.3) and find dynamical properties of the Langevin equations that are inherited by the stochastic numerical methods. A number of interesting papers in this direction are available [7, 6]. Forward Euler is not symplectic for the Hamiltonian system (case $\gamma = \sigma = 0$). We consider now a first order method that does reduce to a symplectic method in the Hamiltonian case. The following generalises the symplectic Euler method to the case $\sigma, \gamma \neq 0$:

$$\begin{aligned} q_{n+1} &= q_n + p_{n+1}\Delta t \\ p_{n+1} &= p_n - (\gamma p_n + V'(q_n))\Delta t + \sigma B_n(\Delta t). \end{aligned} \tag{3.4}$$

It can be shown that the following modified equation satisfies the consistency conditions for the first and second order moments

$$\begin{aligned} dq &= \left[\left(1 - \tfrac{1}{2}\gamma\Delta t\right)p - \tfrac{1}{2}\Delta t V'(q_n)\right] dt - \sigma\,\Delta t\, d\beta(t) \\ dp &= \left[\left(-\gamma + \tfrac{1}{2}\Delta t\gamma^2\right)p - \left(V'(q) - \tfrac{1}{2}\Delta t V''(q)p\right) + \tfrac{1}{2}\gamma V'(q)\Delta t\right] dt \\ &\quad + \sigma(1 + \gamma\Delta t/2)\, d\beta(t). \end{aligned}$$

This system can be written

$$\begin{aligned} dq &= (\tilde{H}_p(q,p) - \gamma\Delta t p_n/2)\, dt \\ dp &= -\tilde{H}_q(q,p)\, dt - \gamma\left(1 + \tfrac{1}{2}\Delta t\gamma + \tfrac{1}{2}\Delta t V'(q)\right)p\, dt + \sigma(1 + \gamma\Delta t/2)\, d\beta(t), \end{aligned} \tag{3.5}$$

where the modified Hamiltonian $\tilde{H}(q,p) = \frac{1}{2}p^2 + V(q) - \frac{1}{2}\Delta t V'(q)p$, as one expects from studying modified equations for the symplectic Euler method. In this case, it can be shown that the moment $\mathbf{E}q(\Delta t)p(\Delta t)^2$ is incorrect in the Δt^2 term (see Appendix C) and therefore weak convergence of the modified equation will only be first order.

4 Conclusions.

We have developed a limited form of backward error analysis for SDEs with additive noise, providing weak second order modified equations for Euler type methods. The analysis does not extend easily to more general situations. For example, we might like to determine higher order modified equations for the Euler methods and modified equations for higher order weak methods. This is not possible in general.

The type of expansion given does not have sufficient degrees of freedom to satisfy all the consistency conditions. It is simple to introduce further degrees of freedom by making $\tilde{f}, \tilde{\sigma}$ random, but I have been unable to achieve any results with such terms. To study this problem further, a better form for the expansion should be introduced, but one which is simple enough for the modified equation to provide understanding of the numerical method. One direction to extend this work is pathwise backward error analysis. It is possible to approximate Stratonovich SDEs by a non autonomous ODE, see for example [1, 9]. A pathwise error analysis could be achieved by modifying this approximate ODE and seeing how the much change is required to describe the numerical method. The approximate ODE technique has been applied to the numerical analysis of SDEs in [2].

A Expansions in one dimension for exact and forward Euler.

We verify the expansions used in Section 2. Start by expanding the true solution

$$\mathbf{E}\phi(X(t)) = \phi(Y) + \mathbf{E}\left[\int_0^t \phi'(X(s))f(X(s))\,ds + \tfrac{1}{2}\int_0^t \phi''(X(s))^2\sigma(X(s))^2\,ds\right].$$

Now,

$$\begin{aligned}\mathbf{E}\phi'(X_t)f(X_t) = \phi'(Y)f(Y) &+ \mathbf{E}\int_0^t (\phi'(X(s))f(X(s)))'f(X(s))\,ds \\ &+ \tfrac{1}{2}\mathbf{E}\int_0^t (\phi'(X(s))f(X(s)))''\sigma(X(s))^2\,ds\end{aligned}$$

and

$$\begin{aligned}\mathbf{E}\phi''(X_t)\sigma(X_t)^2 = \phi''(Y)\sigma(Y)^2 &+ \mathbf{E}\int_0^t \left(\phi''(X(s))\sigma(X(s))^2\right)'f(X(s))\,ds \\ &+ \tfrac{1}{2}\mathbf{E}\int_0^t (\phi''(X(s))\sigma^2(X(s)))''\sigma(X(s))^2\,ds.\end{aligned}$$

Meaning that,

$$\begin{aligned}\phi(X(\Delta t)) = \phi(Y) &+ \phi'(Y)f(Y)\Delta t + \tfrac{1}{2}\phi''(Y)\sigma(Y)^2\Delta t \\ &+ \tfrac{1}{2}\Delta t^2\left[(\phi'(Y)f(Y))'f(Y) + \tfrac{1}{2}(\phi'(Y)f(Y))'\sigma(Y)^2\right] \\ &+ \tfrac{1}{4}\Delta t^2\left[(\phi''(Y)\sigma(Y)^2)'f(Y) + \tfrac{1}{2}(\phi''(Y)\sigma(Y)^2)''\sigma(Y)^2\right] + \mathcal{O}(\Delta t^3)\,.\end{aligned}$$

Similarly, if $\phi(X) = X^p$,

$$\begin{aligned}\phi(X(\Delta t)) = (Y)^p &+ p(Y)^{p-1}\left[f(Y)\Delta t + \tfrac{1}{2}f'f\Delta t^2 + \tfrac{1}{4}f''\sigma^2\Delta t^2\right] \\ &+ p(p-1)(Y)^{p-2}\left[\tfrac{1}{2}\sigma(Y)^2\Delta t + \tfrac{1}{2}f^2\Delta t^2 + \tfrac{1}{4}(\sigma^2)'f\Delta t^2\right. \\ &\quad \left. + \tfrac{1}{8}(\sigma^2)''\sigma^2\Delta t^2 + \tfrac{1}{2}f'\sigma^2\Delta t^2\right] \\ &+ p(p-1)(p-2)Y^{p-3}\left[\tfrac{1}{2}(\sigma^2)'\sigma^2\Delta t^2 + \tfrac{1}{4}f\sigma^2\Delta t^2 + \tfrac{1}{4}f\sigma^2\Delta t^2\right] \\ &+ p(p-1)(p-2)(p-3)Y^{p-4}\left[\tfrac{1}{8}\sigma^4\Delta t^2\right] + \mathcal{O}(\Delta t^3)\,.\end{aligned}$$

Now, for the forward Euler method,

$$\begin{aligned}\mathbf{E}\phi(X_1) &= \mathbf{E}(Y + f(Y)\Delta t + \sigma(Y)N(0,\Delta t))^p \\ &= \mathbf{E}\Bigg[Y^p + pY^{p-1}(f(Y)\Delta t + \sigma(Y)N(0,\Delta t)) \\ &\qquad + \binom{2}{p}Y^{p-2}(f(Y)\Delta t + \sigma(Y)N(0,\Delta t))^2\end{aligned}$$

$$+ \binom{3}{p} Y^{p-3}(f(Y)\Delta t + \sigma(Y)N(0,\Delta t))^3$$
$$+ \binom{4}{p} Y^{p-4}(f(Y)\Delta t + \sigma(Y)N(0,\Delta t))^4\Big].$$

That is,

$$\begin{aligned}\mathbf{E}\phi(X_1) = Y^p &+ pY^{p-1}f(Y)\Delta t \\ &+ p(p-1)Y^{p-2}\big(\tfrac{1}{2}f(Y)^2\Delta t^2 + \tfrac{1}{2}\sigma(Y)^2\Delta t\big) \\ &+ p(p-1)(p-2)Y^{p-3}\big(\tfrac{1}{6}3f(Y)\Delta t^2\sigma(Y)^2\big) \\ &+ p(p-1)(p-2)(p-3)Y^{p-4}\big(\tfrac{3}{4!}\sigma(Y)^4\Delta t^2\big).\end{aligned}$$

B Multiple dimensions-forward Euler.

We verify that the modified equation for forward Euler method in multiple dimensions satisfies the moment conditions up to fifth order. Consider

$$d\tilde{\boldsymbol{X}} = [\boldsymbol{f}(\tilde{\boldsymbol{X}}) + \Delta t\tilde{\boldsymbol{f}}(\tilde{\boldsymbol{X}})]\;dt + \sum_{i,j=1}^{d}(\sigma_i + \Delta t\tilde{\sigma}_{ij}(\tilde{\boldsymbol{X}}))\boldsymbol{e}_i\;d\beta_j(t).$$

The relevant Itô–Taylor expansion for $X(t)$ is

$$\begin{aligned}&\mathbf{E}\phi(\boldsymbol{X}(t)) = \mathbf{E}\phi(\boldsymbol{Y}) + t\,\boldsymbol{\nabla}\phi(\boldsymbol{Y})\cdot\boldsymbol{f}(\boldsymbol{Y}) \\ &+ \tfrac{1}{2}t\sum_{i=1}^{d}\sigma_i^2\partial_i^2\phi(\boldsymbol{Y}) + \tfrac{1}{2}t^2\boldsymbol{\nabla}(\boldsymbol{\nabla}\phi(\boldsymbol{Y})\cdot\boldsymbol{f}(\boldsymbol{Y}))\cdot\boldsymbol{f}(\boldsymbol{Y}) + \tfrac{1}{4}t^2\sigma_i^2\partial_i^2(\boldsymbol{\nabla}\phi(\boldsymbol{Y})\cdot\boldsymbol{f}(\boldsymbol{Y})) \\ &+ \tfrac{1}{4}t^2\sum_{i=1}^{d}\nabla(\partial_i^2\phi(\boldsymbol{Y}))\cdot\boldsymbol{f}(\boldsymbol{Y})\sigma_i^2 + \tfrac{1}{8}t^2\sum_{i,j=1}^{d}\sigma_i^2\sigma_j^2\partial_j^2\partial_i^2\phi(\boldsymbol{Y}) + \mathcal{O}(t^3)\,.\end{aligned}$$

Substitute the modified terms for the forward Euler method,

$$\tilde{f}(\boldsymbol{Y}) = -\tfrac{1}{2}Df(\boldsymbol{Y})\boldsymbol{f}(\boldsymbol{Y}) - \tfrac{1}{4}\sum_{i=1}^{d}\sigma_i^2\partial_i^2\boldsymbol{f}(\boldsymbol{Y}), \quad \tilde{\sigma}_{ij}(\boldsymbol{Y}) = -\sigma_i\partial_i f_j(\boldsymbol{Y})/2,$$

to gain

$$\begin{aligned}\mathbf{E}\phi(\tilde{\boldsymbol{X}}(t)) = \mathbf{E}\phi(\boldsymbol{Y}) &+ t\,\boldsymbol{\nabla}\phi(\boldsymbol{Y})\cdot(\boldsymbol{f}(\boldsymbol{Y}) + \Delta t\tilde{\boldsymbol{f}}(\boldsymbol{Y})) \\ &+ \tfrac{1}{2}t\sum_{i=1}^{d}\sigma_i^2\partial_i^2\phi(\boldsymbol{Y}) + \tfrac{1}{2}t^2\sum_{i,j=1}^{d}2\Delta t\sigma_i\tilde{\sigma}_{ij}\partial_{ij}^2\phi(\boldsymbol{Y}) \\ &+ \tfrac{1}{2}t^2\big(\boldsymbol{\nabla}^2\phi(\boldsymbol{Y})(\boldsymbol{f},\boldsymbol{f}) + (\boldsymbol{\nabla}\phi D\boldsymbol{f}\boldsymbol{f})\big)\end{aligned}$$

$$
\begin{aligned}
&+ \tfrac{1}{4}t^2 \sum_{i=1}^{d} \sigma_i^2 \Big(\big(\boldsymbol{\nabla}\partial_i^2 \phi(\boldsymbol{Y}) \cdot \boldsymbol{f}(\boldsymbol{Y})\big) + 2(\boldsymbol{\nabla}\partial_i \phi(\boldsymbol{Y}) \cdot \partial_i \boldsymbol{f}(\boldsymbol{Y})) \\
&\qquad + \big(\boldsymbol{\nabla}\phi(\boldsymbol{Y}) \cdot \partial_i^2 \boldsymbol{f}(\boldsymbol{Y})\big)\Big) \\
&+ \tfrac{1}{4}t^2 \sum_{i=1}^{d} \boldsymbol{\nabla}\big(\partial_i^2 \phi(\boldsymbol{Y})\big) \cdot \boldsymbol{f}(\boldsymbol{Y})\sigma_i^2 + \tfrac{1}{8}t^2 \sum_{i,j=1}^{d} \sigma_i^2 \sigma_j^2 \partial_j^2 \partial_i^2 \phi(\boldsymbol{Y}) + \mathcal{O}(t^3)\,.
\end{aligned}
$$

Note that

$$
2\sum_{i,j=1}^{d} \sigma_i \tilde{\sigma}_{ij} \partial_{ij}^2 \phi(\boldsymbol{Y}) = -\sum_{i,j=1}^{d} \sigma_i^2(\boldsymbol{Y}) \partial_i f_j \partial_{ij}^2 \phi = -\sum_{i=1}^{d} \sigma_i^2 \partial_i \boldsymbol{f} \cdot \boldsymbol{\nabla}\partial_i \phi.
$$

Thus, we have reduced the expansion to

$$
\begin{aligned}
\mathbf{E}\phi(\tilde{\boldsymbol{X}}(t)) &= \mathbf{E}\phi(\boldsymbol{Y}) + t\,\boldsymbol{\nabla}\phi(\boldsymbol{Y}) \cdot \boldsymbol{f}(\boldsymbol{Y}) + \tfrac{1}{2}t\sum_{i=1}^{d} \sigma_i^2 \partial_i^2 \phi(\boldsymbol{Y}) + \tfrac{1}{2}t^2(\boldsymbol{\nabla}^2\phi(\boldsymbol{Y})(\boldsymbol{f},\boldsymbol{f})) \\
&\quad + \tfrac{1}{4}t^2 \sum_{i=1}^{d} \sigma_i^2 \big(\boldsymbol{\nabla}\partial_i^2 \phi(\boldsymbol{Y}) \cdot \boldsymbol{f}(\boldsymbol{Y})\big) \\
&\quad + \tfrac{1}{4}t^2 \sum_{i=1}^{d} \boldsymbol{\nabla}\big(\partial_i^2 \phi(\boldsymbol{Y})\big) \cdot \boldsymbol{f}(\boldsymbol{Y})\sigma_i^2 + \tfrac{1}{8}t^2 \sum_{i,j=1}^{d} \sigma_i^2 \sigma_j^2 \partial_j^2 \partial_i^2 \phi(\boldsymbol{Y}) + \mathcal{O}(t^3) \\
&= \mathbf{E}\phi(\boldsymbol{Y}) + t\,\boldsymbol{\nabla}\phi(\boldsymbol{Y}) \cdot \boldsymbol{f}(\boldsymbol{Y}) + \tfrac{1}{2}t\sum_{i=1}^{d} \sigma_i^2 \partial_i^2 \phi(\boldsymbol{Y}) + \tfrac{1}{2}t^2(\boldsymbol{\nabla}^2\phi(\boldsymbol{Y})(\boldsymbol{f},\boldsymbol{f})) \\
&\quad + \tfrac{1}{2}t^2 \sum_{i=1}^{d} \sigma_i^2 \big(\boldsymbol{\nabla}\partial_i^2 \phi(\boldsymbol{Y}) \cdot \boldsymbol{f}(\boldsymbol{Y})\big) + \tfrac{1}{8}t^2 \sum_{i,j=1}^{d} \sigma_i^2 \sigma_j^2 \partial_j^2 \partial_i^2 \phi(\boldsymbol{Y}) + \mathcal{O}(t^3)\,.
\end{aligned}
$$

Remarkably, if $\phi(\boldsymbol{Y}) = \prod \phi_i(\boldsymbol{Y})$, where $\phi_i(\boldsymbol{Y})$ has the form Y_i^j, then

$$
\mathbf{E}\phi(\tilde{\boldsymbol{X}}(t)) = \prod \mathbf{E}[\phi_i(\tilde{\boldsymbol{X}}(t))] + \mathcal{O}(t^3)\,.
$$

This is easily verified by multiplying terms together, noting that

$$
\begin{aligned}
\mathbf{E}\phi_i(\tilde{\boldsymbol{X}}(t)) &= \phi_i(\boldsymbol{Y}) + t\,\partial_i\phi_i(\boldsymbol{Y}) f_i(\boldsymbol{Y}) + \tfrac{1}{2}t\sigma_i^2 \partial_i^2 \phi_i(\boldsymbol{Y}) + \tfrac{1}{2}t^2 \partial_i^2 \phi_i f_i(\boldsymbol{Y})^2 \\
&\quad + \tfrac{1}{4}t^2\sigma_i^2 \partial_i^3 \phi_i f_i(\boldsymbol{Y}) + \tfrac{1}{4}\sigma_i^2 t^2\, \partial_i^3 \phi_i(\boldsymbol{Y}) \tilde{f}_i(\boldsymbol{Y}) + \tfrac{1}{8}t^2 \sigma_i^4 \partial_i^4 \phi_i(\boldsymbol{Y}) + \mathcal{O}(t^3)\,.
\end{aligned}
$$

C Symplectic Euler-not consistent.

We derive the modified terms for the symplectic Euler method, and show they do not satisfy the higher order moment conditions. Consider the method given in (3.4),

$$
\begin{aligned}
q_{n+1} &= q_n + p_{n+1}\Delta t \\
p_{n+1} &= p_n - (\gamma p_n + V'(q_n))\Delta t + \sigma B_n(\Delta t).
\end{aligned}
$$

Thus,

$$\mathbf{E}p_{n+1} = p_n - (\gamma p_n + V'(q_n))\Delta t, \tag{C.1}$$

$$\mathbf{E}q_{n+1} = q_n + \mathbf{E}p_{n+1}\Delta t = q_n + p_n\Delta t - \Delta t^2(\gamma p_n + V'(q_n)). \tag{C.2}$$

Further,

$$\begin{aligned}
\mathbf{E}p_{n+1}^2 &= (\mathbf{E}p_{n+1})^2 + \sigma^2\Delta t \\
&= p_n^2 - 2(\gamma p_n + V'(q_n))p_n\Delta t + \Delta t^2(\gamma p_n + V'(q_n))^2 + \sigma^2\Delta t \\
\mathbf{E}q_{n+1}^2 &= (\mathbf{E}q_{n+1})^2 + \mathcal{O}(\Delta t^3) \\
&= q_n^2 + 2\Delta t q_n p_n - 2q_n\Delta t^2(\gamma p_n + V'(q_n)) + \Delta t^2 p_n^2 + \mathcal{O}(\Delta t^3)\,.
\end{aligned}$$

For the cross term, note

$$\mathbf{E}p_{n+1}q_{n+1} = \mathbf{E}(q_n + p_{n+1}\Delta t)p_{n+1} = q_n\mathbf{E}p_{n+1} + \Delta t\mathbf{E}p_{n+1}^2$$

and thus

$$\begin{aligned}
\mathbf{E}p_{n+1}q_{n+1} &= q_n(p_n - (\gamma p_n - V'(q_n))\Delta t) + \Delta t\big(p_n^2 - 2(\gamma p_n + V'(q_n))p_n\Delta t\big) \\
&= q_n p_n - \gamma q_n p_n\Delta t - V'(q_n)q_n\Delta t \\
&\quad + p_n^2\Delta t - 2\gamma p_n^2\Delta t^2 - 2V'(q_n)p_n\Delta t^2.
\end{aligned}$$

Now, we have enough information about the moments of the numerical method over one time step, to identify the terms in the following modified equation

$$\begin{aligned}
dq &= p\,dt + \Delta t\tilde{f}_1(q,p)\,dt + \Delta t\tilde{\sigma}_{12}(q,p)\,d\beta(t), \\
dp &= (-\gamma p - V'(q))\,dt + \Delta t\tilde{f}_2(q,p)\,dt + (\sigma + \Delta t\tilde{\sigma}(q,p))\,d\beta(t),
\end{aligned}$$

with initial data $q(0) = q_0$ and $p(0) = p_0$. We compute the moments over time t and identify the modified drift and diffusion terms. First,

$$\begin{aligned}
\mathbf{E}q(t) &= q_0 + \int_0^t p(s) + \Delta t\tilde{f}_1(q(s),p(s))\,ds. \\
&= q_0 + \int_0^t \Big(p_0 + \int_0^s (-\gamma p(r) - V'(q(r)) + \Delta t\tilde{f}_2(q(r),p(r)))\,dr\Big) \\
&\quad + \Delta t\tilde{f}_1(q_0,p_0)\,ds + \mathcal{O}(t^3 + \Delta t\,t^2) \\
&= q_0 + p_0 t + (-\gamma p_0 - V'(q_0))t^2/2 + \Delta t\tilde{f}_1(q_0,p_0)t + \mathcal{O}(t^3 + \Delta t\,t^2)\,.
\end{aligned}$$

Comparing with (C.2), we see $\tilde{f}_1(q,p) = -\frac{1}{2}(\gamma p + V'(q))$.

$$\begin{aligned}
\mathbf{E}p(t) &= p_0 + \int_0^t (-\gamma p - V'(q))\,ds + \int_0^t \Delta t \tilde{f}_2(q,p))\,ds \\
&= p_0 + \int_0^t (-\gamma(p_0 - \gamma p_0 s - V'(q_0)s) - (V'(q_0) + V''(q_0)p\,s)\,ds \\
&\quad + \int_0^t \Delta t \tilde{f}_2(q(s),p(s))\,ds + \mathcal{O}(t^2)\; + \mathcal{O}(t^3) \\
&= p_0 - \gamma\big(p_0 t - \gamma p_0 t^2/2 - V'(q_0)t^2/2\big) - (V'(q_0)t + V''(q_0)p\,t^2/2) \\
&\quad + \Delta t\, t\, \tilde{f}_2(q,p) + \mathcal{O}(t^3 + \Delta t\, t^2)\,.
\end{aligned}$$

Comparing with (C.1), we see $\tilde{f}_2(q,p) = -\frac{1}{2}(\gamma^2 p + \gamma V'(q) - V''(q)p)$.

$$\begin{aligned}
\mathbf{E}p(t)^2 &= p_0^2 + \int_0^t 2p(s)(-\gamma p(s) - V'(q(s)) + \Delta t \tilde{f}_2(q(s),p(s)))\,ds + \sigma^2 t \\
&\quad + \tfrac{1}{2}\int_0^t 2\Delta t \sigma \tilde{\sigma}(q(s),p(s))\,ds \\
&= p_0^2 + \int_0^t 2(p_0 - \gamma p_0 s - V'(q)s)(-\gamma(p_0 - s\gamma p_0 - sV'(q_0)) \\
&\qquad - (V'(q_0) + V''(q_0)p_0 s))\,ds \\
&\quad + \sigma^2 t + \Delta t \sigma \tilde{\sigma} t + 2p_0 \Delta t\, t \tilde{f}_2 - 2\gamma\sigma^2 t^2/2 + \mathcal{O}(t^3 + \Delta t\, t^2) \\
&= p_0^2 + 2tp_0(-\gamma p_0 - V'(q_0)) \\
&\quad + 2\tfrac{1}{2}t^2\big(\gamma^2 p_0^2 + \gamma V'(q)p_0 + \gamma^2 p_0^2 + p_0\gamma V'(q_0) - p_0^2 V''(q_0)\big) \\
&\quad + \sigma^2 t + 2\Delta t \sigma \tilde{\sigma} t + 2p_0 \Delta t\, t \tilde{f}_2(q_0,p_0) - 2\gamma\sigma^2 t^2/2 + \mathcal{O}(t^3 + \Delta t\, t^2)\,.
\end{aligned}$$

From this we see $\tilde{\sigma} = \gamma\sigma/2$. And

$$\begin{aligned}
\mathbf{E}p(t)q(t) &= p_0 q_0 + \int_0^t q(s)(-\gamma p(s) - V'(q(s)) + \Delta t \tilde{f}_2(q(s),p(s)))\,ds \\
&\quad + \int_0^t p(s)(p(s) + \Delta t \tilde{f}_1(q(s),p(s)))\,ds + \tfrac{1}{2}\tilde{\sigma}_{12}\sigma \Delta t\, t \\
&= p_0 q_0 + \int_0^t (q_0 + sp_0)(-\gamma(p_0 - \gamma p_0 s - V'(q_0)s) \\
&\qquad - (V'(q_0) + V''(q_0)p\,s) + \Delta t \tilde{f}_2(q_0,p_0))\,ds \\
&\quad + \int_0^t (p_0 - \gamma p_0 s - V'(q_0)s)(p_0 - \gamma p_0 s - V'(q_0)s + \Delta t \tilde{f}_1(q_0,p_0))\,ds \\
&\quad + \tfrac{1}{2}\tilde{\sigma}_{12}\sigma \Delta t\, t + \sigma^2 \tfrac{1}{2} t^2 + \mathcal{O}(t^2)
\end{aligned}$$

$$
\begin{aligned}
&= p_0 q_0 - \gamma q_0 p_0\, t - q_0 V'(q_0) t \\
&\quad + \tfrac{1}{2} t^2 \big(\gamma^2 p_0 q_0 + \gamma q_0 V'(q_0) - \gamma p_0^2 - q_0 p_0 V''(q_0) - p_0 V'(q_0)\big) \\
&\quad + q_0 \Delta t \tilde{f}_2(q_0, p_0)\, t + t p_0^2 + \tfrac{1}{2} t^2 \big(- 2\gamma p_0^2 - 2V'(q_0) p_0)\big) \\
&\quad + t \Delta t \tilde{f}_1(q_0, p_0) p_0 + \tfrac{1}{2} \tilde{\sigma}_{12} \sigma \Delta t\, t + \sigma^2 \tfrac{1}{2} t^2.
\end{aligned}
$$

From which, we glean that $\tilde{\sigma}_{12} = -\sigma$. With these terms, the modified equation takes the form

$$
\begin{aligned}
dq &= \big[p - \tfrac{1}{2}\Delta t(\gamma p_n + V'(q_n))\big]\, dt = \big[\big(1 - \tfrac{1}{2}\gamma \Delta t\big) p - \tfrac{1}{2}\Delta t V'(q_n)\big]\, dt - \sigma \Delta t\, d\beta(t) \\
dp &= \big[- \gamma p - V'(q) + \tfrac{1}{2}\Delta t (V''(q) p - \gamma^2 p - \gamma V'(q))\big]\, dt + \sigma(1 + \gamma \Delta t/2)\, d\beta(t) \\
&= \big[- \big(\gamma + \tfrac{1}{2}\Delta t \gamma^2\big) p - \big(V'(q) - \tfrac{1}{2}\Delta t V''(q) p\big) + \tfrac{1}{2}\gamma \Delta t V'(q))\big]\, dt \\
&\quad + \sigma(1 + \gamma \Delta t/2)\, d\beta(t).
\end{aligned}
$$

We have used the second order moment conditions to assign all the free variables. But to guarantee convergence we need to assert that all moments up to order five have the correct order. This is not the case, as can be seen by examining $\phi(q,p) = qp^2$ in the case $\gamma = 0$ and $V = 0$. Note that with $p_{n+1} = p_n + \sigma B_n(\Delta t)$,

$$
\begin{aligned}
\mathbf{E} q_{n+1} p_{n+1}^2 &= \mathbf{E}\big[(q_n + \Delta t p_{n+1}) p_{n+1}^2\big] \\
&= \mathbf{E} q_n p_{n+1}^2 + \mathbf{E} p_{n+1}^3 \Delta t \\
&= q_n \big(p_n^2 + \sigma^2 \Delta t\big) + \Delta t \big(p_n^3 + 3 p_n \sigma^2 \Delta t\big).
\end{aligned}
\tag{C.3}
$$

Now this should match the expansion of $\mathbf{E}\phi(q(t), p(t))$ up to second order:

$$
\begin{aligned}
\mathbf{E}\big[q(t) p(t)^2\big] &= q_0 p_0^2 + \int_0^t p(s)^2 p(s)\, ds + \int_0^t 2p(s) q(s)(0)\, ds \\
&\quad + \tfrac{1}{2} \int_0^t 2q(s)(\sigma + \tilde{\sigma}\Delta t)^2\, ds + \tfrac{1}{2} \int_0^t 2p(s) \Delta t \sigma \tilde{\sigma}_{12}\, ds.
\end{aligned}
$$

Now, $\mathbf{E} p(t)^3 = p_0^3 + \frac{1}{2}(6p_0)\sigma^2 t + \mathcal{O}(t^2)$. Hence,

$$
\begin{aligned}
\mathbf{E}\big[q(t) p(t)^2\big] &= q_0 p_0^2 + \big(p_0^3 t + \tfrac{1}{2} t^2 \big(3 p_0 \sigma^2\big)\big) \\
&\quad + \tfrac{1}{2}\big(2 t q_0 \sigma^2 + \tfrac{1}{2} t^2 2 p_0 \sigma^2 + 2 q_0 2 \sigma \tilde{\sigma} \Delta t\, t\big) \\
&\quad + \tfrac{1}{2}(2 p_0 \Delta t\, t \tilde{\sigma}_{12} \sigma) + \mathcal{O}(t^3) \\
&= q_0 p_0^2 + t q_0 \sigma^2 + \big(\tfrac{1}{2}\sigma^2 + \tilde{\sigma}_{12}\sigma + \tfrac{3}{2}\sigma^2\big) p_0 t^2 + 2\sigma \tilde{\sigma} t^2 q_0 + \mathcal{O}(t^3)\,.
\end{aligned}
$$

We see the coefficient of $p_0 \sigma^2 t^2$ with the coefficient $\tilde{\sigma}_{12} = -\sigma$ is 3, which is inconsistent with the coefficient of 1 in (C.3).

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