Stability-Optimized High Strong Order Methods for Stochastic Differential Equations with Additive and Diagonal Noise

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April 28, 2017

1 Introduction

Stochastic differential equations have seen increasing use in scientific fields such as biology and climate science due to their ability to capture the randomness inherent in physical systems. These equations are of the general form:

$$dX_t = f(t, X_t)dt + g(t, X_t)dW_t$$

where X_t is a d-dimensional vector, where $f : \mathbb{R}^d \to \mathbb{R}^d$ is the drift coefficient and $g : \mathbb{R}^d \to \mathbb{R}^{d\times m}$ is a matrix equation known as the diffusion coefficient which describes the amount and mixtures of the noise process W_t which is a m-dimensional Brownian motion. In many models, noise is added to deterministic equations phenomenologically. In one case, the noise process is modeled as exogenous to the system and thus not dependent the system itself, leading to the assumption that $g(t, X_t) \equiv g(t)$. This case is known as additive noise. Another common case is multiplicative noise, where to each deterministic equation a noise term $\sigma_i X_t^i dW_t$ is added to give proportional noise. This results in $g(t, X_t)$ being the diagonal matrix $\left(\sigma_i X_t^i\right)$ and thus falling into the category of diagonal noise. In contrast to how common models of this form occur, methods which utilize this functional form for increased efficiency are relatively underdeveloped.

The bread-and-butter methods for the integration of ordinary differential equations

$$x'(t) = f(t, x)$$

are adaptive Runge-Kutta methods. Runge first extended the Euler method to greater accuracy in 1895. Later, these methods were extended to a general form resulting in the theory of the Butcher tableau. In this framework, a Runge-Kutta method

$$x_{n+1} = x_n + h_n \sum_{j=1}^{s} b_j k_j, \quad \hat{x}_{n+1} = x_n + h_n \sum_{j=1}^{s} \hat{b}_j k_j$$
$$f_j = f\left(x_n + c_i h_n, y_n + h_n \sum_{j=1}^{s} a_{ij} k_j\right)$$

is defined by a table of coefficients:

$$\begin{array}{c|cccc} c_1 & a_{11} & a_{12} & \dots & a_{1s} \\ c_2 & a_{21} & a_{22} & \dots & a_{2s} \\ \vdots & \vdots & \vdots & & \vdots \\ c_s & a_{s1} & a_{s2} & \dots & a_{ss} \\ \hline & b_1 & b_2 & \dots & b_s \end{array}$$

x_{n+1} is the approximation to $x(t_j + \Delta t)$ where t_j is the ith timepoint, and $\hat{x}_{n+1}$ is an embedded approximation of a different order. Using $E_n = \|x_n - \hat{x}_n\|$ as a local error estimator, the timestep is adaptive using the error estimate. One common algorithm for doing so is

$$h_{n+1} = 0.9h_n \left(\frac{TOL}{E_n}\right)^{\frac{1}{p}}$$

due to optimality results by Cechino where TOL is a user-chosen error tolerance and p is the order of the method.

Early work in Runge-Kutta methods focused on the development of high order methods. Fehlberg developed the first 5th order method with an embedded error estimator. Dormand and Prince expanded the theory by considering the problem as a coefficient optimization problem: choosing coefficients for an order 4/5 method which minimizes the the principle term in the truncation error to maximize the efficiency in each step, while controlling for an enlarged stability region. In order to make the problem tractable, they introduced extra assumptions and the resulting method, known as the RK5(4) or DP5 method (or through the name of its implementations dopri5 or ode45) is the standard method for integrating non-stiff ODEs. More recent work by Tsitouras used a minimal number of simplifying assumptions to generate a more efficient order 4/5 method. As an alternative to the mixed truncation error vs stability region selection, Verner derived methods with extended stability regions for higher orders.

An approach to the integration of stochastic differential equations is the use of adaptive Stochastic Runge-Kutta (SRK) methods. Kloden and Platen developed a theory of stochastic Taylor expansions which allowed the development of high strong order (greater than order 1.0) methods which replace the derivatives by approximations, also known as derivative-free or SRK methods. Burrage and Burrage introduced the use of colored trees for calculating the strong order conditions for SRK methods and thus extended the Butcher tableau theory to SDE with Stratonovich noise. Later work by Rossler extended the approach to Ito SDEs and along with relaxed conditions for commutative, scalar, diagonal, and additive noise. Rackauckas and Nie derived an extension to the Rossler methods which provides a natural embedded order 1.0 method and results in efficient adaptive timestepping for any Rossler method. However, to the author's knowledge, no attempts have been made at deriving optimal sets of coefficients for the high strong order adaptive SRK methods.

In this paper we develop a method for deriving optimal-stability SRK methods. Section 2 recaps the theory of high strong order SRK methods and their adaptive extensions. In Section 3 we derive a optimization problem whose solution is a stability-optimized SRK methods. Also discussed are extended constraints which are required for the stability and locality of the error estimator. In Section 4 we describe the numerical used to solve the optimization problem and the resulting explicit SRK methods. In Section 5 demonstrate the efficiency of our new methods on a set of test problems. We end by discussing the extension of our method of derivation to implicit and non-diagonal SRK methods.

2 Adaptive Strong Order 1.0/1.5 Methods

Rosseler used a colored root tree analysis to developed order conditions for high order SRK methods. The diagonal noise methods utilize the same general form and order conditions as the methods for scalar noise so we use their notation for simplicity. The strong order 1.5 methods for scalar noise are of the form

$$X_{n+1}=X_n+\sum_{i=1}^{s}\alpha_i f\left(t_n+c_i^{(0)}h,H_i^{(0)}\right)+\sum_{i=1}^{s}\left(\beta_i^{(1)}I_{(1)}+\beta_i^{(2)}\frac{I_{(1,1)}}{\sqrt{h}}+\beta_i^{(3)}\frac{I_{(1,0)}}{h}+\beta_i^{(4)}\frac{I_{(1,1,1)}}{h}\right)g\left(t_n+c_i^{(1)}h\right)$$

with stages

$$H_i^{(0)}=X_n+\sum_{j=1}^{s}A_{ij}^{(0)}f\left(t_n+c_j^{(0)}h,H_j^{(0)}\right)h+\sum_{j=1}^{s}B_{ij}^{(0)}g\left(t_n+c_j^{(1)}h,H_j^{(1)}\right)\frac{I_{(1,0)}}{h}$$

$$H_i^{(1)}=X_n+\sum_{j=1}^{s}A_{ij}^{(1)}f\left(t_n+c_j^{(0)}h,H_j^{(0)}\right)h+\sum_{j=1}^{s}B_{ij}^{(1)}g\left(t_n+c_j^{(1)}h,H_j^{(1)}\right)\sqrt{h}$$

where the I_j are the Wiktorsson approximations to the iterated stochastic integrals. In the case of additive noise, this reduces to the form

$$X_{n+1}=X_n+\sum_{i=1}^{s}\alpha_i f\left(t_n+c_i^{(0)}h,H_i^{(0)}\right)+\sum_{i=1}^{s}\left(\beta_i^{(1)}I_{(1)}+\beta_i^{(2)}\frac{I_{(1,0)}}{h}\right)g\left(t_n+c_i^{(1)}h\right)$$

with stages

$$H_i^{(0)}=X_n+\sum_{j=1}^{s}A_{ij}^{(0)}f\left(t_n+c_j^{(0)}h,H_j^{(0)}\right)h+\sum_{j=1}^{s}B_{ij}^{(0)}g\left(t_n+c_j^{(1)}h\right)\frac{I_{(1,0)}}{h}.$$

The tuple of coefficients $\left(A^{(j)},B^{(j)},\beta^{(j)},\alpha\right)$ thus fully determine the SRK method. These coefficients are subject to the constraint equations:

The coefficients
$\left(A_0,B_0,\beta^{(i)},\alpha\right)$ must satisfy the following order conditions to achieve order .5:

1. $\alpha^T e=1$
2. $\beta^{(1)^T}e=1$
3. $\beta^{(2)^T}e=0$
4. $\beta^{(3)^T}e=0$
5. $\beta^{(4)^T}e=0$

additionally, for order 1:

1. $\beta^{(1)^T}B^{(1)}e=0$
2. $\beta^{(2)^T}B^{(1)}e=1$
3. $\beta^{(3)^T}B^{(1)}e=0$
4. $\beta^{(4)^T}B^{(1)}e=0$

and lastly for order 1.5:

1. $\alpha^T A^{(0)} e = \frac{1}{2}$
2. $\alpha^T B^{(0)} e = 1$
3. $\alpha^T \left(B^{(0)} e\right)^2 = \frac{3}{2}$
4. ${\beta^{(1)}}^T A^{(1)} e = 1$
5. ${\beta^{(2)}}^T A^{(1)} e = 0$
6. ${\beta^{(3)}}^T A^{(1)} e = -1$
7. ${\beta^{(4)}}^T A^{(1)} e = 0$
8. ${\beta^{(1)}}^T \left(B^{(1)} e\right)^2 = 1$
9. ${\beta^{(2)}}^T \left(B^{(1)} e\right)^2 = 0$
10. ${\beta^{(3)}}^T \left(B^{(1)} e\right)^2 = -1$
11. ${\beta^{(4)}}^T \left(B^{(1)} e\right)^2 = 2$
12. ${\beta^{(1)}}^T \left(B^{(1)} \left(B^{(1)} e\right)\right) = 0$
13. ${\beta^{(2)}}^T \left(B^{(1)} \left(B^{(1)} e\right)\right) = 0$
14. ${\beta^{(3)}}^T \left(B^{(1)} \left(B^{(1)} e\right)\right) = 0$
15. ${\beta^{(4)}}^T \left(B^{(1)} \left(B^{(1)} e\right)\right) = 1$
16. $\frac{1}{2}{\beta^{(1)}}^T \left(A^{(1)} \left(B^{(0)} e\right)\right) + \frac{1}{3}{\beta^{(3)}}^T \left(A^{(1)} \left(B^{(0)} e\right)\right) = 0$

where $f, g \in C^{1,2}(\mathcal{I} \times \mathbb{R}^d, \mathbb{R}^d)$, $c^{(i)} = A^{(i)} e$, $e = (1,1,1,1)^T$. The reduced constraints for additive noise were derived for order 1:

1. $\alpha^T e = 1$
2. ${\beta^{(1)}}^T e = 1$
3. ${\beta^{(2)}}^T e = 0$

and the additional conditions for order 1.5:

1. $\alpha^T B^{(0)} e = 1$
2. $\alpha^T A^{(0)} e = \frac{1}{2}$
3. $\alpha^T \left(B^{(0)} e\right)^2 = \frac{3}{2}$
4. ${\beta^{(1)}}^T c^{(1)} = 1$
5. ${\beta^{(2)}}^T c^{(1)} = -1$

where $c^{(0)} = A^{(0)} e$ with $f \in C^{1,3}(\mathcal{I} \times \mathbb{R}^d, \mathbb{R}^d)$ and $g \in C^1(\mathcal{I}, \mathbb{R}^d)$.

Rackauckas and Nie showed that for any method of this form, there exists an error estimator

$$E = \delta E_D + E_N$$

where E_D is the deterministic (drift) error estimator and E_N is the noise error estimator, given respectively by

$$E_D = \left| h \sum_{i \in I_1} (-1)^{\sigma(i)} f\left(t_n + c_i^{(0)} h, H_i^{(0)}\right) \right|$$
$$E_N = \left| \sum_{i \in I_1} \left(\beta_i^{(3)} \frac{I_{(1,0)}}{h} + \beta_i^{(4)} \frac{I_{(1,1,1)}}{h} \right) g\left(t_n + c_i^{(1)} h, H_i^{(1)}\right) \right|$$

with some constraints on $\sigma(i)$ and the I_j. Thus unlike in the theory of ordinary differential equations, the choice of coefficients for SRK methods does not require explicitly finding an embedded method.

3 Optimized-Stability High Order SRK Methods with Additive Noise

Using the terms as defined by Kloden and Platen, we define a discrete approximation as numerically stable if for any finite time interval $[t_0, T]$, there exists a positive constant Δ_0 such that for each $\epsilon > 0$ and each $\delta \in (0, \Delta_0)$

$$\lim_{\left|X_0^\delta - \bar{X}_0^\delta\right| \to 0} \sup_{t_0 \le t \le T} P\left(\left|X_t^\delta - \bar{X}_t^\delta\right| \ge \epsilon\right) = 0$$

where X_n^δ is a discrete time approximation with maximum step size $\delta > 0$ starting at X_0^δ and $\bar{X}_n^\delta$ respectively starting at $\bar{X}_n^\delta$. For additive noise, we consider the complex-valued linear test equations

$$dX_t = \mu X_t dt + dW_t$$

where λ is a complex number. In this framework, a scheme which can be written in the form

$$X_{n+1}^h = X_n^h G(\mu h) + Z_n^\delta$$

with a constant step size $\delta \equiv h$ and Z_n^δ are random variables which do not depend on the Y_n^δ, then the region of absolute stability is the set where for $z = \mu h$, $|G(z)| < 1$.

The additive SRK method can be written as

$$X_{n+1}^h = X_n^h + z\left(\alpha \cdot H^{(0)}\right) + \beta^{(1)}\sigma I_{(1)} + \sigma\beta^{(2)}\frac{I_{(1,0)}}{h}$$

where

$$H^{(0)} = \left(I - zA^{(0)}\right)^{-1}\left(\hat{X}_n^h + B^{(0)} e\sigma\frac{I_{(1,0)}}{h}\right)$$

where $\hat{X}_n^h$ is the size s constant vector of elements X_n^h and $e = (1,1,1,1)^T$. By substitution we receive

$$X_{n+1}^h = X_n^h\left(1 + z\left(\alpha \cdot \left(I - zA^{(0)}\right)^{-1}\right)\right) + \left(I - zA^{(0)}\right)^{-1} B^{(0)} e\sigma\frac{I_{(1,0)}}{h} + \beta^{(1)}\sigma I_{(1)} + \sigma\beta^{(2)}\frac{I_{(1,0)}}{h}$$

This set of equations decouples to the form of Equation ## since the iterated stochastic integral approximation I_j are random numbers and are independent of the X_n^h. Thus the stability condition is determined by the equation

$$G(z) = 1 + z\left(\alpha \cdot \left(I - zA^{(0)}\right)^{-1}\right).$$

3.1 Stability-Optimal Explicit Methods

For explicit methods, the $A^{(i)}$ and $B^{(i)}$ are lower diagonal and we receive the simplified stability function

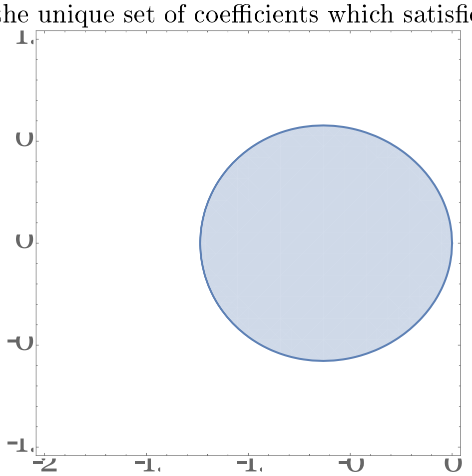
$$G(z) = 1 + A_{21} z^2 \alpha_2 + z(\alpha_1 + \alpha_2)$$

for a two-stage additive noise SRK method. For this method we will find the method which optimizes the stability in the real part of z. Thus we wish to find $A^{(0)}, \alpha$ s.t. the negative real roots of $|G(z)| = 1$ are minimized. By the quadratic equation we see that there exists only a single negative root: $z = \frac{1 - \sqrt{1 + 8\alpha_2}}{2\alpha_2}$. Using Mathematica's minimum function, we determine that the minimum value for this root subject to the order constraints is $z = \frac{3}{4}\left(1 - \sqrt{\frac{19}{3}}\right) \approx -1.13746$. We see that this is achieved when $\alpha = \frac{2}{3}$, meaning that the SRA1 method due to Rossler achieves the maximum stability criteria. However, given extra degrees of freedom, we impose that $c_1^{(0)} = c_1^{(1)} = 0$ and $c_2^{(0)} = c_2^{(1)} = 1$ so that the error estimator spans the whole interval. This can lead to improved robustness of the adaptivity. Under these conditions we find the solution

$$A^{(0)} = \begin{pmatrix} 0 & 0 \\ \frac{3}{4} & 0 \end{pmatrix}, \quad B^{(0)} = \begin{pmatrix} 0 & 0 \\ \frac{3}{2} & 0 \end{pmatrix}, \quad \alpha = \begin{pmatrix} \frac{1}{3} \\ \frac{2}{3} \end{pmatrix}$$

$$\beta^{(1)} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad \beta^{(2)} = \begin{pmatrix} 1 \\ -1 \end{pmatrix}, \quad c^{(0)} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad c^{(1)} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

is the unique set of coefficients which satisfies these constraints, and achieves the optimal value for the root.



3.2 An A-Stable L-Stable Implicit Method For Stiff SDEs with Additive Noise

It's clear that, as in the case for deterministic equations, the explicit methods cannot be made A-stable. However, the implicit two-stage additive noise SRK method is determined by

$$G(z) = \frac{z(A_{11}(A_{22}z - \alpha_2 z - 1) + A_{12}z(\alpha_1 - A_{21}) + A_{21}\alpha_2 z - A_{22}(\alpha_1 z + 1) + \alpha_1 + \alpha_2) + 1}{A_{11}z(A_{22}z - 1) - z(A_{12}A_{21}z + A_{22}) + 1}$$

which is A-stable if

$$A_{11}z(A_{22}z-1)-z(A_{12}A_{21}z+A_{22})+1 > z(A_{11}(A_{22}z-\alpha_2 z-1)+A_{12}z(\alpha_1-A_{21})+A_{21}\alpha_2 z-A_{22}(\alpha_1 z+1)+\alpha_1+\alpha_2)+1.$$

Notice that the numerator equals the denominator if and only if $z = 0$ or

$$z = \frac{\alpha_1 + \alpha_2}{(A_{22} - A_{12})\,\alpha_1 + (A_{11} - A_{21})\,\alpha_2}.$$

From the order conditions we know that $\alpha_1 + \alpha_2 = 1$ which means that no root exists with $Re(z) < 0$ if $(A_{22} - A_{12})\,\alpha_1 + (A_{11} - A_{21})\,\alpha_2 > 0$. Thus under these no roots conditions, we can determine A-stability by checking the inequality at $z = 1$, which gives $1 > (A_{22} - A_{12})\,\alpha_1 + (A_{11} - A_{21})\,\alpha_2$. Using the order condition, we have a total of four constraints on the $A^{(0)}$ and α:

$$\begin{aligned}\left(A_{11}+A_{12}\right)\alpha_1+\left(A_{21}+A_{22}\right)\alpha_2&=\frac{1}{2}\\ \alpha_1+\alpha_2&=1\\ 0<\left(A_{22}-A_{12}\right)\alpha_1+\left(A_{11}-A_{21}\right)\alpha_2&<1\end{aligned}$$

An immediate fact we note is that none of the 2-stage (Order 3) Labatto or Radau methods create stochastically A-stable methods. Instead, we wish to derive methods which have similar properties and have stochastic A-stability. One property we extend is L-stability. The straightforward extension of L-stability is the condition

$$\lim_{z\to\infty} G(z)=0.$$

This implies that

$$\frac{-A_{11}A_{22}+A_{11}\alpha_2+A_{12}A_{21}-A_{12}\alpha_1-A_{21}\alpha_2+A_{22}\alpha_2\alpha_1}{A_{12}A_{21}-A_{11}A_{22}}=0$$

The denominator is $-\det(A^{(0)})$ which implies $A^{(0)}$ must be non-singular. Next, we attempt to impose B-stability on the drift portion of the method. We use the condition due to Burrage and Butcher that for $B=\operatorname{diag}\left(\alpha_1,\alpha_2\right)$ $M=BA^{(0)}+A^{(0)}B-\alpha\alpha^T$, we require both B and M to be non-negative definite. However, in the supplemental Mathematica notebooks we show computationally that there is no 2-stage SRK method of this form which satisfies all three of these stability conditions. Thus we settle for A-stability and L-stability.

Recalling that $c^{(0)}$ and $c^{(1)}$ are the locations in time where f and g are approximated respectively, we wish to impose

$$\begin{aligned}c_2^{(0)}&=1\\ c_2^{(1)}&=1\end{aligned}$$

so that the error estimator covers the entire interval of integration (for robustness to discontinuities). Since $c^{(0)}=A^{(0)}e$, this leads to the condition $A_{21}+A_{22}=1$. Using the constraint-satisfaction algorithm FindInstance in Mathematica, we find the following coefficient set:

$$\begin{aligned}A^{(0)}&=\begin{pmatrix}2&-\frac{7}{2}\\0&\frac{3}{2}\end{pmatrix},\quad B^{(0)}=\begin{pmatrix}0&0\\\frac{3}{2}&0\end{pmatrix},\quad \alpha=\begin{pmatrix}\frac{1}{3}\\\frac{2}{3}\end{pmatrix}\\ \beta^{(1)}&=\begin{pmatrix}0\\1\end{pmatrix},\quad \beta^{(2)}=\begin{pmatrix}1\\-1\end{pmatrix},\quad c^{(0)}=\begin{pmatrix}0\\1\end{pmatrix},\quad c^{(1)}=\begin{pmatrix}0\\1\end{pmatrix}\end{aligned}$$

4 Optimized-Stability Order 1.5 SRK Methods with Diagonal Noise

4.1 A Multivariate Lamperti Transform for Multiplicative Noise to Additive SRK

Given the efficiency of the methods for additive noise, one method for developing efficient methods for more general noise processes is to use a transform of diagonal noise processes to additive noise. This transform is due to Lamperti, which states that the SDE of the form

$$dX_t=f(t,X_t)dt+\sigma(t,X_t)R(t)dW_t$$

where σ a diagonal matrix with diagonal elements $\sigma_i(t, X_{i,t})$ has the transformation

$$Z_{i,t} = \psi_i(t, X_{i,t}) = \int \frac{1}{\sigma_i(x,t)} dx \mid_{x=X_{i,t}}$$

which will result in an Ito process with the ith element given by

$$dZ_{i,t} = \left(\frac{\partial}{\partial t} \psi_i(t,x) \mid_{x=\psi^{-1}(t,Z_{i,t})} + \frac{f_i(\psi^{-1}(t,Z_t),t)}{\frac{1}{2}\frac{\partial}{\partial x}\sigma_i\left(\psi_i^{-1}\left(t,Z_{i,t}\right)\right)} \right) dt + \sum_{j=1}^{n} r_{ij}(t) dw_{j,t}$$

with

$$X_t = \psi^{-1}\left(t, Z_t\right).$$

This is easily verified using Ito's Lemma. An example of such a transformation is multidimensional geometric Brownian motion, where $A = diag(a_1, a_2)$, $\sigma = diag(X_1, X_2)$, and $R = r_{ij}$. Then in this case, $Z = \psi(X) = \log(X)$ and

$$d\begin{bmatrix} Z_1 \\ Z_2 \end{bmatrix} = \begin{bmatrix} a_1 - \frac{1}{2}\left(r_{11}^2 + r_{12}^2\right) \\ a_2 - \frac{1}{2}\left(r_{21}^2 + r_{22}^2\right) \end{bmatrix} dt + \begin{bmatrix} r_{11} & r_{12} \\ r_{21} & r_{22} \end{bmatrix} dW_t.$$

This transformation requires that $\sigma_i^{-1}(t, X_{i,t})$ is one-to-one, and thus does not exist in general for diagonal noise. However, in the case of mixed multiplicative and additive noise:

$$dX_t = f(t, X_t)dt + \sigma X_t dW_t$$

where σ is a constant diagonal matrix, then

$$d \log X_t = \tilde{f}(t, X_t)dt + dW_t$$
$$\tilde{f}(t, X_t) = \frac{f(t, X_t)}{\sigma X_t}$$

where the division is considered element-wise. Thus we can modify the additive SRK method to be in the form

$$\log X_{n+1} = \log X_n + \sum_{i=1}^{s} \alpha_i \tilde{f}\left(t_n + c_i^{(0)}h, H_i^{(0)}\right) + \sum_{i=1}^{s}\left(\beta_i^{(1)} I_{(1)} + \beta_i^{(2)} \frac{I_{(1,0)}}{h}\right)$$

with stages

$$H_i^{(0)} = \log X_n + \sum_{j=1}^{s} A_{ij}^{(0)} \tilde{f}\left(t_n + c_j^{(0)}h, H_j^{(0)}\right) h + \sum_{j=1}^{s} B_{ij}^{(0)} \frac{I_{(1,0)}}{h}.$$

Back-transforming this, we get

$$X_{n+1} = X_n \exp\left(\sum_{i=1}^{s} \alpha_i \tilde{f}\left(t_n + c_i^{(0)}h, H_i^{(0)}\right) + \sum_{i=1}^{s}\left(\beta_i^{(1)} I_{(1)} + \beta_i^{(2)} \frac{I_{(1,0)}}{h}\right)\right)$$

where the exponentiation is interpreted element-wise.

4.2 The Stability Equation for Order 1.5 SRK Methods with Diagonal Noise

For diagonal noise, we will use the mean-square definition of stability. A method is mean-square stable if $\lim_{n\to\infty}\mathbb{E}\left(|X_n|^2\right)=0$ on the test equation

$$dX_t = \mu X_t dt + \sigma X_t dW_t.$$

In matrix form we can re-write our method as given by

$$X_{n+1} = X_n + \mu h\left(\alpha\cdot H^{(0)}\right) + \sigma I_{(1)}\left(\beta^{(1)}\cdot H^{(1)}\right) + \sigma\frac{I_{(1,1)}}{\sqrt{h}}\left(\beta^{(2)}\cdot H^{(1)}\right) + \sigma\frac{I_{(1,0)}}{h}\left(\beta^{(3)}\cdot H^{(1)}\right) + \sigma\frac{I_{(1,1,1)}}{h}\left(\beta^{(4)}\cdot H^{(1)}\right)$$

with stages

$$\begin{aligned}
H^{(0)} &= X_n + \mu\Delta t A^{(0)}H^{(0)} + \sigma\frac{I_{(1,0)}}{h}B^{(0)}H^{(1)},\\
H^{(1)} &= X_n + \mu\Delta t A^{(1)}H^{(0)} + \sigma\sqrt{\Delta t}B^{(1)}H^{(1)}
\end{aligned}$$

where $\hat{X_n}$ is the size s constant vector of X_n.

$$\begin{aligned}
H^{(0)} &= \left(I-hA^{(0)}\right)^{-1}\left(\hat{X_n}+\sigma\frac{I_{(1,0)}}{h}B^{(0)}H^{(1)}\right),\\
H^{(1)} &= \left(I-\sigma\sqrt{h}B^{(1)}\right)^{-1}\left(\hat{X_n}+\mu hA^{(1)}H^{(0)}\right)
\end{aligned}$$

By the derivation in the appendix, we receive the equation

$$\begin{aligned}
S = E\left[\frac{U_{n+1}^2}{U_n^2}\right] &= \{1+\mu ht\left(\alpha\cdot\left[\left(I-\mu\Delta tA^{(0)}-\mu\sigma I_{(1,0)}A^{(1)}B^{(0)}\left(I-\sigma\sqrt{h}B^{(1)}\right)^{-1}\right)^{-1}\left(I+\sigma\frac{I_{(1,0)}}{h}B^{(0)}\left(I-\sigma\sqrt{h}B^{(1)}\right)^{-1}\right)\right]\right)\\
&+\sigma I_{(1)}\left(\beta^{(1)}\cdot\left[\left(I-\sigma\sqrt{h}B^{(1)}-\mu hA^{(1)}\left(I-\mu hA^{(0)}\right)^{-1}\sigma\frac{I_{(1,0)}}{h}B^{(0)}\right)^{-1}\left(I+\mu hA^{(1)}\left(I-\mu hA^{(0)}\right)^{-1}\right)\right]\right)\\
&+\sigma\frac{I_{(1,1)}}{\sqrt{h}}\left(\beta^{(2)}\cdot\left[\left(I-\sigma\sqrt{h}B^{(1)}-\mu hA^{(1)}\left(I-\mu hA^{(0)}\right)^{-1}\sigma\frac{I_{(1,0)}}{h}B^{(0)}\right)^{-1}\left(I+\mu hA^{(1)}\left(I-\mu hA^{(0)}\right)^{-1}\right)\right]\right)\\
&+\sigma\frac{I_{(1,0)}}{h}\left(\beta^{(3)}\cdot\left[\left(I-\sigma\sqrt{h}B^{(1)}-\mu hA^{(1)}\left(I-\mu hA^{(0)}\right)^{-1}\sigma\frac{I_{(1,0)}}{h}B^{(0)}\right)^{-1}\left(I+\mu hA^{(1)}\left(I-\mu hA^{(0)}\right)^{-1}\right)\right]\right)\\
&+\sigma\frac{I_{(1,1,1)}}{h}\left(\beta^{(4)}\cdot\left[\left(I-\sigma\sqrt{h}B^{(1)}-\mu hA^{(1)}\left(I-\mu hA^{(0)}\right)^{-1}\sigma\frac{I_{(1,0)}}{h}B^{(0)}\right)^{-1}\left(I+\mu hA^{(1)}\left(I-\mu hA^{(0)}\right)^{-1}\right)\right]\right)\}^2
\end{aligned}$$

We apply the substitutions from the Appendix and let

$$\begin{aligned}
z &= \mu h,\\
w &= \sigma\sqrt{h}.
\end{aligned}$$

In this space, z is the stability variable for the drift term and w is the stability in the diffusion term. Under this scaling $\left(h,\sqrt{h}\right)$, the equation becomes independent of h and thus becomes a function $S(z,w)$ on the coefficients of the SRK method. The equation $S(z,w)$ in terms of its coefficients for explicit methods ($A^{(i)}$ and $B^{(i)}$ lower diagonal) has millions of terms and is shown in the supplemental Mathematica notebook. Determination of the stability equation for the implicit methods was found to be computationally intractable and is an avenue for further research.

4.3 An Optimization Problem for Determination of Coefficients

We wish to determine the coefficients for the additive and diagonal SRK methods which optimize the stability. To do so, we generate an optimization problem which we can numerically solve for the coefficients. To simplify the problem, we let $z, w \in \mathbb{R}$. Define the function

$$f(z, w; N, M) = \int_{-M}^{M} \int_{-N}^{1} \chi_{S(z,w)\leq 1}(z, w) dz dw.$$

Notice that for $N, M \to \infty$, f is the area of the stability region. Thus we define the stability-optimized diagonal SRK method as the set of coefficients which achieves

$$\max_{A^{(i)}, B^{(i)}, \beta^{(i)}, \alpha} f(z, w)$$
$$\text{subject to: Order Constraints}$$

However, like with the SRK methods for additive noise, we impose a few extra constraints to add robustness to the error estimator. In all cases we impose $0 < c_i^{(0)}, c_i^{(1)} < 1$. Additionally we can prescribe $c_4^{(0)} = c_4^{(1)} = 1$ which we call the End-C Constraint. Lastly, we can prescribe the ordering constraint $c_1^{(j)} < c_2^{(j)} < c_3^{(j)} < c_4^{(j)}$ which we denote as the Inequality-C Constraint.

The resulting problem is a nonlinear programming problem with 44 variables and 42-48 constraint equations. The objective function is the two-dimensional integral of a discontinuous function which is determined by a polynomial of in z and w with approximately 3 million coefficients. To numerically approximate this function, we calculated the characteristic function on a grid with even spacing dx using a CUDA kernel and found numerical solutions to the optimization problem using the JuMP framework with the NLopt backend. A mixed approach using many solutions of the semi-local optimizer LN_AUGLAG_EQ and fewer solutions from the global optimizer GN_ISRES were used to approximate the optimality of solutions.

The parameters N and M are the bounds on the stability region, but also represent a tradeoff between the stability in the drift and the stability in the diffusion. A method which is optimized when M is small would be highly stable in the case of small noise, but would not be guaranteed to have good stability properties in the presence of large noise. Thus these parameters are knobs for tuning the algorithms for specific situations, and thus we solved the problem for different combinations of N and M to determine different algorithms for the different cases.

4.4 Approximately-Optimal Methods

The coefficients generated for approximately-optimal methods fall into three categories. In one category we have the drift-dominated stability methods where large N and small M was optimized. On the other end we have the diffusion-dominated stability methods where large M and small N was optimized. Then we have the mixed stability methods which used some mixed size choices for N and M.

4.4.1 Drift-Dominated Stability Methods

Just a bunch of pictures? Tables?

4.4.2 Diffusion-Dominated Stability Methods

Just a bunch of pictures? Tables?

4.4.3 Mixed Stability Methods

Just a bunch of pictures? Tables?

5 Approximately-Optimal Methods with Stability Detection and Switching Behaviors

- Shampine's method for Jacobian approximation
- Same_C methods
- Stability limit calculations
- Split error estimator

6 Numerical Results

- Convergence charts?
- Efficiency on Oval2 problem?
- Show divergence of SRA1?

7 Discussion

- 3rd stage additive
- Implicit diagonal
- non-commutative and commutative
- principle truncation

8 Appendix: Derivations

$$\begin{aligned}
\Big(I-\mu\Delta tA^{(0)}\Big)H^{(0)} &= U_n+\sigma\frac{I_{(1,0)}}{\Delta t}B^{(0)}\Big(I-\sigma\sqrt{\Delta t}B^{(1)}\Big)^{-1}\Big(U_n+\mu\Delta tA^{(1)}H^{(0)}\Big),\\
\Big(I-\mu\Delta tA^{(0)}\Big)H^{(0)}-\bigg[\sigma\frac{I_{(1,0)}}{\Delta t}B^{(0)}\Big(I-\sigma\sqrt{\Delta t}B^{(1)}\Big)^{-1}\bigg]\mu\Delta tA^{(1)}H^{(0)} &= U_n+\sigma\frac{I_{(1,0)}}{\Delta t}B^{(0)}\Big(I-\sigma\sqrt{\Delta t}B^{(1)}\Big)^{-1}U_n\\
\bigg(I-\mu\Delta tA^{(0)}-\mu\Delta tA^{(1)}\sigma\frac{I_{(1,0)}}{\Delta t}B^{(0)}\Big(I-\sigma\sqrt{\Delta t}B^{(1)}\Big)^{-1}\bigg)H^{(0)} &= \bigg(I+\sigma\frac{I_{(1,0)}}{\Delta t}B^{(0)}\Big(I-\sigma\sqrt{\Delta t}B^{(1)}\Big)^{-1}\bigg)U_n\\
H^{(0)} &= \bigg(I-\mu\Delta tA^{(0)}-\mu\sigma I_{(1,0)}A^{(1)}B^{(0)}\Big(I-\sigma\sqrt{\Delta t}B^{(1)}\Big)^{-1}\bigg)^{-1}\bigg(I+\sigma\frac{I_{(1,0)}}{\Delta t}B^{(0)}\Big(I-\sigma\sqrt{\Delta t}B^{(1}
\end{aligned}$$

$$\begin{aligned}
\Big(I-\sigma\sqrt{\Delta t}B^{(1)}\Big)H^{(1)} &= U_n+\mu\Delta tA^{(1)}\Big(I-\mu\Delta tA^{(0)}\Big)^{-1}\bigg(U_n+\sigma\frac{I_{(1,0)}}{\Delta t}B^{(0)}H^{(1)}\bigg)\\
\bigg(I-\sigma\sqrt{\Delta t}B^{(1)}-\mu\Delta tA^{(1)}\Big(I-\mu\Delta tA^{(0)}\Big)^{-1}\sigma\frac{I_{(1,0)}}{\Delta t}B^{(0)}\bigg)H^{(1)} &= U_n+\mu\Delta tA^{(1)}\Big(I-\mu\Delta tA^{(0)}\Big)^{-1}U_n\\
\bigg(I-\sigma\sqrt{\Delta t}B^{(1)}-\mu\Delta tA^{(1)}\Big(I-\mu\Delta tA^{(0)}\Big)^{-1}\sigma\frac{I_{(1,0)}}{\Delta t}B^{(0)}\bigg)H^{(1)} &= \bigg(I+\mu\Delta tA^{(1)}\Big(I-\mu\Delta tA^{(0)}\Big)^{-1}\bigg)U_n\\
H^{(1)} &= \bigg(I-\sigma\sqrt{\Delta t}B^{(1)}-\mu\Delta tA^{(1)}\Big(I-\mu\Delta tA^{(0)}\Big)^{-1}\sigma\frac{I_{(1,0)}}{\Delta t}B^{(0)}\bigg)^{-1}\bigg(I+\mu\Delta tA^{(1)}\Big(I-\mu\Delta tA^{(0)}\Big)^{-1}\bigg)U
\end{aligned}$$

$$
\begin{aligned}
U_{n+1} \quad = \quad & U_n + \mu\Delta t\left(\alpha \cdot \left[\left(I - \mu\Delta t A^{(0)} - \mu\sigma I_{(1,0)} A^{(1)} B^{(0)}\left(I - \sigma\sqrt{\Delta t}B^{(1)}\right)^{-1}\right)^{-1}\left(I + \sigma\frac{I_{(1,0)}}{\Delta t}B^{(0)}\left(I - \sigma\sqrt{\Delta t}B^{(1)}\right)^{-1}\right)\right] U_n\right) \\
& + \sigma I_{(1)}\left(\beta^{(1)} \cdot \left[\left(I - \sigma\sqrt{\Delta t}B^{(1)} - \mu\Delta t A^{(1)}\left(I - \mu\Delta t A^{(0)}\right)^{-1}\sigma\frac{I_{(1,0)}}{\Delta t}B^{(0)}\right)^{-1}\left(I + \mu\Delta t A^{(1)}\left(I - \mu\Delta t A^{(0)}\right)^{-1}\right)\right] U_n\right) \\
& + \sigma\frac{I_{(1,1)}}{\sqrt{\Delta t}}\left(\beta^{(2)} \cdot \left[\left(I - \sigma\sqrt{\Delta t}B^{(1)} - \mu\Delta t A^{(1)}\left(I - \mu\Delta t A^{(0)}\right)^{-1}\sigma\frac{I_{(1,0)}}{\Delta t}B^{(0)}\right)^{-1}\left(I + \mu\Delta t A^{(1)}\left(I - \mu\Delta t A^{(0)}\right)^{-1}\right)\right] U_n\right) \\
& + \sigma\frac{I_{(1,0)}}{\Delta t}\left(\beta^{(3)} \cdot \left[\left(I - \sigma\sqrt{\Delta t}B^{(1)} - \mu\Delta t A^{(1)}\left(I - \mu\Delta t A^{(0)}\right)^{-1}\sigma\frac{I_{(1,0)}}{\Delta t}B^{(0)}\right)^{-1}\left(I + \mu\Delta t A^{(1)}\left(I - \mu\Delta t A^{(0)}\right)^{-1}\right)\right] U_n\right) \\
& + \sigma\frac{I_{(1,1,1)}}{\Delta t}\left(\beta^{(4)} \cdot \left[\left(I - \sigma\sqrt{\Delta t}B^{(1)} - \mu\Delta t A^{(1)}\left(I - \mu\Delta t A^{(0)}\right)^{-1}\sigma\frac{I_{(1,0)}}{\Delta t}B^{(0)}\right)^{-1}\left(I + \mu\Delta t A^{(1)}\left(I - \mu\Delta t A^{(0)}\right)^{-1}\right)\right] U_n\right)
\end{aligned}
$$

Thus we substitute in the Wiktorsson approximations

$$
\begin{aligned}
I_{(1,1)} &= \frac{1}{2}\left(\Delta W^2 - h\right) \\
I_{(1,1,1)} &= \frac{1}{6}\left(\Delta W^3 - 3h\Delta W\right) \\
I_{(1.0)} &= \frac{1}{2}h\left(\Delta W + \frac{1}{\sqrt{3}}\Delta Z\right)
\end{aligned}
$$

where $\Delta Z \sim N(0,h)$ is independent of $\Delta W \sim N(0,h)$. By the properties of the normal distribution, we have that

$$
E\left[(\Delta W)^n\right] = 0
$$

for any odd n and

$$
\begin{aligned}
E\left[(\Delta W)^2\right] &= h \\
E\left[(\Delta W)^4\right] &= 3h^2 \\
E\left[(\Delta W)^6\right] &= 15h^3 \\
E\left[(\Delta W)^8\right] &= 105h^4.
\end{aligned}
$$