Runge-Kutta Methods

An extra file for Lecture 3

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1 Introduction and General Formulation

Runge-Kutta (RK) methods constitute a powerful class of implicit and explicit iterative algorithms utilized for the numerical approximation of solutions to ordinary differential equations (ODEs). Consider the foundational initial value problem (IVP):

$$\frac{dy}{dt} = f(t, y), \quad y(t_0) = y_0 \tag{1}$$

where $y(t) \in \mathbb{R}^d$ and $f : \mathbb{R} \times \mathbb{R}^d \to \mathbb{R}^d$ is continuous and Lipschitz in y, guaranteeing a unique solution by the Picard-Lindelof theorem.

A general s-stage Runge-Kutta method advances the solution from t_n to $t_{n+1} = t_n + h$ via:

$$y_{n+1} = y_n + h \sum_{i=1}^{s} b_i k_i \tag{2}$$

where the intermediate stage values $k_i \in \mathbb{R}^d$ evaluate the vector field:

$$k_i = f\left(t_n + c_i h,\, y_n + h \sum_{j=1}^{s} a_{ij} k_j\right) \tag{3}$$

The coefficients a_{ij} (stage weights), b_i (quadrature weights), and c_i (nodes) fully characterize the method. They are structured using the standard **Butcher Tableau**:

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

The structure of matrix A determines the classification:

1. **Explicit (ERK)**: $a_{ij} = 0$ for all $j \geq i$. A is strictly lower triangular.
2. **Implicit (IRK)**: $a_{ij} \neq 0$ for some $j \geq i$, requiring nonlinear system solves.
3. **Diagonally Implicit (DIRK)**: $a_{ij} = 0$ for $j > i$ with non-zero diagonal entries.

Row-sum consistency requires that the nodes satisfy: $c_i = \sum_{j=1}^{s} a_{ij}$ for all $i = 1, \dots, s$.

2 Consistency, Accuracy, and Convergence

The local truncation error (LTE), denoted as τ_{n+1}, measures the discrepancy introduced over a single temporal step assuming $y_n = y(t_n)$:

$$\tau_{n+1} = y(t_n + h) - \left[y(t_n) + h \sum_{i=1}^{s} b_i k_i\right] \tag{4}$$

A scheme is **consistent** if $\lim_{h \to 0} \frac{\tau_{n+1}}{h} = 0$, which evaluates directly to:

$$\sum_{i=1}^{s} b_i = 1 \tag{5}$$

Theorem 2.1 (Global Convergence)**.** If an RK scheme is consistent, possesses an LTE of order $\mathcal{O}(h^{p+1})$, and f is Lipschitz continuous, the method is globally convergent of order p, meaning the global error satisfies $||e_n|| = ||y(t_n) - y_n|| = \mathcal{O}(h^p)$.

3 Linear Stability Analysis and A-Stability

To evaluate numerical stability, we apply the scheme to the Dahlquist test equation:

$$\frac{dy}{dt} = \lambda y, \quad \text{Re}(\lambda) \leq 0, \quad y(0) = y_0 \tag{6}$$

Letting $z = \lambda h \in \mathbb{C}$, the numerical advancement step collapses to $y_{n+1} = R(z)y_n$, where $R(z)$ is the rational **Stability Function**:

$$R(z) = 1 + zb^T(I - zA)^{-1}\mathbb{E} = \frac{\det(I - zA + z\mathbb{E}b^T)}{\det(I - zA)} \tag{7}$$

where $\mathbb{E} = [1, \ldots, 1]^T$. For explicit schemes, $R(z)$ is a polynomial of degree s.

Definition 3.1. The **Region of Absolute Stability** is defined as $\mathcal{D} = \{z \in \mathbb{C} : |R(z)| \leq 1\}$. A method is defined as **A-stable** if the entire left half-plane lies within $\mathcal{D}$: $\mathbb{C}^- = \{z \in \mathbb{C} : \text{Re}(z) \leq 0\} \subseteq \mathcal{D}$.

Theorem 3.1 (Dahlquist Barrier)**.** No explicit Runge-Kutta method can be A-stable, because its polynomial stability function satisfies $|R(z)| \to \infty$ as $|z| \to \infty$.

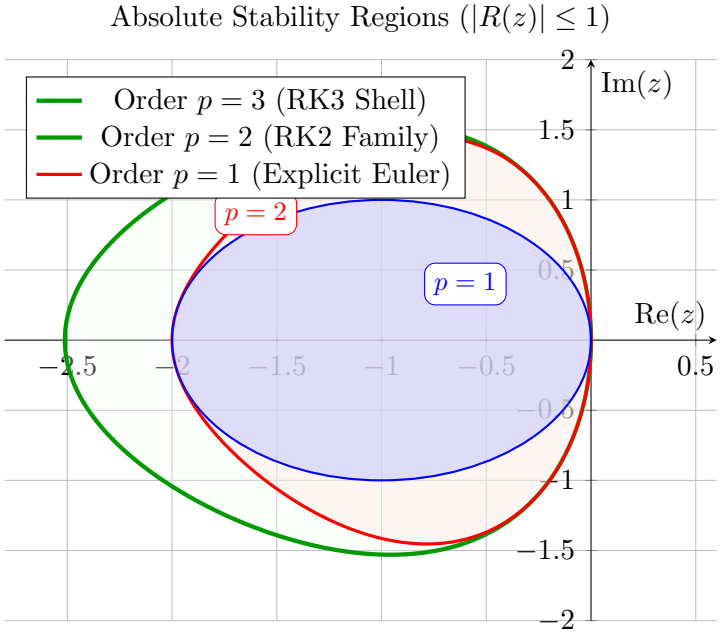


Figure 1: Comparison of nested absolute stability domains ($p = 1, 2, 3$). Higher-order explicit extensions expand the stable step-size ceiling both horizontally and vertically.

4 Derivation of the 2-Stage, 2nd-Order Family

An explicit 2-stage scheme ($s = 2$) uses the coefficients $c_2 = a_{21}$, $a_{22} = a_{12} = 0$. The exact solution expands via multivariate Taylor series around (t_n, y_n) up to $\mathcal{O}(h^2)$ as:

$$y(t_n + h) = y_n + hf + \frac{h^2}{2}(f_t + f_y f) + \mathcal{O}(h^3) \tag{8}$$

The numerical advancement expands identically as:

$$y_{n+1} = y_n + h(b_1 + b_2)f + h^2 c_2 b_2 (f_t + f_y f) + \mathcal{O}(h^3) \tag{9}$$

Matching the coefficients of h and h^2 yields the algebraic order conditions:

$$b_1 + b_2 = 1, \quad c_2 b_2 = \frac{1}{2} \implies b_2 = \frac{1}{2c_2}, \quad b_1 = 1 - \frac{1}{2c_2} \tag{10}$$

Varying the free parameter $c_2 \neq 0$ defines the classical RK2 family realizations:

- **Heun's Method** ($c_2 = 1$): $b_1 = 1/2, b_2 = 1/2, a_{21} = 1$.
- **The Midpoint Method** ($c_2 = 1/2$): $b_1 = 0, b_2 = 1, a_{21} = 1/2$.
- **Ralston's Method** ($c_2 = 2/3$): $b_1 = 1/4, b_2 = 3/4, a_{21} = 2/3$.

5 The Divergence of Order and Stages (Butcher's Barriers)

For lower accuracy requirements, the number of stages equals the order of accuracy ($s = p$). However, for higher orders, this relationship breaks down due to structural limitations known as **Butcher's Order Barriers**:

Target Order (p)	1	2	3	4	5	6
Minimum Stages (s)	1	2	3	4	**6**	7

Table 1: The minimum number of stages s required to resolve explicit order p.

The reason for this divergence is combinatorial. John C. Butcher established a bijective mapping between the partial derivatives of an ODE and graph-theoretical structures known as **Rooted Trees**. Every tree represents an independent non-linear algebraic condition.

While the number of available free parameters in an explicit scheme scales quadratically ($\approx s^2/2$), the number of cumulative order conditions grows explosively: $p = 4$ requires 8 conditions, whereas $p = 5$ requires 17 independent equations. For $s = 5$, the non-linear algebraic system becomes strictly overdetermined, and no real solution exists. Thus, to resolve 17 independent equations for a fifth-order method, a minimum of 6 stages ($s = 6$) is mathematically required.

6 Conclusion

Runge-Kutta methods provide a highly rigid and customizable framework for solving differential systems. Explicit schemes provide simple, uncoupled calculations but are strictly bound by stability regions and Butcher barriers. Implicit schemes overcome stability limits by achieving global A-stability at the expense of solving coupled non-linear systems, making them optimal for stiff ODEs.