Initial value problem (ODE)

$$x' = f(t,x)$$
$$x(t_0) = x_0 \qquad \text{(IVP)}$$

where $f: J \times D \subset \mathbb{R} \times \mathbb{R}^n \to \mathbb{R}$

$(t_0, x_0) \in J \times D$ initial condition

Autonomous ODE: $f(t,x) = f(x)$ $\forall (t,x) \in J \times D$; i.e. f independent of t.

Local Lipschitz continuous: $f: J \times D \to \mathbb{R}^n$ & $f \in C(J \times D, \mathbb{R}^n)$

For each $(t_0, x_0) \in J \times D$ $\exists$ open neighbourhood $\tilde{J} \times \tilde{D}$ of (t_0, x_0) s.t. $f: \tilde{J} \times \tilde{D} \to \mathbb{R}^n$ Lipschitz continuous: $\exists L > 0$ s.t.

$$\|f(t,x) - f(t,y)\| \leq L\|x - y\| \quad \forall t \in \tilde{J}, x, y \in \tilde{D}.$$

Solution: $\exists$ open interval $I \subset J$ containing t_0, $\exists u: \mathbb{R}^n \to \mathbb{R}$, $u \in C^1(I, \mathbb{R}^n)$ s.t. $u'(t) = f(t, u(t))$ and $u(t_0) = x_0$

Flow of vector field $\phi: \mathbb{R} \times \mathbb{R} \times \mathbb{R}^n \to \mathbb{R}^n$:

$$t \in J(t_0, x_0), (t_0, x_0) \in J \times D \to \phi(t, t_0, x_0) = u(t) \in \mathbb{R}^n$$

where $J(t_0, x_0) = (t^-(t_0, x_0), t^+(t_0, x_0))$ interval where maximal solution $u(t)$ exists (no trivial extension)

Second order ODE: - can be written as system of first order:

$$y'' = f(t,y) + g(t,y') \equiv \begin{cases} x_1' = x_2 \\ x_2' = f(t, x_2) + g(t, x_1) \end{cases}$$

One-step methods

- Estimate $u(t) = \Phi(t, t_0, x_0)$ on finite closed interval $t \in [t_0, T]$, $t_0 < T < t^+(t_0, x_0)$.
- Discrete flow of vector field:
  - f locally Lipschitz continuous on $J \times D$
  - $\Psi : J \times D \times \mathbb{R} \to \mathbb{R}^n$

$$t, x, \tau \geq 0 \to \Psi(t+\tau, t, x) \in \mathbb{R}^n$$

s.t. $\Psi(t,t,x) = \lim_{\tau \to 0^+} \frac{\Psi(t+\tau, t, x) - x}{\tau} = f(t,x)$

- Partition interval $[t_0, T]$ into N subintervals:

$$\{t_j\}_{j=0}^{N}, \; t_{j+1} > t_j, \quad t_N = T.$$

Approximation $\{u_j\}_{j=0}^{N}$ by $\underbrace{u_j \mapsto u_{j+1} = \Psi(t_{j+1}, t_j, u_j) \in \mathbb{R}^n}_{\text{one-step method}}$

where $u_j \approx u(t_j)$

Local Discretization Error

f locally Lipschitz cont. on $J \times D$; Φ flow of f
$(t,x) \in J \times D$, $\tau > 0$. Consider

$$t, x, \tau \mapsto \Psi(t+\tau, t, x) \in \mathbb{R}^n$$

Define $d(t+\tau, t, x) = \| \Phi(t+\tau, t, x) - \Psi(t+\tau, t, x) \|$

as local discretization error

If $\exists p > 0$ (integer) st $d(t+\tau, t, x) = \mathcal{O}(\tau^{p+1})$ for $\tau \to 0^+$

then method is of order p at (t,x).

Method	Im/Ex	Order
Euler: $K_1 = f(t,x)$, $\psi \equiv x + \tau K_1$	Explicit	1
Runge: $K_1 = f(t,x)$, $K_2 = f(t+\tau/2, x+\frac{\tau}{2}K_1)$, $\psi = x + \tau K_2$	Explizit	2
Heun: $K_1 = f(t,x)$, $K_2 = f(t+\tau, x+\tau K_1)$, $\psi = x + \frac{\tau}{2}(K_1 + K_2)$	Explizit	2
Runge-Kutta: $K_1 = f(t,x)$, $K_2 = f(t+\frac{\tau}{2}, x+\frac{\tau}{2}K_1)$, $K_3 = f(t+\frac{\tau}{2}, x+\frac{\tau}{2}K_2)$, $K_4 = f(t+\tau, x+\tau K_3)$, $\psi = x + \tau\left(\frac{1}{6}K_1 + \frac{2}{3}K_2 + \frac{2}{3}K_3 + \frac{1}{6}K_4\right)$	Explizit	4
Imp. Euler: $K_1 = f(t+x, x+\tau K_1)$, $\psi = x + \tau K_1$	Implizit	1
Crank-Nicholson: $K_1 = f(t,x)$, $K_2 = f(t+\tau, x+\frac{\tau}{2}K_1 + \frac{\tau}{2}K_2)$, $\psi = x + \frac{\tau}{2}(K_1 + K_2)$	Implizit	2

- Implizit methods require non-linear solver (fixed point, Newton, ...).

Consistency function: $\Phi(t,x,\tau) \equiv \frac{\psi(t+\tau, t, x) - x}{\tau} \in \mathbb{R}^n$

Assumption: $\exists \Lambda > 0$ s.t. $\|\Phi(t,x,\tau) - \Phi(t,x,y)\| \leq \Lambda \|x-y\|$

$\forall t \in [t_0, T]$, $x, y \in D$, $\tau \geq 0$

Theorem 2.23 (Global Error Estimate)

$\exists C > 0, \tau_1 > 0$ sufficiently small s.t.

$$d(t+\tau, t, u(t)) \le C\tau^{p+1} \quad \tau \le \tau_1, t \in [t_0, T]$$

Consider equidistant partition $\{t_j\}_{j=0}^N$ and approximation $\{u_j\}_{j=0}^N$; then

$$\|u(t_j) - u_j\| \le \frac{e^{\Lambda(t_j - t_0)} - 1}{\Lambda} C\tau^p, \; j = 0, \dots, N$$

Adaptive timestepping

Consider "low order method" of order p:

$$t, x, \tau \mapsto \psi(t+\tau, t, x) \in \mathbb{R}^n$$

and "high order method" order $p+1$

$$t, x, \tau \mapsto \overline{\psi}(t+\tau, t, x) \in \mathbb{R}^n$$

$$\Delta(\tau) \equiv \overline{\psi}(t+\tau, t, x) - \psi(t+\tau, t, x)$$

$$\|\Delta(\tau)\| \approx K_0 \tau^{p+1}$$

Can compute optimal time step size τ_{opt} such that

$$\|\Delta(\tau_{opt})\| = K_0 \tau_{opt}^{p+1} \approx tol$$

$$\tau_{opt} = \tau \left(\frac{tol}{\|\Delta(\tau)\|} \right)^{\frac{1}{p+1}}$$

$\hookrightarrow$ gives Algorithm 2.1 for computing optimal stepsize.

Runge-Kutta methods

Butcher tableau: $A \in \mathbb{R}^{s \times s}$, $b, c \in \mathbb{R}^s$, $s \ge 1$

$$\begin{array}{c|ccc} c_1 & a_{11} & \cdots & a_{1s} \\ \vdots & \vdots & \ddots & \vdots \\ c_s & a_{s1} & \cdots & a_{ss} \\ \hline & b_1 & \cdots & b_s \end{array} = \begin{array}{c|c} c & A \\ \hline & b^T \end{array}$$

$$k_i = f\left(t+\tau c_i, x+\tau \sum_{j=1}^{s} a_{ij} k_j\right) \quad i=1,\dots,s$$

$$\psi(t+\tau, t, x) \equiv x + \tau \sum_{i=1}^{s} b_i k_i$$

Aim to derive highest order RK method:

<u>Lemma 2.31 (autonomous ODE, order $p=3$):</u>

$f(t,x) = f(x)$, $f \in C^3(D, \mathbb{R}^n)$; then, if

$$\sum_{i=1}^{s} b_i = 1, \quad 2\sum_{i,j=1}^{s} b_i a_{ij} = 1, \quad 3\sum_{i,j,k=1}^{s} b_j a_{ij} a_{ik} = 1, \quad 6\sum_{i,j,k=1}^{s} b a_{ij} a_{jk} = 1$$

$\Rightarrow$ RK method of order $p=3$ at $x \in D$.

<u>Lemma 2.32 (Invariance w.r.t "autonomisation"):</u>

RK invariant w.r.t automomisation if and only if

$$c_i = \sum_{j=1}^{s} a_{ij} \quad i=1,\dots,s$$

<u>Corollary 2.33 (RK order $p=3$):</u> $f \in C^3(D, \mathbb{R}^n)$

Let 2.32 be satisfied then,

$$\sum_{i=1}^{s} b_i = 1, \quad 2\sum_{i=1}^{s} b_i c_i = 1, \quad 3\sum_{i=1}^{s} b_i c_i^2 = 1, \quad 6\sum_{i,j=1}^{s} b_i a_{ij} c_j = 1$$

$\Rightarrow$ RK method of order $p=3$ at $x \in D$

<u>Explizit RK</u>: $a_{ij} = 0 \quad i \leq j$ (A strictly lower triangular):

$$\begin{array}{c|cccc}
c_1 & & & & \\
c_2 & a_{2s} & & & \\
\vdots & \vdots & \ddots & & \\
c_s & a_{1s} & \cdots & a_{1,s-1} & \\
\hline
 & b_1 & & b_{s-1} & b_s
\end{array}$$

Embedded RK $p(p-1)$: Low order $(p-1)$ RK embedded within high order (p); e.g.

$$\begin{array}{c|ccc} 0 & & & \\ 1 & 1 & & \\ 1/2 & 1/4 & 1/4 & \\ \hline & 1/2 & 1/2 & \\ & 1/6 & 1/6 & 2/3 \end{array}$$

"low order"

"high order"

Multistep Methods

m-step method, $m \geq 1$, given by real coefficients
$$\{a_i\}_{i=0}^{m}, \{b_i\}_{i=0}^{m}, a_m = 1$$
such that $|a_0| + |b_0| \neq 0$, initialised with first m values, $\{u_i\}_{i=0}^{m-1}, u_0 = x_0$; then
$$\sum_{i=0}^{m} a_i u_{j+i} = \tau \sum_{i=0}^{m} b_i f(t_{j+i}, u_{j+i}), \; j = 0, .., N-m$$

Usually use one-step for initialisation.

m-step methods are
- explicit if $b_m = 0$
- implicit if $b_m \neq 0$

Local discretisation error: $f \in C^1(J \times D, \mathbb{R}^n)$

Then $D(t+\tau, t, x) = \sum_{i=0}^{m} a_i u(t+i\tau) - \tau \sum_{i=0}^{m} b_i u'(t+i\tau)$

If $\exists p \geq 1$ (positive integer) such that
$$\|D(t+\tau, t, x)\| = O(\tau^{p+1})$$
then method is of order p at $(t,x) \in J \times D$

If at least order 1 then consistent.

Theorem 3.2 Assume $f \in C^p(J \times D, \mathbb{R}^n)$, $p \geq 1$, and let $\sum_{i=0}^{m} a_i = 0$, $\sum_{i=0}^{m} i^l a_i = l \sum_{i=0}^{m} i^{l-1} b_i$, $l = 1, \dots, p$ $(0^0 = 1)$

Then, m-step method is at least order p at $(t, x) \in J \times D$.

Characteristic polynomials $z \in \mathbb{C}$:

first: $\rho(z) = \sum_{i=0}^{m} a_i z^i$; second: $\sigma(z) = \sum_{i=0}^{m} b_i z^i$

D-stability Method D-stable provided every root $z \in \mathbb{C}$ of first characteristic polynomial $\rho(z) = 0$ satisfies <u>either</u>

- $|z| < 1$ or
- $|z| = 1$, $\rho'(z) \neq 0$ (i.e. algebraic multiplicity $= 1$)

Theorem 3.7 (Global error estimate)

Assume $f \in C^p(J \times D, \mathbb{R}^n)$, $p \geq 1$. Consider D-stable, m-step method of order $p \geq 1$ on equidistant partition: Then, $\exists\, C > 0$ s.t. for sufficiently large N

$$\|u(t_j) - u_j\| \leq C(\varepsilon_0 + \tau^p), \; j = 0, \dots, N, \; \tau = \frac{T - t_0}{N}$$

where $\varepsilon_0 = \max_{l=0,\dots,m-1} \|u(t_l) - u_l\|$ is initialisation error.

Remark One-step method of order k, $k \geq p$, should be chosen for initialisation as then $\varepsilon_0 = O(\tau^k)$.

Dahlquist Barrier D-stable m-step method of order $p \geq 1$. Then, necessary that

$$p \leq \begin{cases} m+2 & \text{if } m \text{ is even} \\ m+1 & \text{if } m \text{ is odd} \\ m & \text{if } \frac{b_m}{a_m} \leq 0 \text{ (e.g. explicit } b_m = 0) \end{cases}$$

m-step methods

Adams: $a_m = 1$, $a_{m-1} = -1$, $a_{m-2} = \dots = a_0 = 0$

$b_m, \dots, b_0$ selected to obtain highest order possible via Theorem 3.2

→ explicit (Adams-Bashford), $b_m = 0$, $p = m$, D-stable

→ implizit (Adams-Moulton), $b_m \neq 0$, $p = m+1$, D-stable

BDF: $b_0 = \dots = b_{m-1} = 0$, $b_m \neq 0$, $a_m = 1$

$a_{m-1}, \dots, a_0$ selected such that highest order possible

→ implizit, $b_m \neq 0$, $p = m$, D-stable for $p \leq 6$ only.

Dynamical Systems

Autonomous ODE: $x' = f(x)$, $x(0) = x_0$

Orbit: $\gamma(x_0) = \bigcup_{t \in (t^-(x_0), t^+(x_0))} \phi(t, x)$

$\gamma^+(x_0) = \bigcup_{t \in (0, t^+(x_0))} \phi(t, x)$ – positive

$\gamma^-(x_0) = \bigcup_{t \in (t^-(x_0), 0)} \phi(t, x)$ – negative

ω-limit: $x_0 \in D$: $\omega(x_0) = \bigcap_{\tau \geq 0} \overline{\gamma^+(\phi(\tau, x_0))}$

Steady state $x^* \in D$. Steady state when $f(x^*) = 0$:

i.e. $\phi(t, x^*) = x^* \quad \forall t \in \mathbb{R}$.

- $x^* \in D$, $f(x^*) = 0$, $\forall \varepsilon > 0 \ \exists \delta > 0$ s.t. if $x \in B_\delta(\bar{x})$ it holds that $\|\phi(t, x) - x^*\| < \varepsilon \quad \forall t \geq 0$

$\Rightarrow x^*$ stable steady state

- additionally if $\exists r > 0$ s.t. $\forall x \in B_r(x)$ it holds $\lim_{t \to +\infty} \phi(t, x) = x^*$ $\Rightarrow x^*$ A-stable steady state

- otherwise unstable

Theorem 4.14 $f \in C^1(D, \mathbb{R}^n)$, $x^* \in D$, $f(x^*) = 0$

$$A = \left(\frac{\partial f_i}{\partial x_j}(x^*)\right)_{i,j=1}^n \in \mathbb{R}^{n\times n}$$

denote Jacobian of f at x^*.

If $\max_{\lambda \in \sigma(A)} Re(\lambda) < 0 \Rightarrow x^*$ A-stable steady state

If $\exists \lambda \in \sigma(A) : Re(\lambda) > 0 \Rightarrow x^*$ unstable

Linearisation of ODE:

$$x' = Ax \qquad x(0) = x_0 \qquad (*)$$

Theorem 4.15 Steady state $x^* = 0 \in \mathbb{R}^n$ of $(*)$ A-stable if and only if $\max_{\lambda \in \sigma(A)} Re(\lambda) < 0$.

Discrete time dynamical system: $t, x, \tau \mapsto \psi(t+\tau, t, x) \in \mathbb{R}^n$, for autonomous ODE $t, \tau \mapsto \psi(\tau, x) \in \mathbb{R}^n$

Iteration: $j \in \mathbb{N}_0 \mapsto t_j = \tau j$, $u_j = \psi^j(\tau, x)$

where $\psi^j(\tau, x) = \psi(\tau, \psi^{j-1}(\tau, x))$, $\psi^1 = \psi$

gives discrete sequence $\{t_j\}_{j=0}^{+\infty}$, $\{u_j\}_{j=0}^{+\infty}$

Fixed point of mapping $x \mapsto \psi(\tau, x)$ is $x^* \in D$ such that $x^* = \psi(\tau, x^*)$.

Proposition 4.23 $x^* \in D$, $\tau > 0$. If $f(x^*) = 0$ (i.e. steady state) then $x^* = \psi(\tau, x^*)$; i.e. fixed point of $x \mapsto \psi(\tau, x)$.

A-stability of F.P. $x^* = \psi(\tau, x^*) \in D$ be f.p. of $x \in D \mapsto \psi(\tau, x) \in \mathbb{R}^n$ for $\tau > 0$:

- stable f.p: $\forall \varepsilon > 0 . \exists \delta > 0$ s.t. if $x \in B_\delta$ it holds $\|\psi^j(\tau, x) - x^*\| < \varepsilon \; \forall j \in \mathbb{N}_0$
- A-stable f.p. - stable f.p and $\exists r > 0$ s.t $\forall x \in B_r$ it holds $\psi^j(\tau, x) \to x^*$ for $j \to \infty$.
- unstable f.p - if not stable

Domain of stability

Autonomous ODE: $x' = f(x)$, $x(0) = x_0$
with steady state $x^* \in D$, $f(x^*) = 0$
Jacobian at x^*: $A = \left(\frac{\partial f_i(x^*)}{\partial x_j} \right)_{i,j=1..n} \in \mathbb{R}^{n \times n}$

Assume $\max\limits_{\lambda \in \sigma(A)} \operatorname{Re}(\lambda) < 0 \Rightarrow A^*$ A-stable.

↳ steady state is fixed point. Is it A-stable?
Consider linearisation: $x' = Ax$, $x(0) = x_0$
- steady state $x^* = 0 \in \mathbb{R}^n$ (A-stab).

↳ Is fixed point A-stable for numerical method?
what value of τ is required?
↳ domain of stability: $S \subset \mathbb{C}$

F.P. A-stable if $\tau\lambda \in S \; \forall \lambda \in \sigma(A)$

Domain of stability (explicit RK):

$s=1$ (Euler): $S = \{\mu \in \mathbb{C} : |1+\mu| < 1\}$
$s=2$ (Runge/Heun): $S = \{\mu \in \mathbb{C} : |1+\mu+\frac{1}{2}\mu^2| < 1\}$
$s=3$ $S = \{\mu \in \mathbb{C} : |1+\mu+\frac{1}{2}\mu^2+\frac{1}{6}\mu^3| < 1\}$
$s=4$ (cl. RK) $S = \{\mu \in \mathbb{C} : |1+\mu+\frac{1}{2}\mu^2+\frac{1}{6}\mu^3+\frac{1}{24}\mu^4| < 1\}$

Domain of stability (implizit one-step)

Implizit Euler: $S = \left\{ \mu \in \mathbb{C} : \frac{1}{|1-\mu|} < 1 \right\}$

Crank-Nichdson: $S = \left\{ \mu \in \mathbb{C} : \frac{|1+\frac{\mu}{2}|}{|1-\frac{\mu}{2}|} < 1 \right\}$

Domain of stability (m-step)

$S = \{ \mu \in \mathbb{C} : \forall z \in \mathbb{C} : \rho(z) - \tau \lambda \sigma(z) = 0 \in \mathbb{C} \Rightarrow |z| < 1 \}$

A-stable RK/m-step methods

S domain of stability; then method A-stable if

$$\{ \mu \in \mathbb{C} : Re(\mu) < 0 \} \subset S$$

(left half-plane of complex domain subset of domain)

i.e. fixed point A-stable regardless of $\tau > 0$ value

A-stable RK/m-step methods

- Implizit Euler, Crank-Nichdson, Gauss & Radau are A-stable
- <u>No</u> explicit RK are A-stable.
- Adams-Moulton 1, BDF1 and BDF2.

Stiff Problems

Consider linear system $x' = Ax$, with $\max_{\lambda \in \sigma(A)} Re(\lambda) < 0$

$\Rightarrow x^* = 0$ A-stable steady state

Stiffness Ratio $L = \frac{\max_{\lambda \in \sigma(A)} |Re(\lambda)|}{\min_{\lambda \in \sigma(A)} |Re(\lambda)|}$

$\hookrightarrow$ stiffness ratio large if $L \gg 1$.

$\hookrightarrow$ stiff problems require a stiff (e.g. implicit) method.