Linear Algebra

Vector norms: $\|\mathbf{x}\|_1 = \sum_i |x_i|$, $\|\mathbf{x}\|_2 = \sqrt{\sum_i x_i^2}$, $\|\mathbf{x}\|_\infty = \max_i |x_i|$
Matrix norms: $\|A\|_1 = \max_j \sum_i |a_{ij}|$ (col sum), $\|A\|_\infty = \max_i \sum_j |a_{ij}|$ (row sum),
$\|A\|_2 = \sqrt{\lambda_{\max}(A^T A)}$, $\|A\|_F = \sqrt{\sum_{i,j} a_{ij}^2}$ (Frobenius)
Eigenvalues: $A\mathbf{v} = \lambda\mathbf{v}$. Characteristic poly: $\det(A - \lambda I) = 0$
SVD: $A = U\Sigma V^T$ with U, V orthogonal, Σ diagonal. $\sigma_{\max} = \|A\|_2$, $\kappa_2(A) = \sigma_{\max}/\sigma_{\min}$
Spectral radius: $\rho(A) = \max_i |\lambda_i| \le \|A\|$ for any matrix norm
Strictly diagonally dominant (SDD): $|a_{ii}| > \sum_{j\neq i} |a_{ij}|$ for all i. Guarantees non-singular matrix and convergence of Jacobi/Gauss-Seidel
Matrix classes: SPD (symmetric positive definite): $A = A^T$ and $\mathbf{x}^T A\mathbf{x} > 0$ for $\mathbf{x} \neq \mathbf{0}$.
Orthogonal: $Q^T Q = I$. Unitary: $U^* U = I$
Rank: $\operatorname{rank}(A)$ = number of linearly independent rows/cols = number of nonzero singular values
Determinant properties: $\det(AB) = \det(A)\det(B)$, $\det(A^T) = \det(A)$, $\det(A^{-1}) = 1/\det(A)$
Trace: $\operatorname{tr}(A) = \sum_i a_{ii} = \sum_i \lambda_i$. $\operatorname{tr}(AB) = \operatorname{tr}(BA)$
Matrix inverses: $(AB)^{-1} = B^{-1}A^{-1}$, $(A^T)^{-1} = (A^{-1})^T$. For SPD: A^{-1} is also SPD

Non-linear Equations & Fixed-Point

Banach FPT: A self map g on a complete metric space X is a contraction if $\exists\, 0 < \kappa < 1$ such that $|g(x) - g(y)| \le \kappa|x - y|$ for all x, y. Then $\mathbf{x}^{(k+1)} = g(\mathbf{x}^{(k)})$ converges to unique fixed point. Error: $|\mathbf{x}^{(k)} - \mathbf{x}^*| \le \frac{\kappa^k}{1-\kappa}|\mathbf{x}^{(1)} - \mathbf{x}^{(0)}|$
General FP: Starting with $\mathbf{x}^{(0)}$, generate $\mathbf{x}^{(k+1)} = g(\mathbf{x}^{(k)})$. Convergence requires g to be a contraction on a region containing the fixed point.
Newton's method: For $f(x) = 0$ with $f : \mathbb{R}^n \to \mathbb{R}^n$: $\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} - J_f(\mathbf{x}^{(k)})^{-1} f(\mathbf{x}^{(k)})$. Scalar: $x_{k+1} = x_k - \frac{f(x_k)}{f'(x_k)}$. Locally quadratically convergent.
Order p: $\lim_{k\to\infty} \frac{|\mathbf{x}^{(k+1)} - \mathbf{x}^*|}{|\mathbf{x}^{(k)} - \mathbf{x}^*|^p} = C \neq 0$
Conditioning: For simple root $\mathbf{x}^*$ of f, relative condition number $\approx \frac{1}{|\mathbf{x}^* f'(\mathbf{x}^*)|}$

Linear Systems

Direct Methods

Gaussian elimination: $O(n^3/3)$ flops for $n \times n$ system. Forward elimination + back substitution
Elimination step: For pivot row k: $l_{j,k} = a_{j,k}/a_{k,k}$ (requires $a_{k,k} \neq 0$). Update: $a_{j,p} \leftarrow a_{j,p} - l_{j,k} a_{k,p}$, $b_j \leftarrow b_j - l_{j,k} b_k$ for $j > k$, $p \ge k+1$
Partial pivoting: Choose largest $|a_{j,k}|$ in column k below diagonal as pivot. Essential for numerical stability
LU factorization: $PA = LU$ with permutation P, unit lower triangular L, upper triangular U. Solve $L\mathbf{y} = P\mathbf{b}$ (forward), then $U\mathbf{x} = \mathbf{y}$ (backward)
Cholesky: For SPD matrix: $A = LL^T$ with L lower triangular, positive diagonal. $O(n^3/6)$ flops, no pivoting needed. Fails if A not SPD
QR decomposition: $A = QR$ with Q orthonormal, R upper triangular. For $A\mathbf{x} = \mathbf{b}$: solve $R\mathbf{x} = Q^T\mathbf{b}$. Cost: $O(2n^3/3)$ flops
Householder reflectors: $H = I - 2\mathbf{v}\mathbf{v}^T/\|\mathbf{v}\|_2^2$ where $\mathbf{v} = \mathbf{x} \pm \|\mathbf{x}\|_2\mathbf{e}_1$ (choose sign to avoid cancellation). More stable than Gram-Schmidt
Givens rotations: Zero element (j, i) using $G_{ij}(\theta)$ where $c = \cos\theta = \frac{a_{ii}}{\sqrt{a_{ii}^2 + a_{ji}^2}}$, $s = \sin\theta = \frac{a_{ji}}{\sqrt{a_{ii}^2 + a_{ji}^2}}$
Gram-Schmidt: $\mathbf{q}_1 = \mathbf{a}_1/\|\mathbf{a}_1\|_2$. For $k \ge 2$: $\mathbf{u}_k = \mathbf{a}_k - \sum_{j=1}^{k-1}(\mathbf{a}_k^T\mathbf{q}_j)\mathbf{q}_j$, $\mathbf{q}_k = \mathbf{u}_k/\|\mathbf{u}_k\|_2$. Numerically unstable; prefer modified GS or Householder
Least squares: Minimize $\|\mathbf{b} - A\mathbf{x}\|_2^2$. Normal equations: $A^T A\mathbf{x} = A^T\mathbf{b}$ (condition number $\kappa_2(A^T A) = \kappa_2(A)^2$). QR method: $R\mathbf{x} = Q^T\mathbf{b}$ (condition number $\kappa_2(A)$). Prefer QR for better stability

Conditioning & Spectra

Condition number: $\kappa(A) = \|A\|\|A^{-1}\|$. Measures sensitivity of x in $Ax = \mathbf{b}$
Gershgorin discs: Each eigenvalue $\lambda \in S_j = \{z \in \mathbb{C} : |z - a_{jj}| \le \sum_{k\neq j}|a_{jk}|\}$

Iterative Methods

General form: Stationary iteration for solving $A\mathbf{x} = \mathbf{b}$:
$$\mathbf{x}^{(k+1)} = B\,\mathbf{x}^{(k)} + \mathbf{f},$$
where B is the iteration matrix and $\mathbf{f}$ is a constant vector. If $\mathbf{x}^*$ is the exact solution and $\mathbf{e}^{(k)} = \mathbf{x}^{(k)} - \mathbf{x}^*$, then
$$\mathbf{e}^{(k+1)} = B\,\mathbf{e}^{(k)} \quad\Rightarrow\quad \mathbf{e}^{(k)} = B^k\mathbf{e}^{(0)}.$$
Convergence: The iteration converges for every initial guess $\mathbf{x}^{(0)}$ iff
$$\rho(B) < 1,$$
where $\rho(B)$ is the spectral radius of B.
Asymptotic error decay (in any matrix norm compatible with B):
$$\|\mathbf{e}^{(k)}\| \le C\,\rho(B)^k\,\|\mathbf{e}^{(0)}\|$$
for some constant C independent of k.
Richardson: For A (typically SPD) and relaxation parameter $\omega > 0$,
$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} + \omega\left(\mathbf{b} - A\mathbf{x}^{(k)}\right) = (I - \omega A)\mathbf{x}^{(k)} + \omega\mathbf{b},$$
so the iteration matrix is $B_R = I - \omega A$.
For A SPD with eigenvalues $0 < \lambda_{\min} \le \lambda_{\max}$,

- Convergence iff $0 < \omega < \dfrac{2}{\lambda_{\max}}$.
- Optimal parameter:
$$\omega_{\text{opt}} = \frac{2}{\lambda_{\min} + \lambda_{\max}}.$$

Jacobi: Use the standard splitting
$$A = D + L + U,$$
where $D = \operatorname{diag}(A)$ is the diagonal of A and L, U are the strictly lower/upper triangular parts.
From $(D + L + U)\mathbf{x} = \mathbf{b}$ we write
$$D\mathbf{x} = \mathbf{b} - (L + U)\mathbf{x}.$$
Replacing the exact $\mathbf{x}$ by iterates:
$$D\mathbf{x}^{(k+1)} = \mathbf{b} - (L + U)\mathbf{x}^{(k)}.$$
Thus
$$B_J = -D^{-1}(L + U),$$
$$\mathbf{x}^{(k+1)} = B_J\,\mathbf{x}^{(k)} + D^{-1}\mathbf{b},$$
$$x_i^{(k+1)} = \frac{1}{a_{ii}}\left[b_i - \sum_{j\neq i} a_{ij}\,x_j^{(k)}\right].$$
Convergence:

- If A is strictly diagonally dominant (SDD) by rows, then Jacobi converges.
- In general, Jacobi converges iff $\rho(B_J) < 1$.

Gauss–Seidel: With the same splitting $A = D + L + U$,
$$(D + L)\,\mathbf{x} = \mathbf{b} - U\,\mathbf{x}.$$
Replacing $\mathbf{x}$ by iterates and using the new iterate on the left:
$$(D + L)\,\mathbf{x}^{(k+1)} = \mathbf{b} - U\,\mathbf{x}^{(k)}.$$
Hence
$$B_{GS} = -(D + L)^{-1}U, \qquad \mathbf{x}^{(k+1)} = B_{GS}\,\mathbf{x}^{(k)} + (D + L)^{-1}\mathbf{b}.$$
Componentwise:
$$x_i^{(k+1)} = \frac{1}{a_{ii}}\left[b_i - \sum_{j<i} a_{ij}\,x_j^{(k+1)} - \sum_{j>i} a_{ij}\,x_j^{(k)}\right].$$
Convergence:

- If A is SPD, Gauss–Seidel is convergent (and error decreases monotonically in the A-norm).

SOR (Successive Over-Relaxation): For $\omega \in \mathbb{R} \setminus \{0\}$, the componentwise form is
$$x_i^{(k+1)} = (1 - \omega)\,x_i^{(k)} + \frac{\omega}{a_{ii}}\left[b_i - \sum_{j<i} a_{ij}\,x_j^{(k+1)} - \sum_{j>i} a_{ij}\,x_j^{(k)}\right].$$
In matrix form (with $A = D + L + U$) one can show
$$(D + \omega L)\,\mathbf{x}^{(k+1)} = ([(1 - \omega)D - \omega U])\mathbf{x}^{(k)} + \omega\mathbf{b},$$
hence
$$B_\omega = (D + \omega L)^{-1}\,([(1 - \omega)D - \omega U]).$$
Convergence (classical results):

- For A SPD (Ostrowski): SOR converges iff $0 < \omega < 2$.
- If A is SDD by rows, SOR converges for $0 < \omega \le 1$.
- Under additional assumptions (e.g. A has the A-property and $\rho(B_J) < 1$), the optimal relaxation parameter is
$$\omega_{\text{opt}} = \frac{2}{1 + \sqrt{1 - \rho(B_J)^2}}.$$

Convergence rates (comparison): For matrices with the A-property (in particular for many SPD tridiagonal problems),
$$\rho(B_{GS}) = \rho(B_J)^2 \quad\text{and}\quad \rho\left(B_{\omega_{\text{opt}}}\right) < \rho(B_{GS}) = \rho(B_J)^2 < \rho(B_J),$$
so SOR with ω_{opt} is fastest, followed by Gauss–Seidel, then Jacobi.

Interpolation & Splines

Lagrange & Newton

Lagrange form: $P_n(x) = \sum_{j=0}^n f(x_j)L_j(x)$, $L_j(x) = \prod_{i\neq j}\frac{x - x_i}{x_j - x_i}$
Newton form: Uses divided differences $f[x_0, x_1, \ldots, x_k]$ recursively:
$P_n(x) = f[x_0] + f[x_0, x_1](x - x_0) + \ldots + f[x_0, \ldots, x_n]\prod_{j=0}^{n-1}(x - x_j)$
Divided differences: $f[x_i] = f(x_i)$, $f[x_i, x_{i+1}] = \frac{f[x_{i+1}] - f[x_i]}{x_{i+1} - x_i}$,
$f[x_i, \ldots, x_{i+k}] = \frac{f[x_{i+1}, \ldots, x_{i+k}] - f[x_i, \ldots, x_{i+k-1}]}{x_{i+k} - x_i}$
Error bound: For $f \in C^{n+1}[a, b]$ and distinct nodes $x_0, \ldots, x_n$:
$$f(x) - P_n(x) = \frac{f^{(n+1)}(\xi)}{(n+1)!}\prod_{j=0}^{n}(x - x_j)$$

Splines

Definition. A (univariate $s : \mathbb{R} \to \mathbb{R}$) spline of degree $k \ge 1$ on the partition $a = x_0 < \cdots < x_n = b$ is
$$\mathcal{S}_k := \left\{ s \in C^{k-1}[a, b] \;:\; s|_{[x_i, x_{i+1}]} \in \mathbb{P}_k \text{ for } i = 0, \ldots, n-1 \right\},$$
$\mathbb{P}_k$ denotes the polynomials $s(x) = p_i(x)$ of $\deg(p_i) \le k$.
Dimension.
$$\dim(\mathcal{S}_k) = n(k + 1) - k(n - 1) = n + k.$$
(There are n pieces, each with $k + 1$ coefficients, and k continuity constraints at each of the $n - 1$ interior knots.)
Knot vector: $\Delta = \{x_0, x_1, \ldots, x_n\}$ with $n + 1$ knots defining n subintervals
Error bound. If $f \in C^{k+1}[a, b]$ and $s \in \mathcal{S}_k$ is an interpolatory spline (made unique by adding $k - 1$ extra conditions), then on a quasi-uniform mesh
$$\|f - s\|_\infty \le C\,h^{k+1}\,\|f^{(k+1)}\|_\infty, \quad h = \max_i h_i, \quad h_i = x_{i+1} - x_i$$
for a const. C indep. of h (but dep. on k).
Piecewise linear ($k = 1$): For $s_1 \in C^0$, $x \in [x_i, x_{i+1}]$,
$$s_1(x) = y_i + \frac{y_{i+1} - y_i}{h_i}(x - x_i), \qquad \|f - s_1\|_\infty = O(h^2).$$
Piecewise quadratic ($k = 2$). $s_2 \in C^1$ and, with one additional condition beyond nodal interpolation (since $k - 1 = 1$),
$$\|f - s_2\|_\infty = O(h^3).$$

Cubic Splines

Definition: $s \in C^2[a, b]$, $s|_{[x_i, x_{i+1}]} \in \mathbb{P}_3$ on $a = x_0 < x_1 < \ldots < x_n = b$
Error bound: For $f \in C^4[a, b]$: $\|f - s\|_\infty \le \frac{5h^4}{384}\|f^{(4)}\|_\infty$ where $h = \max_i h_i$
Second derivative form: Let $h_i = x_{i+1} - x_i$, $z_i = s''(x_i)$:
$$s_i(x) = \frac{z_{i+1}}{6h_i}(x - x_i)^3 + \frac{z_i}{6h_i}(x_{i+1} - x)^3 + \left(\frac{y_{i+1}}{h_i} - \frac{z_{i+1}h_i}{6}\right)(x - x_i) + \left(\frac{y_i}{h_i} - \frac{z_i h_i}{6}\right)(x_{i+1} - x)$$
Tridiagonal system: For $i = 1, \ldots, n-1$:
$$h_{i-1}z_{i-1} + 2(h_{i-1} + h_i)z_i + h_i z_{i+1} = 6\left[\frac{y_{i+1} - y_i}{h_i} - \frac{y_i - y_{i-1}}{h_{i-1}}\right]$$
Boundary conditions:

- Natural: $z_0 = z_n = 0$ ($s''(a) = s''(b) = 0$)
- Clamped: $s'(a), s'(b)$ specified
- Not-a-knot: s''' continuous at x_1, x_{n-1}
- Periodic: $s(a) = s(b)$, $s'(a) = s'(b)$, $s''(a) = s''(b)$

Variational property: Natural cubic spline minimizes $\int_a^b [g''(x)]^2\,dx$ among all $g \in C^2[a, b]$ interpolating the data
Optimality: Cubic splines achieve optimal approximation order $O(h^4)$ for C^4 functions

B-splines

Basis: $\{B_{i,k+1}\}$ forms basis for spline space $\mathcal{S}_k$ of degree k splines
Support: $B_{i,k+1}$ has support on $[t_i, t_{i+k+1}]$ where Δ is extended knot sequence
Properties: Partition of unity: $\sum_i B_{i,k+1}(x) = 1$; Non-negativity: $B_{i,k+1}(x) \ge 0$; Local support

Cox-de Boor recursion: $B_{i,1}(x) = \begin{cases}1 & \text{if } t_i \le x < t_{i+1} \\ 0 & \text{otherwise}\end{cases}$

$$B_{i,k+1}(x) = \frac{x - t_i}{t_{i+k} - t_i} B_{i,k}(x) + \frac{t_{i+k+1} - x}{t_{i+k+1} - t_{i+1}} B_{i+1,k}(x)$$

Representation: Any spline $s(x) = \sum_i c_i B_{i,k+1}(x)$ with control points c_i
Knot insertion: Adding knots refines spline without changing its shape, enabling adaptive approximation

Orthogonal Polynomials & Fourier

Orthogonal Polynomials

Inner product: $(f,g)_w = \int_a^b f(x)g(x)w(x)dx$ with weight $w(x) > 0$
Gram-Schmidt: Orthogonalize $\{1, x, x^2, \ldots\}$ to get $\{p_0, p_1, p_2, \ldots\}$
Three-term recurrence: $p_{k+1}(x) = (a_k x + b_k)p_k(x) - c_k p_{k-1}(x)$
Chebyshev polynomials: $T_k(x) = \cos(k \arccos x)$, $w(x) = 1/\sqrt{1-x^2}$, $[-1,1]$. $T_{k+1} = 2xT_k - T_{k-1}$, $|T_k(x)| \le 1$
Legendre polynomials: $w(x) = 1$ on $[-1,1]$. $(2k+1)P_{k+1} = (2k+1)xP_k - kP_{k-1}$
Zeros property: Orthogonal polynomial p_n has n simple real zeros in (a,b)

Fourier Series

Complex form: $f(x) = \sum_{n=-\infty}^{\infty} c_n e^{in\pi x/L}$, $c_n = \frac{1}{2L}\int_{-L}^{L} f(x)e^{-in\pi x/L}dx$
Real form: $f(x) = \frac{a_0}{2} + \sum_{n=1}^{\infty}[a_n \cos(n\pi x/L) + b_n \sin(n\pi x/L)]$
Parseval's theorem: $\frac{1}{2L}\int_{-L}^{L}|f(x)|^2dx = \sum_{n=-\infty}^{\infty}|c_n|^2 = \frac{|a_0|^2}{2} + \frac{1}{2}\sum_{n=1}^{\infty}(|a_n|^2 + |b_n|^2)$
Gibbs phenomenon: Fourier series exhibits 9% overshoot near discontinuities
Convergence: Pointwise convergence if f piecewise smooth; uniform convergence if f continuous and periodic

Numerical Differentiation

Forward difference: $f'(x) \approx \frac{f(x+h)-f(x)}{h}$ (error $O(h)$)
Backward difference: $f'(x) \approx \frac{f(x)-f(x-h)}{h}$
Central difference: $f'(x) \approx \frac{f(x+h)-f(x-h)}{2h}$ (error $O(h^2)$)
Second derivative: $f''(x) \approx \frac{f(x+h)-2f(x)+f(x-h)}{h^2}$ (error $O(h^2)$)
Optimal step size: Balance truncation $\propto h^p$ and rounding $\propto h^{-1}$: $h \approx \epsilon^{1/(p+1)}$

Numerical Integration

Newton-Cotes

Trapezoidal: $T(a,b) = \frac{b-a}{2}[f(a)+f(b)]$. Error: $I - T = -\frac{(b-a)^3}{12}f''(\xi)$. Composite: error $-\frac{(b-a)h^2}{12}f''(\xi)$
Simpson's:

$$S(a,b) = \frac{b-a}{6}[f(a) + 4f(c) + f(b)], \quad c = \frac{a+b}{2}.$$

Error: $-\frac{(b-a)^5}{2880}f^{(4)}(\xi)$
Composite Simpson:

$$\int_a^b f(x)\,dx \approx \frac{h}{3}\left[f(x_0) + 4\sum_{jextodd} f(x_j) + 2\sum_{jexteven} f(x_j) + f(x_n)\right].$$

Error: $-\frac{(b-a)h^4}{180}f^{(4)}(\xi)$

Richardson & Romberg

Richardson extrapolation: If $Q(h) = I + \alpha_1 h + \alpha_2 h^2 + \ldots$, then $ildeQ(h) = \frac{2Q(h/2)-Q(h)}{2-1}$ eliminates h term
Romberg integration: Recursive Richardson on trapezoidal rule. $\mathcal{A}_{k,j} = \frac{4^j\mathcal{A}_{k,j-1} - \mathcal{A}_{k-1,j-1}}{4^j - 1}$
Accuracy: $\mathcal{A}_{k,k} = I + O(h_k^{2(k+1)})$ with super-geometric convergence

Gaussian Quadrature

Principle: Choose both nodes x_i and weights ω_i optimally. $Q_n(f) = \sum_{i=1}^n \omega_i f(x_i)$ exact for polynomials of degree $\le 2n-1$
Gauss-Legendre: Nodes are zeros of Legendre polynomial $P_n(x)$ on $[-1,1]$
Gauss-Chebyshev: Nodes are zeros of $T_n(x)$, weight $w(x) = 1/\sqrt{1-x^2}$, $\omega_i = \pi/n$

Error: $\frac{f^{(2n)}(\xi)}{(2n)!}\int_a^b w(x)\omega_n(x)^2dx$ where $\omega_n(x) = \prod_{i=1}^n(x - x_i)$

Adaptive & Gauss

Adaptive Simpson: Apply Simpson on $[a,b]$ and halves $[a,c], [c,b]$. Error estimate: $\frac{S_2 - S_1}{15}$. If $|S_2 - S_1|$ below tolerance, accept S_2
Gauss: Choose nodes x_i as zeros of orthogonal polynomial p_n w.r.t. weight w. $Q_{w,n}(f) = \sum_{i=1}^n \omega_i f(x_i)$ has exactness degree $2n-1$. Error: $\frac{f^{(2n)}(\xi)}{(2n)!}\int_a^b w(x)\omega_n(x)^2dx$

ODEs

Initial Value Problems (IVPs)

Solve

$$y'(t) = f(t, y(t)), \quad t \in [t_0, T], \quad y(t_0) = y_0 \in \mathbb{R}^m.$$

Assume f is Lipschitz in y:

$$\|f(t,y) - f(t,z)\| \le L\|y - z\| \quad \Rightarrow \quad \text{existence/uniqueness of solution.}$$

Discretization:

$$t_n = t_0 + nh, \quad h = \frac{T - t_0}{N}, \quad n = 0, \ldots, N, \quad y_n := y(t_n).$$

One-Step Methods

General form:

$$u_{n+1} = u_n + h\,\Phi(t_n, u_n, h), \quad u_0 = y_0.$$

Local truncation error (LTE):

$$\tau_{n+1} := \frac{y_{n+1} - y_n}{h} - \Phi(t_n, y_n, h).$$

Consistency of order p:

$$\|\tau_{n+1}\| = O(h^p) \quad \Leftrightarrow \quad y_{n+1} - y_n - h\,\Phi(t_n, y_n, h) = O(h^{p+1}).$$

Convergence of order p:

$$\max_{0 \le n \le N}\|u_n - y_n\| = O(h^p).$$

Fundamental relation (one-step methods):
Consistency of order p + (zero-)stability $\Rightarrow$ Convergence of order p.

Basic One-Step Methods

Explicit (Forward) Euler

$$u_{n+1} = u_n + hf(t_n, u_n).$$

Properties:
- Explicit, one function evaluation per step.
- LTE $= O(h^2)$, global error $= O(h)$ (order 1).

Implicit (Backward) Euler

$$u_{n+1} = u_n + hf(t_{n+1}, u_{n+1}) \quad \Rightarrow \quad \text{solve nonlinear eqn for } u_{n+1}.$$

Properties:
- Implicit, LTE $= O(h^2)$, global error $= O(h)$ (order 1).
- A-stable (good for stiff problems).

Taylor Methods (Order q)

Use Taylor expansion of exact solution:

$$y(t_{n+1}) = y(t_n) + hy'(t_n) + \frac{h^2}{2}y''(t_n) + \cdots + \frac{h^q}{q!}y^{(q)}(t_n) + O(h^{q+1}).$$

Define u_{n+1} by truncating at h^q and replacing $y^{(k)}$ by expressions involving f and its derivatives. Requires higher derivatives of f.

Runge–Kutta (RK) Methods

General s-stage RK method:

$$k_i = f\left(t_n + c_i h,\ u_n + h\sum_{j=1}^s a_{ij}k_j\right), \quad i = 1, \ldots, s,$$

$$u_{n+1} = u_n + h\sum_{i=1}^s b_i k_i.$$

Butcher tableau:

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

Explicit RK: $a_{ij} = 0$ for $j \ge i$ (no implicit equations).

Examples:
- Explicit midpoint (order 2):

$$k_1 = f(t_n, u_n), \quad k_2 = f\left(t_n + \tfrac{h}{2}, u_n + \tfrac{h}{2}k_1\right),$$
$$u_{n+1} = u_n + hk_2.$$

- Classical RK4 (order 4):

$$\begin{aligned} k_1 &= f(t_n, u_n), \\ k_2 &= f\left(t_n + \tfrac{h}{2}, u_n + \tfrac{h}{2}k_1\right), \\ k_3 &= f\left(t_n + \tfrac{h}{2}, u_n + \tfrac{h}{2}k_2\right), \\ k_4 &= f(t_n + h, u_n + hk_3), \\ u_{n+1} &= u_n + \tfrac{h}{6}(k_1 + 2k_2 + 2k_3 + k_4). \end{aligned}$$

Absolute Stability

Test equation:

$$y' = \lambda y, \quad \lambda \in \mathbb{C}, \quad y(0) = 1.$$

A one-step method gives

$$u_{n+1} = R(z)\,u_n, \quad z = h\lambda,$$

where $R(z)$ is the *stability function*.
Region of absolute stability:

$$\mathcal{S} := \{z \in \mathbb{C} : |R(z)| \le 1\}.$$

Examples:
- Forward Euler: $R(z) = 1 + z$.
- Backward Euler: $R(z) = \frac{1}{1-z}$ (A-stable).

Linear Multistep Methods (LMM)

General k-step LMM:

$$\sum_{j=0}^k \alpha_j u_{n+j} = h\sum_{j=0}^k \beta_j f(t_{n+j}, u_{n+j}),$$

with constants α_j, β_j not depending on h, n.
Define characteristic polynomials:

$$\rho(\xi) := \sum_{j=0}^k \alpha_j \xi^j, \quad \sigma(\xi) := \sum_{j=0}^k \beta_j \xi^j.$$

Consistency and Order of LMM

Consistency (at least order 1):

$$\rho(1) = 0, \quad \rho'(1) = \sigma(1).$$

Order p:

$$\sum_{j=0}^k \alpha_j \frac{(jh)^m}{m!} - h\sum_{j=0}^k \beta_j \frac{(jh)^{m-1}}{(m-1)!} = O(h^{p+1}) \quad \text{for } m = 0, \ldots, p.$$

Equivalently, a set of algebraic "order conditions" relating α_j, β_j.

Zero-Stability and Convergence

Zero-stability (root condition):
- All roots ξ of $\rho(\xi) = 0$ satisfy $|\xi| \le 1$,
- Any root with $|\xi| = 1$ is simple.

Fundamental theorem (LMM):
Consistency of order p + zero-stability $\Rightarrow$ Convergence of order p.

Adams Methods (LMM)

Explicit Adams–Bashforth (AB)

Use past function values $f_n, f_{n-1}, \ldots$.
- AB1 (Forward Euler): $u_{n+1} = u_n + hf_n$.
- AB2 (order 2): $u_{n+1} = u_n + \frac{h}{2}(3f_n - f_{n-1})$.
- AB3 (order 3): $u_{n+1} = u_n + \frac{h}{12}(23f_n - 16f_{n-1} + 5f_{n-2})$.

Implicit Adams–Moulton (AM)

Use f_{n+1} as well (implicit).

- AM1 (Backward Euler): $u_{n+1} = u_n + hf_{n+1}$.
- AM2 (trapezoidal rule, order 2): $u_{n+1} = u_n + \frac{h}{2}(f_{n+1} + f_n)$.
- AM3 (order 3): $u_{n+1} = u_n + \frac{h}{12}(5f_{n+1} + 8f_n - f_{n-1})$.

Predictor–Corrector Methods

- Predictor (explicit, e.g. AB method): compute a provisional value $\tilde{u}_{n+1}$.
- Corrector (implicit, e.g. AM method): use $\tilde{u}_{n+1}$ inside an AM formula to obtain u_{n+1}.

Example (AB2–AM2 PC method):

$$\text{Predict:}\quad \tilde{u}_{n+1} = u_n + \frac{h}{2}(3f_n - f_{n-1}),$$

$$\text{Correct:}\quad u_{n+1} = u_n + \frac{h}{2}(f(t_{n+1}, \tilde{u}_{n+1}) + f_n).$$

Backward Differentiation Formulas (BDF)

Implicit LMM based on backward differences; general form:

$$\sum_{j=0}^{k} \alpha_j u_{n+j} = h\beta f(t_{n+k}, u_{n+k}),$$

with $\beta \neq 0$ and only f_{n+k} on the right.
Standard BDF k (written with u_{n+1} as newest value):

- BDF1 (Backward Euler, order 1):
$$\frac{u_{n+1} - u_n}{h} = f_{n+1}.$$
- BDF2 (order 2):
$$\frac{3u_{n+1} - 4u_n + u_{n-1}}{2h} = f_{n+1}.$$
- BDF3 (order 3):
$$\frac{11u_{n+1} - 18u_n + 9u_{n-1} - 2u_{n-2}}{6h} = f_{n+1}.$$

Remark: BDF methods are stiffly stable up to order 6; higher-order BDFs are not zero-stable.

IVPs & One-step Methods

IVP: $y'(t) = f(t, y(t))$, $y(t_0) = y_0$. If f continuous and Lipschitz in y, unique solution exists
Euler: $y_{n+1} = y_n + hf(t_n, y_n)$. Local error $O(h^2)$, global $O(h)$. Stable for $h|\lambda| \leq 2$
Heun (RK2): $k_1 = f(t_n, y_n)$; $k_2 = f(t_n + h, y_n + hk_1)$; $y_{n+1} = y_n + \frac{h}{2}(k_1 + k_2)$. Order 2
RK4: $k_1 = f(t_n, y_n)$; $k_2 = f(t_n + \frac{h}{2}, y_n + \frac{h}{2}k_1)$; $k_3 = f(t_n + \frac{h}{2}, y_n + \frac{h}{2}k_2)$; $k_4 = f(t_n + h, y_n + hk_3)$; $y_{n+1} = y_n + \frac{h}{6}(k_1 + 2k_2 + 2k_3 + k_4)$. Local $O(h^5)$, global $O(h^4)$
Implicit Euler: $y_{n+1} = y_n + hf(t_{n+1}, y_{n+1})$. A-stable, order 1

Linear Multistep

General: $\sum_{j=0}^{k} \alpha_j y_{n+j} = h\sum_{j=0}^{k} \beta_j f_{n+j}$ (Explicit if $\beta_k = 0$, implicit otherwise).
Adams-Bashforth: $y_{n+1} = y_n + h\sum_{j=0}^{k-1} \gamma_j f_{n-j}$

- AB1: $y_{n+1} = y_n + hf_n$ (Euler)
- AB2: $y_{n+1} = y_n + h[\frac{3}{2}f_n - \frac{1}{2}f_{n-1}]$
- AB3: $y_{n+1} = y_n + h[\frac{23}{12}f_n - \frac{16}{12}f_{n-1} + \frac{5}{12}f_{n-2}]$

Adams-Moulton: $y_{n+1} = y_n + h\sum_{j=0}^{k} \gamma_j^* f_{n+1-j}$

- AM1: $y_{n+1} = y_n + hf_{n+1}$ (Backward Euler)
- AM2: $y_{n+1} = y_n + \frac{h}{2}(f_{n+1} + f_n)$ (Trapezoidal, A-stable)
- AM3: $y_{n+1} = y_n + \frac{h}{12}(5f_{n+1} + 8f_n - f_{n-1})$

Method of Order q: Local truncation error $\tau_{n+1} = C_q h^{q+1} y^{(q+1)}(\xi) + O(h^{q+2})$ where

$$C_q = \frac{1}{q!}\left(\sum_{j=0}^{k} \alpha_j j^q - q\sum_{j=0}^{k} \beta_j j^{q-1}\right)$$

If $C_0 = C_1 = \cdots = C_{q-1} = 0$ and $C_q \neq 0$, method has order q.
Zero stability: If roots of char. poly $\rho(z) = \sum_{j=0}^{k} \alpha_j z^j = 0$ satisfy $|z_j| \leq 1$ and roots on unit circle have multiplicity 1 (i.e., $\rho'(z_j) \neq 0$ for $|z_j| = 1$), method is zero stable
Convergence: Zero stability + consistency ⇒ convergence (Dahlquist equivalence theorem)
A-stability: Method stable for all $h\lambda$ with $\Re(\lambda) \leq 0$. AM2 (trapezoidal) is A-stable

Optimization (Brief)

Gradient: $\nabla f(x)$ gives steepest ascent direction
Hessian: $H(x)$ contains second derivatives
Steepest descent: $x_{k+1} = x_k - \alpha_k \nabla f(x_k)$ with line search for α_k
Newton: Solve $H(x_k)p_k = -\nabla f(x_k)$, set $x_{k+1} = x_k + p_k$. Requires positive definite H

Error Analysis & Stability

Error sources: Modelling, discretization (truncation), rounding
Floating point: $\mathrm{fl}(a \circ \mathbf{b}) = (a \circ \mathbf{b})(1 + \delta)$, $|\delta| \leq \varepsilon_{\text{mach}}$
Absolute vs relative: Absolute: $|\tilde{x} - x|$, Relative: $\frac{|\tilde{x}-x|}{|x|}$
Algorithm stability: Small perturbations ⇒ small changes in result
Conditioning vs stability: Conditioning = problem sensitivity to data; Stability = algorithm sensitivity