DKE Numerical Mathematics 2017
Formula Sheet

Algebraic equations

Bisection Method f is continuous on $[a,b]$, $\operatorname{sgn}(f(a) \neq \operatorname{sgn}(f(b))$.
Set $c = (a+b)/2$. If $\operatorname{sgn}(f(a)) = \operatorname{sgn}(f(c))$, set $a = c$, else set $b = c$.

Secant method

$$p_{n+1} = p_n - \frac{p_n - p_{n-1}}{f(p_n) - f(p_{n-1})} f(p_n).$$

Newton's method $p_{n+1} = p_n - f(p_n)/f'(p_n)$.

Polynomial Interpolation

Lagrange Form Interpolating polynomial

$$p(x) = \sum_{k=0}^{n} y_k \, l_{n,k}(x) \text{ where } l_{n,k}(x) = \prod_{\substack{j\neq k\\ j=0}}^{n} \left(\frac{x - x_j}{x_k - x_j} \right)$$

Divided Differences $f[x_i] = f(x_i)$; recurrence relation

$$f[x_i, \ldots, x_{i+k}] = \frac{f[x_{i+1}, \ldots, x_{i+k}] - f[x_i, \ldots, x_{i+k-1}]}{x_{i+k} - x_i}$$

Theorem (Divided differences and derivatives) If $f^{(n)}$ is continous on $[a,b]$ and $x_0, \ldots, x_n$ are distinct points in $[a,b]$, there exists $\xi \in [a,b]$ with

$$f[x_0, \ldots, x_n] = f^{(n)}(\xi)/n!$$

Nested Form Let $a_k = f[x_0, \ldots, x_k]$. Then

$$p(x) = a_0 + (x - x_0)\big(a_1 + (x - x_1)\big(a_2 + \cdots + (x - x_{n-2})\big(a_{n-1} + (x - x_{n-1})a_n\big)\big)\big)$$

Theorem (Error of polynomial interpolation) If p is the degree-n polynomial of interpolating f at the $n+1$ distinct nodes $x_0, x_1, \ldots, x_n$ in $[a,b]$, and $f^{(n+1)}$ is continuous, then for each x in $[a,b]$, there is a ξ in (a,b) for which

$$f(x) - p(x) = \frac{1}{(n+1)!} f^{n+1}(\xi) \prod_{i=0}^{n} (x - x_i)$$

If p is the interpolating polynomial of f with $n+1$ equally-spaced nodes, then

$$|f(x) - p(x)| \leq \frac{(b-a)^{n+1}}{4n^{n+1}(n+1)} \max_{x\in[a,b]} |f^{(n+1)}(\xi)|$$

If p is the interpolating polynomial of f with $n+1$ Chebyshev nodes, then

$$|f(x) - p(x)| \leq \frac{(b-a)^{n+1}}{2^{2n+1}(n+1)!} \max_{x\in[a,b]} |f^{(n+1)}(\xi)|$$

Cubic spline interpolation

Knots Interpolate $(x_0, y_0), \ldots, (x_n, y_n)$ with knots x_j. Set $h_j = x_{j+1} - x_j$.

Interpolant $s(x) = s_j(x) = a_j + b_j(x - x_j) + c_j(x - x_j)^2 + d_j(x - x_j)^3$ for $x_j \leq x < x_{j+1}$.

Coefficients

$$a_j = y_j, \; b_j = \frac{1}{h_j}(a_{j+1} - a_j) - \frac{h_j}{3}(2c_j + c_{j+1}), \; d_j = \frac{1}{3h_j}(c_{j+1} - c_j).$$

Knot conditions

$$h_{j-1}c_{j-1} + 2(h_{j-1} + h_j)c_j + h_j c_{j+1} = \frac{3}{h_j}(a_{j+1} - a_j) - \frac{3}{h_{j-1}}(a_j - a_{j-1}).$$

Derivatives

$$s_j'(x_j) = b_j = \frac{1}{h_j}(a_{j+1} - a_j) - \frac{h_j}{3}(2c_j + c_{j+1}); \qquad s_j''(x_j) = 2c_j.$$

Natural spline $s''(x_0) = s''(x_n) = 0$, so $c_0 = c_n = 0$.

Clamped boundary $s'(x_0) = w_0$, $s'(x_n) = w_n$, so $b_0 = w_0$; $b_n = w_n$;

$$2h_0c_0 + h_0c_1 = 3\big(\frac{a_1 - a_0}{h_0} - b_0\big); \quad h_{n-1}c_{n-1} + 2h_{n-1}c_n = 3\big(b_n - \frac{a_n - a_{n-1}}{h_{n-1}}\big).$$

Not-a-knot s''' is continuous at x_1 and x_{n-1}, so

$$h_1c_0 - (h_0 + h_1)c_1 + h_0c_2 = 0; \quad h_{n-1}c_{n-2} - (h_{n-1} + h_{n-2})c_{n-1} + h_{n-2}c_n = 0.$$

Equally-spaced $c_{j-1} + 4c_j + c_{j+1} = \frac{3}{h^2}(a_{j-1} - 2a_j + a_{j+1})$;

$$2c_0 + c_1 = \tfrac{3}{h^2}\big(a_1 - a_0 - hb_0\big); \quad c_{n-1} + 2c_n = \tfrac{3}{h^2}\big(hb_n - a_n + a_{n-1}\big).$$

Differentiation

Two-point forward difference $f'(x) = (f(x+h) - f(x))/h - f''(\xi)h/2$.

Three-point centred difference $f'(x) = (f(x+h) - f(x-h))/2h - f'''(\xi)h^2/6$.

Three-point forward difference
$f'(x) = (-f(x+2h) + 4f(x+h) - 3f(x))/2h + f'''(\xi)h^2/3$.

Five-point centred difference
$f'(x) = \big(-f(x+2h) + 8f(x+h) - 8f(x-h) + f(x-2h)\big)/12h + f^{(5)}(\xi)h^4/30$.

Second derivative $f''(x) = \big(f(x+h) - 2f(x) + f(x-h)\big)/h^2 - f^{(4)}(\xi)\, h^2/12$.

Integration

Midpoint rule $M(f,P) = h \sum_{j=1}^{n} f(c_j)$ where $c_j = (x_{j-1} + x_j)/2 = a + (j - \frac{1}{2})h$.
Error $I(f) - M(f,P) = (b-a)\, h^2 f^{(2)}(\xi)/24$.

Trapezoid rule $T(f,P) = h\big(\frac{1}{2}f(x_0) + f(x_1) + \cdots + f(x_{n-1}) + \frac{1}{2}f(x_n)\big)$.
Error $I(f) - T(f,P) = -(b-a)\, h^2 f^{(2)}(\xi)/12$.

Simpson's rule

$S(f,P) = \frac{1}{3}h\big(f(x_0)+4f(x_1)+2f(x_2)+4f(x_3)+\cdots+2f(x_{n-2})+4f(x_{n-1})+f(x_n)\big)$.

Error $I(f) - S(f,P) = -(b-a)\,h^4\,f^{(4)}(\xi)/180$.

Error estimate $|I(f) - S(f,P_4)| \approx |S(f,P_2) - S(f,P_4)|/15$
$= \big|f(a) - 4f(\frac{3a+b}{4}) + 6f(\frac{a+b}{2}) - 4f(\frac{a+3b}{4}) + f(b)\big|\,(b-a)/180$

where $P_2 = (a, \frac{a+b}{2}, b)$, $P_4 = (a, \frac{3a+b}{4}, \frac{a+b}{2}, \frac{a+3b}{4}, b)$.

Romburg integration $\int_a^b f(x)\,dx \approx R_{n,n}$. Let $h_k = (b-a)/2^{k-1}$.

$$R_{k,1} = T_{2^{k-1}}; \quad R_{k,j} = R_{k,j-1} + (R_{k,j-1} - R_{k-1,j-1})/(4^{j-1} - 1).$$

$$T_1 = \tfrac{b-a}{2}\big(f(a) + f(b)\big); \quad T_{2^k} = \tfrac{1}{2}\big(T_{2^{k-1}} + \tfrac{b-a}{2^{k-1}}\textstyle\sum_{i=1}^{2^{k-1}} f(a + (2i-1)h_k)\big).$$

Differential Equations

Euler's method $w_{i+1} = w_i + hf(t_i, w_i)$. Local error $O(h^2)$; global error $O(h)$.

Error $w_{i+1} - y(t_{i+1}) = \frac{1}{2}\ddot{y}(\tau_i)h^2$ for some τ_i in (t_i, t_{i+1}) if $w_i = y(t_i)$.

Taylor method Local error $O(h^3)$.

$w_{i+1} = w_i + hf(t_i, w_i) + \frac{1}{2}h^2\big(f_{,t}(t_i, w_i) + f_{,y}(t_i, w_i)f(t_i, w_i)\big)$.

Trapezoid (modified Euler) method Local error $O(h^3)$.

$w_{i+1} = w_i + \frac{1}{2}h\big(f(t_i, w_i) + f(t_{i+1}, w_i + hf(t_i, w_i))\big)$.

Midpoint method Local error $O(h^3)$.

$w_{i+1} = w_i + hf(t_i + \frac{1}{2}h, w_i + \frac{1}{2}hf(t, w_i))$.

Ralston's 2nd-order method Local error $O(h^3)$.

$w_{i+1} = w_i + \frac{1}{4}h\big(f(t_i, w_i) + 3f(t_i + \frac{2}{3}h, w_i + \frac{2}{3}hf(t_i, w_i))\big)$.

$k_{i,1} = hf(t_i, w_i)$; $k_{i,2} = hf(t_i + \frac{2}{3}h, w_i + \frac{2}{3}k_{i,1})$; $w_{i+1} = w_i(t) + \frac{1}{4}(k_{i,1} + 3k_{i,2})$.

Heun's 3rd-order method Local error $O(h^4)$.

$k_{i,1} = hf(t_i, w_i)$; $k_{i,2} = hf(t_i + \frac{1}{3}h, w_i + \frac{1}{3}k_{i,1})$; $k_{i,3} = hf(t_i + \frac{2}{3}h, w_i + \frac{2}{3}k_{i,2})$;
$w_{i+1} = w_i(t) + \frac{1}{4}(k_{i,1} + 3k_{i,3})$.

Classical 4th-order Runge-Kutta method Local error $O(h^5)$.

$k_{i,1} = hf(t_i, w_i)$; $k_{i,2} = hf(t_i + \frac{1}{2}h, w_i + \frac{1}{2}k_{i,1})$;
$k_{i,3} = hf(t_i + \frac{1}{2}h, w_i + \frac{1}{2}k_{i,2})$; $k_{i,4} = hf(t_i + h, w_i + k_{i,3})$;
$w_{i+1} = w_i + k_i = w_i + \frac{1}{6}(k_{i,1} + 2k_{i,2} + 2k_{i,3} + k_{i,4})$.

2-stage Adams-Bashforth method Local error $O(h^3)$.

$w_{i+1} = w_i + \frac{1}{2}h\big(3f(t_i, w_i) - f(t_{i-1}, w_{i-1})\big)$.

3-stage Adams-Bashforth method Local error $O(h^4)$.

$w_{i+1} = w_i + \frac{1}{12}h\big(23f(t_i, w_i) - 16f(t_{i-1}, w_{i-1}) + 5f(t_{i-2}, w_{i-2})\big)$.

2-stage Adams-Moulton method Local error $O(h^4)$.

$w_{i+1} = w_i + \frac{1}{12}h\big(5f(t_{i+1}, w_{i+1}) + 8f(t_i, w_i) - f(t_{i-1}, w_{i-1})\big)$.

Bogacki-Shampine adaptive method Local error $O(h^4)$.

$k_1 = hf(t_i, w_i)$; $k_2 = hf(t_i + \frac{1}{2}h, w_i + \frac{1}{2}k_1)$; $k_3 = hf(t_i + \frac{3}{4}h, w_i + \frac{3}{4}k_2)$;
$w_{i+1} = w_n + \frac{2}{9}k_1 + \frac{3}{9}k_2 + \frac{4}{9}k_3$;
$k_4 = hf(t_i + h, w_{i+1})$; $\hat{w}_{i+1} = w_i + \frac{7}{24}k_1 + \frac{1}{4}k_2 + \frac{1}{3}k_3 + \frac{1}{8}k_4$.
Set $q = (\epsilon h/|w_{i+1} - \hat{w}_{i+1}|)^{1/2}$. Step size estimate qh.

Least-squares approximation

Linear least squares $g(x) = ax + b$ fitting data $(x_1, y_1), \ldots, (x_m, y_m)$ where

$$a = (\overline{XY} - \overline{X}\cdot\overline{Y})/(\overline{X^2} - \overline{X}^2); \quad b = \overline{Y} - a\,\overline{X}.$$

Nonlinear least squares If $g(x) = \sum_{k=0}^n c_k\phi_k(x)$ then for $j = 0, \ldots, n$:

$$\sum_{k=0}^{n} c_k \sum_{i=1}^{m} \phi_j(x_i)\phi_k(x_i) = \sum_{i=1}^{m} \phi_j(x_i)y_i.$$

Continuous least squares If $g(x) = \sum_{k=0}^n c_k\phi_k(x)$ fits $f(x)$, then for $j = 0, \ldots, n$:

$$\sum_{k=0}^{n} c_k \int_a^b w(x)\,\phi_j(x)\,\phi_k(x)\,dx = \int_a^b w(x)\,\phi_j(x)\,f(x)\,dx.$$

Least-squares for orthogonal functions

$$c_k = \frac{\int_a^b w(x)\,\phi_k(x)\,f(x)\,dx}{\int_a^b w(x)\,\phi_k(x)^2\,dx} \quad \text{if} \quad \int_a^b w(x)\,\phi_j(x)\,\phi_k(x)\,dx = 0 \text{ for } j \neq k.$$

Generating orthogonal polynomials $\phi_k(x) = (x - B_k)\phi_{k-1}(x) - C_k\phi_{k-2}(x)$

$$\text{with } B_k = \frac{\int_a^b x\,w(x)\,(\phi_{k-1}(x))^2\,dx}{\int_a^b w(x)\,(\phi_{k-1}(x))^2\,dx}, \quad C_k = \frac{\int_a^b x\,w(x)\,\phi_{k-1}(x)\,\phi_{k-2}(x)\,dx}{\int_a^b w(x)\,(\phi_{k-2}(x))^2\,dx}.$$

Legendre polynomials

$$P_0(x) = 1; \quad P_1(x) = x; \quad (k+1)P_{k+1}(x) = (2k+1)xP_k(x) - kP_{k-1}(x).$$

$$\textstyle\int_{-1}^{1} P_j(x)\,P_k(x)\,dx = 0,\ j \neq k, \quad \int_{-1}^{+1} P_k^2(x)\,dx = \frac{k}{2k+1}; \quad c_k = (k + \frac{1}{2})\int_{-1}^{1} P_k(x)\,f(x)\,dx.$$

$$P_0(x) = 1;\ P_1(x) = x;\ P_2(x) = \tfrac{3}{2}x^2 - \tfrac{1}{2};\ P_3(x) = \tfrac{5}{2}x^3 - \tfrac{3}{2}x;\ P_4(x) = \tfrac{35}{8}x^4 - \tfrac{15}{4}x^2 + \tfrac{3}{8}.$$

Chebyshev polynomials $T_k(x) = \cos(k\,\mathrm{acos}(x))$

$$T_0(x) = 1; \quad T_1(x) = x; \quad T_{k+1}(x) = 2xT_k(x) - T_{k-1}(x)$$

$$\int_{-1}^{1} \frac{T_j(x)\,T_k(x)}{\sqrt{1-x^2}}\,dx = \begin{cases} 0,\ j \neq k; \\ \pi/2,\ j = k \neq 0; \\ \pi,\ j = k = 0. \end{cases}$$

Fourier series

$$f(x) \approx \frac{a_0}{2} + \sum_{k=1}^{n}\big(a_k\cos(kx) + b_k\sin(kx)\big);$$

$$a_k = \frac{1}{\pi}\int_{-\pi}^{\pi}\cos(kx)f(x)\,dx; \quad b_k = \frac{1}{\pi}\int_{-\pi}^{\pi}\sin(kx)f(x)\,dx.$$

Discrete Fourier transform If $x_j = (j/m - 1)\pi$ for $j = 0, 1, \ldots, 2m-1$, then

$$f(x) \approx \frac{a_0}{2} + \sum_{k=1}^{n}\big(a_k\cos(kx) + b_k\sin(kx)\big);$$

$$a_k = \frac{1}{m}\sum_{j=0}^{2m-1} f(x_j)\cos(kx_j), \quad b_k = \frac{1}{m}\sum_{j=0}^{2m-1} f(x_j)\sin(kx_j).$$