DACS KEN1540 & BCS2540 Numerical Methods 2025 Formula Sheet

Algebraic equations

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

$$p(x) = \sum_{i=0}^{n} y_i l_i(x) \text{ where } l_i(x) = \prod_{\substack{j \neq i \\ j=0}}^{n} \left(\frac{x - x_j}{x_i - x_j} \right)$$

Divided Differences Recurrence relation

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

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

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

Chebyshev nodes $x_k = \frac{a+b}{2} - \frac{b-a}{2} \cos\big(\frac{2k+1}{2(n+1)}\pi\big)$ for $k = 0, \ldots, n$.

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

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

Theorem (Maximum error of polynomial interpolation) If p is the interpolating polynomial of f with $n+1$ equally-spaced nodes, then for any $x \in [a, b]$,

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

If p is the interpolating polynomial of f with $n+1$ Chebyshev nodes, then for any $x \in [a, b]$,

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

Differential Equations

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

Ralston's 2nd-order method Local error $O(h^3)$.
$w_{i+1} = w_i + \frac{1}{4} h_i \big(f(t_i, w_i) + 3f(t_i + \frac{2}{3}h_i, w_i + \frac{2}{3}h_i f(t_i, w_i))\big)$.
$k_{i,1} = h_i f(t_i, w_i)$; $k_{i,2} = h_i f(t_i + \frac{2}{3}h_i, w_i + \frac{2}{3}k_{i,1})$; $w_{i+1} = w_i + \frac{1}{4}(k_{i,1} + 3k_{i,2})$.

Heun's 3rd-order method Local error $O(h^4)$.
$k_{i,1} = h_i f(t_i, w_i)$; $k_{i,2} = h_i f(t_i + \frac{1}{3}h_i, w_i + \frac{1}{3}k_{i,1})$; $k_{i,3} = h_i f(t_i + \frac{2}{3}h_i, w_i + \frac{2}{3}k_{i,2})$;
$w_{i+1} = w_i + \frac{1}{4}(k_{i,1} + 3k_{i,3})$.

Kutta's 3rd-order method Local error $O(h^4)$.
$k_{i,1} = h_i f(t_i, w_i)$; $k_{i,2} = h_i f(t_i + \frac{1}{2}h_i, w_i + \frac{1}{2}k_{i,1})$; $k_{i,3} = h_i f(t_i + h_i, w_i - k_{i,1} + 2k_{i,2})$;
$w_{i+1} = w_i + \frac{1}{6}(k_{i,1} + 4k_{i,2} + k_{i,3})$.

Classical 4th-order Runge-Kutta method Local error $O(h^5)$.
$k_{i,1} = h_i f(t_i, w_i)$; $k_{i,2} = h_i f(t_i + \frac{1}{2}h_i, w_i + \frac{1}{2}k_{i,1})$;
$k_{i,3} = h_i f(t_i + \frac{1}{2}h_i, w_i + \frac{1}{2}k_{i,2})$; $k_{i,4} = h_i f(t_i + h_i, w_i + k_{i,3})$;
$w_{i+1} = w_i + \frac{1}{6}(k_{i,1} + 2k_{i,2} + 2k_{i,3} + k_{i,4})$.

2-stage Adams-Bashforth method Local error $O(h^3)$.
$w_{i+1} = w_i + (h/2)\big(3f(t_i, w_i) - f(t_{i-1}, w_{i-1})\big)$.

3-stage Adams-Bashforth method Local error $O(h^4)$.
$w_{i+1} = w_i + (h/12)\big(23f(t_i, w_i) - 16f(t_{i-1}, w_{i-1}) + 5f(t_{i-2}, w_{i-2})\big)$.

2-stage Adams-Moulton method Local error $O(h^4)$.
$w_{i+1} = w_i + (h/12)\big(5f(t_{i+1}, w_{i+1}) + 8f(t_i, w_i) - f(t_{i-1}, w_{i-1}))\big)$.

Backward Euler method $w_{i+1} = w_i + h_i\, f(t_{i+1}, w_{i+1})$.

2-stage backward-difference method Local error $O(h^4)$.
$w_{i+1} = \frac{4}{3}w_i - \frac{1}{3}w_{i-1} + \frac{2}{3}hf(t_{i+1}, w_{i+1})$.

Bogacki-Shampine adaptive method Local error $O(h^4)$.
$k_{i,1} = hf(t_i, w_i)$; $k_{i,2} = hf(t_i + \frac{1}{2}h, w_i + \frac{1}{2}k_{i,1})$; $k_{i,3} = hf(t_i + \frac{3}{4}h, w_i + \frac{3}{4}k_{i,2})$;
$w_{i+1} = w_i + \frac{2}{9}k_{i,1} + \frac{3}{9}k_{i,2} + \frac{4}{9}k_{i,3}$;
$k_{i,4} = hf(t_i + h, w_{i+1})$; $\hat{w}_{i+1} = w_i + \frac{7}{24}k_{i,1} + \frac{1}{4}k_{i,2} + \frac{1}{3}k_{i,3} + \frac{1}{8}k_{i,4}$.
Set $q = (\epsilon h / s|w_{i+1} - \hat{w}_{i+1}|)^{1/2}$. Step size estimate qh.

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

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 $M_n(f;a,b) = h\big(f(x_{1/2}) + f(x_{1+1/2}) + \cdots + f(x_{n-1/2})\big)$
Error $\int_a^b f(x)dx - M(f;P) = (b-a)\,h^2\,f^{(2)}(\xi)/24$.

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

Simpson's rule
$$S_n(f;a,b) = \tfrac{1}{3}h\big(f(x_0) + 4f(x_1) + 2f(x_2) + 4f(x_3) + \cdots + 2f(x_{n-2}) + 4f(x_{n-1}) + f(x_n)\big).$$
Error $\int_a^b f(x)dx - S(f;P) = -(b-a)\,h^4\,f^{(4)}(\xi)/180$.

Romburg integration $R_{k,0} = T_{2^k}$; $\quad R_{k,j} = R_{k,j-1} + (R_{k,j-1} - R_{k-1,j-1})/(4^j - 1)$.

Adaptive trapezoid rule Error estimate
$$\Big|\int_a^b f(x)\,dx - T_2(f;a,b)\Big| \lessapprox \tfrac{1}{3}\big|T_2(f;a,b) - T_1(f;a,b)\big| = \tfrac{b-a}{12}\big|f(a) - 2f(\tfrac{a+b}{2}) + f(b)\big|.$$

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 $g(x) = \sum_{i=0}^n c_i\,\phi_i(x)$ then for $i = 0,\ldots,n$:
$$\textstyle\sum_{j=0}^n c_j \sum_{k=1}^m \phi_i(x_k)\,\phi_j(x_k) = \sum_{k=1}^m \phi_i(x_k)\,y_k.$$

Continuous least-squares $g(x) = \sum_{i=0}^n c_i\phi_i(x)$
$$\textstyle\sum_{j=0}^n c_j \int_a^b \phi_i(x)\,\phi_j(x)\,dx = \int_a^b \phi_i(x)\,f(x)\,dx.$$

Orthogonal basis $\int_a^b w(x)\,\phi_i(x)\,\phi_j(x)\,dx = 0$ for $i \neq j$.

Least-squares approximation in orthogonal basis $g(x) = \sum_{i=0}^n c_i\phi_i(x)$
$$\text{with } c_i = \big(\textstyle\int_a^b w(x)\,\phi_i(x)\,f(x)\,dx\big)/\big(\int_a^b w(x)\,(\phi_i(x))^2\,dx\big)$$

Square error for orthogonal functions With $\alpha_k = \int_a^b w(x)\phi_k(x)^2\,dx$,
$$\textstyle\int_a^b w(x)(f(x) - g(x))^2\,dx = \int_a^b w(x)f(x)^2\,dx - \sum_{k=0}^n \alpha_k c_k^2.$$

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
$$P_0(x) = 1; \quad P_1(x) = x; \quad P_k(x) = (2 - 1/k)xP_{k-1}(x) - (1 - 1/k)P_{k-2}(x).$$
$$\textstyle\int_{-1}^1 P_i(x)\,P_j(x)\,dx = 0,\ i \neq j, \quad \int_{-1}^{+1} P_k^2(x)\,dx = \frac{2}{2k+1}.$$

Chebyshev polynomials
$$T_0(x) = 1;\ T_1(x) = x;\ T_{k+1}(x) = 2xT_k(x) - T_{k-1}(x); \quad T_k(x) = \cos(k\,\mathrm{acos}(x)).$$
$$\int_{-1}^1 \frac{T_i(x)\,T_j(x)}{\sqrt{1-x^2}}\,dx = 0,\ i \neq j; \quad \int_{-1}^1 \frac{T_i(x)^2}{\sqrt{1-x^2}} = \begin{cases}\pi,\ i = 0,\\ \pi/2,\ i \neq 0\end{cases}$$

Fourier series
$$f(x) \approx \frac{a_0}{2} + \sum_{k=1}^n a_k\cos(kx) + b_k\sin(kx);$$
$$a_k = \frac{1}{\pi}\int_{-\pi}^{\pi}\cos(kx)f(x)\,dx; \quad b_k = \frac{1}{\pi}\int_{-\pi}^{\pi}\sin(kx)f(x)\,dx.$$

Discrete Fourier transform If $x_i = (i/m)\pi$ for $i = -m, -(m-1), \ldots, m-1$, then
$$a_k = \frac{1}{m}\sum_{i=-m}^{m-1} f(x_i)\cos(kx_i), \quad b_k = \frac{1}{m}\sum_{i=-m}^{m-1} f(x_i)\sin(kx_i).$$

Linear Algebraic Equations

Conditioning $K(A) = ||A|| \cdot ||A^{-1}||$;
$$||\mathbf{x} - \tilde{\mathbf{x}}|| \leq ||A^{-1}|| \cdot ||\mathbf{b} - A\tilde{\mathbf{x}}||; \qquad \frac{||\mathbf{x} - \tilde{\mathbf{x}}||}{||\mathbf{x}||} \leq K(A)\,\frac{||\mathbf{b} - A\tilde{\mathbf{x}}||}{||\mathbf{b}||}$$

LU factorization $PA = LU$; $A\mathbf{x} = \mathbf{b}$ if $L\mathbf{y} = P\mathbf{b}$, $U\mathbf{x} = \mathbf{y}$.

Cholesky factorization $S = U^T\,U = L\,L^T$.

Jacobi method $x_i^{(n+1)} = \big(b_i - \sum_{j\neq i} a_{i,j}x_j^{(n)}\big)/a_{i,i} = \mathbf{x}^{(n)} - D^{-1}\big(A\mathbf{x}^{(n)} - \mathbf{b}\big)$

Gauss-Seidel method $x_i^{(n+1)} = \big(b_i - \sum_{j<i} a_{i,j}x_j^{(n+1)} - \sum_{j>i} a_{i,j}x_j^{(n)}\big)/a_{i,i}$

Successive over-relaxation
$$x_i^{(n+1)} = (1-\omega)x_i^{(n)} + \omega\big(b_i - \textstyle\sum_{j<i} a_{i,j}x_j^{(n+1)} - \sum_{j>i} a_{i,j}x_j^{(n)}\big)/a_{i,i}$$

Conjugate gradient method $\mathbf{x}^{(0)} = \mathbf{0}$, $\mathbf{r}^{(0)} = \mathbf{b} - A\mathbf{x}^{(0)}$; $\mathbf{v}^{(1)} = \mathbf{r}^{(0)}$,
$t^{(k)} = \langle\mathbf{r}^{(k-1)}, \mathbf{r}^{(k-1)}\rangle/\langle\mathbf{v}^{(k)}, A, \mathbf{v}^{(k)}\rangle$, $\mathbf{x}^{(k)} = \mathbf{x}^{(k-1)} + t^{(k)}\mathbf{v}^{(k)}$, $\mathbf{r}^{(k)} = \mathbf{r}^{(k-1)} - t^{(k)}A\mathbf{v}^{(k)}$;
$s^{(k+1)} = \langle\mathbf{r}^{(k)}, \mathbf{r}^{(k)}\rangle/\langle\mathbf{r}^{(k-1)}, \mathbf{r}^{(k-1)}\rangle$, $\mathbf{v}^{(k+1)} = \mathbf{r}^{(k)} + s^{(k+1)}\mathbf{v}^{(k)}$.

Orthogonality and Eigenvalues

Gram-Schmidt orthogonalisation
$$r_{i,i} = ||\mathbf{v}_i||_2,\ r_{j,i} = \mathbf{u}_j \cdot \mathbf{x}_i\ (j < i),\ \mathbf{v}_i = \mathbf{x}_i - \textstyle\sum_{j=1}^{i-1} r_{j,i}\mathbf{u}_j,\ \mathbf{u}_i = \mathbf{v}_i/r_{i,i}.$$

Power method $\mathbf{y}^{(n)} = A\mathbf{x}^{(n)}$, $\mathbf{x}^{(n+1)} = \mathbf{y}^{(n)}/||\mathbf{y}^{(n)}||$; $\quad \mathbf{y}^{(n)}/\mathbf{x}^{(n)} \to \lambda_{\max}$.

Inverse power method $\mathbf{y}^{(n)} = (A - \mu I)^{-1}\mathbf{x}^{(n)}$, $\mathbf{x}^{(n+1)} = \mathbf{y}^{(n)}/||\mathbf{y}^{(n)}||$.

Householder matrix $H = I - 2\mathbf{v}\mathbf{v}^T/\mathbf{v}^T\mathbf{v}$; $\quad H = I - 2\mathbf{u}\mathbf{u}^T$ if $||\mathbf{u}||_2 = 1$.

Givens rotation ($\mathbf{2} \times \mathbf{2}$) $G = \begin{pmatrix}\cos\theta & -\sin\theta\\ \sin\theta & \cos\theta\end{pmatrix} = \begin{pmatrix}a & -b\\ b & a\end{pmatrix}$ where $a^2 + b^2 = 1$.

Upper Hessenburg If $\alpha = \big(\sum_{i=2}^n a_{i,1}^2\big)^{1/2}$, $v_1 = 0$, $v_2 = a_{2,1} \pm \alpha$, $v_i = a_{i,1}$ $(i \geq 3)$,
$H = I - 2\mathbf{v}\mathbf{v}^T/\mathbf{v}^T\mathbf{v}$, $A' = H^T AH$. Then $A'_{i,1} = 0$ for $i \geq 3$.