

## 1. (Gaussian Elimination and Schur Complement)

Let  $A \in \mathbb{R}^{m \times m}$  be nonsingular. Suppose that for each  $k$  with  $1 \leq k \leq m$ , the upper-left  $k \times k$  block of  $A$  is nonsingular. Assume that  $A$  is written in the block form  $A = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix}$  where  $A_{11}$  is  $n \times n$  and  $A_{22}$  is  $(m - n) \times (m - n)$ .

(a) Verify the formula

$$\begin{pmatrix} I & 0 \\ -A_{21}A_{11}^{-1} & I \end{pmatrix} \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} = \begin{pmatrix} A_{11} & A_{12} \\ 0 & A_{22} - A_{21}A_{11}^{-1}A_{12} \end{pmatrix}$$

for “elimination” of the block  $A_{21}$ . The matrix  $A_{22} - A_{21}A_{11}^{-1}A_{12}$  is known as the *Schur complement* of  $A_{11}$  in  $A$ .

(b) Suppose now that  $A_{21}$  is eliminated row by row by means of  $n$  steps of Gaussian elimination without pivoting:

$U = A, L = I$ <p>for <math>k = 1</math> to <math>n</math></p> <p>for <math>j = m - n + 1</math> to <math>m</math></p> $l_{jk} = u_{jk}/u_{kk}$ $u_{j,k:m} = u_{j,k:m} - l_{jk}u_{k,k:m}$
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Show that the bottom-right  $(m - n) \times (m - n)$  block of the result is again  $A_{22} - A_{21}A_{11}^{-1}A_{12}$ .

## 2. (Exponential Interpolation)

Some modeling considerations have mandated a search for a function

$$u(x) = c_0 e^{c_1 x + c_2 x^2}$$

where the unknown coefficients  $c_1$  and  $c_2$  are expected to be nonpositive. Given are data pairs to be interpolated,  $(x_0, z_0)$ ,  $(x_1, z_1)$ , and  $(x_2, z_2)$ , where  $z_i > 0$ ,  $i = 0, 1, 2$ . Thus, we require  $u(x_i) = z_i$ .

The function  $u(x)$  is not linear in its coefficients, but  $v(x) = \ln(u(x))$  is linear in its.

Find a quadratic polynomial  $v(x)$  that interpolates appropriately defined three data pairs, and then give a formula for  $u(x)$  in terms of the original data.

3. The gradient method (the steepest descent method) for solving a linear system,  $\mathbf{Ax} = \mathbf{b}$ , where  $\mathbf{A}$  is a real and symmetric positive definite  $n \times n$  matrix, is given as follows:

<p>Given initial guess <math>\mathbf{x}_0</math>, for <math>k \geq 0</math>, we compute</p> <p>(i) <math>\mathbf{g}_k = \mathbf{Ax}_k - \mathbf{b}</math>,</p> <p>(ii) <math>\rho_k = \mathbf{g}_k^t \mathbf{g}_k / \mathbf{g}_k^t \mathbf{A} \mathbf{g}_k</math>,</p> <p>(iii) <math>\mathbf{x}_{k+1} = \mathbf{x}_k - \rho_k \mathbf{g}_k</math>.</p>
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(a) Verify that  $\mathbf{g}_k \cdot \mathbf{g}_{k+1} = 0$  for  $k = 0, 1, \dots$

(b) Via the result in (a), can we prove that the gradient method always converges at most in  $n$  iterations? Justify your answer.

(c) For the following descent method,

<p>Given initial guess <math>\mathbf{x}_0</math>, for <math>k \geq 0</math>, we compute</p> <p>(i) <math>\mathbf{g}_k = \mathbf{Ax}_k - \mathbf{b}</math>,</p> <p>(ii) <math>\mathbf{x}_{k+1} = \mathbf{x}_k - \alpha \mathbf{g}_k</math>,</p>
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find the conditions on  $\alpha$  so that the revised descent method converges.

4. For computing the integral  $\int_{-\pi/2}^{\pi/2} \cos(x)f(x) dx$ , find a two point quadrature formula

$$S_2(f) = c_1 f(x_1) + c_2 f(x_2),$$

which is exact for all polynomials of a maximal possible degree.

5. The modified Euler method for the approximation of the Cauchy problem is defined as:

$$\begin{cases} u_{n+1} = u_n + hf(t_{n+1}, u_n + hf(t_n, u_n)) \\ u_0 = y_0 \end{cases}$$

Find the region of stability for this method when applied to the test problem

$$\begin{cases} y'(t) = \lambda y(t), & t > 0 \\ y(0) = 1, \end{cases}$$

where  $\lambda \in \mathbb{R}^-$ .

6. Consider the matrix

$$\begin{bmatrix} 2 & -1 \\ -1 & 2 \end{bmatrix}.$$

Is it possible to find the Cholesky factorization of  $A$ ? If so, find the unique upper triangular matrix  $H$  such that  $A = H^T H$ .

Assume that you have computed the upper triangular matrix affected by rounding errors  $\tilde{H}$  with  $\tilde{H}^T \tilde{H} = A + \delta A$ . Find an estimate of  $\|\delta A\|_2$  for the given matrix  $A$ .

7. Find all the functions  $f(x) = a_2 x^2 + a_1 x + a_0$  whose polynomial of best approximation of degree 1 on the interval  $[2, 4]$  is  $p_1^*(x) = 0$ .

8. **(Interpolation and Weak Line Search)**

A popular technique arising in methods for minimizing functions in several variables involves a *weak line search*, where an approximate minimum  $x^*$  is found for a function in one variable,  $f(x)$ , for which the values of  $f(0)$ ,  $f'(0)$ , and  $f(1)$  are given. The function  $f(x)$  is defined for all nonnegative  $x$ , has a continuous second derivative, and satisfies  $f(0) < f(1)$  and  $f'(0) < 0$ . We then interpolate the given values by a quadratic polynomial and set  $x^*$  as the minimum of the interpolant.

- Find  $x^*$  for the values  $f(0) = 1$ ,  $f'(0) = -1$ ,  $f(1) = 2$ .
- Show that the quadratic interpolant has a unique minimum satisfying  $0 < x^* < 1$ . Can you show the same for the function  $f$  itself?

9. **(Gaussian Elimination)**

Given an  $m$ -by- $m$  nonsingular matrix  $A$ , how do you efficiently solve the following problems, using Gaussian elimination with partial pivoting?

- Solve the linear system  $A^k x = b$ , where  $k$  is a positive integer.
- Compute  $\alpha = c^T A^{-1} b$ .
- Solve the matrix equation  $AX = B$ , where  $B$  is  $m$ -by- $n$ .

You should: (1) describe your algorithms, (2) present them in pseudocode (using a Matlab-like language), and (3) give the required flops.

10. Let  $\mathbf{A}$  be a strictly diagonally dominant  $n \times n$  matrix. Show that the Jacobi iterative method generates a convergent sequence of approximate solutions when applying it to solve the linear system  $\mathbf{Ax} = \mathbf{B}$  for any initial guess  $\mathbf{x}_0$ .

11. Find solutions of the two systems of equations:

$$\begin{cases} x_1 + 3x_2 = 4 \\ x_1 + 3.00001x_2 = 4.00001 \end{cases} \iff A_1x = b.$$

and

$$\begin{cases} y_1 + 3y_2 = 4 \\ y_1 + 2.99999y_2 = 4.00001 \end{cases} \iff A_2y = b.$$

Compute  $\|A_1 - A_2\|_\infty$  and  $\|x - y\|_\infty$ . Using the notion of the matrix condition number, explain why  $\|x - y\|_\infty$  is much larger than  $\|A_1 - A_2\|_\infty$ .

12. Consider the following two fixed point methods to find the root  $z \approx 0.6$  of the equation  $x + \ln x = 0$ :

$$1) x_{n+1} = -\ln x_n, \quad 2) x_{n+1} = \exp(-x_n).$$

Study the convergence of the methods and argue which one you would prefer.

13. Find the polynomial of best approximation  $p_1^*(x)$  for  $f(x) = |x|$  on  $[-1, 3]$ .

14. For the solution of the linear system  $A\mathbf{x} = \mathbf{b}$  with

$$A = \begin{bmatrix} 1 & 2 \\ 2 & 3 \end{bmatrix}, \quad \mathbf{b} = \begin{bmatrix} 3 \\ 5 \end{bmatrix},$$

consider the following iterative method: given  $\mathbf{x}^{(0)} \in \mathbb{R}^2$ , find

$$\mathbf{x}^{(k+1)} = B(\theta)\mathbf{x}^{(k)} + \mathbf{g}(\theta) \quad \text{for } k \geq 0,$$

where  $\theta$  is a real parameter and

$$B(\theta) = \frac{1}{4} \begin{bmatrix} 2\theta^2 + 2\theta + 1 & -2\theta^2 + 2\theta + 1 \\ -2\theta^2 + 2\theta + 1 & 2\theta^2 + 2\theta + 1 \end{bmatrix}, \quad \mathbf{g} = \begin{bmatrix} \frac{1}{2} - \theta \\ \frac{1}{2} - \theta \end{bmatrix}.$$

Address the following points:

- (a) Check that the method is consistent  $\forall \theta \in \mathbb{R}$ .
- (b) Determine the values of  $\theta$  for which the method is convergent.
- (c) Find the optimal value of  $\theta$ , i.e. the value of  $\theta$  for which  $\rho(B(\theta))$  is minimum.

15. Consider the function  $f(x) = \ln(x) + 6\sqrt{x} - 9$ , which has a zero on the interval  $[1, 2]$ . Given two fixed point methods  $x = \phi_i(x)$ ,  $i = 1, 2$ , where

$$\phi_1(x) = \frac{(9 - \ln(x))^2}{36} \quad \text{and} \quad \phi_2(x) = e^{9-6\sqrt{x}},$$

verify that the zero of  $f$  is a fixed point for  $\phi_1$  and  $\phi_2$ . Which method would you use to calculate the zero of  $f$ ? Justify your answer.

16. Consider  $f(x) = \sin(\pi x)$  on the interval  $[-1, 1]$ . Find the polynomial  $\Pi_2 f(x)$  interpolating  $f(x)$  at the Chebyshev nodes.

17. Given a nonsingular matrix  $A \in \mathbb{R}^{n \times n}$ , consider the preconditioned nonstationary Richardson method:

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} + \alpha_k P^{-1}(\mathbf{b} - A\mathbf{x}^{(k)}),$$

where  $P \in \mathbb{R}^{n \times n}$  is nonsingular. Find a formula for the parameter  $\alpha_k$  such that  $\mathbf{x}^{(k+1)}$  minimizes the Euclidean norm of the preconditioned residual  $\|P^{-1}(A\mathbf{y} - \mathbf{b})\|_2$  among all vectors  $\mathbf{y} \in \mathbb{R}^n$  of the form:

$$\mathbf{y} = \mathbf{x}^{(k)} + \alpha P^{-1}(\mathbf{b} - A\mathbf{x}^{(k)}).$$

18. **(Cholesky Factorization)**

Given an  $m$ -by- $m$  symmetric and positive definite matrix  $A$ , how do you efficiently solve the following problems, using the Cholesky factorization of  $A$ ?

- (a) Solve the linear system  $A^k x = b$ , where  $k$  is a positive integer.
- (b) Compute  $\alpha = c^T A^{-1} b$ .
- (c) Solve the matrix equation  $AX = B$ , where  $B$  is  $m$ -by- $n$ .

You should: (1) describe your algorithms, (2) present them in pseudocode (using a Matlab-like language), and (3) give the required flops.

19. **(Orthogonal Polynomials)**

Let  $\phi_0(x), \phi_1(x), \phi_2(x), \dots$  be a sequence of orthogonal polynomials on an interval  $[a, b]$  with respect to a positive weight function  $w(x)$ . Let  $x_1, \dots, x_n$  be the  $n$  zeros of  $\phi_n(x)$ ; it is known that these roots are real and  $a < x_1 < \dots < x_n < b$ .

- (a) Show that the Lagrange polynomials of degree  $n - 1$  based on these points are orthogonal to each other, so we can write

$$\int_a^b w(x) L_j(x) L_k(x) dx = 0, \quad j \neq k,$$

where

$$L_j(x) = \prod_{k \neq j} \frac{(x - x_k)}{(x_j - x_k)}, \quad 1 \leq j \leq n.$$

- (b) For a given function  $f(x)$ , let  $y_k = f(x_k)$ ,  $k = 1, \dots, n$ . Show that the polynomial  $p_{n-1}(x)$  of degree at most  $n - 1$  that interpolates the function  $f(x)$  at the zeros  $x_1, \dots, x_n$  of the orthogonal polynomial  $\phi_n(x)$  satisfies

$$\|p_{n-1}\|^2 = \sum_{k=1}^n y_k^2 \|L_k\|^2$$

in the weighted least squares norm. This norm for any suitably integrable function  $g(x)$  is defined by

$$\|g\|^2 = \int_a^b w(x) [g(x)]^2 dx.$$

- 20. Given a function  $f(x) = \sin x$  on  $[-\pi, \pi]$ , we want to approximate  $f$  by Lagrange interpolating polynomials  $P_n(x)$  with equally spaced nodes,  $x_i = -\pi + \frac{2i\pi}{n}$ , for  $i = 0, 1, \dots, n$ , i.e., the supporting pairs are  $\{(x_i, f(x_i))\}_{i=0}^n$ , and we have  $P_n(x_i) = f(x_i)$ , for  $i = 0, 1, \dots, n$ . Does  $P_n(x)$  converge to  $f(x)$  on  $[-\pi, \pi]$  as  $n \rightarrow \infty$ ?

- 21. We consider the initial value problem

$$\begin{cases} y'(t) = f(t, y(t)), & t > 0 \\ y(0) = \alpha. \end{cases}$$

Define  $h > 0$  and  $t_i = ih$  for  $i = 0, 1, \dots$ . Let  $w_i$  be the approximate solution of  $y(t_i)$  obtained with the following Trapezoidal method:

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

for  $i = 0, 1, \dots$ , and  $w_0 = \alpha$ . Find the stability condition on  $h$  so that the modified Trapezoidal method is stable when applying it to the stiff problem

$$\begin{cases} y' = -\lambda y, \\ y(0) = \alpha \end{cases}$$

with positive  $\lambda$ .

22. Find a parameter  $\tau \in \mathbb{R}$  such that the Richardson method

$$x^{k+1} = x^k - \tau(Ax^k - b)$$

converges to a solution of  $Ax = b$ , if

$$A = \begin{pmatrix} 3 & 1 & & & \mathbf{0} \\ 1 & 3 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & & 1 & 3 & 1 \\ \mathbf{0} & & & & 1 & 3 \end{pmatrix} \in \mathbb{R}^{N \times N}.$$

23. Check if the following scheme approximates the equation  $y' = f(x, y)$ :

$$\frac{1}{2h}(y_k - y_{k-2}) = \frac{1}{2}(f(x_k, y_k) + f(x_{k-2}, y_{k-2})).$$

Find the stability region for the scheme.

24. Consider the matrix

$$A = \begin{bmatrix} \epsilon & 1 \\ 1 & 0 \end{bmatrix}$$

where  $\epsilon$  is a very small number (e.g.,  $10^{-15}$ ). Prove that the matrices  $L$  and  $U$  have entries very large in absolute value.

If rounding errors are accounted for, the  $LU$  factorization yields matrices  $\widehat{L}$  and  $\widehat{U}$ , such that  $A + \delta A = \widehat{L}\widehat{U}$ . Explain why for the given matrix  $A$ , we do not have control on the size of the perturbation matrix  $\delta A$ .

Finally, check that by using GEM with pivoting we have control on the size of  $\delta A$ .

25. To compute numerically the integral  $I(f) = \int_0^2 f(x) dx$  with  $f(x) = \frac{1}{1+x}$ , consider the composite quadrature formula:

$$I_c(f) = \frac{1}{10}[f(0) + 2f(0.2) + 2f(0.4) + \dots + 2f(1.8) + f(2)].$$

Find an estimate for:

$$|I(f) - I_c(f)|.$$

26. Let  $\{P_0(x), P_1(x), \dots, P_n(x)\}$  be the set of Legendre polynomials satisfying the following properties:

- i. For each  $n$ ,  $P_n(x)$  is a polynomial of degree  $n$ .
- ii.  $\int_{-1}^1 P(x)P_n(x) dx = 0$  for any polynomial  $P(x)$  of degree less than  $n$ .

Suppose that  $x_1, x_2, \dots, x_n$  are the roots of the  $n^{\text{th}}$  Legendre polynomial  $P_n(x)$  and

$$c_i = \int_{-1}^1 \prod_{\substack{j=1 \\ j \neq i}}^n \frac{x - x_j}{x_i - x_j} dx$$

for  $i = 1, 2, \dots, n$ .

- (a) Show that if  $P(x)$  is any polynomial of degree less than  $2n$ , then

$$\int_{-1}^1 P(x) dx = \sum_{i=1}^n c_i P(x_i).$$

(b) For  $n = 2$ , we have

$$\int_{-1}^1 P(x) dx = P(x_1) + P(x_2),$$

for any polynomial  $P(x)$  of degree at most three with  $x_1 = -\sqrt{3}/3$  and  $x_2 = \sqrt{3}/3$ . Verify that

$$\int_{-1}^1 \int_{-1}^1 P(x, y) dx dy = P(x_1, x_1) + P(x_1, x_2) + P(x_2, x_1) + P(x_2, x_2)$$

where the degree of  $P(x, y)$  in  $x$  (resp.,  $y$ ) is at most three (resp., three).

27. Let  $\mathbf{A}$  be a real and symmetric positive definite  $n \times n$  matrix. The linear system  $\mathbf{Ax} = \mathbf{b}$  is solved by the conjugate gradient method as follows:

Given initial guess  $\mathbf{x}_0$ , we compute  
 $\mathbf{g}_0 = \mathbf{Ax}_0 - \mathbf{b}$ , and  $\mathbf{w}_0 = -\mathbf{g}_0$ .  
 For  $k \geq 0$ , knowing  $\mathbf{x}_k$  we compute  $\mathbf{x}_{k+1}$  as follows:

- (a).  $\rho_k = \mathbf{g}_k^t \mathbf{g}_k / \mathbf{w}_k^t \mathbf{A} \mathbf{w}_k$ ,
- (b).  $\mathbf{x}_{k+1} = \mathbf{x}_k + \rho_k \mathbf{w}_k$ ,
- (c).  $\mathbf{g}_{k+1} = \mathbf{g}_k + \rho_k \mathbf{A} \mathbf{w}_k$ ,
- (d).  $\beta_k = \mathbf{g}_{k+1}^t \mathbf{g}_{k+1} / \mathbf{g}_k^t \mathbf{g}_k$ ,
- (e).  $\mathbf{w}_{k+1} = -\mathbf{g}_{k+1} + \beta_k \mathbf{w}_k$

Suppose that with a given initial guess  $\mathbf{x}_0$ , the initial error  $\mathbf{x}_0 - \mathbf{x}$  has an expression of the form

$$\mathbf{x}_0 - \mathbf{x} = \sum_{i=1}^n c_i \mathbf{v}_i = \mathbf{A}^{-1} \mathbf{g}_0$$

where  $\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_n$  are eigenvectors of  $\mathbf{A}$ . Let  $m$  be the number of nonzero coefficients in the set  $\{c_1, \dots, c_n\}$ . Prove that the conjugate gradient method converges in  $m$  iterations with the initial guess  $\mathbf{x}_0$ .

28. To obtain an approximate solution of the initial value problem

$$y'(x) = 0, \quad y(0) = \alpha,$$

we apply the following linear multistep method:

$$\eta_{j+2} = -9\eta_{j+1} + 10\eta_j + \frac{h}{2}(13f(x_{j+1}, \eta_{j+1}) + 9f(x_j, \eta_j)), \quad j \geq 0.$$

Let the starting values be  $\eta_0 = \alpha$  and  $\eta_1 = \alpha + \epsilon$  ( $\epsilon =$  machine precision). What values  $\eta_j$  are to be expected for arbitrary  $h$ ? Is this linear multistep method convergent?

29. **(Runge-Kutta Method and Numerical Solution of ODEs)**

Consider Heun's method

$$y_{n+1} = y_n + \frac{h}{2}[f_n + f(t_{n+1}, y_n + hf_n)].$$

- (a) Show that Heun's method is an explicit two-stage Runge-Kutta method.
- (b) Prove that Heun's method has order 2 with respect to  $h$ .
- (c) Sketch the region of absolute stability of the method in the complex plane.