Homework Problems for the Proseminar in Numerical Mathematics I
Summer Semester 2009

1. For $\Omega = (0,1)$ let $u \in C^2(\bar{\Omega})$ be a solution to the boundary value problem,

$$\begin{cases} -Tu'' &= f, \quad \Omega \\ u &= 0, \quad \partial\Omega \end{cases}$$

for $T > 0$ and $f \in C^0(\bar{\Omega})$, and show that

$$\delta(x,h) = -T\frac{u(x+h) - 2u(x) + u(x-h)}{h^2} - f(x)$$

satisfies $\delta(x,h) = \mathcal{O}(h^2)$.

2. Consider images defined on a domain $\Omega \subset \boldsymbol{R}^N$. Suppose that $\tilde{u}$ is a measured image corresponding to an exact image $u^\star$ according to $\tilde{u} = Ku^\star + \nu$, where ν represents noise and K represents blurring. Specifically, the operator K is a convolution,

$$Ku = \kappa * u, \quad [Ku](x) = \int_\Omega \kappa(x-y)u(y)dy$$

and κ is the so-called point-spread function. For instance,

$$\kappa(z) = \begin{cases} (2\epsilon)^{-N}, & z \in [-\epsilon,\epsilon]^N \\ 0, & \text{else} \end{cases}$$

is a possibility. In any case, assume that κ satisfies $\kappa(z) = \kappa(-z)$ and show that:

$$\int_\Omega vKudx = \int_\Omega uKvdx$$

holds for all sufficiently regular u and v. Now the image $u^\star$ is estimated from the measurement $\tilde{u}$ by minimizing the functional:

$$J(u) = \int_\Omega [Ku - \tilde{u}]^2 dx + \int_\Omega \phi(|\nabla u|^2)dx$$

For instance, $\phi(s) = \mu s^{p/2}$, $\mu > 0$, $1 \le p \le 2$, is a possibility. Show that the necessary optimality condition for a minimizer u is:

$$\begin{cases} -\nabla \cdot [\phi'(|\nabla u|^2)\nabla u] + K^2 u &= K\tilde{u}, \quad \Omega \\ \partial u/\partial n &= 0, \quad \partial\Omega \end{cases}$$

3. Consider the case in the last problem that $\Omega = (0,1)$ $(N = 1)$ is discretized by the grid with cells having centers $x_i = h(i - 1/2)$, $i = 1,\ldots,n$, $h = 1/n$. Also suppose κ is given by:

$$\kappa(z) = \begin{cases} 1/(2h), & z \in [-h,h] \\ 0, & \text{else} \end{cases}$$

and show that with an appropriate integration rule, Ku can be approximated by:

$$[Ku](x_i) \approx \frac{u_{i+1} + 2u_i + u_{i-1}}{4}, \quad 1 < i < N, \quad [Ku](x_1) \approx \frac{3u_1 + u_2}{4}, \quad [Ku](x_n) \approx \frac{u_{n-1} + 3u_n}{4}$$

Denote this discretization by $[Ku](x_i) \approx (K_h U)_i$ where $U = \{u_i\}$. Now assume that $\phi(s) = \mu s$ with $\mu > 0$ and develop a discretization of the optimality condition in example 2 for which the coefficient matrix A_h is symmetric and positive definite.

Note that the corresponding operator $A = -\mu\Delta + K^2$ with a domain

$$\mathcal{D}(A) = \{\text{sufficiently smooth } u \text{ satisfying } \partial u/\partial n = 0 \text{ on } \partial\Omega\}$$

satisfies the counterparts to the desired properties of A_h:

$$\int_\Omega vAudx = \int uAvdx, \quad \forall u, v \in \mathcal{D}(A)$$

$$\int_\Omega uAudx = \int_\Omega \left(\mu|u'|^2 + |Ku|^2\right) dx > 0, \quad u \neq 0.$$

4. Newton's method for minimizing J in example 2 takes the form:

$$\left\{\begin{array}{rcll} \dfrac{\delta^2 J}{\delta u^2}(u_k; \bar{u}, \delta u) & = & -\dfrac{\delta J}{\delta u}(u_k; \bar{u}), & \forall \bar{u} \text{ (sufficiently smooth)} \\ u_{k+1} & = & u_k + \alpha\delta u & \end{array}\right. \qquad k = 1, 2, \ldots$$

for a given step size $\alpha > 0$. By neglecting ϕ'', a modified Newton's method is given by:

$$\left\{\begin{array}{rcll} -\nabla\cdot[\phi'(|\nabla u_k|^2)\nabla\delta u] + K^2\delta u & = & \nabla\cdot[\phi'(|\nabla u_k|^2)\nabla u_k] - K^2 u_k + K\tilde{u}, & \Omega \\ \partial\delta u/\partial n & = & 0, & \partial\Omega \\ u_{k+1} & = & u_k + \alpha\delta u, \quad k = 1, 2, \ldots & \end{array}\right.$$

For $N = 1$ and $\Omega = (0, 1)$ develop a symmetric discretization of this problem using the discretization K_h given in example 3. (Hint: Express $\phi'(|\nabla u_k|^2)\nabla\delta u$ at cell interfaces before differencing with $\nabla\cdot$) Write a MATLAB code to implement this method for $\phi(s) = \mu s^{p/2}$, $\mu > 0$, $1 < p \leq 2$. As a test case, let $u^\star$ be a step function and set $\tilde{u} = Ku^\star + \nu$ according to a certain noise level ν. Then determine the parameters μ and p for which the numerical reconstruction U comes closest to $U^\star = \{u^\star(x_i)\}$.

5. Now for the functional J in example 2, let $\phi = 0$ and consider the following spectral approach to estimating $u^\star$ from $\tilde{u}$. Let $K_h = PSQ^{\mathrm{T}}$ be the singular value decomposition of K_h, where P and Q are unitary matrices and S is a diagonal matrix of the singular values $\{\sigma_i\}$ of K_h. (Note that the squared singular values are the eigenvalues of $K_h^{\mathrm{T}}K_h = (QSP^{\mathrm{T}})(PSQ^{\mathrm{T}}) = QS^2Q^{\mathrm{T}}$. Also, in the present case, the symmetry of K_h means that $P = Q$ holds, and the singular values of K_h are also the eigenvalues.) Without regularization, the minimizer of $\|K_hU - \tilde{U}\|_{\ell_2}^2$ is given by $U = K_h^{-1}\tilde{u} = QS^{-1}P^{\mathrm{T}}\tilde{U}$, where $\tilde{U} = \{\tilde{u}_i\}$. Define a regularized estimator by

$$U_\chi = QS_\chi^{-1}P^{\mathrm{T}}\tilde{U}$$

where:

$$S_\chi^{-1} = \mathrm{diag}\left\{\frac{(\sigma_i > \chi\cdot\bar{\sigma})}{\sigma_i}\right\}, \quad \bar{\sigma} = \max\{\sigma_i\}$$

That is, the ith entry on the diagonal of S_χ^{-1} is $1/\sigma_i$ when $\sigma_i > \chi\cdot\bar{\sigma}$ holds, and otherwise the ith entry is zero. Write a MATLAB code to implement this spectral estimation method and determine the value of χ for which the reconstruction U comes closest to $U^\star$. Compare these results with those of the previous example.

6. Consider the model transport problem for $\Omega = (0, 1)$, $\Gamma = \{0\} \subset \partial\Omega$,

$$\left\{\begin{array}{rcllr} u_t + cu + fu_x & = & du_{xx}, & \Omega, & t > 0 \\ u & = & 0, & \Gamma, & t > 0 \\ u_x & = & 0, & \partial\Omega\backslash\Gamma, & t > 0 \\ u & = & u_0, & \Omega, & t = 0 \end{array}\right.$$

where $c, f, d > 0$. This problem can be expressed as $u_t = Au$ for the operator $Au = du_{xx} - fu_x - cu$ with a domain

$$\mathcal{D}(A) = \{\text{sufficiently smooth } u \text{ satisfying } u = 0, \Gamma, u_x = 0, \partial\Omega \backslash \Gamma\}$$

Note that A satisfies

$$\int_\Omega uAudx = duu_x|_0^1 - \int_\Omega [du_x^2 + \tfrac{1}{2}f(u^2)_x + cu^2]dx =$$

$$-\tfrac{1}{2}fu^2|_0^1 - \int_\Omega [du_x^2 + cu^2]dx = -\tfrac{1}{2}fu^2(1) - \int_\Omega [du_x^2 + cu^2]dx < 0, \quad u \neq 0.$$

Develop a spatial discretization A_h of A which analogously has only eigenvalues with negative real parts. (Hint: Discretize fu_x with backward differences when $f > 0$. If the problem were turned around with $f < 0$, $u_x(0) = 0$ and $u(1) = 0$, one would discretize fu_x with forward differences. This manner of differencing flux terms is called *upwinding.*)

Let $u_t = Au$ be discretized temporally, $U_i^n \approx u(x_i, t^n)$, $t^n = n\tau$, using the forward Euler method,

$$\frac{U^{n+1} - U^n}{\tau} = A_h U_h^n, \qquad U^{n+1} = [I + \tau A_h]U_h^n$$

Show that a stability condition, $\|U^{n+1}\|_\infty \leq \|U^n\|_\infty$, holds when the spatial and temporal discretization parameters satisfy the highly restrictive condition that τh^{-2} be sufficiently small and in particular bounded independently of τ and h.

On the other hand, when the backward Euler method is used for temporal discretization,

$$\frac{U^{n+1} - U^n}{\tau} = A_h U_h^{n+1}, \qquad [I - \tau A_h]U^{n+1} = U_h^n$$

the stability condition $\|U^{n+1}\|_2 \leq \|U^n\|_2$ holds independently of τh^{-2}.

7. For $A \in \boldsymbol{R}^{N\times N}$ and $b, x, x^\star = A^{-1}b \in \boldsymbol{R}^N$ show that the error $x - x^\star$ in an induced norm $\|\cdot\|$ can be estimated in terms of the residual $b - Ax$ according to:

$$\frac{\|x - x^\star\|}{\|x^\star\|} \leq \kappa(A)\frac{\|b - Ax\|}{\|b\|}$$

where $\kappa(A) = \|A\|\|A^{-1}\|$ is the condition number of A.

8. Show that if $\rho(M) \geq 1$ then there are x_0 and c such that the iteration $x_{k+1} = Mx_k + c$ fails to converge.

9. Let $M \in \boldsymbol{R}^{N\times N}$. Prove that the iteration $x_{k+1} = Mx_k + c$ converges for all $c \in \boldsymbol{R}^N$ and for all $x_0 \in \boldsymbol{R}^N$ if and only if $\rho(M) < 1$.

10. Derive the approximate inverse B for the SSOR method and show that it is symmetric and positive definite when the matrix A is symmetric and positive definite.

11. Write a MATLAB code to solve problem 3 above in $\boldsymbol{R}^2$ using a Jacobi iteration. When the problem size is sufficiently small, backslash can be used to solve the linear system directly instead of iteratively. Use this direct solution to plot the accuracy of your Jacobi iteration with respect to iteration number.

12. Write a MATLAB code to solve problem 3 above in $\boldsymbol{R}^2$ using an SSOR iteration. Let the unknowns be numbered according to the lexicographic ordering. Again use a direct solution with backslash to determine the accuracy of your SSOR iteration with respect to iteration number. Also determine by experimentation the best relaxation parameter ω.

13. Repeat the last exercise using the red-black ordering of unknowns.

14. Use the QR algorithm to solve problem 5 in one and in two dimensions.

15. For Theorem 5.10 in Deuflhard and Hohmann, show that it is unnecessary to assume that Q in $AQ = Q\Lambda$ can be decomposed as $Q^{\mathrm{T}} = LR$ without permuting or else find a counterexample showing that the assumption is necessary.

16. Prove that the QR decomposition is unique if the diagonal entries of R are positive.

17. In the proof of Theorem 5.10 in Deuflhard and Hohmann, A^k is expressed in terms of two QR decompositions. Show that a difference in signs of the diagonal entries of these decompositions can in general cause Q_k, R_k or A_k to oscillate instead of converging, or else show that these sign differences never prevent convergence.

18. Prove that for a given matrix A and $\varepsilon > 0$ there exists an induced norm $|A|$ satisfying $|A| < \rho(A) + \varepsilon$.

19. Give an example of a matrix A for which $\|\lambda'(A)\|$ is arbitrarily large.

20. For a real symmetric matrix A whose eigenvalue λ_1 with largest magnitude is simple, state and prove an estimate on the convergence rate of the power method in terms of λ_2/λ_1, where λ_2 is an eigenvalue with the next largest magnitude.

21. Write a MATLAB code to compute the spectral radius of $[I+\tau A_h]$ in problem 6 using the power method.

22. Show that if the SVD decomposition of a matrix $A \in \boldsymbol{R}^{m\times n}$ is formed iteratively according to

$$A_{k+1} = U_k^{\mathrm{T}} A_k V_k = \begin{pmatrix} \sigma_1 & 0 & 0 & 0 \\ 0 & \ddots & 0 & 0 \\ 0 & 0 & \sigma_k & 0 \\ 0 & 0 & 0 & B_k \end{pmatrix}$$

$$U_k \in O(m), \quad V_k \in O(n), \quad A_1 = A, \quad B_0 = A, \quad \sigma_k = \|B_{k-1}\|_2$$

then for $p = \min\{m, n\}$, $A_{p+1} = \mathrm{diag}\{\sigma_1, \ldots, \sigma_p\} \in \boldsymbol{R}^{m\times n}$ holds with $\sigma_1 \geq \cdots \geq \sigma_p$.

23. For a real symmetric $n \times n$ matrix A with eigenvalues $\{\lambda_i\}$ satisfying $|\lambda_1| > \cdots > |\lambda_n| > 0$, state and prove an estimate on the convergence rate of the QR method in terms of λ_i/λ_j.

24. For a polynomial $p(z)$ and a positive definite symmetric matrix A with spectrum $\sigma(A)$ show that

$$\|p(A)\|_2 = \max_{z\in\sigma(A)} |p(z)|$$

25. Let A be a symmetric positive definite $N \times N$ matrix, and suppose that there are exactly $k \leq N$ distinct eigenvalues of A. Show that the CG iteration terminates in at most k iterations.

26. Let $u \in H^2(\Omega)$ (u and its derivatives up to second order are in $L^2(\Omega)$) be the exact solution to a boundary value problem $Lu = f$. For a given approximation space $S_h(\Omega)$, let P_h be the orthogonal projection of $L^2(\Omega)$ onto $S_h(\Omega)$, and let L_h be an approximation of L. Then define $f_h = P_h f$ and let $u_h \in S_h(\Omega)$ be the solution of the discretized problem $L_h u_h = f_h$ which is assumed to satisfy

$$\|u - u_h\|_{L^2(\Omega)} \leq c_1 h^2$$

For the explicit solution to the discretized problem define the matrices A_N and B_N by

$$h(A_N \chi_i, \chi_j)_{\ell_2} = (L_h \chi_i, \chi_j)_{L^2(\Omega)}, \quad h(B_N \chi_i, \chi_j)_{\ell_2} = (\chi_i, \chi_j)_{L^2(\Omega)}, \qquad \forall \chi_i, \chi_j \in S_h(\Omega)$$

where $(U,F)_{\ell_2}$ is the Euclidean inner product on $\boldsymbol{R}^N$. Assume that A_N and B_N satisfy $0 < \gamma < \lambda_{\min}(A_N)$, $\lambda_{\max}(A_N) \le c_2 h^{-2}$, $0 < \beta \le \lambda_{\min}(B_N)$ and $\lambda_{\max}(B_N) \le \delta$ for positive constants γ, δ and c_2. Then with the basis $\{\chi_i\}_{i=1}^{N(h)}$ for $S_h(\Omega)$, $u_h = \sum_{i=1}^N U_i \chi_i$ and $f_h = \sum_{i=1}^N F_i \chi_i$, the problem $L_h u_h = f_h$ in $S_h(\Omega)$ becomes $A_N U = B_N F$ in $\boldsymbol{R}^N$. Let $U^{(k)}$ be the approximate solution to this linear system obtained by k conjugate gradient iterations. Determine the number k required for $u_h^{(k)} = \sum_{i=1}^N U_i^{(k)} \chi_i$ to satisfy:

$$\|u - u_h^{(k)}\|_{L^2(\Omega)} \le c_4 h^2$$

for some positive constant c_4.

27. Write a MATLAB code to solve problem 3 above in $\boldsymbol{R}^2$ using a conjugate gradient iteration. Let the unknowns be numbered according to the lexicographic ordering. Compare the result using (a) no preconditioning, (b) Jacobi preconditioning and (c) SSOR preconditioning. Use a direct solution with backslash to determine the accuracy of your CG iteration with respect to iteration number.

28. Write a MATLAB code to solve problem 4 above in $\boldsymbol{R}^2$ using a conjugate gradient iteration for each Newton step. Let the unknowns be numbered according to the lexicographic ordering. Compare the result using (a) no preconditioning, (b) Jacobi preconditioning and (c) SSOR preconditioning. Use a direct solution with backslash to determine the accuracy of your CG iteration with respect to iteration number.

29. For the matrices,

$$A = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 4 & 0 \\ 0 & 0 & 9 \end{bmatrix} \quad b = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} \quad x_0 = \begin{bmatrix} 3 \\ 2 \\ 1 \end{bmatrix}$$

implement the CG algorithm until the exact solution to $Ax = b$ is obtained, and plot the vectors $\{x_k\}$, $\{r_k\}$ and $\{p_k\}$ in relation to level surfaces of $\phi(x) = \frac{1}{2} x^{\mathrm{T}} A x - b^{\mathrm{T}} x$.

30. Construct a Krylov space $\mathcal{K}_n$ spanned by vectors $\{v_k\}$ and $\{\tilde{v}_k\}$, obtained respectively by the classical Gram-Schmidt method and the modified Gram-Schmidt method, where $v_k \ne \tilde{v}_k$ even with exact arithmetic, or else show that the sets are always identical in exact arithmetic. In any case, show that the vectors $\{\tilde{v}_k\}$ obtained by the the modified Gram-Schmidt method are orthonormal.

31. Apply the GMRES Algorithm to implement the backward Euler method for solving problem (6) above. Note that the associated linear system is non-symmetric for $f \ne 0$.

32. Write a MATLAB code to implement the QR Algorithm for the determination of the eigenvalues of a real symmetric $n \times n$ matrix A with eigenvalues $\{\lambda_i\}$ satisfying $|\lambda_1| > \cdots > |\lambda_n| > 0$.

33. Write a MATLAB code to implement the LU Algorithm for the determination of the eigenvalues of a real symmetric $n \times n$ matrix A with eigenvalues $\{\lambda_i\}$ satisfying $|\lambda_1| > \cdots > |\lambda_n| > 0$. In case A is positive definite, use the Cholesky decomposition instead of the LU decomposition.

34. Write a MATLAB code to implement the implicit QR Algorithm for the determination of the singular values of a real matrix.