CS556 Iterative Methods Fall 2024 Homework 3.

Due Tuesday, Oct. 8, 5 PM.

1. Conjugate Gradient Convergence. Consider the $n \times n$ SPD matrix

$$A = VDV^T, \qquad (1)$$

where V is orthonormal and D=diag(1, 2 ... $n-1$, M), with $M := n^2$. Let A_n be defined in the same way as A, save that $M = n$.

- What is the condition number of A_n?
- What is the condition number of A?
- Using the CG error bound (e.g., Eq. (25) of the "projection2a.pdf" from the 9-24-2024 notes on Relate), estimate the number of iterations k required to reach a *relative* error tolerance, *tol*=2×10^{-8} in the A-norm or A_n-norm when solving a system in A or A_n, respectively. (Use actual logarithms, rather than the quick estimates we used in class.) Please show the steps used to reach your given estimate.
- **Challenge.** Let $k_{\max}$ and k_n denote your estimated iteration counts from the preceding question. Use the best-fit principles of CG to show that the number of CG iterations for solving $A\underline{x} = \underline{b}$ to tolerance *tol* is bounded by $k_n + 1$. *Hint: Think carefully about a polynomial that would solve the discrete minimax problem.*
- Code up CG Saad (2nd Ed.) **Alg. 6.18** and solve $A\underline{x} = \underline{b}$ with random rhs $\underline{b}$ with $n = 101$. What number of iterations do you find to reach a relative A-norm error tolerance of *tol*=2×10^{-8}? (Note that V can be generated as `[V,R]=qr(rand(n,n));`.
- Make a semilogy plot of $\|\underline{e}_k\|_A / \|\underline{x}\|_A$ and $\|\underline{r}_k\|_2 / \|\underline{b}\|_2$ vs. k, both on the same graph, and comment on your observations for the graph and the overall analysis.

2. Coarse-Grid + Diagonal Preconditioning.

- Extend your CG code from **Q1** to support preconditioned search directions, $z = M^{-1}r$, where

$$M^{-1} = D^{-1} + M_c^{-1} \tag{2}$$

$$M_c^{-1} = J A_c^{-1} J^T \tag{3}$$

$$A_c = J^T A J. \tag{4}$$

  Here, A is the SPD, second-order finite difference, matrix that approximates the 2D Poisson (homogeneous-Dirichlet) operator with $n = (N-1)^2$ interior grid points and uniform grid spacing $h = L/N$ in each direction. Take $J = \hat{J} \otimes \hat{J}$ to be the tensor product of 1D piecewise linear interpolants from N_c to N, where N_c is the number of coarse-grid spacings and N is the number of fine-grid spacings. (An matlab example to generate $\hat{J}$ is provided.)
  (**Note:** do not form M_c, as it will be completely full.)

- Run the code for $N = 256$ and relative residual tolerance 10^{-8} and plot, on a *loglog* scale, the relative residual-norm, $res := \|\underline{r}_k\|/\|\underline{b}\|$ vs. k until $res < 10^{-8}$.

- Generate the relative residual history for $N_c = 2, 4, 8, 16, 32, 64$ and plot each on the same figure. **Also,** plot the relative residual history for the *unpreconditioned case.*

- How does the required number of iterations, $k_{\max}$, vary with N_c?

3. Preconditioned Spectra.

- For insight into the behavior of this preconditioner, we look at its impact on the spectrum of A. Recall the following set of tensor-product decompositions

$$\begin{aligned}
A &= S\Lambda S^T \\
S &= S_y \otimes S_x \\
\Lambda &= I_y \otimes \Lambda_x \;+\; \Lambda_y \otimes I_x \\
S_x &= [\underline{s}_{x,1}\; \underline{s}_{x,2}\; \dots\; \underline{s}_{x,N-1}] \;=\; [\dots \sin(k\pi x_j)\, \dots] \\
\Lambda_x &= \text{diag}(\lambda_k); \;\; \lambda_k = \frac{2}{\Delta x^2}(1-\cos(\pi k/N)) \\
&\textit{etc.}
\end{aligned}$$

  Specifically,

$$\lambda_j(A) = \lambda_k(A_x) \;+\; \lambda_l(A_y) \tag{5}$$

$$= \frac{\underline{s}_j^T A \underline{s}_j}{\underline{s}_j^T \underline{s}_j} \tag{6}$$

$$= \frac{\underline{s}_{k,l}^T A \underline{s}_{k,l}}{\underline{s}_{k,l}^T \underline{s}_{k,l}} \;=:\; \lambda_{k,l}(A) \tag{7}$$

  Here, $\underline{s}_j \in \mathbb{R}^n$, with $n = (N-1)^2$ is the jth eigenvector of A. It can be viewed as a matrix of mesh values given $\underline{s}_{k,l} := \underline{s}_j = \underline{s}_{x,k}\underline{s}_{y,l}^T$.

  Make a 2D mesh plot of $\lambda_{k,l}$ for $k, l \in \{1, \dots, N-1\}^2$ using (7), with $N = 32$.

- Make a similar mesh plot with

$$\mu_{kl} = \frac{\underline{s}_{k,l}^T M^{-1} A \underline{s}_{k,l}}{\underline{s}_{k,l}^T \underline{s}_{k,l}}, \tag{8}$$

  which approximates the spectra of the preconditioned operator, $M^{-1}A$. (This approximation is exact if $\mathcal{R}(\hat{J})$ =span$\{\underline{s}_{x,1}\, \underline{s}_{x,1} \dots \underline{s}_{x,c}\}$.)

- Plot the two distributions on the *same* mesh plot.
- Comment on the implications for the condition number in the preconditioned case and on the sensitivity of the condition number to the choice of A_c.

- The condition number for the unpreconditioned case is

$$\kappa(A) = \frac{\max(\lambda_k + \lambda_l)}{\min(\lambda_k + \lambda_l)} \tag{9}$$

$$= \frac{2 \cdot 4(N-1)^2}{2\pi^2}. \tag{10}$$

- Based on observations from your 2D spectra, what is the condition number for the preconditioned case as a function of N_c?
- What is the expected iteration count for PCG as a function of N_c?
- How does this estimate compare with the results of your *loglog* plot of **Q2**?