MA3227 Numerical Analysis II

Topics for Midterm Exam

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Topics for Midterm Exam

Finite differences

- Consistency and stability implies convergence theorem:

$$\|u - u_n\| \le \|\Delta_n^{-1}\| \, \|\Delta_n u + f\|.$$

- Taylor expansion for computing the consistency error $\|\Delta_n u + f\|$.

Sparse LU

- Graph of sparse matrices, structural nonzeros, fill-in.
- Path theorems for matrix powers, inverses and the LU factorisation.
  Application only, no proofs.
- Runtimes of dense and sparse LU factorisation:

$$\text{dense: } \mathcal{O}(N^3), \qquad \text{sparse: } \begin{cases} \mathcal{O}(N) & \text{if } d = 1, \\ \mathcal{O}(N^{3/2}) & \text{if } d = 2, \\ \mathcal{O}(N^2) & \text{if } d = 3. \end{cases}$$

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Orthogonal matrices

- Basic orthogonalisation procedure $\hat{b} = b - \frac{a^T b}{a^T a}\, a$.
- Use of the basic orthogonalisation procedure in the Gram-Schmidt, Arnoldi and Lanczos algorithms.
- Arnoldi relation $AQ_k = Q_{k+1} H_k$.
- Lanczos theorem: A symmetric $\implies$ H_k tridiagonal.
- QR factorisation $A = QR$.
- $x = \arg\min \|Ax - b\|_2 \quad \iff \quad x = R^{-1}\, Q^T b$

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Krylov methods

- Krylov algorithms:

$$x_k = p_{k-1}(A)\, b \qquad \text{where} \qquad p_{k-1} = \operatorname*{arg\,min}_{p_{k-1} \in \mathcal{P}_{k-1}} \left\| \big(A p_{k-1}(A) - I\big)\, b \right\|.$$

- GMRES and MinRes minimise 2-norm, CG minimises A^{-1} norm.
- Runtime GMRES is N matvecs plus $\mathcal{O}(Nk^2)$ other operations.
  Runtime MinRes and CG is N matvecs plus $\mathcal{O}(Nk)$ other operations.
- GMRES is applicable to any matrix. MinRes requires symmetry.
  CG requires symmetric positive definite.

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Krylov methods (continued)

- Convergence estimate

  $$\|Ax_k - b\| \le C \min_{q_k \in \mathcal{P}} \max_{\lambda_\ell} \frac{|q_k(\lambda_\ell)|}{|q_k(0)|}$$

  and its corollaries regarding scale-invariance, outliers and finite termination.

  Application only, no proofs.

  You may ignore `alternating_eigenvalues()` from lab 2.
- Convergence bound for intervals: if $\lambda_\ell \in [1, \kappa]$, then $\|Ax_k - b\| \le C\,\rho^k$ and $\rho \in (0, 1)$ is closer to 0 for κ closer to 1.

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Jacobi and multigrid

- Jacobi and Gauss-Seidel iterations:

$$\begin{aligned} \text{Jacobi:} \quad & x_{k+1} = D^{-1}\left(b - (A - D)\, x_k\right), \\ \text{Gauss-Seidel:} \quad & x_{k+1} = (D + U)^{-1}\left(b - Lx_k\right). \end{aligned}$$

  You should know these formulae and be able to perform the iterations by hand.

- Error recursion formula

$$x_{k+1} = x_k + B\,(b - Ax_k) \quad \Longrightarrow \quad x_{k+1} - x = (I - BA)\,(x_k - x)$$

  and its consequences regarding convergence.

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Root-finding algorithms

- You should be able to perform bisection, false position, Newton and secant methods by hand.
- You should be able to show the convergence result for Newton's method, but you may ignore secant and false position.
- Be informed about Broyden and gradient descent. No need to remember the formulae for Broyden's method.

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Example question

Consider the 2×2 matrix

$$A = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \quad \text{where} \quad a, d \neq 0.$$

Show that Gauss-Seidel converges at least twice as fast as Jacobi.

For an actual exam question, I would clarify more precisely what is meant by twice as fast. Here, it will be clear once you see the answer on the next slide.

Hint. We have

$$x_k - x = R^k\,(x_0 - x) \qquad \text{where} \qquad R = \begin{cases} -D^{-1}\,(A - D) & \text{(Jacobi)}, \\ -(U + D)^{-1} L & \text{(Gauss-Seidel)}. \end{cases}$$

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Answer. We know that $\|x_k - x\| \leq C\,|\lambda_{\max}|^k$ where $\lambda_{\max}$ is the eigenvalue of largest magnitude of the two matrices R given above.

For Jacobi, we compute

$$-D^{-1}(A - D) = -\begin{pmatrix} 0 & \frac{b}{a} \\ \frac{c}{d} & 0 \end{pmatrix}$$

and thus $|\lambda_{\max}| = \sqrt{\frac{bc}{ad}}$.

For Gauss-Seidel, we compute

$$-(U + D)^{-1} L = -\begin{pmatrix} 0 & \frac{b}{a} \\ 0 & \frac{bc}{ad} \end{pmatrix}$$

and thus $|\lambda_{\max}| = \frac{bc}{ad}$.

We conclude $|\lambda_{\max}^{(Jac)}|^2 = |\lambda_{\max}^{(GS)}|$, i.e. Jacobi requires two steps to achieve the same error reduction as Gauss-Seidel achieves in a single step.

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Example question

Let $A \in \mathbb{R}^{N \times N}$ be a dense and symmetric matrix with eigenvalues in the interval $[1, \kappa]$. Determine $\alpha \in \mathbb{R}$ such that if $\kappa = \mathcal{O}\big(N^{\tilde{\alpha}}\big)$ with $\tilde{\alpha} < \alpha$, then MinRes is asymptotically faster than LU factorisation, and if $\tilde{\alpha} > \alpha$ then MinRes is asymptotically slower than LU factorisation.

Hint. Under the assumptions above, the MinRes iterates x_k satisfy

$$\|Ax_k - b\| \leq C\,\rho^k \text{ with } \rho = 1 - \mathcal{O}\big(\kappa^{-1/2}\big),$$

and

$$k = \mathcal{O}\big(\log(\varepsilon)\,(1-\rho)^{-1}\big) = \mathcal{O}\big(\log(\varepsilon)\,\kappa^{1/2}\big)$$

steps are required to achieve $\|Ax_k - b\| \leq \varepsilon$.

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Answer. Since A is dense, the runtime of LU is $\mathcal{O}(N^3)$.

For MinRes, the runtime is k matrix-vector products and $\mathcal{O}(Nk)$ other operations. Since A is dense, the matrix-vector products dominate and the runtime is $\mathcal{O}(N^2 k)$.

We know that MinRes requires $k = \mathcal{O}\big(\kappa^{1/2}\big)$ to achieve a fixed error. The critical α is therefore $\alpha = 2$.

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Example question

Consider the inner product

$$\langle p, q \rangle = \int_0^1 p(x)\, q(x)\, dx$$

defined for all polynomials $p, q \in \mathcal{P}_k = \{p(x) \mid p(x) = \sum_{\ell=0}^{k} c_k x^k\}$.
Determine three polynomials p_0, p_1, p_2 such that $\langle p_k, p_\ell \rangle = 0$ if $k \neq \ell$ and

$$\operatorname{span}\{p_0\} = \mathcal{P}_0, \qquad \operatorname{span}\{p_0, p_1\} = \mathcal{P}_1, \qquad \operatorname{span}\{p_0, p_1, p_2\} = \mathcal{P}_2.$$

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Answer. The polynomials can be found by applying the Gram-Schmidt algorithm to $1, x, x^2$. We compute:

$$p_0(x) = 1, \qquad p_1(x) = x - \frac{\langle 1, x\rangle}{\langle 1, 1\rangle}\, 1 = x - \tfrac{1}{2}$$

$$\begin{aligned} p_2(x) &= x^2 - \frac{\langle x - \frac{1}{2}, x^2\rangle}{\langle x - \frac{1}{2}, x - \frac{1}{2}\rangle}\left(x - \tfrac{1}{2}\right) - \frac{\langle 1, x^2\rangle}{\langle 1, 1\rangle}\, 1 \\ &= x^2 - \left(x - \tfrac{1}{2}\right) - \tfrac{1}{3} \\ &= x^2 - x + \tfrac{1}{6}. \end{aligned}$$

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Example question

Perform a single step of Newton's method for

$$f(x,y) = \begin{pmatrix} x^2 - xy + 1 \\ 2xy - 2x - y + 5 \end{pmatrix}$$

and initial guess $(x_0, y_0) = (0, 1)$.

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Answer. We compute

$$\nabla f(x,y) = \begin{pmatrix} 2x-y & -x \\ 2y-2 & 2x-1 \end{pmatrix} \quad \Longrightarrow \quad \nabla f(0,1) = \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}$$

and

$$f(0,1) = \begin{pmatrix} 1 \\ 4 \end{pmatrix}.$$

Thus,

$$\begin{pmatrix} x_1 \\ y_1 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} - \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}^{-1} \begin{pmatrix} 1 \\ 4 \end{pmatrix} = \begin{pmatrix} 1 \\ 5 \end{pmatrix}$$