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Programming assignment #2: electrostatics on a lattice

Let $N > 0$ be a positive integer, and consider a uniform grid of points:

$$\mathbf{x}_{i,j} = (i, j) \in \mathbb{R}^2, \quad 0 \leq i \leq N, \quad 0 \leq j \leq N. \quad (1)$$

We will consider an equilibrium electrostatics problem on this grid, thinking of it as a lattice of nodes, with each node being connected to its four nearest neighbors in the cardinal directions (north, south, east, and west). Let $\mathbf{u} \in \mathbb{R}^{(N+1)^2}$ be a vector which contains the electric potentials at each grid node, assuming that the nodes are inserted row-by-row, from top to bottom and left to right so that:

$$\mathbf{u}_k = u(\mathbf{x}_{i,j}), \quad k = (N+1)i + j, \quad 0 \leq k < (N+1)^2. \quad (2)$$

If \mathbf{u}_k and \mathbf{u}_l give the potential for two connected grid points, the flux through the edge that connects them is $\pm(\mathbf{u}_k - \mathbf{u}_l)$. We require the fluxes to balance. That is, for each k such that $0 \leq k < (N+1)^2$, we require:

$$\sum_{l \sim k} (\mathbf{u}_k - \mathbf{u}_l) = 4\mathbf{u}_k - \sum_{l \sim k} \mathbf{u}_k = 0, \quad (3)$$

where “ $l \sim k$ ” means that the grid points indexed by the l and k are neighbors.

Next, we assume that the electric potential u is equal to zero on the boundary nodes of the grid:

$$u(\mathbf{x}_{i,j}) = 0 \quad \text{if } i = 0, N \quad \text{or} \quad j = 0, N. \quad (4)$$

If we let the remaining values of u be variables, then we are left with a matrix equation of the form:

$$\mathbf{A}\mathbf{u} = \mathbf{0}, \quad (5)$$

where $\mathbf{A} \in \mathbb{R}^{(N-1)^2 \times (N-1)^2}$ and $\mathbf{u} \in \mathbb{R}^{(N-1)^2}$.

Problem 1. Compute \mathbf{A} for $N = 10$ and use `matplotlib`'s `imshow` command to make a plot of its entries. Be sure to include a `colorbar` and choose an appropriate colormap so that is easy to visualize. In particular, make sure that the zero entries of \mathbf{A} are colored in white. *Hint: note very carefully the size of \mathbf{A} and the consequence of assuming that the boundary values of u equal zero. Work from (3).*

Problem 2. Write a function with the signature:

$$L, U, P = \text{lu}(A)$$

which computes the LU decomposition of a (possibly non-symmetric!) matrix A using partial pivoting, and so that afterwards $PA = LU$ holds. *Hint: test this on some small matrices and compare the result with `np.linalg.lu` as you go.*

Problem 3. Using `lu`, compute the LU decomposition of \mathbf{A} for $N = 10, 20, 30, 40$, and 50. Plot \mathbf{L} in the same way you plotted \mathbf{A} in Problem 1. Count the number of nonzeros of the L factor, and find its *lower bandwidth* (the number of diagonals of the matrix that contain nonzero values). Make two plots of the number of nonzeros of \mathbf{L} and the lower bandwidth of \mathbf{L} , each with N on the horizontal axis.

Problem 4. Write two functions:

$$\mathbf{x} = \text{fsolve}(\mathbf{L}, \mathbf{b}) \quad \mathbf{x} = \text{bsolve}(\mathbf{U}, \mathbf{b})$$

which do forward substitution (solve a linear system $\mathbf{L}\mathbf{x} = \mathbf{b}$ where L is lower-triangular) and backwards substitution (solve a linear system $\mathbf{U}\mathbf{x} = \mathbf{b}$ where U is upper-triangular), respectively. For $N = 50$, use these functions and your function `lu` to solve:

$$\mathbf{A}\phi_{i,j} = \mathbf{e}_{i,j}, \tag{6}$$

where $\mathbf{e}_{i,j}$ is the (k, l) standard basis vector—i.e., it has a 1 in the position corresponding to $\mathbf{x}_{i,j}$, and 0s everywhere else. Make a 3D plot of $\phi_{i,j}$ as the graph of a function using `mplot3d` for a few different choices of (i, j) after rearranging the entries of ϕ to lie on a square grid (so that they match the 2D layout of the grid nodes $\mathbf{x}_{i,j}$).