Problem Set 7

Due Wednesday Nov. 15, 10 am

Comments

- No late submissions. Given the timing of the second quiz, I will hand out solutions in class November 15.
- This covers material in Unit 10.
- It's due at 10 am (Pacific) on November 15, both submitted as a PDF to Gradescope as well as committed to your GitHub repository.
- Please see PS1 for formatting and attribution requirements.
- Note that is is fine to hand-write solutions to the the non-coding questions, but make sure your writing is neat and insert any hand-written parts in order into your final submission.

Problems

- 1. Details of the Cholesky decomposition presented in Unit 10. Work out the operation count (total number of multiplications plus divisions) for the Cholesky decomposition, including the constant c, not just the order, for terms involving n^3 or n^2 (e.g., $5n^3/2 + 8n^2$, not $O(n^3)$). You can ignore the square root and any additions/subtractions. You can ignore pivoting for the purpose of this problem. Remember not to count any steps that involve multiplying by 0 or 1. Compare your result to that given in the notes.
- 2. Compare the speed of $x = A^{-1}b$ using: (i) np.linalg.inv(A) @ b, (ii) np.linalg.solve(A, b), and (iii) Cholesky decomposition followed by solving triangular systems. To ensure that A is positive definite (needed of course for the Cholesky), you can construct a matrix A as $A = W^{\top}W$, with the elements of the $n \times n$ matrix W generated randomly. Note that if your Python/numpy installation is not using a fast BLAS package, all three of these approaches will likely take a lot longer than if you are using a fast BLAS (e.g., on the SCF). See Section 6.1 of Unit 10 and/or Section 5 of Unit 6.
 - a. Using a single thread, how do the timing and relative ordering amongst methods compare to the order of computations we discussed in class and the notes using n = 5000? Note that if one works out the complexity of the full inversion using the LU decomposition, it is $4n^3/3$.
 - b. Show how the timing scales with n for a few values up through n=5000 for all three of the approaches.

- c. Are the results for the solution x the same numerically for methods (ii) and (iii) (up to machine precision)? Comment on how many digits in the elements of x agree, and relate this to the condition number of the calculation. You can do this for one of the smaller values of n to reduce the time to compute the condition number.
- 3. The following calculation arises in solving a least squares regression problem where the coefficients are subject to an equality constraint, in particular, we want to minimize $(Y X\beta)^{\top}(Y X\beta)$ with respect to β subject to the m constraints $A\beta = b$ for an $m \times p$ matrix A. (Each row of A represents a constraint that a linear combination of β equals the corresponding element of b.) Solving this problem is a form of optimization called *quadratic programming*. Some derivation using the Lagrange multiplier approach (we'll see this in Unit 11) gives the following solution:

$$\hat{\beta} = C^{-1}d + C^{-1}A^{\top}(AC^{-1}A^{\top})^{-1}(-AC^{-1}d + b),$$

where $C = X^{\top}X$ and $d = X^{\top}Y$. X is $n \times p$.

- a. Describe how you would implement this in pseudo-code, taking account of the principles discussed in class in terms of matrix inverses and factorizations
- b. Write a Python function to efficiently compute $\hat{\beta}$, using numpy or scipy's matrix manipulation/factorization functions. Note: in reality a very efficient solution is only important when the number of regression coefficients, p, is large.