MTH 373/573:
Scientific Computing
Monsoon 2018

Homework 3

IIIT-Delhi
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Due: October 25, 2018 (Friday) by 23.59 **Total: 150 points.**

Before you start, please read General Submission Guidelines on Page 2.

Problem 1: Orthogonalization procedures (150 points)

(a) Implement both the classical and modified Gram-Schmidt procedures and use each to generate an orthogonal matrix **Q** whose columns form an orthonormal basis for the column space of the Hilbert matrix H, with entries $h_{ij} = 1/(i+j-1)$, for $n = 2, 3, \ldots, 12$.

As a measure of quality of the results (specifically the potential loss of orthogonality), plot the quantity $-\log_{10}(\|I_n - Q^T Q\|)$, which can be interpreted as *digits of accuracy* and I_n is the $n \times n$ identity matrix. Compute this measure for each method as a function of n.

In addition, try applying the classical procedure twice (that is, apply your classical Gram-Schmidt routine to its own output Q to obtain a new $\widehat{Q}$), and again plot the resulting departure from orthogonality. How do the three methods compare in accuracy?

(b) Repeat the previous experiment but this time use the Householder method, that is, use the explicitly-computed orthogonal matrix Q resulting from Householder QR factorization of the Hilbert matrix. For this you can either use the NumPy function `numpy.linalg.qr` or Julia's `qr` (via `(using LinearAlgebra)`). Again, plot the departure from orthogonality for this method and compare it with that of the previous methods.

(c) Yet another way to compute an orthonormal basis is to use the normal equations. If we form the cross-product matrix and compute its Cholesky factorization $A^T A = LL^T$, then we have:

$$\begin{aligned} I_n &= L^{-1} \left(A^T A\right) L^{-T} \\ &= \left(A\, L^{-T}\right)^T \left(A\, L^{-T}\right), \end{aligned}$$

which means that $Q = A\, L^{-T}$ is orthogonal, and its column space is the same as that of A. Repeat the previous experiment using Hilbert matrices again, this time using the Q obtained in this way from the normal equations. Again, plot the resulting departure from orthogonality and compare it with that of the previous methods.

(d) Can you explain the relative quality of the results you obtained for the various methods used in these experiments?

General Submission Guidelines

- **This assignment should be answered individually.**
- **You will be penalized for copying or any plagiarism with an automatic zero.**
- The points for each problem is roughly indicative of effort needed for answering that problem. Your mileage may vary!
- IIIT-Delhi academic policies on honesty and integrity apply to all HWs. This includes not copying from one another, from the internet, a book, or any other online or offline source. A repeat offense will be reported to academic administration.
- If you discuss or read secondary sources (other than class notes), please list all your discussion partners and/or secondary sources in your writeup. Failure to do so will constitute violation of honor code.
- All files should be submitted via Google Classroom.
- If your code generates an output figure or table, please provide all such results in a single PDF file along with your code submission.
- You will need to write a separate code for each problem and sometimes for each subproblem as well. You should name each such file as `problem_`n`.py` where n is the problem number. For example, your files could be named `problem_1.py`, `problem_4a.py` and `problem_4b.py` in this HW.
- *Python tip:* You can import Python modules as follows:

```
from __future__ import division
import numpy as np
import scipy as sp
import matplotlib.pyplot as plt
import numpy.linalg as npla
import scipy.linalg as spla
```

Every code you write will have one or more of these import statements.