HPC for numerical methods and data analysis

Fall Semester 2023

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Session 10 – November 21, 2023

Deterministic rank revealing factorizations for low rank approximation

Exercise 0 (Optional): Numerical stability of randomized Nystrom

Just as in last week's exercise, consider the MNIST data set and the matrix A as defined in the project or in last week's exercise sheet (with a fixed value of c). **You'll have to be careful with this data set here and in your project because you have to make sure the data set is normalized, i.e. all the entries are between 0 and 1**. Take a relatively small sample of the training set. In this section you can use either last week's code or your code from your project. Consider two different types of sketching matrices, Ω_1, Ω_2. For different sketching dimensions of both types of matrices, compute the relative error of the low rank approximation in terms of the nuclear norm. Provide a graph that compares these errors. Comment on your findings.

Exercise 1: Tournament pivoting

The truncated SVD provides the best low rank approximation in terms of the Frobenius and L2 norms. Recall that the QR decomposition with column pivoting relies on a permutation matrix Π and computes the decomposition $A\Pi = QR$. There are many ways of building such permutation matrix. Let

$$\rho_i(W) = \frac{1}{\|W^{-1}[i,:]\|}$$
$$\chi_j(W) = \|W[:,j]\|$$

Consider the following theorem from `https://inria.hal.science/hal-02947991v2/document`:

Theorem 1 *Let A be an $m \times n$ matrix, $1 \leq k \leq \min(m,n)$. For any $f > 1$ there exists a permutation matrix Π such that the decomposition $A\Pi = QR$ verifies for all $(i,j) \in [1,k] \times [1,n-k]$,*

$$(R_{11}^{-1}R_{12})_{ij}^2 + \rho_i^2(R_11)\chi_j^2(R_22) \leq f^2.$$

Such factorization is called a strong RRQR factorization.

Recall tournament pivoting for deterministic column selection. (Refer to the image below).

a) Consider a matrix A partitioned into 4 column blocks. Each processor has one of these blocks.

b) Implement strong RRQR (there is a MATLAB implementation, you can use that as a template for building your own Python implementation).

c) For each block of columns, select k columns using strong RRQR, save their indices are given in I_{i0}. Be careful with these indices, you might have to deal with "global" and "local" indices.

d) In each processor output these indices $I_{00}, I_{10}, I_{20}, I_{30}$.

e) Test your method with three different matrices:

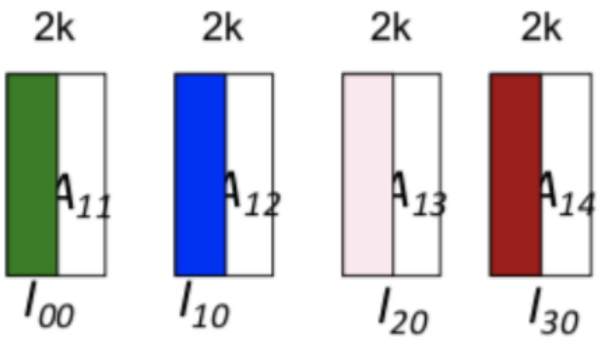
- $A = H_n D H_n^\top$, where H_n is the normalized Hadamard matrix of dimension n, D is a diagonal matrix of your choice. Pick n to be "small".
- Load the normalized MNIST data set and build A as in the project (or last week's exercises). Select a few columns and rows.
- Build A from the MNIST data set with 2^{11} data points.

f) Comment your results with the different matrices. Do you notice a problem when you take more rows and columns using the MNIST data set?

g) Using $I_{00}, I_{10}, I_{20}, I_{30}$ build a low rank approximation of A. Check the L2 norm of the error with respect to the error of the truncated SVD.

h) Check if the singular values of these selected columns approximate well the singular values of A.

i) Check if the diagonal elements of R_{11} approximate well the singular values of A.



A Python implementation for strong RRQR is found below (adapted after the MATLAB implementation found in `https://www.mathworks.com/matlabcentral/fileexchange/69139-strong-rank-revealing-q`

```
# Implementation of the strong rank revealing QR with fixed rank 'k'
```

```
import numpy as np
from math import sqrt
from scipy.linalg import solve_triangular
import pdb
from numpy.linalg import norm
from scipy.linalg import qr
import pdb

def givens(a, b):
    '''
    Submatrix for a Givens rotation
    '''
    if b == 0:
        c = 1;
        s = 0;
    elif abs(b) ≥ abs(a):
        cotan = a/b;
        s = 1/sqrt(1 + cotan**2)
        c = s*cotan
    else:
        tang = b/a;
        c = 1/sqrt(1 + tang**2)
        s = c*tang
    G = np.array([[c, s], [-s, c]])
    return G


def sRRQR_rank(A, f, k):
    '''
    Strong Rank Revealing QR with fixed rank 'k'. The name of the variables
    are the same as in the paper. (Combination of algorithm 4 and 5).
    A is R11, B is R12, C is R22
    gamma is the norm of R22's columns
    omega is the reciproval of R11^-1's row norm

    Reference:
       Gu, Ming, and Stanley C. Eisenstat. "Efficient algorithms for
       computing a strong rank-revealing QR factorization." SIAM Journal
       on Scientific Computing 17.4 (1996): 848-869.
    Paper found in: https://math.berkeley.edu/~mgu/MA273/Strong_RRQR.pdf
    Translated from matlab implementation
    https://www.mathworks.com/matlabcentral/fileexchange/69139-strong-rank-revealing-qr-decompositior
    '''
        # Check constant bound f
    if f < 1:
        print("Parameter f is less than 1. Automatically set f = 2")
        f = 2

    # Dimension of the given matrix
    m, n = A.shape

    # Modify rank k if necessary
    k = min(k, m, n)

    # Pivoting QR first (generally most time-consuming step)
    Q, R, p = qr(A, pivoting = True, mode='economic')
    # Check special case: rank equals the number of columns.
    if k == n:
        # No need for SRRQR.
        return Q, R, p

    # Make diagonals of R positive
    ss = np.sign(np.diag(R))
    ss = np.diag(ss)
    R = ss@R
    Q = Q@ss

    # Initialization of A^{-1}B (A refers to R11, B refers to R12)
    AB = np.linalg.solve(R[:k, :k], R[:k, k:])

    # Initialization of gamma, i.e., norm of C's columns (C refers to R22)
    gamma = np.zeros(n - k)
    if k != R.shape[0]:
        gamma = np.linalg.norm(R[k:, k:], axis=0)

    # Initialization of omega, i.e., reciprocal of inv(A)'s row norm
    tmp = np.linalg.solve(R[:k, :k], np.eye(k, k))
    omega = np.reciprocal(np.sqrt(np.sum(tmp**2, axis=1)))
    omega = np.reshape(omega, (len(omega), 1))
    gamma = np.reshape(gamma, (len(gamma), 1))

    # KEY STEP in Strong RRQR:
    # "while" loop for interchanging the columns from the first k columns and
    # the remaining (n-k) columns.
    Rm, _ = R.shape
    while True:
        # Identify interchanging columns
        tmp = (1 / omega * np.transpose(gamma))**2 + AB**2
        i, j = np.unravel_index(np.argmax(tmp > f**2), tmp.shape)

        # If no entry of tmp greater than f*f, no interchange needed and the
        # present Q, R, p is a strong RRQR.
        if tmp[i, j] ≤ f**2:
            #print("NO ENTRY OF TMP GREATER")
            break

        # Interchange the i-th and (k+j)-th column of the target matrix A and
        # update QR decomposition (Q, R, p), AB, gamma, and omega.
        # First step: interchanging the k+1 and k+j-th columns
        if j > 0:
            AB[:, [0, j]] = AB[:, [j, 0]]
            gamma[[0, j]] = gamma[[j, 0]]
            R[:, [k, k+j]] = R[:, [k+j, k]]
            p[[k, k+j]] = p[[k+j, k]]

        # Second step: interchanging the i and k-1-th columns
        if i < k:
            #print("USING SECOND STEP")
            ind = list(range(i+1, k)) + [i]
            p[i:k] = p[ind]
            R[:, i:k] = R[:, ind]
            omega[i:k] = omega[ind]
            AB[i:k, :] = AB[ind, :]
            # Givens rotation for the triangulation of R(1:k, 1:k)
            for ii in range(i, k-1):
                G = np.array([[R[ii, ii] / np.sqrt(R[ii, ii]**2 + R[ii+1, ii]**2),
                                R[ii+1, ii] / np.sqrt(R[ii, ii]**2 + R[ii+1, ii]**2)],
                               [-R[ii+1, ii] / np.sqrt(R[ii, ii]**2 + R[ii+1, ii]**2),
                                R[ii, ii] / np.sqrt(R[ii, ii]**2 + R[ii+1, ii]**2)]])
                if G[0, :] @ np.array([R[ii, ii], R[ii+1, ii]]) < 0:
                    G = -G  # guarantee R(ii,ii) > 0
                R[ii:ii+2, :] = G @ R[ii:ii+2, :]
                Q[:, ii:ii+2] = Q[:, ii:ii+2] @ G.T
            if R[k-1, k-1] < 0:
                R[k-1, :] = -R[k-1, :]
                Q[:, k-1] = -Q[:, k-1]

        # Third step: zeroing out the below-diagonal of k-th columns
        if k < Rm-1:
            #print("USING THIRD STEP")
            for ii in range(k+1, Rm):
                G = np.array([[R[k-1, k-1] / np.sqrt(R[k-1, k-1]**2 + R[ii, k-1]**2),
                                R[ii, k-1] / np.sqrt(R[k-1, k-1]**2 + R[ii, k-1]**2)],
                               [-R[ii, k-1] / np.sqrt(R[k-1, k-1]**2 + R[ii, k-1]**2),
                                R[k-1, k-1] / np.sqrt(R[k-1, k-1]**2 + R[ii, k-1]**2)]])
                if G[0, :] @ np.array([R[k, k], R[ii, k]]) < 0:
                    G = -G  # guarantee R(k,k) > 0
                R[[k, ii], :] = G @ R[[k, ii], :]
                Q[:, [k, ii]] = Q[:, [k, ii]] @ G.T

        # Fourth step: interchanging the k and k+1-th columns
        #print("USING FOURTH STEP")
        p[[k-1, k]] = p[[k, k-1]]
        ga = R[k-1, k-1]
        mu = R[k-1, k] / ga
        if k-1 < Rm:
            nu = R[k, k] / ga
        else:
            nu = 0
        rho = np.sqrt(mu**2 + nu**2)
        ga_bar = ga * rho
        b1 = R[:k-1, k-1]
        b2 = R[:k-1, k]
        c1T = R[k, k+1:]
        if k+1 > Rm:
            c2T = np.zeros(len(c1T))
        else:
            c2T = R[k, k+1:]
        c1T_bar = (mu * c1T + nu * c2T) / rho
        c2T_bar = (nu * c1T - mu * c2T) / rho
        c1T_bar = np.reshape(c1T_bar, (1, -1))
        c2T_bar = np.reshape(c2T_bar, (1, -1))

        # Modify R
        R[:k-1, k-1] = b2
        R[:k-1, k] = b1
        R[k-1, k-1] = ga_bar
        R[k-1, k] = ga * mu / rho
        R[k, k] = ga * nu / rho
        R[k-1, k+1:] = c1T_bar
        R[k, k+1:] = c2T_bar

        # Update AB
        u = np.linalg.solve(R[:k-1, :k-1], b1)
        u = np.reshape(u, (-1, 1))
        u1 = AB[:k-1, 0]
        u1 = np.reshape(u1, (-1, 1))
```

```
        AB[:k-1, 0] = ((nu * nu * u - mu * u1) / rho**2)[:, 0]
        AB[k-1, 0] = mu / rho**2
        AB[k-1, 1:] = (c1T_bar / ga_bar)[0, :]
        AB[:k-1, 1:] = AB[:k-1, 1:] + (nu * u*c2T_bar - u1*c1T_bar ) / ga_bar

        # Update gamma
        gamma[0] = ga * nu / rho
        gamma[1:, 0] = np.sqrt( np.power(gamma[1:], 2)[:, 0] + np.power(np.transpose(c2T_bar), 2)[:,

        # Update omega
        u_bar = u1 + mu * u
        omega[k-1] = ga_bar
        omega[:k-1] = np.reciprocal(np.sqrt(omega[:k-1]**(-2) + u_bar**2 / ga_bar**2 - u**2 / ga**2))

        # Eliminate new R(k+1, k) by orthogonal transformation
        Gk = np.array([[mu/rho, nu/rho], [nu/rho, -mu/rho]])
        if k < Rm:
            Q[:, [k-1, k]] = Q[:, [k-1, k]] @ Gk.T

    # Only return the truncated version of the strong RRQR decomposition
    Q = Q[:, :k]
    R = R[:k, :]

    return Q, R, p




# Implementation of deterministic column selection: tournament pivoting

import numpy as np
from numpy.linalg import norm
import matplotlib.pyplot as plt
from copy import deepcopy
from scipy.linalg import hadamard
from math import ceil, log, exp
import pandas as pd


plt.ion()

# Functions to build the matrix A (see last week's exercises)
def readData(filename, size = 784, save = False):
    '''
    Read MNIST sparse data from filename
    and transforms this into a dense
    matrix, each line representing an entry
    of the database (i.e. a "flattened" image)
    '''
    dataR = pd.read_csv(filename, sep=',', header = None)
    n = len(dataR)
    data = np.zeros((n, size))
    labels = np.zeros((n, 1))
    # Format accordingly
    for i in range(n):
        l = dataR.iloc[i, 0]
        labels[i] = int(l[0]) # We know that the first digit is the label
        l = l[2:]
        indices_values = [tuple(map(float, pair.split(':'))) for pair in l.split()]
        # Separate indices and values
        indices, values = zip(*indices_values)
        indices = [int(i) for i in indices]
        # Fill in the values at the specified indices
        data[i, indices] = values
    if save:
        data.tofile('./denseData.csv', sep = ',',format='%10.f')
        labels.tofile('./labels.csv', sep = ',',format='%10.f')
    return data, labels

def buildA_sequential(data, c = 1e3, save = False):
    '''
    Function to build A out of a data base
    using the RBF exp( -||x_i - x_j||/c)
    Notice that we only need to fill in the
    upper triangle part of A since it's symmetric
    and its diagonal elements are all 1.
    '''
    n = data.shape[0]
    A = np.zeros((n, n))
    for j in range(n):
        for i in range(j):
            A[i,j] = exp( -norm( data[i, :] - data[j, :])**2/c)
    A = A + np.transpose(A)
    np.fill_diagonal(A, 1.0)
    if save:
        A.tofile('./A.csv',sep=',',format='%10.f')
    return A


filename = "mnist_780"
data, labels = readData(filename)
A = buildA_sequential(data)
A = A[0:16, 0:32]


Q, R, P = sRRQR_rank(A, 1.05, 5)
```

The tournament pivoting for deterministic column selection can be found below:

```
# Implementation of deterministic column selection: tournament pivoting


from mpi4py import MPI
import numpy as np
from numpy.linalg import norm, svd
import matplotlib.pyplot as plt
from copy import deepcopy
from scipy.linalg import hadamard
from math import ceil, log, exp, sqrt
import pandas as pd
from scipy.linalg import qr

# Custom library
from sRRQR import sRRQR_rank

plt.ion()
np.set_printoptions(precision=5)
```

```
# Functions to build the matrix A (see last week's exercises)
def readData(filename, size = 784, save = False):
    '''
    Read MNIST sparse data from filename
    and transforms this into a dense
    matrix, each line representing an entry
    of the database (i.e. a "flattened" image)
    '''
    dataR = pd.read_csv(filename, sep=',', header = None)
    n = len(dataR)
    data = np.zeros((n, size))
    labels = np.zeros((n, 1))
    # Format accordingly
    for i in range(n):
        l = dataR.iloc[i, 0]
        labels[i] = int(l[0]) # We know that the first digit is the label
        l = l[2:]
        indices_values = [tuple(map(float, pair.split(':'))) for pair in l.split()]
        # Separate indices and values
        indices, values = zip(*indices_values)
        indices = [int(i) for i in indices]
        # Fill in the values at the specified indices
        data[i, indices] = values
    if save:
        data.tofile('./denseData.csv', sep = ',',format='%10.f')
        labels.tofile('./labels.csv', sep = ',',format='%10.f')
    return data, labels

def buildA_sequential(data, c = 1e3, save = False):
    '''
    Function to build A out of a data base
    using the RBF exp( -||x_i - x_j||/c)
    Notice that we only need to fill in the
    upper triangle part of A since it's symmetric
    and its diagonal elements are all 1.
    '''
    n = data.shape[0]
    A = np.zeros((n, n))
    for j in range(n):
        for i in range(j):
            A[i,j] = exp( -norm( data[i, :] - data[j, :])**2/c)
    A = A + np.transpose(A)
    np.fill_diagonal(A, 1.0)
    if save:
        A.tofile('./A.csv',sep=',',format='%10.f')
    return A

def matTranspose(A, n):
    '''
    Since we want to distribute A's columns
    we need to manipulate our data into the correct
    order before sending it.
    '''
    arrs = np.split(A, n, axis = 1)
    raveled = [np.ravel(arr) for arr in arrs]
    A_transpose = np.concatenate(raveled)
    return A_transpose
```

```
# Initialize MPI (world)

comm = MPI.COMM_WORLD
rank = comm.Get_rank()
size = comm.Get_size()

A = None
m = None
n = None
local_sizeCols = None
A_T = None
f = 1.0005
k = 4
Pend = None

if rank == 0:
    # Read the files and build the matrix A here (see last week's exercises)
    filename = "mnist_780"
    data, labels = readData(filename)
    A = buildA_sequential(data)
    A = A[0:16, 0:16]
    # D = np.diag([1, 0.9, 0.8, 0.7, 0.65, 0.4, 0.1, 0.001])
    # H = hadamard(8)
    # H = 1/norm(H[:, 0])*H
    # A = H@D@np.transpose(H)
    # A = np.arange(0, 108)
    # A = np.reshape(A, (9, 12)) + 0.0
    m = A.shape[0]
    n = A.shape[1]
    print("m: ", m, "n: ", n)
    local_sizeCols = n//size # number of columns
    A_T = matTranspose(A, n)
    Pend = np.empty((k*size, 1), dtype = 'i')

# Step one: partition A into 4 column blocks
local_sizeCols = comm.bcast(local_sizeCols, root=0)
m = comm.bcast(m, root=0)
A_local = np.empty((local_sizeCols, m))
comm.Scatter(A_T, A_local, root = 0)
# Step 0
# From each column block A1i, i = 1, . . . , 4, k columns are selected by using
# strong RRQR, and their indices are given in Ii0.
Q, R, P = sRRQR_rank(np.transpose(A_local), f, k)
P = P[0:k]
Pall = deepcopy(P) + rank*local_sizeCols
Q, R, P = sRRQR_rank(np.transpose(A_local), f, k)
print("Rank: ", rank)
print("Columns selected: ", P[0:k])
comm.Gather(Pall, Pend, root = 0)
comm.Barrier()

if rank == 0:
    # Here we make our low rank approximation here and all
    # Make the low rank approximation. Note: this is
    # not an efficient way of making this, next week
    # we'll see a better way of doing this
    Pend = Pend.flatten()
    Atilde = A[:, Pend] # Selected columns
    U, Sigma, V = svd(Atilde)
    U = U[:, 0:k]
    Sigma = Sigma[0:k]
    V = V[0:k, 0:k]
    appsRRQR = U@np.diag(Sigma)@V
    print(appsRRQR.shape)
    # Singular values of full A
    Uf, Sigmaf, Vf = svd(A)
    # Compare them
    Uf = Uf[:, 0:k]
    Sigmaf = Sigma[0:k]
    Vf = Vf[0:k, 0:k]
    appfull = Uf@np.diag(Sigmaf)@Vf
    print(appfull.shape)
    # Compute the theoretical bound
    gamma = sqrt( 1 + f**2*k*(n-k) )
    print("L2 error with truncated SVD: ",
          norm( appsRRQR - appfull)  )
    print(r'$\gamma (n, k) = $')
    print(gamma)
    print(r'$\sigma_i(A)/\sigma_i(R_{11}) = $')
    print(np.divide(Sigma,Sigmaf))
    # We also plot the decay on the actual singular values vs estimate
    plt.figure(figsize=(8, 6), dpi=80)
    plt.loglog(range(0, k), Sigma, c = "#b200ff", marker = 'o', label = "sRRQR")
    plt.loglog(range(0, k), Sigmaf, c = "#004dff", marker = 'o', label = "Exact")
    plt.title("Singular values with sRRQR vs exact")
    plt.xlabel("i")
    plt.ylabel(r'$\sigma_i$')
    plt.show()
```

Note that all the solutions are uploaded to the following github repository: `https://github.com/mtzmarianaa/MATH-HPC`