Homework 2: Local and Far field expansions of the Gaussian

CMSC8789R/AMSC698R/MAIT 627

Due: September 19, 2006

This week's assignment uses the ideas of using Taylor series and far field expansions to achieve factorizations suitable for use in FMM type algorithms. Using the efficient global factorization of the Gaussian function discussed in class, one can develop an algorithm for the fast summation of Gaussians. Let

$$\Phi_{ji} = e^{-(y_j - x_i)^2}, \quad i = 1, ..., N, \quad j = 1, ..., M$$

$$\mathbf{\Phi} = \begin{pmatrix} \Phi_{11} & \Phi_{12} & ... & \Phi_{1N} \\ \Phi_{21} & \Phi_{22} & ... & \Phi_{2N} \\ ... & ... & ... & ... \\ \Phi_{M1} & \Phi_{M2} & ... & \Phi_{MN} \end{pmatrix}, \quad \mathbf{u} = \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ ... \\ u_N \end{pmatrix}, \quad \mathbf{v} = \begin{pmatrix} v_1 \\ v_2 \\ v_3 \\ ... \\ v_M \end{pmatrix}, \tag{1}$$

where $x_1, ..., x_N$, $y_1, ..., y_M, u_1, ..., u_N$, are random numbers distributed uniformly in $[0, 1]$. Compute the matrix-vector product

$$\mathbf{v} = \mathbf{\Phi u}, \qquad v_j = \sum_{i=1}^{N} \Phi_{ji} u_i, \quad j = 1, ..., M, \tag{2}$$

with absolute error $\epsilon < 10^{-6}$. The matrix sizes, $N, M > 0$ are given (fixed) positive integers.

1. Using the example from Lecture #2, write down a factored expression. Estimate the error in truncating the series using residual term evaluation for the Taylor series, and evaluate the truncation number, p,as a function of the required accuracy and N. Provide a formula that can be used for the "fast" ($O(N + M)$) method.

2. Write a program that implements both the straightforward computation based on Eq. (2) (using for loops) and the "fast" method.

3. Plot the absolute maximum error between the straightforward and "Fast" method for $N = 10^3$ and $M = 2N$ and p varying between 1 and 11. Compare the results with your evaluations of the accuracy.

4. Provide a graph that compares the CPU time required by the straightforward and the "Fast" method for N varying between 10^2 and 10^3 for the straightforward and N varying between 10^2 and 10^4 for the "Fast" method. Take $M = 2N$ and the theoretical value of the truncation number that ensures that the required accuracy is achieved. Use logarithmic axes.

5. Provide a graph of the abs. max. error (between the standard and fast methods) for N varying between 10^2 and 10^3, $M = 2N$ and the truncation numbers used for each N.

Hints/Notes.

1. Note that each source contributes to the error. So the truncation number p,corresponding to a required accuracy ϵ, depends on N . This relationship is an implicit function of p and you can either solve for p (write a Matlab function to do that) or determine it by developing a table of values and interpolating.

2. Use Matlab.

3. The maximum absolute error is defined as

$$error = \max_{i=1,\ldots,N} \left| v_i^{straightforward} - v_i^{fast} \right| . \tag{3}$$

   Plot the theoretical error bound on the same graph (use hint 1).

4. You may keep the truncation number constant (using the one evaluated for $N \leqslant 10^4$) or vary it with N according to the theoretical estimate for the error. In this case the function calculated in hint 1 will be helpful.

5. This version of the fast Gauss transform has been developed further in Raykar et al. (2005) to develop an improved fast Gauss transform (IFGT). (see https://drum.umd.edu/dspace/handle/1903/3020)