Fast CUR Approximation of Average Matrix and Extensions

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Abstract

CUR and low-rank approximations are among most fundamental subjects of numerical linear algebra, with a wide range of applications to a variety of highly important areas of modern computing, which range from the machine learning theory and neural networks to data mining and analysis. We first dramatically accelerate computation of such approximations for the average input matrix, then show some narrow classes of hard inputs for our algorithms, and finally point out a tentative direction to narrowing such classes further by means of preprocessing with quasi Gaussian structured multipliers. Our extensive numerical tests with a variety of real world inputs for regularization from Singular Matrix Database have consistently produced reasonably close CUR approximations at a low computational cost. There is a variety of efficient applications of our results and our techniques to important subjects of matrix computations. Our study provides new insights and enable design of faster algorithms for low-rank approximation by means of sampling and oversampling, for Gaussian elimination with no pivoting and block Gaussian elimination, and for the approximation of railing singular spaces associated with the \( \nu \) smallest singular values of a matrix having numerical nullity \( \nu \). We conclude the paper with novel extensions of our acceleration to the Fast Multipole Method and the Conjugate Gradient Algorithms. (This report is an outline of our paper [PSZA].)

Keywords: CUR approximation, Low-rank approximation, Average input, Gaussian matrices, Cross-approximation, Maximal volume, Fast Multipole Method, Conjugate Gradient Algorithms, Gaussian elimination with no pivoting, Block Gaussian elimination, Trailing singular spaces

1 Background: CUR and low-rank approximation

Low-rank approximation of an \( m \times n \) matrix \( W \) having a small numerical rank \( r \), that is, having a well-conditioned rank-\( r \) matrix nearby, is one of the most fundamental problems of numerical linear algebra [HMT11], with a variety of applications to highly important areas of modern computing, which range from the machine learning theory and neural networks [DZBLCF14, JVZ14] to numerous problems of data mining and analysis [M11].

*This report is an outline of our paper [PSZA].
One of the most studied approaches to the solution of this problem is given by CUR approximation where \(C\) and \(R\) are a pair of \(m \times l\) and \(k \times n\) submatrices formed by \(l\) columns and \(k\) rows of the matrix \(W\), respectively, and \(U\) is a \(k \times l\) matrix such that \(W \approx CUR\).

Every low-rank approximation allows very fast approximate multiplication of the matrix \(W\) by a vector, but CUR approximation is particularly transparent and memory efficient.

The algorithms for computing it are characterized by the two main parameters:

(i) their complexity and
(ii) bounds on the error norms of the approximation.

We assume that \(r \ll \min\{m, n\}\), that is, the integer \(r\) is much smaller than \(\min\{m, n\}\), and we seek algorithms that use \(o(mn)\) flops, that is, much fewer than the information lower bound \(mn\).

## 2 State of the art and our progress

The algorithms of [GE96] and [P00] compute CUR approximations by using order of \(mn \min\{m, n\}\) flops. [BW14] do this in \(O(mn \log(mn))\) flops by using randomization.

These are record upper bounds for computing a CUR approximation to any input matrix \(W\), but the user may be quite happy with having a close CUR approximations to many matrices \(W\) that make up the class of his/her interest. The information lower bound \(mn/2\) (a flop involves at most two entries) does not apply to such a restricted input classes, and we go well below it in our paper [PSZa] (we must refer to that paper for technical details because of the limitation on the size of this submission).

We first formalize the problem of CUR approximation of an average \(m \times n\) matrix of numerical rank \(r \ll \min\{m, n\}\), assuming the customary Gaussian (normal) probability distribution for its \((m + n)r\) i.i.d. input parameters.

Next we consider a two-stage approach: (i) first fix a pair of integers \(k \leq m\) and \(l \leq n\) and compute a CUR approximation (by using the algorithms of [GE96] or [P00]) to a random \(k \times l\) submatrix and then (ii) extend it to computing a CUR approximation of an input matrix \(W\) itself.

We must keep the complexity of Stage (i) low and must extend the CUR approximation from the submatrix to the matrix \(W\). We prove that for a specific class of input matrices \(W\) these two tasks are in conflict (see Example 11 of [PSZa]), but such a class of hard inputs is narrow, because we prove that our algorithm produces a close approximation to the average \(m \times n\) input matrix \(W\) having numerical rank \(r\). (We define such an average matrix by assuming the standard Gaussian (normal) probability distribution.)

By extending our two-stage algorithms with the technique of [GOSTZ10], which we call cross-approximation, we will narrow the class of hard inputs of Example 11 of [PSZa], and moreover deduce a sharper bounds on the error of approximation by maximizing the volume of an auxiliary \(k \times l\) submatrix that defines a CUR approximation.

In our extensive tests with a variety of real world input data for regularization of matrices from Singular Matrix Database, our fast algorithms consistently produce close CUR approximation.

Since our fast algorithms produce reasonably accurate CUR approximation to the average input matrix, the class of hard input matrices for these algorithms must be narrow, and we studied a tentative direction towards further narrowing this input class. We prove that the algorithms are expected to output a close CUR approximation to any matrix \(W\) if we pre-process it by applying Gaussian multipliers. This is a nontrivial result of independent interest (proven on more than three pages), but its formal support is only for application of Gaussian multipliers, which is quite costly.

We hope, however, that we can still substantially narrow the class of hard inputs even if we replace Gaussian multipliers with the products of reasonable numbers of random bidiagonal matrices and if we partly curb the permutation of these matrices. If we achieve this, then preprocessing would become non-costly. This direction seems to be quite promising, but still requires further work.

Finally, our algorithms can be extended to the acceleration of various computational problems that are known to have links to low-rank approximation, but in our concluding Section 3 we describe a novel and rather unexpected extensions to the acceleration of the Fast Multipole Method and

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1 Here and hereafter “flop” stands for “floating point arithmetic operation”.

2 State of the art and our progress
Conjugate Gradient Algorithms\footnote{Hereafter we use the acronyms FMM and CG.}, both being among the most celebrated achievements of the 20th century in Numerical Linear Algebra.

\section*{2.1 Some related results on matrix algorithms and our progress on other fundamental subjects of matrix computations}

A huge bibliography on CUR and low-rank approximation, including the known best algorithms, which we already cited, can be accessed from the papers [HMT11], [M11], [BW14] and [W14].

Our main contribution is dramatic acceleration of the known algorithms.

Some of our techniques extend the ones of [PZ16], [PZ17], and [PZa], where we also show duality of randomization and derandomization and apply it to fundamental matrix computations.

In [PZ16] we prove that preprocessing with almost any well-conditioned multiplier of full rank is as efficient on the average for low-rank approximation as preprocessing with a Gaussian one, and then we propose some new highly efficient sparse and structured multipliers. Besides providing a new insight into the subject, this motivates the design of more efficient algorithms and shows specific direction to this goal.

We obtain similar progress in [PZa] for and [PZ17] for preprocessing Gaussian elimination with no pivoting and block Gaussian elimination. We recall that Gaussian elimination with partial pivoting is performed millions times per day, where pivoting, required for numerical stabilization, is frequently a bottleneck because it interrupts the stream of arithmetic operations with foreign operations of comparison, involves book-keeping, compromises data locality, and increases communication overhead and data dependence.

Randomized preprocessing is a natural substitution for pivoting, and in [PZa] we show that Gaussian elimination with no pivoting as well as block Gaussian elimination (which is another valuable algorithm and which also requires protection against numerical problems) are efficient on the average input with preprocessing by any nonsingular and well-conditioned multipliers.

[PZ17] obtains similar progress for the important subject of the approximation of trailing singular spaces associated with the $\nu$ smallest singular values of a matrix having numerical nullity $\nu$.

Our current progress greatly supersedes these earlier results, however, in terms of the scale of the acceleration of the known algorithms.

Our technique of representing random Gaussian multipliers as a product of random bidiagonal factors, our extension of CUR approximation to FMM and CG algorithms, and our analysis of CUR approximation for the average input are new and can have some independent interest.

\section*{3 Conclusions}

We dramatically accelerated the known algorithms for the fundamental problems of CUR and low-rank approximation in the case of the average input matrix and then pointed out a direction towards heuristic extension of the resulting fast algorithm to a wider class of inputs by applying quasi Gaussian preprocessing. Our extensive tests for benchmark matrices of discretized PDEs have consistently supported the results of our formal analysis.

Our study can be extended to a variety of important subjects of matrix computations. Some of such extensions have been developed in papers [PZ10], [PZ17] and [PZa], and there are various challenging directions for further progress. In particular our accelerated CUR and low-rank approximation enables faster solution of some new important computational problems, thus extending the long list of the known applications. In the concluding section of [PSZa], we add two new highly important subjects to this long list.
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