Computational Math Project

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0 Introduction

In this paper we discuss what motivates the study of banded matrices and show several results regarding their properties. We will also consider the application of these properties to find a more efficient implementation of the Modified Gram-Schmidt Algorithm. Finally, we will discuss potential future work.

1 Origin of the problem and its applications

In this part of the project we explain the motivation behind our ideas and examine the applications of our results. First, we consider the standard elliptic equation in two dimensions

$$-\Delta u = f \quad \text{in } \Omega$$
$$u = 0 \quad \text{on } \partial\Omega.$$

Then the discretised equation on a grid is

$$-\Delta_h u_{ij} = f_{ij} \;\forall\, (x_i, y_i) \in \Omega_h,\;\; f_{ij} = f(x_i, y_j)$$
$$u_{ij} = 0 \;\forall\, (x_i, y_i) \in \partial\Omega_h,$$

where we use the second-order central differencing to represent the Laplace operator

$$-\Delta_h u_{ij} = \frac{1}{h^2}\begin{pmatrix} 0 & -1 & 0 \\ -1 & 4 & -1 \\ 0 & -1 & 0 \end{pmatrix} u_{ij} = \frac{1}{h^2}\big(- u_{ij+1} - u_{i-1j} + 4u_{ij} - u_{i+1j} - u_{ij_1}\big)$$

If we assume that the domain Ω is a square, ordering the grid points from left to right and bottom to top yields the following matrix of the system $A \in \mathbb{R}^{(h-1)^{-2} \times (h-1)^{-2}}$:

$$A = h^2 \begin{pmatrix} 4 & -1 & 0 & \dots & 0 & -1 & & \\ -1 & 4 & -1 & & & & \ddots & \\ 0 & -1 & 4 & \ddots & & & & -1 \\ \vdots & & \ddots & \ddots & & & & 0 \\ 0 & & & & & & & \vdots \\ -1 & & & & & \ddots & \ddots & 0 \\ & \ddots & & & & \ddots & 4 & -1 \\ & & -1 & 0 & \dots & 0 & -1 & 4 \end{pmatrix}$$

And, the problem we need to solve is the linear system $Au = f$.

Therefore, it is important to understand how the structure of A affects the structure of the QR decomposition. Note that in this case the highest and lowest off-diagonal has a distance of order h from the diagonal.

Another example where these banded matrices show up is in the following: consider the parabolic equation in two dimensions

$$\frac{\partial u}{\partial t} = \sigma \Delta u,\;\; 0 \leq x \leq X,\, 0 \leq y \leq Y\, 0 \leq t \leq T$$

with Dirichlet boundary condition and given initial data $u(x,y,0) = U^0(x,y)$. For the numerical implementation we consider the implicit Crank-Nicolson scheme

$$
\begin{aligned}
&-\frac{\mu_x}{2}\big(U^{n+1}_{j-1,l} + U^{n+1}_{j+1,l}\big) - \frac{\mu_y}{2}\big(U^{n+1}_{j,l-1} + U^{n+1}_{j,l+1}\big) + \big(1+\mu_x+\mu_y\big)U^{n+1}_{j,l} \\
=&\frac{\mu_x}{2}\big(U^{n}_{j-1,l} + U^{n}_{j+1,l}\big) + \frac{\mu_y}{2}\big(U^{n}_{j,l-1} + U^{n}_{j,l+1}\big) + \big(1-\mu_x-\mu_y\big)U^{n}_{j,l},
\end{aligned}
$$

for $0 \le j \le J_x$, $0 \le l \le J_y$ and $n > 0$. Again, we can rewrite this as a linear system $AU^{n+1} = U^n$, with

$$
A = \begin{pmatrix}
1+\mu_x+\mu_y & -\frac{\mu_x}{2} & 0 & \dots & 0 & -\frac{\mu_y}{2} & & \\
-\frac{\mu_x}{2} & 1+\mu_x+\mu_y & -\frac{\mu_x}{2} & & & & \ddots & \\
0 & -\frac{\mu_x}{2} & 1+\mu_x+\mu_y & \ddots & & & & -\frac{\mu_y}{2} \\
\vdots & & \ddots & \ddots & & & & 0 \\
0 & & & & & & & \vdots \\
-\frac{\mu_y}{2} & & & & & \ddots & \ddots & 0 \\
& \ddots & & & & \ddots & 1+\mu_x+\mu_y & -\frac{\mu_x}{2} \\
& & -\frac{\mu_y}{2} & 0 & \dots & 0 & -\frac{\mu_x}{2} & 1+\mu_x+\mu_y
\end{pmatrix}
$$

and $A \in \mathbb{R}^{(J_x-1)(J_y-1)\times(J_x-1)(J_y-1)}$ where the highest and lowest off-diagonal band have the distance $J_x - 1$ from the diagonal.

Remark 1. In the case of three dimension, we would obtain one more non-zero sub/super-diagonal, now with a distance of $\mathcal{O}(J_x * J_y)$ from the diagonal.

2 Matrix Properties

2.1 Tridiagonal Matrices

Theorem 2.1. *If A is a tridiagonal matrix, then R in the product $A = QR$ is an upper triangular matrix with non-zero entries only in the diagonal and first two superdiagonals.*

$$A = \begin{pmatrix} a_{11} & a_{12} & & \\ a_{21} & a_{22} & a_{23} & \\ & \ddots & \ddots & \ddots \\ & & a_{mm-1} & a_{mm} \end{pmatrix}, \ R = \begin{pmatrix} r_{11} & r_{12} & r_{13} & \\ & \ddots & \ddots & \ddots \\ & & \ddots & \ddots \\ & & & r_{mm} \end{pmatrix}$$

Pf. To prove the statement we will use the classical Gram-Schmidt (CGS) method for the QR decomposition.

Step 1: show that q_j has the form $q_j = \begin{pmatrix} * \\ \vdots \\ * \\ 0 \\ \vdots \end{pmatrix} \leftarrow j+1$-th entry.

We prove this by induction:

Base step: For $j = 1$, if we assume that $\|a_1\| = 1$, then $q_1 = a_1$. Thus

$$q_1 = \begin{pmatrix} a_{11} \\ a_{21} \\ 0 \\ \vdots \end{pmatrix}$$

Induction step: Assume that the statement holds for $j - 1$. Then

$$v_j = a_j - \sum_{k=1}^{j-1} (q_k^* a_j) q_k \quad \text{and } q_j = v_j / \|v\|_j$$

and by using the form of q_{j-1} we obtain

$$q_j = \begin{pmatrix} 0 \\ \vdots \\ a_{j-1,j} \\ a_{jj} \\ a_{j+1,j} \\ 0 \\ \vdots \end{pmatrix} - \sum_{k=1}^{j-1} \begin{pmatrix} * \\ \vdots \\ \vdots \\ * \\ 0 \\ \vdots \\ \vdots \end{pmatrix} \leftarrow k+1\text{-th entry} = \begin{pmatrix} * \\ \vdots \\ \vdots \\ * \\ 0 \\ \vdots \\ \vdots \end{pmatrix} \leftarrow j+1\text{-th entry}$$

Step 2: compute r_{ij} in the CGS method.

For j from 1 to n and for i from 1 to $j-1$, we have $r_{ij} = q_i^* a_j$. Then by step 1, if $i \leq j-3$, we obtain $r_{ij} = 0$ from the form of the vectors q_{j-3} and a_j:

$$0 = \begin{pmatrix} * \\ \vdots \\ * \\ 0 \\ 0 \\ 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix}^* \begin{pmatrix} 0 \\ \vdots \\ 0 \\ * \\ * \\ * \\ 0 \\ \vdots \\ 0 \end{pmatrix} \leftarrow j\text{-th enttry}$$

Since, the above argument holds for all $i \leq j-3$, R is non-zero only for the main diagonal and first two superdiagonals. ■

2.2 General Banded Matrices

Theorem 2.2. *If A is a banded matrix with bandwidth $2p+1$, then R in the orthogonalization $A = QR$ is an upper triangular matrix with non-zero entries only in the main diagonal and first $2p$ superdiagonals.*

Pf. If A has bandwidth $2p+1$ then for $i-j>p$,

$$0 = a_{ij} = \sum_{k=1}^{m} q_{ik} r_{kj}$$

For $k>j$, since R is upper triangular, $r_{kj}=0$. Then, when $i>j+p$,

$$0 = a_{ij} = \sum_{k=1}^{j} q_{ik} r_{kj}$$

This gives $q_{ij}=0$. Hence, for each j

$$q_j = \begin{pmatrix} q_{1,j} \\ q_{2,j} \\ \vdots \\ q_{j+p,j} \\ 0 \\ \vdots \\ 0 \end{pmatrix} \tag{1}$$

From (1), when $i+p<j-p$ (i.e., $j-i>2p$):

$$r_{ij} = q_i^* a_j = \begin{pmatrix} q_{1,i} & q_{2,i} & \dots & q_{i+p,i} & 0 & \dots & 0 \end{pmatrix} \begin{pmatrix} 0 \\ \vdots \\ 0 \\ a_{j-p,j} \\ \vdots \\ a_{j+p,j} \\ 0 \\ \vdots \\ 0 \end{pmatrix} = 0$$

Therefore, R is upper triangular with its only non-zero entries in the main diagonal and $2p$ super-diagonals. ■

2.3 Sparse Diagonal Matrices

Now we want to generalize the ideas from Theorems 2.1 and 2.2 to the case where A still has only three non-zero bands, but the lower band is distance $k-1$ from the diagonal and the upper band is distance $l-1$ from the diagonal. Consider the following example for A:

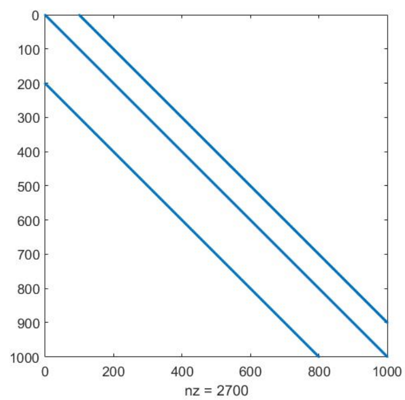
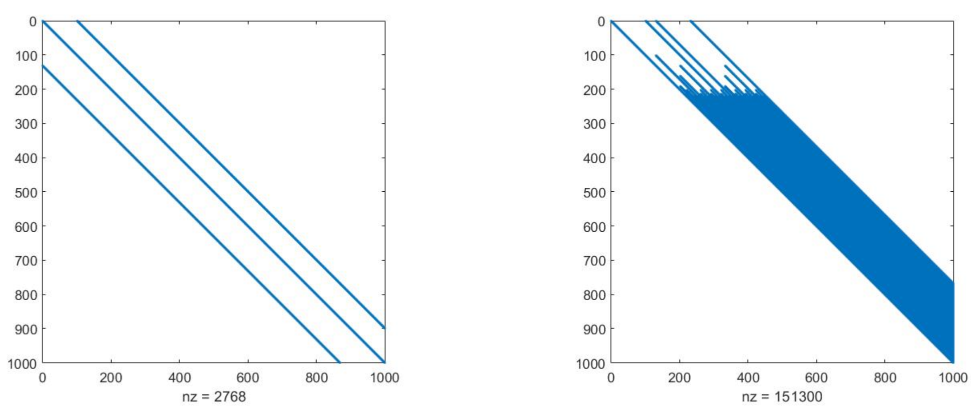


Figure 1: $k = 200$ and $l = 100$

Theorem 2.3 (General case)**.** *The upper triangular matrix R in the QR decomposition of A has a $k+l$-band structure.*

Pf. From the CGS method we immediately see, in the worst case, the first $j+k$ entries are non zero. Therefore, the inner product in the computation of the entries r_{ij} is only zero if $i < j-l-k+2$. ■

To illustrate this, consider the example of a matrix close to the worst case, where the number of non-zero entries (nz) increases by order 50:

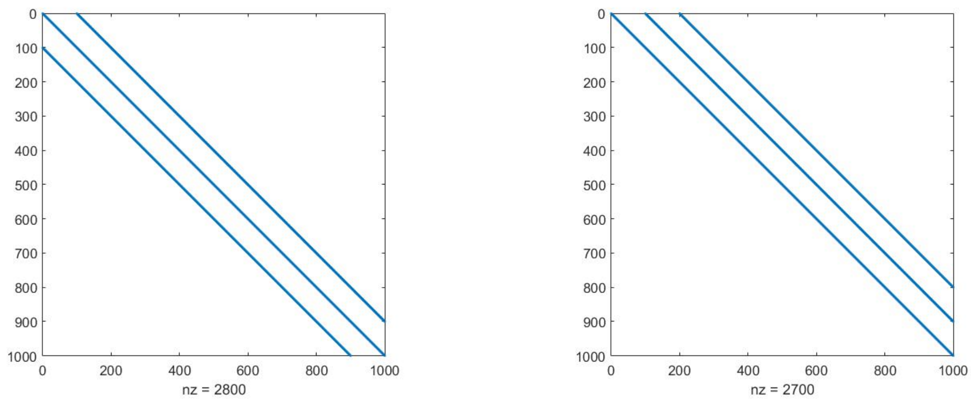


(a) A

(b) R

Figure 2: $k = 131$ and $l = 101$

A special case occurs when $k = l$. Again, R has only three non-zero bands: the main diagonal, the superdiagonal that has a distance k to the main diagonal, and the superdiagonal that has a distance $2k$ to the main diagonal. For $k = l = 100$:



(a) A

(b) R

Figure 3: $k = l = 100$

3 Algorithms and Results

Based on the properties proved in section 2, it is fairly straightforward to modify existing algorithms for finding the QR-factorization of a matrix, to exploit sparsity patterns.

3.1 General Banded Matrices

Suppose $A \in C^{m \times n}$ with bandwidth $2p + 1$. Consider the QR-factorization of A, $A = QR$. Then by Theorem 2.2, we know that if $j > i + 2p$, $r_{ij} = 0$. We can alter the well-known *Modified Gram-Schmidt* (MGS) algorithm to take advantage of this fact, as seen in Algorithm 1. Below are some results for the performance of **MGS for Banded Matrices** and the performance of the standard MGS algorithm applied to the same random banded matrices.

Performance of *Modified Gram-Schmidt* **NOT COMPLETE!**

Algorithm 1 MGS for Banded Matrices

1: **for** $i = 1$ **to** n **do**

2: $r_{ii} \leftarrow ||\mathbf{a_i}||_2$

3: $q_i \leftarrow \mathbf{a_i}/r_{ii}$

4: **for** $j = i + 1$ **to** $\min\{i + 2p, n\}$ **do**

5: $r_{ij} \leftarrow \mathbf{q_i}^*\mathbf{a_j}$

6: $\mathbf{v_j} \leftarrow \mathbf{v_j} - r_{ij}\mathbf{q_i}$

[Note that this is based on the *Modified Gram-Schmidt* algorithm as described in [1]]

$\mathbb{C}^{10\times10}$	0.0024461	0.0023396	0.0023416	0.0023403	0.0023373	0.0023707
$\mathbb{C}^{500\times500}$	5.1399053	5.0569402	5.0526341	5.0476353	5.0430921	5.3553525
$\mathbb{C}^{750\times750}$	12.0286885	12.1555834	12.3704160	12.0967193	12.5868144	12.2757503
$\mathbb{C}^{1000\times1000}$	21.6673735	21.1107465	21.1824376	21.3300323	21.0178360	22.8876292

3.2 Special Cases

In the special case of the symmetric tridiagonal matrix A, where the super and sub diagonal have a distance k from the diagonal, we can improve the **Algorithm 1** even further using **Theorem** and **Corollary**.

Algorithm 2 MGS for special tridiagonal Matrices

```
for i = 1 to n do
    v_i ← a_i
for i = 1 to n do
    r_ii ← ||v_i||_2
    q_i ← v_i/r_ii
    if i + 2k + 2 ≤ n then
        r_{i,i+2k+2} ← q_i^* a_{i+2k+2}
        v_{i+2k+2} ← v_{i+2k+2} − r_{i,i+2k+2} q_i
        r_{i,i+k+} ← q_i^* a_{i+k+1}
        v_{i+k+1} ← v_{i+k+1} − r_{i,i+k+1} q_i
    else if i + k + 1 ≤ n then
        r_{i,i+k+} ← q_i^* a_{i+k+1}
        v_{i+k+1} ← v_{i+k+1} − r_{i,i+k+1} q_i
```

3.3 Flop count

Here, we are going to give the theoretical flop count of the two algorithms and compare it with the MGS algorithm in [1].

Recall that the MGS requires $\sim 2n^3$ operations, where the most amount of work is due to an inner *for*-loop. In both of the above algorithms we can eliminate/ heavily reduce the the size of the inner *for*-loop. Therefore the first algorithm has a flop count of $\sim 8 * 2pn^2$ and the second one for the special case tridiagonal matrices we have $\sim 8n^2$ flops.

4 Further Study

There are several avenues for future work on this topic. Other algorithms, such as Householder triangularization, may be able to take advantage of the properties of banded matrices and address the poor stability of Modified Gram-Schmidt. Our report also never considers memory optimization with the use of a compressed storage format, such as Compressed Sparse Row (CSR) or diagonal form. Finally, further work may investigate the application of banded matrix properties to algorithmic parallelization of Modified Gram-Schmidt and other algorithms.

References

[1] Lloyd N. Trefethen and III David Bau. *Numerical Linear Algebra*. SIAM, Philadelphia, Pennsylvania, 1997.