Computational Math Project

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Contents

0 Introduction

1 Origin of the problem and its applications

In this part of the project we explain the motivation behind our ideas and consider the applications of the 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 and 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

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

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

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

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 the product $A = QR$ is a upper triangular matrix with non zero entries only in the diagonal and the two super diagonals.*

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

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

Step 1: we want to 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 $j = 1$ the 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 $j = 1$ to n and for $i = 1$ to $j-1$: $r_{ij} = q_i^* a_j$. Then by step 1 we obtain that $r_{ij} = 0$ if $i \leq j-3$

since then by the form of the vectors q_{j-3} and a_j

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

The above argument holds for all $i \leq j-3$. ■

2.2 General Banded Matrices

Pf. Let $A = QR$ for $A, Q \in \mathbb{C}^{m\times m}$, $R \in \mathbb{C}^{m\times m}$, unitary Q, and upper triangular R. If A has bandwidth $2p+1$ then for $i-j > p$,

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

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

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

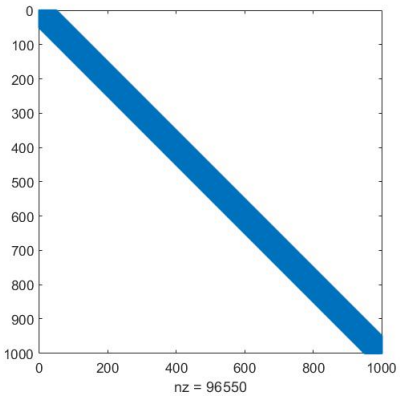
so $q_{ij} = 0$. Hence

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

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

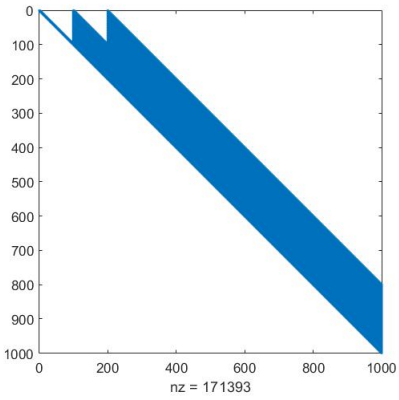
$$r_{ij} = q_i^* a_j = \begin{pmatrix} q_{1,i} & q_{2,i} & \dots & q_{i+p,i} & 0 & \dots & 0 \end{pmatrix} \begin{pmatrix} 0 \\ \vdots \\ 0 \\ a_{j-p-1,j} \\ \vdots \\ a_{j+p+1,j} \\ 0 \\ \vdots \\ 0 \end{pmatrix} = 0$$

Hence R is upper triangular with its only nonzero entries in the diagonal and $2p$ super diagonals. ■



8.jpg

(a) A

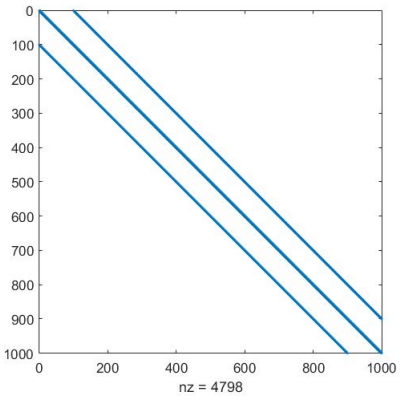


9.jpg

(b) R

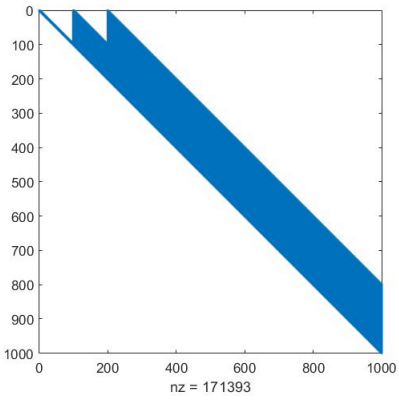
Figure 1: bandwith 101, i.e $p = 50$

Remark 2. This results also holds for the matrices considered in the first part, i.e. the matrices derived from finite difference methods.



6.jpg

(a) A



7.jpg

(b) R

Figure 2: A has the special form as in Section 1

2.3 Sparse Diagonal Matrices

Now we want to generalize the above ideas to the case where A still has only three non-zero bands. But now, the lower band has the distance $k-1$ from the diagonal and the upper band has the distance $l-1$ from the diagonal.

Consider the following example for A:

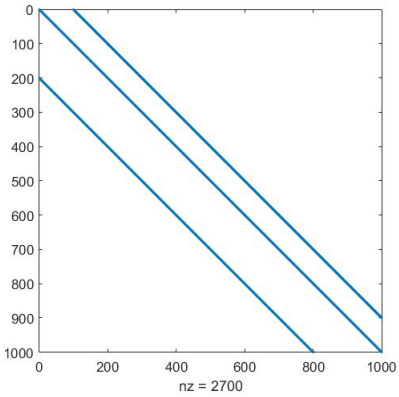


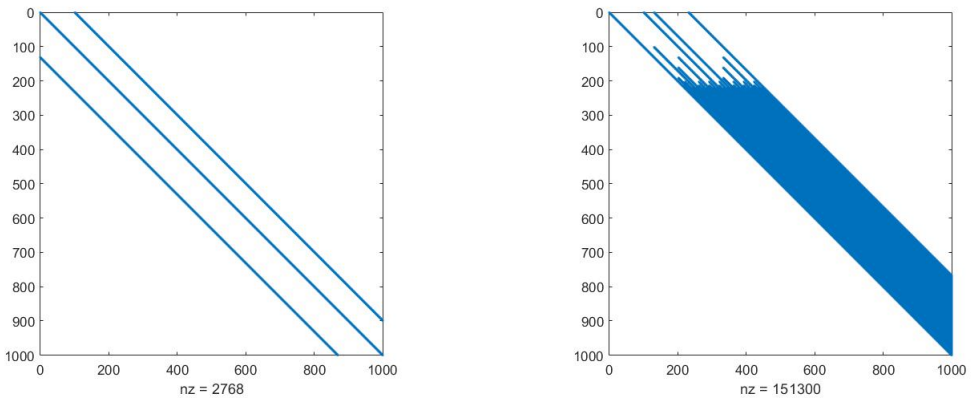
Figure 3: $k = 200$ and $l = 100$

Theorem 2.2 (General case)**.** *The upper triangular matrix R in the QR decomposition of A has*

a $k+l$-band structure.

Pf. From the classical Gram Schmidt method we immediately see, that 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 $i < j-l-k+2$. ■

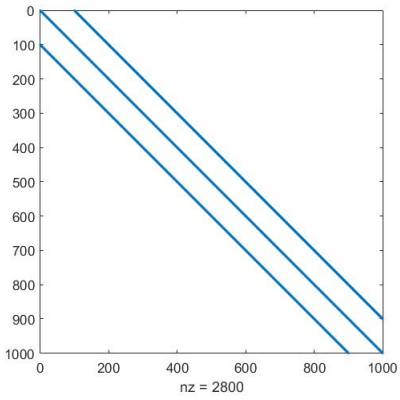
Example of a matrix close to the worst case, where the number of non-zero entries (nz) increases by order 50:



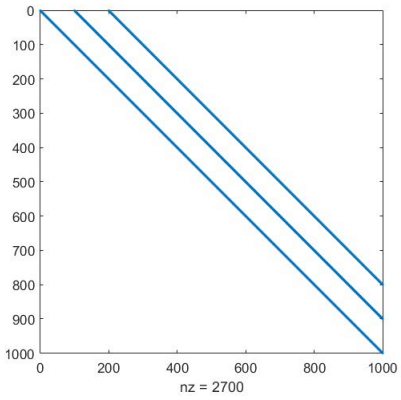
(a) A (b) R

Figure 4: $k = 131$ and $l = 101$

A special case occurs when $k = l$. Then again R has only three non-zero band, i.e the diagonal, the band on the upper diagonal that has a distance k to the diagonal and the upper diagonal that has a distance $2k$ to the diagonal.
Again we have an example for this case:



(a) A



(b) R

Figure 5: $k = l = 100$

Corollary 2.1. *Let the square matrix A have the form as mentioned in the example. Then R of the QR decomposition has the form $r_{ij} \neq 0$ only for the cases $i = j$, $i + k + 1$ and $i + 2k + 2$.*

Pf. From the ideas of the theorems before, the column vector q_i of Q in the QR decomposition has the form $q_i^* = (\underbrace{0 \dots 0}_{i \mod k} * \underbrace{0 \dots 0}_{k} * | \dots | * \underbrace{0 \dots 0}_{k} \underbrace{*}_{i-th} 0 \dots 0 * 0, \dots)$. Therefore $r_{ij} = q_i^* a_j = 0$ for $i \neq j$ or $i + k + 1 \neq j$ or $i + 2k + 2 \neq j$. ■

3 Algorithms and Results

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

3.1 General Banded Matrices

Suppose $A \in C^{m \times n}$ with bandwidth p. Consider some QR-factorization of A, $A = QR$. Then by **THEOREM**, we know that if $j > i + 2p$, $r_{ij} = 0$. We can alter the well-known *Modified Gram-Schmidt* algorithm to take advantage of the above fact in the following way.

Algorithm 1 MGS for Banded Matrices

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

2: $\quad v_i \leftarrow a_i$

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

4: $\quad r_{ii} \leftarrow ||\mathbf{v_i}||_2$

5: $\quad q_i \leftarrow \mathbf{v_i}/r_{ii}$

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

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

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

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

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!**

$\mathbb{C}^{10\times10}$	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

1: **for** $i = 1$ **to** n **do**
2: $\quad v_i \leftarrow a_i$
3: **for** $i = 1$ **to** n **do**
4: $\quad r_{ii} \leftarrow ||\mathbf{v_i}||_2$
5: $\quad q_i \leftarrow \mathbf{v_i}/r_{ii}$
6: $\quad$ **if** $i + 2k + 2 \leq n$ **then**
7: $\quad\quad r_{i,i+2k+2} \leftarrow \mathbf{q_i}^* \mathbf{a_{i+2k+2}}$
8: $\quad\quad \mathbf{v_{i+2k+2}} \leftarrow \mathbf{v_{i+2k+2}} - r_{i,i+2k+2}\mathbf{q_i}$
9: $\quad\quad r_{i,i+k+} \leftarrow \mathbf{q_i}^* \mathbf{a_{i+k+1}}$
10: $\quad\quad \mathbf{v_{i+k+1}} \leftarrow \mathbf{v_{i+k+1}} - r_{i,i+k+1}\mathbf{q_i}$
11: $\quad$ **else if** $i + k + 1 \leq n$ **then**
12: $\quad\quad r_{i,i+k+} \leftarrow \mathbf{q_i}^* \mathbf{a_{i+k+1}}$
13: $\quad\quad \mathbf{v_{i+k+1}} \leftarrow \mathbf{v_{i+k+1}} - r_{i,i+k+1}\mathbf{q_i}$

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

References

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