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Note

On the ordering of sparse linear systems [1]

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Abstract

In this paper we consider the algorithms for transforming an $n \times n$ sparse matrix A into another matrix B such that Gaussian elimination applied to B takes time asymptotically less than n^3. These algorithms take the sparse matrix A as input, and return a pair of permutation matrices P, Q such that $B = PAQ$ has a small bandwidth, or some other desirable form. We study the average effectiveness of these algorithms by using random matrices with $\Theta(n)$ nonzero elements. We prove that with high probability these algorithms cannot produce a reduction of the asymptotic cost of the standard Gaussian elimination algorithm.

We also study the effectiveness of these algorithms for ordering very sparse matrices. We show that there exist matrices with $3n$ nonzeros for which reordering rows and columns does not reduce the asymptotic cost of Gaussian elimination. We also prove that each matrix with at most two nonzeros in each row and in each column, can be transformed into a banded matrix with bandwidth five.

1. Introduction

In this paper we consider the problem of solving the linear system $A\boldsymbol{x} = \boldsymbol{b}$, where A is an $n \times n$ sparse matrix. A classical method for solving this problem is Gaussian elimination that basically computes the LU factorization of the coefficient matrix A. If A is sparse, Gaussian elimination is usually applied to the matrix PAQ, where P and Q are permutation matrices chosen to guarantee numerical stability, and to reduce the computational cost. In fact, during the elimination process, new nonzero elements are generated, and the coefficient matrix tends to become less sparse. Introducing the matrices P and Q changes the order in which equations and unknowns are numbered. Different orderings yield different sets of new nonzero elements, and

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also different operation counts for the elimination algorithm. The set of new nonzeros generated during the elimination process is called the *fill-in*. The problem of finding an ordering that minimizes the fill-in is NP-complete [10, 12], but many heuristic algorithms have been suggested, with the goal of reducing, if not minimizing, the fill-in.

If the matrix A is symmetric and positive definite, then, by taking $Q = P^{\mathrm{T}}$, we have the guarantee that no pivoting is needed. For this class of matrices, the performance of the ordering algorithms has been extensively studied. Lipton et al. [7] proved that there exists a good ordering for A only if the graph associated with A has good separators. This result implies that "almost all" sparse symmetric matrices *do not* have good orderings, i.e. for any permutation matrix P, PAP^{T} has fill-in of size $\Theta(n^2)$, i.e. the Cholesky factor is essentially dense. In the same paper, Lipton et al. proved that, if the graph associated with A is planar, the factorization of A can be computed in $\mathrm{O}(n^{3/2})$ time. Their algorithm is a variant of the nested dissection algorithm [3], and produces an ordering yielding a fill-in of size $\mathrm{O}(n \log n)$. Recently, Agrawal et al. [1] presented a nested dissection algorithm that finds an ordering yielding a fill-in which is within a factor $\mathrm{O}(\log^4 n)$ of the optimum. Moreover, for the same ordering, the operation count for Gaussian elimination is within a factor $\mathrm{O}(\log^6 n)$ of the optimum.

If the matrix A is not symmetric, fewer results are known on the performance of the ordering algorithms. Although the concepts of "separator" and "nested dissection" can be extended to the unsymmetric case (see for example [8]), numerical stability has to be taken into account, and the "best" ordering depends also on the values of the nonzero elements of A.

The algorithms for reordering an unsymmetric matrix A can be broadly divided into two classes. The algorithms of the first class [2, 4, 5] build the ordering during the elimination process. More precisely, at each elimination step, the pivot is chosen so that the number of new nonzero elements is small. The algorithms of the second class [2, 4, 9, 11] find two permutation matrices P and Q so that PAQ has a small bandwidth, or some other desirable form (see Fig. 1). When Gaussian elimination – with partial pivoting – is executed, the fill-in may occur only in a small area, and the operation count can be much smaller than $\Theta(n^3)$ (which is the cost of Gaussian elimination for a dense matrix).

In this paper we analyze the average performance of the algorithms of the second class. We introduce four different probability measures on the set of sparse matrices, and we estimate the probability that these algorithms allow one to compute sparse Gaussian elimination in $\mathrm{o}(n^3)$ time. We prove that for matrices with more than $10n$ nonzero elements such probability is very small. More precisely, for a random matrix A, we prove that, with high probability, *for each* pair of permutation matrices P, Q, Gaussian elimination applied to PAQ takes $\Theta(n^3)$ time. This result holds only for the standard elimination algorithm, i.e. we do not consider algorithms that take advantage of the presence of zero elements *within* the shaded areas of the matrices of Fig. 1. The proof of this result follows from the fact that, with probability $1 - 2^{-n/2}$,

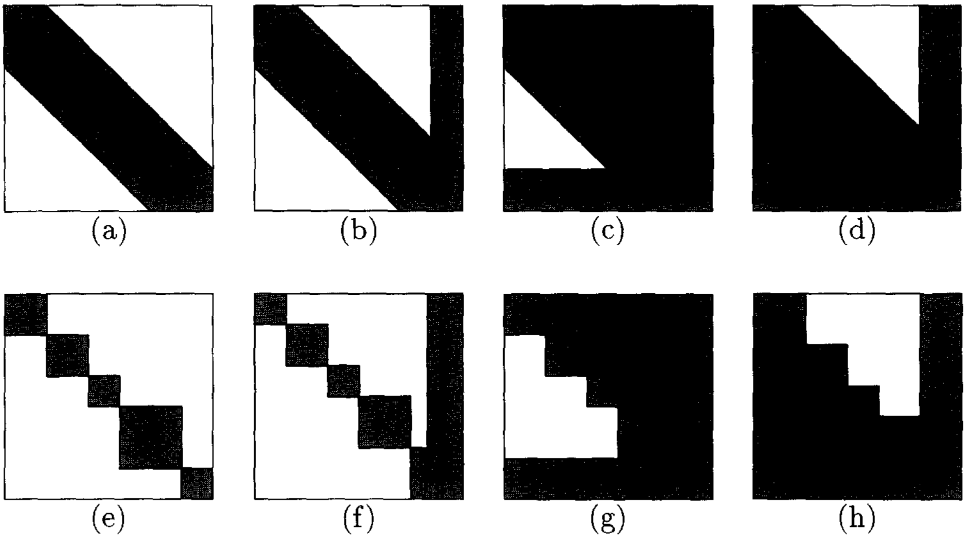

Fig. 1. Some desirable forms for Gaussian elimination. (a) band form, (b) bordered band form, (c) upper triangular bordered band form, (d) lower triangular bordered band form, (e) block diagonal form, (f) bordered block diagonal form, (g) upper triangular bordered block diagonal form, (h) lower triangular bordered block diagonal form.

the graph associated with a random sparse matrix has the property of being a *weak-expander*.

We also study the effectiveness of these algorithms for reordering very sparse matrices. We prove that each matrix containing at most two nonzeros in each row and in each column, can be transformed, in $O(n)$ time, into a banded matrix with bandwidth five. Unfortunately, a similar result does not hold when the number of nonzero elements increases. We show that there exist matrices with three nonzeros in each row and in each column, for which these ordering algorithms do not produce a reduction in the computational cost of Gaussian elimination. This completes a result obtained by Gilbert [6] for the symmetric case. He proved that there exists a symmetric positive definite matrix A with four nonzeros per row that does not have good orderings, i.e. for any permutation matrix P, PAP^T has fill-in $\Theta(n^2)$.

Throughout the paper, we use the standard O-notation, i.e. we say $f(n) = O(g(n))$ if $f(n)/g(n)$ is bounded for $n \to \infty$; we say $f(n) = \Theta(g(n))$ if both $f(n)/g(n)$ and $g(n)/f(n)$ are bounded for $n \to \infty$; we say $f(n) = o(g(n))$ if $\lim_{n\to\infty} f(n)/g(n) = 0$.

The rest of this paper is organized as follows. In Section 2 we introduce four probability measures on the set of sparse matrices, and we prove some properties of random matrices. This section is rather technical and the reader can skip the proofs of the lemmas without affecting his/her comprehension of the material presented next. In Section 3 we analyze the average effectiveness of the ordering algorithms, and in Section 4 we study the behavior of ordering algorithms for very sparse matrices. Section 5 contains some concluding remarks.

2. Preliminaries

In order to study the average effectiveness of the ordering algorithms, we introduce four probability measures on the set of $n \times n$ sparse matrices. Each measure represents a different type of sparse matrix. Since the behavior of the ordering algorithms does not depend on the numerical values, all measures are defined on the set of 0–1 matrices, where 1 represents a generic nonzero. Note that this set contains 2^{n^2} elements.

1. Let $0 \leqslant d_1 \leqslant n$ such that $d_1 n$ is an integer. We denote by $\mathscr{M}_1$ the probability measure such that $\Pr\{A\} \neq 0$ only if the matrix A has exactly $d_1 n$ nonzero elements; moreover, all $\binom{n^2}{d_1 n}$ matrices with $d_1 n$ nonzeros are equally likely.
2. Let $0 \leqslant d_2 \leqslant n$, $p = d_2/n$. We denote by $\mathscr{M}_2$ the probability measure such that for all i,j $\Pr\{a_{ij} \neq 0\} = p$. Hence, we have $\Pr\{A\} = p^k(1-p)^{n^2-k}$, where k is the number of nonzero elements of A.
3. Let d_3 be an integer s.t. $0 \leqslant d_3 \leqslant n$. We denote by $\mathscr{M}_3$ the probability measure such that $\Pr\{A\} \neq 0$ only if each row of A contains exactly d_3 nonzero elements; moreover, all $\binom{n}{d_3}^n$ matrices with d_3 nonzeros per row are equally likely.
4. Let d_4 be an integer s.t. $0 \leqslant d_4 \leqslant n$. We denote by $\mathscr{M}_4$ the probability measure such that $\Pr\{A\} \neq 0$ only if each column of A contains exactly d_4 nonzero elements; moreover, all $\binom{n}{d_4}^n$ matrices with d_4 nonzeros per column are equally likely.

In the following, the expression "random matrix" will denote a matrix chosen according to one of the probability measures $\mathscr{M}_1$–$\mathscr{M}_4$.

Let $X = \{x_1, \ldots, x_n\}$, and $Y = \{y_1, \ldots, y_n\}$. Given an $n \times n$ matrix A, we consider the formal product $\boldsymbol{y} = A\boldsymbol{x}$, and we associate with the matrix A a directed bipartite graph $G(A)$, called the *dependency graph*. The vertex set of $G(A)$ is $X \cup Y$ and (x_i, y_j) is an edge of $G(A)$ if and only if $a_{ji} \neq 0$. In other words, the vertices of $G(A)$ represent the components of $\boldsymbol{x}$ and $\boldsymbol{y}$, and the edge $(x_i, y_j) \in G(A)$ if and only if the value y_j depends on x_i. Given $U \subseteq X$, we define $\mathrm{Adj}(U) = \{y \in Y \mid y \text{ is adjacent to } x \in U\}$.

Let $1 < \beta < 2$. We say that the graph $G(A)$ is a *β-weak-expander* if, for each set $U \subseteq X$, the following property holds:

$$|U| = \lfloor n/2 \rfloor \implies |\mathrm{Adj}(U)| > \beta |U|.$$

The notion of weak-expander is similar to the well known notion of expander graph (we remind that a graph is an (α, β, n)-expander if $|U| \leqslant n\alpha$ implies $|\mathrm{Adj}(U)| > \beta|U|$).

Given a random matrix A we want to estimate the probability that the graph $G(A)$ is a β-weak-expander. In this section we prove that, for the measures $\mathscr{M}_1$–$\mathscr{M}_4$ previously defined, such probability is very close to one.

We will make use of some well known inequalities. For $n \geqslant 1$, we have

$$\sqrt{2\pi n}(n/\mathrm{e})^n < n! < \sqrt{2\pi n}(n/\mathrm{e})^n \mathrm{e}^{1/12}, \tag{1}$$

which is a sharp form of Stirling's formula. For $0 \leqslant k \leqslant n$, we have

$$\binom{n}{k} \leqslant \left(\frac{\mathrm{e}n}{k}\right)^k, \tag{2}$$

and, for any real number $x \geqslant 1$, we have

$$\left(1 - \frac{1}{x}\right)^x < e^{-1}. \tag{3}$$

Lemma 2.1. *Let N, Z, m be positive integers such that $Z + m \leqslant N$. Then*

$$\binom{N-Z}{m} \cdot \binom{N}{m}^{-1} \leqslant \left(1 - \frac{m}{N}\right)^Z.$$

Proof. We have

$$\begin{aligned}
\binom{N-Z}{m} \cdot \binom{N}{m}^{-1} &= \frac{(N-Z)!(N-m)!}{N!(N-Z-m)!} \\
&= \frac{(N-m)(N-m-1)\cdots(N-m-Z+1)}{N(N-1)\cdots(N-Z+1)} \\
&= \left(1 - \frac{m}{N}\right)\left(1 - \frac{m}{N-1}\right)\cdots\left(1 - \frac{m}{N-Z+1}\right) \\
&\leqslant \left(1 - \frac{m}{N}\right)^Z. \quad \square
\end{aligned}$$

Lemma 2.2. *Let $1 \leqslant i \leqslant 4$, and let A be a random matrix chosen accordingly to the probability measure $\mathcal{M}_i$. If $U \subseteq X$, $V \subseteq Y$, then*

$$\Pr\{\mathrm{Adj}(U) \cap V = \emptyset\} \leqslant \left(1 - \frac{d_i}{n}\right)^{|U|\,|V|}. \tag{4}$$

Proof. Let $Q = \{a_{ji} \mid x_i \in U, y_j \in V\}$. We have $|Q| = |U|\,|V|$ and $\mathrm{Adj}(U) \cap V = \emptyset$ if and only if $a_{ji} = 0$ for all $a_{ji} \in Q$. For the probability measure $\mathcal{M}_1$, using Lemma 2.1, we have

$$\Pr\{\mathrm{Adj}(U) \cap V = \emptyset\} = \binom{n^2 - |Q|}{d_1 n}\binom{n^2}{d_1 n}^{-1} \leqslant \left(1 - \frac{d_1}{n}\right)^{|U|\,|V|}$$

For the probability measure $\mathcal{M}_2$ we have trivially

$$\Pr\{\mathrm{Adj}(U) \cap V = \emptyset\} = \left(1 - \frac{d_2}{n}\right)^{|U|\,|V|}.$$

For the probability measure $\mathcal{M}_3$ we have $\mathrm{Adj}(U) \cap V = \emptyset$ only if the $|V|$ rows corresponding to V do not contain nonzeros in the $|U|$ columns corresponding to U. Using Lemma 2.1 we have

$$\Pr\{\mathrm{Adj}(U) \cap V = \emptyset\} = \left[\binom{n - |U|}{d_3}\binom{n}{d_3}^{-1}\right]^{|V|} \leqslant \left(1 - \frac{d_3}{n}\right)^{|U|\,|V|}$$

An analogous reasoning yields for the probability measure $\mathcal{M}_4$

$$\Pr\{\mathrm{Adj}(U) \cap V = \emptyset\} = \left[\binom{n-|V|}{d_4}\binom{n}{d_4}^{-1}\right]^{|U|} \leqslant \left(1 - \frac{d_4}{n}\right)^{|U||V|}. \qquad \Box$$

Lemma 2.3. *If $n > 1, n \geqslant d$, then*

$$\left(1 - \frac{d}{n}\right)^{\lfloor n/2 \rfloor} < \mathrm{e}^{1/2 - d/2}.$$

Proof. If $1 - d/n < \mathrm{e}^{-1}$, then

$$\left(1 - \frac{d}{n}\right)^{\lfloor n/2 \rfloor} < \mathrm{e}^{-(n-1)/2} \leqslant \mathrm{e}^{1/2 - d/2}.$$

If $1 - d/n \geqslant \mathrm{e}^{-1}$, using (3) we have

$$\left(1 - \frac{d}{n}\right)^{\lfloor n/2 \rfloor} \leqslant \left(1 - \frac{d}{n}\right)^{-1/2}\left(1 - \frac{d}{n}\right)^{n/2} < \mathrm{e}^{1/2 - d/2}. \qquad \Box$$

Lemma 2.4. *Let $U \subseteq X$, $|U| = \lfloor n/2 \rfloor$, and assume that* (4) *holds. If*

$$d_i \geqslant 2\left[\tfrac{3}{2} + \log\gamma + \gamma(\log 2 + \tfrac{1}{2})\right], \qquad \gamma = \frac{1}{1 - \beta/2}, \tag{5}$$

then

$$\Pr\{|\mathrm{Adj}(U)| \leqslant \beta|U|\} < \left(2\mathrm{e}^{1/2}\right)^{-n}.$$

Proof. First note that

$$\Pr\{|\mathrm{Adj}(U)| \leqslant \beta|U|\} = \Pr\{|\mathrm{Adj}(U)| \leqslant \lfloor \beta|U| \rfloor\}.$$

We have that $|\mathrm{Adj}(U)| \leqslant \lfloor \beta|U| \rfloor$ only if there exists a set $\tilde{V} \subseteq Y$, with $|\tilde{V}| = n - \lfloor \beta|U| \rfloor$, such that $\mathrm{Adj}(U) \cap \tilde{V} = \emptyset$. Since there are $\binom{n}{n - \lfloor \beta|U| \rfloor}$ sets V of size $n - \lfloor \beta|U| \rfloor$, if (4) holds then

$$\Pr\{|\mathrm{Adj}(U)| \leqslant \beta|U|\} \leqslant \binom{n}{n - \lfloor \beta|U| \rfloor}\left(1 - \frac{d_i}{n}\right)^{|U|(n - \lfloor \beta|U| \rfloor)}.$$

From (2), using Lemma 2.3, we have

$$\begin{aligned}
\Pr\{|\mathrm{Adj}(U)| \leqslant \beta|U|\} &\leqslant \left(\frac{\mathrm{e}n}{n - \lfloor \beta|U| \rfloor}\right)^{n - \lfloor \beta|U| \rfloor}\left(1 - \frac{d_i}{n}\right)^{|U|(n - \lfloor \beta|U| \rfloor)} \\
&\leqslant \left[\frac{\mathrm{e}}{1 - \beta/2}\left(1 - \frac{d_i}{n}\right)^{\lfloor n/2 \rfloor}\right]^{n - \lfloor \beta|U| \rfloor} \\
&\leqslant \left[\gamma \mathrm{e}^{3/2 - d_i/2}\right]^{n - \lfloor \beta|U| \rfloor}.
\end{aligned}$$

From (5) it follows that

$$\gamma e^{3/2-d_i/2} \leqslant \left(2e^{1/2}\right)^{-\gamma} < 1,$$

hence

$$\begin{aligned}\Pr\{|\mathrm{Adj}(U)| \leqslant \beta|U|\} &< \left(2e^{1/2}\right)^{-n(1-\beta/2)\gamma} \\ &= \left(2e^{1/2}\right)^{-n}. \quad \square\end{aligned}$$

Lemma 2.5. *Let A be an $n \times n$ random matrix for which* (4) *holds. If d_i satisfies* (5), *then the graph $G(A)$ is a β-weak-expander with probability greater than $1-(\sqrt{2})^{-n}$.*

Proof. The graph $G(A)$ is not a β-weak-expander only if there exists a set $U \subseteq X$ with $|U| = \lfloor n/2 \rfloor$ such that $|\mathrm{Adj}(U)| \leqslant \beta|U|$. The probability that a set of size $\lfloor n/2 \rfloor$ is connected to less than $\beta\lfloor n/2 \rfloor$ vertices is given by Lemma 2.4. Since there are $\binom{n}{\lfloor n/2 \rfloor}$ such sets, we have

$$\begin{aligned}\Pr\{G(A) \text{ is not a } \beta\text{-weak-expander}\} &< \binom{n}{\lfloor n/2 \rfloor}\left(2e^{1/2}\right)^{-n} \\ &\leqslant \left(\frac{en}{\lfloor n/2 \rfloor}\right)^{\lfloor n/2 \rfloor}\left(2e^{1/2}\right)^{-n}.\end{aligned}$$

Let $f(t) = (m/t)^t$, since $f'(t) > 0$ for $m/t > e$, we have

$$\begin{aligned}\Pr\{G(A) \text{ is not a } \beta\text{-weak-expander}\} &< (2e)^{n/2}\left(2e^{1/2}\right)^{-n} \\ &= (\sqrt{2})^{-n}.\end{aligned}$$

This completes the proof. $\square$

From Lemmas 2.2 and 2.5 we obtain the main results of this section.

Theorem 2.6. *Let A be a matrix chosen at random from distribution $\mathcal{M}_i$ $i = 1,\ldots,4$. If d_i satisfies* (5), *then the graph $G(A)$ is a β-weak-expander with probability greater than $1-(\sqrt{2})^{-n}$.*

For example, for $\beta = 16/15$ inequality (5) becomes $d_i \geqslant 9.63\ldots$. If this condition is met, $G(A)$ is a 16/15-weak-expander with probability greater than $1-(\sqrt{2})^{-n}$. Similarly, if $d_i \geqslant 11.32\ldots$ $G(A)$ is a 5/4-weak-expander with very high probability.

If $G(A)$ is a β-weak-expander, given $U \subseteq X$ such that $|U| = \lfloor n/2 \rfloor$, there are more than $\beta|U|$ values y_j's that depend on the values $x_i \in U$. It is interesting to note that, if $G(A^{\mathrm{T}})$ is a β-weak-expander, given $V \subseteq Y$ $|V| = \lfloor n/2 \rfloor$ the values $y_j \in V$ depend on more than $\beta|V|$ values x_i's. The following theorem gives a lower bound to the probability that both these properties hold.

Theorem 2.7. *Let A be a matrix chosen at random from distribution $\mathcal{M}_i$ $i = 1, \ldots, 4$. If d_i satisfies* (5), *then the probability that both $G(A)$ and $G(A^{\mathrm{T}})$ are β-weak-expanders is greater than $1 - 2(\sqrt{2})^{-n}$.*

Proof. It is straightforward to verify that Lemma 2.2 holds also for the matrix A^{T}. By Lemma 2.5, we know that $G(A^{\mathrm{T}})$ is a β-weak-expander with probability greater than $1 - (\sqrt{2})^{-n}$. The theorem follows from elementary properties of probability measures. □

The following result justifies the use of weak-expanders in the study of ordering algorithms.

Theorem 2.8. *Let A be an $n \times n$ matrix, and let P, Q be permutation matrices. Then*

$$G(A) \text{ is a } \beta\text{-weak-expander} \iff G(PAQ) \text{ is a } \beta\text{-weak-expander.}$$

Proof. The proof is straightforward since the graphs $G(A)$ and $G(PAQ)$ are isomorphic, i.e. they differ only in the labeling of the vertices. □

3. The average effectiveness of ordering algorithms

In this section we analyze the average effectiveness of the ordering algorithms described in Section 1. These algorithms take a sparse matrix A as input, and return a pair of permutation matrices P, Q such that PAQ has one of the forms shown in Fig. 1. When Gaussian elimination – with partial pivoting – is applied to PAQ, we have the following well known behaviors.

1. If PAQ is in band or bordered band form, during Gaussian elimination the size of the band at most doubles. If the bands have size $\Theta(m)$, then Gaussian elimination takes $\Theta(m^2 n)$ time.
2. If PAQ is in block or bordered block form, the fill-in occurs only within the shaded area. If bands and blocks have size $\Theta(m)$, then Gaussian elimination takes $\Theta(m^2 n)$ time.
3. If PAQ is in upper or lower triangular bordered band (or bordered block) form, the fill-in occurs only within the shaded area. If bands and blocks have size $\Theta(m)$, then Gaussian elimination takes $\Theta(mn^2)$ time.

These results hold for the standard elimination algorithm that does not take advantage of the presence of zero elements within the shaded regions of the matrices of Fig. 1. In this section we prove that, with high probability, reordering rows and columns does not allow one to execute Gaussian elimination in $o(n^3)$ time. We consider only the algorithms for transforming a matrix into upper or lower triangular bordered band form, since all other special forms are clearly more difficult to achieve.

We say that an $n \times n$ matrix A is in upper triangular (d, b)-bordered band form, if $a_{ij} \neq 0$ implies $i < j + d$ or $i > n - b$. We say that A is in lower triangular (d, b)-bordered band form, if A^{T} is in upper triangular (d, b)-bordered band form.

Lemma 3.1. *Let A be a matrix such that $G(A)$ is a β-weak-expander. Suppose that there exist two permutation matrices P, Q such that $B = PAQ$ is in upper triangular (d,b)-bordered band form. Then $d + b > 1 + (\beta - 1)\lfloor n/2 \rfloor$.*

Proof. Let $k = \lfloor n/2 \rfloor$ and consider the set $U \subseteq G(B)$, $U = \{1,2,\ldots,k\}$. By Theorem 2.8, we know that $G(B)$ is a β-weak-expander, hence $|\mathrm{Adj}(U)| > \beta\lfloor n/2 \rfloor$.

Since B is in upper triangular (d,b)-bordered band form we have

$$\mathrm{Adj}(U) = \{1,2,\ldots,k\} \cup \{k+1, k+2, \ldots, k+d-1\} \cup \{n-b+1, n-b+2, \ldots, n\},$$

hence $|\mathrm{Adj}(U)| \leqslant k + d + b - 1$. It follows that $\lfloor n/2 \rfloor + d + b - 1 > \beta\lfloor n/2 \rfloor$, that implies $d + b > 1 + (\beta - 1)\lfloor n/2 \rfloor$. □

Suppose for example that $G(A)$ is a 5/4-weak-expander. Then, if $B = PAQ$ is in upper triangular (d,b)-bordered band form, $b + d > 1 + \frac{1}{4}\lfloor \frac{n}{2} \rfloor \approx \frac{n}{8}$. In other words, even if we try all $(n!)^2$ pairs of permutation matrices it is not possible to reduce $b+d$ below this threshold.

Lemma 3.2. *Let A be a matrix such that $G(A^{\mathrm{T}})$ is a β-weak-expander. Suppose that there exist two permutation matrices P, Q such that $B = PAQ$ is in lower triangular (d,b)-bordered band form. Then $d + b > 1 + (\beta - 1)\lfloor n/2 \rfloor$.*

Proof. We have that $B^{\mathrm{T}} = Q^{\mathrm{T}}A^{\mathrm{T}}P^{\mathrm{T}}$ is in upper triangular (d,b)-bordered band form. The thesis follows from Lemma 3.1. □

From Lemmas 3.1, 3.2, and Theorem 2.7 we have the following result.

Theorem 3.3. *Let A be a matrix chosen at random from distribution $\mathscr{M}_i$ $i = 1,\ldots,4$, and assume that d_i satisfies (5). The probability that there exists a pair of permutation matrices P, Q such that PAQ is in lower or upper triangular (d,b)-bordered band form with $b + d \leqslant 1 + (\beta - 1)\lfloor n/2 \rfloor$, is less than $2^{1-n/2}$. In particular, if $d_i \geqslant 9.63\ldots$ we have $d + b > n/30$ with probability greater than $1 - 2^{1-n/2}$.*

This theorem implies that any ordering algorithm will leave most of the matrices with $\approx 10n$ nonzero elements in (d,b)-bordered band form with $b + d = \Theta(n)$. Since $b + d = \Theta(n)$ implies that Gaussian elimination takes $\Theta(n^3)$ time, we have that the asymptotic cost of the elimination algorithm cannot be reduced by reordering the rows and columns of the coefficient matrix.

4. Ordering matrices with at most two or three nonzeros per row

By Theorem 3.3 we know that, with high probability, we cannot transform a matrix with more than $10n$ nonzeros into (d,b)-bordered band form with $b + d = \mathrm{o}(n)$. In

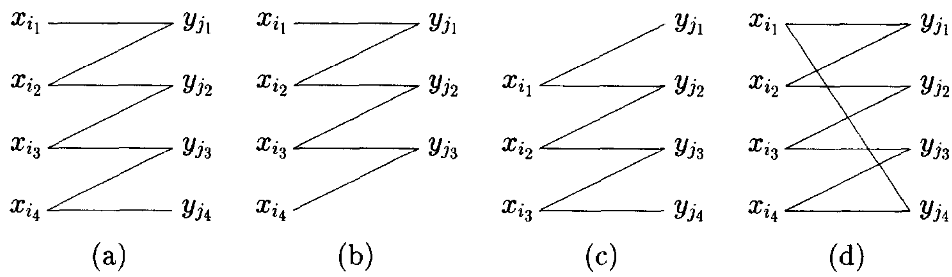

Fig. 2. The four possible types of connected components of $G(A)$. (a) Balanced chain, (b) X-chain, (c) Y-chain, (d) ring.

this section we study the effectiveness of the ordering algorithms for matrices with $2n$ and $3n$ nonzero elements.

We need a preliminary lemma.

Lemma 4.1. *For any integer $m \geqslant 1$ there exists a one-to-one function $f_m : \{1,\dots,m\} \to \{1,\dots,m\}$ such that, for $i = 1,\dots,m-1$, $|f_m(i+1) - f_m(i)| \leqslant 2$ and $|f_m(m) - f_m(1)| = 1$.*

Proof. Take $f_m(i) = 2i - 1$ for $i \leqslant \lceil m/2 \rceil$, and $f_m(i) = 2m - 2i + 2$ for $i > \lceil m/2 \rceil$. □

Theorem 4.2. *Let A be a matrix in which each row and each column contains at most two nonzero elements. Then, there exists a pair of permutation matrices P, Q such that $B = PAQ$ is a banded matrix with bandwidth five (i.e. $b_{ij} = 0$ if $|i-j| > 2$). Moreover, the matrices P and Q can be computed in $O(n)$ time.*

Proof. Clearly, it suffices to prove that there exist two permutations τ, σ such that $a_{ji} \neq 0$ implies $|\tau(j) - \sigma(i)| \leqslant 2$. Since there is a one-to-one correspondence between nonzeros of A and edges of $G(A)$, this is equivalent to proving that $(x_i, y_j) \in G(A)$ implies $|\tau(j) - \sigma(i)| \leqslant 2$.

We consider the connected components of $G(A)$. Since each vertex has degree at most two, there are only four possible types of connected components (see Fig. 2).

1. The *balanced chain*, which is composed of an even number of vertices.
2. The *X-chain*, which is composed of an odd number of vertices; the first and the last vertex both belong to X.
3. The *Y-chain*, which is composed of an odd number of vertices; the first and the last vertex both belong to Y. Note that the number of Y-chains is equal to the number of X-chains.
4. The *ring*, in which each vertex has degree two.

Note that, by inserting a dummy edge, an X-chain and a Y-chain can be linked together to form a balanced chain. This allows us to consider only two types of connected components: rings and balanced chains.

Let $\gamma = \langle x_{i_1}, y_{j_1}, x_{i_2}, y_{j_1}, \ldots, x_{i_m}, y_{i_m} \rangle$ a balanced chain of size $2m$, and let $z \leqslant n - m$. By taking $\sigma(i_k) = z + k$, and $\tau(j_k) = z + k$ all nonzeros of γ are moved into an $m \times m$ diagonal block. Moreover, $(x_i, y_j) \in \gamma$ implies $|\tau(j) - \sigma(i)| \leqslant 1$.

Similarly, if $\gamma' = \langle x_{i_1}, y_{j_1}, x_{i_2}, y_{j_1}, \ldots, x_{i_m}, y_{i_m} \rangle$ is a ring of size $2m$, by taking $\sigma(i_k) = z' + f_m(k)$, and $\tau(j_k) = z' + f_m(k)$ all nonzeros of γ' are moved into a diagonal block, and $(x_i, y_j) \in \gamma'$ implies $|\tau(j) - \sigma(i)| \leqslant 2$.

In other words, by permuting rows and columns of A, the nonzeros of each connected component can be moved into a diagonal block of bandwidth at most five. By combining these permutations the whole matrix A can be transformed into a block diagonal matrix of bandwidth at most five.

It is straightforward to verify that the connected components of $G(A)$, and the permutations τ, σ can be determined in $O(n)$ time. □

From Theorem 4.2, we do not obtain a new result on the complexity of Gaussian elimination. In fact, it is already known that the factorization of a matrix with two nonzeros in each column takes $O(n)$ time. However, Theorem 4.2 shows that, when the number of nonzeros is small, it is possible to significantly reduce the bandwidth of the matrix. Unfortunately, this is no longer true when the number of nonzero elements increases. The following theorem establishes that there exist matrices with $3n$ nonzeros for which reordering rows and columns does not allow us to execute Gaussian elimination in $o(n^3)$ time.

Theorem 4.3. *For all $n \geqslant 5$, there exists an $n \times n$ matrix $\tilde{A}$ such that*
1. *each row and each column of $\tilde{A}$ contains at most three nonzero elements,*
2. *for all pair of permutation matrices P, Q, if $P\tilde{A}Q$ is in lower or upper triangular (d,b)-bordered band form, then $b + d > n/16$.*

Proof. Let Π denote the set of the $n \times n$ permutation matrices. We consider the set $\mathscr{P}_3$ of the matrices of the form $\pi_1 + \pi_2 + \pi_3$, where $\pi_1, \pi_2, \pi_3 \in \Pi$. Clearly $\mathscr{P}_3$ contains $(n!)^3$ matrices, although some of them are equal, and some of them have the same nonzero pattern.

We prove that $\mathscr{P}_3$ contains at least one matrix $\tilde{A}$ such that both $G(\tilde{A})$ and $G(\tilde{A}^{\mathrm{T}})$ are 9/8-weak-expanders. This result, together with Lemmas 3.1 and 3.2, will prove the theorem.

In order to prove that $\mathscr{P}_3$ contains at least one 9/8-weak-expander, we count the number of matrices in $\mathscr{P}_3$ that *are not* 9/8-weak-expanders, and we show that they are less than $(n!)^3$. We start by observing that given a set U of size m, the number of matrices $B \in \mathscr{P}_3$ such that $|\mathrm{Adj}_B(U)| \leqslant \beta|U|$ is at most

$$\binom{n}{\lfloor \beta m \rfloor} \left[\binom{\lfloor \beta m \rfloor}{m} (n-m)!m! \right]^3,$$

since for each set V of size $\lfloor \beta m \rfloor$ there are $\binom{\lfloor \beta m \rfloor}{m}(n-m)!m!$ matrices $\pi \in \Pi$ such that $\mathrm{Adj}_\pi(U) \subseteq V$.

Let $m = \lfloor n/2 \rfloor$, and β be such that $\beta m = \lfloor 9m/8 \rfloor$. The number $W(n)$ of matrices in $\mathscr{P}_3$ that are not 9/8-weak-expanders, is at most

$$W(n) \leqslant \binom{n}{m}\binom{n}{\beta m}\left[\binom{\beta m}{m}(n-m)!\,m!\right]^3$$

$$= (n!)^3 \frac{[(n-m)!\,(\beta m)!]^2}{n!\,m!\,(n-\beta m)!\,[(\beta m - m)!]^3},$$

For $5 \leqslant n \leqslant 31$, a direct calculation shows that $W(n) < (n!)^3/10$. For $n \geqslant 32$, we bound $W(n)$ using Stirling's formula. If n is even, we have $n = 2m$, hence

$$W(n) \leqslant (n!)^3 \frac{m!\,[(\beta m)!]^2}{(2m)!\,(2m-\beta m)!\,[(\beta m - m)!]^3}. \tag{6}$$

If n is odd, we have $n = 2m+1$, and

$$W(n) \leqslant (n!)^3 \frac{[(m+1)!\,(\beta m)!]^2}{m!\,(2m+1)!\,(2m-\beta m+1)!\,[(\beta m - m)!]^3}$$

$$= (n!)^3 \frac{(m+1)^2}{(2m+1)(2m-\beta m+1)} \frac{m![(\beta m)!]^2}{(2m)!\,(2m-\beta m)!\,[(\beta m - m)!]^3}$$

$$\leqslant (n!)^3 \frac{m!\,[(\beta m)!]^2}{(2m)!\,(2m-\beta m)!\,[(\beta m - m)!]^3},$$

where the last inequality holds because $(m+1)^2 < (2m+1)(2m-\beta m+1)$ for $\beta \leqslant 9/8$ and $m \geqslant 1$. It follows that (6) holds for all n. By using (1) we obtain

$$W(n) < (n!)^3 \frac{e^{1/4}\beta}{2\pi m\sqrt{2(2-\beta)(\beta-1)^3}} \left(\frac{\beta^{2\beta}}{4(2-\beta)^{2-\beta}(\beta-1)^{3(\beta-1)}}\right)^m.$$

Since $9/8 - 1/m \leqslant \beta \leqslant 9/8$, and $m \geqslant 16$, we have

$$\frac{e^{1/4}\beta}{2\pi m\sqrt{2(2-\beta)(\beta-1)^3}} \leqslant \frac{e^{1/4}\left(\frac{9}{8}\right)}{32\pi\sqrt{2\left(\frac{7}{8}\right)\left(\frac{1}{16^3}\right)}} < 1;$$

hence

$$W(n) < (n!)^3 \left(\frac{\beta^{2\beta}}{4(2-\beta)^{2-\beta}(\beta-1)^{3(\beta-1)}}\right)^m.$$

The function $f(t) = t^{2t}/(2-t)^{2-t}(t-1)^{3t-3}$ increases for $1 < t < 3/2$, hence $f(\beta) < f(9/8) < 16/5$. It follows that

$$W(n) < (n!)^3 \left(\frac{4}{5}\right)^m < (n!)^3 \left(\frac{4}{5}\right)^{16} < \frac{(n!)^3}{30}.$$

This computation can be repeated verbatim to show that the same bound holds also for the number $W'(n)$ of matrices $B \in \mathscr{P}_3$ such that $G(B^{\mathrm{T}})$ is not a 9/8-weak-expander.

Since $W(n) + W'(n) < (n!)^3$, we have proved that $\mathscr{P}_3$ contains a matrix $\tilde{A}$ such that both $G(\tilde{A})$ and $G(\tilde{A}^{\mathrm{T}})$ are 9/8-weak-expanders. By Lemmas 3.1 and 3.2, $\tilde{A}$ cannot be transformed into upper or lower triangular (d, b)-bordered band form with $b+d \leqslant n/16$. □

As a consequence of the preceding analysis, we have that, for $n \geqslant 32$, if A is chosen randomly in $\mathscr{P}_3$ the probability that both $G(A)$ and $G(A^{\mathrm{T}})$ are 9/8-weak-expanders is greater than $1 - 2\left(\frac{4}{5}\right)^{\lfloor n/2 \rfloor}$. For this reason, we conjecture that a result analogous to Theorem 3.3 holds for $d_i \geqslant 3$, i.e. for matrices with $\approx 3n$ nonzero elements.

5. Conclusions

In this paper we have considered a class of ordering algorithms designed for reducing the computational cost of sparse Gaussian elimination. In particular, we have analyzed the probability that such algorithms allow us to compute the factorization of an $n \times n$ sparse matrix in $o(n^3)$ time. We have shown that for the matrices with more than $10n$ nonzeros, such probability is less than $2^{1-n/2}$.

We conjecture that, when the number of nonzero elements is greater than $3n$, the probability of computing Gaussian elimination in $o(n^3)$ time is 2^{-cn}.

Our next step is to study the average effectiveness of the algorithms that reorder rows and columns during Gaussian elimination. We also plan to extend our probabilistic analysis to random Toeplitz matrices.

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