

## ON NUMERICAL PROPERTIES OF COMPLEX SYMMETRIC HOUSEHOLDER MATRICES

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**ABSTRACT.** Analysis is given of construction and stability of complex symmetric analogues of Householder matrices, with applications to the eigenproblem for such matrices. We investigate numerical properties of the deflation of complex symmetric matrices by using complex symmetric Householder transformations. The proposed method is very similar to the well-known deflation technique for real symmetric matrices (Cf. [16], pp. 586–595). In this paper we present an error analysis of one step of the deflation of complex symmetric matrices.

### 1. INTRODUCTION

The set of all  $n$ -by- $n$  matrices over  $\mathbf{C}$  is denoted by  $\mathcal{M}_n$ . We remind that  $A \in \mathcal{M}_n$  is symmetric iff  $A = A^T$ .  $A^* \in \mathcal{M}_n$  stands for the matrix formed by conjugating each element and taking the transpose. If  $A = A^*$  then  $A$  is called Hermitian. We say that  $A \in \mathcal{M}_n$  is complex orthogonal iff  $A^T A = I$ .

Complex symmetric matrices occur frequently, particularly in algebraic eigenvalue problem (Cf. [3], [4], [5]). However, the mathematical properties of complex symmetric matrices are quite different from those of real symmetric matrices (Cf. [6], [11], [12]). For example, a complex symmetric matrix may not be diagonalizable. A complex symmetric matrix  $A \in \mathcal{M}_n$  is diagonalizable if and only if its eigenvector matrix,  $Q$ , can be chosen complex orthogonal,  $Q^T Q = I$  and  $Q^T A Q = \text{diag}(\lambda_1, \lambda_2, \dots, \lambda_n)$  (Cf. [12], p. 233). It is known that any general complex matrix is similar to some complex symmetric matrix (Gantmacher's theorem, see [2]). Lately, the new algorithms for

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solving the eigenproblem of complex symmetric matrices that exploit the symmetry were proposed (Cf. [2], [3], [4], [5]). However, the accuracy guarantee is not quite as good as for real symmetric matrices. In order to improve the accuracy of the computed eigenpairs of a complex symmetric matrices, like for real symmetric matrices, we can apply Newton's method as considered in [15]. The problem of evaluating an eigenpair  $(\lambda, z)$ , where  $z$  is not an isotropic vector (i.e.  $z^T z \neq 0$  and  $\lambda$  is a single eigenvalue of  $A$ ), is equivalent to this of solving the nonlinear system  $F(z, \lambda) = 0$ , where

$$F(z, \lambda) = \begin{pmatrix} Az - \lambda z \\ (1 - z^T z) / 2 \end{pmatrix}.$$

In this paper we present an error analysis of the deflation of complex symmetric matrices using complex symmetric Householder transformations instead of Hermitian Householder transformations. The algorithms given here are based upon Wilkinson's ideas from [16], pp. 586–595. We discuss the conditioning of complex symmetric Householder matrices and give the detailed error analysis of the deflation.

To illustrate our results we present some numerical experiments. All tests were carried out in *MATLAB* in double precision  $\epsilon_M \approx 2.2 \cdot 10^{-16}$ .

## 2. COMPLEX SYMMETRIC HOUSEHOLDER TRANSFORMATIONS

A complex symmetric Householder matrix is a matrix of the form

$$(1) \quad H = I - \frac{2}{u^T u} uu^T,$$

where  $0 \neq u^T u$  and  $u \in \mathbf{C}^n$ .

A complex symmetric matrix  $H$  has the following properties (Cf. [1], [2]):

- (1)  $H$  is symmetric:  $H = H^T$ .
- (2)  $H$  is orthogonal:  $H^T H = I$ .
- (3) The eigenvalues of  $H$  are equal to:

$$\lambda_1 = -1, \lambda_2 = \dots = \lambda_n = 1.$$

- (4)  $\det(H) = -1$ .

This is because  $\det(H) = \lambda_1 \lambda_2 \dots \lambda_n = -1$ .

(5) The singular values  $\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_n$  of  $H$  are equal to

$$\begin{aligned}\sigma_2 &= \dots = \sigma_{n-1} = 1, \\ \sigma_1 &= c(u) + \sqrt{c^2(u) - 1}, \\ \sigma_n &= \frac{1}{\sigma_1} = c(u) - \sqrt{c^2(u) - 1},\end{aligned}$$

where

$$(2) \quad c(u) = \frac{u^*u}{|u^T u|}.$$

(6) The condition number of a matrix  $H$  equals

$$\text{cond}(H) = \|H\|_2 \|H^{-1}\|_2 = \{c(u) + \sqrt{c^2(u) - 1}\}^2.$$

(7) The product of  $H$  with a given vector  $z \in \mathbf{C}^n$  can be computed as follows:

$$Hz = z - \left(\frac{2u^T z}{u^T u}\right)u.$$

The main application of complex symmetric Householder transformations is reducing a given matrix to a special form to zero some elements.

**Theorem 2.1.** *For a given vector  $z \in \mathbf{C}^n$  such that  $z^T z \neq 0$  there exists a symmetric Householder transformation  $H = I - \frac{2}{u^T u} u u^T$  such that  $Hz = \rho e_1$  and  $\rho^2 = z^T z$ .*

*Moreover, it is possible to choose  $u$  such that  $1 \leq c(u) \leq c(z)$ .*

*Proof.*

The first part of this theorem is known (Cf. [2]).

Notice that  $H$  is independent of the scaling of  $u$  ( $u := \alpha u$  where  $\alpha \neq 0$ ), so we can take

$$(3) \quad u = z - \rho e_1.$$

Then

$$(4) \quad u^T u = z^T z + \rho^2 - 2\rho z_1 = 2\rho(\rho - z_1).$$

Since  $\rho = \theta\beta$  with  $\beta = \sqrt{z^T z}$  and  $\theta = \pm 1$ , we need to show that  $u^T u \neq 0$ , that is that  $u_1 = z_1 - \rho \neq 0$ . We will choose the sign  $\theta$  as follows. If we let  $\beta = a + ib$  and  $z_1 = c + id$  where  $a, b, c, d \in \mathbf{R}$ , then  $|u_1|^2 = (\theta a - c)^2 + (\theta b - d)^2 = |\beta|^2 + |z_1|^2 - 2\theta(ac + bd)$ . If  $ac + bd < 0$  then we choose  $\theta = 1$  else  $\theta = -1$ .

If we let

$$(5) \quad t = \frac{z_1}{\rho},$$

then under this choice of a sign we have

$$(6) \quad |u_1|^2 = |\rho|^2 \{1 + |t|^2 + 2 |Re(t)|\}.$$

Hence  $u_1 \neq 0$  and, consequently,  $u^T u \neq 0$ .

Now we prove that under this choice of sign the inequality  $c(u) \leq c(z)$  holds.

From (3) we get

$$(7) \quad u^* u = |\rho|^2 \{1 - 2Re(t) + c(z)\},$$

which together with (6) gives the formula

$$(8) \quad c(u) = \frac{1 - 2Re(t) + c(z)}{2 \sqrt{1 + |t|^2 + 2 |Re(t)|}}.$$

It can be easily verified that

$$(9) \quad c(u) \leq \frac{1 + 2 |Re(t)| + c(z)}{2 (1 + |Re(t)|)},$$

hence

$$c(u) \leq \frac{1 + c(z)}{2} \leq c(z),$$

because  $c(z) \geq 1$ . This finishes the proof. ■

#### ALGORITHM I.

Given vector  $z \in \mathbf{C}^n$  such that  $z^T z \neq 0$  this algorithm computes a vector  $0 \neq u \in \mathbf{C}^n$  and  $R = \frac{u^T u}{2}$  such that  $H z = \rho e_1$ ,  $\rho^2 = z^T z$ , where  $H = I - \frac{1}{R} u u^T$ .

- :  $\beta = \sqrt{z^T z}$ ,
- :  $\rho_1 = \beta$ ,  $\rho_2 = -\beta$ ,
- : if  $|z_1 - \rho_1| \geq |z_1 - \rho_2|$  then  $\rho = \rho_1$  else  $\rho = \rho_2$ ,
- :  $u_1 = z_1 - \rho$ ,

- :  $u_j = z_j$  for  $j = 2, \dots, n$ ,
- :  $R = (u^T u)/2$ . ■

### 3. DEFLATION USING COMPLEX SYMMETRIC HOUSEHOLDER TRANSFORMATIONS

We consider now a deflation which depends on similarity Householder transformations. We adopt the methods developed in [16], pp. 586–595.

Suppose that we find an eigenvalue  $\lambda_1$  and a corresponding eigenvector  $z$  of a complex symmetric matrix  $A(n \times n)$ . We are interested in computation of eigenvectors and further eigenvalues of  $A$ . We use the reduction of  $A$ , where  $A$  is used to generate an  $(n - 1) \times (n - 1)$  matrix with the eigenvalues  $\lambda_2, \dots, \lambda_n$ .

Suppose  $H = I - \frac{2}{u^T u} u u^T$  is such that  $H z = \rho e_1$ ,  $A z = \lambda_1 z$ . We assume additionally that  $z$  is not an isotropic vector, that is  $z^T z \neq 0$ . Then  $H A H e_1 = \lambda_1 e_1$ .

We see that the first column of  $B = H A H$  is equal to  $\lambda_1 e_1$ , hence  $B$  is symmetric and has the following form:

$$(10) \quad B = \begin{bmatrix} \lambda_1 & 0^T \\ 0 & C \end{bmatrix}.$$

We see that the deflated matrix is also complex symmetric. Here  $C$  is a symmetric matrix of order  $(n - 1)$  which has the eigenvalues  $\lambda_2, \dots, \lambda_n$ . If  $p \in \mathbf{C}^{n-1}$  is an eigenvector of  $C$  corresponding to  $\lambda_2$  then we can take  $[0; p^T]^T$  as an eigenvector of  $B$  and  $H[0; p^T]^T$  as an eigenvector of  $A$ .

In order to take advantage of symmetry in calculation  $B = H A H$  we write a matrix  $H$  as

$$H = I - \frac{1}{R} u u^T, \quad R = \frac{u^T u}{2}.$$

We remark that in the construction of  $u$  the special choice of sign can be used as described in Algorithm I.

We have

$$B = \left( I - \frac{1}{R} u u^T \right) A \left( I - \frac{1}{R} u u^T \right).$$

This equation may be written in the form

$$B = A - (p - Lu) u^T - u (p - Lu)^T,$$

where  $p = Au/R$ ,  $L = u^T p/(2R)$ .

## ALGORITHM II.

Given vector  $z \in \mathbf{C}^n$  such that  $z^T z \neq 0$  and  $Az = \lambda_1 z$ , where  $A(n \times n)$  is complex symmetric, this algorithm computes a symmetric matrix  $B$  defined in (10).

- : Find  $u$  and  $R$  by Algorithm I,
- :  $p = (Au)/R$ ,
- :  $L = (u^T p)/(2R)$ ,
- :  $q = p - Lu$ ,
- : for  $i = 1, \dots, n$ ,  $j = 1, \dots, i$  compute
 
$$b_{i,j} = a_{i,j} - q_i u_j - u_i q_j, \quad b_{j,i} = b_{i,j}. \quad \blacksquare$$

We see that the number of arithmetic operations involved in the computation of  $B$  is of order  $O(n^2)$ .

## 4. ERROR ANALYSIS

We consider complex arithmetic (cfl) (Cf. [9]) implemented using real arithmetic with machine unit  $\epsilon_M$ . We assume that for  $x, y \in \mathbf{C}$  we have

$$(11) \quad cfl(x \odot y) = (x \odot y)(1 + \delta), \quad |\delta| \leq \tilde{\gamma}_1, \quad \odot = +, -, *, /,$$

and

$$(12) \quad cfl(\sqrt{x}) = \sqrt{x}(1 + \delta), \quad |\delta| \leq \tilde{\gamma}_1.$$

Here

$$(13) \quad \tilde{\gamma}_1 = \frac{c\epsilon_M}{1 - c\epsilon_M}, \quad \tilde{\gamma}_n = \frac{cn\epsilon_M}{1 - cn\epsilon_M},$$

where  $c$  is a small constant whose exact value is unimportant in error analysis (Cf. [9]).

**4.1. Error analysis of Algorithm I..** From (12) we get

$$cfl(z^T z) = \sum_{j=1}^n z_j^2 (1 + \delta_j), \quad |\delta_j| \leq \tilde{\gamma}_n.$$

From this it follows that

$$(14) \quad cfl(z^T z) = (z^T z) (1 + \mu_1), \quad |\mu_1| \leq c(z) \tilde{\gamma}_n.$$

We see that  $c(z)$  may be interpreted as a condition number of evaluating  $z^T z$ .

From (13)–(14) we get

$$\tilde{\beta} = \sqrt{z^T z} (1 + \mu_2), \quad |\mu_2| \leq c(z) \tilde{\gamma}_n.$$

Then  $\tilde{u}_j = z_j$  for  $j = 2, \dots, n$ . From (6) it follows that  $|u_1| \geq |\rho|$  and  $|u_1| \geq |z_1|$ , so without loss of generality we can assume that

$$\tilde{u}_1 = u_1 (1 + \mu_3), \quad |\mu_3| \leq c(z) \tilde{\gamma}_n.$$

Thus,

$$(15) \quad \tilde{u} = (I + \phi)u, \quad \phi = \text{diag}(\mu_3, 0, \dots, 0), \quad \|\phi\|_F \leq c(z) \tilde{\gamma}_n.$$

Here, the computed  $\tilde{R} = \text{cfl}((u^T u)/2)$  satisfies

$$\tilde{R} = \sum_{j=1}^n \tilde{u}_j^2 (1 + \Delta_j)/2, \quad |\Delta_j| \leq \tilde{\gamma}_n.$$

Combining this with (15) we get

$$\tilde{R} = \frac{u^T (I + D) u}{2},$$

where  $D$  is diagonal such that

$$I + D = (I + \phi) (I + \text{diag}(\Delta_1, \dots, \Delta_n)) (I + \phi).$$

This equation may be rewritten

$$\tilde{R} = \frac{u^T u}{2} (1 + \mu_4), \quad |\mu_4| \leq c(u) \tilde{\gamma}_n.$$

Since  $c(u) \leq c(z)$  and by Th. 2.1

$$(16) \quad \tilde{R} = \frac{u^T u}{2} (1 + \mu_4), \quad |\mu_4| \leq c(z) \tilde{\gamma}_n.$$

4.2. **Error analysis of Algorithm II.** We prove the following theorem.

**Theorem 4.1.** *Assume that  $c^A(z) \tilde{\gamma}_n \leq \frac{1}{2}$  and*

$$(17) \quad \text{cfl}(A\tilde{u}) = (A + E_1)\tilde{u}, \quad \|E_1\|_F \leq \tilde{\gamma}_n \|A\|_F.$$

Let  $\tilde{B}$  denote the computed deflated matrix  $B(n \times n)$  in cfl. Then there exists matrix  $\Delta A$  such that

$$(18) \quad \tilde{B} = H(A + \Delta A)H,$$

where  $H = I - \frac{2}{u^T u} u u^T$ , and

$$(19) \quad \|\Delta A\|_F \leq c^A(z) \tilde{\gamma}_n \|A\|_F.$$

*Proof.*

From (16)–(17) we get

$$\tilde{p} = \frac{1}{R} (A + E_2)u, \quad \|E_2\|_F \leq c(z) \tilde{\gamma}_n \|A\|_F.$$

Similarly, the computed quantity  $L$  in cfl can be written as

$$\tilde{L} = \frac{1}{2R^2} u^T (A + E_3)u, \quad \|E_3\|_F \leq c(z) \tilde{\gamma}_n \|A\|_F.$$

From (11) and (13) it follows that

$$\tilde{B} = A + E_4 + \tilde{q}\tilde{u}^T + \tilde{u}\tilde{q}^T,$$

where

$$\|E_4\|_F \leq \tilde{\gamma}_1 (\|A\|_F + \|\tilde{q}\|_2 \|\tilde{u}\|_2).$$

Using elementary calculations we get

$$\tilde{q} = \frac{1}{R} (A + E_6)u - \frac{1}{2R^2} u (u^T (A + E_5)u),$$

where

$$\|E_k\|_F \leq c(z) \tilde{\gamma}_n \|A\|_F, \quad k = 5, 6.$$

We see that

$$\tilde{q} = \hat{q} + \delta q,$$



where

$$\hat{q} = \frac{1}{R}(A + E_5)u - \frac{1}{2R^2}u(u^T(A + E_5)u),$$

and

$$\|u\|_2 \|\delta q\|_2 \leq c^2(z) \tilde{\gamma}_n \|A\|_F.$$

We have

$$\tilde{B} = E_7 + (A + E_5) + \hat{q}u^T + u\hat{q}^T,$$

where

$$\|E_7\|_F \leq c^2(z) \tilde{\gamma}_n \|A\|_F.$$

This equation can be rewritten

$$\tilde{B} = H(A + \Delta A)H, \quad \Delta A = E_5 + HE_7H.$$

Thus,

$$\|\Delta A\|_F \leq c(z) \tilde{\gamma}_n \|A\|_F + \text{cond}(H) \|E_7\|_F.$$

From this and Th. 2.1 it follows that

$$\|\Delta A\|_F \leq c^4(z) \tilde{\gamma}_n \|A\|_F.$$

This completes the proof. ■

We conclude that if  $c(z)$  is small, eg.  $c(z) \leq 5$  then the computed matrix  $\tilde{B}$  is similar to a slightly perturbed matrix  $A$ , and the deflation algorithm is numerically stable. However, the real problem here is the possible exponential growth of the condition number of the Householder matrix  $H$  and the algorithm may become unstable and the spectrum of the deflated matrices may be completely unrelated to the original ones. However, in practice, this exponential growth in the condition number of  $H$  is very unlikely to happen.

## 5. NUMERICAL TESTS

To illustrate our results we give some numerical experiments. All computations were carried out in *MATLAB* with unit roundoff  $\epsilon_M \approx 2.2 \cdot 10^{-16}$ . The computed results for a wide class of complex symmetric matrices  $A$  were very good. Here we present special examples to show that the accuracy of Algorithm II in floating point arithmetic depends on conditioning of a Householder matrix  $H$ .

In order to have an eigenpair of the matrix  $A$  we use *MATLAB* function "eigs". For example,  $[X,D] = \text{eigs}(A,2)$  returns a diagonal matrix  $D$  of  $A$ 's 2 largest magnitude eigenvalues and a matrix  $X$  whose columns are the corresponding eigenvectors.

A simple way to test the error bounds is to compute  $B = HAH$  and  $M = HBH$  by Algorithm II, and to evaluate the error

$$(20) \quad \text{err} = \frac{\|A - M\|_2}{\|A\|_2}.$$

**Example 5.1.** *The first example is the problem with a matrix*

$$A = b b^T, \quad b = [1, i, -i, -1]^T.$$

*Note that  $A$  has an isotropic vector  $z = b$  as an eigenvector, that is,  $Az = 0$  and  $z^T z = 0$ . The Algorithm II fails.*

**Example 5.2.** *The second example is the problem with a slightly perturbed matrix from Example 5.1.*

*The following code finds the error defined in (20).*

```
i=sqrt(-1);
A=b*b.'+rand(4)*(2*i-1)*1.1e-10
[X,D]=eigs(A,2);
d=D(1,1)
z=X(:,1)
c=(z'*z)/abs(z.'*z)
```

*We performed Algorithm II for the matrix  $A = A_1 + iA_2$ , where*

$$A_1 = \begin{bmatrix} 1.0000e+000 & -9.8043e-011 & -9.0355e-011 & -1.0000e+000 \\ -2.5425e-011 & -1.0000e+000 & 1.0000e+000 & -8.1203e-011 \\ -6.6753e-011 & 1.0000e+000 & -1.0000e+000 & -1.9389e-011 \\ -1.0000e+000 & -2.0354e-012 & -8.7113e-011 & 1.0000e+000 \end{bmatrix}$$

$$A_2 = \begin{bmatrix} 2.0903e-010 & 1.0000e+000 & -1.0000e+000 & 2.0280e-010 \\ 1.0000e+000 & 1.6766e-010 & 9.7835e-011 & -1.0000e+000 \\ -1.0000e+000 & 1.0042e-010 & 1.3540e-010 & 1.0000e+000 \\ 1.0692e-010 & -1.0000e+000 & 1.0000e+000 & 8.9255e-011 \end{bmatrix}$$

The results are given by

$$c = 1.7408e + 005,$$

$$err = 1.0612e - 005.$$

We see that the accuracy guarantee is not quite as good as the deflation for real symmetric matrices and depends on condition number of a complex symmetric Householder matrix  $H$ .

**Remark 5.1.** In practice, we should apply one step of the deflation for an approximate eigenpair  $(\tilde{\lambda}, \tilde{z})$  such that the backward error

$$\eta = \frac{\|A\tilde{z} - \tilde{\lambda}\tilde{z}\|_2}{\|A\|_F \|\tilde{z}\|_2}$$

is small (of order  $\epsilon_M$ ). It is well-known (Cf. [16]) that then the computed eigenpair  $(\tilde{\lambda}, \tilde{z})$  is an exact eigenpair of a slightly perturbed matrix, i.e.

$$(A + E)\tilde{z} = \tilde{\lambda}\tilde{z}, \|E\|_F \leq \eta \|A\|_F.$$

## 6. PRESERVING SYMMETRY IN PERTURBATIONS

In some numerical applications it is important that the perturbed matrix  $A + E$  has the same structure as  $A$ . This property helps to guarantee that one has solved a problem with the same physical connectivity as the original problem.

First, we adopt a result of a J.R.Bunch, J.W.Demmel and C.V.Loan (Cf. [8], [9], [10]).

**Theorem 6.1.** Assume that  $A \in \mathcal{M}_n$  is symmetric. If  $(A + E)z = \lambda z$ , where  $z^T z \neq 0$ , then there exists a matrix  $F = F^T \in \mathcal{M}_n$  such that  $(A + F)z = \lambda z$  and  $\|F\|_2 \leq 3 c(z) \|E\|_2$  where  $c(z) = \frac{z^* z}{|z^T z|}$ .

*Proof.*

Let  $r = \lambda z - Az$ . Then  $r = Ez$ , so it is sufficient to prove that there exists a complex symmetric matrix  $F$  such that  $Ez = Fz$ .

If we let

$$F = \frac{rz^T + zr^T}{z^T z} - \frac{r^T z}{z^T z} I,$$

then  $Fz = r$ , and

$$\|F\|_2 \leq \frac{2\|r\|_2\|z\|_2 + |r^T z|}{|z^T z|}.$$

By the Cauchy–Schwartz inequality we have

$$|r^T z| \leq \|r\|_2 \|z\|_2$$

and

$$\|r\|_2 \leq \|E\|_2 \|z\|_2.$$

Therefore we obtain the desired inequality. ■

We see that if  $c(z)$  is small enough then the symmetry in perturbations is preserved. However, we can prove the following theorem using the similar idea as in [13], [14].

**Theorem 6.2.** *Assume that  $A \in \mathcal{M}_n$  is symmetric. If  $(A + E)z = \lambda z$ , where  $z \neq 0$ , then there exists a matrix  $F = F^T \in \mathcal{M}_n$  such that  $(A + F)z = \lambda z$  and  $\|F\|_2 \leq (2n - 1)n \|E\|_2$ .*

*Proof.*

It is sufficient to prove that there exists a complex symmetric matrix  $F$  such that  $Ez = Fz$ . We can assume, without loss of generality, that

$$|z_1| \leq |z_2| \leq \dots \leq |z_n|.$$

Let  $f_{1,1} = e_{1,1}$  and  $f_{i,j} = f_{j,i} = e_{i,j}$  for  $i = 1, \dots, n$  and  $j = i + 1, \dots, n$ . We need to determine  $f_{i,i}$  for  $i = 2, \dots, n$  so that

$$f_{i,i}z_i = e_{i,i}z_i + \sum_{j=1}^{i-1} (e_{i,j} - e_{j,i})z_j.$$

If  $z_i = 0$ , set  $f_{i,i} = 0$ . Otherwise, set

$$f_{i,i} = e_{i,i} + \sum_{j=1}^{i-1} (e_{i,j} - e_{j,i}) \frac{z_j}{z_i}.$$

Since  $|e_{i,j}| \leq \|E\|_2$  for all  $i, j$ , we have

$$|f_{i,i}| \leq \|E\|_2 + \sum_{j=1}^{i-1} (2\|E\|_2) \leq (2i-1)\|E\|_2.$$

It is well-known that  $\|F\|_2 \leq n \max_{i,j} |f_{i,j}|$ , so

$$\|F\|_2 \leq (2n-1)n \|E\|_2. \blacksquare$$

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