The distance of an eigenvector to a Krylov subspace and the convergence of the Arnoldi method for eigenvalue problems

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We consider the eigenvalue problem

 $Ax = \lambda x$ 

The Krylov subspace and matrix are defined as

$$\mathcal{K}_k(A, v) = \operatorname{span}\{v, Av, \dots, A^{k-1}v\}$$
$$\mathcal{K}_k = \begin{pmatrix} v & Av & \dots & A^{k-1}v \end{pmatrix}$$

## The Arnoldi algorithm

The residual vectors are orthogonal to the Krylov subspace

$$(A x^{(k)} - \lambda^{(k)} x^{(k)}, A^{i} v) = 0$$
 for  $i = 0, ..., k - 1$ 

The orthonormal basis of  $\mathcal{K}_k(A, v)$  is computed using

- $AV_k = V_k H_k + h_{k+1,k} v_{k+1} e_k^T$ ,  $v_1 = v / ||v||$
- $H_k = V_k^* A V_k$

The approximate eigenvalue problem can now be written as

$$V_k^* A V_k y^{(k)} = H_k y^{(k)} = \lambda^{(k)} y^{(k)}$$

which is equivalent to

 $V_k^*(A-\lambda^{(k)}I)V_ky^{(k)}=0$ 

Approximate eigenvalues (the so-called Ritz values) are the eigenvalues of  $H_k$  which is upper Hessenberg

Let  $\mathcal{P}_k$  be the orthogonal projector onto  $\mathcal{K}_k(A, v)$ It can be written as  $\mathcal{K}_k(\mathcal{K}_k^*\mathcal{K}_k)^{-1}\mathcal{K}_k^*$  or  $\mathcal{V}_k\mathcal{V}_k^*$  depending on the basis we consider

Then, the approximate eigenvalue problem amounts to solving

 $\mathcal{P}_k(Ax - \lambda x) = 0, \quad x \in \mathcal{K}_k(A, v)$ 

or in operator form

 $\mathcal{P}_k A \mathcal{P}_k x = \lambda x$ 

Let us define  $A_k \equiv \mathcal{P}_k A \mathcal{P}_k$ . Note that  $A_k = V_k H_k V_k^*$ 

## Convergence analysis

#### Theorem

Let x be an eigenvector of A associated with the eigenvalue  $\lambda$  and  $\gamma_k = \|\mathcal{P}_k \mathcal{A}(I - \mathcal{P}_k)\|$ 

Then the residual norms of the pairs  $(\lambda, \mathcal{P}_k x)$  and  $(\lambda, x)$  for the linear operator  $A_k$  satisfy

$$\|(A_k - \lambda I)\mathcal{P}_k x\| \le \gamma_k \|(I - \mathcal{P}_k)x\|$$
  
 $\|(A_k - \lambda I)x\| \le \sqrt{|\lambda|^2 + \gamma_k^2} \|(I - \mathcal{P}_k)x\|$ 

Y. Saad, Numerical methods for large eigenvalue problems, Halstead Press, (1992). Revised edition, SIAM (2011) Note that  $\gamma_k \leq \|A\|$ 

Therefore, the coefficients on the right-hand sides of these inequalities are at most of the order of  $\|(I - \mathcal{P}_k)x\|$ 

The Theorem states how accurate the *exact eigenpair* is with respect to the *approximate problem*. This is stated in terms of the distance of the exact eigenvector x to the Krylov subspace.

The remaining issue is to compute or to estimate  $\|(I - \mathcal{P}_k)x\|$ 

Upper bounds for the norm have been obtained in

M. Bellalij, Y. Saad and H. Sadok, *Further analysis of the Arnoldi process for eigenvalue problems*, SIAM J. Numer. Anal., v 48 n 2 (2010), pp. 393–407

using several tools: the eigenvectors, the Schur vectors and an approximation theory viewpoint

We remark that  $\|(I - P_k)x\|$  is also involved in the analysis of convergence of harmonic Ritz values and harmonic and refined Ritz vectors

#### The minimum distance to a subspace

We consider the minimum distance  $\min_{x \in \mathcal{X}} ||w - x||$  of a vector w to  $\mathcal{X}$  which is an arbitrary subspace of dimension k ( $w \notin \mathcal{X}$ ) Given any matrix W whose columns give a basis of the subspace  $\mathcal{X}, x \in \mathcal{X}$  can be written as Wy, where  $y \in \mathbb{C}^k$ . Hence,

$$\|w - x\|^{2} = \|w - Wy\|^{2} = w^{*}w - w^{*}Wy - y^{*}W^{*}w + y^{*}W^{*}Wy$$
$$\|w - x\|^{2} = \begin{pmatrix} 1 \\ -y \end{pmatrix}^{*} \underbrace{\begin{pmatrix} w^{*}w & w^{*}W \\ W^{*}w & W^{*}W \end{pmatrix}}_{\equiv C} \begin{pmatrix} 1 \\ -y \end{pmatrix}$$
$$\underset{x \in \mathcal{X}}{\min} \|w - x\|^{2} = \min_{y \in \mathbb{C}^{k}} \|w - Wy\|^{2} = \min_{y \in \mathbb{C}^{k}} \begin{pmatrix} 1 \\ y \end{pmatrix}^{*} C \begin{pmatrix} 1 \\ y \end{pmatrix}$$

Lemma

Let  $\mathcal{X}$  be an arbitrary subspace of dimension k in  $\mathbb{C}^N$  with a basis  $W = [w_1, \cdots, w_k]$  and let  $w \notin \mathcal{X}$ . Let  $\mathcal{P}$  be the orthogonal projector onto  $\mathcal{X}$ . Then,

$$\|(I - \mathcal{P})w\|^2 = \frac{1}{e_1^T C^{-1} e_1}$$

where

$$C = \left(\begin{array}{cc} w^*w & w^*W \\ W^*w & W^*W \end{array}\right)$$

We have

$$||(I - \mathcal{P})w||^2 = w^*w - w^*\mathcal{P}w = w^*w - w^*W(W^*W)^{-1}W^*w$$

The right-hand side is the Schur complement of the (1,1) entry of C which is the inverse of the (1,1) entry of  $C^{-1}$ 

# The minimum distance of an eigenvector to a Krylov subspace

Hypothesis H:

Let k < N. The matrix A is diagonalizable as  $A = X\Lambda X^{-1}$  where X is the matrix of the normalized eigenvectors and  $\Lambda$  is the diagonal matrix of the eigenvalues denoted as  $\lambda_i$ , i = 1, ..., NWe assume that there are at least k + 1 distinct eigenvalues (which we number from 1 to k + 1) and that the first k + 1 components of  $\alpha = X^{-1}v$  are different from zero

We are interested in the convergence to a given simple eigenvalue which is indexed by 1, that is, we consider  $x_1$ , the first column of X corresponding to  $\lambda_1$ . We have assumed that  $[X^{-1}v]_1 \neq 0$  and  $||x_j|| = 1$  for all j

We would like to compute  $||(I - P_k)x_1||$  where  $P_k$  is the orthogonal projector onto  $\mathcal{K}_k(A, v)$ 

Noting that  $C = [w, W]^*[w, W]$  and applying the previous lemma we obtain

#### Corollary

Let A be a general square matrix,  $x_1 \notin \mathcal{K}_k(A, v)$  be an eigenvector of A and  $L_{k+1}$  be the rectangular matrix of  $\mathbb{C}^{N \times (k+1)}$ 

$$L_{k+1} = \begin{pmatrix} \alpha_1 \ x_1, \quad v, \quad A \ v, \quad \dots, \quad A^{k-1} \ v \end{pmatrix}$$

We assume that  $\alpha \in \mathbb{C}$ ,  $\alpha_1 \neq 0$  and  $L_{k+1}$  is of rank k + 1. Then

$$\|(I - \mathcal{P}_k) \alpha_1 x_1\|^2 = \frac{1}{e_1^T (L_{k+1}^* L_{k+1})^{-1} e_1}$$

Theorem Let A be a diagonalizable matrix satisfying hypothesis H,  $\alpha$  a vector of  $\mathbb{C}^k$  with components  $\alpha_j$  such that the starting vector is  $\mathbf{v} = X\alpha$  and  $D_\alpha$  be a diagonal matrix with  $(D_\alpha)_{i,i} = \alpha_i$  and

$$W_{k+1} = \begin{pmatrix} 1 & 1 & \lambda_1 & \dots & \lambda_{k-1}^{k-1} \\ 0 & 1 & \lambda_2 & \dots & \lambda_2^{k-1} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 1 & \lambda_i & \dots & \lambda_i^{k-1} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 1 & \lambda_N & \dots & \lambda_N^{k-1} \end{pmatrix}$$

Let 
$$\tilde{M}_{k+1} = L_{k+1}^* L_{k+1}$$
. Then  
 $\|(I - \mathcal{P}_k) \alpha_1 x_1\|^2 = \frac{1}{(\tilde{M}_{k+1}^{-1})_{1,1}} = \frac{1}{e_1^T (W_{k+1}^* D_{\alpha}^* (X^* X) D_{\alpha} W_{k+1})^{-1} e_1}$ 

When A is normal the preceding formula simplifies to

$$\|(I - \mathcal{P}_k) \alpha_1 x_1\|^2 = \frac{1}{e_1^T (W_{k+1}^* D_\alpha^* D_\alpha W_{k+1})^{-1} e_1}$$

The proof is obtained by factoring  $L_{k+1}$ 

$$L_{k+1} = [\alpha_1 x_1, v, A v, \dots, A^{k-1} v]$$
  
=  $X [\alpha_1 e_1, \alpha, \Lambda \alpha, \dots, \Lambda^{k-1} \alpha]$   
=  $X D_{\alpha} W_{k+1}$ 

Now, using Cramer's rule, we have

$$( ilde{M}_{k+1}^{-1})_{1,1} = rac{\det(\hat{M}_{k+1})}{\det( ilde{M}_{k+1})}$$

where  $\hat{M}_{k+1}$  is equal to  $\tilde{M}_{k+1}$  except for the first column which is replaced by the first column of the identity matrix

Obviously  $\det(\tilde{M}_{k+1}) = \det((\tilde{M}_{k+1})_{[2:k+1],[2:k+1]})$  and

$$(\tilde{M}_{k+1})_{[2:k+1],[2:k+1]} = \begin{pmatrix} 0 \\ \vdots & I_k \\ 0 \end{pmatrix} \tilde{M}_{k+1} \begin{pmatrix} 0 & \cdots & 0 \\ & I_k \end{pmatrix}$$
$$= \begin{pmatrix} 0 \\ \vdots & I_k \\ 0 \end{pmatrix} W_{k+1}^* D_{\alpha}^* (X^* X) D_{\alpha} W_{k+1} \begin{pmatrix} 0 \\ & I_k \end{pmatrix}$$
$$= \mathcal{V}_k^* D_{\alpha}^* (X^* X) D_{\alpha} \mathcal{V}_k$$

with

$$\mathcal{V}_k = \begin{pmatrix} 1 & \lambda_1 & \cdots & \lambda_1^{k-1} \\ 1 & \lambda_2 & \cdots & \lambda_2^{k-1} \\ \vdots & \vdots & & \vdots \\ 1 & \lambda_N & \cdots & \lambda_N^{k-1} \end{pmatrix}$$

But

$$\mathcal{V}_k^* D_{lpha}^* (X^* X) D_{lpha} \mathcal{V}_k = M_k \equiv K_k^* K_k$$

Lemma (J. Duintjer Tebbens and G.M.)

Let A be a diagonalizable matrix with a spectral decomposition  $A = X\Lambda X^{-1}$  Then

$$\det(M_k) = \sum_{I_k} \left| \sum_{J_k} \det(X_{I_k,J_k}) \alpha_{j_1} \cdots \alpha_{j_k} \prod_{\substack{j_1 \leq j_\rho < j_q \leq j_k \\ j_\rho, j_q \in J_k}} (\lambda_{j_q} - \lambda_{j_\rho}) \right|^2$$

where the summations are over all sets of indices  $I_k$  and  $J_k$ defined as  $I_\ell$  to be a set of  $\ell$  indices  $(i_1, i_2, \ldots, i_\ell)$  such that  $1 \le i_1 < \cdots < i_\ell \le N$  and  $J_\ell$  is similar with *i* replaced by *j*,  $X_{I_\ell,J_\ell}$ is the submatrix of *X* whose row and column indices of entries are defined respectively by  $I_\ell$  and  $J_\ell$  and  $\alpha = X^{-1}v$ . The product is on all pairs of indices that belong to  $J_k$  (the product being equal to 1 if k = 1)

If the matrix A is normal then with  $\alpha = X^* v$ 

$$\det(M_k) = \sum_{I_k} \left[ \prod_{j=1}^k |\alpha_{i_j}|^2 \right] \prod_{\substack{i_1 \leq i_p < i_q \leq i_k \\ i_p, i_q \in I_k}} |\lambda_{i_q} - \lambda_{i_p}|^2$$

Lemma Let A be a diagonalizable matrix with a spectral decomposition  $A = X\Lambda X^{-1}$ . Then

$$\det(\tilde{M}_{k+1}) = |\alpha_1|^2 \sum_{I_{k+1}} \left| \sum_{\hat{j}_{k+1}} \det(X_{I_{k+1}, \hat{j}_{k+1}}) \alpha_{j_2} \cdots \alpha_{j_{k+1}} \prod_{\substack{1 < j_2 \le j_p < j_q \le j_{k+1} \\ j_p, j_q \in \hat{J}_{k+1}}} (\lambda_{j_q} - \lambda_{j_p}) \right|$$

where the summation with  $\hat{J}_{k+1}$  is over all sets of indices  $\{1, j_2, \ldots, j_{k+1}\}$  such that  $1 < j_2 < \cdots < j_{k+1} \le N$ If the matrix A is normal then

$$\det(\tilde{M}_{k+1}) = |\alpha_1|^2 \sum_{\hat{l}_{k+1}} \left[ \prod_{j=2}^{k+1} |\alpha_{i_j}|^2 \right] \prod_{\substack{1 < i_2 \le i_p < i_q \le i_{k+1} \\ i_p, i_q \in \hat{l}_{k+1}}} |\lambda_{i_q} - \lambda_{i_p}|^2$$

and the summation with  $\hat{l}_{k+1}$  is over all sets of indices  $\{i_2, \ldots, i_{k+1}\}$  such that  $1 < i_2 < \cdots < i_{k+1} \le N$ 

Let  $G = XD_{\alpha}W_{k+1}$ , then

$$\tilde{M}_{k+1} = G^*G$$

We use the Cauchy-Binet formula

$$\det(\tilde{M}_{k+1}) = \sum_{I_{k+1}} |\det(G_{I_{k+1},:})|^2$$

It yields

$$\det(G_{I_{k+1},:}) = \sum_{J_{k+1}} \det(X_{I_{k+1},J_{k+1}}) \alpha_{j_1} \cdots \alpha_{j_{k+1}} \det(\mathcal{W}(j_1,\ldots,j_{k+1}))$$

where  $\mathcal{W}(j_1, \ldots, j_{k+1})$  is obtained from the rows  $j_1, \ldots, j_{k+1}$  of  $W_{k+1}$ 

## $\det(\mathcal{W}(j_1, ..., j_{k+1})) = 0 \text{ if } 1 \notin \{j_1, j_2, ..., j_{k+1}\}$

But the indices in  $J_{k+1}$  are strictly ordered, so the determinant is different from zero only if  $j_1 = 1$ 

The sum over the sets  $J_{k+1}$  reduces to a sum over sets of indices  $\hat{J}_{k+1}$  which are  $\{1, j_2, \dots, j_{k+1}\}$  with  $1 < j_2 < \dots < j_{k+1} \le N$ 

$$\det(\mathcal{W}(1, j_2, \dots, j_{k+1})) = \det\begin{pmatrix} 1 & \lambda_{j_2} & \cdots & \lambda_{j_2}^{k-1} \\ 1 & \lambda_{j_3} & \cdots & \lambda_{j_3}^{k-1} \\ \vdots & \vdots & & \vdots \\ 1 & \lambda_{j_{k+1}} & \cdots & \lambda_{j_{k+1}}^{k-1} \end{pmatrix}$$

It yields

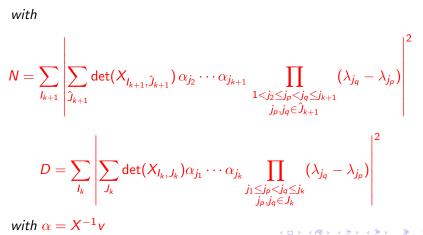
$$\prod_{1 < j_2 \le j_p < j_q \le j_{k+1}} (\lambda_{j_q} - \lambda_{j_p})$$

where the indices  $j_p, j_q$  have to belong to the set  $\{j_2, j_3, \ldots, j_{k+1}\}$ 

## Main result

Let A be a diagonalizable matrix satisfying hypothesis H. The distance of the eigenvector  $x_1$  to the Krylov subspace  $\mathcal{K}_k(A, v)$  is given by

$$\|(I-\mathcal{P}_k)x_1\|^2 = \frac{N}{D}$$



If, in addition, A is normal we have

$$N = \sum_{\hat{j}_{k+1}} \left[ \prod_{j=2}^{k+1} |\alpha_{i_j}|^2 \right] \prod_{\substack{1 \le i_2 \le i_p < i_q \le i_{k+1} \\ i_p, i_q \in \hat{j}_{k+1}}} |\lambda_{i_q} - \lambda_{i_p}|^2$$
$$D = \sum_{l_k} \left[ \prod_{j=1}^k |\alpha_{i_j}|^2 \right] \prod_{\substack{i_1 \le i_p < i_q \le i_k \\ i_p, i_q \in l_k}} |\lambda_{i_q} - \lambda_{i_p}|^2$$

with  $\alpha = X^* v$ 

The formula for the non-normal case is difficult to interpret since there is a strong dependence on the eigenvectors through determinants of submatrices of X

The result for normal matrices can be written in a different way. Let

 $I_k = \mathcal{I}_1 \cup \mathcal{I}_k, \quad \mathcal{I}_1 = \{1, i_2, \dots, i_k\}, \quad \mathcal{I}_k = \{i_1, i_2, \dots, i_k, |i_1 > 1\}.$ Let us denote the sums over these two sets of indices by  $S_{\mathcal{I}_1}$  and  $S_{\mathcal{I}_k}$ 

$$S_{\mathcal{I}_1} = |\alpha_1|^2 \sum_{\substack{\{i_2,\dots,i_k\}\\i_2>1}} \left[\prod_{j=2}^k |\alpha_{i_j}|^2\right] \prod_{\substack{1\le i_p < i_q \le i_k\\i_p, i_q \in \{1, i_2, \dots, i_k\}}} |\lambda_{i_q} - \lambda_{i_p}|^2$$
$$S_{\mathcal{I}_k} = \sum_{\mathcal{I}_k} \left[\prod_{j=1}^k |\alpha_{i_j}|^2\right] \prod_{\substack{1\le i_1\le i_p \le i_q \le i_k\\i_p, i_q \in \mathcal{I}_k}} |\lambda_{i_q} - \lambda_{i_p}|^2$$

 $S_{\mathcal{I}_k}$  is equal to the numerator N

$$\frac{N}{D} = \frac{S_{\mathcal{I}_k}}{S_{\mathcal{I}_1} + S_{\mathcal{I}_k}} = \frac{1}{1 + \frac{S_{\mathcal{I}_1}}{S_{\mathcal{I}_k}}}$$

as long as  $S_{\mathcal{I}_k} \neq 0$ 

The eigenvalue of interest  $\lambda_1$  does not appear in  $S_{\mathcal{I}_k}$ 

We see that the distance of  $x_1$  to the Krylov subspace is equal to 1 if and only if  $S_{I_1} = 0$ 

It is small if  $S_{\mathcal{I}_1}/S_{\mathcal{I}_k}$  is large

## A small example

We consider a normal matrix A of order 4 with eigenvalues  $\lambda_1, \lambda_2, \lambda_3, \lambda_4$  and k = 2

The sets of indices in  $l_3$  are (1, 2, 3), (1, 2, 4), (1, 3, 4)Therefore, the sets of indices in  $\hat{l}_3$  are (2, 3), (2, 4), (3, 4). The sets of indices in  $l_2$  are

$$(1,2), (1,3), (1,4), (2,3), (2,4), (3,4)$$

The three first pairs are in  $\mathcal{I}_1$  and the four last ones are in  $\mathcal{I}_2$ We see that  $\mathcal{I}_2$  is identical to  $\hat{I}_3$  Let  $\beta_i = |\alpha_i|^2$ . We have  $\begin{aligned} S_{\mathcal{I}_1} &= \beta_1 \left[ \beta_2 |\lambda_2 - \lambda_1|^2 + \beta_3 |\lambda_3 - \lambda_1|^2 + \beta_4 |\lambda_4 - \lambda_1|^2 \right] \\ S_{\mathcal{I}_2} &= \beta_2 \beta_3 |\lambda_3 - \lambda_2|^2 + \beta_2 \beta_4 |\lambda_4 - \lambda_2|^2 + \beta_3 \beta_4 |\lambda_4 - \lambda_3|^2 \end{aligned}$ 

The term  $S_{\mathcal{I}_1}$  will be large if at least one of the other eigenvalues is "far" from  $\lambda_1$  and the projection of v on the corresponding eigenvector is not too small

The other term  $S_{I_2}$  is small if the products of the pairwise distances between the other eigenvalues with the moduli of the projections of v are small

If only one of the terms in the sum is not small,  $S_{\mathcal{I}_2}$  cannot be small

Let us assume that we have a cluster of three distinct eigenvalues  $\lambda_2, \lambda_3, \lambda_4$  whose small pairwise distances are of order  $\varepsilon$  and another complex eigenvalue  $\lambda_1$  whose pairwise distances to the three other ones are of order 1

Assume also that all the  $\beta_i$ 's are non zero and that no one is very small

Then  $S_{I_2} = c\varepsilon^2$  where  $c \gg \varepsilon$  and the ratio N/D is equal to

$$\frac{1}{1+\frac{S_{\mathcal{I}_1}}{c\varepsilon^2}} = \frac{c\varepsilon^2}{c\varepsilon^2 + S_{\mathcal{I}_1}} = \mathcal{O}(\varepsilon^2)$$

since  $S_{\mathcal{I}_1}$  is of order 1

We see that with this distribution of eigenvalues  $\|(I - P_2) x_1\|$  is small of order  $\varepsilon$ 

Let us now assume that A is real. Then the eigenvalues arise as real numbers or complex conjugate pairs

Let  $\lambda_1$  be a complex eigenvalue with  $\lambda_2 = \overline{\lambda_1}$ 

Assume that  $\lambda_3$  and  $\lambda_4$  are complex conjugate or real with  $|\lambda_4 - \lambda_3| = \varepsilon$  and the distances to  $\lambda_1$  and  $\lambda_2$  are of order 1

Then,  $S_{I_2}$  is not small unless  $\beta_2$  is small. Generally, the ratio N/D is not small

Let us consider the normal matrix

$$A = \begin{pmatrix} 1.894 & 0.09975 & -0.2124 & -0.3811 \\ 0.4172 & 1.137 & 0.3024 & 0.8461 \\ 0.1531 & -0.7204 & 1.649 & -0.1911 \\ 0.05344 & -0.6726 & -0.6651 & 1.32 \end{pmatrix}$$

 $\mathsf{and}$ 

$$v = \begin{pmatrix} -0.3019\\ -0.2286\\ -0.8316\\ 0.4063 \end{pmatrix}$$

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The eigenvalues of A are

(1+i, 1-i, 2-0.01i, 2+0.01i)

The distance is  $||x_1 - \mathcal{P}_2 x_1|| = 0.67682$ The two sums are

 $S_{I_1} = 0.15514, \quad S_{I_2} = 0.13115$ 

 $S_{I_1}$  is not large and  $S_{I_2}$  is not small The two Ritz values at iteration 2 are real, being (1.8123, 1.1039)

 $\|(A_2 - (1+i)I)P_2 x_1\| = 0.67421, \gamma_2 = 0.99644, \|x_1 - \mathcal{P}_2 x_1\| = 0.67682$  $\gamma_2 \|x_1 - \mathcal{P}_2 x_1\| = 0.67441$ 

and

$$\|(A_2 - (1+i)I)x_1\| = 1.1708, \quad \sqrt{1 + \gamma_2^2} = 1.7300$$
  
 $\sqrt{1 + \gamma_2^2} \|x_1 - \mathcal{P}_2 x_1\| = 1.1709$ 

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The two bounds are close to the values of the residual norms

## Conclusion

- We exhibited an exact expression for the distance of an eigenvector to a Krylov subspace
- It depends in an intricate way on the eigenvalues, the eigenvectors and the starting vector
- The expression is simpler when the matrix is normal
- This gives some bounds for residual norms in the Arnoldi algorithm

Finally, let us remember the happy days...



Marrakech, 2011