# Part II

# Spectral information and convergence of GMRES

## From Hermitian through normal to non-normal

Normal matrices have a full set of eigenvectors forming a basis of $\mathbb{C}^N$ which can be chosen orthonormal. Therefore the change to (orthonormal) eigenvector coordinates does not involve any distortion of geometry.

Substantial difference from the Hermitian case which causes enormous technical difficulties in proofs and in deriving bounds - the eigenvalues are not real. However, principal difficulties come with nonnormality.

We restrict ourselves to the GMRES method.

Given $A \in \mathbb{C}^{N \times N}$, $b \in \mathbb{C}^N$, $A$ nonsingular, we wish to solve $Ax = b$.

Consider $x_0 \in \mathbb{C}^N$, $r_0 = b - Ax_0$,

construct the sequence of Krylov subspaces

$$K_j(A, r_0) = \text{span } \left\{ r_0, Ar_0, \ldots, A^{j-1} r_0 \right\}, \quad j = 1, 2, \ldots$$

and look for $\quad x_j \in x_0 + K_j(A, r_0)$.

Minimal residual methods

$$\|r_n\| = \min_{u \in x_0 + K_n(A, r_0)} \|b - Au\| = \min_{z \in AK_n(A, r_0)} \|r_0 - z\|$$

$$\Leftrightarrow \; r_n \perp AK_n(A, r_0)\,.$$

(Hermitian) MINRES [Paige, Saunders - 75]
and GMRES [Saad, Schultz - 86];
mathematically equivalent to GCR analyzed in [Elman - 1982]
and to many other (mostly numerically inferior) methods.

MINRES is not a symmetric variant of GMRES.

**Implementation of GMRES** [Saad, Schultz - 86]

Arnoldi basis : $v_1 \equiv r_0 \|r_0\|\,, \qquad AV_n \;=\; V_{n+1} H_{n+1,n}\,.$

$$x_n \;=\; x_0 + V_n\, y_n\,,$$

$$\| \|r_0\| e_1 - H_{n+1,n}\, y_n \| \;=\; \min_y \| \|r_0\| e_1 - H_{n+1,n}\, y \|\,.$$

Other iplementations (GCR, simpler GMRES, ORTHODIR) suffer from possible numerical difficulties.

**Bound by Elman step by step for $A$ normal :**

$$\|r_n\| = \|p_n(A)r_0\| = \min_{p\in\Pi_n} \|p(A)r_0\| = \min_{p\in\Pi_n} \| S\,[p(\Lambda)\,S^* r_0]\|$$

$$= \min_{p\in\Pi_n} \|p(\Lambda)\,S^* r_0\| = \min_{p\in\Pi_n} \{\sum_i |\,(s_i^* r_0)\,p(\lambda_i)\,|^2\}^{\frac{1}{2}}$$

$$\leq \|r_0\| \min_{p\in\Pi_n} \max_i |p(\lambda_i)|\,.$$

$|p_n(\lambda_i)|$ represents a multiplicative correction to the absolute values $|s_i^* r_0|$ of the individual components of $r_0$ in the orthonormal basis $\{y_1, \ldots, y_N\}$ in order to minimize the sum of squares.

For a general $S$, some of the components $S^{-1}r_0$ in $S\,[p(J)\,S^{-1}r_0]$ can become very large. In such case $S\,[\,p(J)\,S^{-1}r_0]$ represents a significant cancelation. The minimization problem

$$\|r_n\| \;=\; \min_{p \in \Pi_n} \|\, S\;[\,p(J)\,S^{-1}r_0]\|$$

reflects that, while the term in the bound

$$\|S\| \;\min_{p \in \Pi_n} \|\, p(J)\,S^{-1}r_0\,\|$$

does not (cf. [Trefethen-97]).

In practical computations the rate of convergence// is often automatically linked to// the distribution of eigenvalues of the matrix $A$.

There are, however, examples showing that any (nonincreasing) convergence curve is possible for GMRES with matrix $A$ having any given (nonzero) eigenvalues.

[Greenbaum, S - 94], [Greenbaum, Pták, S - 96]

Assume convergence exactly in $N$ steps (generalization to $m < N$ possible). For simplicity of notation $r_0 = b$ ($x_0 = 0$).

**Question I:**

Given convergence curve, describe the set of all $\{A, b\}$ such that GMRES $(A, b)$ generates the prescribed curve.

**Question II:**

Given convergence curve, given $N$ nonzero eigenvalues (not necessarily distinct), describe the set of all $\{A, b\}$ such that GMRES $(A, b)$ generates the curve while the spectrum of $A$ is prescribed.

**Question III:**

Given $A$, denote by $\widehat{m}$ the degree of the minimal polynomial of $A$. Describe those $b$ for which GMRES $(A, b)$ converges in $\widehat{m}$ steps.

# Convergence curve

$$\|r_0\| \geq \|r_1\| \geq \cdots \geq \|r_{N-1}\| > \|r_N\| = 0,$$

$$h \equiv (\eta_1, \ldots, \eta_N)^T, \quad \eta_j \equiv ((\|r_{j-1}\|)^2 - \|r_j\|^2)^{1/2}.$$

$$d \equiv (\nu_1, \ldots, \nu_N), \quad \nu_1 = \frac{1}{\eta_N}, \; \nu_2 = -\frac{\eta_1}{\eta_N}, \; \ldots, \; \nu_N = -\frac{\eta_{N-1}}{\eta_N}.$$

Meaning? Let $W = (w_1, \ldots, w_j)$ be the orthonormal basis of $AK_j(A, r_0)$. Then

$$r_n = r_0 - \sum_{j=1}^{n} w_j \eta_j, \quad r_0 = \sum_{j=1}^{n} w_j \eta_j + r_n, \quad \|r_0\|^2 = \sum_{j=1}^{n} \eta_j^2 + \|r_n\|^2$$

## Convergence curve companion matrix

$$\widehat{H} = \begin{pmatrix} 0 & & & 1/\eta_N \\ 1 & \ddots & & -\eta_1/\eta_N \\ & \ddots & 0 & \vdots \\ & & 1 & -\eta_{N-1}/\eta_N \end{pmatrix} = \begin{pmatrix} 0 & & & \\ 1 & \ddots & & \boxed{d} \\ & \ddots & 0 & \\ & & 1 & \end{pmatrix}$$

$$\widehat{H}^{-1} = \begin{pmatrix} \eta_1 & 1 & & \\ \vdots & 0 & \ddots & \\ \vdots & & \ddots & 1 \\ \eta_N & & & 0 \end{pmatrix} = \begin{pmatrix} & 1 & & \\ \boxed{h} & 0 & \ddots & \\ & & \ddots & 1 \\ & & & 0 \end{pmatrix}$$

## Eigenvalues:

$$\{\lambda_1, \lambda_2, \ldots, \lambda_N\}, \quad \lambda_j \neq 0, \qquad j = 1, \ldots, n\,.$$

$$q_N(z) \;\equiv\; z^N - \sum_{j=0}^{N-1} \alpha_j z^j = (z-\lambda_1)(z-\lambda_2)\ldots(z-\lambda_N),$$

$$p_N(z) \;\equiv\; 1 - \sum_{j=1}^{N} \xi_j z^j = -\frac{1}{\alpha_0}\, q_N(z), \qquad \xi_N = \frac{1}{\alpha_0}, \quad \xi_j = -\frac{\alpha_j}{\alpha_0}\,,$$

$$s \;\equiv\; (\xi_1, \ldots, \xi_N)^T\,, \qquad a = (\alpha_0, \ldots, \alpha_{N-1})^T$$

**Spectral companion matrix:** $q_N(z) = \det(zI - C)$

$$C = \begin{pmatrix} 0 & & & \alpha_0 \\ 1 & \ddots & & \alpha_1 \\ & \ddots & 0 & \vdots \\ & & 1 & \alpha_{N-1} \end{pmatrix} = \begin{pmatrix} 0 & & & \\ 1 & \ddots & & \\ & \ddots & 0 & \boxed{a} \\ & & 1 & \end{pmatrix}$$

$$C^{-1} = \begin{pmatrix} -\alpha_1/\alpha_0 & 1 & & \\ -\alpha_2/\alpha_0 & 0 & \ddots & \\ \vdots & & \ddots & \\ \vdots & & & 1 \\ 1/\alpha_0 & & & 0 \end{pmatrix} = \begin{pmatrix} & 1 & & \\ & 0 & \ddots & \\ \boxed{s} & & \ddots & 1 \\ & & & 0 \end{pmatrix}$$

**Theorem 1 (Question I)**

*The following assertions are equivalent:*

1° *Residual vectors norms of GMRES*$(A, b)$ *form a prescribed nonincreasing sequence* $\|r_0\| \geq \|r_1\| \geq \cdots \geq \|r_{N-1}\| > \|r_N\| = 0$.

2° *Matrix* $A$ *is of the form* $A = W\widehat{R}\widehat{H}W^*$ *and* $b$ *satisfies* $W^*b = h$, *where* $W$ *is a unitary matrix,* $\widehat{R}$ *is a nonsingular upper triangular matrix and*

$$\widehat{H} = \begin{pmatrix} 0 & & & \\ 1 & \ddots & & \\ & \ddots & 0 & \\ & & 1 & \end{pmatrix} \boxed{d} .$$

**Proof.** Consider the QR decomposition

$$B \equiv (Ab, A^2b, \ldots, A^N b) = \tilde{W}\tilde{R}$$

.

Then the columns $\tilde{W}_j = (\tilde{w}_1, \ldots, \tilde{w}_j)$ represent an orthonormal basis of

$$AK_j = A\,\mathrm{span}\{b, \ldots, A^{j-1}b\} = \mathrm{span}\{Ab, \ldots, A^j b\}.$$

therefore

$$\eta_j = |\tilde{\eta}_j| = \left(\|r_{j-1}\|^2 - \|r_j\|^2\right)^{1/2} .$$

Rescaling

$$b = \tilde{W}(\Gamma h) = (\tilde{W}\Gamma)h = Wh$$

where

$$\Gamma = \text{diag}\,(\gamma_i),\; |\gamma_i| = 1,$$

we can write

$$B = WR, \quad R = \Gamma^* \tilde{R}.$$

$1^\circ$ is equivalent to

$$A\,(b, W_{N-1}) = A\,W \begin{pmatrix} \boxed{\begin{matrix} \\ \\ h \\ \\ \end{matrix}} & 1 & & \\ & 0 & \ddots & \\ & & \ddots & 1 \\ & & & 0 \end{pmatrix} = AW\widehat{H}^{-1}\,.$$

Since for some nonsingular upper triangular $\widehat{R}$

$$A\,(b, W_{N-1}) \;=\; (Ab, AW_{N-1}) \;=\; W\widehat{R}\,,$$

the identity $\quad AW\widehat{H}^{-1} = W\widehat{R} \quad$ finishes the proof.

**Theorem 2 (Question II)**

*The following two assertions are equivalent:*

1° *The spectrum of* $A$ *is* $\{\lambda_1, \ldots, \lambda_N\}$ *and GMRES*$(A, b)$ *yields residuals with the prescribed nonincreasing sequence*

$$\|r_0\| \geq \|r_1\| \geq \cdots \geq \|r_{N-1}\| > \|r_N\| = 0\,.$$

2° *Matrix* $A$ *is of the form* $A = WRCR^{-1}W^*$ *and* $b = Wh$ *where* $C$ *is the companion matrix corresponding to the polynomial* $q_N(z)$*,* $W$ *is unitary and* $R$ *a nonsingular upper triangular matrix such that* $Rs = h$*.*

**Corollary**: Any noninreasing convergence curve can be generated by GMRES for a matrix having any prescribed eigenvalues.

**Proof.** Assume 1°. $A$ is annihilated by $q_N(z)$,

$A^N - \sum_{j=0}^{N-1} \alpha_j A^j = 0$, therefore

$$B = (Ab, \ldots, A^N b) \; = \; (b, \ldots, A^{N-1} b)\, C \; = \; (A^{-1} B)\, C \,,$$

$$AB = BC \quad \text{and} \quad b = BC^{-1} e_1 = Bs.$$

Similarly to Theorem 1, $b = Wh$, $B = WR$, i.e. $b = Wh = WRs$, which gives $Rs = h$ , and

$$AWR = AB = BC = WRC$$

proves 2°.

Assume 2°.

Then $\mathrm{sp}(A) = \{\lambda_1, \ldots, \lambda_N\}$, and, by induction, $\{w_1, \ldots, w_k\}$ represents the unitary basis of $AK_k$, which proves 1°. Indeed,

$$Ab = W(RC^{-1}R^{-1}h) = W(RC^{-1}s) = W(Re_1) = (R_{1,1})w_1 \,.$$

Assume $A^j b = W(Re_j)$. Then

$$A^{j+1}b = A(A^j b) = A(WRe_j) = W(RCe_j) = W(Re_{j+1}) \,.$$

**Remark:** $W$ represents a change of the basis.

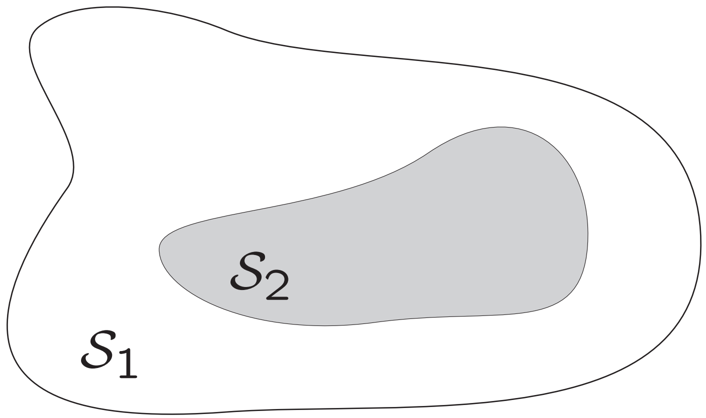
Denote

$\mathcal{S}_1 = \mathcal{S}_1(f)$ the set of all pairs $\{A, b\}$ determined by Theorem 1,

$\mathcal{S}_2 = \mathcal{S}_2(f, \{\lambda_1, \ldots, \lambda_N\})$ the set of all pairs $\{A, b\}$ determined by Theorem 2.

Clearly $\mathcal{S}_2 \subset \mathcal{S}_1$.

**Parametrization ?**




$\mathcal{S}_2 : A = WRCR^{-1}W,\ Rs = h,\ b = Wh,$

$\mathcal{S}_2$ is determined by $s$ and $h$.

$\mathcal{S}_1 : A = W\widehat{R}\widehat{H}W^*,\ b = Wh,$

$\mathcal{S}_1$ is determined by $h$.

**Proposition 1**

*The set $\mathcal{S}_2$ is parametrized by $W$ and by the nonsingular upper triangular matrix $R$ satisfying the relation*

$$Rs = h.$$

*The set $\mathcal{S}_1$ is parametrized by $W$ and an arbitrary nonsingular upper triangular matrix $\hat{R}$. If, in addition, the spectrum of the matrix $A$ is prescribed, then this additional condition is equivalent to*

$$RCR^{-1} = \hat{R}\widehat{H},$$

*where $\hat{R}$ is given by*

$$\hat{R} = R \begin{pmatrix} 1 & 0 \\ 0 & \boxed{R_{N-1}^{-1}} \end{pmatrix}, \quad \mathbf{Rs} = \mathbf{h}\,.$$

**Proof.**

$$\{A,b\} \in \mathcal{S}_2 \quad \Rightarrow \quad \{A,b\} \in \mathcal{S}_1 \text{ with the specific form of } \widehat{R}$$

$$\underbrace{RCR^{-1}} = \widehat{R}\widehat{H} \text{ while } Rs = h$$

$$R\,(RC^{-1})^{-1} = R \begin{pmatrix} h, & \boxed{R_{N-1}} \\ & 0 \end{pmatrix}^{-1}$$

$$= R \left( \widehat{H}^{-1} \begin{pmatrix} 1 & 0 \\ 0 & \boxed{R_{N-1}} \end{pmatrix} \right)^{-1}$$

$$= R \begin{pmatrix} 1 & 0 \\ 0 & \boxed{R_{N-1}^{-1}} \end{pmatrix} \widehat{H}$$

$$\Rightarrow \quad \widehat{R} = R \begin{pmatrix} 1 & 0 \\ 0 & \boxed{R_{N-1}^{-1}} \end{pmatrix} \quad \text{where} \quad Rs = h\,.$$

**Proposition 2**

$\{A, b\} \in \mathcal{S}_1$ and the spectrum, i.e. the vector $s$ , is given as the additional requirement.

[0.5cm] Then $\{A, b\} \in \mathcal{S}_2$ $R$ is determined by

the decomposition $\widehat{R} = R \begin{pmatrix} 1 & 0 \\ 0 & \boxed{R_{N-1}^{-1}} \end{pmatrix}$ and

it satisfies $Rs = h$.

**Proof.** $\widehat{R}$ determines uniquely $R$ by the given decomposition. For this uniquely determined $R$ define $\tilde{s}$ such that $R\,\tilde{s} = h$. Then

$$\widehat{R}\widehat{H} = R \begin{pmatrix} 1 & 0 \\ 0 & \boxed{R_{N-1}^{-1}} \end{pmatrix} \widehat{H} = R \left( \boxed{h} \begin{matrix} \boxed{R_{N-1}} \\ \\ 0 \end{matrix} \right)^{-1}$$

$$= R \left( R \left( \boxed{\tilde{s}} \begin{matrix} 1 & & \\ & \ddots & \\ & & 1 \end{matrix} \right) \right)^{-1}$$

$$= R\,(R\widetilde{C}^{-1})^{-1} = R\,\widetilde{C}^{-1}R^{-1}\,.$$

Since $A$ has the given spectrum ($s$ is given), $\tilde{s} = s$.

Since $\xi_N = (s, e_N) \neq 0$, any nonsingular upper triangular matrix $R$ satisfying

$$R\,s = h$$

has its last column uniquely determined by the entries in the left principal submatrix $R_{N-1}$ representing free parameters.

Denoting

$$Y \equiv RC^{-1} = R \begin{pmatrix} \boxed{\begin{matrix} \\ s \\ \\ \end{matrix}} & \begin{matrix} 1 & & \\ 0 & \ddots & \\ & \ddots & 1 \\ & & 0 \end{matrix} \end{pmatrix} = \begin{pmatrix} \boxed{\begin{matrix} \\ h \\ \\ \end{matrix}} & \begin{matrix} \boxed{R_{N-1}} \\ \\ 0 \end{matrix} \end{pmatrix},$$

Then

$$\begin{aligned} A &= WRCR^{-1}W^* = W(RC^{-1})C(CR^{-1})W^* = \\ &= W(RC^{-1})C(RC^{-1})^{-1}W^* = WYCY^{-1}W^* \end{aligned}$$

Assertions 1° and 2° of Theorem 2 are equivalent to

**Theorem 2 (continuation)**

3° *Matrix* $A$ *is of the form* $A = WYCY^{-1}W^*$ *and* $b = Wh$ *where* $C$ *is the companion matrix corresponding to the polynomial* $q(\lambda)$ *,* $W$ *is unitary and* $R_{N-1}$ *part of* $Y$ *is* **any** $(N-1)$ *by* $(N-1)$ *nonsingular upper triangular matrix.*

**Proof.** It remains to prove $3^\circ \Rightarrow 2^\circ$. Using $3^\circ$, we construct the last column of $R$ such that $R\,s = h$. Then

$$Y = \widehat{H}^{-1} \begin{pmatrix} 1 & 0 \\ 0 & \boxed{R_{N-1}} \end{pmatrix} = RC^{-1}$$

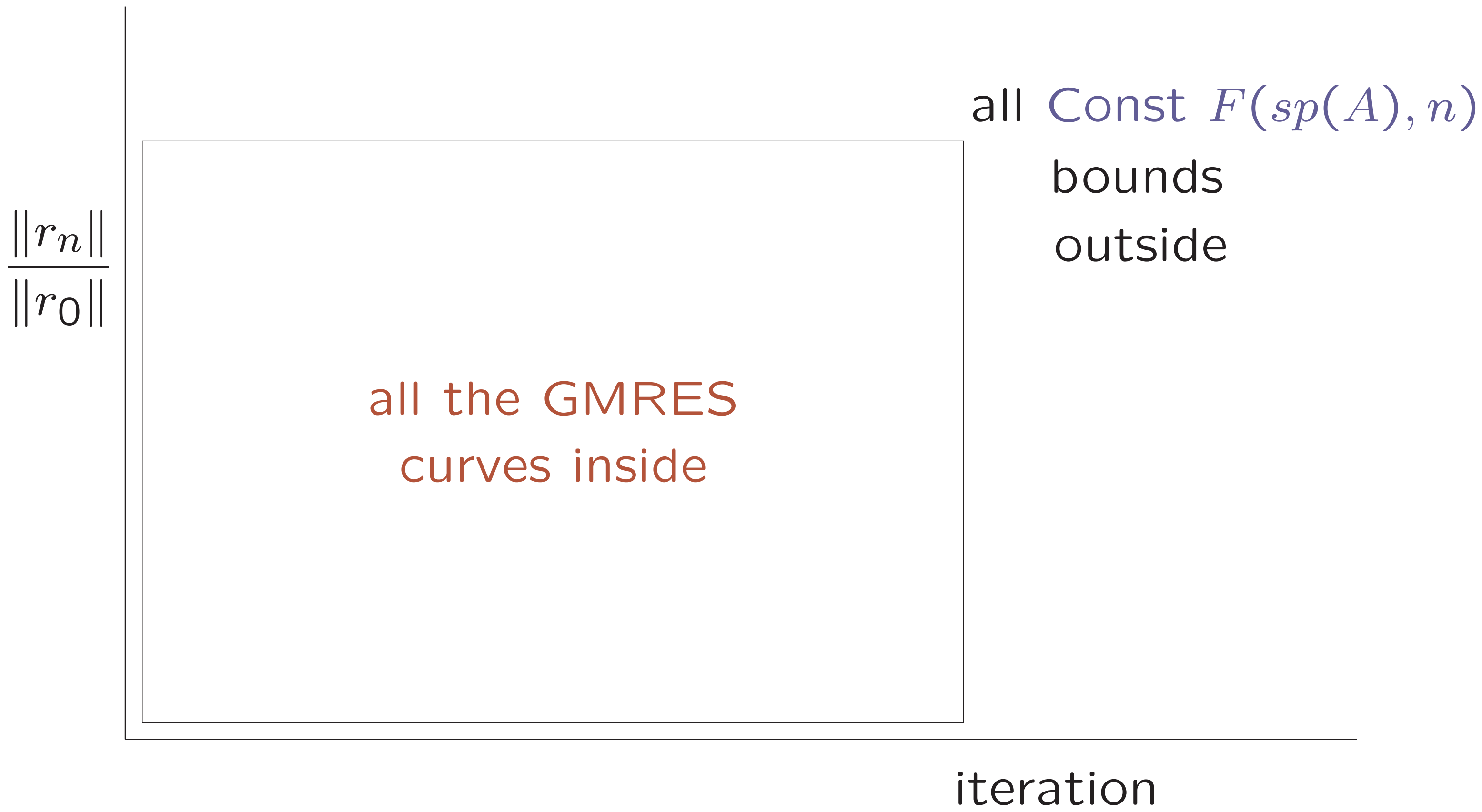
and the substitution finishes the proof.

**The problem of "constants" in the bounds of the type**

$$\| r_n \| \leq \omega(A, r_0) \, F_n(sp(A), N) \, .$$

If conclusion is based only on $F_n(sp(A), N)$ and the dependence of $\omega(A, r_0)$ on the data is not included, then the bound must hold for any data. Consequently, the bound is for any finite dimensional problem irrelevant, otherwise we get a contradiction with the given Theorems.

The bound Const $F_n(sp(A), N)$ does not intersect the rectangle $(1,0) - (1,N) - (0,N) - (0,0)$.



## Relationship to minimal polynomial

### Theorem 3

*Let $m$ denotes the degree of the minimal polynomial $q_A(\lambda)$ of the matrix $A$. Then, for any right hand side $b$, GMRES$(A, b)$ converges to the exact solution $x$ on or before the step $m$. Moreover, there exist a right hand side $\tilde{b}$, for which GMRES$(A, \tilde{b})$ converges to $x$ exactly in $m$ steps.*

Characterization of right hand sides, for which Krylov sequences have the maximal length?

Minimal polynomial $q_A(\lambda) = (\lambda - \lambda_1)^{n_1} \ldots (\lambda - \lambda_{\tilde{k}})^{n_{\tilde{k}}}$.

Denote the nullspaces of $(\lambda_j I - A)^{n_j}$ by $E(\lambda_j)$.

Then any $b$ can be decomposed as

$$b = t_1 + t_2 + \cdots + t_{n_{\tilde{k}}}, \quad t_j \in E(\lambda_j).$$

The vector $b$ yields the Krylov sequence of the length $m$ if and only if

$$(\lambda_j I - A)^{n_j - 1}\, t_j \neq 0$$

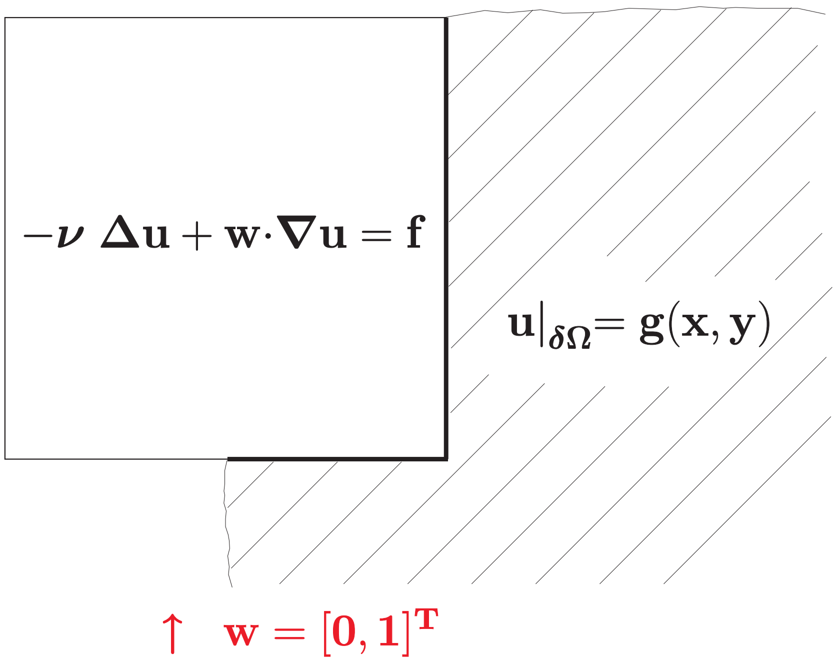
for each $j$, $j = 1, \ldots, \tilde{k}$. Equivalently, the vector $b$ have for each $j$ nonzero component in the direction of at least one last Jordan principal vector conformed to any of the Jordan blocks largest in size corresponding to $\lambda_j$.

# Pathological initial residuals?

The presented cautious view seems to be in conflict with the common wisdom – convergence is commonly related to eigenvalue distribution even for general matrices without examining eigenvectors. The proved facts should not be ignored (even a common knowledge can be wrong). They need a correct interpretation. There are good reasons for linking convergence to eigenvalues in many cases, but the reasons **must be given and examined** (contrary to common practice).

The role of "pathological initial residuals"; just academic examples ? Not true. Convection-diffusion examples were described by Trefethen long ago, see also [Ernst - 00].

# Convection-diffusion model problem




Convection dominated: $\nu \ll \|w\|$

## Discretization

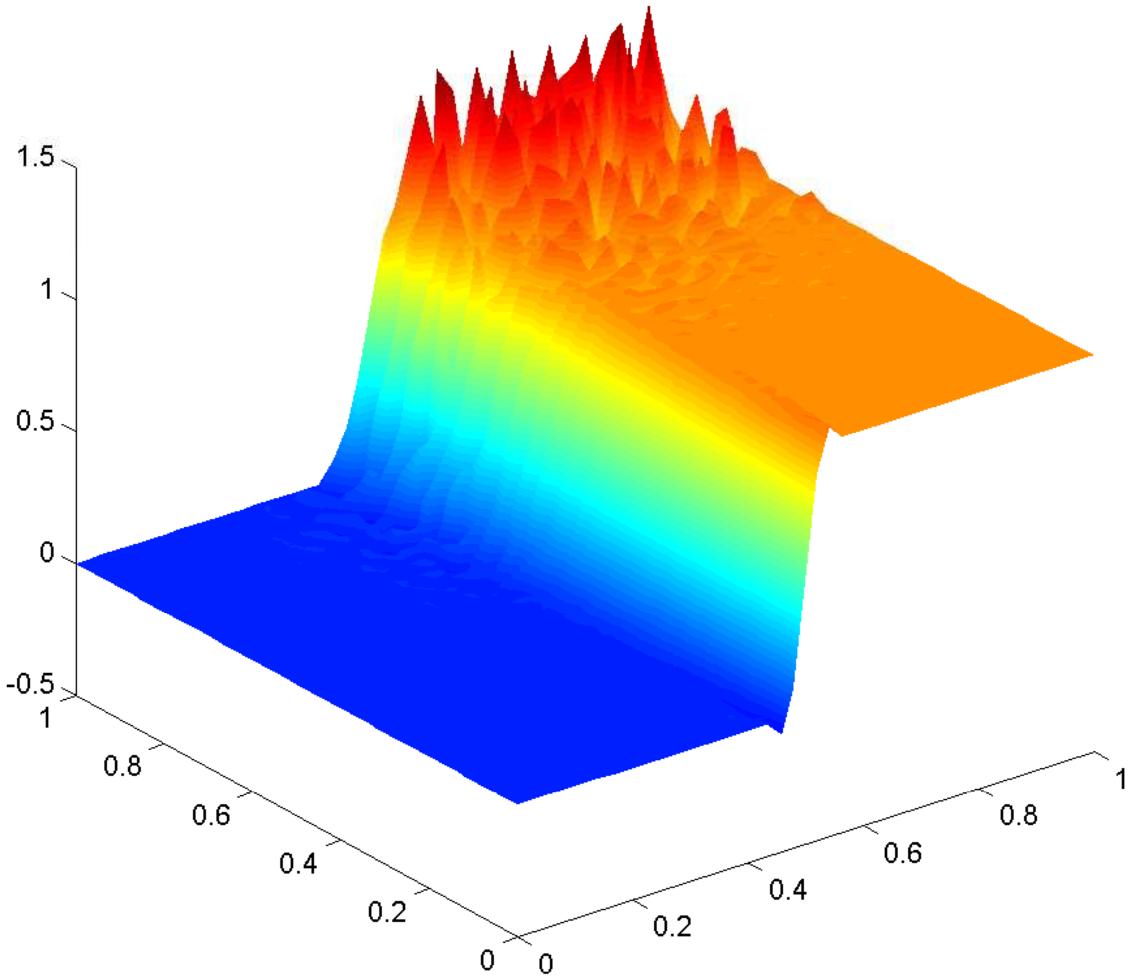
- regular $h \times h$ grid, $h = 1/(N+1)$, bilinear finite elements, mesh Peclet number $P_h \equiv (h\|w\|)/(2\nu)$;

- $P_h > 1$, then Galerkin discretization produces wiggles (non-physical oscillations near the boundary layers);

- Streamline Upwind Petrov Galerkin (SUPG) equivalent to adding stabilizing diffusion in the direction of the flow (wind);

- wind parallel to the mesh; here the vertical wind

$$w = [0,1]^T .$$


1.5
1
0.5
0
-0.5
1
0.8
0.6
0.4
0.2
0
0
0.2
0.4
0.6
0.8
1

The coefficient matrix of the linear algebraic system is

$$A \;=\; \nu\, A_d + A_c + \widehat{\delta}\, A_s\,,$$

$$\begin{aligned} A_d &= (\nabla \phi_j,\ \nabla \phi_i)\,, \\ A_c &= (w \cdot \nabla \phi_j,\ \phi_i)\,, \\ A_s &= (w \cdot \nabla \phi_j,\ w \cdot \nabla \phi_i)\,, \qquad \widehat{\delta} = \delta_* \, h/\|w\|\,. \end{aligned}$$

$$A = \Big( (\nu\, I + \widehat{\delta}\, w\, w^T)\, \nabla\phi_j,\ \nabla \phi_i \Big) \;+\; (w \cdot \nabla \phi_j,\ \phi_i)\,.$$

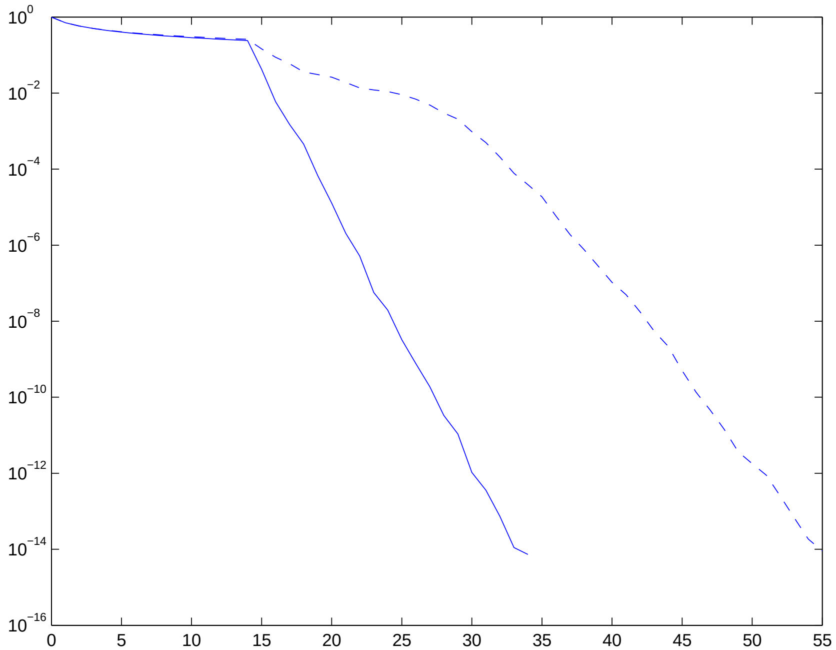
$\approx$ optimal stabilization parameter $\delta_* \equiv \frac{1}{2}\left(1 - \frac{1}{P_h}\right)$ affects

- smoothing of the discretized solution,
- behavior of the linear algebraic solver (convergence behavior of GMRES).

Example of boundary conditions:

- Raithby (discontinuous inflow).

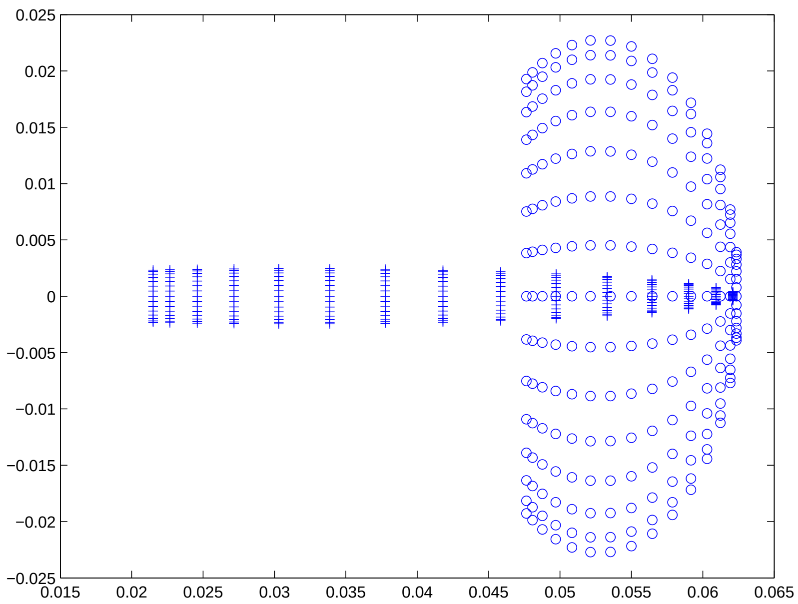
Discontinuous inflow boundary conditions (Raithby), two different values of the diffusion coefficient $\nu = 0.01$ and $\nu = 0.0001$ correspond to the solid and to the dashed line, respectively.



$$\sigma_{jk} = \lambda_j + (\gamma_j \mu_j)^{1/2} \omega_k \,,\; \omega_k = 2\cos(kh\pi),\; k = 1, \ldots, N\,.$$

Which spectrum corresponds to which convergence curve?

$$\lambda_j > 0\,, \quad \gamma_j \mu_j < 0\,.$$



## Concluding remarks

- initial phase is important, it depends on the right hand side!

- technique: orthonormal transformation to Jordan-like-structure
  (for the convection-diffusion model problem
  the matrix is diagonalizable!)

- generalizations? Many ways . . . ?

- analytical study of preconditioning?

**Thank you !**