

Asymptotic diagonalization of Hilbert-Schmidt operators

Benjamin BOUTIN



University of Rennes 1

Joint work with N. RAYMOND

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A little history

Hint around the power method : Consider $A \in M_n(\mathbb{C})$, $x_0, y_0 \in \mathbb{C}^n$.

For z sufficiently large :

$$f(z) = \langle x_0, (zI - A)^{-1} y_0 \rangle = \sum_{\nu=0}^{+\infty} \frac{\overbrace{\langle x_0, A^\nu y_0 \rangle}^{=: s_\nu}}{z^{\nu+1}} = \frac{\langle x_0, \text{adj}(zI - A)y_0 \rangle}{\det(zI - A)}.$$

Under some assumptions on x_0, y_0 and on A :

$$\frac{s_{\nu+1}}{s_\nu} \xrightarrow{\nu \rightarrow \infty} \lambda_1, \text{ eigenvalue of maximum modulus.}$$

More generally : *Being given the sequence of moments (s_ν) , find all the eigenvalues of a matrix A ?*

1892 Hadamard extended the above idea to obtain any of the pole of a meromorphic function from its moments, using the sequence of Hankel determinants of the form $|s_{\nu+i+j}|_{0 \leq i, j \leq k}$.

1931 Aitken rediscovered a more algorithmic version of the method.

1954 Rutishauser introduced **qd (quotient-difference) algorithm**, avoiding Hankel determinants, reducing ill-posedness of the method, and then reformulated (first for tridiagonal matrices) into the **LR algorithm** (Gauss LU decomposition)

$$L_k R_k := A_k, \quad A_{k+1} := R_k L_k$$



Hadamard



Rutishauser

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1961 Francis, Kublanovskaya : **QR algorithm**

$$Q_k R_k := A_k, \quad A_{k+1} := R_k Q_k$$

$$A_{k+1} = Q_k^* A_k Q_k = (Q_1 \dots Q_k)^* A (Q_1 \dots Q_k)$$

$$\text{spec } A_k = \text{spec } A$$

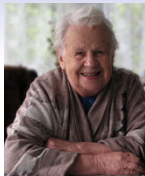
Francis, Wilkinson : Fast variants with shifts

$$Q_k R_k := A_k - \sigma_k I_n, \quad A_{k+1} := R_k Q_k + \sigma_k I_n$$

1968 Colette Lebaud :

Remarques sur la convergence de la méthode Q.R., Publications mathématiques et informatique de Rennes, Tome (1967-1968), Exposé no. 5, p.1–17.

PhD Univ. Rennes : *Contribution à l'étude de l'algorithme QR*, 1971.



Kublanovskaya



Francis



Lebaud

Common convergence results for the QR algorithm

Theorem

Let $A \in M_n(\mathbb{C})$ and $P \in GL_n(\mathbb{C})$ such that $PAP^{-1} = \text{diag}(\lambda_1, \dots, \lambda_n) = D$ with

$$|\lambda_1| > |\lambda_2| > \dots > |\lambda_n| > 0.$$

Assume moreover that P admits a LU factorization. Then

$$A_k \xrightarrow[k \rightarrow \infty]{} \begin{pmatrix} \lambda_1 & & \color{red}{(\star)_k} \\ & \ddots & \\ (0) & & \lambda_n \end{pmatrix}.$$

The lower part converge as $\mathcal{O}(\mu^k)$ with $\mu = \max_{1 \leq \ell \leq n-1} \left| \frac{\lambda_{\ell+1}}{\lambda_\ell} \right|$.

- In presence of "same modulus" distinct eigenvalues: convergence "by block".
- Iterations preserve symmetry and Hessenberg structure.
- Convergence is quadratic for the Wilkinson shifted version, and then cubic for symmetric matrices.
- The algorithm is equivalent to the orthogonal simultaneous power iteration (this makes the assumption $P = LU$ and improved convergence rates more intelligible)

Continuous dynamical systems

- 1988 Chu and Norris, *Isospectral flows and abstract matrix factorizations*, SIAM J. Numer. Anal.
- 1991 Brockett, *Dynamical systems that sort lists, diagonalize matrices and solve linear programming problems*, Linear Algebra Appl.
- 1994 Wegner, *Flow equations for Hamiltonians*, Ann. Physik.
- 2010 Bach and Bru, *Rigorous foundations of the Brockett-Wegner flow for operators*, J. Evol. Equ.
- 2016 Bach and Bru, *Diagonalizing quadratic bosonic operators by non-autonomous flow equation*, Memoirs AMS.

References for some history :

Gutknecht and Parlett, *From qd to LR, or, How were the qd and LR algorithms discovered?*, IMA J. Numer. Anal. 31 (2011).

Golub and van der Vorst, *Eigenvalue computation in the 20th century*, J. Comput. Appl. Math. 123 (2000).

Our aim :

Get a unified proof for different bracket flow ODEs : $H' = [H, G(H)]$, acting on Hilbert-Schmidt operators, and understand the QR method !

Outline

Introduction

Main result

Bracket flows

- Global existence and isospectrality

- Quadratic bracket flows

- Several examples

The Toda's choice

- A more specific result

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Some notations

$\mathcal{L}(\mathcal{H})$ bounded operators on a separable Hilbert space \mathcal{H}

$\mathcal{S}(\mathcal{H}), \mathcal{A}(\mathcal{H}), \mathcal{U}(\mathcal{H})$ symmetric, skew-symmetric and unitary operators respectively

$\mathcal{L}_2(\mathcal{H})$ Hilbert-Schmidt (compact) operators on \mathcal{H} , with the norm $\|\cdot\|_{\text{HS}}$:

$$\|H\|_{\text{HS}}^2 = \text{tr}(H^*H) = \sum_{n \geq 0} \|He_n\|^2 = \sum_{n=0}^{+\infty} |\lambda_n(H)|^2$$

$$\mathcal{S}_2(\mathcal{H}) = \mathcal{S}(\mathcal{H}) \cap \mathcal{L}_2(\mathcal{H})$$

$$\mathcal{A}_2(\mathcal{H}) = \mathcal{A}(\mathcal{H}) \cap \mathcal{L}_2(\mathcal{H})$$

$(e_n)_{n \in \mathbb{N}}$ a Hilbert basis of \mathcal{H}

$$h_{i,j} = \langle He_i, e_j \rangle, \text{ for any } H \in \mathcal{L}(\mathcal{H})$$

$\mathcal{D}(\mathcal{H})$ bounded diagonal operators with respect to the Hilbert basis:

$$T \in \mathcal{D}(\mathcal{H}) \Leftrightarrow \forall n \in \mathbb{N}, \exists \lambda_n \in \mathbb{R}, Te_n = \lambda_n e_n$$

$E_{i,j}$ ($i \leq j$) canonical Hilbert basis of $\mathcal{S}_2(\mathcal{H})$

$E_{i,j}^{\pm}$ ($i < j$) canonical Hilbert basis of $\mathcal{A}_2(\mathcal{H})$

Main result

Consider $H \in \mathcal{C}^1(\mathbb{R}, \mathcal{L}_2(\mathcal{H}))$ such that

- i) the function $t \mapsto \|H(t)\|_{\text{HS}}$ is bounded,
- ii) the family $(h_{i,j})_{i,j \in \mathbb{N}}$ is balanced (symmetry-like property, uniform in t)
- iii) there exists a pointwise bounded and balanced family of measurable functions $(g_{i,j})_{i,j \in \mathbb{N}}$ defined on \mathbb{R} such that

$$\forall t \in \mathbb{R}, \forall i \in \mathbb{N}, \quad h'_{i,i}(t) = \sum_{j=0}^{+\infty} g_{i,j}(t) |h_{i,j}(t)|^2.$$

Suppose that there exists $T > 0$ and a sign sequence $(\epsilon_\ell)_{\ell \in \mathbb{N}} \in \{-1, 1\}^{\mathbb{N}}$, such that

$$\forall t \geq T, \forall k, \ell \in \mathbb{N}, k \geq \ell, \quad \epsilon_\ell g_{\ell,k}(t) \geq 0. \quad (\text{sign})$$

Then we have the **integrability property**

$$\forall \ell \in \mathbb{N}, \quad \sum_{j=0}^{+\infty} \int_T^{+\infty} |g_{\ell,j}(t)| |h_{\ell,j}(t)|^2 dt < +\infty,$$

and the **diagonal terms** $h_{\ell,\ell}(t)$ converges at infinity.

Ideas of the proof

- Proof by induction on $\ell \in \mathbb{N}$, using monotonicity arguments
- Limit of the $h_{\ell, \ell}$ coefficient and integrability of the series is controlled from the next lemma

Lemma

Consider $h \in \mathcal{C}^1(\mathbb{R}_+)$ a real-valued bounded function, $F \in L^1(\mathbb{R}_+)$ and G a nonnegative measurable function defined on \mathbb{R}_+ such that

$$\forall t \geq 0, h'(t) = F(t) + G(t).$$

Then, the function G is integrable and h converges to a finite limit at infinity.

$$\int_0^x G(t) dt = h(x) - h(0) - \int_0^x F(t) dt \leq 2 \sup_{\mathbb{R}_+} |h| + \int_0^{+\infty} |F(t)| dt.$$

Therefore $G \in L^1(\mathbb{R}_+)$ and $\lim_{x \rightarrow +\infty} h(x) = h(0) + \int_0^{+\infty} (F(t) + G(t)) dt.$

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Main result (2)

Under the additional semi-uniform lower bound condition

$$\forall \ell \in \mathbb{N}, \exists c_\ell > 0, \forall j \neq \ell, \forall t \geq T, |g_{\ell,j}(t)| \geq c_\ell, \quad (\text{lower bound})$$

we have [the stronger integrability result](#)

$$\sum_{j \neq \ell} \int_T^{+\infty} |h_{\ell,j}(t)|^2 dt = \int_T^{+\infty} \|H(t)e_\ell - h_{\ell,\ell}(t)e_\ell\|^2 dt < +\infty.$$

Suppose moreover that, for any $\ell \in \mathbb{N}$, the function $t \mapsto \|H'(t)e_\ell\|$ is bounded, then for any $\ell \in \mathbb{N}$, $H(t)e_\ell$ converges to $h_{\ell,\ell}(\infty)e_\ell$.

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Global existence and isospectrality

Theorem

Suppose $G : \mathcal{S}(\mathcal{H}) \rightarrow \mathcal{A}(\mathcal{H})$ is locally Lipschitz, then any solution to the following Cauchy problem

$$H' = [H, G(H)], \quad H(0) = H_0 \in \mathcal{S}_2(\mathcal{H}).$$

admits a unique global solution $H \in \mathcal{C}^1(\mathbb{R}, \mathcal{S}_2(\mathcal{H}))$ and there exists $U \in \mathcal{C}^1(\mathbb{R}, \mathcal{U}(\mathcal{H}))$ such that

$$H(t) = U(t)^* H_0 U(t), \quad t \in \mathbb{R}.$$

Proof: As long $H(t)$ is defined, consider the following Cauchy problem:

$$\begin{cases} U'(t) = U(t)G(H(t)), \\ U(0) = \text{Id}. \end{cases}$$

Then $U(t) \in \mathcal{U}(\mathcal{H})$ and $H(t) = U^*(t)H_0U(t)$.

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$$\begin{aligned} \frac{d}{dt}(UU^*) &= U'U^* + UU'^* \\ &= UG(H)U^* + U(\underbrace{U G(H)}_{\in \mathcal{A}(\mathcal{H})})^* = UG(H)U^* - UG(H)U^* = 0. \end{aligned}$$

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Then $U(t) \in \mathcal{U}(\mathcal{H})$ and $H(t) = U^*(t)H_0U(t)$.

$$\begin{aligned} \frac{d}{dt}(UHU^*) &= U'HU^* + UH'U^* + UHU'^* \\ &= UG(H)HU^* + U[H, G(H)]U^* - UHG(H)U^* \\ &= U\left(G(H)H - HG(H) + [H, G(H)]\right)U^* = 0. \end{aligned}$$

Quadratic bracket flows

Consider $H' = [H, G(H)]$, in the case $G \in \mathcal{L}(S_2(\mathcal{H}), \mathcal{A}_2(\mathcal{H}))$.

The map G is said to be **diagonalizable** when there exists a Hilbertian basis $(e_n)_{n \in \mathbb{N}}$ and a skew-symmetric family $(g_{i,j})$ such that $G(E_{i,j}) = g_{i,j} E_{i,j}^\pm$.

We then have

$$h'_{i,i}(t) = -2 \sum_j g_{i,j} |h_{i,j}(t)|^2,$$

and prove from the main result :

Corollary

Let $G \in \mathcal{L}(S_2(\mathcal{H}), \mathcal{A}_2(\mathcal{H}))$ be a diagonalizable map such that its matrix-eigenvalue satisfies **(sign)** and **(lower bound)**.

Then the unique global solution $H \in \mathcal{C}^1(\mathbb{R}, S_2(\mathcal{H}))$ converges weakly in $S_2(\mathcal{H})$ to some $H_\infty \in \mathcal{D}_2(\mathcal{H})$.

Moreover, any diagonal term α of H_∞ with multiplicity m is an eigenvalue of H_0 of multiplicity at least m .

Example 1: Brockett's choice

$$G_{\text{Br}}(H) = [H, A], \quad \text{where } A = \text{diag}(a_1, \dots) \in \mathcal{D}(\mathcal{H}), \quad a_1 > a_2 > \dots > 0$$

- skew-symmetric matrix-eigenvalue :

$$g_{i,j} = a_j - a_i$$

- (sign) assumption :

$$\forall k, \ell \in \mathbb{N}, k \geq \ell, -g_{\ell,k} \geq 0$$

- (lower bound) assumption :

$$\forall \ell \in \mathbb{N}, \forall j \neq \ell, |g_{\ell,j}| \geq \min(|a_\ell - a_{\ell-1}|, |a_\ell - a_{\ell+1}|)$$

Example 2: Toda's choice

$$G_{\text{Tod}}(H) = H^- - (H^-)^*, \quad H^- = \sum_{1 \leq i < j} h_{i,j} e_i^* e_j$$

- skew-symmetric matrix-eigenvalue :

$$g_{i,j} = -1, \quad i < j$$

- (sign) assumption :

$$\forall k, \ell \in \mathbb{N}, k \geq \ell, -g_{\ell,k} \geq 0$$

- (lower bound) assumption :

$$\forall \ell \in \mathbb{N}, \forall j \neq \ell, |g_{\ell,j}| \geq 1$$

Example 3: Wegner's choice

$$G_{\text{Weg}}(H) = [H, \text{diag}(H)]$$

- $G_{\text{Weg}} \notin \mathcal{L}(\mathcal{S}_2(\mathcal{H}), \mathcal{A}_2(\mathcal{H}))$
- but $G_{\text{Weg}}(\mathcal{S}_2(\mathcal{H})) \subset \mathcal{A}_2(\mathcal{H})$ therefore the flow is unitarily equivalent and global.
- diagonal terms follow the dynamic:

$$h'_{i,i} = \sum_{j=0}^{+\infty} \underbrace{(h_{i,i} - h_{j,j})}_{g_{i,j}(t)} |h_{ij}|^2.$$

- What about (sign) and (lower bound) assumptions ?
If for large time, the diagonal terms $(h_{\ell,\ell})$ become "sufficiently" distinct, both assumptions are valid.

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More about the Toda flow : $G(H) = H^- - (H^-)^*$.

Proposition

Assume that $H_0 \in \mathcal{L}_2(\mathcal{H})$ (not necessarily symmetric) is diagonalizable with eigenvalues $(\lambda_j)_{j \geq 0}$ such that

$$\operatorname{Re} \lambda_0 > \operatorname{Re} \lambda_1 > \dots$$

Let us also assume that we may find $P \in \mathcal{L}(\mathcal{H})$ such that $PH_0P^{-1} = \operatorname{diag}(\lambda_j)$ and such that all the minors of $P : P_J = (\langle Pe_i, e_j \rangle)_{0 \leq i, j \leq J}$ are invertible.

For $\ell \in \mathbb{N}$, we denote $\delta_\ell = \min_{0 \leq j \leq \ell} \operatorname{Re}(\lambda_j - \lambda_{j+1})$, then

$$H(t)e_\ell - \sum_{j=\ell+1}^{+\infty} \langle H(t)e_\ell, e_j \rangle e_j = \lambda_\ell e_\ell + \mathcal{O}\left(e^{-t\delta_\ell}\right) .$$

- Find exponentially fast eigenvalues of any Hilbert-Schmidt operator
- If $H(0)$ is symmetric, then $H(t)$ converges to a diagonal operator H_∞ that has exactly the same eigenvalues as H_0
- Even in infinite dimension no eigenvalue is lost in the limit !

Relation with the discrete QR algorithm

1988 Chu and Norris proposed an abstract decomposition of the flow

$$H'(t) = [H(t), G_{\text{Tod}}(H(t))], \quad H(0) = H_0 \in \mathcal{L}_2(\mathcal{H}),$$

$$\begin{aligned} g_1'(t) &= g_1(t)G_{\text{Tod}}(H(t)), & g_1(0) &= \text{Id}, \\ g_2'(t) &= (H(t) - G_{\text{Tod}}(H(t)))g_2(t), & g_2(0) &= \text{Id}. \end{aligned}$$

so that

$$\begin{aligned} H(t) &= g_1(t)^{-1}H_0g_1(t) = g_2(t)H_0g_2^{-1}(t) \\ e^{tH_0} &= g_1(t)g_2(t), \quad e^{tH(t)} = g_2(t)g_1(t). \end{aligned}$$

- $G_{\text{Tod}}(H) = H_- - H_+^* \in \mathcal{A}(\mathcal{H})$ therefore $g_1(t) \in \mathcal{U}(\mathcal{H})$
- $H - G_{\text{Tod}}(H) = H_+ + H_-^*$ is upper triangular and so is $g_2(t)$
- at $t = 1$: $e^{H_0} = g_1(1)g_2(1)$ is a QR factorization of e^{H_0}
and $e^{H(1)} = g_2(1)g_1(1)$ is then the first iterate of the QR algorithm
- Toda flow \simeq sampling of the discrete algorithm (up to a change in $g_2(0)$ to ensure corresponding normalization choices in the diagonal of $g_2(1)$)
- $\text{spec}(e^{H_0}) = \{e^{\lambda_j}\}$ with decreasing moduli (convergence rate)
- *Remark* : this can be done for many matrix factorization : QR, LU, Cholesky.

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- at $t = 1$: $e^{H_0} = g_1(1)g_2(1)$ is a QR factorization of e^{H_0}
and $e^{H(1)} = g_2(1)g_1(1)$ is then the first iterate of the QR algorithm
- Toda flow \simeq sampling of the discrete algorithm (up to a change in $g_2(0)$ to ensure corresponding normalization choices in the diagonal of $g_2(1)$)
- $\text{spec}(e^{H_0}) = \{e^{\lambda_j}\}$ with decreasing moduli (convergence rate)
- *Remark* : this can be done for many matrix factorization : QR, LU, Cholesky.

Numerical examples

Finite dimension case :

- strong convergence to the limit
- alternative : compactness of $\mathcal{U}(\mathcal{H})$
- linearization of the flow in $\mathcal{U}(\mathcal{H})$ around U_∞ , parameterized by its Lie algebra $\mathcal{A}(\mathcal{H})$
- \Rightarrow exponential convergence, whatever is the stable manifold in consideration.

Datas for the computations :

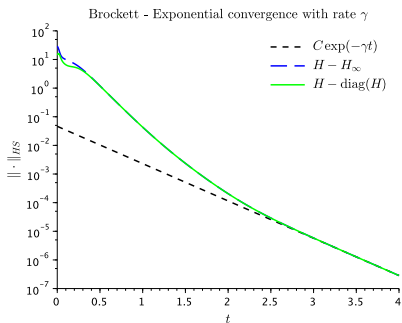
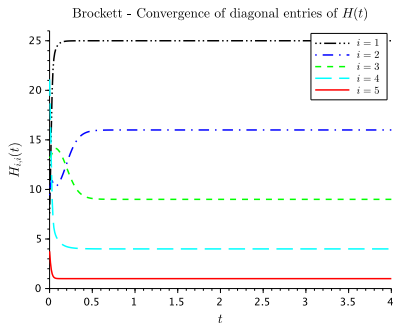
- **Initial data** : $H_0 = Q \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 4 & 0 & 0 & 0 \\ 0 & 0 & 9 & 0 & 0 \\ 0 & 0 & 0 & 16 & 0 \\ 0 & 0 & 0 & 0 & 25 \end{pmatrix} Q^*$ where $Q = \exp \begin{pmatrix} 0 & -1 & -1 & -1 & -1 \\ 1 & 0 & -1 & -1 & -1 \\ 1 & 1 & 0 & -1 & -1 \\ 1 & 1 & 1 & 0 & -1 \\ 1 & 1 & 1 & 1 & 0 \end{pmatrix}$
- G_{Br} is defined from $A = \begin{pmatrix} 5 & 0 & 0 & 0 & 0 \\ 0 & 4 & 0 & 0 & 0 \\ 0 & 0 & 3 & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}$
- The numerical solutions are computed using adaptive 4th-order Runge-Kutta scheme.
- Test the three flows presented before.

Brockett's choice

$$H(t) \rightarrow H_\infty = \text{diag}([25, 16, 9, 4, 1])$$

Diagonal terms are sorted in a descending order, w.r.t to A

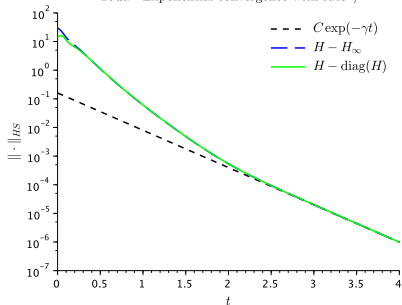
$$\text{spec } dF_{H_\infty} = \begin{pmatrix} 0 & -9 & -32 & -63 & -96 \\ -9 & 0 & -7 & -24 & -45 \\ -32 & -7 & 0 & -5 & -16 \\ -63 & -24 & -5 & 0 & -3 \\ -96 & -45 & -16 & -3 & 0 \end{pmatrix}.$$



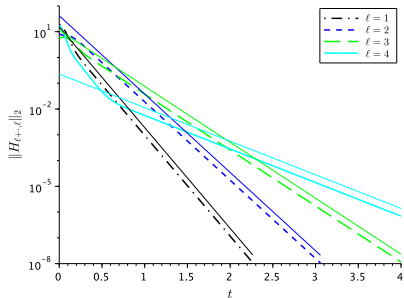
Toda's choice

$$\text{spec } dF_{H_\infty} = \begin{pmatrix} 0 & -9 & -16 & -21 & -24 \\ -9 & 0 & -7 & -12 & -15 \\ -16 & -7 & 0 & -5 & -8 \\ -21 & -12 & -5 & 0 & -3 \\ -24 & -15 & -8 & -3 & 0 \end{pmatrix}.$$

Toda - Exponential convergence with rate γ



Toda - Convergence of extradiagonal entries

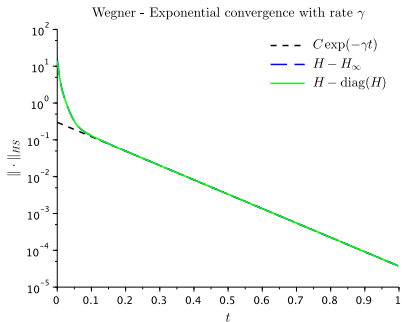
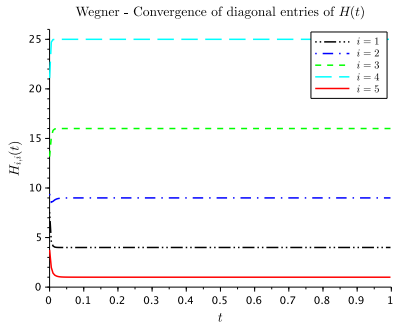


Wegner's choice

$$H(t) \rightarrow H_\infty = \text{diag}([4, 9, 16, 25, 1])$$

$$dF_{H_\infty}(E_{i,j}) = -(\lambda_i - \lambda_j)^2 E_{i,j}.$$

$$\text{spec } dF_{H_\infty} = \begin{pmatrix} 0 & -25 & -144 & -441 & -9 \\ -25 & 0 & -49 & -256 & -64 \\ -144 & -49 & 0 & -81 & -225 \\ -441 & -256 & -81 & 0 & -576 \\ -9 & -64 & -225 & -576 & 0 \end{pmatrix}.$$



Brockett's choice – other stable manifold

Other initial data : $\tilde{H}_0 = \tilde{Q} \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 4 & 0 & 0 & 0 \\ 0 & 0 & 9 & 0 & 0 \\ 0 & 0 & 0 & 16 & 0 \\ 0 & 0 & 0 & 0 & 25 \end{pmatrix} \tilde{Q}^*$, where $Q = \exp \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & -1 & -1 \\ 0 & 1 & 0 & -1 & -1 \\ 0 & 1 & 1 & 0 & -1 \\ 0 & 1 & 1 & 1 & 0 \end{pmatrix}$.

- $\tilde{H}(t) = \begin{pmatrix} 1 & (0) \\ (0) & K(t) \end{pmatrix}$ with $\text{spec}(K(t)) = \{4, 9, 16, 25\}$.
- The (floating-point arithmetic) numerical method preserves this particular subspace
- $H(t) \rightarrow H_\infty = \text{diag}([1, 25, 16, 9, 4])$ with exponential rate $\mathcal{O}(e^{-5t})$

$$\text{spec } dF_{H_\infty} = \begin{pmatrix} 0 & 24 & 30 & 24 & 12 \\ 24 & 0 & -9 & -32 & -63 \\ 30 & -9 & 0 & -7 & -24 \\ 24 & -32 & -7 & 0 & -5 \\ 12 & -63 & -24 & -5 & 0 \end{pmatrix}.$$

Grub's up !

À table !

Ăn trưa được phục vụ !

午餐已送达