Computable error bounds for nonlinear eigenvalue problems allowing for a minmax characterization

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Outline

Linear eigenvalue problems

Theorem (Krylov, Bogoliubov 1929, Weinstein 1934)
Let $A = A^H$, $x \neq 0$, and $R(x) := x^H Ax / x^H x$. Then here exists an eigenvalue η of A such that

$$|\eta - R(x)| \leq \frac{\|Ax - R(x)x\|}{\|x\|}.$$

Theorem (Kato 1949, Temple 1929, 1952)
Let $A = A^H$ with eigenvalues $\eta_1 \geq \eta_2 \geq \cdots \geq \eta_n$, and let $\alpha < \beta$ such that $\eta_{j+1} \leq \alpha \leq \eta_j \leq \beta \leq \eta_{j-1}$.
Let

$$\|Ax - R(x)x\|^2 \leq (R(x) - \alpha)(\beta - R(x))\|x\|^2.$$

Then it holds that

$$R(x) - \frac{\|Ax - R(x)x\|^2}{(\beta - R(x))\|x\|^2} \leq \eta_j \leq R(x) + \frac{\|Ax - R(x)x\|^2}{(R(x) - \alpha)\|x\|^2}.$$

Nonlinear Eigenvalue Problem

Let $J \subset \mathbb{R}$ be an open interval (which may be unbounded), and $T(\lambda)$, $\lambda \in J$ be a family of Hermitian matrices.

Nonlinear eigenvalue Problem:
Find $\lambda \in J$ and $x \neq 0$ such that

$$T(\lambda)x = 0.$$

Then λ is called an eigenvalue of $T(\cdot)$, and x a corresponding eigenvector.

Problems of this type arise in damped vibrations of structures, conservative gyroscopic systems, lateral buckling problems, problems with retarded arguments, fluid-solid vibrations, and quantum dot heterostructures, e.g.

Nonlinear minmax theory

Assume that for fixed $x \in \mathbb{C}^n$, $x \neq 0$ the real equation

$$f(\lambda, x) := x^H T(\lambda) x = 0$$

has at most one solution $\lambda =: p(x)$ in J.

Then equation $f(\lambda, x) = 0$ implicitly defines a functional p on some subset D of $\mathbb{C}^n$ which we call the Rayleigh functional.

Let

$$(\lambda - p(x)) f(\lambda, x) > 0 \quad \text{for every } \lambda \neq p(x) \text{ and every } x \in D.$$

Overdamped problems

If p is defined on $D = \mathbb{C}^n \setminus \{0\}$ then the problem $T(\lambda)x = 0$ is called overdamped.

Notation is motivated by the finite dimensional quadratic eigenvalue problem

$$T(\lambda)x = \lambda^2 Mx + \lambda Cx + Kx = 0$$

where M, C and K are Hermitian and positive definite matrices.

Theorem (Duffin 1955, Rogers 1964)
Under the conditions above an overdamped problem has exactly n eigenvalues $\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n$ which can be characterized by

$$\lambda_j = \min_{\dim V = j} \max_{x \in V \setminus \{0\}} p(x).$$

Nonoverdamped problems

For nonoverdamped eigenproblems the natural ordering to call the smallest eigenvalue the first one, the second smallest the second one, etc., is not appropriate.

This is obvious if we make a linear eigenvalue

$$T(\lambda)x := (\lambda I - A)x = 0$$

nonlinear by restricting it to an interval J which does not contain the smallest eigenvalue of A.

Then all conditions are satisfied, p is the restriction of the Rayleigh quotient R_A to

$$D := \{x \neq 0 \; : \; R_A(x) \in J\},$$

and $\inf_{x \in D} p(x)$ will in general not be an eigenvalue.

Enumeration of eigenvalues

If $\lambda \in J$ is an eigenvalue of $T(\cdot)$ then $\mu = 0$ is an eigenvalue of the linear problem $T(\lambda)y = \mu y$, and therefore there exists $\ell \in \mathbb{N}$ such that

$$0 = \max_{V \in H_\ell} \min_{v \in V \setminus \{0\}} \frac{v^H T(\lambda) v}{\|v\|^2}$$

where H_ℓ denotes the set of all ℓ–dimensional subspaces of $\mathbb{C}^n$.

In this case λ is called an ℓ-th eigenvalue of $T(\cdot)$.

Minmax characterization (V., Werner 1982, V. 2009)

Under the conditions given above it holds:

(i) For every $\ell \in \mathbb{N}$ there is at most one ℓ-th eigenvalue of $T(\cdot)$ which can be characterized by

$$\lambda_\ell = \min_{V \in H_\ell,\ V \cap D \neq \emptyset} \ \sup_{v \in V \cap D} p(v). \qquad (*)$$

The set of eigenvalues of $T(\cdot)$ in J is at most countable.

(ii) $\tilde{\lambda}$ is an ℓ-th eigenvalue if and only if $\mu = 0$ is the ℓ largest eigenvalue of the linear eigenproblem $T(\tilde{\lambda})x = \mu x$.

(iii) The minimum in (*) is attained for the invariant subspace of $T(\lambda_\ell)$ corresponding to its ℓ largest eigenvalues.

(iv) If $T(\cdot)$ has an ℓth eigenvalue $\lambda_\ell \in J$, then it holds for $\lambda \in J$

$$\lambda \left\{ \begin{array}{c} < \\ = \\ > \end{array} \right\} \lambda_\ell \iff \eta_\ell(\lambda) := \sup_{\dim V = \ell} \ \min_{x \in V, x \neq 0} \frac{x^H T(\lambda) x}{x^H x} \left\{ \begin{array}{c} < \\ = \\ > \end{array} \right\} 0.$$

Assume that $T : J \to \mathbb{C}^{n\times n}$ allows for a minmax characterization of its eigenvalues in J, and let $\eta_j(\lambda)$ be the jth largest eigenvalue of the linear eigenproblem

$$T(\lambda)y = \eta_j(\lambda)y,\ j = 1,\dots,n,\ \lambda \in J.$$

Lemma

For $\lambda, \tilde\lambda \in J$, $\lambda \neq \tilde\lambda$ it holds that

$$\frac{\eta_j(\lambda) - \eta_j(\tilde\lambda)}{\lambda - \tilde\lambda} \geq \min_{y\neq 0} \frac{y^H(T(\lambda) - T(\tilde\lambda))y}{(\lambda - \tilde\lambda)y^H y} =: \phi(\lambda, \tilde\lambda).$$

Follows easily from the monotonicity result for eigenvalues of sums of Hermitian matrices A and B

$$\lambda_{j+k-1}(A + B) \leq \lambda_j(A) + \lambda_k(B),\ j,k = 1,\dots,n,\ j + k \leq n + 1,$$

$$\lambda_{j+k-n}(A + B) \geq \lambda_j(A) + \lambda_k(B),\ j,k = 1,\dots,n,\ j + k \geq n + 1,$$

Krylov,Bogoliubov, Weinstein

Theorem
Under the conditions of the minmax characterization let $x \in \mathcal{D}(p)$, and assume that for $\gamma \le p(x) \le \delta$ it holds that

$$\phi(p(x),\gamma)(p(x)-\gamma) \ge \frac{\|T(p(x))x\|}{\|x\|}$$

and

$$\phi(\delta,p(x))(\delta-p(x)) \ge \frac{\|T(p(x))x\|}{\|x\|}.$$

Then $T(\lambda)x = 0$ has an eigenvalue λ such that

$$\gamma \le \lambda \le \delta.$$

Krylov,Bogoliubov, Weinstein

Proof
The Rayleigh quotient for $T(p(x))y = \eta y$ at x is 0, and hence the (linear) Krylov, Bogoliubov, Weinstein Theorem yields the existence of some eigenvalue $\eta_j(p(x))$ such that

$$|\eta_j(p(x))| \le \frac{\|T(p(x))x\|}{\|x\|}.$$

If $\eta_j(p(x)) > 0$, then it follows from the Lemma

$$\frac{\|T(p(x))x\|}{\|x\|} \ge \eta_j(p(x)) \ge \eta_j(\gamma) + \phi(p(x))(p(x) - \gamma) \ge \eta_j(\gamma) + \frac{\|T(p(x))x\|}{\|x\|},$$

i.e. $\eta_j(\gamma) \le 0$, and there exists $\lambda_j \in [\gamma, p(x)]$ such that $\eta_j(\lambda_j) = 0$.

Likewise for $\eta_j(p(x)) < 0$ we get the existence of an eigenvalue $\lambda_j \in [p(x), \delta]$.

Kato, Temple

Theorem
Under the conditions of the minmax characterization let $\lambda_j, \beta \in J$ and $x \in \mathcal{D}(p)$. Assume that $\lambda_j \le p(x) \le \beta$, let $\eta_{j+1}(\beta) \le 0$, and

$$\phi(\lambda, \tilde{\lambda}) \ge 0 \quad \text{for } \lambda, \tilde{\lambda} \in [\lambda_j, \beta],\ \lambda \ne \tilde{\lambda}.$$

Then it holds that

$$\phi(p(x), \lambda_j)(p(x) - \lambda_j) \le \frac{\|T(p(x))x\|^2}{\phi(\beta, p(x))(\beta - p(x))\|x\|^2}.$$

Remarks 1. If $\lambda_{j+1} \in J$ then $\eta_{j+1}(\beta) \le 0$ holds for $\beta \le \lambda_{j+1}$; otherwise it is trivial for $\beta \in J$.
2. For $T(\lambda) := \lambda I - K$ it holds $\phi(\lambda, \tilde{\lambda}) = 1$, and with $p(x) = x^H K x / x^H x$ one gets

$$(p(x) - \lambda_j)(\beta - p(x)) \le \|T(p(x))x\|^2 / \|x\|^2,$$

i.e. the Kato-Temple Theorem for linear problems.

Kato, Temple

Proof

From the Lemma we get

$$-\eta_{j+1}(p(x)) \geq \eta_{j+1}(\beta) - \eta_{j+1}(p(x)) \geq \phi(\beta, p(x))(\beta - p(x)) \geq 0.$$

From $\lambda_j \leq p(x) \leq \beta$ and property (vi) of the minmax Theorem it follows that the conditions of the (linear) Kato- Temple Theorem are satisfied, and therefore

$$\eta_j(p(x)) \leq \frac{\|T(p(x))x\|^2}{(-\eta_{j+1}(p(x))\|x\|^2} \leq \frac{\|T(p(x))x\|^2}{\phi(\beta, p(x))(\beta - p(x))\|x\|^2}$$

and applying the Lemma again yields

$$\begin{aligned} \frac{\|T(p(x))x\|^2}{\phi(\beta, p(x))(\beta - p(x))\|x\|^2} &\geq \eta_j(p(x)) = \eta_j(p(x)) - \eta_j(\lambda_j) \\ &\geq \phi(p(x), \lambda_j)(p(x) - \lambda_j). \end{aligned}$$

Kato, Temple for differentiable T

Theorem

Let $T(\cdot)$ be differentiable and let the conditions of the minmax characterization be satisfied. Let $x \in \mathcal{D}(p)$, and assume that $\lambda_j, \beta \in J$ with $\lambda_j \le p(x) \le \beta$, that $\eta_{j+1}(\beta) \le 0$, and

$$\psi(\lambda) := \min_{y \neq 0} \frac{y^H T'(\lambda) y}{y^H y} \ge 0 \quad \text{for every } \Lambda \in [\lambda_1, \lambda_2].$$

Then it holds that

$$\int_{\lambda_j}^{p(x)} \psi(\lambda)\, d\lambda \int_{p(x)}^{\beta} \psi(\lambda)\, d\lambda \le \frac{\|T(p(x))x\|^2}{\|x\|^2}.$$

For overdamped problems and the maximal eigenvalue of $T(\cdot)$ this Kato-Temple bound was proved by Hadeler (1969).

Proof

$\eta_j(\lambda) : J \to \mathbb{R}$, the j largest eigenvalue of

$$T(\lambda)y(\lambda) = \eta(\lambda)y(\lambda)$$

is a continuous and piecewise continuously differentiable function, and the corresponding eigenvector $y(\lambda)$ can be chosen continuous and piecewise continuously differentiable.

Multiplying

$$T'(\lambda)y(\lambda) + T(\lambda)y'(\lambda) = \eta_j'(\lambda)y(\lambda) + \eta_j(\lambda)y'(\lambda)$$

by $y(\lambda)^H$ from the left yields

$$\eta_j'(\lambda) = \frac{y(\lambda)^H T'(\lambda)y(\lambda)}{y(\lambda)^H y(\lambda)}.$$

Proof

Hence,

$$\begin{aligned}\eta_{j+1}(p(x)) &= \eta_{j+1}(\beta) - \int_{p(x)}^{\beta} \eta_j'(\lambda)d\lambda \le - \int_{p(x)}^{\beta} \frac{y(\lambda)^H T'(\lambda) y(\lambda)}{y(\lambda)^H y(\lambda)} d\lambda \\ &\le - \int_{p(x)}^{\beta} \psi(\lambda) d\lambda =: \gamma \le 0.\end{aligned}$$

If $\gamma = 0$, then nothing is left to be shown. Otherwise, we have

$$\eta_{j+1}(p(x)) \le \gamma < 0 \le \eta_j(p(x))$$

where the last inequality follows from the minmax characterization, (iv).

Proof

From the (linear) Kato-Temple Theorem for $T(p(x))$ (notice that the Rayleigh quotient of $T(p(x))$ at x is 0) we get

$$\eta_j(p(x)) \le -\frac{\|T(p(x))x\|^2}{\gamma\|x\|^2},$$

and therefore

$$0 = \eta_j(\lambda_j) = \eta_j(p(x)) + \int_{p(x)}^{\lambda_j} \eta_j'(\lambda)d\lambda \le -\frac{\|T(p(x))x\|^2}{\gamma\|x\|^2} + \int_{p(x)}^{\lambda_j} \psi(\lambda)d\lambda,$$

i.e.

$$\phi(p(x),\lambda_j)(p(x)-\lambda_j) \le \frac{\|T(p(x))x\|^2}{\phi(\beta,p(x))(\beta-p(x))\|x\|^2}.$$

Quadratic eigenproblem

$$Q(\lambda)x := (\lambda^2 I + 2\lambda B + C)x = 0, \quad B = B^T > 0, \ C = C^T > 0.$$

Assume that $Q(\sigma)$ is indefinite for some $\sigma < 0$. Then there exist intervals $J_- := (-\infty, \sigma_-)$ and $J_+ := (\sigma_+, 0)$ such that all eigenvalue $\lambda_1^- \le \lambda_2^- \le \dots \le \lambda_k^-$ in J_- are minmax values of p_-, and all eigenvalues $\lambda_1^+ \ge \lambda_2^+ \ge \dots \ge \lambda_\ell^+$ are maxmin values of p_+ where

$$p_\pm(x) = (-x^T Bx \pm \sqrt{(x^T Bx)^2 - x^T Cx \cdot x^T x})/\|x\|^2.$$

Let $x \in D(p_-)$ and $\lambda_j^- \le p(x) \le \beta \le \lambda_{j+1}^-$ such that $\beta \le -\lambda_{max}(B)$. Then for $T(\cdot) = -Q(\cdot)$ we have

$$\phi(\lambda, \tilde\lambda) = -\lambda - \tilde\lambda - 2\lambda_{\max}(B) \ge 0 \quad \text{for } \lambda, \tilde\lambda \le -\lambda_{\max}(B),$$

and one gets

$$(\lambda_j^- + \lambda_{\max}(B))^2 \le (p_-(x) + \lambda_{\max}(B))^2 + \frac{\|Q(p_-(x))x\|^2}{\|x\|^2(-\beta - p_-(x) - 2\lambda_{\max}(B))(\beta - p_-(x))}$$

Numerical Example

$A = \text{eye}(20); \quad B = \text{randn}(20); B = 0.5 * B^T * B; \quad C = \text{randn}(20); C = C^T * C;$

Then $Q(\lambda)x = 0$ has 26 real eigenvalues, 13 of either type, and the maximum of the eigenvalues of negative type is less than the minimum of the eigenvalue of positive type. So, all of them are minmax and maxmin values of p_- and p_+, respectively.

Only 4 real eigenvalues satisfy $\lambda_j^- < -\lambda_{\max}(B)$ such that the Kato-Temple bound applies.

For a random vector y and $p = p_-(y)$ we projected $-Q(\cdot)$ to the invariant subspace of $-Q(p)$ corresponding to the 4 largest eigenvalues, and chose as ansatz vectors the corresponding Ritz vectors.

For the Kato-Temple bound of the kth eigenvalue we chose $\beta = 0.5 * (\lambda_k^- + \lambda_{k+1}^-)$.

Numerical Example

	l.bound	e.val	u.bound	e.val-l.b.	u.b.-e.val
1	-64.8808	-64.8638	-64.8607	1.70e-2	3.05e-3
2	-45.4187	-44.8673	-44.8595	5.51e-1	7.87e-3
3	-42.0779	-41.7205	-41.7143	3.57e-1	6.18e-3
4	-37.0017	-36.2613	-36.2587	7.40e-1	2.63e-3

Quadratic eigenproblem

In a similar way one can prove a Kato-Temple Theorem yielding upper bounds for nonlinear eigenproblems allowing for a maxmin characterization of its eigenvalues.

For $Q(\lambda) = \lambda^2 + 2\lambda B + C$ as before let $x \in D(p_+)$, $\lambda_{j+1}^+ \le \beta \le p_+(x) \le \lambda_j^+$, and $\beta > -\lambda_{\min}(B)$. Then it holds that

$$(\lambda_j^+ + \lambda_{\min}(B))^2 \le (p_+(x) + \lambda_{\min}(B))^2 + \frac{\|Q(p_+(x))x\|^2}{\|x\|^2(\beta + p_+(x) + 2\lambda_{\min}(B))(p_+(x) - \beta)}.$$

In our numerical example only one eigenvalue $\lambda_1^+ = -3.66e-3$ satisfies $\lambda_j^+ > -\lambda_{\min}(B) = -6.52e-3$, and a very good lower bound $p_+(x)$ is needed to obtain a negative upper bound from the Kato-Temple Theorem.

	l.bound	e.val-l.b.	u.bound	u.b.-e.val
1	-3.5479e-2	3.18e-2	5.9067e+2	
2	-6.3189e-3	2.66e-3	4.3382e+3	
3	-3.7373e-3	7.66e-5	2.5967e+1	
4	-3.6608e-3	7.91e-8	7.4345e-1	
5	-3.6607e-3	8.59e-14	-3.5576e-3	1.03e-4

Plateproblem

Consider vertical vibrations of a clamped plate with k identical elastically attached loads. Discretization with finite elements (with Bogner, Fox, Schmit elements) yields a rationale eigenvalue problem

$$T(\lambda)x := \lambda Mx - Kx + \frac{\lambda}{\sigma - \lambda} CC^T x = 0$$

where $K, M \in \mathbb{R}^{n\times n}$ are symmetric and positive definite, and $C \in \mathbb{R}^{n\times k}$, which is equivalent to

$$A(\lambda)x := (\lambda I - E^{-1}KE^{-T} + \frac{\lambda}{\sigma - \lambda}(E^{-1}C)(E^{-1}C)^T)x = 0, \ M = EE^T.$$

All eigenvalues allow for a minmax characterization, and for $\lambda, \tilde{\lambda} < \sigma$

$$\phi(\lambda, \tilde{\lambda}) = 1 + \frac{\sigma}{(\sigma - \lambda)(\sigma - \tilde{\lambda})} \lambda_{\min}(E^{-1}CC^T E^{-T}) = 1 > 0.$$

Plateproblem

j	$[\lambda_l, \lambda_u]$	$\lambda_u - \lambda_l$	$\\|A(\lambda_u)x\\|/\\|x\\|$
1	$[0, 1294.946254361]$	$1.29e+03$	$3.04e+02$
1	$[1294.940212116, 1294.941039746]$	$8.28e-04$	$1.84e+00$
1	$[1294.941039550, 1294.941039557]$	$7.24e-09$	$5.44e-03$
1	$[1294.941039557, 1294.941039557]$	≈ 0	$1.13e-05$
2	$[1294.941039557, 5386.761205603]$	$4.07e+03$	$8.59e+01$
2	$[5326.150980044, 5386.760800508]$	$6.06e+01$	$3.42e-01$
2	$[5386.759576233, 5386.760800501]$	$1.22e-03$	$1.54e-03$
2	$[5386.759470012, 5386.760800501]$	$1.33e-03$	$1.60e-03$
2	$[5386.760369240, 5386.760800501]$	$4.31e-04$	$9.12e-04$
2	$[5386.760800501, 5386.760800501]$	$5.02e-10$	$9.84e-07$
2	$[5386.760800501, 5386.760800501]$	$1.00e-11$	$1.40e-07$
3	$[5386.760800501, 5387.480359789]$	$7.11e-01$	$3.99e+03$
3	$[5386.762494844, 5386.762727965]$	$2.33e-04$	$1.21e+00$
3	$[5386.762727350, 5386.762727353]$	$2.79e-09$	$4.20e-03$
3	$[5386.762727352, 5386.762727352]$	≈ 0	$7.25e-06$

Plateproblem

j	$[\lambda_l, \lambda_u]$	$\lambda_u - \lambda_l$	$\|A(\lambda_u)x\|/\|x\|$
4	[5386.762727352, 11711.132378606]	$6.32e+03$	$6.34e+01$
4	[11711.131988297, 11711.132013564]	$2.53e-05$	$3.76e-01$
4	[11711.132013556, 11711.132013556]	$1.09e-10$	$7.80e-04$
4	[11711.132013556, 11711.132013556]	≈ 0	$6.85e-07$
5	[11711.132013556, 17314.691936356]	$5.40e+03$	$3.91e+02$
5	[17314.683054949, 17314.683982005]	$9.27e-04$	$3.91e-01$
5	[17314.683981950, 17314.683981955]	$5.52e-09$	$9.53e-04$
5	[17314.683981955, 17314.683981955]	≈ 0	$1.24e-06$
6	[17314.683981955, 17479.083431959]	$1.64e-02$	$5.70e+01$
6	[17479.083270569, 17479.083271900]	$1.33e-06$	$1.14e-01$
6	[17479.083271900, 17479.083271900]	≈ 0	$1.15e-04$