

# NSF DAY AT DARTMOUTH

September 11, 2008

MPS for  
EVPs find eigenpairs  $(\lambda, u)$  for nontrivial  $u$ ,  $\begin{cases} -\Delta u = \lambda u & \text{in } \Omega \\ u=0 & \text{on } \partial\Omega \end{cases}$ .

Pick an freq.  $\lambda$ .

Basis rep.  $u = \sum \alpha_n \phi_n(x)$  set of basis func.  $(\lambda + \epsilon) \phi_n = 0$  in  $\Omega$ .  $\forall n$

$$\text{bdry norm } \|u\|_{L^2(\partial\Omega)}^2 = \int_{\partial\Omega} |u(y)|^2 ds_y$$

$$= \sum_{nm} \alpha_n \bar{\alpha}_m \underbrace{\int_{\partial\Omega} \phi_n(y) \overline{\phi_m(y)} ds_y}_{\text{matrix } F_{mn}, \text{ Hermitian}} = \vec{\alpha}^* F \vec{\alpha}$$

$$\text{interior norm } \|u\|_{L^2(\Omega)}^2 = \vec{\alpha}^* G \vec{\alpha}$$

called quadratic form.  
note  $\vec{\alpha}^* F \vec{\alpha} = 1$  is an ellipsoid

If  $u$  sat.  $(\lambda + \epsilon)u = 0$  in  $\Omega$ ,

$$t[u] = \frac{\|u\|_{\Omega}}{\|u\|_{\partial\Omega}}$$

measures how 'close'  $u$  is to eigenfunc of laplacian.

Why?

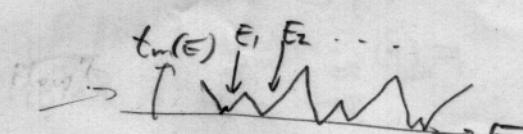
Remark: also will see  $t[u]$  small.  $\Leftrightarrow \lambda$  close to eigen.

Method: i) guess  $\lambda$

$t[u] = 0 \Leftrightarrow u$  is eigfunc & eigen

ii) Find  $\min_{u \in \text{Span}\{\phi_n\}} t[u] =: t_m(\lambda)$

iii) search along  $\lambda$  axis for minimum where  $t_m(\lambda) \approx 0$ .



How do ii)?  $t_m(\lambda) = \min_{\vec{\alpha} \in \mathbb{C}^n} \frac{\vec{\alpha}^* F \vec{\alpha}}{\vec{\alpha}^* G \vec{\alpha}}$  Rayleigh quotient for matrices  $(F, G)$

$$= \min_{\substack{\vec{\alpha}^* G \vec{\alpha} = 1}} \vec{\alpha}^* F \vec{\alpha}$$

Thm.: Let  $G$  be positive definite Hermitian,  $F$  Hermitian, both  $N \times N$ . generalized Min. value of Rayleigh quot.  $(F, G)$  is the minimum eigenval.  $\lambda_1$  of  $Fv = \lambda_1 Gv$  (GEP)

and is achieved at  $\vec{\alpha} = v_1$  the corresp. eigenv.

i) Lemma: spectral thm for pair  $(F, G)$ : GEP has complete set  $\{v_i\}_{i=1}^N$  eigenectors which sat.  $v_i^* G v_j = \delta_{ij}$ , ie  $G$ -orthog. Remark: GEP common in structural engineering.

PF: spectral thm. for  $G$ :  $G = W \Lambda W^*$   $W$  unitary,  $\Lambda$  diagonal.

coordinate change  $x = \underbrace{\Lambda^{1/2} W^* v}_\text{invertible}$  ie  $v = W \Lambda^{-1/2} x$  (positive entries)

$$x, v \in \mathbb{C}^N$$

$$\text{So } Fv = \lambda_1 Gv \quad (\text{GEP}) \quad \Leftrightarrow \quad FW^* \Lambda^{1/2} x = NGW \Lambda^{-1/2} x \quad (\text{cancels.}) \quad \Leftrightarrow \underbrace{\Lambda^{-1/2} W^* F W \Lambda^{1/2} x}_\text{Hermitian since F is.} = \mu x$$

By spectral thm  $\lambda^{1/2} W^* F W \lambda^{-1/2}$ ,  $\exists X \in \mathbb{C}^N$  for some unitary  $X = [x_1 \dots x_N]$   
 Then  $v_i = \underbrace{W \lambda^{1/2}}_{\text{inv.}} x_i$   $i=1 \dots N$  are eigenvectors of GEP, basis for  $\mathbb{C}^N$ , complete set, eigenvectors  
 $v_i^* G v_i = x_i \underbrace{\lambda^{-1/2} W^* G W \lambda^{1/2}}_I x_i = \delta_{ij}$  QED.

Now pf thm:

any  $\alpha$  can be written  $\sum_{i=1}^N \beta_i v_i$  since  $v_i$  basis.

$$F\alpha = \sum \beta_i \mu_i G v_i$$

$$\alpha^* F\alpha = \sum_{ij} \overline{\beta_j} \beta_i \mu_i \underbrace{v_j^* G v_i}_{\delta_{ij}} = \sum_i \mu_i |\beta_i|^2$$

$$\alpha^* G\alpha = \sum_i \overline{\beta_j} \beta_i \underbrace{v_j^* G v_i}_{\delta_{ij}} = \sum_i |\beta_i|^2$$

$$\text{so } \frac{\alpha^* F\alpha}{\alpha^* G\alpha} = \frac{\sum \mu_i |\beta_i|^2}{\sum |\beta_i|^2}$$

minimized by choosing  $\beta_i = 0$  for  $i \neq 1 \dots N$ .  
 (obvious or prove it).

May also prove via Lagrange multipliers.

$G$ 's ellipsoid because sphere.  
 $F$ 's aligned w/ axes.

In practice, we find as  $N$  incr,  $\phi_n$  not close to 100% deg.

ie nontriv. lin. comb of  $\phi_n$  exp. small in  $\mathcal{L}$  & on  $\mathcal{D}\Omega$ .

$\Rightarrow F, G$  acquire common numerical nullspace, not full rank. (in floating pt. arith.)

recipe (based on Fix & Heiberger, 1972,

diag.  $\hookrightarrow W, \Lambda$

$$\begin{matrix} N \\ \square \\ \approx \\ \leq N \end{matrix}$$

$$\text{diag. } \tilde{\Lambda}^{-1/2} \tilde{W}^* F \tilde{W} \tilde{\Lambda}^{-1/2} \rightarrow X, D$$

Vergili-Szarek (1994) = code I gave you, put in  $\tilde{\Lambda}$

keep only  $\lambda_i > 10^{-14} \lambda_{\max}, \lambda_i$ , kill corresponding cols of  $W$ .

$\tilde{W}$  may now be rect.

a regularizing parameter.

How fill  $F, G$  entries?

$$F_{mn} \approx \sum_{j=1}^M w_j \phi_m(y_j) \phi_n(y_j) \text{ mostly each needs } O(N^2) \text{ integrals, each w/ quadrature}$$

$$\text{ie } F = A^* A \quad \text{where } A_{jn} = \int_{\Omega} \phi_n(y_j)$$

sim

$$G = B^* B$$

, the 'square' of  $A$ .

$$B_{jm} = \sqrt{w_j} \phi_n(z_j)$$

$z_j$  interior pt,  $j=1 \dots J$

last time.

Note  $t_m(\epsilon) = \min_{x \neq 0} \frac{\alpha^* F x}{\alpha^* G x} = \min_{x \neq 0} \frac{\|Ax\|}{\|Bx\|} = \min$  generalized svd. ( $A, B$ ), GSVD.

Betcke's papers use this ... since no squaring, is actually more accurate.

$$w_j^2 = \frac{\text{Vol } \Omega}{J}$$

may be v. crud approx

• we need convergence in  $M \leq N$ : usually  $M > N$  but same order, e.g.  $2N$ . got to here.

Error analysis: if  $t[u]$  small, how close is  $\epsilon$  to eigen  $E_j$  of domain?

(Moler-Payne, 1967)  
 Still, 1989

Kuttler-Sigillito, 1978

Let  $(A+\epsilon I)u=0$  in  $\Omega$ ,

$$\text{then } \frac{|E - E_j|}{E_j} \leq C_{\alpha} t[u]$$

const dep. only on domain  $\Omega$ .

relative error in eigenvalue

means.

$$\sqrt{\alpha}$$

smaller  $t$   
 $\Rightarrow$  closer to  $E_j$

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State Thm. on WS, give example of domain:  $A = \frac{d^2}{dx^2}$  in  $[0, 1]$  may act on func. in  $C^2$ .  
 \* self-adjointness of  $A$  in  $L^2(\Omega)$  only w/ ~~some~~ homog. BCs. (p. 44) 11/18.  
 → do WS.

$$\text{eg. } A = -\Delta \text{ with } D(A) = \{u \in C^2(\Omega) \cap C(\bar{\Omega}), u|_{\partial\Omega} = 0\}$$

Thm. Let  $\tilde{A}$  be extension of operator  $A$  to larger domain, i.e.  $D(A) \subset D(\tilde{A}) \subset \mathcal{H}$   
 we will apply to  $\tilde{A} = -\Delta$  on  $L^2(\Omega)$  with no BCs. and  $\tilde{A}^* = A$  in  $D(A)$   
prove Thm. Let  $u \in D(\tilde{A})$ , and  $w$  be st.  $\begin{cases} u-w \in D(A) \\ \tilde{A}w = 0 \end{cases}$ , i.e.  $w$  has same bdry values as  $u$ .

$$u-w = \sum c_i \phi_i \quad \text{ie } u \text{ sat Helm. in } \Omega, \text{ bdry. not nec. 0 on bdry.}$$

$$\sum c_i E_i = A(u-w) \stackrel{\text{extension}}{=} \tilde{A}(u-w) \stackrel{(*)}{=} Eu \quad (*)$$

$$\text{and. } \sum c_i^2 (E-E_i)^2 = \| \underbrace{\sum c_i (E-E_i) \phi_i}_\text{since} \|_2^2 = E^2 \|w\|^2$$

$$\| \tilde{A}(u-w) - (E-A)w \|_2^2 = (\tilde{A}-E)w = -Ew$$

$$\sum c_i^2 \frac{(E-E_i)^2}{E_i^2} \geq \min_i \left( \frac{E-E_i}{E_i} \right)^2 \cdot \underbrace{\sum c_i^2 E_i^2}_{E^2 \|w\|^2} \quad \text{since. (*)}$$

$$\text{so } \min_i \frac{|E-E_i|}{E_i} \leq \frac{\|w\|}{\|u\|}$$

A-posteriori estimate.

$$\text{Finally } \|w\|_2 \leq C \underbrace{\|w\|_\infty}_{= \|u\|_\infty}$$

(Similar bound on eigenmode.)

Use for error bounds on dist. to eigenvalue.

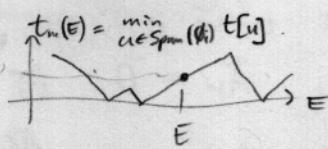
Error anal. of MPS for eigenmodes:  $\phi_j$  & eigenval  $E_j$  of domain  $\Omega$ .

If  $t[u]$  small.  
Thm (Moler-Payne '67, Kuttler-Sigillito '78) Let  $(A+E)u=0$  in  $\Omega$ ,

$$\text{then } \exists j \text{ st. } \frac{|E - E_j|}{E_j} \leq C_\alpha t[u] \quad \text{const. dep only on domain., } O(1).$$

rel. err. in eigen.

Usage:  
MPS errors



then smaller  $t[u]$  is, smaller closer there must be to true eigen.  $E_j$ .  
eg.  $10^{-6}$  rel. err.

Domain of op.  $A$   $= D(A) \subset \mathcal{H}$  Hilbert space: complete banach space w/ 2-norm.

eg.  $\mathcal{H} = L^2(\Omega)$ ,  $A = -\Delta$ , may define  $D(A) = \{u \in C^2(\Omega) \cap C(\bar{\Omega}), u|_{\partial\Omega} = 0\}$  vanish on boundary  
with  $C_{\delta_0}^2$  2nd deriv cont.

note  $D(A) \neq \mathcal{H}$  since  $A$  not bounded, so can't act on every element of  $\mathcal{H}$  (since  $\mathcal{H}$  complete, contains its limit points is closed).

Such  $u \in D(A)$  are 'classical solns' to PDE, may expand to a Sobolev space of weak solns.  
We assume  $A$  has point spectrum, i.e. countable set of eigenvals  $E_j$ , whose eigenvectors are complete o.n.b. for  $\mathcal{H}$

sufficient condition is:  $A^{-1}$  opt, true for diff. ops since Kernel of  $A^{-1}$  is Greens func, continuous or weakly singular

Thm: define residual  $r := Au - Eu$ , for  $u \in D(A)$ .

then i)  $\exists j$  st.  $|E - E_j| \leq \frac{\|r\|}{\|u\|}$

WS.

note:  $\|r\|$  is size of failure of

similarly may prove ii)  $\exists$  eigenfunc  $\phi_j$  st.  $\frac{\|u - \phi_j\|}{\|u\|} \leq \varepsilon \sqrt{1 + \varepsilon^2} \|r\|$ , where  $\varepsilon := \frac{\|r\|}{\|u\|} d(E)$

Application: from above  $A$ ,  $D(A)$ , say  $\{E_k\}$  trial eigenvals, mode produced by some method (eg FEM), with correct (nonay) BCs. but not satisfying PDE, i.e.  $(A+E)u = -r$ ,  $\|r\| \neq 0$ , then  $\|r\|$  bounds dist. to nearest true  $E_j$  'a-posteriori' error bound, common in num. anal.

From Moler-Payne: choose  $A, D(A)$  as above, and  $\tilde{A}$  an extension of  $A$  to larger domain  $\tilde{D}(A) \subset D(A) \subset \mathcal{H}$ .

this means  $\tilde{A}|_{D(A)} = A$ , i.e.  $\tilde{A}u = Au \quad \forall u \in D(A)$ .

choose  $D(\tilde{A}) = C^2(\Omega) \cap C(\bar{\Omega})$  with no BCs on  $u$ .

Approximation theory for MPS for Laplace BVP.

$\Omega$  bounded domain; analytic simply-connected in  $\mathbb{R}^2$ . Basis func  $\phi_n(r, \theta) = e^{in\theta} r^{1/n}$  regular sols to  $\Delta \phi_n = 0$  in  $\mathbb{R}^2$ .

Thm:  $\phi_n$  are dense in the space of solutions to  $\Delta u = 0$ , in  $L^2(\Omega)$  norm.  
I.e., for any soln.  $\Delta u = 0$  in  $\Omega$ ,

$$\min_{\sum c_n \phi_n} \left\| \sum_{n \in N} c_n \phi_n - u \right\|_{L^2(\Omega)} \rightarrow 0 \quad \text{as } N \rightarrow \infty.$$

proof: Gaier book.

- Same result in sup norm.
- Example of Runge's Thm (1885): approximation of any analytic func on  $\Omega$  by poly's  $P^{(i)} = a_0 + a_1 z + a_2 z^2 + \dots$  Weierstrass thm, special case of  $\Omega = [a, b]$  on real axis.
- connection to analytic funcs & every harm.  $u(r, \theta)$  may be written as  $Re[g]$  for  $g(z)$  analytic.  $z = x + iy$ ,  $\phi_n = \phi_{n+1}$ ,  $\phi_n$  are then  $Re, Im$  parts of  $z^n$ , i.e. complex polynomials.
- if not simply-conn, need basis funcs to include singularities in each conn. component of  $\mathbb{R}^2 \setminus \bar{\Omega}$ .

If soln.  $u$  may be analytically continued beyond  $\bar{\Omega}$  a finite distance,

e.g. if  $f$  analytic on  $\partial\Omega$ ,  $u$  analytic today.

then  $\exists p > 1$ :  $\min_{\sum c_n \phi_n} \left\| \sum_{n \in N} c_n \phi_n - u \right\|_{L^\infty(\Omega)} = O(R^{-N})$

for every  $R < p$ ,  
but no  $R > p$ .

Furthermore,  $p$  is conformal dist. of nearest singularity of  $u$  to  $\partial\Omega$ .

singularities

Defn of conf. dist  $p(\vec{x})$  for pny.  $\vec{x} \in \mathbb{R}^2 \setminus \bar{\Omega}$ : solve  $\begin{cases} \Delta v = 0 \text{ in } \mathbb{R}^2 \setminus \bar{\Omega} \\ v = 0 \text{ on } \partial\Omega \\ v - \ln|\vec{x}| = O(1) \end{cases}$

then  $p(\vec{x}) := e^{v(\vec{x})}$

ext BVP w/ soln. asymp. to ln r.

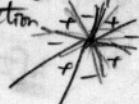
note how similar to interpolation convergence rates.



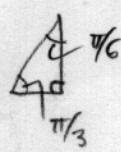
Through theory of Vekua, (see Betti's theory, Henrici review), convergence rates carry over to 2nd order elliptic PDE w/ analytic coeffs, e.g.  $(\Delta + E)u = 0$  Helmholtz - convergence rates carry over to 2nd order elliptic EVP behavior at corners:

$\beta = \frac{\pi}{n}$   $n \in \mathbb{Z}$  called regular: straight lines (not curves).

otherwise singular: modes  $\phi_j$  analytically continuable beyond corner, by  $2n$ -fold reflection



Note HW7



all regular  $\Rightarrow$  eigenmode analytically continued, in fact to  $\mathbb{R}^2$  since tiles they are

singular corners:



to regain exponential convergence need  $J_\nu(kr) \sin \nu \theta$  for  $\nu = \frac{\pi}{\beta} n$  fractional-order bessels, show mushroom pics?