Some Unusual Eigenvalue Problems

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Problem of Computing Bilinear Form

Given $\mathbf{u}, \mathbf{v} \in \Re^n$, $n \times n$ matrix A and a "smooth" function f, find γ_l and γ_u such that

$$\gamma_l \leq \mathbf{u}^T f(A)\mathbf{v} \leq \gamma_u.$$

or <u>estimate</u>

$$\mathbf{u}^T f(A)\mathbf{v}$$

Difficulties:

- A is large, from $O(10^3)$ to $O(10^6)$
- A is only referenced via matrix-vector products
- function f is $1/x$, $\ln x$, e^x, ...

No loss of generality by letting $u = v$. Otherwise

$$\mathbf{u}^T f(A)\mathbf{v} = \frac{1}{4}\left(\mathbf{y}^T f(A)\mathbf{y} - \mathbf{z}^T f(A)\mathbf{z}\right),$$

where $\mathbf{y} = \mathbf{u} + \mathbf{v}$ and $\mathbf{z} = \mathbf{u} - \mathbf{v}$.

Some eigenvalue problems.

1.

$$\min_{\mathbf{x}\neq\mathbf{0}} \frac{\mathbf{x}^T A\mathbf{x}}{\mathbf{x}^T\mathbf{x}}$$

$$s.t. \quad \mathbf{c}^T\mathbf{x} = 0, (\|\mathbf{c}\|_2 = 1).$$

Lagrangian:

$$\phi(\mathbf{x}; \lambda, \mu) = \mathbf{x}^T A\mathbf{x} - \lambda\mathbf{x}^T\mathbf{x} - 2\mu\mathbf{x}^T\mathbf{c}.$$

$\nabla\phi = 0$ when

$$A\mathbf{x} - \lambda\mathbf{x} = \mu\mathbf{c}$$

$$\mathbf{x} = \mu(A - \lambda I)^{-1}\mathbf{c}$$

$$\mathbf{c}^T\mathbf{x} = 0 \Longrightarrow \boxed{\mathbf{c}^T(A - \lambda I)^{-1}\mathbf{c} = 0}$$

2. Solve for the eigenvalues of

$$A\mathbf{x} = \lambda\mathbf{x}$$

and

$$(A + \mathbf{c}\mathbf{c}^T)\mathbf{x} = \bar{\lambda}\mathbf{x}$$

$$(A - \bar{\lambda}I)\mathbf{x} = -\mathbf{c}\mathbf{c}^T\mathbf{x}$$

$$\boxed{1 + \mathbf{c}^T(A - \bar{\lambda}I)^{-1}\mathbf{c} = 0}$$

3.

$$\min \mathbf{x}^T A\mathbf{x} - 2\mathbf{b}^T\mathbf{x}, \quad A \ p.d.$$

$$s.t. \quad \mathbf{x}^T\mathbf{x} = \alpha^2.$$

$$\phi(\mathbf{x};\lambda) = \mathbf{x}^T A\mathbf{x} - 2\mathbf{b}^T\mathbf{x} + \lambda(\mathbf{x}^T\mathbf{x} - \alpha^2)$$

$\nabla\phi = 0 \Longrightarrow$

$$(A + \lambda I)\mathbf{x} = \mathbf{b}$$

$$\boxed{\mathbf{b}^T(A + \lambda I)^{-2}\mathbf{b} = \alpha^2}$$

4.

Estimate $tr(A^{-1}) = \sum_{i=1}^{n} \frac{1}{\lambda_i}$.

Estimate $det(A)$.

$$E\{u_i\} = 0$$

$$E\{u_i u_j\} = 0, \quad (i \neq j)$$

$$E\{u_i^2\} = 1$$

$$\boxed{E\{\mathbf{u}^T A^{-1} \mathbf{u}\} = tr(A^{-1})}$$

$$\boxed{E\{\mathbf{u}^T ln(A) \mathbf{u}\} = tr(ln(A)) = ln(det(A)).}$$

$$P_r\{u_i = +1\} = \tfrac{1}{2}$$

$$P_r\{u_i = -1\} = \tfrac{1}{2}$$

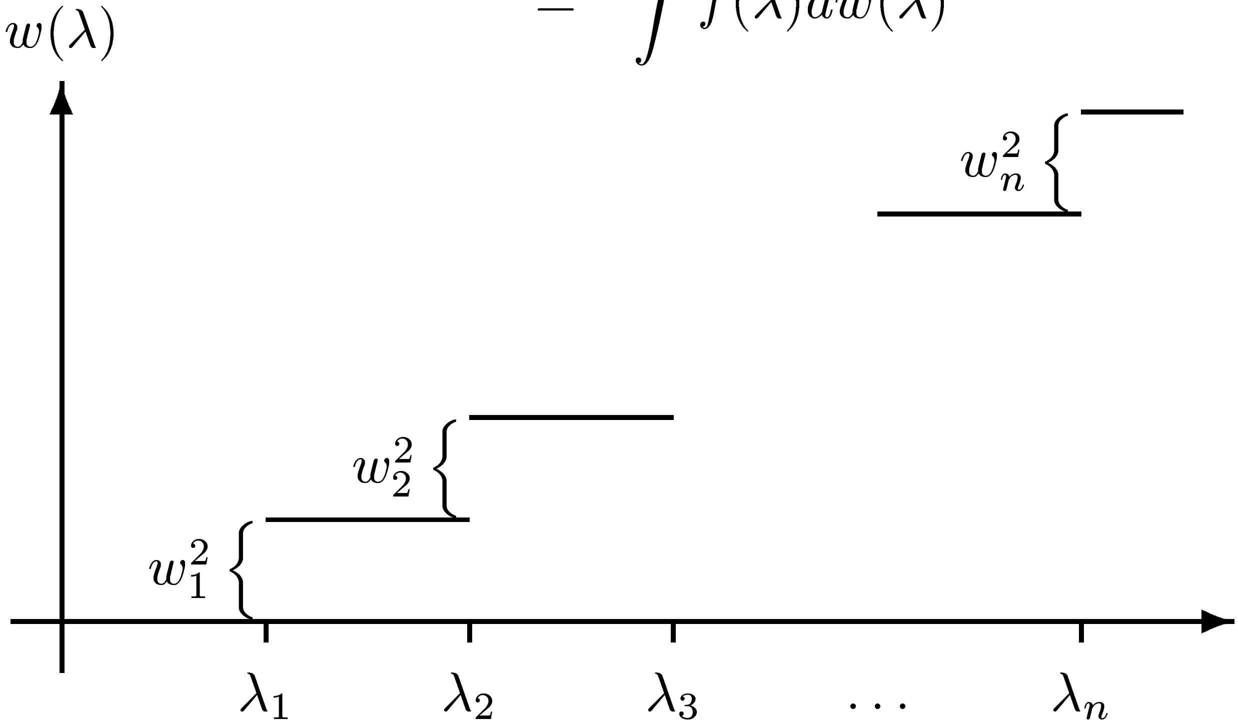
<u>Hutchinson</u>

$$A = Q\Lambda Q^T$$

$$\begin{aligned}
\mathbf{u}^T f(A)\mathbf{u} &= \mathbf{u}^T f(Q\Lambda Q^T)\mathbf{u} \\
&= \mathbf{u}^T Q f(\Lambda) Q^T \mathbf{u} \\
&= \mathbf{w}^T f(\Lambda)\mathbf{w}
\end{aligned}$$

$$\boxed{\mathbf{w} = Q^T \mathbf{u}}$$

$$\begin{aligned}
\mathbf{u}^T f(A)\mathbf{u} &= \sum_{i=1}^{n} f(\lambda_i) w_i^2 \\
&= \int f(\lambda) dw(\lambda)
\end{aligned}$$



$$\gamma_l \leq \int_a^b f(\lambda) dw(\lambda) \leq \gamma_u$$

Gauss-Radau Rules

$$\mu_r = \int \lambda^r dw(\lambda) \qquad (r = 0, 1, \ldots, 2k+m-1)$$

$$\int_a^b f(\lambda) dw(\lambda) = I[f] + R[f]$$

$$I[f] = \sum_{i=1}^{k} A_i f(t_i) + \sum_{j=1}^{m} B_j f(z_j)$$

$\{A_i, t_i\}_{i=1}^{k}$	unknown weights and nodes
$\{z_j\}_{j=1}^{m}$	prescribed
$\{B_j\}_{j=1}^{m}$	must be calculated

$$I[\lambda^r] = \mu_r$$

$$\mu_r = \sum_{i=1}^{k} A_i t_i^r + \sum_{j=1}^{m} B_j z_j^r$$

System of Non-linear Equations

$$R[f] = \frac{f^{(2k+m)}(\eta)}{(2k+m)!} \int_a^b \prod_{j=1}^{m} (\lambda - z_j) \left[\Pi(\lambda - t_i)\right]^2 dw(\lambda)$$

$$a < \eta < b$$

$$\underline{m = 1}$$

$$f^{(2k+1)}(\eta) \leq 0 \text{ and } z_1 = a,\ R[f] \leq 0$$

$$\Rightarrow I[f] = \gamma_u$$

$$f^{(2k+1)}(\eta) \leq 0 \text{ and } z_1 = b,\ R[f] \geq 0$$

$$\Rightarrow I[f] = \gamma_l$$

Gauss Quadrature

$$\int p_r(\lambda) p_s(\lambda) d\omega(\lambda) = 0, \qquad j \neq k$$

$$(r, s = 0, 1, \ldots, k)$$

$$p_{j+1}(\lambda) = (\lambda - \xi_{j+1}) p_j(\lambda) - \eta_j^2 p_{j-1}(\lambda)$$

$$p_k(t_i) = 0, \qquad i = 1, 2, \ldots, k$$

$$J_k = \begin{pmatrix} \xi_1 & \eta_1 & & & \\ \eta_1 & \xi_2 & \eta_2 & & \\ & \eta_2 & \ddots & \ddots & \\ & & \ddots & \ddots & \eta_{k-1} \\ & & & \eta_{k-1} & \xi_k \end{pmatrix}$$

$$\mu_0 = 1$$

$$\begin{aligned} J_k \mathbf{v}_j &= t_j \mathbf{v}_j, \qquad j = 1, 2, \ldots, k \\ A_j &= v_{1j}^2, \qquad j = 1, 2, \ldots, k \end{aligned}$$

Gauss-Radau

$$\bar{J}_{k+1} = \begin{pmatrix} & & & 0 \\ & J_k & & \vdots \\ & & & \eta_k \\ 0 & \dots & \eta_k & \bar{\xi}_{k+1} \end{pmatrix}$$

$$0 = p_{k+1}(t_0) = (t_0 - \bar{\xi}_{k+1})p_k(t_0) - \eta_k^2 p_{k-1}(t_0)$$

$$\bar{\xi}_{k+1} = t_0 - \eta_k^2 \frac{p_{k-1}(t_0)}{p_k(t_0)}$$

or

$$(J_k - t_0 I)\delta = \eta_k^2 \mathbf{e}_k$$

$$\bar{\xi}_{k+1} = t_0 + \delta_k$$

Evaluate

$$I[f] = \sum_{i=0}^{k} v_{1i}^2 f(t_i)$$

$$\bar{J}_{k+1} = VTV^T$$

$$V^T \mathbf{e}_1 = \langle \text{ first component of } V \ \rangle$$

$$\begin{aligned} I[f] &= \mathbf{e}_1^T V f(T) V^T \mathbf{e}_1 \\ &= \mathbf{e}_1^T f(VTV^T) \mathbf{e}_1 \\ &= \mathbf{e}_1^T f(\bar{J}_{k+1}) \mathbf{e}_1 \end{aligned}$$

How can we determine the orthogonal polynomials w.r.t. the measure $w(\lambda)$?

Now

$$\begin{aligned} p_{j+1}(\lambda) &= (\lambda - \xi_{j+1})p_j(\lambda) - \eta_j^2 p_{j-1}(\lambda) \\ p_{j+1}(A) &= (A - \xi_{j+1}I)p_j(A) - \eta_j^2 p_{j-1}(A) \\ p_{j+1}(A)\mathbf{u} &= (A - \xi_{j+1}I)p_j(A)\mathbf{u} - \eta_j^2 p_{j-1}(A)\mathbf{u} \end{aligned}$$

Set $\mathbf{w}_j = p_j(A)\mathbf{u}$

We define ξ_{j+1} and η_j^2 so that

$$\begin{aligned} \mathbf{w}_{j+1}^T \mathbf{w}_j &= 0 \\ \mathbf{w}_{j+1}^T \mathbf{w}_{j-1} &= 0 \end{aligned}$$

$$\Rightarrow \mathbf{w}_{j+1}^T \mathbf{w}_r = 0 \qquad \text{for } r < j-1$$

$$
\begin{aligned}
\xi_{j+1} &= \frac{(\mathbf{w}_j, A\mathbf{w}_j)}{(\mathbf{w}_j, \mathbf{w}_j)} \\
\eta_j^2 &= \frac{(\mathbf{w}_j, \mathbf{w}_j)}{(\mathbf{w}_{j-1}, \mathbf{w}_{j-1})}
\end{aligned}
$$

<u>LANCZOS METHOD</u>

$$
\begin{aligned}
(\mathbf{w}_j, \mathbf{w}_k) &= 0 \\
&= (p_j(A)\mathbf{u}, p_k(A)\mathbf{u}) \\
&= \int p_j(\lambda) p_k(\lambda) dw(\lambda)
\end{aligned}
$$

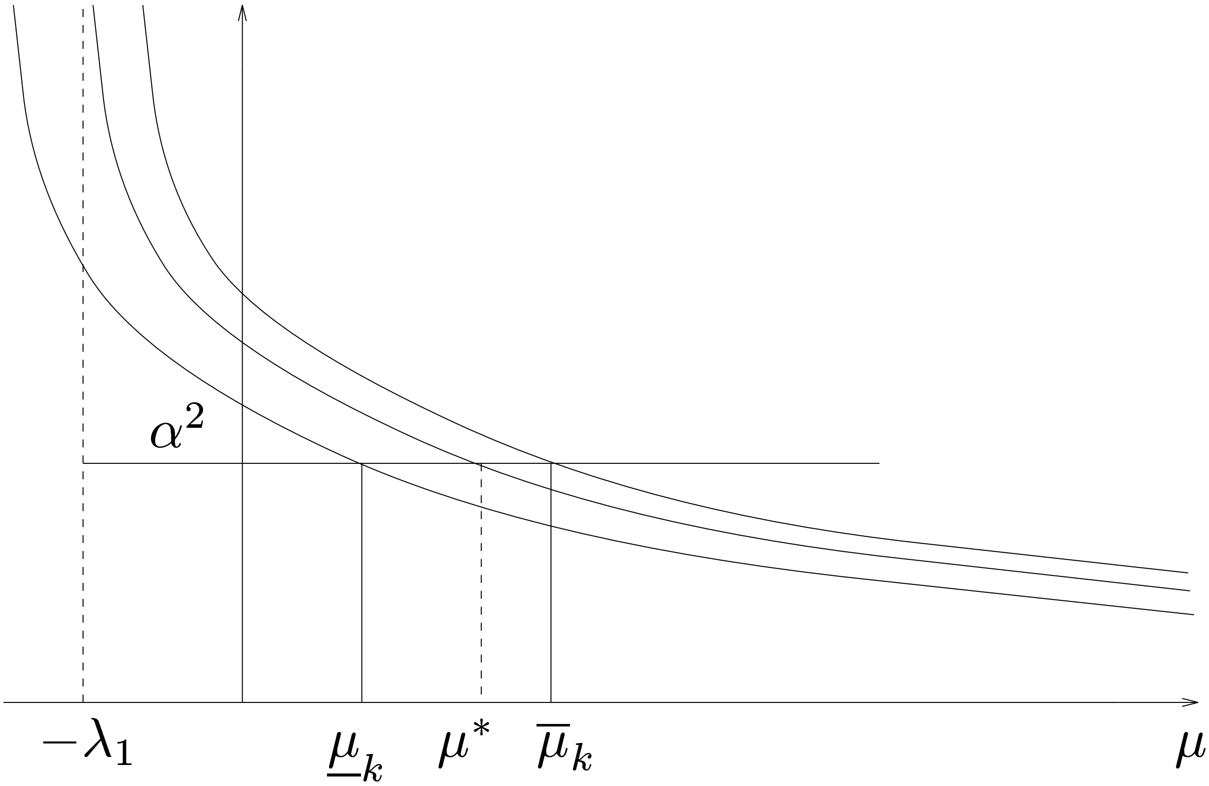
Problem 3. We need to solve

$$\mathbf{b}^T (A + \mu I)^{-2} \mathbf{b} = \alpha^2$$

a) Begin Lanczos process with $\mathbf{u} = \mathbf{b}$.

b) Construct $\bar{J}_{k+1}$.

c) Solve $\mathbf{e}_1^T (\bar{J}_{k+1} + \mu I)^{-2} \mathbf{e}_1 = \alpha^2$



$$\underline{\mu}_1 \leq \underline{\mu}_2 \leq \ldots \mu^* \leq \ldots \leq \overline{\mu}_2 \leq \overline{\mu}_1$$

5.

$$A\mathbf{x} = \lambda B\mathbf{x}$$

- Compute

$$\tau_\mu = \sum_{\lambda_i < \mu} \lambda_i \qquad \text{or} \qquad \tau_{\alpha,\beta} = \sum_{\alpha < \lambda_i < \beta} \lambda_i$$

Application: Total energy of an electronic system in molecular dynamics

Problem: Given generalized sym.-def. eigenproblem

$$Hx = \lambda Sx$$

where $H^T = H$ and $S^T = S > 0$, $n \times n$ and eigenvalues λ_i are ordered:

$$\lambda_1 \leq \cdots \leq \lambda_m < \mu < \lambda_{m+1} \leq \cdots \leq \lambda_n,$$

Find

$$\tau_\mu = \lambda_1 + \lambda_2 + \cdots + \lambda_m$$

The number m is unknown and could be $\approx n/2$

Available methods:

- QR algorithm for all eigenvalues $\to O(n^3)$
- Bisection method for partial eigenvalues $\to O(n^3)$
- Trace minimization method

$$\lambda_1 + \lambda_2 + \cdots + \lambda_m = \min_{U \in \mathcal{U}} tr(U^T H U),$$

where $\mathcal{U} = \{U \ : \ n \times m \text{ and } U^T S U = I_m\}$

$\to$ *m is unknown and too large to use*

- Sparse matrix eigensolvers, such as Lanczos method

$\to$ *m is too large*

Key issue for using bilinear form approach: find f

$$f(\lambda) = \begin{cases} \lambda, & \text{if } \lambda < \mu \\ 0, & \text{if } \lambda > \mu, \end{cases}$$

Then

$$tr(f(S^{-1}H)) = \lambda_1 + \lambda_2 + \cdots + \lambda_m.$$

We use a function of the form

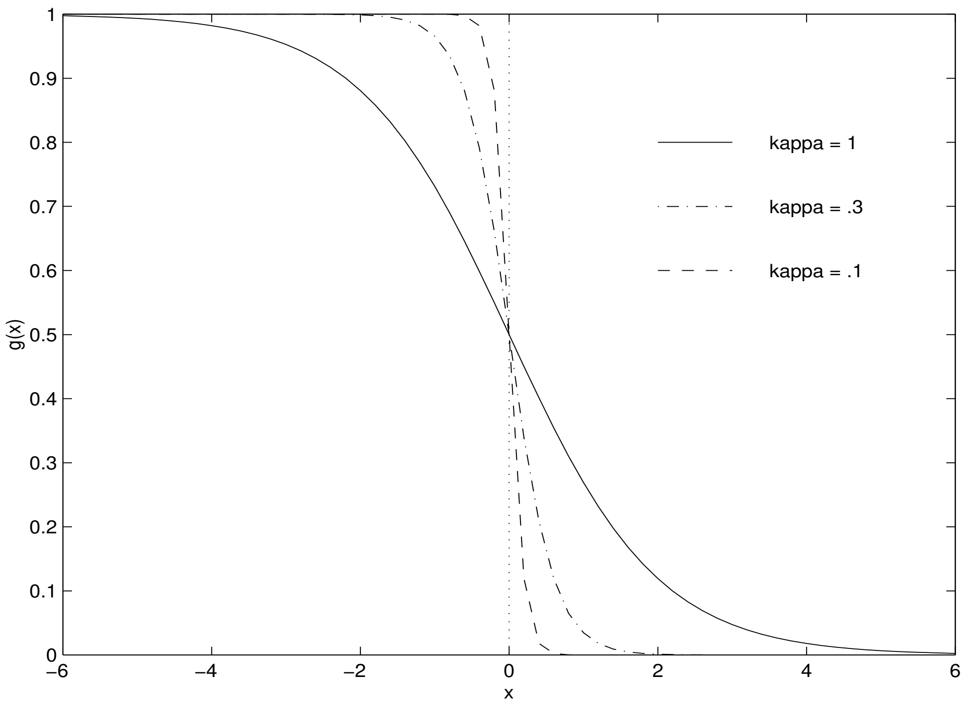
$$f(\lambda) = \lambda g(\lambda),$$

where

$$g(\lambda) = \frac{1}{1 + \exp\left(\frac{\lambda - \mu}{\kappa}\right)},$$

μ and κ constants, $g(\lambda)$ is Femi-Dirac distribution in thermodynamics, $\kappa \sim T$ (temperature).

$$g(\lambda) \to \chi(\lambda) = \begin{cases} 1 & \text{if} \quad \lambda < \mu \\ \frac{1}{2} & \text{if} \quad \lambda = \mu \\ 0 & \text{if} \quad \lambda > \mu. \end{cases}$$


kappa = 1
kappa = .3
kappa = .1
g(x)
x
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
−6
−4
−2
0
2
4
6

Probabilistic Error Bounds

By Hoeffding's Inequality, we have

$$P\left(\left|\frac{1}{m}\sum_{i=1}^{m}\mathbf{u}_i^T f(A)\mathbf{u}_i - tr(f(A))\right| \geq \frac{\eta}{m}\right) \leq 2\exp\left(\frac{-2\eta^2}{d}\right)$$

where

$$d = m(u_{\max} - l_{\min})^2,$$

and

$$l_{\min} = \min\{\gamma_l^{(i)}\}, \quad u_{\max} = \max\{\gamma_u^{(i)}\}.$$

Probabilistic error bounds:

$$tr(f(A)) \in \left(\frac{1}{m}\sum_{i=1}^{m}\gamma_l^{(i)} - \frac{\eta}{m}, \quad \frac{1}{m}\sum_{i=1}^{m}\gamma_l^{(i)} + \frac{\eta}{m}\right)$$

with probability $1 - 2\exp(-2\eta^2/d)$.

MC Method for Estimating $tr(f(A))$

(Bai, Fahey and Golub '96)

- For $j = 1, 2, \cdots, m$
  1. generate "random" vector $\mathbf{u}_j$
  2. apply the basic algorithm to compute bounds $\gamma_l^{(j)}$ and $\gamma_u^{(j)}$ of $\mathbf{u}_j^T f(A)\mathbf{u}_j$
  3. $I_p^{(j)} = \frac{1}{2j} \sum_{k=1}^{j} (\gamma_l^{(j)} + \gamma_u^{(j)})$
  4. $l_{\min} = \min\{l_{\min}, \gamma_l^{(j)}\}$
  5. $u_{\max} = \max\{u_{\max}, \gamma_u^{(j)}\}$
  6. $\eta^2 = -\frac{1}{2} j (u_{\max} - l_{\min})^2 \ln(\frac{1-p}{2})$
  7. $l_p^{(j)} = \frac{1}{j} \sum_{k=1}^{j} \gamma_l^{(k)} - \frac{\eta}{j}$
  8. $u_p^{(j)} = \frac{1}{j} \sum_{k=1}^{j} \gamma_u^{(k)} + \frac{\eta}{j}$

▷ $I_p^{(m)}$ is an unbiased estimation of $tr(f(A))$

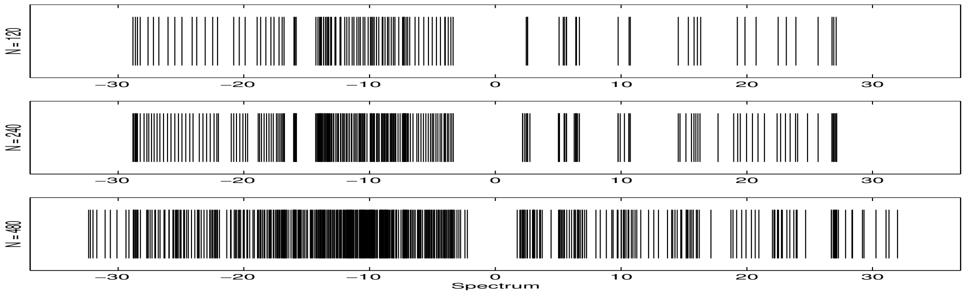
▷ $tr(f(A)) \in (l_p^{(m)}, u_p^{(m)})$ with probability p

Numerical Examples

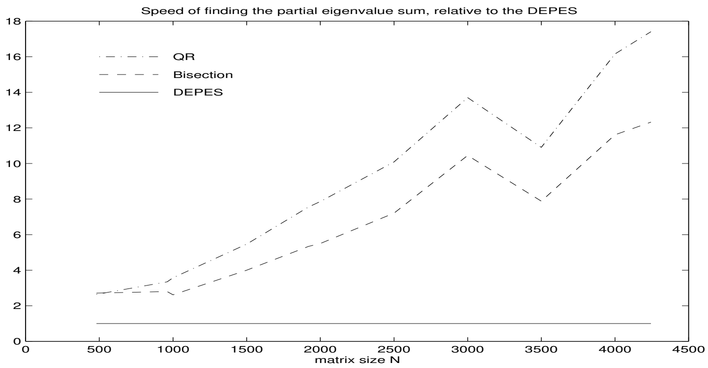
- Stopping criterion: $tol = 10^{-4}$.
- Gerschgorin circle theorem to estimate A's eigenvalue bounds a and b.
- LAPACK and sparse matrix reordering, factorization and solver routines
- On HP workstations and Convex Exemplar SPP1200 supercomputer

Partial Eigenvalue Sum in Tight-binding Molecular Dynamics

- Spectra distribution of Carbon Fullerene Systems



- Relative errors are within 0.5% to 2.2% (10 random samples) to the "exact values".
- *Low accuracy requirement*
- Speed (vs. QR and bisection methods)



- No competitive sparse eigensolvers for computing such large number of eigenvalues.

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