The Envelope Method

for computing orthogonal eigenvectors belonging to isolated clusters of very close eigenvalues of a symmetric tridiagonal matrix

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IWASEP7
June 2008

Eigenvectors - The pure mathematician's solution

Givens' method

$$(T - \lambda I)\mathbf{x} = \mathbf{0}$$

$$\begin{bmatrix} \alpha_1 - \lambda & \beta_1 & & & & \\ \beta_1 & \alpha_2 - \lambda & \beta_2 & & & \\ & \beta_2 & \alpha_3 - \lambda & \beta_3 & & \\ & \ddots & \ddots & \ddots & & \\ & & \beta_{n-2} & \alpha_{n-1} - \lambda & \beta_{n-1} \\ & & & \beta_{n-1} & \alpha_n - \lambda \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_{n-1} \\ x_n \end{bmatrix} = \mathbf{0}$$

Assumption: $\beta_i \neq 0$, all i [for the all talk]

Theorem 1. $\beta_i \neq 0$, all $i \implies$ eigenvalues distinct

Theorem 2. $\beta_i \neq 0$, all $i \implies x_1 x_n \neq 0$

Givens method: set $x_1 = 1$

Eqn. 1	determines	x_2
Eqn. 2	"	x_3
	$\cdots$	
Eqn. $n-1$	"	x_n

[Eqn. n is redundant]

Normalize, if required

$\langle$could start with $x_n = 1$ and proceed in reverse$\rangle$

Properties. Perfect in exact arithmetic with exact λ.

Defect 1. What if 2 eigs agree to working precision?
What if 4 eigs agree too working precision?

Defect 2. Can fail even for an isolated eigenvalue (W_{21}^{-})

Is it difficult to compute numerically orthogonal eigenvectors belonging to an isolated cluster of very close eigenvalues?

Ans: yes, if you compute them one by one.

Ans: no , if you compute them all together.

Envelopes

The envelope of a vector v is

$$|v| = \left[|v_1|, |v_2|, \ldots, |v_n|\right]^t .$$

Let Q be any orthonormal basis for a subspace $S \subseteq \mathbb{R}^n$ of dimension p. Then its envelope $\mathcal{E}_s$ is given by

$$\mathcal{E}_s(i) = \|Q(i, 1:p)\|_2 , \quad i = 1, 2, \ldots, n$$

$$\|\mathcal{E}_s\|_2 = \|Q\|_F = \sqrt{p}.$$

The envelopes of invariant subspaces belonging to isolated clusters of very close eigenvalues of tridiagonal T have hills and valleys.

The smaller is

$$\frac{\text{cluster width}}{\text{cluster gap}}$$

the deeper are the valleys.

The number of hills $\leq$ the number of eigenvalues in the cluster.

Distinguished sparse basis

To each hill associate a vector that is zero except for the hill (suitably extended).

Some hills may have two vectors assigned to them.

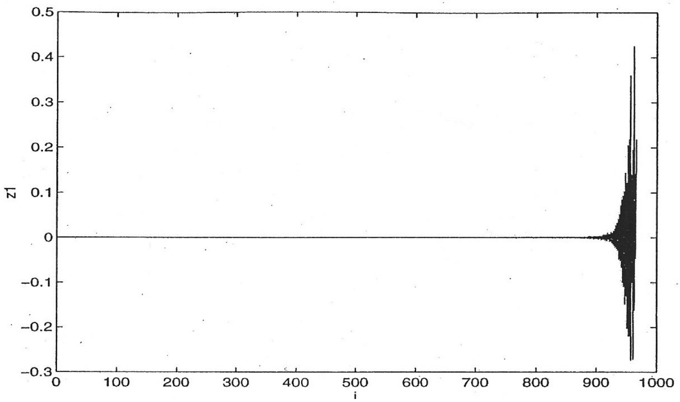


Figure: *An eigenvector of a tridiagonal: most of its entries are negligible*

Matrix comes from nuclear chemistry
George Fann matrix, $n = 966$

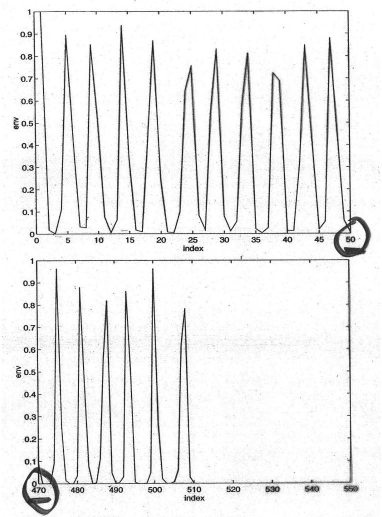


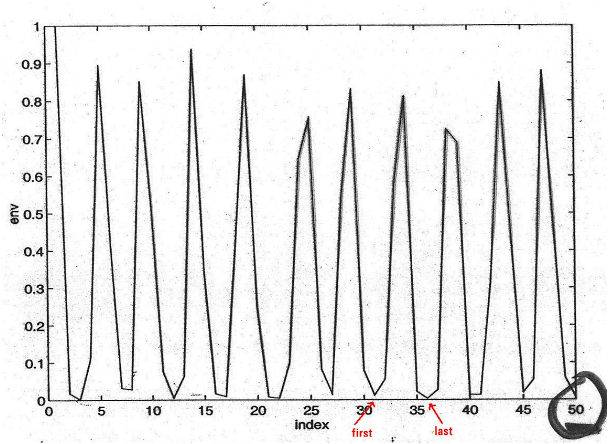
Figure: *Snapshot of Envelope (108 eigenvalues)*

$n = 2053$, cluster size 108

Cluster determined by submatrix 1:515

How to construct a distinguished basis from the envelope

Take each hill down to the valley on each side and extend smoothly to zero to obtain the indices *first* and *last*



This gives one submatrix $T(first : last)$ per hill.

In pratice, we will not have the envelope.

We want to create the index pair (first:last)
from the tridiagonal itself.

There are several methods.

We will describe a new inexpensive one later.

To create the basis vector(s)

- Use the submatrix $T(first.last)$
- Compute the eigenpair(s) with eigenvalue in the cluster interval.

λ_{21}	10.746194182903393..
λ_{20}	10.746194182903322..
.	.
.	.
λ_{13}	6.0002340..
λ_{12}	6.0002175..
.	.
.	.
λ_3	0.9475..
λ_2	0.2538..
λ_1	-1.1254..

Table: *Selected eigenvalues of W_{21}^{+}*

$$W_{21}^{+} = \begin{bmatrix} 10 & 1 & & & & & & & & & \\ 1 & 9 & 1 & & & & & & & & \\ & 1 & 8 & 1 & & & & & & & \\ & & \ddots & \ddots & \ddots & & & & & & \\ & & & 1 & 1 & 1 & & & & & \\ & & & & 1 & 0 & 1 & & & & \\ & & & & & 1 & 1 & 1 & & & \\ & & & & & & \ddots & \ddots & \ddots & & \\ & & & & & & & 1 & 8 & 1 & \\ & & & & & & & & 1 & 9 & 1 \\ & & & & & & & & & 1 & 10 \end{bmatrix}$$

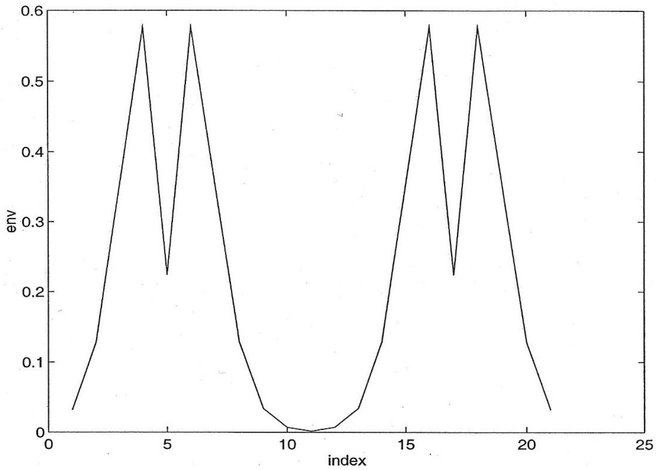


Figure: *Envelope for* λ_{12}, λ_{13} *from* W_{21}^{+}

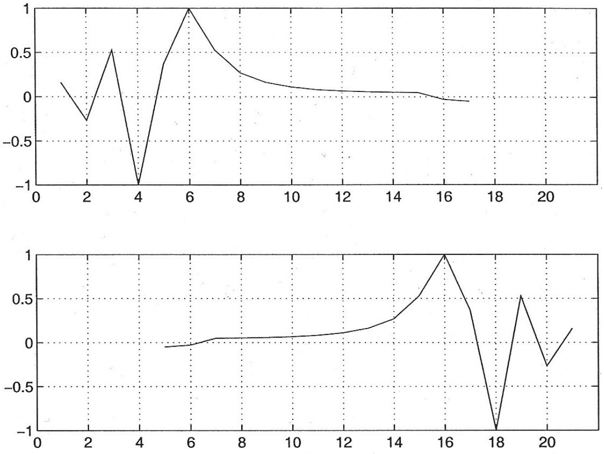


Figure: *Vectors* z_+ *and* z_- *for the pair near 6 on a* log *scale*

$0 < x < 1, \quad x \longrightarrow -1/\log_{10} x, \quad$ correct sign

normalized

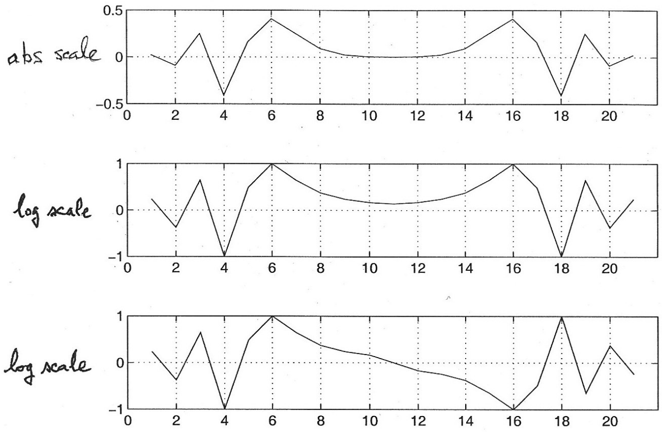


Figure: *Bisectors of z_+ and z_- on a* log *scale*

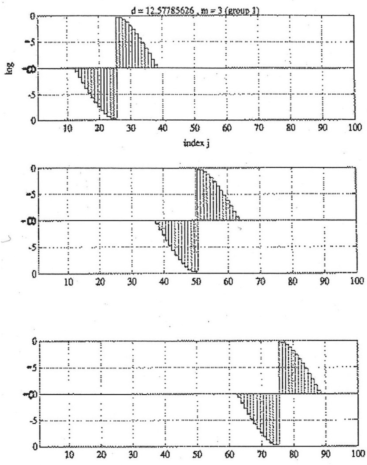


Figure: *Basis eigenvectors of* W_{100} *for* $\{\lambda_{93}, \lambda_{94}, \lambda_{95}\}$

Glued Wilkinson matrix $\quad G_2(W_{25}^{+}, 4, 0.3)$

4 copies of W_{25}^{+}, glue$= 0.3$

Cluster structure $3 - 2 - 3$

12.5778 . . .	3
12.74619 . . .	2
12.93911 . . .	3

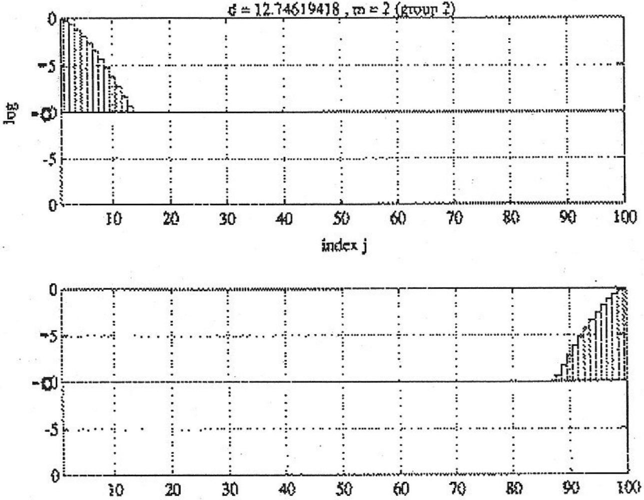


Figure: *Basis eigenvectors of* W_{100} *for* $\{\lambda_{96}, \lambda_{97}\}$

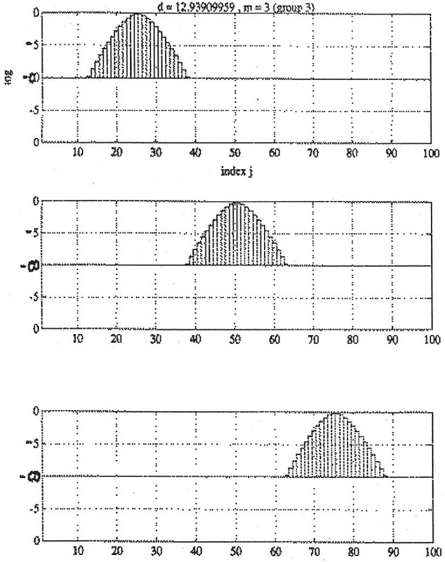


Figure: *Basis eigenvectors of* W_{100} *for* $\{\lambda_{98}, \lambda_{99}, \lambda_{100}\}$

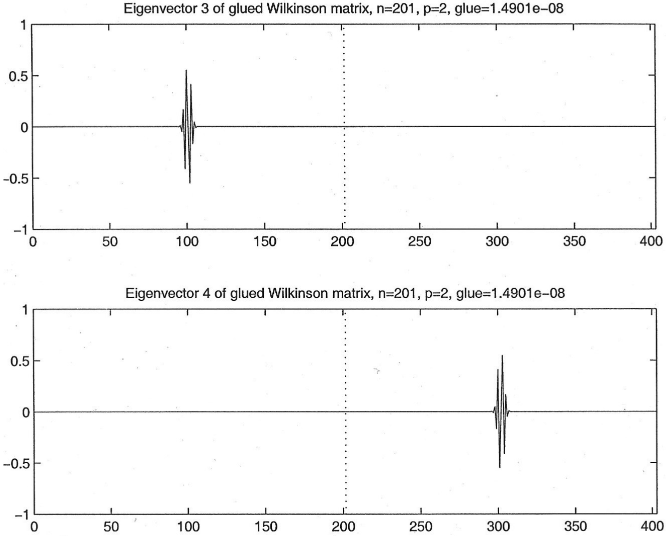


Figure: $G_2(W_{201}^{+}, 2, \sqrt{\varepsilon}), \quad \lambda_3, \lambda_4 \sim 0.25$

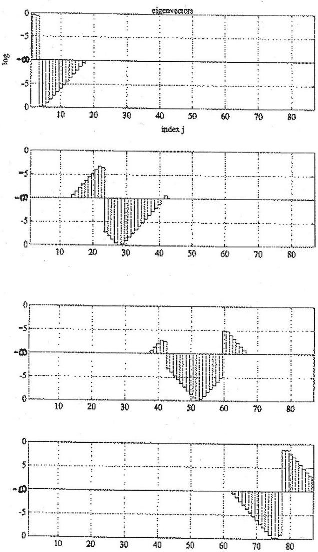


Figure: *Eigenvectors* $x_{79}, x_{80}, x_{81}, x_{82}$ *for* T_{87} *on a* log *scale*

Wanted:

a cheap way to approximate the submatrices

Results complementary to Gersgorin's Circle Theorem

$B \in \mathbb{C}^{n \times n}$

$$G_j^{row} := \left\{ \zeta : |\zeta - b_{jj}| \leq \sum_{k \neq j} |b_{jk}| \right\}$$

G's Theorem. Each $\lambda \in \text{eig}(B)$ is located in at least one G-disk.

A complementary result

If

$$\lambda \notin G_j^{row} \text{ for } j = p : q, \quad p < q,$$

then

λ's column eigenvector decays in entries $p : q$.

(the direction of decay varies, sometimes from p to q, sometimes q to p)

Corollary. The (local) maximal elements of an eigenvector occur only for indices k for which $\lambda \in G_k$.

For large n this corollary makes searching for a maximal entry more efficient.

E.g.
If $\lambda \notin G_i, \; i = 1, \ldots, 500$, then start computing at index 501.

Are there any uses for indices i for which $\lambda \notin G_i$?

Symmetric Tridiagonal Case

$$T = \begin{bmatrix} \alpha_1 & \beta_1 & & & & \\ \beta_1 & \alpha_2 & \beta_2 & & & \\ & \beta_2 & \alpha_3 & \beta_3 & & \\ & & \ddots & \ddots & \ddots & \\ & & & \beta_{n-2} & \alpha_{n-1} & \beta_{n-1} \\ & & & & \beta_{n-1} & \alpha_n \end{bmatrix}$$

Suppose that

$$T - \lambda I = LDL^t$$

$$L := \begin{bmatrix} 1 & & & & \\ l_1 & 1 & & & \\ & l_2 & 1 & & \\ & & \ddots & \ddots & \\ & & & l_{n-1} & 1 \end{bmatrix}, \qquad D := \begin{bmatrix} d_1 & & & & \\ & d_2 & & & \\ & & \ddots & & \\ & & & d_{n-1} & \\ & & & & 0 \end{bmatrix}$$

$$(T - \lambda I)z = \mathbf{0} \Longrightarrow L^t z = \mathbf{e}_n z_n \Longrightarrow z_j = -l_j z_{j+1}, \quad j = n-1, \ldots, 1$$

Lemma. If $\lambda \notin G_j$ and $|l_{j-1}| < 1$ then $|l_j| < 1$.

Proof.

$$
\begin{aligned}
l_j &= \frac{\beta_j}{d_j} \\
d_j &= \alpha_j - \lambda - l_{j-1}\beta_{j-1}
\end{aligned}
$$

$$
\begin{aligned}
|d_j| &\geq |\alpha_j - \lambda| - |l_{j-1}||\beta_{j-1}| \\
&> |\alpha_j - \lambda| - |\beta_{j-1}|, \qquad \text{since} |l_{j-1}| < 1
\end{aligned}
$$

$$
\begin{aligned}
|l_j| &< \frac{|\beta_j|}{|\alpha_j - \lambda| - |\beta_{j-1}|} \\
&< 1, \qquad \text{since} \lambda \notin G_j \quad \square
\end{aligned}
$$

Theorem. If $\lambda \notin G_j$ for $j = p : q,\ p < q$, and $|l_{p-1}| < 1$ then

$$|l_j| < 1 \qquad \text{for } \ j = p-1 : q$$

and

$$|z_j| < \left(\prod_{i=j}^{q} |l_i| \right) |z_{q+1}| \qquad \text{for } \ j = p-1 : q.$$

Similar results for $T - \lambda I = U\mathring{D}U^t$.

Heuristic: replace d_i^+ and d_i^- by $\alpha_i - \lambda$

Hence

$$\prod_{i=j}^{q} |l_i| \approx \frac{\prod_{i=j}^{q} \beta_i}{\prod_{i=j}^{q} (\alpha_i - \lambda)} =: \frac{\mathrm{num}}{\mathrm{den}}$$

Test: $\mathrm{num} \leq tol.\mathrm{den}$ $\qquad tol = 10^{-12}$ or 10^{-15}

General Case

$$B - \lambda I = L^+ D^+ U^+$$

$$\begin{aligned} u_{kj}^+ &= \frac{b_{kj}}{d_k^+}, \qquad k = 1, 2, \ldots, j-1 \\ d_j^+ &= (b_{jj} - \lambda) - \sum_{k<j} b_{jk} u_{kj}^+ \\ u_{jl}^+ &= \frac{b_{jl}}{d_j^+}, \qquad l = j+1 : n \end{aligned}$$

$$\begin{aligned} \sum_{l>j} |u_{jl}^+| = \frac{1}{|d_j^+|} \sum_{l>j} |b_{jl}| &\leq \frac{\sum_{l>j} |b_{jl}|}{|b_{jj} - \lambda| - \left(\sum_{k<j} |b_{jk}|\right) \max_{k<j} |u_{kj}^+|} \\ &< \frac{\sum_{l>j} |b_{jl}|}{|b_{jj} - \lambda| - \sum_{k<j} |b_{jk}|}, \quad \text{if } \max_{k<j} |u_{kj}^+| < 1 \\ &< 1, \quad \text{if } \lambda \notin G_j^{row} \end{aligned}$$

Theorem. If $\max_{k<p} |u_{kp}^{+}| < 1$ and $\lambda \notin G_j^{row}$ for $j = p : q$ then

$$\sum_{l>m} |u_{ml}^{+}| < 1 \quad \text{for} \quad m = p : q.$$

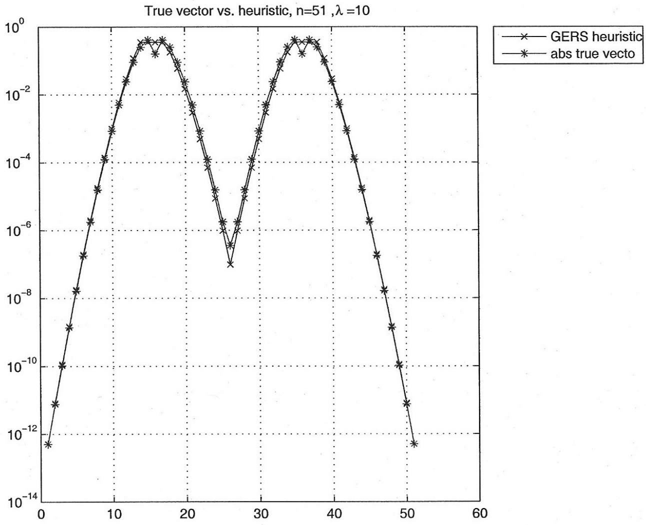


Figure: $W_{51}^{+}, \quad \lambda_{21}$

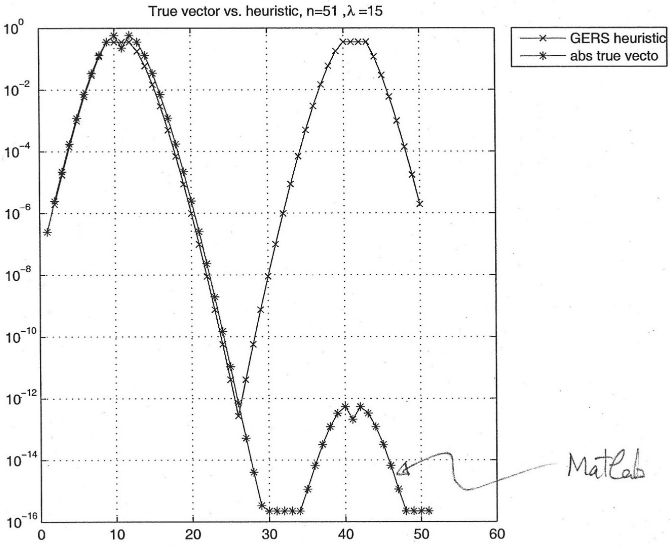


Figure: $W_{51}^{+}, \quad \lambda_{31}$

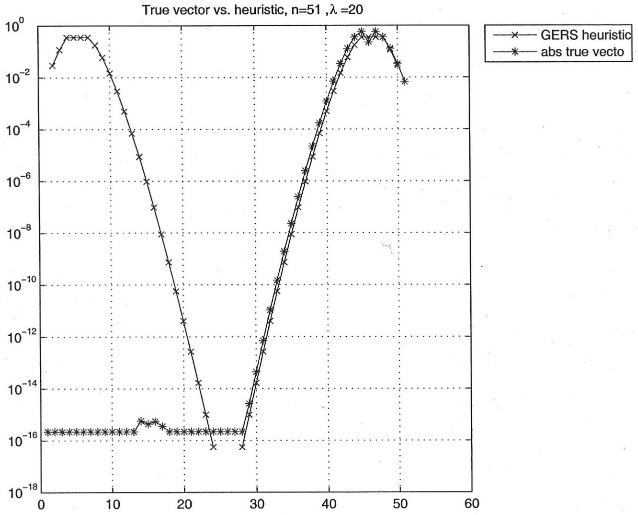


Figure: W_{51}^{+}, λ_{41}

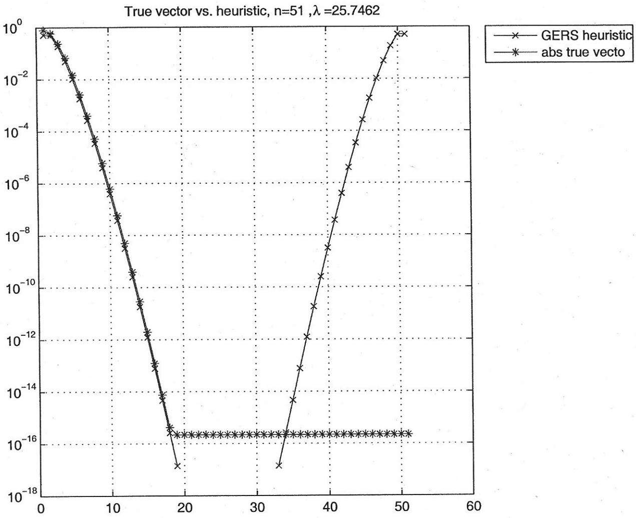


Figure: W_{51}^{+}, λ_{51}

Conclusion

For symmetric tridiagonal matrices the computation of numerically orthogonal eigenvectors for

isolated cluster of close eigenvalues

is

easy and rapid

if the cluster is treated as a whole and

almost impossible

if they are computed one by one.