Orthogonal Eigenvectors and Gram-Schmidt

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One of FOUR main papers on this work

Algorithm $\text{MR}^3$ or MRRR
- Acronym for Multiple Relatively Robust Representations
- Accurate but turgid title
- Jim Demmel has a more catchy title...

Guiding Principle: No Gram-Schmidt
interest very close to 0. The middle part of this paper presents the relevant error analysis. Although essential for our results, this analysis will be indigestible for most readers, but it tells us that changes of only 3 or 4 units in the last digit of each entry of the input \( L, D \) and the output twisted factors suffice to give the exact relation.
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- Theorems, Proofs
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- Theorems, Proofs
- Performance Numbers
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What this talk will not do

- Roundoff Error Analysis
- Theorems, Proofs
- Performance Numbers
- Stick closely to the paper
Diagonal of the Inverse

- Let $J$ be a tridiagonal that is irreducible and invertible
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- Perform triangular factorization “down” and “up” (no pivoting)

\[ J = L_+ D_+ U_+ = U_- D_- L_- \]

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Beautiful identity:

$$D_+ + D_- = \text{diag}(J) + \text{diag}(J^{-1})^{-1}$$
FOUR New Ideas
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Replace the tridiagonal with a bidiagonal
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- Shift close to clusters, but with differential transforms
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- Replace the tridiagonal with a bidiagonal
- Shift close to clusters, but with differential transforms
- Twist, again with differential transforms
- Analyze with a Representation Tree
Difficulties

- All eigenvalues of $T$ are easily computed in $O(n^2)$ time
- Given $\hat{\lambda}$, inverse iteration computes the eigenvector:

$$
(T - \hat{\lambda}I)x_{i+1} = x_i, \quad i = 0, 1, 2, \ldots
$$

- Costs $O(n)$ per iteration
- Typically, 1-3 iterations are enough

**BUT**, inverse iteration only guarantees

$$
\|T\hat{v} - \hat{\lambda}\hat{v}\| = O(\varepsilon\|T\|)
$$
Fundamental Limitations

Gap Theorem:

\[
\sin \angle (v, \hat{v}) \leq \frac{\|T \hat{v} - \hat{\lambda} \hat{v}\|}{\text{Gap}(\hat{\lambda})}
\]

Gap(\hat{\lambda}) can be small:

\[
\begin{bmatrix}
1 & \varepsilon_1 \\
\varepsilon_1 & 1 & \varepsilon_2 \\
\varepsilon_2 & 1 & \varepsilon_3 \\
\varepsilon_3 & 1
\end{bmatrix}
\]

When eigenvalues are close, independently computed eigenvectors WILL NOT be mutually orthogonal.
Symmetric positive definite eigenproblem, $n = 966$

Occurs in Møller-Plesset theory in the modeling of biphenyl

Eigenvalue Distribution:

LAPACK “clusters” — numbered 1, . . . , 939 and smaller ones
Example from Quantum Chemistry

Plot of $\text{Absgap}(i) = \log_{10}\left(\min(\lambda_{i+1} - \lambda_i, \lambda_i - \lambda_{i-1})/||T||\right)$ versus $i$ :

Plot of $\text{Relgap}(i) = \log_{10}\left(\min(\lambda_{i+1} - \lambda_i, \lambda_i - \lambda_{i-1})/|\lambda_i|\right)$ versus $i$ :
First Steps

- Factor $T = LDL^T$
- Compute eigenvalues of $LDL^T$ — by dqds or bisection
- For each eigenvalue $\lambda$, compute eigenvector by inverse iteration
Computing Eigenvector #1

\( \hat{\lambda}_1 = 4.1338 \times 10^{-08}, \hat{\lambda}_2 = 4.3417 \times 10^{-08}, \hat{\lambda}_3 = 4.5 \ldots \times 10^{-08} \)

Factor \( T_1 = LDL^T - \hat{\lambda}_1 I = L_+ D_+ L_+^T = U_- D_- U_-^T \) (up & down)

Compute \( \gamma(i) = D_+(i) + D_-(i) - T_1(i, i) \)

Solve \( T_1 z_1 = \gamma_r e_r \), where \( \gamma_r = \min_k |\gamma_k| \)
Computing Eigenvector #2

- $\hat{\lambda}_1 = 4.1338 \times 10^{-08}$, $\hat{\lambda}_2 = 4.3417 \times 10^{-08}$, $\hat{\lambda}_3 = 4.5\ldots \times 10^{-08}$
- Factor $T_2 = LDL^T - \hat{\lambda}_2 I = L_+ D_+ L_+^T = U_- D_- U_-^T$ (up & down)
- Compute $\gamma(i) = D_+(i) + D_-(i) - T_2(i, i)$

Solve $T_2z_2 = \gamma_r e_r$, where $\gamma_r = \min_k |\gamma_k|$
Accuracy of the vectors

- $|z_1^T z_2| < 2\varepsilon$
- Residual norms are $< \varepsilon \|T\|$.

In general,

- $\min_k |\gamma_k| \approx \varepsilon |\hat{\lambda}|$
- Dot Product between two vectors $\propto \frac{\varepsilon |\hat{\lambda}|}{\text{Gap}}$
- If two eigenvalues share $d$ leading digits, then dot product $\approx 10^d \varepsilon$
Smaller Relative Gaps

\[ \hat{\lambda}_{280} \text{ to } \hat{\lambda}_{303} \text{ are:} \]

- 0.2852950617
- 0.2877656004
- ...
- 0.2901068244
- 0.2901514166
- 0.2901480490

Some eigenvalues agree in 5 digits
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Compute new shifted representations:

\[
LDL^T - 0.2852950617I = L_1D_1L_1^T
\]

\[
0.60738244647 \times 10^{-15} \\
0.24705386756 \times 10^{-02} \\
\vdots \\
0.4811762683 \times 10^{-02} \\
0.4852987244 \times 10^{-02} \\
0.4855354851 \times 10^{-02}
\]
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\[
L_1D_1L_1^T - 0.4855354851 \times 10^{-02}I = L_2D_2L_2^T \\
-0.4459216793 \times 10^{-04} \\
-0.3367607591 \times 10^{-05} \\
-0.1463151420 \times 10^{-17}
\]
The computed vectors

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- Maximum Dot Product $< 3\varepsilon$. 
Key Idea 1 — Replace the tridiagonal with a bidiagonal

Bidirectional Factorization

\[ T \rightarrow LDL^T \]
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- Bidiagonal Factorization

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- Relative condition number

\[
\text{relcond}(\lambda) = \frac{v^T L |D| L^T v}{v^T LDL^T v}
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- Seminal 1991 Demmel-Kahan paper (SIAG/LA Prize)
  - Small relative changes in the entries of a bidiagonal cause small relative changes in all its singular values
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- \( L \) and \( D \) almost always define the small eigenvalues of \( LDL^T \) to high relative accuracy
  - Even in the face of element growth!
Key Idea 2 — Shift close to clusters

Connection between residuals and orthogonality. Let

\[ r = Ax - x\hat{\lambda} \neq 0, \quad s = Ay - y\hat{\mu} \neq 0, \]
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\[ x^T y (\hat{\mu} - \hat{\lambda}) = y^T r - x^T s \]
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Suppose, by some miracle, \( \|r\| \leq \varepsilon_1|\hat{\lambda}| \) and \( \|s\| \leq \varepsilon_2|\hat{\mu}| \), then
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\[ |x^T y| \leq \max(\varepsilon_1, \varepsilon_2) \left/ \frac{|\hat{\lambda} - \hat{\mu}|}{|\hat{\lambda}| + |\hat{\mu}|} \right. \]

Thus, orthogonality depends on the relative separation
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- Thus, orthogonality depends on the relative separation

- Relative Gaps can be made larger by shifting

$$LDL^T - \xi I = \tilde{L}\tilde{D}\tilde{L}^T$$

- Different representations for different clusters!

  - Essential to use differential transforms
Differential Transforms

\[ LDL^T - \hat{\lambda} I = L_+ D_+ L_+^T \]

### Simple qd:

\[ D_+(1) := d_1 - \hat{\lambda} \]

for \( i = 1, n - 1 \)

\[ L_+(i) := (d_i l_i) / D_+(i) \]

\[ D_+(i + 1) := d_i l_i^2 + d_{i+1} - L_+(i) d_i l_i - \hat{\lambda} \]

end for

### Differential qd:

\[ s_1 := -\hat{\lambda} \]

for \( i = 1, n - 1 \)

\[ D_+(i) := s_i + d_i \]

\[ L_+(i) := (d_i l_i) / D_+(i) \]

\[ s_{i+1} := L_+(i) l_i s_i - \hat{\lambda} \]

end for

\[ D_+(n) := s_n + d_n \]
Key Idea 3 — Twist, again with differential transformations

- Godunov et al. [1985], Fernando [1995]
- Compute the appropriate Twisted Factorization:

\[
LDL^T - \hat{\lambda} I = N_r D_r N_r^T,
\]

where \( N_r = \)

\[
\begin{bmatrix}
\times & \times & \times & & \\
\times & \times & \times & & \\
& & \ddots & \times & \times \\
& & \times & \times & \\
& & & \times & \\
& & & & \times
\end{bmatrix}
\]

- Solve for \( z \), \( N_r D_r N_r^T z = \gamma_r e_r \) (\( \Rightarrow N_r^T z = e_r \)):

\[
z(i) = \begin{cases} 
1, & i = r, \\
-L_+(i) \cdot z(i + 1), & i = r - 1, \ldots, 1, \\
-U_-(i - 1) \cdot z(i - 1), & i = r + 1, \ldots, n.
\end{cases}
\]
Key Idea 4 — Representation Tree

Eigenvalues: $\varepsilon, 1 + \sqrt{\varepsilon}, 1 + 2\sqrt{\varepsilon}, 2$
Key Idea 4 — Representation Tree

Eigenvalues: \( \varepsilon, 1 + \sqrt{\varepsilon}, 1 + 2\sqrt{\varepsilon}, 2 \)

Extra representation needed at \( \sigma = 1 \): \[
L_p D_p L_p^T - I = L_0 D_0 L_0^T
\]
Key Idea 4 — Representation Tree

- Eigenvalues: \( \varepsilon, 1 + \sqrt{\varepsilon}, 1 + 2\sqrt{\varepsilon}, 2 \)

- Extra representation needed at \( \sigma = 1 \):

\[
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\]

- Following **Representation Tree** captures the steps of the algorithm:
Caveats

- BLAS
  - Complexity is $O(nk)$ to compute $k$ eigenpairs
  - However, all operations are BLAS 1
  - Closest competitor D&C — $O(n^3)$, but BLAS 3

- Very tight eigenvalue clusters
  - C. Vömel’s torture tests
\( W_{21}^+ \)

\[ \lambda_{20} \text{ and } \lambda_{21} \text{ are identical to working precision} \]
Wilkinson’s Matrix $W_{21}^+$

- $\lambda_{20}$ and $\lambda_{21}$ are identical to working precision
- Form new representation:

$$L_p D_p L_p^T - \hat{\lambda}_{21} I = L_0 D_0 L_0^T$$
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- Form new representation:

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- Roundoff to the rescue:

$$\lambda_{20} (L_0 D_0 L_0^T) \& \lambda_{21} (L_0 D_0 L_0^T) \quad \text{— no digits in common!}$$

$$-7.28 \times 10^{-14} \& -1.22 \times 10^{-15}$$
Wilkinson’s Matrix $W_{21}^+$

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- Form new representation:
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  \]
  \[
  -7.28 \times 10^{-14} \quad \& \quad -1.22 \times 10^{-15}
  \]
- Computed Eigenvectors $\hat{v}_{20}$ and $\hat{v}_{21}$ (inner product is $1.0 \times 10^{-16}$):
Caveats

- **BLAS**
  - Complexity is $O(nk)$ to compute $k$ eigenpairs
  - However, all operations are BLAS 1
  - Closest competitor D&C — $O(n^3)$, but BLAS 3

- Very tight eigenvalue clusters
  - C. Vömel’s torture tests — 5 copies of $W_{101}^+$ with glue of $\sqrt{\varepsilon}$
  - Required a tweak — Perturb base representation