Highlights of Paul Willems' thesis

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Notation for error analysis

Need to bound

$$\sqrt{(1+\alpha_1)(1+\alpha_2)(1+\alpha_3)(1+\alpha_4)}, |\alpha_i| \le \varepsilon.$$

Get

$$1 + 2\varepsilon + O(\varepsilon^2)$$

Question

How to avoid $O(\cdot)$ but keep it simple?

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Higham. $\gamma_n = n\varepsilon/(1 - n\varepsilon)$.
Good for sums and products, but

$$\sqrt{1+\gamma_4} \ne 1 + \gamma_2 \text{ !!}$$

Willems. $\varepsilon^{[k]}(n) := n\varepsilon/(1 - kn\varepsilon)$.
Top expression $\le 1 + \varepsilon^{[2]}(2) = 1 + 2\varepsilon/(1 - 4\varepsilon)$.

In general,

$$
\begin{aligned}
(1+\varepsilon^{[k]}(n))^{s} &= 1+\varepsilon^{[k/s]}(sn),\ 0<s<1,\\
(1+\varepsilon^{[k]}(n))^{-1} &= 1+\varepsilon^{[k+1]}(n).
\end{aligned}
$$

Representations of T (without twists)

1. (T) matrix entries $\{c_i, e_i\}$
2. (N) $\{d_i, l_i\}$, $T = LDL^*$.

   Pro: defines tiny eigenvalues to high relative accuracy.

   Con: does not always exist. Element growth.
3. (e) $\{d_i, e_i\}, e_i = l_i d_i$.
4. (Z) $\{d_i, lld_i\}, lld_i = d_i {l_i}^2 =$ Schur complements.

   $c_{i+1} = d_{i+1} + lld_i$.

Can convert between representations with **no** adds or subtracts.
Square Roots for (Z).

Comparison of Representations

The computation of eigenvectors is organized in the Representation Tree.

Each internal node requires a new representation which defines a specific subset of `shifted` eigenvalues to high relative accuracy.

Accuracy: (Z) is best. max is 3 ulps for (Z) versus 4 for (e).

Speed: (e) , when properly optimized. (N) almost as good.

Conclusion: Always use (Z) but switch to (N) or (e) when a node contains a singleton.

Shift of Origin

$$L_+D_+(L_+)^T = LDL^T - \tau I$$

$$\begin{aligned}(l^+{}_i)^2 d^+{}_i + d^+{}_{i+1} &= l_i{}^2 d_i + d_{i+1} - \tau \\ d^+{}_{i+1} &= e_i{}^2/d_i + d_{i+1} - e_i{}^2/d^+{}_i - \tau\end{aligned}$$

Define s_i by $s_i - \tau = d^+{}_i - d_i$ to find

$$s_{i+1} = e_i{}^2(s_i - \tau)/d_i d^+{}_i,$$

an important recurrence.

a sample error analysis

Algorithm dstqds, unblocked, e-rep

1. ${d_i}^+ = d_i + (s_i - \tau)$
2. ${e_i}^+ = e_i$
3. $s_{i+1} = {e_i}^2(s_i - \tau)/d_i {d_i}^+$

Keep the computed s_i sacred.

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$$1.\ {d_i}^+/(1+\alpha_+) = d_i + (s_i - \tau)(1+\sigma),$$

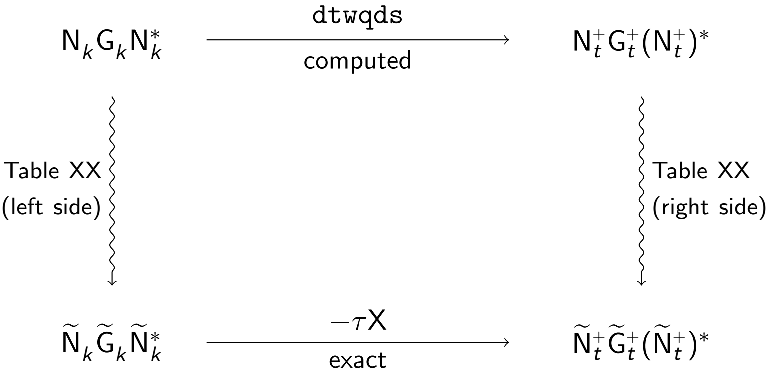
$$\left(\frac{{d_i}^+}{(1+\alpha_+)(1+\sigma)}\right) = \left(\frac{d_i}{1+\sigma}\right) + (s_i - \tau).$$

$$3.\ s_{i+1} = {e_i}^2(s_i - \tau)(1+\sigma)(1+\alpha_s)/d_i {d_i}^+$$

$$1+\alpha_s = (1+\varepsilon)^4, \quad \text{3 mults, 1 divide.}$$

$$\tilde{e}_i = e_i \sqrt{\frac{(1+\alpha_s)(1+\sigma)}{(1+\sigma)^2(1+\alpha_+)}}, \quad \text{cancel } 1+\sigma,$$

$$= e_i[1+\varepsilon^{[4]}(3)], \quad \text{Willems notation .}$$



$$\mathsf{X} = \mathsf{I} + \delta_k \mathsf{e}_k \mathsf{e}_k^* + \delta_t \mathsf{e}_t \mathsf{e}_t^*, \quad \delta_k, \delta_t \doteq \epsilon(1)$$

Figure: Mixed relative error analysis for `dtwqds`.

Perturbing the shift

Outer Perturbations
$NGN^* \to DNGN^*D,\ D \approx I$

Inner Perturbations
$NGN^* \to NDGDN^*,\ D \approx I$

Ostrowski's Theorem. $A^* = A$
$|\lambda(FAF^*) - \lambda(A)| \leq |\lambda(A)| \cdot ||FF^* - I||.$
Outer perturbations make tiny relative changes.

Application. $X \approx I,\ Y = X^{-1/2}$

$$N_+G_+(N_+)^* = NGN^* - \tau X$$
$$Y(N_+G_+(N_+)^*)Y = YNGN^*Y - \tau I$$

$G \to YGY, N \to YNY^{-1}.$

Preserving Tridiagonal Form

Allow 2×2 blocks in D

$$LDL^T$$

$$L = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ k_1 & l_2 & 1 & 0 \\ 0 & 0 & l_3 & 1 \end{bmatrix}, D = \begin{bmatrix} d_1 & 1 & 0 & 0 \\ 1 & c_2 & 0 & 0 \\ 0 & 0 & d_3 & 0 \\ 0 & 0 & 0 & d_4 \end{bmatrix}.$$

$(3,1)$ entry: $k_1 d_1 + l_2 \cdot 1 + 1 \cdot 0$

Cannot perturb k_1 and l_2 *independently* and preserve tridiagonal form

Blocks in LDL*

Example. $T = GK - \alpha I, \quad \alpha = O(\varepsilon)$.

$$T = \begin{bmatrix} -\alpha & 1 & 0 & 0 \\ 1 & -\alpha & 1 & 0 \\ 0 & 1 & -\alpha & \alpha \\ 0 & 0 & \alpha & -\alpha \end{bmatrix}, L = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ k_1 & l_2 & 1 & 0 \\ 0 & 0 & l_3 & 1 \end{bmatrix}$$

$$D = \begin{pmatrix} d_1 & 1 \\ 1 & c_2 \end{pmatrix} \oplus \begin{pmatrix} d_3 & 0 \\ 0 & d_4 \end{pmatrix}.$$

$k_1 = 1/(1-\alpha^2),\ l_2 = \alpha/(1-\alpha^2)\ l_3 = -(2-\alpha^2)/(1-\alpha^2),\ \Omega = \{2\}$.

Willems Representation: $D, e, and\ \Omega = \{$ i where a 2×2 ends $\}$.
Secondary Data: $k_i, l_j, \Delta_i = d_i c_{i+1} - {e_i}^2, inv_D(i)$.

Auxiliary Quantities: $s_i = D_+(i,i) - D(i,i) + \tau$ (straightforward)
BUT

s_{i+1} is much more commplicated (9 cases).

What did I miss?

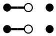
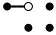
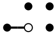
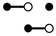
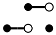
Case	Description	i $\downarrow$	s_{i+1}
S1	$i, i+1 \notin \Omega$ $i, i+1 \notin \Omega^+$		$e_i^2/d_i - e_i^2/d_i^+$
S2	$i+1 \in \Omega$ $i+1 \in \Omega^+$		0
S3	$i \in \Omega$ $i \in \Omega^+$		$e_i^2 d_{i-1}/\Delta_{i-1} - e_i^2 d_{i-1}^+/\Delta_{i-1}^+$
S4	$i+1 \in \Omega$ $i, i+1 \notin \Omega^+$		$-e_i^2/d_i^+$
S5	$i, i+1 \notin \Omega$ $i+1 \in \Omega^+$		e_i^2/d_i
S6	$i \in \Omega$ $i, i+1 \notin \Omega^+$		$e_i^2 d_{i-1}/\Delta_{i-1} - e_i^2/d_i^+$
S7	$i, i+1 \notin \Omega$ $i \in \Omega^+$		$e_i^2/d_i - e_i^2 d_{i-1}^+/\Delta_{i-1}^+$
S8	$i \in \Omega$ $i+1 \in \Omega^+$		$e_i^2 d_{i-1}/\Delta_{i-1}$
S9	$i+1 \in \Omega$ $i \in \Omega^+$		$-e_i^2 d_{i-1}^+/\Delta_{i-1}^+$

Table: Standard formulae for the next adjustment s_{i+1}.

LDL^*	
$d_i \rightsquigarrow \widetilde{d}_i$	1
$c_i \rightsquigarrow \widetilde{c}_i$	4

$\mathrm{L}^+\mathrm{D}^+(\mathrm{L}^+)^*$	$i \notin \Omega$	$i \in \Omega$
$d_i^+ \rightsquigarrow \widetilde{d}_i^+$	2	5

	$i \notin \Omega$	$i \in \Omega$
$e_i \rightsquigarrow \widetilde{e}_i$	3	10
$\tau \rightsquigarrow \widetilde{\tau}_i$	0	12

Table: Error bounds to achieve mixed relative stability for Algorithm 4.5, for the concrete parameters $R = 3, K_\square = 1/8$, cf. Theorem 4.11 and Figure 4.2. Only first-order bounds are shown, i.e., an entry p stands for a bound $p\epsilon_\diamond + \mathcal{O}(\epsilon_\diamond^2)$.

Recap on MRRR

- Users want orthogonality among eigenvectors.
  Constraint. No Gram-Schmidt (distributive computing)
  George Fann example.
- Extravagant accuracy delivers orthogonality.
- How to achieve $||Tz - z\lambda|| = O(n\varepsilon)|\lambda|$?
  Replace T with an RRR (for λ).
  Not enough. Need $relgap(\lambda) \geq 10^{-3}$.
- Make relgaps large by shifting origin (to clusters).
  Hence `Multiple Representations`.
- Organize computation in a Representation Tree.
- Twisted factors permit residual norms proportional to $|\lambda|$.
  Solve $N_k G_k {N_k}^T z = e_k \gamma_k$. ${N_k}^T z = e_k$.
  It is e_k that yields z by products only. Can check that $|\gamma_k| = O(n\varepsilon)|\lambda|$.
- Differential qd algorithms allow for roundoff between representations.
  Eigenvectors invariant under exact shifts.