Enclosing interval matrix decompositions

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Robex, dec. 2024

Goal of this work

Well-known linear algebra algorithms:

- Matrix inversion $(A^{-1}),$
- LU decomposition $(A = LU)$;
- Cholesky decomposition $(A = LL^T)$;
- QR decomposition $(A = QR)$;
- (others ?)

The precision and stability of these algorithms have been widely studied. Nevertheless, the design of interval guaranteed results is not so clear.

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Example

Let's consider:

$$
A = \left(\begin{array}{rrrr} 1 & 1 & 1 & 1 \\ 1.25 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 3 & 3 & 3.5 & 3 \end{array}\right)
$$

Inverting A by "full pivot" LU decomposition gives (approximated):

$$
A^{-1} \simeq B = \left(\begin{array}{rrrr} 0 & 4 & -4 & 0 \\ 7 & 1.94 \cdot 10^{-16} & -1 & -2 \\ -6 & 0 & 0 & 2 \\ 0 & -4 & 5 & 0 \end{array}\right)
$$

We know that B is "almost" an inverse of A , but how much should it be inflated to guarantee the inclusion of $\mathcal{A}^{-1}.$

LU decomposition problem

The PLUQ-decomposition (as represented by Eigen) is PLUQ with :

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$$
P = \left(\begin{array}{cccc} 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \end{array}\right) \quad Q = \left(\begin{array}{cccc} 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \end{array}\right)
$$

$$
L \simeq \left(\begin{array}{cccc} 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0,8 & 1 & 0 \\ 0.285 & 0.114 & 0.143 & 1 \end{array}\right) \quad U \simeq \left(\begin{array}{cccc} 3.5 & 3 & 3 & 3 \\ 0 & 1.25 & 1 & 0 \\ 0 & 0 & 0.2 & 0 \\ 0 & 0 & 0 & 0.143 \end{array}\right)
$$

Inflate L and U , keeping them low-triangular and up-triangular to ensure the equality $A \in P[L][U]Q$ (P and Q cannot change as permutation matrices)?

And if we start with an interval matrix $[A]$, can we use the LU decomposition of $mid([A])$ to compute a decomposion $[A] \subseteq P[L][U]Q$?

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General approach

To compute an operation on a matrix, or give a bound on its result, we can use:

- **1** a known algorithm, e.g. Gauss-Jordan algorithm;
- **2** infinite development, e.g. we know that, when $||Id A|| \le 1$:

$$
(\mathrm{Id} - A)^{-1} = \sum_{k \geq 0} A^k
$$

 \bullet infinite iteration, e.g. when $\|\mathrm{Id} - A\| \leq 1$, the sequence:

$$
S_0 = \text{Id} \quad S_{n+1} = \text{Id} + AS_n
$$

(of course, these approaches are not mutually exclusive)

Using Gauss-Jordan

Direct Gauss-Jordan algorithm on intervals does not work well. Using preconditionning works better: from B approximating the inverse of A , we look for Δ such that $\mathcal{A}^{-1}=(\mathrm{Id}-\Delta)\cdot B.$ Then, we have:

$$
\Delta = \mathrm{Id} - (B A)^{-1}
$$

We can then try to inverse $(B\!A)^{-1}$, which is (hopefully) a near-identity matrix. If $(BA)^{-1}$ is (almost) centered to ${\rm Id}$, we may just have to bound the radius if $(B\overline{A})^{-1}$ around Id.

Gauss-Jordan algorithm (bound)

```
Inplace Gauss-Jordan algorithm to compute S(M) = (\mathrm{Id} - M)^{-1} - \mathrm{Id}(without row-pivoting).
  procedure GaussJordanBound(M: (interval) Matrix)
     for all ind indices do
         pivot \leftarrow 1/(1-M(ind,ind)) \triangleright Suppose M(ind,ind)\lt1for all row : indices\neqind, col : indices\neqind do
            M(row,col) \leftarrow M(row,col) + M(row,ind)*pivot*M(ind,col)end for
        for all ind2 \, indices\neqind do
            M(ind,ind2) \leftarrow M(ind,ind2)*pivotM(ind2, ind) \leftarrow M(ind2, ind)*pivotend for
        M(ind, ind) \leftarrow M(ind, ind)*pivotend for
  end procedure
When M is non-negative and ||M|| < 1, the algorithm succeeds and all
operations are monotonic (assuming x \mapsto 1/(1-x) is atomic). We can
compute a safe bound with floating-point computations (rounding up) on
the matrix of magnitudes.
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Example

Let's consider:

$$
[A] = \left(\begin{array}{cccc} 1 & 1 & 1 & 1 \\ 1 & 0 & 0 & -1 \\ 1.25 & 0 & 0 & [-1, -0.9] \\ 3 & 3 & [3.3, 3.5] & 3 \end{array}\right)
$$

Using the bound version of Gauss-Jordan algorithm:

$$
[A^{-1}] = \left(\begin{array}{ccccc} 0 & [-4, -2.34] & [2.67, 4] & 0 \\ [6, 11] & [5.66, 9] & [-8, -5.33] & [-3.33, -1.67] \\ [-10, -5] & [-\varepsilon, \varepsilon] & [-\varepsilon, \varepsilon] & [1.67, 3.33] \\ 0 & [-5, 3.33] & [2.66, 4] & 0 \end{array}\right)
$$

Discussion

- $+$ Easy to apply, at least for some decompositions (inversion, LU)
- $+$ Quite fast (cubic complexity, no successive iterations),
- Result dependent on the order of traversal of the indices
- − Probable accumulation of errors on big matrices

Norm-based bound

The norm-based bound is used to directly enclose:

$$
S(M) = \sum_{i \geq 1} M^i = (\text{Id} - M)^{-1} - \text{Id}
$$

Using a multiplicative matrix norm:

$$
||A + B|| \le ||A|| + ||B|| \qquad ||AB|| \le ||A|| \cdot ||B||
$$

then:

$$
||M|| < 1 \Rightarrow ||S(M)|| \leq \frac{||M||}{1 - ||M||}
$$

If $||M|| \geq \max_{ii} |M_{ii}|$, we can bound $S(M)$ inside the box $||S(M)|| * E$ where E is the interval matrix in which all coefficients are $[-1,1]$.

Discussion

- $+$ Can be applied on most problems
- $+$ Fastest, independant of order of traversal
- $+$ No accumulation of errors for big matrices
- − Not precise, mostly useful on punctual matrices
- Does not handle 0 values well on block matrices

Path-based algorithm

"Intermediate" algorithm: consider $\mathcal{S}(M)=\sum_{i\ \geq 1} M^i$. The coefficients of $S(M)$ can be linked to paths on the graph associated to the matrix M. E.g. let's consider $[M]$:

$$
[M] \simeq \left(\begin{array}{cccc} \varepsilon & 0 & 0 & \varepsilon \\ \varepsilon & \varepsilon & [-0.6, 0.6] & \varepsilon \\ \varepsilon & \varepsilon & [-0.6, 0.6] & \varepsilon \\ \varepsilon & 0 & 0 & \varepsilon \end{array} \right)
$$

Example of path from 2 to 4 of length 4: $2 \rightarrow 2 \rightarrow 1 \rightarrow 4 \rightarrow 4$. This path "defines" the term $M_{2,2}M_{2,1}M_{1,4}M_{4,4}$ which is a "part" of $(M^4)_{2,4}$.

Paths

Then:

$$
(S(M))_{i,j}=\sum_{\ell\geq 1}\ \left(\sum_{\pi\in\Pi_{ij}^{\ell}}\prod_{k=0}^{l-1}M_{\pi_k,\pi_{k+1}}\right)
$$

where $\mathsf{\Pi}_{ij}^\ell$ is the set of paths from i to j of length ℓ (each path π being of the form):

$$
\pi_0 = i \to \pi_1 \to \ldots \to \pi_\ell = j
$$

Example of path from 2 to 4 of length 4. This path defines the term $M_{2,2}M_{2,1}M_{1,4}M_{4,4}$. The sum of these terms for all paths of length 4 from 2 to 4 is $(M^4)_{2,4}$.

Path-based bounding algorithm

Possible algorithm to bound $S(M)$ (with $M \geq 0$) based on this.

- **O** For each i, j, compute the maximum term $M_{u,v}$ appearing in all paths from i to j (hence a product of length l is bounded by $(M_{u,v})^{\prime})$. This is a (max,max) Floyd algorithm (cubic complexity).
- ² Bound the number of paths, for example by bounding the number $k(i, j)$ of indices which can appear from i to j (easly obtained from the Floyd algorithm).

³ Then:

$$
(S(M))_{i,j} \leq \frac{M_{u,v}}{1 - k(i,j)M_{u,v}}
$$

Comparison Let's consider:

 $[A] =$ $\sqrt{ }$ $\overline{}$ 1 1 1 1 $1 \quad 0 \quad 0 \quad -1$ 1.25 0 0 $[-1, -0.9]$ 3 3 [3.3, 3.5] 3 \setminus $\Big\}$ normbased bounding $\sqrt{2}$ $\overline{}$ $[-8, 8]$ $[-10.5, 4.17]$ $[-3.33, 10]$ $[-2.5, 2.5]$ $[0.5, 16.5] \qquad [-5.15, 14.67] \qquad [-13.33, \varepsilon] \qquad [-5, \varepsilon]$ $[\, - \, 15.5, 0.5] \quad [\, - \, 7.33, 7.33] \quad [\, - \, 6.67, 6.67] \quad [\, - \, \varepsilon, 5]$ $[-8, 8]$ $[-11.5, 3.17]$ $[-3.33, 10]$ $[-2.5, 2.5]$ \setminus $\Big\}$ Floydbased bounding (refined) $\sqrt{2}$ \vert 0 [− 4.17, 2.17] [2.5, 4.17] 0 $[4.63, 12.38]$ $[0.75, 13.92]$ $[-12.5, -0.83]$ $[-3.75, -1.25]$ $[-11.375, -3.62]$ $[-4.59, 4.59]$ $[-4.17, 4.17]$ $[1.25, 3.75]$ 0 [− 5.17, 3.17] [2.5, 4.17] 0 \setminus $\Big\}$ Gauss-Jordan bounding $\sqrt{ }$ $\overline{}$ 0 [− 4, −2.34] [2.67, 4] 0 $[6, 11]$ $[5.66, 9]$ $[-8, -5.33]$ $[-3.33, -1.67]$ $[-10, -5]$ $[-\varepsilon, \varepsilon]$ $[-\varepsilon, \varepsilon]$ $[1.67, 3.33]$ 0 [− 5, 3.33] [2.66, 4] 0 \setminus $\Big\}$

Discussion

- $+$ A bit faster than Gauss-Jordan
- $+$ No accumulation of errors for big matrices
- $+$ Handles 0 values well on block matrices
- Slower than norm-based bounds
- − Precision depends on the form of the matrix (sometimes worse than the norm).

LU decomposition

Full-pivot LU decomposition decomposes a matrix M into:

$$
M = P^{-1} L U Q^{-1}
$$

where P and Q are permutation matrices, L is lower-triangular and U is upper-triangular. In Eigen decomposition, L is unit-lower-triangular and the diagonal coefficients of U are sorted with the 0 at the end. Not unique and not "stable": given a existing decomposition of M , P and Q may not be kept for all matrices "close" to M.

$$
\left(\begin{array}{c} 0 \\ 0 \end{array}\right) = \mathrm{Id}_2 \left(\begin{array}{c} 1 \\ 0 \end{array}\right) (0) \, \mathrm{Id}_1
$$

$$
\left(\begin{array}{c} 0 \\ \varepsilon \end{array}\right) \neq \mathrm{Id}_2 \left(\begin{array}{c} 1 \\ \alpha \end{array}\right) (\beta) \, \mathrm{Id}_1
$$

Approximation

Let's consider M and (P, L, U, Q) an approximate decomposition:

$$
M \simeq P^{-1} L U Q^{-1} \qquad PMQ = LU
$$

To handle rectangular matrices, we extend PMQ with a Id-block, and adapt L and U adequately.

$$
\left(\begin{array}{c}2\\1\end{array}\right)=\left(\begin{array}{c}1\\0.5\end{array}\right)(2)\ \Rightarrow\ \left(\begin{array}{cc}2&0\\1&1\end{array}\right)=\left(\begin{array}{cc}1&0\\0.5&1\end{array}\right)\left(\begin{array}{cc}2&0\\0&1\end{array}\right)
$$

We look for a slight modification of L and U to enclose a "correct" decomposition of M:

$$
PMQ = L(\mathrm{Id} - \Delta L)(\mathrm{Id} - \Delta U)U
$$

 (ΔL) is stricly lower, ΔU is upper)

Triangular inversion

From

$$
PMQ = L(\mathrm{Id} - \Delta L)(\mathrm{Id} - \Delta U)U
$$

to

$$
[L^{-1}]P M Q [U^{-1}] = (\mathrm{Id} - \Delta L)(\mathrm{Id} - \Delta U)
$$

But while L is non-singular, U can be singular. \Rightarrow we modify its diagonal to make it non-singular (replacing too small coefficients on the diagonal by a threshold e).

Note that L and U are punctual, we can expect $[L^{-1}]$ and $[U^{-1}]$ to be quasi-punctual (e.g. computed by substitution). The result should be close to Id (for punctual, non-singular matrices).

Example

$$
[M] = \left(\begin{array}{cccc} 1 & 1 & 1 & 1 \\ 1 & 0 & 0 & -1 \\ 1.25 & 0 & 0 & [-1, -0.9] \\ 3 & 3 & [3.3, 3.5] & 3 \end{array}\right)
$$

$$
\mathrm{Id}-[L^{-1}]PMQ[U^{-1}]\simeq\left(\begin{array}{cccccc}[-0.03,0.03] & [-0.07,0.07] & [-0.64,0.64] & [-0.75,0.75] \\ 0 & 0 & [-0.21,0.21] & 0 \\ 0 & [0,\varepsilon] & [-0.17,0.17] & 0 \\ [-0.01,0.01] & [-0.02,0.02] & [-0.35,0.35] & [-0.22,0.22]\end{array}\right)
$$

With $\mathrm{E}=\mathrm{Id}-[L^{-1}]PMQ[U^{-1}],$ We want to solve:

 $(\mathrm{Id} - \Delta L)(\mathrm{Id} - \Delta U) = \mathrm{Id} - \mathrm{E}$

Lower coefficients $(i > j)$:

$$
(\Delta L)_{i,j} = E_{i,j} + E_{i,[1,j]}\left(\sum_{\ell \geq 0} (E_{[1,j],[1,j]})^{\ell}\right) E_{[1,j],j}
$$

Upper coefficients $(2 \le i \le j)$:

$$
(\Delta U)_{i,j} = E_{i,j} + E_{i,[1,i-1]}\left(\sum_{\ell \geq 0} (E_{[1,i-1],[1,i-1]})^{\ell}\right) E_{[1,i-1],j}
$$

Application

To enclose the inverse, we needed to bracket

 $\mathcal{S}(E) = (\mathrm{Id} - E)^{-1} = \sum_{\ell \geq 1} E^{\ell}.$ Here, we need to enclose

- $\mathcal{S}_k = \mathcal{S}(E_{[1,k],[1,k]})$ with k varying from 1 to $\mathcal{N}-1 \longrightarrow$ same techniques. Both Gauss-Jordan and Floyd-Based algorithms compute bounds for
	- successive S_k incrementally;
	- \bullet In the case of ∞ coefficients, we should consider 0 $\ast \infty = 0$. It works well for Id-blocks on the right/bottom of the decomposition.
	- No need to compute $S(E)$ itself (the last step).

Example

$$
E\simeq\left(\begin{array}{cccc} \left[\begin{array}{ccc} -0.03,0.03\right] & \left[\begin{array}{ccc} -0.07,0.07\right] & \left[\begin{array}{ccc} -0.64,0.64\right] & \left[\begin{array}{ccc} -0.75,0.75\right] \\ 0 & 0 \end{array}\right] \\ 0 & \left[\begin{array}{ccc} -0.21,0.21\right] & 0 \\ \left[\begin{array}{ccc} -0.087,0.087\right] & \left[\begin{array}{ccc} -0.020,0.020\right] & \left[\begin{array}{ccc} -0.35,0.35\right] & \left[\begin{array}{ccc} -0.22,0.22\right] \end{array}\right] \end{array}\right)\end{array}\right)
$$

With Gauss-Jordan-based bounds:

$$
\Delta L \simeq \left(\begin{array}{ccccc} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \left[-0.089, 0.089\right] & \left[-0.021, 0.021\right] & \left[-0.44, 0.44\right] & 0\end{array}\right)
$$

$$
\Delta U \simeq \left(\begin{array}{ccccc} \left[-0.03, 0.03\right] & \left[-0.07, 0.07\right] & \left[-0.64, 0.64\right] & \left[-0.75, 0.75\right] \\ 0 & 0 & \left[-0.21, 0.21\right] & 0 \\ 0 & 0 & \left[-0.17, 0.17\right] & 0 \\ 0 & 0 & 0 & \left[-0.23, 0.23\right] \end{array}\right)
$$

Example (cont'd)

$$
[M] = \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 0 & 0 & -1 \\ 1.25 & 0 & 0 & [-1, -0.9] \\ 3 & 3 & [3.3, 3.5] & 3 \end{pmatrix}
$$

$$
P^{-1}[L][U]Q^{-1} \simeq \begin{pmatrix} [0.89, 1.11] & [0.89, 1.11] & [0.94, 1.06] & [0.74, 1.30] \\ 1 & 0 & 0 & [-1.08, -0.91] \\ 1.25 & 0 & 0 & [-1, -0.9] \\ [2.82, 3.18] & [2.82, 3.18] & [3.3, 3.5] & [2.69, 3.31] \end{pmatrix}
$$

Note: Eigen may not select the "best" pivot w.r.t. to the uncertainties (it used 4th line, 3rd column as the first pivot), but it knows only the midpoint. Implanting a different strategy (based on the absolute value of the midpoint and the radius of the interval) may be possible but not easy.

Cholesky decomposition (LL^T)

Cholesky decomposition decompose a symmetric positive matrix M in the form of :

$$
M = LL^T
$$

where L is lower-triangular.

A similar approach to the LU can be considered, in which we would have to solve:

$$
(\mathrm{Id} - \Delta L)(\mathrm{Id} - \Delta L^{\mathcal{T}}) = (\mathrm{Id} - \mathrm{Err})
$$

However the diagonal "shared" by ΔL and $\Delta L^{\mathcal{T}}$ modify slightly the computation.

Cholesky decomposition (LDL^T)

Another Cholesky decomposition (which avoids square root computations) is of the form:

$$
M = LDL^T
$$

where L is unit-lower-triangular, and D is diagonal. We consider an approximative decomposition $\mathcal{M}\simeq L D_0L^{\mathcal{T}}$. Our goal is to enclose ΔL (stricly lower triangular) and D such that:

$$
M = L(\mathrm{Id} - \Delta L)D(\mathrm{Id} - \Delta L^T)L^T
$$

(D is not built from D_0 , in fact D_0 will not be used).

Problem formulation

From:

$$
M = L(\mathrm{Id} - \Delta L)D(\mathrm{Id} - \Delta L^T)L^T
$$

we get:

$$
[L^{-1}]M[(L^{\mathcal{T}})^{-1}] = (\mathrm{Id} - \Delta L)D(\mathrm{Id} - \Delta L^{\mathcal{T}})
$$

We can expect $A=[L^{-1}]M[(L^\mathcal{T})^{-1}]$ to be "almost diagonal". With V the diagonal of A, we pose:

$$
A = V(\mathrm{Id} - E)
$$

where the diagonal of E is 0 (note that E is *not* symmetric).

Result

$$
(\mathrm{Id} - \Delta L)D(\mathrm{Id} - \Delta L^T) = A = V(\mathrm{Id} - E)
$$

Diagonal coefficients:

$$
D_j = V_j \left(E_{j,[1,j-1]} \left(\sum_{\ell \geq 0} (E_{[1,j-1],[1,j-1]})^{\ell} \right) E_{[1,j-1],j} \right)
$$

Lower coefficients $(i > j)$:

$$
(\Delta L)_{i,j} = V_j^{-1}(A_{i,j} + A_{i,[1,j]}) \left(\sum_{\ell \geq 0} (E_{[1,j],[1,j]})^{\ell} \right) E_{[1,j],j})
$$

"Upper" coefficients (transpose) $(i > j)$:

$$
(\Delta L)_{i,j} = (\Delta L)_{j,i}^T = E_{j,i} + E_{j,[1,j]} \left(\sum_{\ell \geq 0} (E_{[1,j],[1,j]})^{\ell} \right) E_{[1,j],i}
$$

Example

$$
[M] = \left(\begin{array}{ccccc} 4 & 1 & 1 & -1 \\ 1 & [4,4.5] & 0 & 0 \\ 1 & 0 & 3 & [-0.2,0] \\ -1 & 0 & [-0.2,0] & [2,3] \end{array}\right)
$$

$$
P^{-1}[L][D][L^{T}]P \simeq \left(\begin{array}{ccccc} [3.94,4.06] & [0.88,1.13] & [0.98,1.02] & [-1.02,-0.98] \\ [0.87,1.13] & [4,4.5] & [-0.04,0.04] & [-0.04,0.04] \\ [0.98,1.02] & [-0.04,0.04] & [2.99,3.01] & [-0.21,0.01] \\ [-1.02,-0.98] & [-0.04,0.04] & [-0.21,0.01] & [1.96,3.04] \end{array}\right)
$$

Application to orthogonal matrices

An orthogonal matrix $Q \in \text{SO}_n(\mathbb{R})$ satisfies $QQ^{\mathcal{T}} = \text{Id}$. "Almost orthogonal" matrix would be $QQ^T \simeq \mathrm{Id}$. If a (non-singular) matrix A satisfies $Q Q^{\mathcal{T}} = A A^{\mathcal{T}}$ then $A^{-1} Q \in \mathrm{SO}_n(\mathbb{R})$ (with a Cholesky decomposition $QQ^T = LDL^T$, $D^{-0.5}L^{-1}Q \in \text{SO}_n(\mathbb{R})$).

We can use this approach to enclose a orthogonal matrix "around" Q (e.g. when Q is the "quasi-orthogonal" result of a floating-point computation).

Example

We consider:

$$
Q = \left(\begin{array}{ccc} 0.8 & -0.3 & -0.1 \\ 0.3 & 0.6 & -0.6 \\ -0.2 & -0.4 & -0.7 \end{array}\right)
$$

We use here only the enclosing algorithm developed for decomposing $\mathrm{Id}-E$ on QQ^T (i.e. no preliminary Cholesky decomposition). The result is:

$$
[Q'] \simeq \left(\begin{array}{ccc} 0.93 & -0.35 & -0.12 \\ 0.19 & 0.73 & -0.66 \\ [-0.32, -0.31] & [-0.59, -0.58] & [-0.75, -0.74] \end{array}\right)
$$

This approach does not find the "closest" orthogonal matrix, but can be used to "terminate" approximate methods.

More general approach

Instead of trying to solve $(\mathrm{Id} - \Delta)(\mathrm{Id} - \Delta^T) = \mathrm{Id} - E$, we can decompose Λ as a sum of infinite terms:

$$
(\mathrm{Id}-\Delta_1-\Delta_2\ldots)(\mathrm{Id}-\Delta_1^T-\Delta_2^T\ldots)=\mathrm{Id}-E,
$$

each term being of decreasing order. Then, we have:

$$
\Delta_1 + \Delta_1^T = E
$$

$$
\forall n \ge 2, \ \Delta_n + \Delta_n^T = \sum_{i=1}^{n-1} \Delta_i \Delta_{n-i}^T
$$

 $+$ we can select whatever we want to decompose E to $\Delta_1+\Delta_1^T$ (e.g. $\Delta_1 = \Delta_1^{\bm{\mathcal{T}}}$, since E is symmetric)

exact expression of Δ_n is harder, bounding relies more on norms.

Norm-based bounding

Looking for symmetric Δ_i (i.e. matrix square root):

$$
\Delta_1 = \Delta_1^T = \frac{E}{2}
$$

$$
\forall n \ge 2, \ \Delta_n = \Delta_n^T = \frac{\sum_{i=1}^{n-1} \Delta_i \Delta_{n-i}}{2}
$$

To bound $||\Delta_i||$, we look for a formula of the form:

$$
\Delta_i = \Phi(i) \frac{E^i}{2^{2i-1}}
$$

We can achieve that if $\Phi(n)$ satisfies for $n \geq 2$:

$$
\Phi(n)=\sum_{i=1}^{n-1}\Phi(i)\Phi(n-i)
$$

Norm-based bounding

With $\Phi(1) = 1$ and

$$
\forall n \geq 2, \Phi(n) = \sum_{i=1}^{n-1} \Phi(i)\Phi(n-i)
$$

$$
\Phi_n = C_{n-1}
$$
 where $C_n = \frac{(2n)!}{(n+1)!n!}$ are the Catalan numbers.

To conclude (matrix square root development):

$$
\Delta_i \leq C_{i-1} \frac{E^i}{2^{2i-1}}
$$

and we want to bound $\sum_{i\geq N}\|\Delta_i\|.$

Bounding (cont'd)

Theorem

if
$$
\rho \le 1/4
$$
, then $\sum_{i\ge 0} \rho^i C_i = \frac{1}{2\rho} (1 - \sqrt{1 - 4\rho})$

Hence, with $||E|| \leq 1$:

$$
\sum_{i\geq 0}\|\Delta_i\|\leq 1-\sqrt{1-\|E\|}
$$

Two bounds for the residual $\sum_{i\geq N}\|\Delta_i\|$:

• the "exact" one (with $||E|| \le 1$) (hard to compute):

$$
\sum_{i\geq N} \|\Delta_i\| \leq 1 - \sqrt{1 - \|E\|} - \sum_{i=1}^{N-1} \frac{C_{i-1}}{2^{2i-1}} \|E\|^i
$$

 \bullet the "approximate" one (with $||E|| < 1$):

$$
\sum_{i\geq N} \|\Delta_i\| \leq \frac{C_{N-1} \|E\|^N}{2^{2N-1} (1 - \|E\|)} \leq \frac{\|E\|^N}{2(1 - \|E\|)}
$$

QR decomposition

QR decomposition decomposes a rectangular matrix A into $A = QR$ where Q is orthogonal and R is upper-triangular (with pivoting, the decomposition is $AP = QR$ where P is a permutation matrix). From an existing approximate decomposition $A \simeq QR$:

- if the goal is to find $A\in [Q'][R']$ with $Q'\in \mathrm{SO}_n({\mathbb R})$ and $[R']$ is *almost* upper-triangular, just compute $[Q']$ from Q , then $[R']=[Q']^{\mathcal{T}} A$.
- To get a "real" QR decomposition, we can use an "infinite"-sum approach with a norm-based bound.

Equations

From an approximate decompositon $A \simeq QR$, we look for an equality of the form:

$$
A = Q(\mathrm{Id} - \Delta Q_1 - \Delta Q_2 - \ldots) \ldots (\mathrm{Id} - \Delta R_1 - \Delta R_2 - \ldots)R
$$

where the ΔR_i are upper-triangular, and $Q(\text{Id} - \Delta Q_1 - \Delta Q_2 - \ldots)$ is orthogonal.

I.e.

$$
(\mathrm{Id}-\Delta Q_1-\Delta Q_2-\ldots)\ldots(\mathrm{Id}-\Delta R_1-\Delta R_2-\ldots)=Q^{-1}AR^{-1}
$$

$$
(\mathrm{Id}-\Delta Q_1-\Delta Q_2-\ldots)(\mathrm{Id}-\Delta Q_1^T-\Delta Q_2^T-\ldots)=(Q^TQ)^{-1}
$$

Note: case A not square or R singular should be more formalised.

Let's pose $E_r = \mathrm{Id} - Q^{-1} A R^{-1}$ and $E_q = \mathrm{Id} - (Q^T Q)^{-1}$ (note that E_q is symmetric).

Systems

Then we have the following systems:

$$
\begin{cases}\n\Delta Q_1 + \Delta Q_1^T = E_q \\
\Delta Q_1 + \Delta R_1 = E_r\n\end{cases}
$$
\n
$$
\begin{cases}\n\Delta Q_n + \Delta Q_n^T = \sum_{k=1}^{n-1} \Delta Q_k \Delta Q_{n-k}^T \quad \text{(symmetric)} \\
\Delta Q_n + \Delta R_n = \sum_{k=1}^{n-1} \Delta Q_k \Delta R_{n-k}\n\end{cases}
$$

This systems enable to compute Q_i and R_i , e.g. for $i=1$:

- \bullet we have $\Delta Q_1 = E_r$ for the lower triangular part
- using $\Delta Q_1 + \Delta Q_1^{\mathcal{T}} = \mathit{E_{q}}$ we deduce the upper triangular part and diagonal
- back to $\Delta Q_1 + \Delta R_1 = E_r$ we compute R_1 .
- If N is the maximum of $||E_{a}||_{\alpha}$, $||E_{r}||_{\alpha}$ with $\alpha \in \{1, \infty\}$.

$$
\text{for all } \alpha \in \{1, \infty\}, \|\textit{Q}_1\|_{\alpha} \leq 3\mathcal{N} \qquad \|\textit{R}_1\|_{\alpha} \leq 3\mathcal{N}
$$

Error bounds

Extending the result to successive products, we get:

$$
\sum_{i\geq N} \|\Delta Q_i\| \leq \frac{(3\mathcal{N})^N}{2(1-3\mathcal{N})}
$$

$$
\sum_{i\geq N} \|\Delta R_i\| \leq \frac{(3\mathcal{N})^N}{2(1-3\mathcal{N})}
$$

The bound is quite rough, but can be used for punctual decompositions.

$$
[A] = \left(\begin{array}{cccc} [0.2, 0.21] & -2.3 & -0.1 & -0.6 \\ 1.3 & 0.6 & -0.6 & -1.2 \\ -0.2 & -1.4 & -0.7 & 1.3 \\ -0.2 & -1.5 & -0.2 & 1.4 \end{array}\right)
$$

$$
[Q][R]P^{-1}\simeq\left(\begin{array}{cccc} [0.17,0.23] & [-2.32,-2.27] & [-0.16,-0.03] & [-0.65,-0.54] \\ [1.28,1.32] & [0.58,0.62] & [-0.65,-0.55] & [-1.24,-1.16] \\ [-0.22,-0.18] & [-1.42,-1.38] & [-0.75,-0.65] & [1.26,1.34] \\ [-0.22,-0.18] & [-1.52,-1.48] & [-0.25,-0.15] & [1.36,1.44] \end{array}\right)
$$

Future work

- Implementation into Codac. \bullet
- More tests, larger and complex matrices. \bullet
- Comparison with other tools (Intlab). \bullet
- Better boundings (e.g. for QR decomposition). \bullet
- Specific applications, on the contraction of matrix product, linear \bullet programming, etc.
- Other computations. \bullet