# (Q)OR Krylov Methods in Finite Precision: Inherent Characteristics.

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## OR and QOR (Krylov Subspace) Methods.

- o Lanczos based methods (short–term methods)
- o Arnoldi based methods (long–term methods)

- o eigensolvers: $Av = v\lambda$
- o linear system solvers: $Ax = b$
  - o (quasi-) orthogonal residual approaches: (Q)OR
  - o (quasi-) minimal residual approaches: (Q)MR

Extensions:

- o Lanczos based methods:
  - o look-ahead
  - o product-type (LTPMs)
  - o applied to normal equations (CGN)
- o Arnoldi based methods:
  - o restart (thin/thick, explicit/implicit)
  - o truncation (standard/optimal)

Krylov method: compute approximations from Krylov subspace

$$\mathcal{K}_m \equiv \mathcal{K}_m(A, q) \equiv \mathsf{span}\{q, Aq, \ldots, A^{m-1}q\}, \quad K_m = [q, Aq, \ldots, A^{m-1}q]$$

*All* Krylov methods based on Hessenberg decomposition

$$\begin{aligned} AQ_m &= Q_m C_m, \\ AQ_k &= Q_{k+1}\underline{C}_k = Q_k C_k + q_{k+1} c_{k+1,k} e_k^T \quad \forall\ k < m \end{aligned}$$

of Krylov subspace ($C_k$ Hessenberg).

Linear system context: $Ax = r_0$, $q \equiv q_1 \equiv r_0 / \|r_0\|$.

$k$th approximation $x_k \in \mathcal{K}_k$ for $x \equiv A^{-1}r_0$ expressed in terms of new basis:

$$x_k = Q_k z_k, \quad z_k \in \mathbb{K}^k.$$

Task: find *computable* expression for $z_k$.

Essentially two approaches: (Q)OR and (Q)MR.

Observe

$$
\begin{aligned}
-r_k = Ax_k - r_0 &= AQ_k z_k - Q_k e_1 \|r_0\| \\
&= Q_k(C_k z_k - e_1\|r_0\|) + q_{k+1} c_{k+1,k} z_{kk}.
\end{aligned}
$$

$\widehat{Q}_k^H$ defined by partition of pseudo-inverse:

$$
Q_{k+1}^{\dagger} Q_{k+1} = \begin{pmatrix} \widehat{Q}_k^H \\ \widehat{q}_{k+1}^H \end{pmatrix} \left[ Q_k, q_{k+1} \right] = I_{k+1}.
$$

Apply $\widehat{Q}_k^H$ to the left:

$$
-\widehat{Q}_k^H r_k = C_k z_k - e_1 \|r_0\|.
$$

When possible, set $z_k = C_k^{-1} e_1 \|r_0\|$:

$\Rightarrow$ annihilate projected residual.

Reason for notion (quasi)-orthogonal residual method, (Q)OR.

Galërkin approach. Project linear system onto smaller linear system:

$$\begin{aligned}(A, r_0) &\rightarrow (AQ_k, Q_k\|r_0\|e_1)\\ &\rightarrow (\widehat{Q}_k^H AQ_k, \widehat{Q}_k^H Q_k\|r_0\|e_1) = (C_k, \|r_0\|e_1),\end{aligned}$$

$\Rightarrow$ second matrix $\widehat{Q}_k$ (bi)orthogonal to $Q_k$.

(Q)OR related to small square matrix $C_k$.

Variety of (Q)OR methods:

OR ($\widehat{Q}_k = Q_k$, *Bubnov*-Galërkin): FOM, Orthores, CG-Ores, CG-Omin, CG-Odir, SymmLQ

QOR ($\widehat{Q}_k \neq Q_k$, *Petrov*-Galërkin): Biores, Biomin, Biodir, QOR

(Q)OR relies on iterated solution of small systems with system matrix $C_k$. Hessenberg structure of $C_k$ admits computation of decomposition along with computation of coefficients.

**Example:** LR decomposition

$$C_k = B_k R_k, \quad c_{k+1,k} = b_{k+1,k} r_{kk}.$$

$B_k$ bidiagonal since $C_k$ Hessenberg. Matrix of *direction vectors* $P_m \equiv Q_m R_m^{-1}$. Split Hessenberg decomposition:

$$\begin{aligned} AP_m &= Q_m B_m, \\ AP_k &= Q_k B_k + q_{k+1} b_{k+1,k} e_k^T \quad \forall\ k < m. \end{aligned}$$

Split Hessenberg decomposition and $Q_k = P_k R_k$ define two *coupled* recurrences.

Methods based on LR (LDLT, LDMT): CG-Omin, Biomin (BiCG)
Methods based on QR (LQ): FOM, SymmLQ, QOR

## Finite Precision Issues.

Finite precision analog of Hessenberg decomposition:

$$AQ_k - Q_k C_k = M_k - F_k, \qquad M_k = q_{k+1} c_{k+1,k} e_k^T.$$

Error term $F_k$ depends on method and implementation.

Orthores, Ores and Biores:

$$|f_k| \leq \gamma_n |A||q_k| + \gamma_g |Q_{k+1}||c_k|, \qquad g = \text{nnz}(c_k).$$

Omin, Biomin:

$$-F_k = AF_k^{(P)} + F_k^{(R)} L_k^{-1} C_k^{(0)}.$$

$(P)$ errors from direction vector recurrence,
$(R)$ errors from residual recurrence,
$L_k$ certain bidiagonal matrix, $C_k^{(0)}$ scaled Hessenberg.

Some methods: a priori bound, often: only a posteriori bounds possible.

**Inherent Characteristics.**

Inherent: We suppose no errors made in solution of small systems, i.e., we think of "best solution" possible with information at hand.
Characteristics: Behaviour common to *all* (Q)OR methods, indicators of potential drawbacks and traps.

**Assumption:** $A$, $C_k$ diagonalisable.

**Notation:** Eigendecompositions defined as

$$\begin{aligned} AV &= V\Lambda, & \hat{V}^H &\equiv V^{-1}, & \check{V}^T &\equiv V^{-1} \\ C_k S_k &= S_k \Theta_k, & \hat{S}_k^H &\equiv S_k^{-1}, & \check{S}_k^T &\equiv S_k^{-1} \end{aligned}$$

Characteristic polynomials: $\chi_{C_k}(z) \equiv \det(zI - C_k)$.

**Toolkit:** Lagrange, Hessenberg eigenvalue-eigenvector-relations ($i \leq j$)

$$\check{s}_{il} s_{jl} = \frac{\chi_{C_{i-1}}(\theta_l) \left( \prod_{\ell=i}^{j-1} c_{\ell+1,\ell} \right) \chi_{C_{j+1:k}}(\theta_l)}{\chi'_{C_k}(\theta_l)}$$

## Inherent Characteristics: "best iterates".

Diagonalised (slightly re-written) form of $AQ_k - Q_k C_k = M_k - F_k$:

$$\widehat{v}_i^H q_{k+1} = \widehat{v}_i^H Q_k \left[ \frac{\lambda_i - \theta_j}{c_{k+1,k} s_{kj}} \right] s_j + \widehat{v}_i^H F_k \left[ \frac{1}{c_{k+1,k} s_{kj}} \right] s_j.$$

"Best solution" coefficients in terms of Ritz values and Ritz vectors:

$$\begin{aligned} \frac{z_k}{\|r_0\|} &= C_k^{-1} e_1 = S_k \Theta_k^{-1} \check{S}_k^T e_1 \\ &= \sum_{j=1}^{k} \frac{\check{s}_{1j}}{\theta_j} s_j = \sum_{j=1}^{k} \left( \frac{c_{k+1,k} \check{s}_{1j} s_{kj}}{(\lambda_i - \theta_j)\,\theta_j} \right) \left( \frac{\lambda_i - \theta_j}{c_{k+1,k} s_{kj}} \right) s_j \end{aligned}$$

Thus "best iterate" defined by

$$\frac{x_k}{\|r_0\|} = Q_k \frac{z_k}{\|r_0\|} = \sum_{j=1}^{k} \left( \frac{c_{k+1,k} \check{s}_{1j} s_{kj}}{(\lambda_i - \theta_j)\,\theta_j} \right) \left[ Q_k \left( \frac{\lambda_i - \theta_j}{c_{k+1,k} s_{kj}} \right) s_j \right].$$

**Theorem:** Expression for (left) eigenpart of "best iterate":

$$\frac{\hat{v}_i^H x_k}{\|r_0\|} = \left[\sum_{j=1}^{k} \frac{c_{k+1,k}\check{s}_{1j}s_{kj}}{(\lambda_i - \theta_j)\,\theta_j}\right] \hat{v}_i^H q_{k+1} - \hat{v}_i^H F_k \left[\sum_{j=1}^{k} \left(\frac{\check{s}_{1j}}{(\lambda_i - \theta_j)\,\theta_j}\right) s_j\right].$$

Interpretation based on Hessenberg EER:

$$\sum_{j=1}^{k} \frac{c_{k+1,k}\check{s}_{1j}s_{kj}}{(\lambda_i - \theta_j)\theta_j} = \prod_{l=1}^{k} c_{l+1,l} \left(\sum_{j=1}^{k} \frac{1}{\chi'_{C_k}(\theta_j)(\lambda_i - \theta_j)} \cdot \frac{1}{\theta_j}\right)$$

Lagrange interpolation of $x^{-1}$ at knots $\theta_j$, $j \in \underline{k}$.

$$\sum_{j=1}^{k} \frac{\check{s}_{1j}s_{\ell j}}{(\lambda_i - \theta_j)\,\theta_j} = \prod_{l=1}^{\ell} c_{l+1,l} \left(\sum_{j=1}^{k} \frac{1}{\chi'_{C_k}(\theta_j)(\lambda_i - \theta_j)} \cdot \frac{\chi_{C_{\ell+1:k}}(\theta_j)}{\theta_j}\right)$$

Lagrange interpolation of $x^{-1}$ weighted by $\chi_{C_{\ell+1:k}}(\theta_j)$.

**Inherent Characteristics: "best errors".**

Similar expression for error $x - x_k$:

$$\begin{aligned}\hat{v}_i^H (x - x_k) &= \hat{v}_i^H A^{-1} r_0 - \|r_0\| \hat{v}_i^H Q_k z_k \\ &= \|r_0\| \hat{v}_i^H Q_k \left(\lambda_i^{-1} I_k - C_k^{-1}\right) e_1\end{aligned}$$

Representation in terms of Ritz vectors $s_j$:

$$\begin{aligned}\left(\lambda_i^{-1} I_k - C_k^{-1}\right) e_1 &= \left(S \lambda_i^{-1} \check{S}^T - S \Theta_k^{-1} \check{S}^T\right) e_1 \\ &= \sum_{j=1}^{k} \left(\frac{\check{s}_{1j}}{\lambda_i} - \frac{\check{s}_{1j}}{\theta_j}\right) s_j.\end{aligned}$$

Thus, we obtain

$$\begin{aligned}\frac{\hat{v}_i^H (x - x_k)}{\|r_0\|} &= \hat{v}_i^H Q_k \left( \sum_{j=1}^{k} \left(\frac{\check{s}_{1j}}{\lambda_i} - \frac{\check{s}_{1j}}{\theta_j}\right) s_j \right) \\ &= \hat{v}_i^H Q_k \left( \sum_{j=1}^{k} \left(\frac{c_{k+1,k} \check{s}_{1j} s_{kj}}{(0 - \theta_j)\lambda_i}\right) \left(\frac{\lambda_i - \theta_j}{c_{k+1,k} s_{kj}}\right) s_j \right).\end{aligned}$$

**Theorem:** Expression for (left) eigenpart of "best error":

$$\frac{\widehat{v}_i^H(x-x_k)}{\|r_0\|} = \left[\sum_{j=1}^{k} \frac{c_{k+1,k}\check{s}_{1j}s_{kj}}{0-\theta_j}\right] \frac{\widehat{v}_i^H q_{k+1}}{\lambda_i} - \frac{\widehat{v}_i^H F_k}{\lambda_i} \left[\sum_{j=1}^{k} \left(\frac{\check{s}_{1j}}{0-\theta_j}\right) s_j\right].$$

Reformulation again based on Hessenberg EER:

$$\sum_{j=1}^{k} \frac{c_{k+1,k}\check{s}_{1j}s_{kj}}{0-\theta_j} = \sum_{j=1}^{k} \frac{\prod_{p=1}^{k} c_{p+1,p}}{\chi'_{C_k}(\theta_j)(0-\theta_j)} = \frac{\prod_{p=1}^{k} c_{p+1,p}}{\chi_{C_k}(0)}.$$

$$\sum_{j=1}^{k} \frac{\check{s}_{1j}s_{lj}}{0-\theta_j} = \sum_{j=1}^{k} \frac{\left(\prod_{p=1}^{l-1} c_{p+1,p}\right)\chi_{C_{l+1:k}}(\theta_j)}{\chi'_{C_k}(\theta_j)(0-\theta_j)} = \frac{\left(\prod_{p=1}^{l-1} c_{p+1,p}\right)\chi_{C_{l+1:k}}(0)}{\chi_{C_k}(0)}.$$

## Inherent Characteristics: "basis vectors".

Influence of errors $f_l$ on the computed "basis" vectors given by

$$\frac{\hat{v}_i^H q_{k+1}}{\lambda_i} = \frac{\chi_{C_k}(0)}{\prod_{p=1}^k c_{p+1,p}} \left( \frac{\hat{v}_i^H (x - x_k)}{\|r_0\|} \right) + \sum_{l=1}^k \left[ \frac{\chi_{C_{l+1:k}}(0)}{\prod_{p=l+1}^k c_{p+1,p}} \left( \frac{\hat{v}_i^H f_l}{\lambda_i c_{l+1,l}} \right) \right].$$

Mixture of Krylov methods:

$$A^{-1} q_{k+1} = \frac{\chi_{C_k}(0)}{\prod_{p=1}^k c_{p+1,p}} \left( \frac{x - x_k}{\|r_0\|} \right) + \sum_{l=1}^k \left[ \frac{\chi_{C_{l+1:k}}(0)}{\prod_{p=l+1}^k c_{p+1,p}} \left( \frac{A^{-1} f_l}{c_{l+1,l}} \right) \right].$$

In terms of residual vectors:

$$q_{k+1} = \frac{\chi_{C_k}(0)}{\prod_{p=1}^k c_{p+1,p}} \left( \frac{r_k}{\|r_0\|} \right) + \sum_{l=1}^k \left[ \frac{\chi_{C_{l+1:k}}(0)}{\prod_{p=l+1}^k c_{p+1,p}} \left( \frac{f_l}{c_{l+1,l}} \right) \right].$$

## Inherent Characteristics: "best residuals".

The $k$th *true error* $x - x_k$ is composed of two terms, namely

$$\frac{x - x_k}{\|r_0\|} = \frac{\prod_{p=1}^{k} c_{p+1,p}}{\chi_{C_k}(0)} A^{-1} q_{k+1} - \sum_{l=1}^{k} \left[ \frac{\left(\prod_{p=1}^{l-1} c_{p+1,p}\right) \chi_{C_{l+1:k}}(0)}{\chi_{C_k}(0)} A^{-1} f_l \right].$$

This implies that the *true residual* $r_k$ can be expressed by

$$\frac{r_k}{\|r_0\|} = \frac{\prod_{p=1}^{k} c_{p+1,p}}{\chi_{C_k}(0)} q_{k+1} - \sum_{l=1}^{k} \left[ \frac{\left(\prod_{p=1}^{l-1} c_{p+1,p}\right) \chi_{C_{l+1:k}}(0)}{\chi_{C_k}(0)} f_l \right].$$

$\Rightarrow$ stopping criteria based on characteristics of $C_k$ and size of $f_l$.

**Idea:** model error behaviour by (one) Krylov method.

**Examples.**

Orthores and Orthomin variants are based on scaled Hessenberg decompositions:

$$e^T \underline{C}_m = 0, \qquad e = (1, \ldots, 1)^T.$$

(Orthores directly, Orthomin based on split Hessenberg decomposition.)

This implies:

$$\chi_{C_k}(0) = \prod_{\ell=1}^{k} c_{\ell+1,\ell} \quad \forall\ k \leq m.$$

(follows by induction; similar to Hyman's computation of determinant)

Very pleasant feature:

holds true in finite precision: Orthomin variants.

holds approximately true: Orthores variants.

## Examples: CG (Omin), BiCG (Biomin).

Formula for true residual:

$$\frac{r_k}{\|r_0\|} = \frac{\prod_{p=1}^{k} c_{p+1,p}}{\chi_{C_k}(0)} q_{k+1} - \sum_{l=1}^{k} \left[ \frac{\left(\prod_{p=1}^{l-1} c_{p+1,p}\right) \chi_{C_{l+1:k}}(0)}{\chi_{C_k}(0)} f_l \right].$$

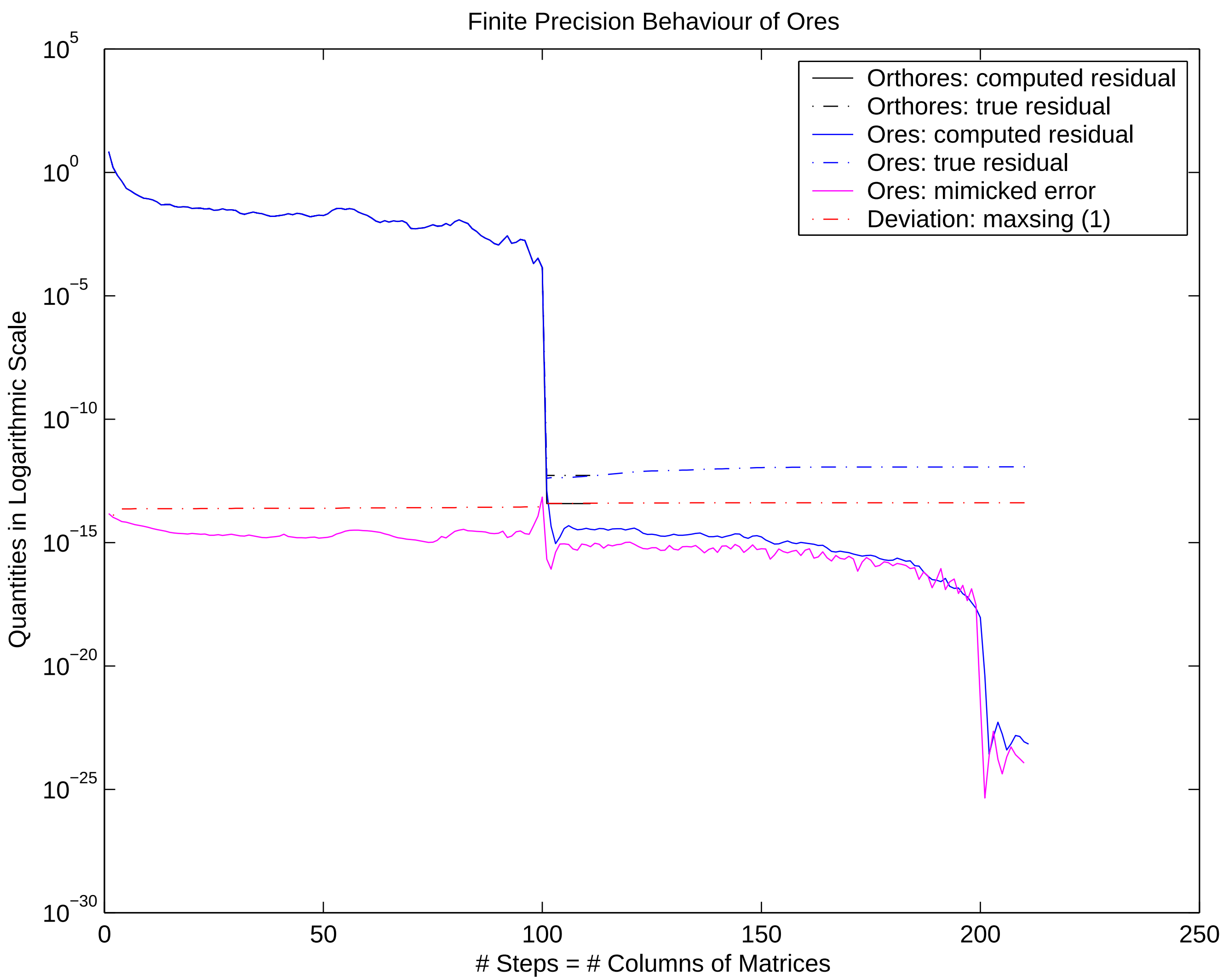
Due to underlying nice feature:

$$\begin{aligned} q_{k+1} - \frac{r_k}{\|r_0\|} &= \sum_{l=1}^{k} \frac{\chi_{C_{1:l-1}}(0)\chi_{C_{l+1:k}}(0)}{\chi_{C_k}(0)} f_l \\ &= \sum_{l=1}^{k} \left(-C_k^{-1}\right)_{ll} f_l. \end{aligned}$$

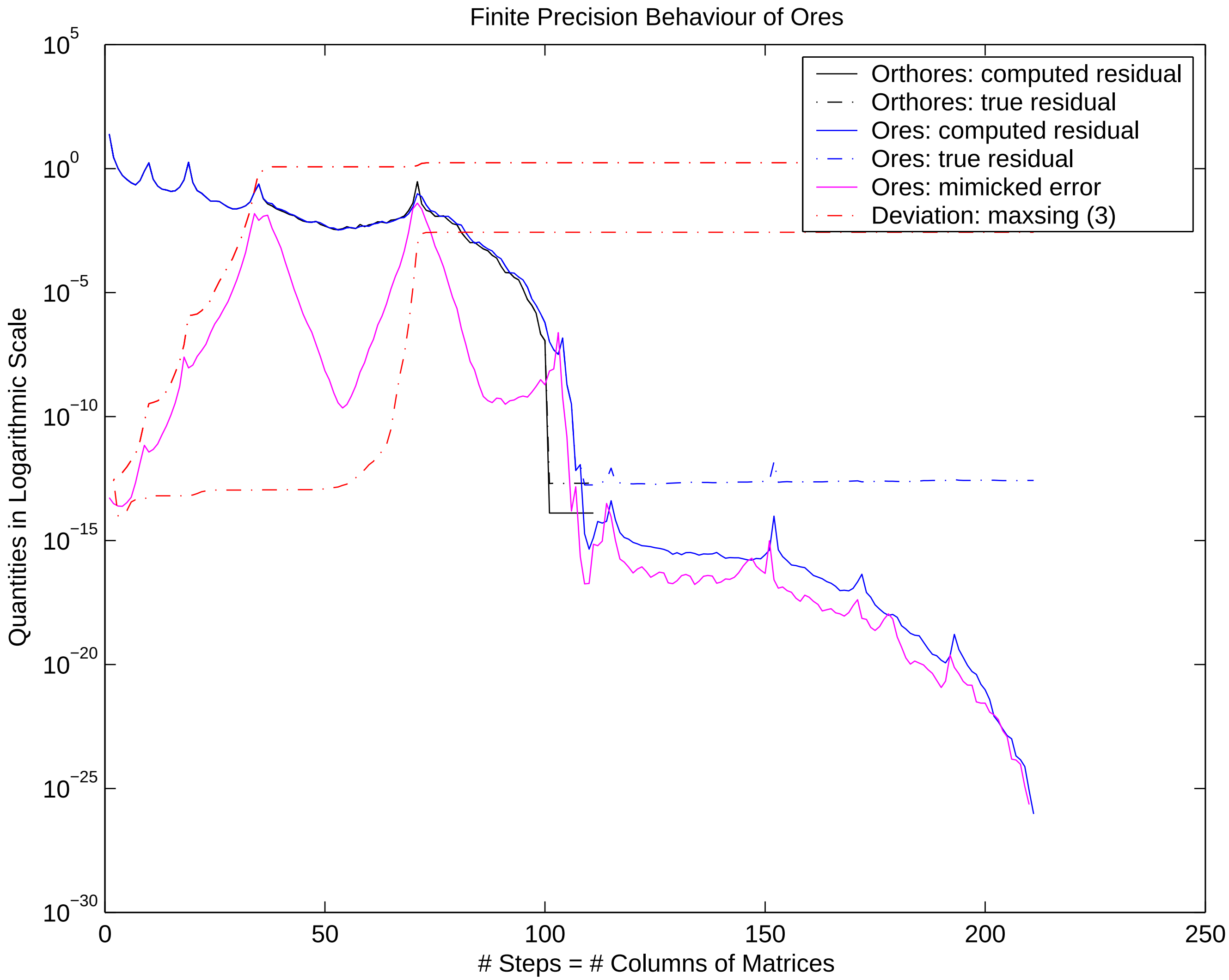
Computable bounds (twisted factorisation?):

$$\left\|\frac{r_k}{\|r_0\|} - q_{k+1}\right\| = \left\|\sum_{l=1}^{k} \left(C_k^{-1}\right)_{ll} f_l\right\| \le \operatorname{tr}\left|C_k^{-1}\right| \cdot \max_l \|f_l\|.$$

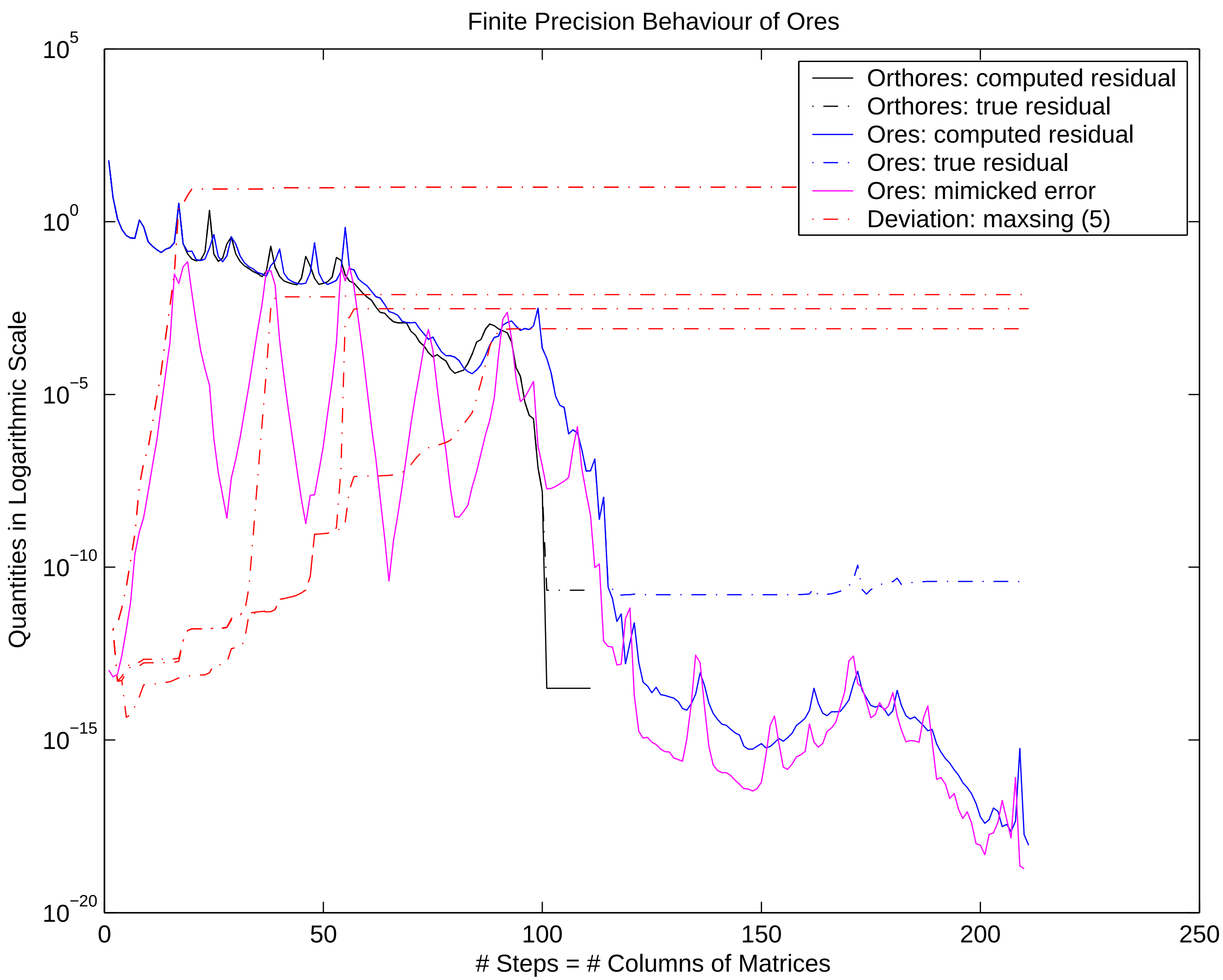
## Examples: Orthores and Ores. $T + \sigma A$, $\sigma = 0.0$



# Examples: Orthores and Ores. $T + \sigma A$, $\sigma = 0.1$



# Examples: Orthores and Ores. $T + \sigma A$, $\sigma = 0.2$



# Examples: Orthores and Ores. $T + \sigma A$, $\sigma = 1.0$