

(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**

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

All Krylov methods based on **Hessenberg decomposition**

$$AQ_m = Q_m C_m,$$

$$AQ_k = Q_{k+1} \underline{C}_k = Q_k C_k + q_{k+1} c_{k+1,k} e_k^T \quad \forall k < m$$

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

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

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

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

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

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

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.

Galärkin approach. Project linear system onto smaller linear system:

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

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

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

Variety of (Q)OR methods:

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

QOR ($\hat{Q}_k \neq Q_k$, Petrov-Galärkin): 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:

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

Error term F_k depends on method and implementation.

Orthores, Ores and Biores:

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

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 $AQ_k - Q_kC_k = M_k - F_k$:

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

“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”:

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

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 θ_j , $j \in \underline{k}$.

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

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

Inherent Characteristics: “best errors”.

Similar expression for error $x - x_k$:

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

Representation in terms of Ritz vectors s_j :

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

Thus, we obtain

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

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:

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

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

Inherent Characteristics: “basis vectors”.

Influence of errors f_l on the computed “basis” vectors given by

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

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

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

⇒ 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:

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

(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:

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

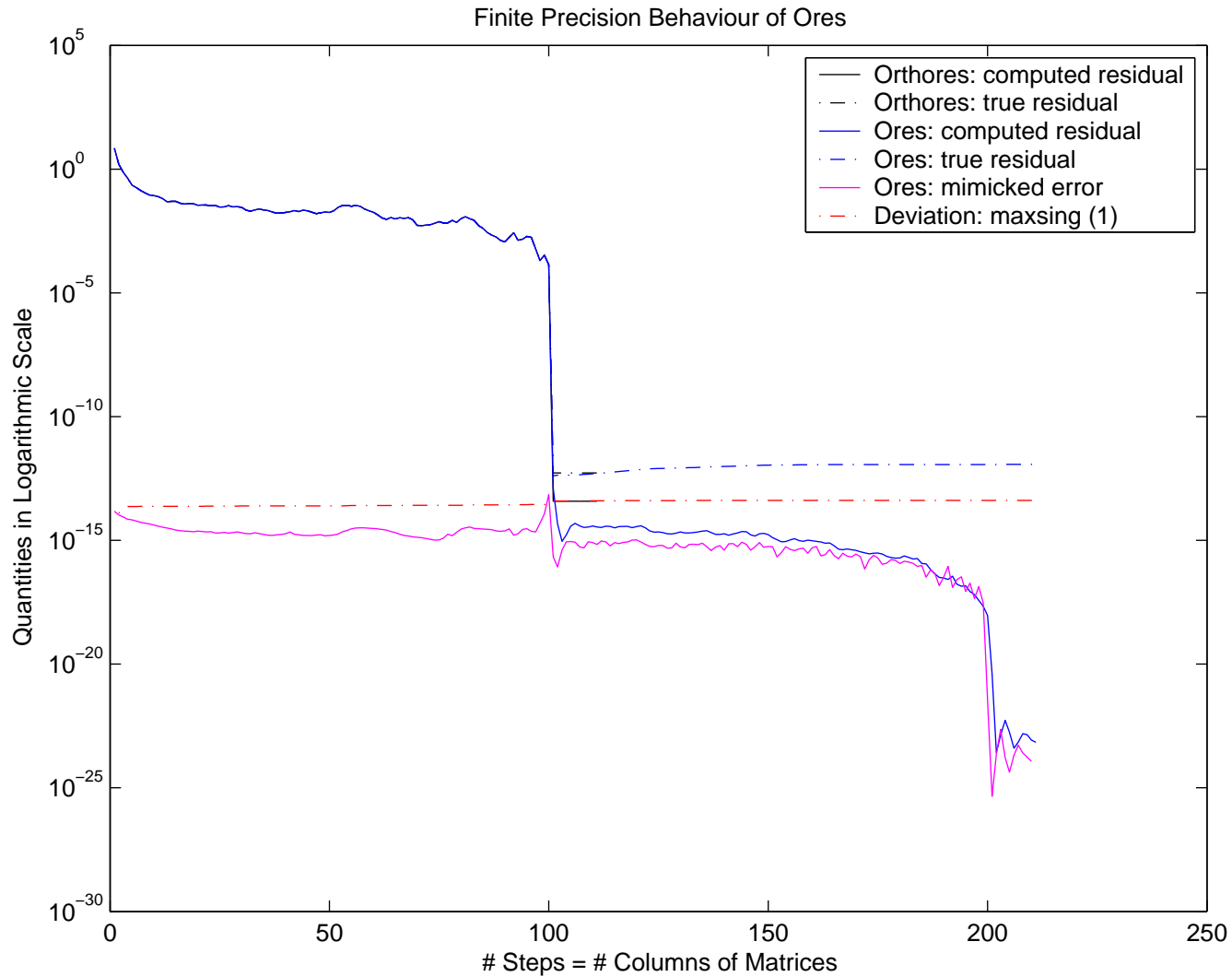
Due to underlying nice feature:

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

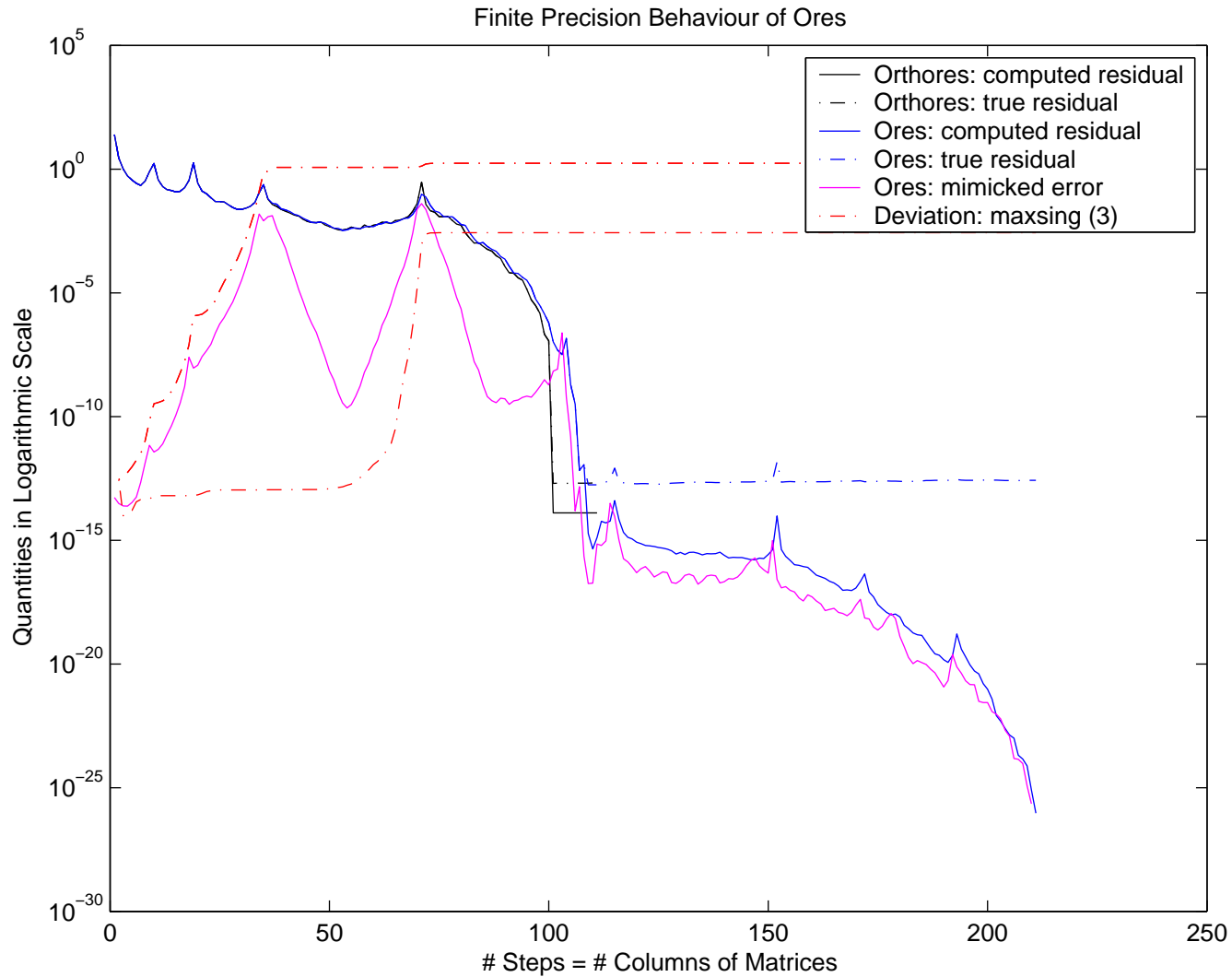
Computable bounds (twisted factorisation?):

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

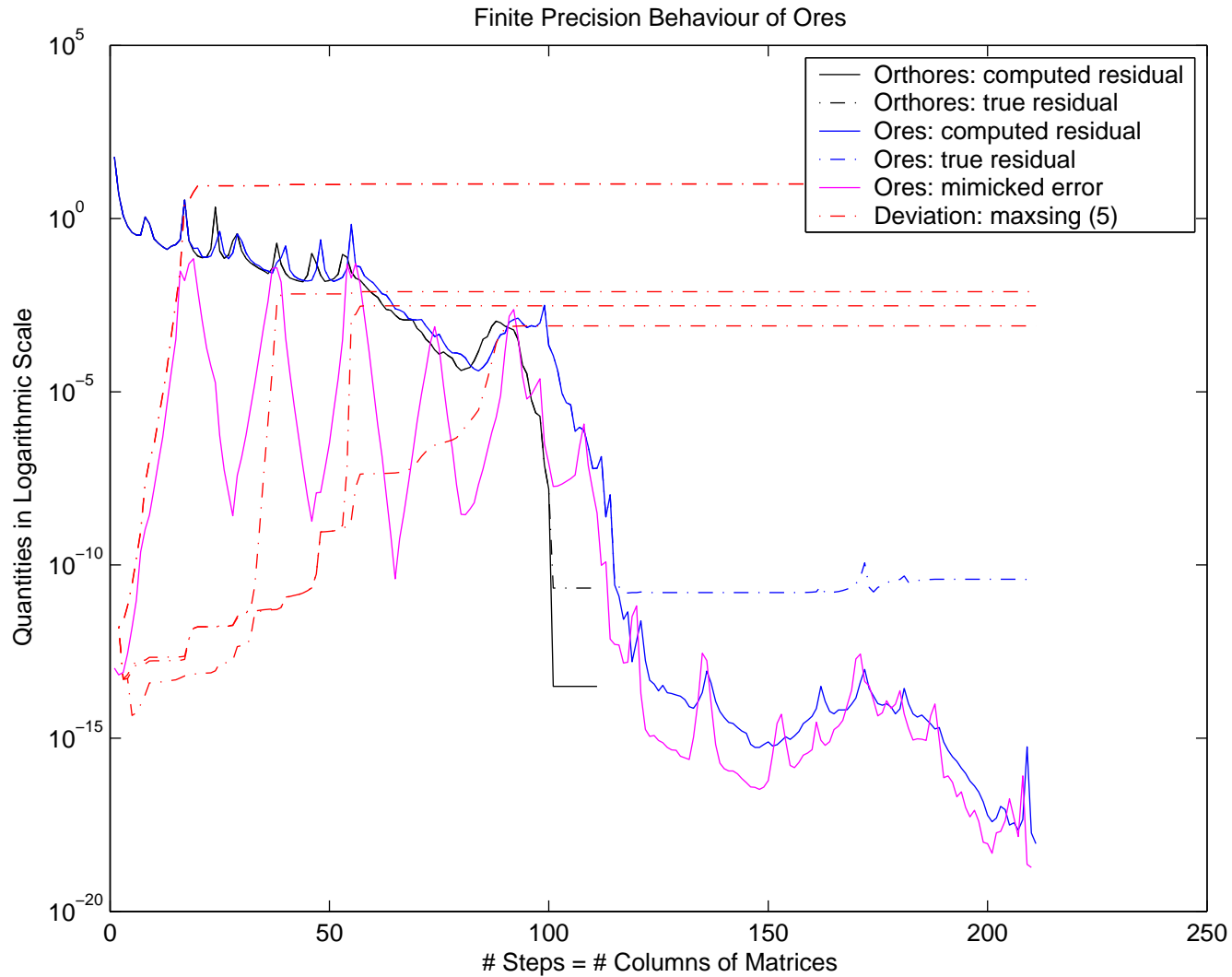
Examples: Orthores and Ores. $T + \sigma A$, $\sigma = 0.0$



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



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



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

