Truncation of Optimal Krylov Subspace Methods

Eric de Sturler

sturler@uiuc.edu http://www.csar.uiuc.edu/~sturler

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Overview

1. Truncation: why and how (not)
2. Neglecting orthogonality and generalized truncation
3. GMRES(m): Analysis and preserving a subspace
4. GCRO with optimal truncation
5. Numerical examples
6. Conclusions
7. An application in lattice QCD (multiple right hand sides)
8. An application in Jacobi-Davidson eigenvalue solvers
9. An application in matrix-free nonlinear solvers (adaptive grid pde package)

Truncation: why and how (not)

- **Full GMRES/GCR too expensive in general: memory / work**
- **GMRES-like method, close to optimal with limited resources**
- **Standard strategies: restart GMRES(m), all previous info lost**
  truncate GCR(m), oldest vectors removed
- **VERY CRUDE!**
- **Better to make some compromise: GMRESR / GCRO / FGMRES**
  eventually these methods still need some truncation
- **How to truncate:**
  - **careful select what to keep**
  - **don't think about vectors, think about spaces**

(truncation: why and how (not))

How to select the subspace to keep?

1. Make assumptions on system (normal, nice spectrum): restrictive
2. No assumptions, only use information from iteration process

- **No general convergence theory for GMRES (GCR)**
- **Worst case exists : bad spectrum**
  non-normality

- **Optimality is obtained through orthogonality: the old 'search space' (after making update) is used only to maintain orthogonality.**

- **So importance of a subspace is determined by its contribution to maintaining orthogonality**

GCR and nested methods

GCR: $Ax = b$

$r_0 = b - Ax_0$; $i = 0$
while $2\ r_i\ 2 > tol$
  $i \;= i+1$
  $u_i = r_{i-1}$; $c_i = Au_i$

  $u_i = <_i (u_i - U_{i-1}C_{i-1}^H c_i)$
  $c_i = <_i (I - C_{i-1}C_{i-1}^H)c_i$

  $r_i = r_{i-1} - c_i\, c_i^H r_i$
  $x_i = x_{i-1} + u_i\, c_i^H r_{i-1}$

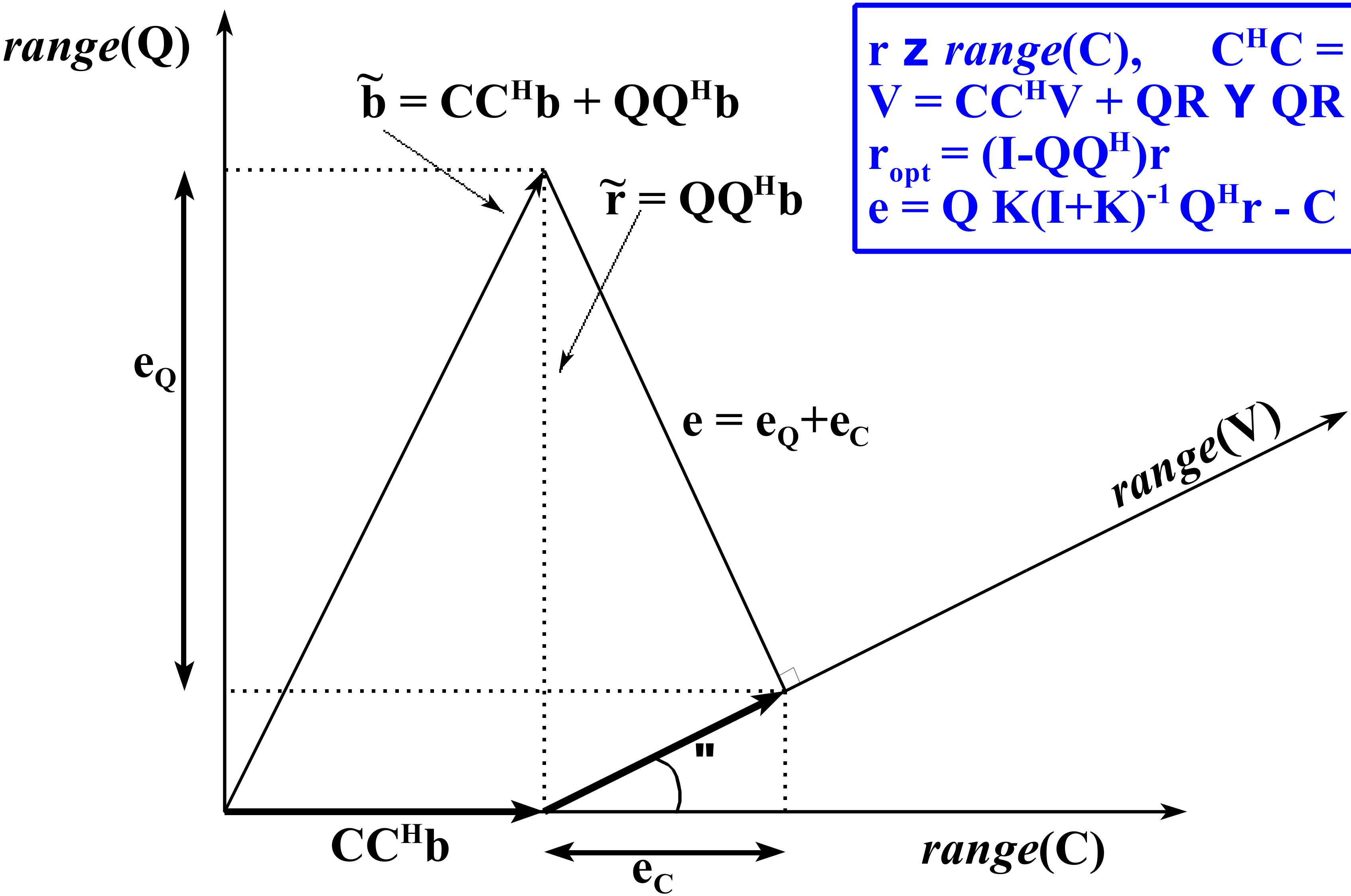
after k iterations:

$range(U_k) = K^k(A,r_0)$
$AU_k = C_k \qquad C_k^H C_k = I$

$r_k = (I-C_kC_k^H)r_0$
$x_k = x_0 + U_kC_k^H r_0$

GMRESR: replace $u_i = r_{i-1}$ by GMRES approx. sol. of $Ae_{i-1} = r_{i-1}$
Ignores orthogonality / optimality w.r.t. $range(C_{i-1})$
GCRO: maintain orthogonality; use $(I-C_{i-1}C_{i-1}^H)A$ for inner iteration

Neglecting Orthogonality & Generalized Truncation



r z *range*(C), $\quad$ **$C^H C = I$**

$V = CC^H V + QR$ Y $QR = V - CB$

$r_{opt} = (I - QQ^H) r$

$e = Q\, K(I+K)^{-1} Q^H r - C\, Z(I+K)^{-1} Q^H r$

(neglecting orthogonality & generalized truncation)

$$V = CB + QR = CC^H V + QQ^H V$$

$$r_{opt} = (I - QQ^H)r$$

$$e = Q\,K(I+K)^{-1}\,Q^H r - C\,Z(I+K)^{-1}\,Q^H r$$

$$Z = BR^{-1} = X_Z \Sigma_Z Y_Z^{\,H}, \qquad K = Z^H Z, \qquad \gamma_i = y_i^{\,H} Q^H r$$

$$e = \sum_{i=1}^{\min(k,m)} \left(\frac{\gamma_i \sigma_i^2}{1+\sigma_i^2}\, Qy_i - \frac{\gamma_i \sigma_i}{1+\sigma_i^2}\, Cx_i \right) \qquad \|e\| = \left(\sum_{i=1}^{\min(k,m)} \frac{|\gamma_i|^2 \sigma_i^2}{1+\sigma_i^2} \right)^{1/2}$$

(neglecting orthogonality & generalized truncation)

$[T^{*}T_c]$ unitary and *rank*($[T^{*}T_c]$) = *rank*(C), $\bar{V} = [CT^{*}V]$ and $\bar{C} = [CT_c]$

$$\bar{Z} = \bar{B}\bar{R}^{-1} = [0^{*}T_c^{H}Z] = [0^{*}T_c^{H}X_Z G_Z Y_Z^{H}]$$

Select T_c^{H} so that singular values of $\bar{Z}$ minimal:

$$\min_{\dim S=k-p} \Big(\max_{u \theta S} {**}u^{H}Z{**} \,/\, {**}u{**} \Big) = F_{p+1} \quad \text{and} \quad S = \mathit{span}\{x_{p+1}, \ddot{y}, x_k\}$$

Set $T_c = [x_{p+1}\ x_{p+2}\ \ddot{y}\ x_k]$ Y $T = [x_1\ \ddot{y}\ x_p]$

$$e = \mathop{E}_{i=p+1}^{\min(k,m)} \left(\frac{<_i F_i^2}{1+F_i^2} Qy_i - \frac{<_i F_i}{1+F_i^2} Cx_i \right)$$

$$2e2\ '\ \ddagger \mathop{E}_{i=p+1}^{\min(k,m)} \frac{{*}<_i{*}^2 F_i^2}{1+F_i^2} \check{Z}^{1/2}$$

GMRES(m) Analysis & Selecting a Subspace

GMRES: $AW_m \;=\; W_{m+1}\overline{H}_m \;=\; W_{m+1}Q_m\overline{R}_m \;=\; W_{m+1}\overline{Q}_mR_m$

How would convergence have been after restarting after s < m iterations?
What was influence on later iterations of orthogonality against *range*(AW_s)?

$r_s = W_{s+1}D_s$ with $D_s = (I - \overline{Q}_s\overline{Q}_s^H)2r2e_1$

C_s : orthogonal basis for *range*(AW_s) ! $C_s = W_{m+1}\overline{Q}_s$

V_s : any basis for $AK^{m-s}(A,r_s) = W_{m+1}\overline{H}_mK^{m-s}(\overline{H}_m,D_s) = \tilde{V}_s$

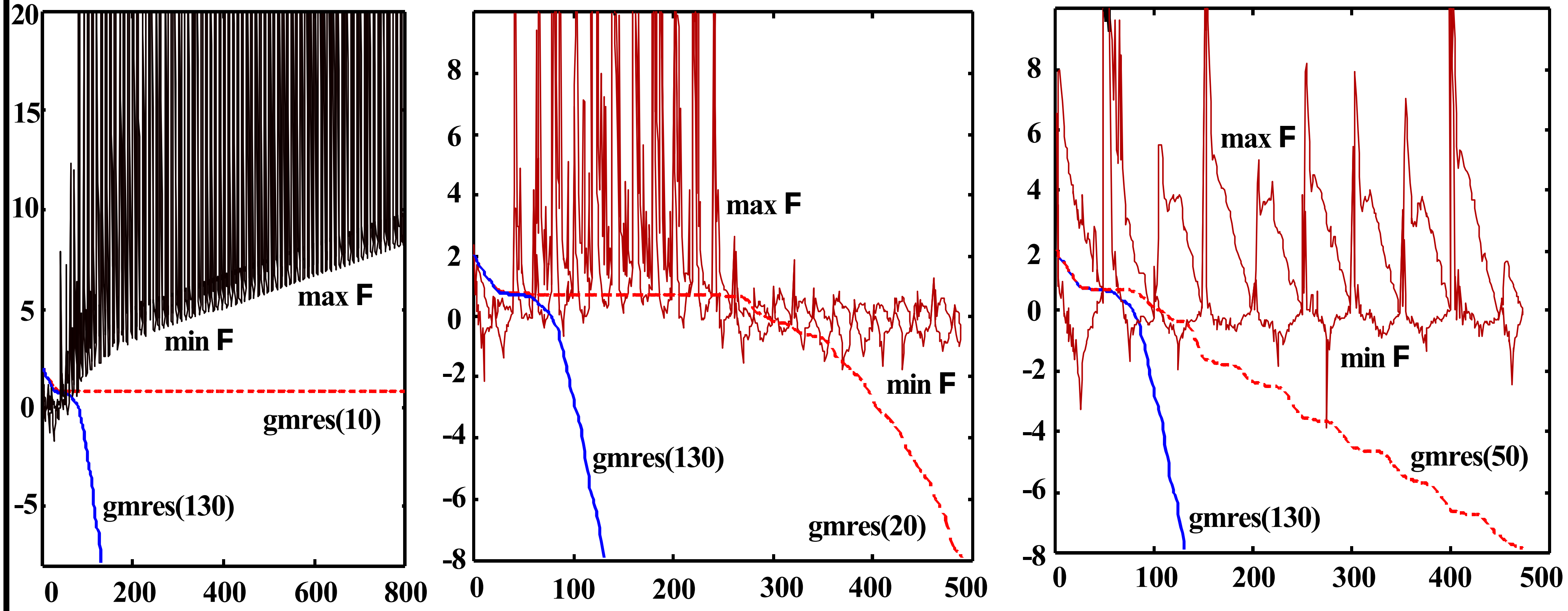
Q_s : orthogonal complement of C_s in *range*(AW_m)

$[C_s|Q_s] = W_{m+1}\overline{Q}_m$

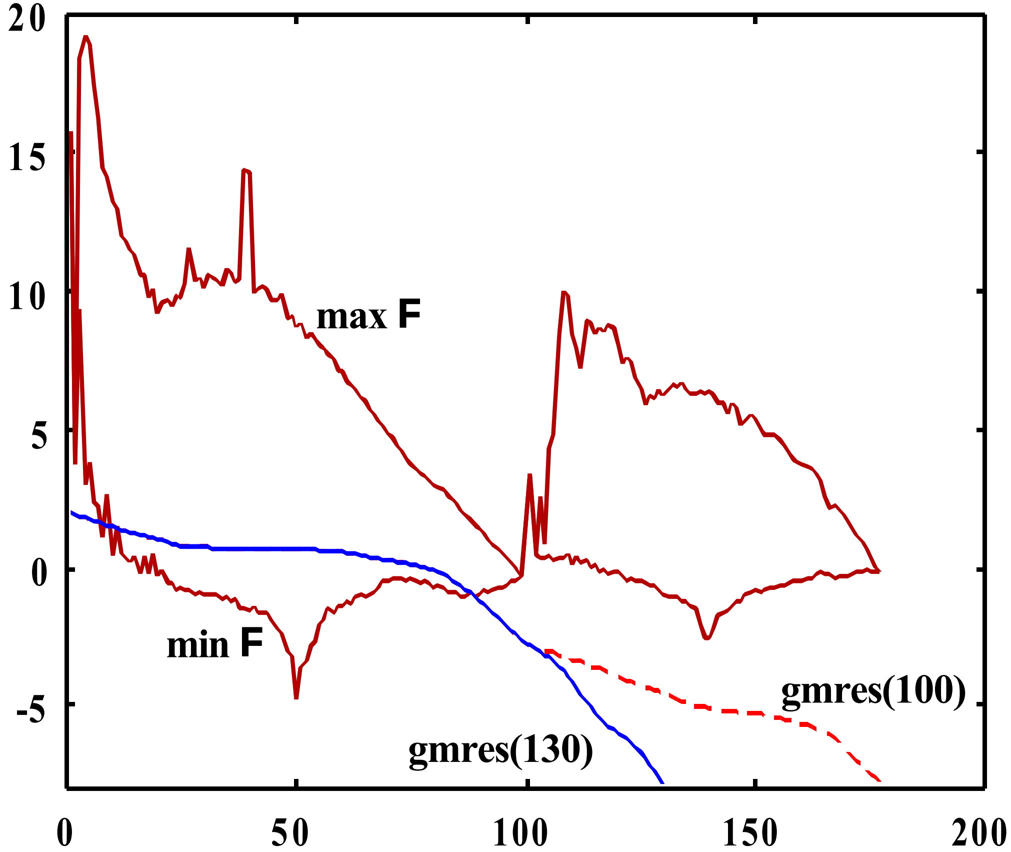
$\overline{Q}_m^H\tilde{V}_s = \left(\begin{array}{c} B_s \\ \hline R_s \end{array}\right)$! Z_s

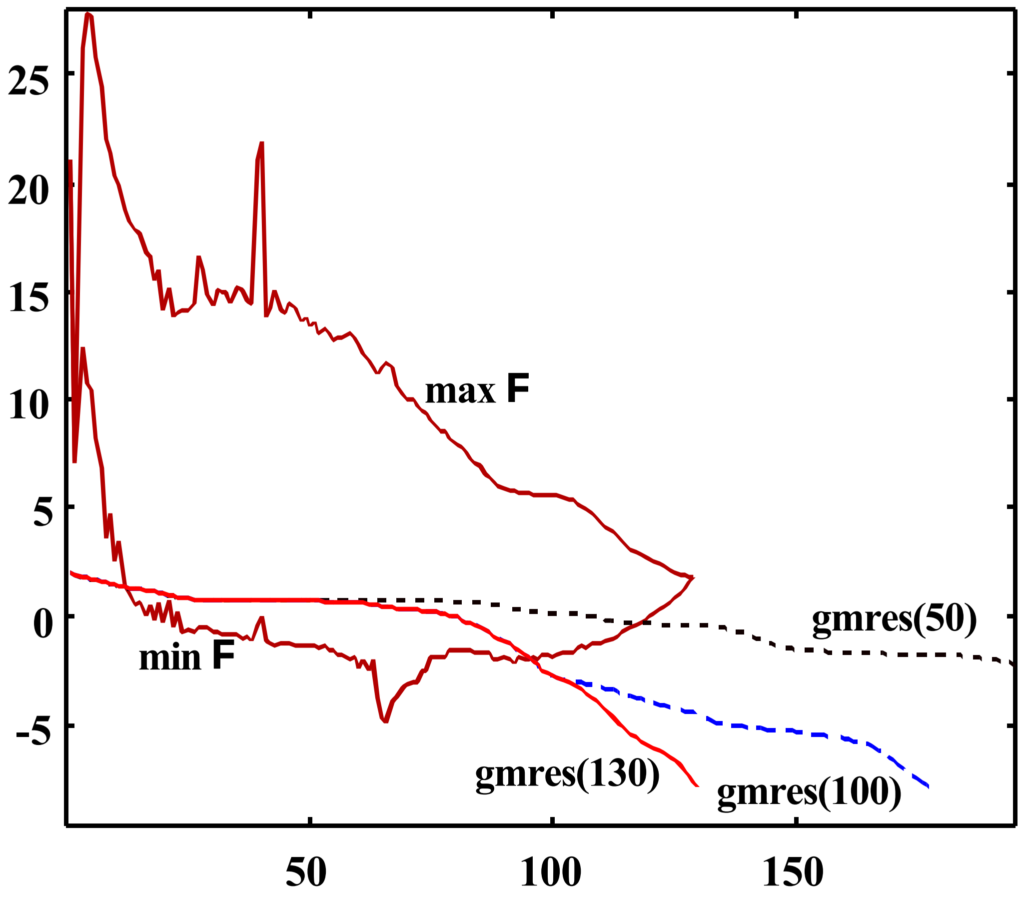
1. difference between optimal residual r_m and residual after restart
2. important vectors for setting V 'orthogonal' to C (useful to keep)

(GMRES(m) analysis & selecting a subspace)



(GMRES(m) analysis & selecting a subspace)





GCRO with Optimal Truncation

Outer method: U_k, C_k such that

$$AU_k = C_k \qquad C_k^H C_k = I_k \qquad \text{(cf. GCR)}$$
$$r_k = (I - C_k C_k^H) b \qquad x_k = U_k C_k^H b$$

Inner GMRES (optimal solution over range(U_k) r range(V_m)):

$$AV_m = C_k B_m + V_{m+1} H_m \qquad \text{where } B_m = C_k^H AV_m$$
$$(I - C_k C_k^H) AV_m = V_{m+1} H_m$$

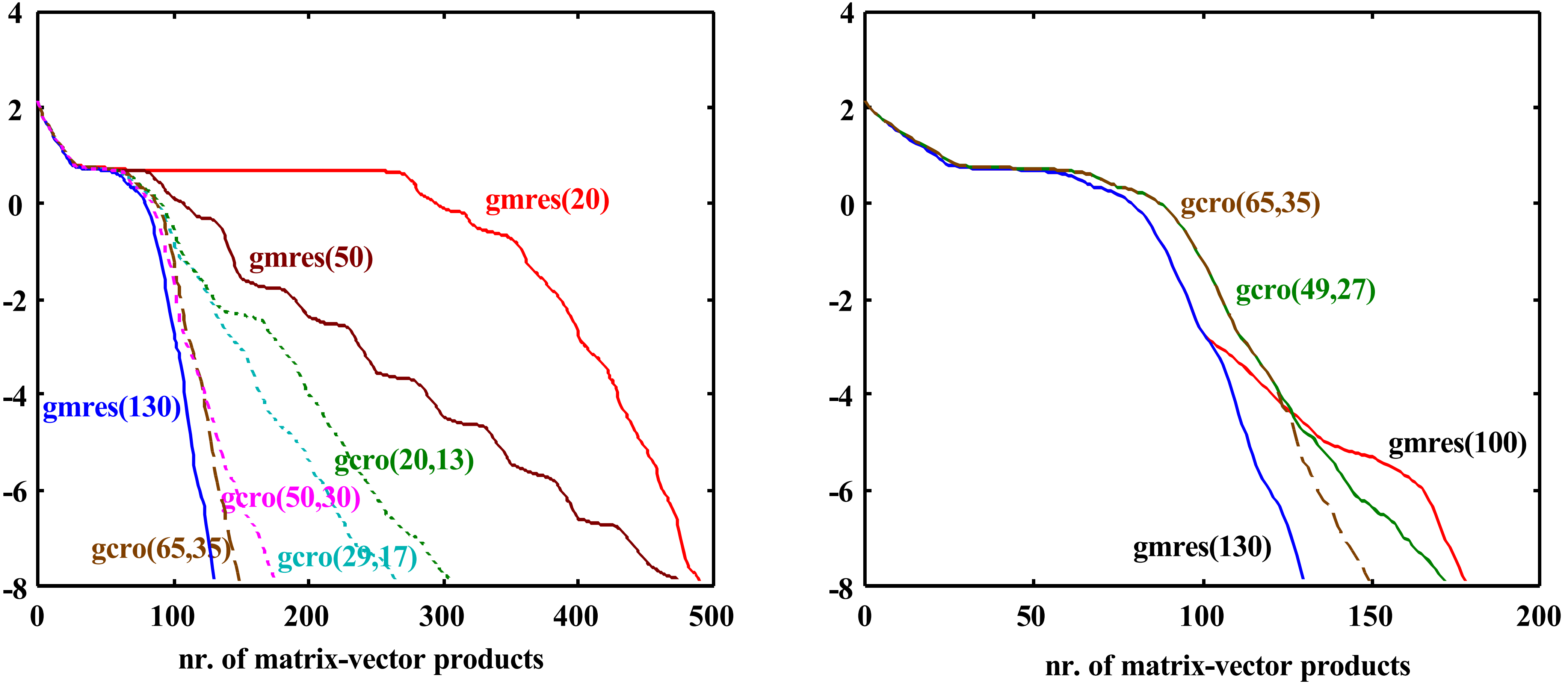
$$y = \text{arg min } {**}r_k - V_{m+1} H_m y{**}$$

$$r_{k+1} = r_k - V_{m+1} H_m y$$

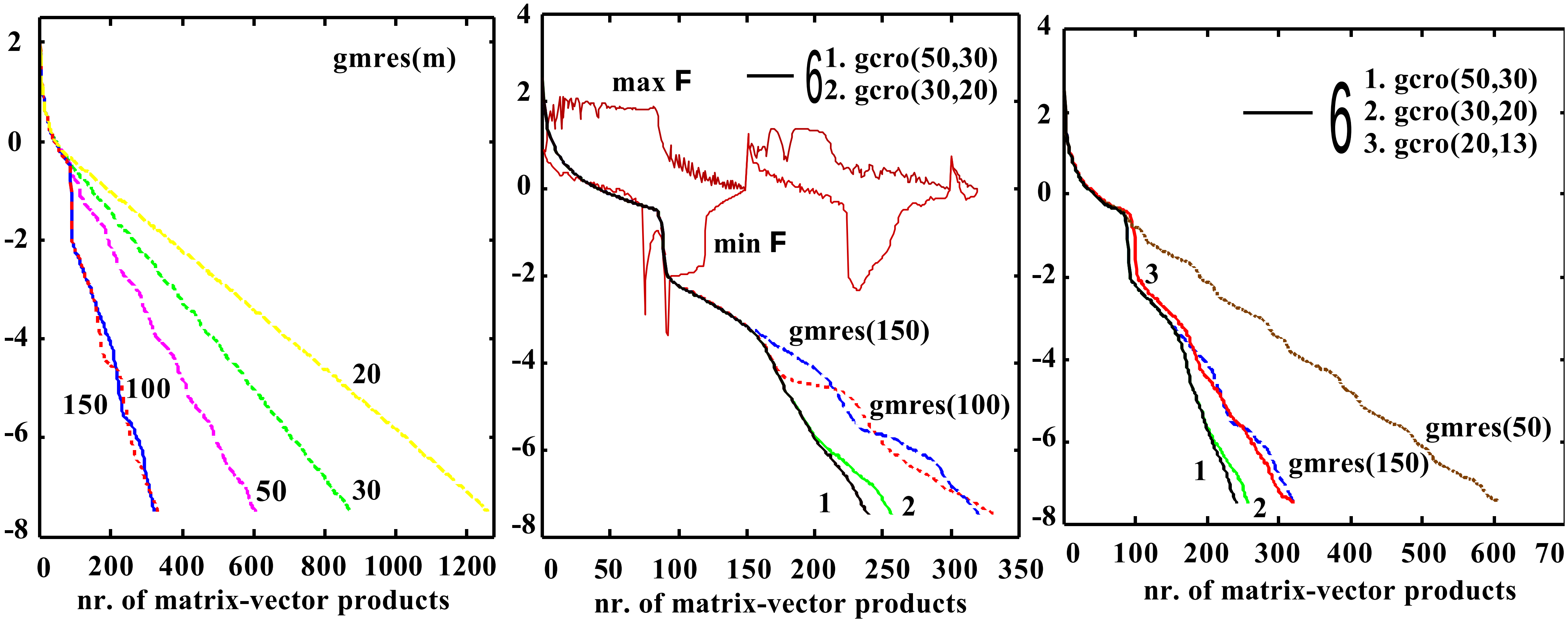
$$c_{k+1} = V_{m+1} H_m y \qquad = (I - C_k C_k^H) AV_m y$$

$$u_{k+1} = A^{-1} V_{m+1} H_m \qquad = A^{-1} (I - C_k C_k^H) AV_m y \qquad = V_m y - U_k C_k^H AV_m y$$

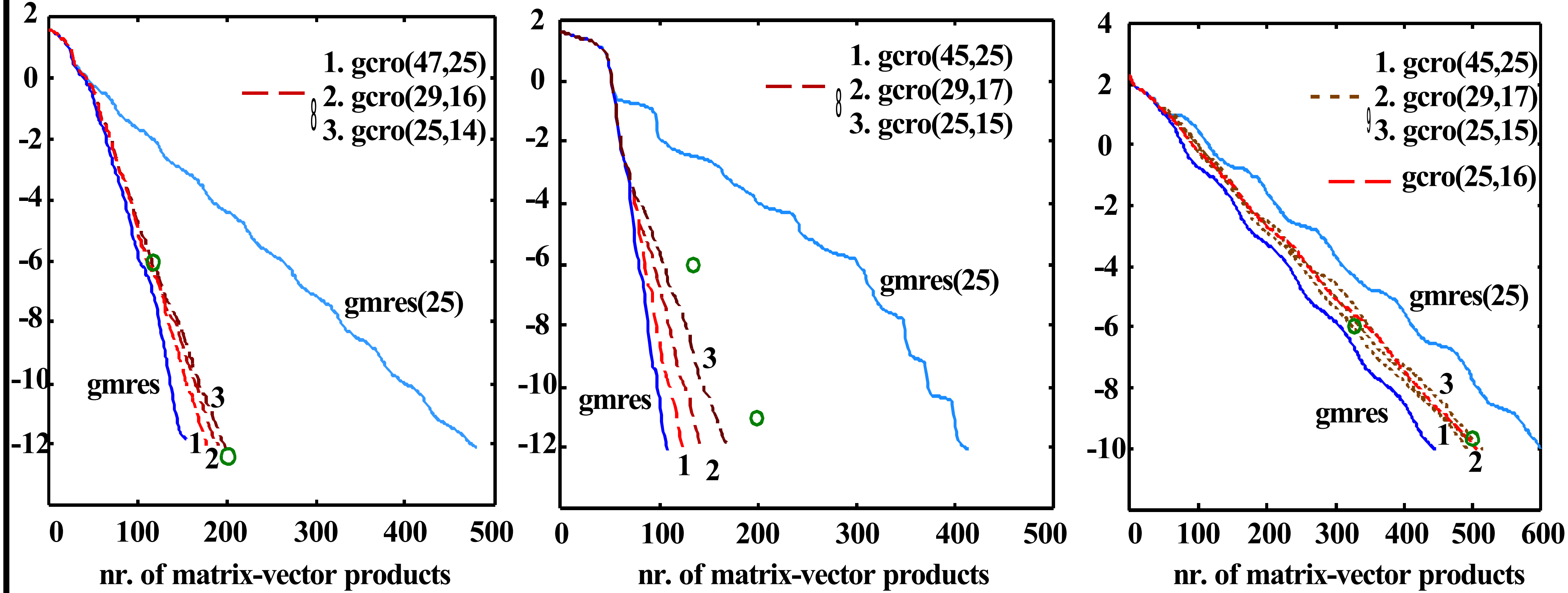
(GCRO with optimal truncation)



(GCRO with optimal truncation)



(GCRO with optimal truncation)

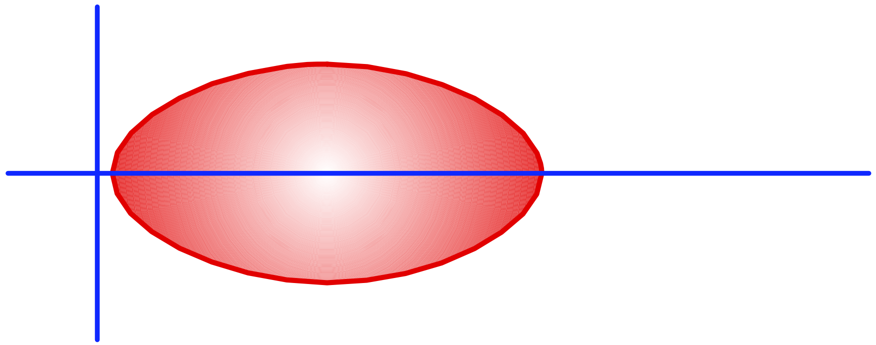


Conclusions and Future Work

- Almost optimal convergence with very small number of vectors
- Minimizing over selected subspaces of very small dimension works better than GMRES(m) with large m
- Methods seems to select right subspaces to keep
- Initial tests indicate comparable or better than Morgan's Augm. GMRES
- Method insensitive to small changes in parameters, and gradual improvement for increase in number of vectors
- Theoretical implications / Analysis
- More flexible and adaptive algorithm; theory / heuristics

Lattice QCD

- 4D Space-time lattice, particles move in 4 directions and change color (3 colors)
- Matrix looks like a 4D Laplacian where each off-diagonal element is replaced by 12x12 (random) unitary matrix (complex).
- These unitary matrices are different for each off-diagonal element: no smoothness.
- A = (I-kM), with parameter k; most interesting case when A almost singular.
- Eigenvalues of M uniformly distributed in (known) ellipse (depending on other parm).
- We need to solve for multiples of 12 right hand sides (sometimes consecutive).

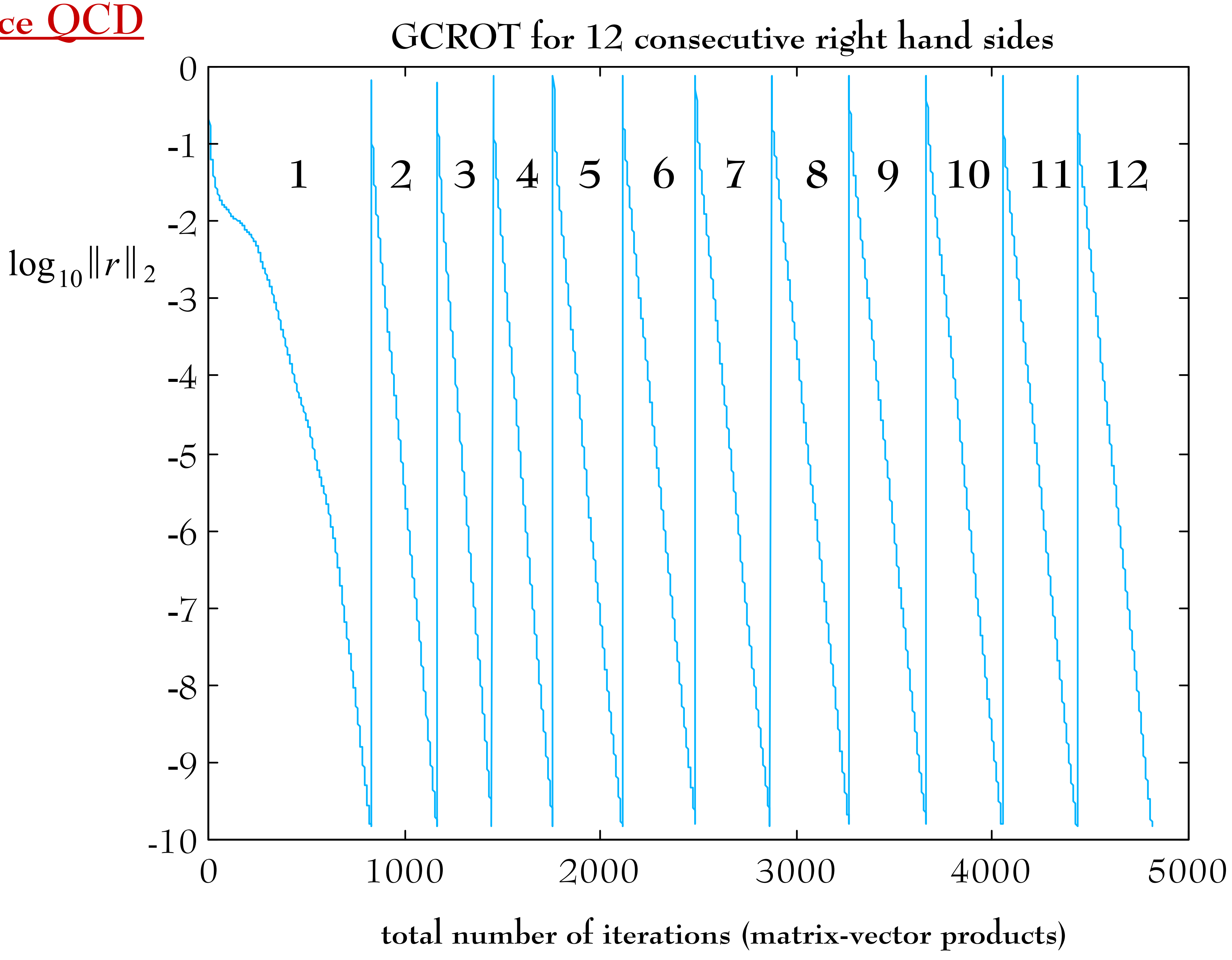


Use U and C matrices (approx. inverse) from previous iteration(s) to speed up convergence.
To solve $Ax^{(k)}=b^{(k)}$ we set

$x_0=UC^*b$ and $r_0=(I-CC^*)b$

Iterate with method described (continuing truncation).

Lattice QCD



GCROT for 12 consecutive right hand sides
$\log_{10}\|r\|_2$
0
-1
-2
-3
-4
-5
-6
-7
-8
-9
-10
1
2
3
4
5
6
7
8
9
10
11
12
0
1000
2000
3000
4000
5000
total number of iterations (matrix-vector products)

Jacobi-Davidson

Given V_k ; $V_k^*V_k = I_k$;$W_k=AV_k$; $H_k=V_k^*W_k$ **6** eigenpair (q_k,s_k) **6**

Ritz pair (q_k,u_k), $u_k=V_ks_k$: $r_k=Au_k-q_ku_k = (A - q_kI)u_k$

Extend the search space and compute better approximate eigenpair

Solve: $(I-u_ku_k^*)(A - q_kI)(I-u_ku_k^*)t=-r$, t **z** u_k

$t = (I-V_kV_k^*)t/2(I-V_kV_k^*)t2$; $V_{k+1}=[V_k|t]$; $W_{k+1}=[W_k|At]$; $H_{k+1}=V_{k+1}^*W_{k+1}$

- Condition number of $(I-u_ku_k^*)(A - q_kI)(I-u_ku_k^*)$?
- Angle **p**(t,*range*(V_kS_c))? Extension of space *range*(V_k)?
- Repeatedly solving 'almost' same system (change (q_k,u_k))
- Efficiency/Stability

Jacobi-Davidson