Minimizing convex quadratics with variable precision Krylov methods

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The (simple?) problem

We consider the unconstrained quadratic optimization (QO) problem:

$$\text{minimize} \quad q(x) = \tfrac{1}{2}x^T A x - b^T x$$

for $x, b \in \mathbb{R}^n$ and A an $n \times n$ symmetric positive-definite matrix.

A truly "core" problem in optimization (and linear algebra)

- the simplest nonlinear optimization problem
- subproblem in many methods for general nonlinear unconstrained optimization
- central in linear algebra (including solving elliptic PDEs)

Working assumptions

For what follows, we assume that

- the problem size n is large enough and A is dense enough to make factorization of A unavailable
- a Krylov iterative method (Conjugate Gradients, FOM) is used
- the cost of running this iterative method is dominated by the products Av

Focus on an optimization point of view: look at decrease in q rather than at decrease in the associated system's residual

ex: ensuring sufficient decrease in trust-region methods

Our aim, for x_* solution of QO,

$$\boxed{\text{Find } x_k \text{ such that } |q(x_k) - q(x_*)| \leq \epsilon |q(x_0) - q(x_*)|.}$$

A first motivating example: weather forecasting (1)

The $\boxed{\text{weakly-constrained 4D-Var}}$ formulation:

$$\min_{x \in \mathbb{R}^n} \frac{1}{2}\|x_0 - x_b\|^2_{B^{-1}} + \frac{1}{2}\sum_{j=0}^{N} \|\mathcal{H}_j(x_j) - y_j\|^2_{R_j^{-1}} + \frac{1}{2}\sum_{j=1}^{N} \|\underbrace{x_j - \mathcal{M}_j(x_{j-1})}_{q_j}\|^2_{Q_j^{-1}}$$

- $x = (x_0, \ldots, x_N)^T$ is the state control variable (with $x_j = x(t_j)$)
- x_b is the background given at the initial time (t_0).
- $y_j \in \mathbb{R}^{m_j}$ is the observation vector over a given time interval
- $\mathcal{H}_j$ maps the state vector x_j from model space to observation space
- $\mathcal{M}_j$ is an integration of the numerical model from time t_{j-1} to t_j
- B, R_j and Q_j are the covariance matrices of background, observation and model error. B and Q_j impractical to "invert"

A first motivating example: weather forecasting (2)

Solve by a Gauss-Newton method whose subproblem (at iteration k) is

$$\min_{\delta x} \frac{1}{2}\|\delta x_0 - b^{(k)}\|^2_{\mathbf{B}^{-1}} + \frac{1}{2}\sum_{j=0}^{N}\left\|H_j^{(k)}\delta x_j - d_j^{(k)}\right\|^2_{\mathbf{R}_j^{-1}} + \frac{1}{2}\sum_{j=1}^{N}\|\underbrace{\delta x_j - M_j^{(k)}\delta x_{j-1}}_{\delta q_j} - c_j^{(k)}\|^2_{\mathbf{Q}_j^{-1}}$$

- δx is the increment in x.
- The vectors $b^{(k)}$, $c_j^{(k)}$ and $d_j^{(k)}$ are defined by

$$b^{(k)} = x_b - {x_0}^{(k)}, \quad c_j^{(k)} = q_j^{(k)}, \quad d_j^{(k)} = \mathcal{H}_j({x_j}^{(k)}) - y_j$$

and are calculated at the outer loop.

A first motivating example: weather forecasting (3)

Can be rewritten as

$$\min_{\delta x} \; q_{\rm st} = \frac{1}{2}\|L\delta x - b\|^2_{D^{-1}} + \frac{1}{2}\|H\delta x - d\|^2_{R^{-1}}$$

where

- $L = \begin{pmatrix} I & & & & \\ -M_1 & I & & & \\ & -M_2 & I & & \\ & & \ddots & \ddots & \\ & & & -M_N & I \end{pmatrix}$
- $d = (d_0, d_1, \dots, d_N)^T$ and $b = (b, c_1, \dots, c_N)^T$
- $H = \mathrm{diag}(H_0, H_1, \dots, H_N)$
- $D = \mathrm{diag}(B, Q_1, \dots, Q_N)$ and $R = \mathrm{diag}(R_0, R_1, \dots, R_N)$

A first motivating example: weather forecasting (3)

$$\min_{\delta x} \; q_{\rm st} = \frac{1}{2}\|L\delta x - b\|^2_{D^{-1}} + \frac{1}{2}\|H\delta x - d\|^2_{R^{-1}}$$

This is a standard QO, but **HUGE!** Note that

$$\nabla^2 q_{\rm st} = L^T D^{-1} L + H^T R^{-1} H$$

In addition $\boxed{D^{-1} = \mathrm{diag}(B^{-1}, Q_1^{-1}, \ldots, Q_N^{-1}) \text{ is unavailable!}}$

Thus $\nabla^2 q_{st} v$ (a Hessian times vector product) must be computed by

- $w = Lv$,
- solve $Dz = w$ using some (preconditioned) Krylov method
- $v = L^T z + H^T R^{-1} H v$

A second motivating example: variable precision arithmetic

Next barrier in hyper computing: energy dissipation!

Heat production is proportional to chip surface, hence

$$\text{energy output} \;\approx \left(\;\text{number of digits used}\;\right)^2$$

Architectural trend: use multiprecision arithmetic

- graphical processing units (GPUs)
- hierarchy of specialized CPUs (double, single, half, ...)

How to use this hierarchy optimally for fully accurate results?

Inaccuracy frameworks

Our proposal;

> Make the Krylov methods for QO more efficient by allowing error on the matrix-vector product (the dominant computation)

Two frameworks of interest:

- Continuous accuracy levels
  ex: WC-4D-VAR, where accuracy in the inversion $Dz = w$ can be continuously chosen
- Discrete accuracy levels
  ex: double-single-half precision arithmetic

Considered here:

> - Full orthonormalisation method (FOM)
> - Conjugate Gradients (CG)

with (wlog) $x_0 = 0$ and $q(x_0) = 0$.

A central equality

Define $r(x) \stackrel{\rm def}{=} Ax - b = \nabla q(x)$ and $Ax_* = b$.

$$\boxed{q(x) - q(x_*) = \tfrac{1}{2}\|r(x)\|^2_{A^{-1}}}$$

$$\begin{aligned}
\tfrac{1}{2}\|r(x)\|^2_{A^{-1}} &= \tfrac{1}{2}(Ax-b)^T A^{-1}(Ax-b) \\
&= \tfrac{1}{2}(x-x_*)^T A(x-x_*) \\
&= \tfrac{1}{2}(x^T Ax - 2x^T Ax_* + x_*^T Ax_*) \\
&= q(x) - q(x_*)
\end{aligned}$$

Hence

Decrease in q can be monitored by considering the A^{-1} norm of its gradient

The primal-dual norm

$\Rightarrow$ natural to consider the inaccuracy on the product Av by measuring the backward error

$$\|E\|_{A^{-1},A} \stackrel{\text{def}}{=} \sup_{x\neq 0} \frac{\|Ex\|_{A^{-1}}}{\|x\|_A} = \|A^{-1/2}EA^{-1/2}\|_2$$

(primal-dual norm)

Let A be a symmetric and positive definite matrix and E be any symmetric perturbation. Then, if $\|E\|_{A^{-1},A} < 1$, the matrix $A + E$ is symmetric positive definite.

The main idea

Krylov methods reduce the (internally recurred) residual r_k on successive nested Krylov spaces

$\Rightarrow$ can expect r_k to converge to zero

$\Rightarrow$ keep $r(x_k) - r_k$ small in the appropriate norm

For FOM and CG, if

$$\max\left[\|r_k - r(x_k)\|_{A^{-1}}, \|r_k\|_{A^{-1}}\right] \leq \frac{\sqrt{\epsilon}}{2}\|b\|_{A^{-1}}$$

then

$$|q(x_k) - q(x_*)| \leq \epsilon |q(x_*)|$$

The inexact FOM algorithm

Theoretical inexact FOM algorithm

1. Set $\beta = \|b\|_2$, and $v_1 = [b/\beta]$,
2. For k=1, 2, . . . , do
3. $\quad w_k = (A + E_k) v_k$
4. $\quad$ For $i = 1, \ldots, k$ do
5. $\quad\quad h_{i,k} = v_i^T w_k$
6. $\quad\quad w_k = w_k - h_{i,k} v_i$
7. $\quad$ EndFor
8. $\quad h_{k+1,k} = \|w_k\|_2$
9. $\quad y_k = H_k^{-1}(\beta e_1)$
10. $\quad$ if $|h_{k+1,k} e_k^T y_k|$ is small enough then go to 13
11. $\quad v_{k+1} = w_k / h_{k+1,k}$
12. EndFor
13. $x_k = V_k y_k$

Results for the inexact FOM

Let $\epsilon_\pi > 0$ and let $\phi \in \mathbb{R}^k_+$ such that $\sum_{j=1}^k \phi_j^{-1} \leq 1$. Suppose also that, for all $j \in \{1, \ldots, k\}$,

$$\|E_j\|_{A^{-1},A} \leq \omega_j^{\rm FOM} \stackrel{\rm def}{=} \min\left[1, \frac{\epsilon_\pi \, \|b\|_{A^{-1}}}{\phi_j \|v_j\|_A \|H_k^{-1}\|_2 \|r_{j-1}\|_2}\right] \quad (2.1)$$

Then

$$\|r(x_k) - r_k\|_{A^{-1}} \leq \epsilon_\pi \, \|b\|_{A^{-1}}.$$

Let $\epsilon > 0$ and suppose that, at iteration $k > 0$ of the FOM algorithm,

$$\|r_k\|_{A^{-1}} \leq \tfrac{1}{2}\sqrt{\epsilon}\, \|b\|_{A^{-1}}$$

and the product error matrices E_j satisfy (2.1) with $\epsilon_\pi = \frac{1}{2}\sqrt{\epsilon}$ for some $\phi \in \mathbb{R}^k$ (as above). Then

$$|q(x_k) - q(x_*)| \leq \epsilon |q(x_*)|$$

The inexact Conjugate Gradients algorithm

Theoretical inexact CG algorithm

1. Set $x_0 = 0$, $\beta_0 = \|b\|_2^2$, $r_0 = -b$ and $p_0 = r_0$
2. For k=0, 1, . . . , do
3. $\quad c_k = (A + E_k)p_k$
4. $\quad \alpha_k = \beta_k / p_k^T c_k$
5. $\quad x_{k+1} = x_k + \alpha_k p_k$
6. $\quad r_{k+1} = r_k + \alpha_k c_k$
7. $\quad$ if r_{k+1} is small enough then stop
8. $\quad \beta_{k+1} = r_{k+1}^T r_{k+1}$
9. $\quad p_{k+1} = -r_{k+1} + (\beta_{k+1}/\beta_k) p_k$
10. EndFor

Results for the inexact CG

Let $\epsilon_\pi > 0$ and let $\phi \in \mathbb{R}^k_+$ such that $\sum_{j=1}^k \phi_j^{-1} \leq 1$. Suppose also that, for all $j \in \{0, \dots, k-1\}$,

$$\|E_j\|_{A^{-1},A} \leq \omega_j^{\text{CG}} \stackrel{\text{def}}{=} \frac{\epsilon_\pi \, \|b\|_{A^{-1}} \|p_j\|_A}{\phi_{j+1}\|r_j\|_2^2 + \epsilon_\pi \, \|b\|_{A^{-1}} \|p_j\|_A} \tag{2.2}$$

Then

$$\|r(x_k) - r_k\|_{A^{-1}} \leq \epsilon_\pi \, \|b\|_{A^{-1}}.$$

Let $\epsilon > 0$ and suppose that, at iteration $k > 0$ of the CG algorithm,

$$\|r_k\|_{A^{-1}} \leq \tfrac{1}{2}\sqrt{\epsilon} \, \|b\|_{A^{-1}}$$

and the product error matrices E_j satisfy (2.2) with $\epsilon_\pi = \frac{1}{2}\sqrt{\epsilon}$ for some $\phi \in \mathbb{R}^k$ (as above). Then

$$|q(x_k) - q(x_*)| \leq \epsilon |q(x_*)|$$

Achieved vs optimal decrease

Let q be the value of the quadratic recurred internally by FOM or CG.

Let x be the result of applying the FOM or CG algorithm with inexact products and suppose that the above error bounds hold with $\epsilon_\pi = \frac{1}{2}\sqrt{\epsilon}$. Then

$$\frac{|q(x) - q|}{|q(x_*)|} \leq \sqrt{\epsilon}(1 + \sqrt{\epsilon}).$$

Can one trust the internally computed decrease? Rather pessismistic!

Managing the inaccuracy budget

Assume $k_{\max}$, an estimate of the maximum number of iterations, is known.

At iteration j of FOM/CG:

$$\left.\begin{matrix} v_j \\ r_{j-1} \\ \phi_j \end{matrix}\right\} \rightarrow \left.\begin{matrix} v_j \\ \omega_j \end{matrix}\right\} \rightarrow \boxed{\begin{matrix}\text{product} \\ \text{routine}\end{matrix}} \rightarrow \begin{matrix} \boxed{(A+E_j)v_j} \\ \|E_j\|_{A^{-1},A} \end{matrix} \rightarrow \hat{\phi}_j \rightarrow \phi_{j+1}$$

where

$$\hat{\phi}_j^{\rm FOM} = \frac{\epsilon_\pi \, \|b\|_{A^{-1}}}{\|E_j\|_{A^{-1},A}\|v_j\|_A\|H_k^{-1}\|_2\|r_{j-1}\|_2}$$

$$\hat{\phi}_j^{\rm CG} = \frac{(1-\|E_j\|_{A^{-1},A})\,\epsilon_\pi \, \|b\|_{A^{-1}}\|p_j\|_A}{\|E_j\|_{A^{-1},A}\|r_j\|_2^2}$$

and $\quad \phi_{j+1} = \dfrac{k_{\max} - j}{1-\sum_{p=1}^{j} \hat{\phi}_p^{-1}}$

So what?

- The primal-dual norm $\|E_j\|_{A^{-1},A}$ is sometimes difficult to evaluate
- The error bounds remain unfortunately impractical (they involve $\|b\|_{A^{-1}}$, $\|v_j\|_A$ or $\|p_j\|_A$, which cannot be computed readily in the course of the FOM or CG algorithm).
- The termination test $\|r_k\|_{A^{-1}} \leq \frac{1}{2}\sqrt{\epsilon}\,\|b\|_{A^{-1}}$ also involves the unavailable $\|r_k\|_{A^{-1}}$

Give up? Not quite...

- the FOM error bound allows a growth of the error in $\|r_j\|^{-1}$ while (2.2) allows a growth of the order of $\|r_j\|^{-2}\|p_j\|_A$ instead.
- The ϕ_j may be viewed as an error management strategy. A simple choice is to define $\phi_j = n$ for all j but there may be better options (discussed later).

Using the true (unavailable) quantities (1)

Would this work at all if using the true $\|b\|_{A^{-1}}$, $\|v_j\|_A$ and $\|p_j\|_A$?

Consider 6 algorithms:

- FOM: the standard full-accuracy FOM
- iFOM: the inexact FOM (with exact bounds, for now)
- CG: the standard full-accuracy CG
- CGR: the full-accuracy CG *with reorthogonalization*
- iCG: the inexact CG (with exact bounds, for now)
- iCGR: the inexact CGR (with exact bounds, for now)

Continuous accuracy levels (1)

Comparing equivalent numbers of full accuracy products:

- Assume obtaining full accuracy is a linearly convergent process of rate ρ
  (realistic for our weather prediction data assimilation example)
- Cost of an ϵ-accurate solution:

$$\frac{\log(\epsilon)}{\log(\rho)}$$

- Cost of an ω-accurate solution

$$\frac{\log(\omega)}{\log(\rho)}$$

$\Rightarrow$ sum these values during computing and compare them.

Continuous accuracy levels (2)

Compare on:

- synthetic matrices of size 1000×1000 with varying conditioning (from 10^1 to 10^8) and log-linearly spaced eigenvalues
- "real" matrices from the NIST Matrix Market (paper only)
- use different levels of final accuracy ($\epsilon = 10^{-3},\ 10^{-5},\ 10^{-7}$)

Note that

> Continuous accuracy levels $\Rightarrow$ no room for inaccuracy budget management!

Continuous accuracy levels (3)

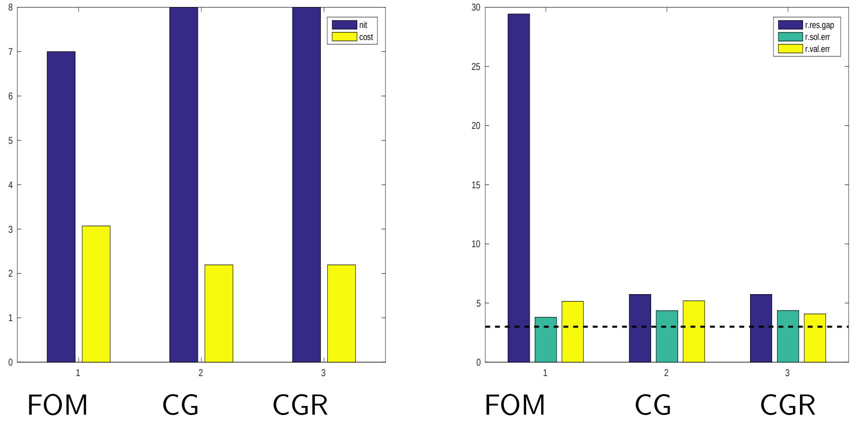


Figure: Exact bounds, $\kappa(A) = 10^1$, $\epsilon = 10^{-3}$ (continuous case)

Continuous accuracy levels (4)

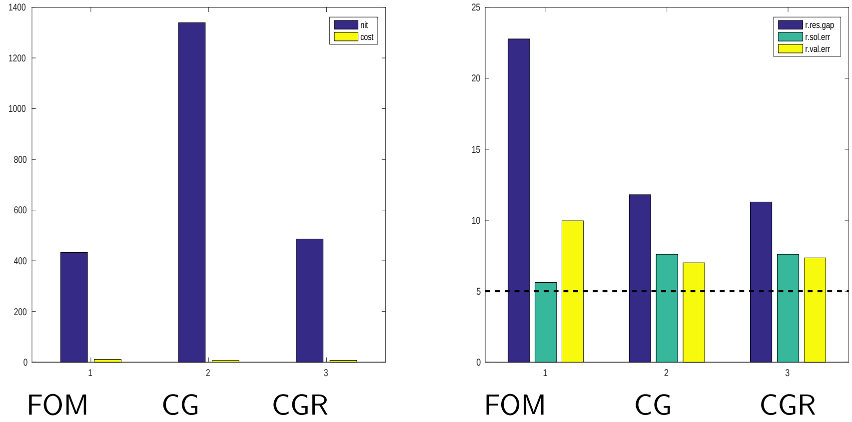


Figure: Exact bounds, $\kappa(A) = 10^5$, $\epsilon = 10^{-5}$ (continuous case)

Continuous accuracy levels (5)

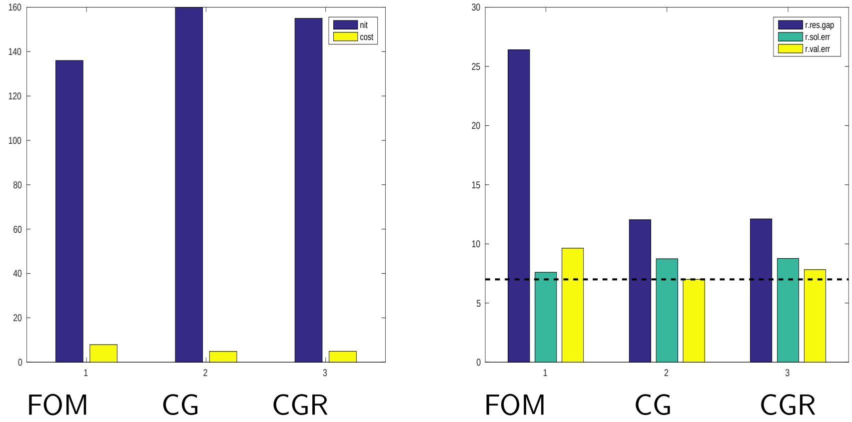


Figure: Exact bounds, $\kappa(A) = 10^3$, $\epsilon = 10^{-7}$ (continuous case)

Discontinuous accuracy levels (1)

Focus on $\boxed{\text{multiprecision arithmetic}}$. Assume

- 3 levels of accuracy (double, single, half)
- a ratio of 4 in efficiency when moving from one level to the next

Use the sames matrices and final accuracies as above.

Apply the inaccuracy budget management!

Discontinuous accuracy levels (2)

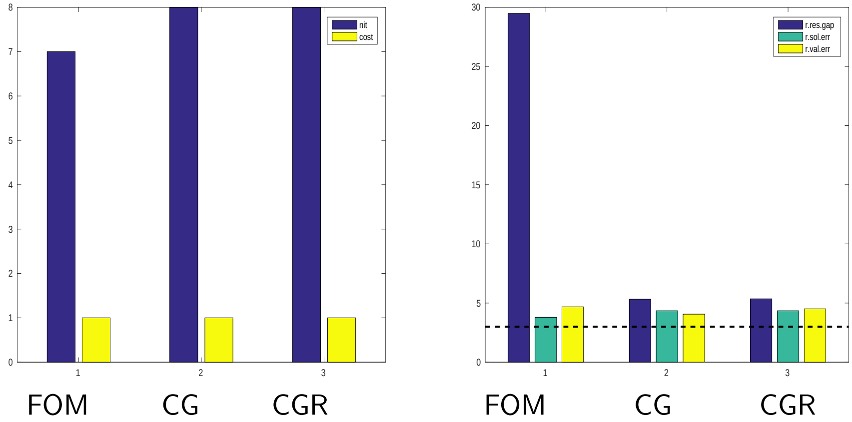
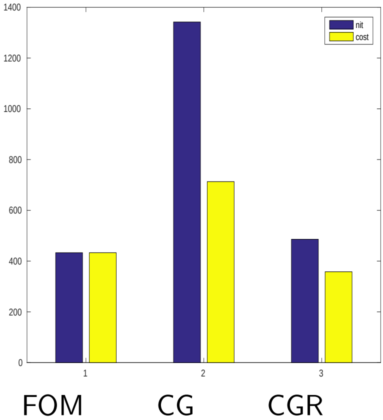


Figure: Exact bounds, $\kappa(A) = 10^1$, $\epsilon = 10^{-3}$ (continuous case)

Discontinuous accuracy levels (3)



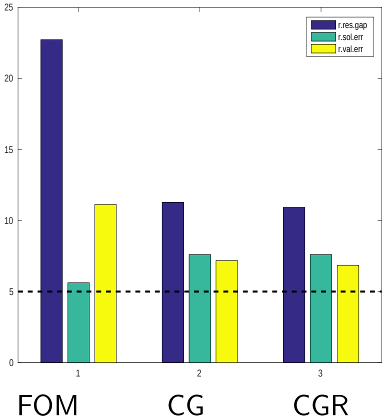
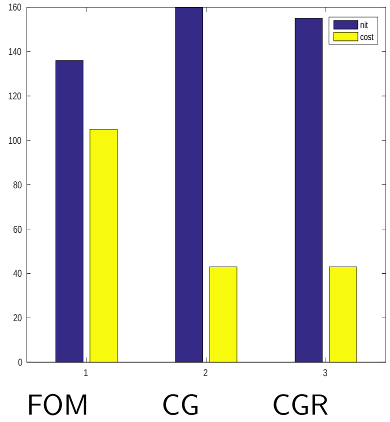


Figure: Exact bounds, $\kappa(A) = 10^5$, $\epsilon = 10^{-5}$ (continuous case)

Discontinuous accuracy levels (4)



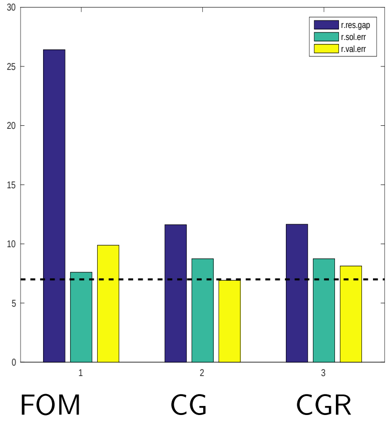


Figure: Exact bounds, $\kappa(A) = 10^3$, $\epsilon = 10^{-7}$ (continuous case)

Adhoc approximations

Abandon theoretical but unavailable quantities $\rightarrow$ approximate them:

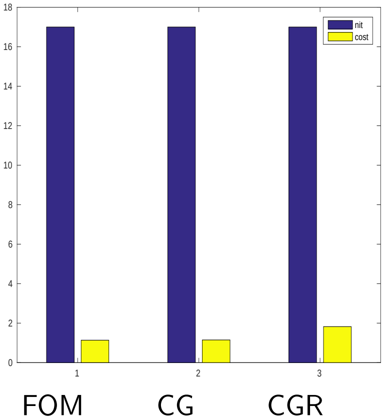
- $\|E\|_{A^{-1},A} \geq \lambda_{\min}(A)^{-1}\|E\|_2$
- $\|p\|_A \approx \frac{1}{n}\mathrm{Tr}(A)\|p\|_2$
  (ok for p with random independent components)
- $\|b\|_{A^{-1}} = |q(x_*)| \approx q_k \approx \frac{1}{2}|b^T x_k|$
- $\|H_k^{-1}\| = \frac{1}{\lambda_{\min}(H_k)} \leq \frac{1}{\lambda_{\min}(A)}$ (FOM only)
- $k_{\max} \approx \frac{\log(\epsilon)}{\log(\rho)}$ with $\rho \stackrel{\text{def}}{=} \frac{\sqrt{\lambda_{\max}/\lambda_{\min}}-1}{\sqrt{\lambda_{\max}/\lambda_{\min}}+1}$

Termination test (Arioli & Gratton):

$$q_{k-d} - q_k \leq \tfrac{1}{4}\epsilon|q_k|$$

for some stabilization delay d (e.g. 10)

Does it still work (continuous accuracy levels, 1)?



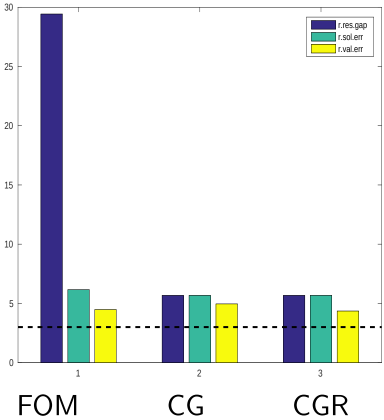


Figure: Approximate bounds, $\kappa(A) = 10^1$, $\epsilon = 10^{-3}$ (continuous case)

Does it still work (continuous accuracy levels, 2)?

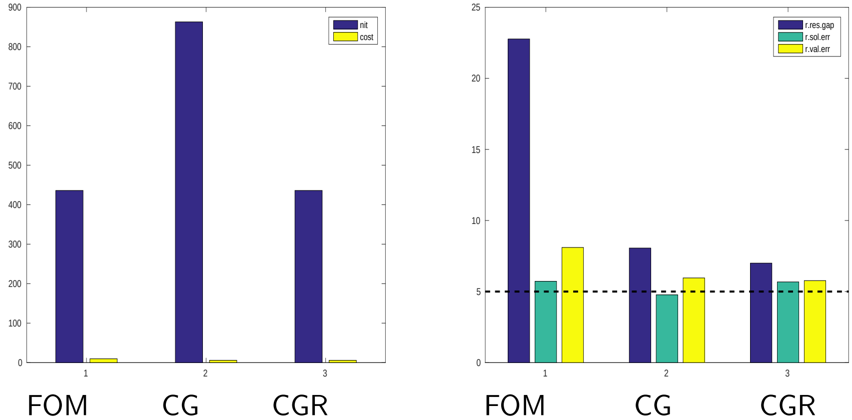


Figure: Approximate bounds, $\kappa(A) = 10^5$, $\epsilon = 10^{-5}$ (continuous case)

Does it still work (continuous accuracy levels, 3)?

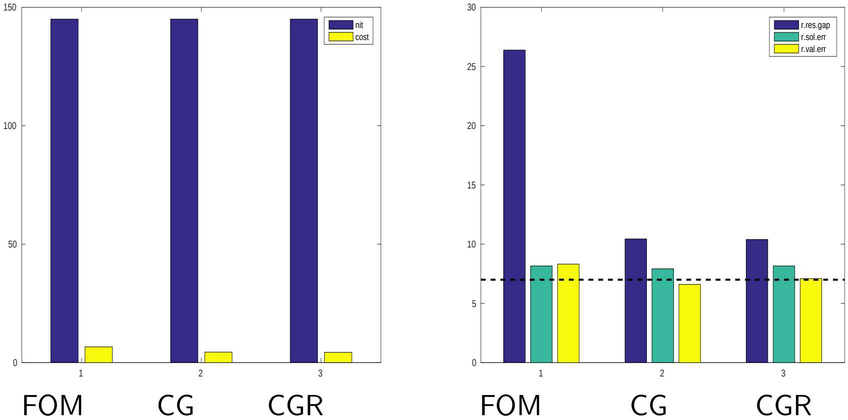


Figure: Approximate bounds, $\kappa(A) = 10^3$, $\epsilon = 10^{-7}$ (continuous case)

Does it still work (multiprecision, 1)?

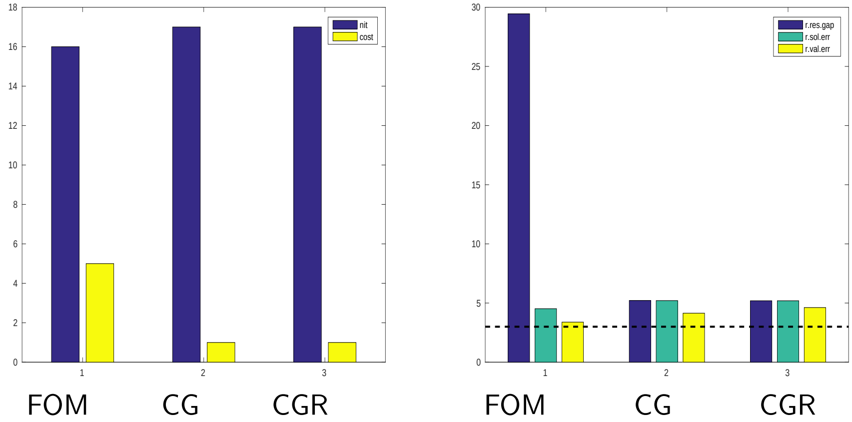
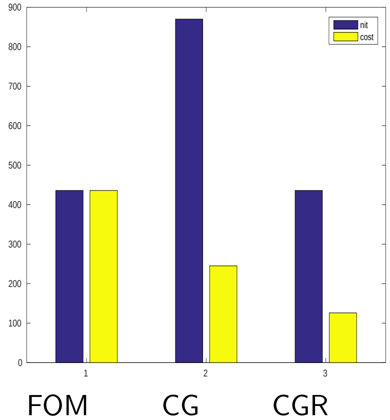


Figure: Approximate bounds, $\kappa(A) = 10^1$, $\epsilon = 10^{-3}$ (continuous case)

Does it still work (multiprecision, 2)?



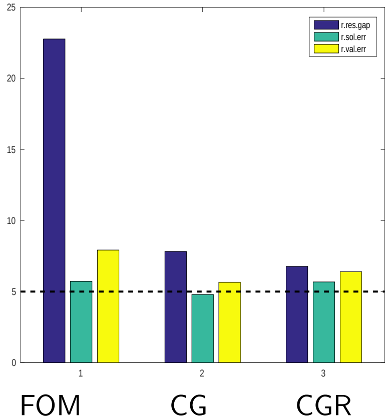


Figure: Approximate bounds, $\kappa(A) = 10^5$, $\epsilon = 10^{-5}$ (continuous case)

Does it still work (multiprecision, 3)?

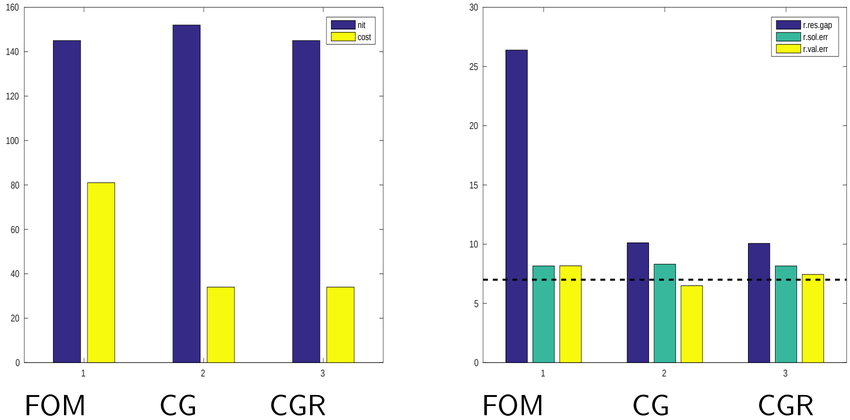


Figure: Approximate bounds, $\kappa(A) = 10^3$, $\epsilon = 10^{-7}$ (continuous case)

Conclusions and perspectives

Summary:

- Optimization-focused theory for iterative QO with inexact products
- Theoretical gains substantial
- Translates well to practice after approximations

Perspectives:

- More general (controlable) inexactness in optimization (inexactly weighted least-squares, . . .)

Thank your for your attention!

Reference

- S. Gratton, E. Simon, Ph. L. Toint,
  Minimizing convex quadratics with variable precision Krylov methods,
  arXiv:1807.07476