A proportional derivative control strategy for varying the restart parameter in GMRES(m)

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Abstract

GMRES(m) is a popular algorithm for solving large linear systems $Ax = b$ where A is a general matrix, possibly nonsymmetric. GMRES(m) consumes less computational resources than GMRES, but its convergence is not guaranteed. We propose a new proportional-derivative control-inspired law for updating the parameter m adaptively, resulting in the method PD-Gmres(m). Numerical experiments using problems from the University of Florida Matrix Collection show that PD-Gmres(m) has good convergence properties, as well as, robustness when it encounters a very slow convergence.

Introduction

Restarted GMRES, denoted as GMRES(m) was proposed by Saad and Schultz [1] to reduce GMRES high computational costs. Normally, at each cycle, the restart parameter m is set to a constant value. However, if the appropriate m is not chosen, the convergence of GMRES(m) is not guaranteed [2].

To improve GMRES(m) several authors modify m using adaptive strategies. These could be classified into three groups:

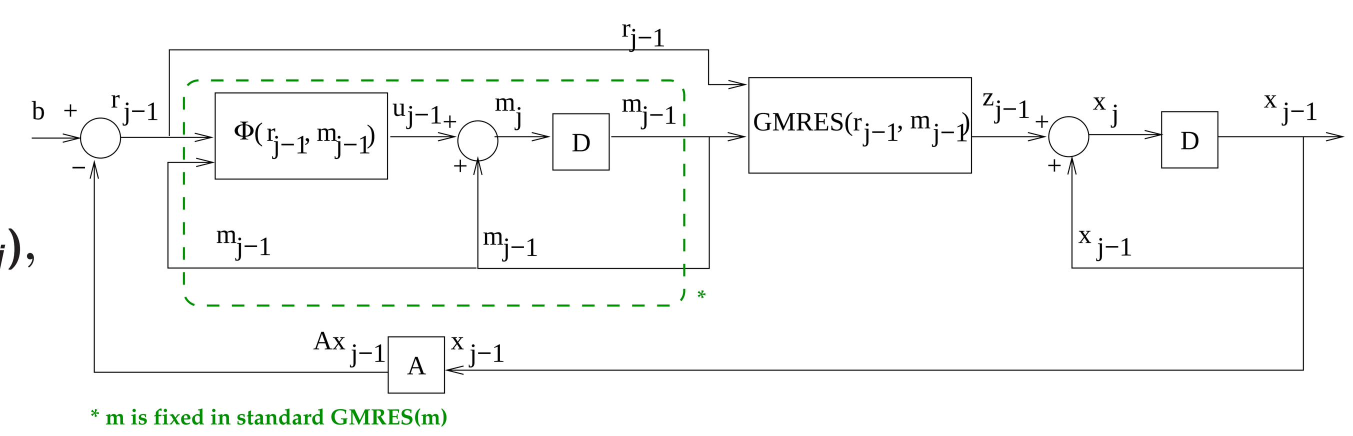
- simple rules, which however contain empirically chosen parameters that are hard to guess/estimate [3, 4];
- rules involving non-trivial calculations of eigenvalues or zeros of polynomials [5, 6]
- simple empirical rules [7, 8].

Why changing m gives good results? The answer is experimental. Baker et al. observed experimentally that GMRES(m) residual vectors may alternate directions ($r_{j+1} \approx \gamma r_{j-1}$ with $\gamma \leq 1$). Furthermore, GMRES(m) slow convergence can often be attributed to this alternating behavior [9]. Heuristically, changing m tries to avoid this, even using a random m gives better time to solution than a fixed m.

GMRES(m) and PD-GMRES(m)

Using the recurrences in GMRES(m) and a feedback law $m_j = \Phi(r_{j-1}, m_{j-1})$ yields a control model and the block diagram below.

$$\begin{cases} m_j &= \Phi(r_{j-1}, m_{j-1}) \\ z_{j-1} &= \text{GMRES}(A, r_{j-1}, m_j), \\ x_j &= x_{j-1} + z_{j-1}, \\ r_j &= b - Ax_j. \end{cases}$$



Block diagram for ***GMRES***(m)

The proposed PD-GMRES(m) updates m using a discrete PD (proportional-derivative) inspired controller. So the function $\Phi(r_{j-1}, m_{j-1})$ takes the form:

$$m_{j+1} = m_j + \alpha \frac{\|r_j\|}{\|r_{j-1}\|} + \beta \frac{\|r_j\| - \|r_{j-2}\|}{2\|r_{j-1}\|} \qquad (1)$$

where $\alpha, \beta \in \mathbb{R}$.

The advantage of (1) is that only a few additional vectors need to be stored and the controller has the capacity to increase the dimension of the Krylov subspace if any convergence problem is detected. Note that if the function $\Phi(r_{j-1}, m_{j-1})$ is a constant value, then we obtain standard GMRES(m).

In this work we consider $\cos(\angle(r_{j-1}, r_{j-2})) = \frac{\|r_{j-1}\|}{\|r_{j-2}\|}$ (see [9]) as a measure of convergence. $\cos(\angle(r_{j-1}, r_{j-2})) \approx 0$, i.e. near orthogonal residuals, means good convergence. $\cos(\angle(r_{j-1}, r_{j-2})) \approx 1$, i.e. near parallel residuals, means poor convergence.

The derivative $\frac{\|r_j\| - \|r_{j-2}\|}{2\|r_{j-1}\|}$ in (1) measures the rate of convergence.

The action of the proportional and derivative parts can be summarized as follows:

- If GMRES(m) has good convergence, the derivative part is important and β updates m.
- If GMRES(m) has poor convergence, the proportional part $\cos(\angle(r_{j-1}, r_{j-2})) \approx 1$ and α updates m.

The parameters α, β have the values:

- $\alpha = -3$ because the proportional part acts like the rule in [7]. There decreasing m in -3 showed good results.
- $\beta = 5$ because in many of the experiments, the derivative is small and we want to amplify its effect. Note that residual norms have decreasing values. Because of that a value of **5** decreases m.

Proposed Rule

Input: m_{j-1} last m value, $m_{initial}$ last m initial value , m_{min} minimum m value,
r residual vectors, j cycle for which m will be computed,
step value to use for increasing m when m_{min} is reached
Output: m_j restart value for cycle j
if $(j > 3)$ **then**

$$m_j = m_{j-1} + \left\lfloor \left(-3\frac{\|r_{j-1}\|}{\|r_{j-2}\|} + 5\frac{\|r_{j-1}\| - \|r_{j-3}\|}{2\|r_{j-2}\|} \right) \right\rfloor$$

else if $(j > 2)$ **then**

$$m_j = m_{j-1} + \left\lfloor -3\frac{\|r_{j-1}\|}{\|r_{j-2}\|} \right\rfloor$$

else
  $m_j = m_{initial}$
end
if $(m_j < m_{min})$ **then**
  $m_{initial} = m_{initial} + m_{step}$
  $m_j = m_{initial}$
end
return m_j

Problems

The solved linear systems $Ax = b$ use A from the University of Florida Matrix Collection [10] which includes problems from Matrix Market. For problems without a right hand side b, it was randomly generated using a uniform distribution with values between the minimum and the maximum $(A)_{i,j}$.

Problem List, n is the size of A, nnz is the number of nonzero elements

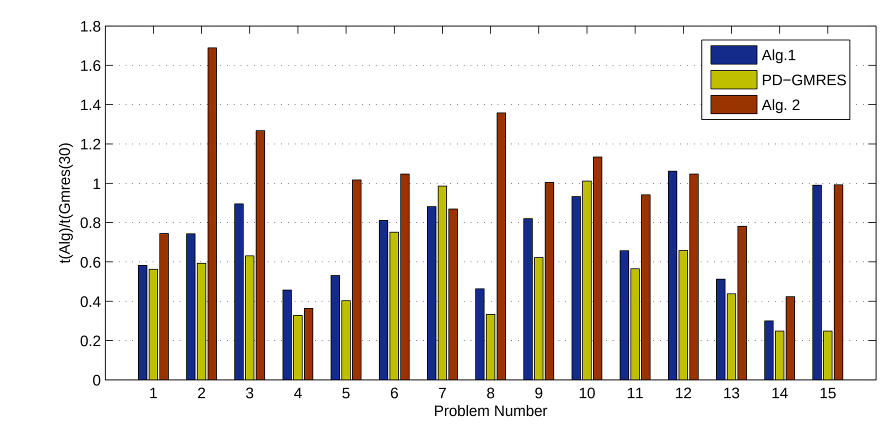
	Problem	n	nnz	Application area
1	add20	2395	17319	Computer component design
2	cdde1	961	4681	2D convection-diffusion operator
3	circuit_2	4510	21199	Circuit simulation
4	fpga_trans_01	1220	7382	Circuit simulation
5	orsirr_1	1030	6858	Oil reservoir simulation
6	orsreg_1	2205	14133	Oil reservoir simulation
7	pde2961	2961	14585	Model PDE equation
8	raefsky1	3242	294276	Incompressible fluid flow
9	raefsky2	3242	293551	Incompressible fluid flow
10	rdb2048	2048	12032	Reaction-diffusion Brusselator model
11	sherman4	1104	3786	Oil reservoir simulation
12	steam2	600	13760	Injected steam oil recovery
13	wang2	2903	19093	Electron continuity equations
14	watt_1	1856	11360	Petroleum engineering
15	young3c	841	3988	Acoustic scattering

Results

We solved the system $Ax = b$ using: standard GMRES(m), Baker's rule (obtained from [7]), Goncalez's rule (obtained from [8]) and PD-GMRES(m).

Algorithms' configurations:

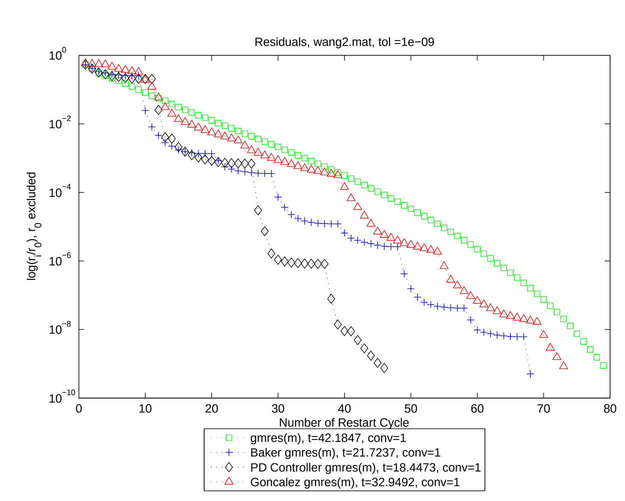
- The initial solution is $x_0 = 0$ or equivalently $r_0 = b$.
- The stopping criterion at the jth iteration is $\frac{\|r_j\|}{\|r_0\|} < 10^{-9}$.
- Standard GMRES(m): $m = 30$.
- PD-GMRES(m): $m_{initial} = 30$, $m_{step} = 3$, $m_{min} = 1$.
- Alg. 1 (Baker's rule): $m_{min} = 1$, $m_{max} = 30$, $m_{step} = 3$.
- Alg. 2 (Goncalez's rule): $m_{ini} = 10$, $m_{max} = 30$, $tolerance = 10^{-9}$.

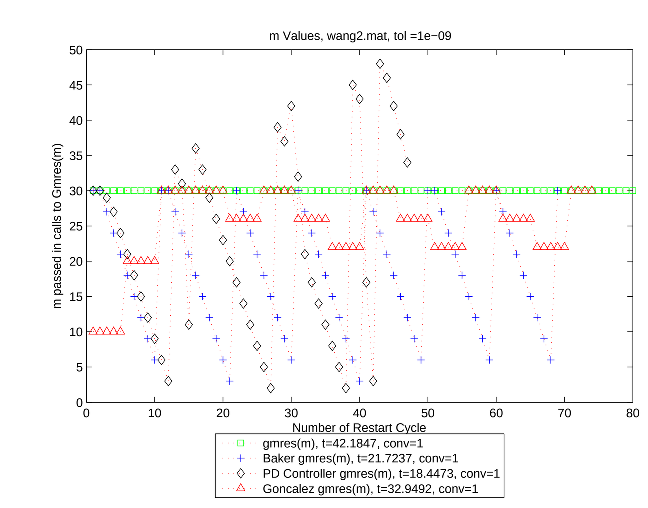


Relative Execution Times. Bars are grouped by problems. The lower the bar, the best the time to solution. In problem 15, only the PD-GMRES(m) converged.

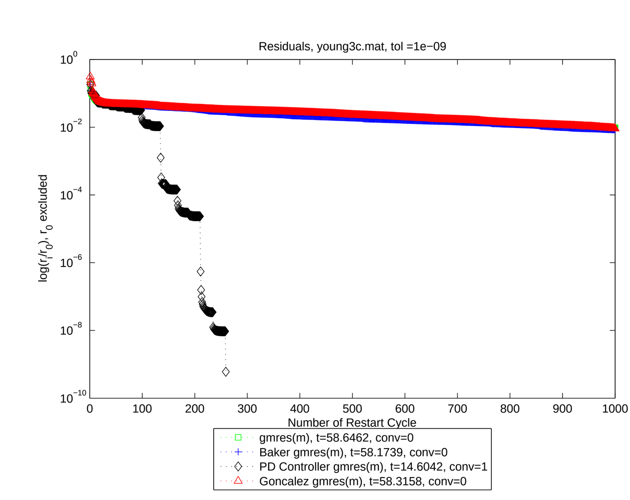
Examples

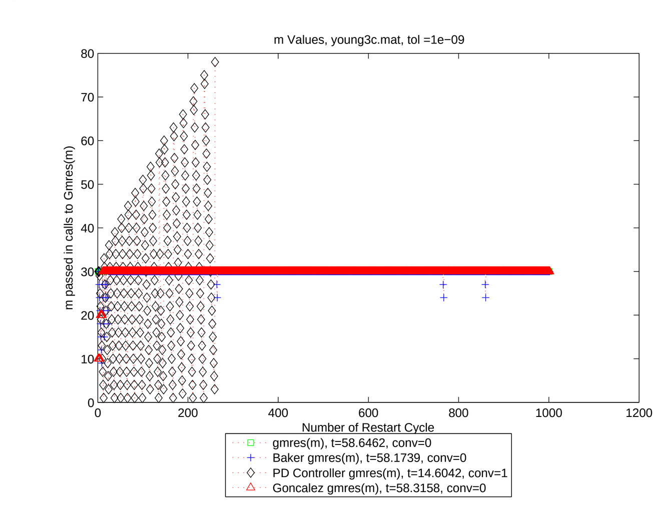
Problem 13: Wang2





Problem 15: Young3c





Relative residual norms $\|r_j\|/\|r_0\|$ Vs. cycle number j. $\|r_0\|$ excluded.

Restart value m_j Vs. cycle number j.

Conclusions

- For all but two (problems 7 and 10) of the 15 test problems, PD-GMRES(m) has a better rate of convergence than GMRES(30), Baker's and Goncalez's algorithms.
- For problem 15, only PD-GMRES(m) converged, the other tested methods presented slow convergence.
- PD-GMRES(m) is simple to implement.
- Future work may find better heuristics for α, β in (1)

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