Gene computation using algebraic multigrid

(Three multigrid schemes)

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Outline

1. Algebraic MG for SPD problems

Let us solve

$$Ax = b,$$

$A \in \mathscr{R}^{N\times N}$, SPD and sparse.
Iterative methods act as "smoothers": residual $r^n := b - Ax^n \ll x - x^n =: e^n$, error.
Let (prolongation matrix) $P \in \mathscr{R}^{N\times N_c}$, $N_c < N$,

$$P^T A P u_c^n = P^T r^n$$

Vector

$$x_{new}^n = x^n + P u_c^n$$

is a better approximation to x in A-norm than x^n,

$$P^T A e^n = 0.$$

We need $P^T AP$ sparse, thus P must contain many zeros,

$$P^T = \begin{pmatrix} 1 & 1 & 0 & 0 & \dots & \dots & 0 \\ 0 & 0 & 1 & 1 & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & \dots & \dots & \dots & 0 & 1 & 1 \end{pmatrix}.$$

AMG algorithm

AMG cycle (input y, output $\tilde{y}$)

1. q-times $\tilde{y} := (I-A)y + b$
2. solve $P^T APu = P^T(b - A\tilde{y})$ for u
3. prolong and add $\tilde{y} := \tilde{y} + Pu$

Step 2. can be solved in a multilevel fashion.

Residual based MG scheme. Stationary method.

Error matrix $(x^{n+1} - x = M(x^n - x))$ for two levels is

$$M = (I-A)^q (I - P(P^T AP)^{-1} P^T A).$$

Always

$$\rho(M) \leq \rho(I-A) < 1.$$

[A. Brandt, Algebraic multigrid theory: The symmetric case, 1983]
[J. H. Bramble, J. E. Pasciak, J. Xu, 1991]

2. AMG - Exact interpolation scheme (EIS)

Exact interpolation scheme (EIS) in [A. Brandt, D. Ron, Multigrid solvers and multilevel optimization strategies, 2003]

Especially, in AMG for Markov chains:

$$Bx = x$$

where B is nonnegative $B_{ij} \geq 0$ and $e^T B = e^T$, e is a vector of all ones.
Coarse problem:

$$RBP(y)u = u,$$

where reduction matrix R and prolongation matrix $P(y)$, $P(y) \neq R^T$ are, for example,

$$R = \begin{pmatrix} 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 1 \end{pmatrix}, \qquad P(y) = \begin{pmatrix} 1/3 & 0 \\ 2/3 & 0 \\ 0 & 2/6 \\ 0 & 3/6 \\ 0 & 1/6 \end{pmatrix} \quad \text{for} \quad y = \begin{pmatrix} 2/12 \\ 4/12 \\ 2/12 \\ 3/12 \\ 1/12 \end{pmatrix}.$$

Full reconstruction matrix $P(y)$: there exists v that $P(y)v = y$,
no residual is transfered between levels.

AMG - EIS algorithm

AMG - EIS cycle (input y, output $\tilde{y}$)

1. q steps of basic iteration $y := T^q y$
2. solve $RAP(y)u = u$ for u
3. prolong $\tilde{y} := P(y)u$

Step 2. can be solved in a multilevel fashion.
No residual is transfered.
Complete reconstruction of the approximation to x in every cycle.
Non-stationary method $x^{n+1} - x = M(x^n)(x^n - x)$.

Error matrix for two level method is

$$M(y) = T^q \left(I - P(y)R(B - xe^T)\right)^{-1} (I - P(y)R).$$

What about $\rho(M(y))$?
[W. J. Stewart, Introduction to the Numerical Solution of Markov Chains, 1994]

AMG - EIS for Markov chains - error formula

Theorem. [P, 2012] Let $L \geq 2$ and let one pre- and post-smoothing step be in all levels up to the coarsest one, $m = 1, 2, \ldots, L-1$. Let T commute with B. The error in $n+1$-th cycle is

$$x^{n+1} - \hat{x} = M(x^n)(x^n - \hat{x}),$$

where

$$\begin{aligned} M(x^n) &= T \prod_{k=2}^{L-1} (Q_k T)(I - Q_L Z)^{-1} \sum_{k=1}^{L-1} (Q_k - Q_{k+1}) J_{k-1} \\ &\quad + T \sum_{m=1}^{L-2} \prod_{k=2}^{m} (Q_k T) \sum_{k=1}^{m} (Q_k - Q_{k+1}) J_{k-1}, \end{aligned}$$

where $J_0 = T$, and for $k = 1, 2, \ldots, L-2$

$$J_k = \Big(T + \sum_{j=2}^{k} T Q_j (T - I)\Big) T, \qquad Q_k = P(x^n)_1 P(x^n)_2 R_2 R_1$$

where R_k and $P(y)_k$ maps from level k to level $k-1$ and vice versa.

Convergence / divergence

Divergence in general, even in local sense.

Especially for "the most nonsymmetric matrices", e.g. $\tilde{C}_4 = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$.

Theorem. [P., 2012] Consider $B = \tilde{C}_{4n}$, $L = 2$. Suppose $2n$ aggregation groups, each containing two elements. Let $T = \tilde{C}_{4n}$ and $q = n$. Then

$$\rho(M(x)) \geq n.$$

Ordering according to strong connections. Let C_N be defined by $[C_N]_{k+1,k} = 1$, $[C_N]_{1,N} = 1$ and $[C_N]_{i,j} = 0$ otherwise, e.g.

$$C_4 = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}.$$

Theorem. [P., 2009] For any N there exists a choice of the aggregation groups and q such that $\limsup_{N \to \infty} \rho(M(x)) = 2$.

Fourier analysis

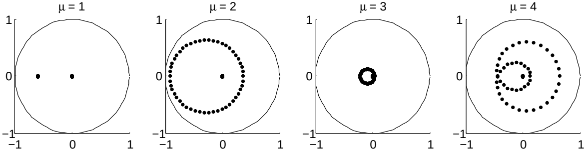
Fourier analysis enables quantitative estimates and optimal choice of parameters. B must have some structure - circulant.

First results for B cyclic. $B = C_N$, where $[C_N]_{i+1,i} = 1$ and $[C_N]_{1,N} = 1$.

Theorem. [P, 2012] Let $B = C_N$, (then $\hat{x} = e/N$). $T = \alpha B + (1-\alpha)I$, $\#G_i = 2$. Then spectrum of the error propagation matrix $J(\hat{x})$ is

$$\sigma(M(\hat{x})) = \{0, \nu_0, \nu_1, \dots, \nu_{n-1}\},$$

where $\nu_k =$
$$\frac{1}{2}\left(\left(1-e^{2\pi ki/N}\right)\left(1-\alpha+\alpha e^{-2\pi ki/N}\right)^{\mu} + \left(1+e^{2\pi ki/N}\right)\left(1-\alpha-\alpha e^{-2\pi ki/N}\right)^{\mu}\right).$$



Example. $N = 100$, $T = \alpha B + (1-\alpha)I$, $\alpha = 0.8$ and $\mu + \nu \in \{1,2,3,4\}$. Spectra of $M(x)$. (The solid lines represent reference unit cycles.)

Numerical example - Genetics

Matrix of transitions of genes (with a perturbation 10^{-5}), $N = 1200$.

Left: original B
Middle: reordered B
Right: $\sigma(B)$

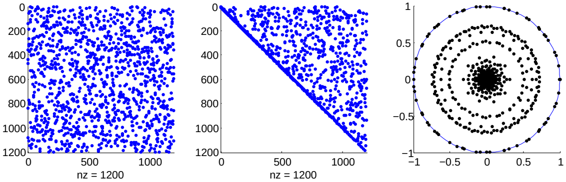
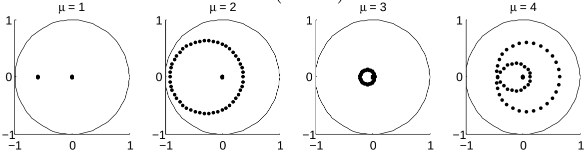


Table: Number of IAD cycles and solution times for obtaining the accuracy 10^{-6}.

steps of basic it., $T = 0.8B + 0.2I$	1	2	**3**	4	5	6
time	8.2	28.5	**3.6**	8.2	3.7	4.9
cycles	25	83	**10**	22	9	12

Fourier analysis: Three steps of basic iteration are the best (among $\{1, \ldots, 4\}$ for $\alpha = 0.8$ in the iteration matrix $T = \alpha T + (1 - \alpha)I$:

Spectra of M for B cyclic:



3. AMG - Adaptive coarse space (ACS)

P. Vaněk and R. Kužel, 2013, ”evolving coarse space multigrid” for eigenvalue problem (of nuclear reaction) and possibly for other nonlinear problems.

Special matrix $P(y)$ - current approximation is augmented to P, for example,

$$P(y) = [y|P] = \begin{pmatrix} y_1 & 1 & 0 \\ y_2 & 1 & 0 \\ y_3 & 0 & 1 \\ y_5 & 0 & 1 \\ y_5 & 0 & 1 \end{pmatrix} \in \mathscr{R}^{N\times(N_c+1)}.$$

Solve

$$A(x) = f(x).$$

Coarse problem:

$$\Big(P(u)z, A\left(P(u)u_c\right) - f\left(P(u)u_c\right)\Big) = 0, \quad \text{for all} \quad z \in \mathscr{R}^{N_c+1}$$

in some scalar product.

AMG - ACS algorithm

The problem: $A(x) = f(x)$.

AMG - ACS cycle (input y, output $\tilde{y}$)

1. q-times $y := S(y)y$ for the underlying problem
2. solve (approximatelly) $P(y)^T A\left(P(y)u\right) = P(y)^T f\left(P(y)u\right)$ for u
3. prolong $\tilde{y} := P(y)u$

Step 2. can be solved in a multilevel fashion.

Error matrix only for linear problems

$$M(y) = (I-A)^q \left(I - P(y)(P(y)^T AP(y))^{-1} P(y)^T A\right) = M\left(I - \frac{1}{y^T AHy} yy^T AH\right)$$

where

$$H = I - P(P^T AP)^{-1} P^T A.$$

Then

$$\rho(M(y)) \leq \rho(M) < 1.$$

AMG - ACS - Example

Equation, $a > 0$,

$$\frac{d^2u}{dx^2} + u(a-u) = f, \quad u(0) = 0, \quad u(1) = a,$$

finite difference discretization

$$Au + B(u) = f(u).$$

Let $P(y) = [y|P]$.

AMG - ACS cycle (input y, output $\tilde{y}$)

1. solve (q-times) $y := A^{-1}(f(y) - B(y))$
2. set $u = (1, 0, \ldots, 0)^T$ and iterate r-times
   $u := \left(P(y)^T A P(y)\right)^{-1} P^T(y)\left(f(P(y)u) - B(P(y)u)\right)$ for u
3. prolong $\tilde{y} := P(y)u$

accuracy 10^{-8}
$N_1 = N = 2000$
N_2 size of the coarse problem

* residual based AMG with
smoothed $P := |A| * P$

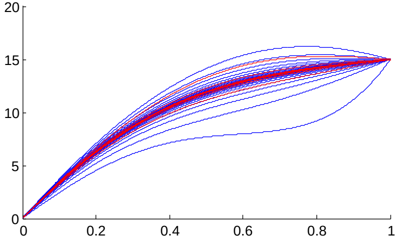


Table: Number of AMG - ACS cycles; (stationary iterations: 141)

$N_2 =$	1000	500	400	200	100	40	20
1 coarse step	9	24	31	54	79	107	120
3 coarse steps	17	32	37	58	81	107	121
30 coarse steps	18	32	37	58	81	107	121
*	72	16	10	29	53	87	108

Table: Time; (stationary iterations: 11.5)

$N_2 =$	1000	500	400	200	100	40	20
1 coarse step	1.8	2.7	3.2	5.1	7.2	9.5	10.5
3 coarse steps	9.6	5.7	5.4	5.9	7.5	9.7	10.7
30 coarse steps	51.9	18.8	14.5	9.0	9.0	10.5	11.1
*	12.3	1.5	1.0	2.5	4.7	7.6	9.5

Questions

AMG - EIS for Markov chains

Main question:

Does local convergence always imply global convergence ?

AMG - ACS

Analysis of local / global convergence for

- eigenvalue problem

- other nonlinear problems.