Smoothed Aggregation and Algebraic Multigrid Methods for Markov Chains

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1. Simple Markov Chain Example

- start in one state with probability 1: what is the stationary probability vector after $\infty$ number of steps?

$$x_{i+1} = B \cdot x_i$$

- stationary probability:

$$B \cdot x = x \quad \|x\|_1 = 1$$

$$x^T = [2/19 \ 6/19 \ 4/19 \ 6/19 \ 1/19]$$
Applications of Markov Chains

- information retrieval and web ranking
- performance modelling of computer systems
- analysis of biological systems
- dependability and security analysis
- …
2. Problem Statement

\[ B x = x \quad \|x\|_1 = 1 \quad x_i \geq 0 \ \forall i \]

- \( B \) is column-stochastic

\[ 0 \leq b_{ij} \leq 1 \ \forall i, j \quad 1^T B = 1^T \]

- \( B \) is irreducible (every state can be reached from every other state in the directed graph)

\[ \exists! \ x : \quad B x = x \quad \|x\|_1 = 1 \quad x_i > 0 \ \forall i \]

(no probability sinks!)
3. Power Method

\[ Bx = x \quad \text{or} \quad (I - B)x = 0 \quad \text{or} \quad Ax = 0 \]

- largest eigenvalue of \( B \): \( \lambda_1 = 1 \)

- power method: \( x_{i+1} = Bx_i \)
  
  - convergence factor: \( |\lambda_2| \)
  
  - convergence is very slow when \( |\lambda_2| \approx 1 \)
    (slowly mixing Markov chain) (JAC, GS also slow)
Why/When is Power Method Slow? Why Multilevel Methods?
Principle of Multigrid (for PDEs)

\[-u_{xx} - u_{yy} = f(x, y) \quad Ax = b\]

- high-frequency error is removed by relaxation (weighted Jacobi, Gauss-Seidel, ... power method)
- low-frequency-error needs to be removed by coarse-grid correction
Multigrid Hierarchy: V-cycle

- multigrid V-cycle:
  - relax (=smooth) on successively coarser grids
  - transfer error using restriction \((R=P^T)\) and interpolation \((P)\)
- \(W=O(n)\) : (optimally) scalable method
4. Aggregation for Markov Chains

- form three coarse, aggregated states

\[ x_{c,I} = \sum_{i \in I} x_i \]

\[ x_c^T = [8/19 \ 10/19 \ 1/19] \]

\[ B_c x_c = x_c \]

\[ b_{c,IJ} = \frac{\sum_{j \in J} x_j \left( \sum_{i \in I} b_{ij} \right)}{\sum_{j \in J} x_j} \]

\[ B_c = \begin{bmatrix} 1/4 & 3/5 & 0 \\ 5/8 & 2/5 & 1 \\ 1/8 & 0 & 0 \end{bmatrix} \]

(Simon and Ando, 1961)
Aggregation for Markov Chains

\[ B_c x_c = x_c \]

\[ b_{c,I,J} = \frac{\sum_{j \in J} x_j \left( \sum_{i \in I} b_{i,j} \right)}{\sum_{j \in J} x_j} \]

\[ B_c = Q^T B \text{ diag}(x) Q \text{ diag}(Q^T x)^{-1} \]

\[ x_{c,I} = \sum_{i \in I} x_i \]

\[ x_c = Q^T x \]

(Krieger, Horton, ... 1990s)
Error Equation

• multiplicative error: \( x = \text{diag}(x_i) e_i \)
• error equation: \( A \text{diag}(x_i) e_i = 0 \)
• coarse grid equation: \( Q^T A \text{diag}(x_i) Q e_c = 0 \)
  \( A_c e_c = 0 \)
• restriction and interpolation:
  \( R = Q^T \quad P = \text{diag}(x_i) Q \)
  \( A_c = R A P \)
• coarse grid correction: \( x_{i+1} = P e_c \)
Error Equation

- important properties of $A_c$:

1. $\mathbf{1}_c^T A_c = 0 \quad \forall \mathbf{x}_i$

   (since $\mathbf{1}_c^T R = \mathbf{1}_c^T$ and $\mathbf{1}_c^T A = 0$)

2. $A_c \mathbf{1}_c = 0 \quad$ for $\mathbf{x}_i = \mathbf{x}$
Multilevel Aggregation Algorithm

Algorithm: Multilevel Adaptive Aggregation method (V-cycle)

\[ x = AM\_V(A, x, \nu_1, \nu_2) \]

\[
\begin{align*}
\text{begin} \\
x &\leftarrow \text{Relax}(A, x) \quad \nu_1 \text{ times} \\
\text{build } Q \text{ based on } x \text{ and } A \quad (Q \text{ is rebuilt every level and cycle}) \\
R &= Q^T \quad \text{and} \quad P = \text{diag}(x) Q \\
A_c &= RAP \\
x_c &= AM\_V(A_c \text{ diag}(P^T 1)^{-1}, P^T 1, \nu_1, \nu_2) \quad (\text{coarse-level solve}) \\
x &= P (\text{diag}(P^T 1))^{-1}x_c \quad (\text{coarse-level correction}) \\
x &\leftarrow \text{Relax}(A, x) \quad \nu_2 \text{ times} \\
\text{end}
\end{align*}
\]

(Krieger, Horton 1994, but no good way to build Q, convergence not good)
Algebraic Aggregation Mechanism

\[ \tilde{A} = A \text{diag}(x_i) \]  
(scaled problem matrix)

\[ S_{jk} = \begin{cases} 
1 & \text{if } j \neq k \text{ and } -\tilde{a}_{jk} \geq \theta \max_{l \neq j} (-\tilde{a}_{jl}) \\
0 & \text{otherwise,}
\end{cases} \]  
(strength matrix)

**Algorithm. Aggregation based on strength matrix S**

repeat
- among the unassigned states, choose state \( j \) which has the largest value in current iterate \( x_i \) as the seed point of a new aggregate
- add all unassigned states \( k \) that are strongly influenced by seed point \( j \) (i.e., \( S_{kj} = 1 \)) to the new aggregate
until all states are assigned to aggregates
Well-posedness: Singular M-matrices

- singular M-matrix:

\[ A \in \mathbb{R}^{n \times n} \text{ is a singular M-matrix } \iff \exists B \in \mathbb{R}^{n \times n}, b_{ij} \geq 0 \forall i, j : A = \rho(B)I - B \]

- our \( A = I - B \) is a singular M-matrix on all levels

1. Irreducible singular M-matrices have a unique solution to the problem \( Ax = 0 \), up to scaling. All components of \( x \) have strictly the same sign (i.e., scaling can be chosen s.t. \( x_i > 0 \forall i \)). (This follows directly from the Perron-Frobenius theorem.)

3. Irreducible singular M-matrices have nonpositive off-diagonal elements, and strictly positive diagonal elements \((n > 1)\).

4. If \( A \) has a strictly positive element in its left or right nullspace and the off-diagonal elements of \( A \) are nonpositive, then \( A \) is a singular M-matrix (see also [21]).
Well-posedness: Unsmoothed Method

**Theorem 3.1** (Singular M-matrix property of AM coarse-level operators). $A_c$ is an irreducible singular M-matrix on all coarse levels, and thus has a unique right kernel vector $e_c$ with strictly positive components (up to scaling) on all levels.

\[
\begin{align*}
(1) \quad & 1_c^T A_c = 0 \quad \forall x_i \\
(\text{since} \quad & 1_c^T R = 1^T \quad \text{and} \quad 1^T A = 0) \\
A &= \begin{bmatrix}
+ & - & - & - & - \\
- & + & - & - & - \\
- & - & + & - & - \\
- & - & - & + & - \\
- & - & - & - & + 
\end{bmatrix}
\end{align*}
\]

**Theorem 3.2** (Fixed-point property of AM V-cycle). *Exact solution* $x$ *is a fixed point of the AM V-cycle.*

\[
\begin{align*}
(2) \quad & A_c 1_c = 0 \quad \text{for} \quad x_i = x \\
A_c e_c &= 0 \\
x_{i+1} &= P e_c
\end{align*}
\]
We Need ‘Smoothed Aggregation’...

(Vanek, Mandel, and Brezina, Computing, 1996)

after smoothing:
coarse grid correction with $Q$:
coarse grid correction with $Q_s$:
Smoothed Aggregation

\[ A = D - (L + U) \]

- smooth the columns of \( P \) with weighted Jacobi:

\[ P_s = (1 - w) \text{diag}(x_i) Q + w D^{-1} (L + U) \text{diag}(x_i) Q \]

- smooth the rows of \( R \) with weighted Jacobi:

\[ R_s = R (1 - w) + R w (L + U) D^{-1} \]
Smoothed Aggregation

• smoothed coarse level operator:

\[
A_{cs} = R_s (D - (L + U)) P_s = R_s D P_s - R_s (L + U) P_s
\]

\[
1^T_c A_{cs} = 0 \quad \forall x_i,
\]

\[
A_{cs} 1_c = 0 \quad \text{for } x_i = x
\]

• problem: \( A_{cs} \) is not a singular M-matrix (signs wrong)

• solution: lumping approach on \( S \) in

\[
A_{cs} = S - G
\]

\[
\hat{A}_{cs} = \hat{S} - G
\]
**Smoothed Aggregation**

\[ A_{cs} = S - G \quad \hat{A}_{cs} = \hat{S} - G \]

- we want as little lumping as possible
- only lump ‘offending’ elements \((i,j)\):
  \[ s_{ij} \neq 0, \ i \neq j \quad \text{and} \quad s_{ij} - g_{ij} \geq 0 \]
  (we consider both off-diagonal signs and reducibility here!)
- for ‘offending’ elements \((i,j)\), add \(S_{\{i,j\}}\) to \(S\):
  \[
  S_{\{i,j\}} = \begin{bmatrix}
  \vdots & \vdots & \vdots \\
  \vdots & \beta_{(i,j)} & \vdots \\
  \vdots & \beta_{(i,j)} & \beta_{(i,j)} \\
  \end{bmatrix}
  \]

\[
\begin{bmatrix}
+ & - & - & - & - \\
- & + & - & - & - \\
- & - & + & - & - \\
- & - & - & + & - \\
\end{bmatrix}
\]

\[ A_{cs}^T \hat{A}_{cs} = 0 \quad \forall \mathbf{x}_i, \quad \hat{A}_{cs} \mathbf{1}_c = 0 \quad \text{for} \ \mathbf{x}_i = \mathbf{x} \]

\[ s_{ij} - g_{ij} - \beta_{\{i,j\}} < 0 \]
\[ s_{ji} - g_{ji} - \beta_{\{i,j\}} < 0 \]

conserves both row and column sums
Lumped Smoothed Method is Well-posed
(A-SAM: Algebraic Smoothed Aggregation for Markov Chains)

**Theorem 4.1** (Singular M-matrix property of lumped SAM coarse-level operators). \( \hat{A}_{cs} \) is an irreducible singular M-matrix on all coarse levels, and thus has a unique right kernel vector \( e_c \) with strictly positive components (up to scaling) on all levels.

**Theorem 4.2** (Fixed-point property of lumped SAM V-cycle). Exact solution \( x \) is a fixed point of the SAM V-cycle (with lumping).

\[
\begin{align*}
1_c^T \hat{A}_{cs} &= 0 \quad \forall x_i, \\
\hat{A}_{cs} 1_c &= 0 \quad \text{for } x_i = x
\end{align*}
\]

(De Sterck et al., SISC (accepted, 2009), ‘Smoothed aggregation multigrid for Markov chains’)
5. Algebraic Multigrid for Markov Chains

- scaled problem matrix: \( \tilde{A} := A \text{diag}(x_i) \)

- multiplicative error equation: \( \tilde{A} e_i = 0 \)
  At convergence, 1 lies in the nullspace of \( \tilde{A} \)

- we can use ‘standard’ AMG on

- define AMG coarsening and interpolation

\[
R \tilde{A} P e_c = 0 \quad \text{or} \quad \tilde{A}_c e_c = 0
\]

\[
R = P^T
\]
AMG (two-pass) Coarsening and Interpolation

\[(P \text{e}_c)_i = \begin{cases} 
(e_c)_i & \text{if } i \in C, \\
\sum_{j \in C_i} w_{ij} (e_c)_j & \text{if } i \in F.
\end{cases}\]

\[
\bar{w}_{ij} = \frac{\bar{a}_{ij} + \sum_{m \in D_i^c} \left( \frac{\bar{a}_{im} \bar{a}_{mj}}{\sum_{k \in C_i} \bar{a}_{mk}} \right)}{\sum_{j \in C_i} \bar{a}_{ij} + \sum_{r \in D_i^c} \bar{a}_{ir}}
\]
AMG Properties

- we can show: all elements of $P \geq 0$
- lumping can be done as in the Smoothed Aggregation case:

\[
\bar{A}_c = P^T \bar{A} P = P^T D P - P^T (L + U) P = S - G
\]

\[
\hat{A}_c = \hat{S} - G
\]

- lumping conserves row and column sums:

\[
1_c^T \hat{A}_c = 1_c^T \bar{A}_c + 1_c^T (\hat{S} - S) 1_c = 1_c^T \bar{A}_c = 0 \quad \forall \ x_i,
\]

\[
\hat{A}_c 1_c = \bar{A}_c 1_c + (\hat{S} - S) 1_c = \bar{A}_c 1_c = 0 \quad \text{for } x_i = x
\]
Algorithm 1: MCAMG($A$, $x$, $\nu_1$, $\nu_2$), AMG for Markov chains (V-cycle)

if not at the coarsest level then
    $x \leftarrow \text{Relax}(A, x) \ nu_1 \text{ times}$
    $\tilde{A} \leftarrow A \ \text{diag}(x)$
    Compute the set of coarse-level points $C$
    Construct the interpolation operator $P$
    Construct the coarse-level operator $\tilde{A}_c \leftarrow P^T \tilde{A} \ P$
    Obtain the lumped coarse-level operator $\hat{A}_c \leftarrow \text{Lump}(\tilde{A}_c, \eta)$
    $e_c \leftarrow \text{MCAMG}(\hat{A}_c, 1_c, \nu_1, \nu_2) \ /\!\!*/ \text{coarse-level solve} \ /\!\!*/$
    $x \leftarrow \text{diag}(x) \ \text{P} e_c \ /\!\!*/ \text{coarse-level correction} \ /\!\!*/$
    $x \leftarrow \text{Relax}(A, x) \ \nu_2 \text{ times}$
else
    $x \leftarrow \text{direct solve of } K x = z \ /\!\!*/ \text{see Section 4.4} \ /\!\!*/$
end
MCAMG Properties

THEOREM 4.2 (Singular M-matrix property of lumped coarse-level operator).
\(\hat{A}_c\) is an irreducible singular M-matrix on all coarse levels and, thus, has a unique right-kernel vector with positive components (up to scaling) on all levels.

\[
A = \begin{bmatrix}
+ & - & - & - & - \\
- & + & - & - & - \\
- & - & + & - & - \\
- & - & - & + & - \\
- & - & - & - & + \\
\end{bmatrix}
\]

THEOREM 4.3 (Fixed-point property of MCAMG V-cycle).
The exact solution, \(x\), is a fixed point of the MCAMG V-cycle.

(De Sterck et al., ‘Algebraic Multigrid for Markov Chains’, preprint)
6. Test Problems

(De Sterck et al., SISC, 2008, ‘Multilevel adaptive aggregation for Markov chains, with application to web ranking’)
6.1 Uniform 1D Chain

- random walk on (undirected) graph
- all edges have the same weight
- transition probability for directed edge = weight of edge / sum of weights of outgoing edges
- solution trivial - test problem
- random walk on undirected graph gives real-spectrum $B$
6.2 Uniform 2D Lattice
6.3 Anisotropic 2D Lattice
6.4 Unstructured Planar Graph
Size of Subdominant Eigenvalue

Fig. 5.1. Magnitude of subdominant eigenvalue as a function of problem size.
6.5 Tandem Queueing Network

**Fig. 5.6.** Tandem queueing network.

**Fig. 5.7.** Graph for tandem queueing network.
6.6 ATM Queueing Network

Class 1 arrivals

Class 2 arrivals

Finite waiting room

2 server station

ATM queueing network, $n = 1940$

ATM queueing network, $p = 0.48508$
7. Numerical Results

7.1 Uniform 1D Chain

<table>
<thead>
<tr>
<th>$n$</th>
<th>$\gamma$</th>
<th>$it$</th>
<th>$C_{op}$</th>
<th>$\gamma_{eff}$</th>
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Table 5.1
Uniform chain.
### 7.2 Uniform 2D Lattice

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**Table 5.2**

*Uniform 2D lattice.*

![Diagram of a 2D lattice](image)
7.3 Anisotropic 2D Lattice

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<th>MCAMG</th>
<th></th>
<th>A-SAM [8] distance-two</th>
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Table 5.3
Anisotropic 2D lattice ($\varepsilon = 1e - 6$).
7.4 Unstructured Planar Graph

|    | MCAMG |         |         |         |         |         |         |         |         |         |         | A-SAM [8] distance-one |         |         |         |         |         |         |         |         |         |         |
|----|-------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------------------------------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|
|    | n     | γ      | it      | $C_{op}$ | $\gamma_{eff}$ | lev | $R_l$ | γ      | it      | $C_{op}$ | $\gamma_{eff}$ | lev | $R_l$ |
|----|-------|---------|---------|---------|---------|-------|-------|---------|---------|---------|---------|-------|-------|---------|---------|         |         |         |         |         |         |         |         |         |         |         |
| 1024| 0.40  | 15      | 2.13    | 0.65    | 6       | 0     | 0.53  | 20      | 1.69    | 0.68    | 5      | 2.6e-2 |
| 2048| 0.33  | 14      | 2.22    | 0.61    | 7       | 6.3e-5| 0.52  | 19      | 1.68    | 0.68    | 5      | 2.1e-2 |
| 4096| 0.40  | 15      | 2.19    | 0.66    | 7       | 6.3e-5| 0.61  | 21      | 1.80    | 0.76    | 5      | 2.4e-2 |
| 8192| 0.40  | 15      | 2.25    | 0.66    | 8       | 9.3e-5| 0.64  | 22      | 1.92    | 0.79    | 7      | 2.5e-2 |
| 16384| 0.37  | 14      | 2.26    | 0.65    | 9       | 7.0e-5| 0.76  | 30      | 2.03    | 0.87    | 7      | 2.4e-2 |
| 32768| 0.37  | 14      | 2.28    | 0.65    | 9       | 1.3e-4| 0.74  | 28      | 2.08    | 0.86    | 7      | 2.4e-2 |

Table 5.4

Unstructured planar graph.
### 7.5 Tandem Queueing Network

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**Table 5.5**

Tandem queueing network.

**Fig. 5.6** Tandem queueing network.

**Fig. 5.7** Graph for tandem queueing network.
7.6 ATM Queueing Network (MCAMG)

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**Table 5.7**

ATM queueing network.

Diagram of an ATM queueing network with two classes of arrivals, a finite waiting room, and two servers.
8. Conclusions

• A-SAM (Smoothed Aggregation for Markov Chains) and MCAMG (Algebraic Multigrid for Markov Chains) are scalable: they are algorithms for calculating the stationary vector of slowly mixing Markov chains with near-optimal complexity
• smoothing is essential for aggregation for many problems
• appropriate theoretical framework (well-posedness)
• no theory yet on (optimal) convergence (non-symmetric matrices)
• this can be done in parallel
• other presentations in this mini-symposium: other multilevel methods for the stationary Markov problem

• Questions?