# Smoothed Aggregation and Algebraic Multigrid Methods for Markov Chains

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### 1. Simple Markov Chain Example



$$B = \begin{bmatrix} 0 & 1/3 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 1/2 & 1/3 & 0 & 0 & 1 \\ 0 & 1/3 & 1 & 0 & 0 \\ 1/2 & 0 & 0 & 0 & 0 \end{bmatrix}$$

 start in one state with probability 1: what is the stationary probability vector after ∞ number of steps?

$$\mathbf{x}_{i+1} = B \mathbf{x}_i$$

• stationary probability:

$$B\mathbf{x} = \mathbf{x} \qquad \|\mathbf{x}\|_1 = 1$$

$$\mathbf{x}^T = [2/19 \,\, 6/19 \,\, 4/19 \,\, 6/19 \,\, 1/19]$$



**Applications of Markov Chains** 

- information retrieval and web ranking
- performance modelling of computer systems
- analysis of biological systems
- dependability and security analysis





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# 2. Problem Statement

 $B\mathbf{x} = \mathbf{x} \qquad \|\mathbf{x}\|_1 = 1 \qquad x_i \ge 0 \,\forall i$ 

• *B* is column-stochastic

 $0 \leq b_{ij} \leq 1 \ \forall i, j \qquad \mathbf{1}^T B = \mathbf{1}^T$ 

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

$$\Rightarrow \\ \exists ! \mathbf{x} : B \mathbf{x} = \mathbf{x} \qquad \|\mathbf{x}\|_1 = 1 \qquad x_i > 0 \ \forall i$$

(no probability sinks!)







### 3. Power Method

 $B\mathbf{x} = \mathbf{x}$  or  $(I - B)\mathbf{x} = 0$  or  $A\mathbf{x} = 0$ 

- largest eigenvalue of *B*:  $\lambda_1 = 1$
- power method:  $\mathbf{x}_{i+1} = B\mathbf{x}_i$

– 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?











- 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

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

$$\mathbf{x}_c^T = [8/19 \ 10/19 \ 1/19]$$

 $B_c \mathbf{x}_c = \mathbf{x}_c$ 







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

(Simon and Ando, 1961)



$$B_c = Q^T B \operatorname{diag}(\mathbf{x}) Q \operatorname{diag}(Q^T \mathbf{x})^{-1}$$

$$\begin{aligned} x_{c,I} &= \sum_{i \in I} x_i \\ \mathbf{x}_c &= Q^T \, \mathbf{x} \end{aligned}$$

(Krieger, Horton, ... 1990s)



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 $Q = \begin{bmatrix} 1 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$ 

# **Error Equation**

- multiplicative error:
- error equation:

 $\mathbf{x} = \operatorname{diag}(\mathbf{x}_i) \mathbf{e}_i$  $A \operatorname{diag}(\mathbf{x}_i) \mathbf{e}_i = 0$ 

$$Q^T A \operatorname{diag}(\mathbf{x}_i) Q \mathbf{e}_c = 0$$
  
 $A_c \mathbf{e}_c = 0$ 

 $R = Q^T \qquad P = \operatorname{diag}(\mathbf{x}_i) Q$  $A_c = R A P$ 

• coarse grid correction:  $\mathbf{x}_{i+1} = P \mathbf{e}_c$ 



# **Error Equation**

• important properties of  $A_c$ :

(1) 
$$\mathbf{1}_{c}^{T} A_{c} = 0 \quad \forall \mathbf{x}_{i}$$
  
(since  $\mathbf{1}_{c}^{T} R = \mathbf{1}^{T}$  and  $\mathbf{1}^{T} A = 0$ )  
(2)  $A_{c} \mathbf{1}_{c} = 0$  for  $\mathbf{x}_{i} = \mathbf{x}$ 



# **Multilevel Aggregation Algorithm**

**Algorithm:** Multilevel Adaptive Aggregation method (V-cycle)



$$\mathbf{x} = \mathsf{AM}_{-}\mathsf{V}(A, \mathbf{x}, \nu_1, \nu_2)$$

#### begin

 $\mathbf{x} \leftarrow \text{Relax}(A, \mathbf{x})$   $\nu_1$  times build Q based on  $\mathbf{x}$  and A (Q is rebuilt every level and cycle)  $R = Q^T$  and  $P = \text{diag}(\mathbf{x}) Q$  $A_c = R A P$  $\mathbf{x}_c = \text{AM}_- \text{V}(A_c \text{diag}(P^T \mathbf{1})^{-1}, P^T \mathbf{1}, \nu_1, \nu_2)$  (coarse-level solve)  $\mathbf{x} = P (\text{diag}(P^T \mathbf{1}))^{-1} \mathbf{x}_c$  (coarse-level correction)  $\mathbf{x} \leftarrow \text{Relax}(A, \mathbf{x})$   $\nu_2$  times end

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

# **Algebraic Aggregation Mechanism**

 $\bar{A} = A \operatorname{diag}(\mathbf{x}_i)$  (scaled problem matrix)

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

Algorithm. Aggregation based on strength matrix S repeat

• among the unassigned states, choose state j which has the largest value in current iterate  $\mathbf{x}_i$  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:

 $A = \begin{bmatrix} + & - & - & - & - \\ - & + & - & - & - \\ - & - & + & - & - \\ - & - & - & + & - \\ - & - & - & - & + \end{bmatrix}$ 

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

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

(1) Irreducible singular M-matrices have a unique solution to the problem  $A \mathbf{x} = 0$ , up to scaling. All components of  $\mathbf{x}$  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  $\mathbf{e}_c$  with strictly positive components (up to scaling) on all levels.

THEOREM 3.2 (Fixed-point property of AM V-cycle). Exact solution  $\mathbf{x}$  is a fixed point of the AM V-cycle.

(2) 
$$A_c \mathbf{1}_c = 0$$
 for  $\mathbf{x}_i = \mathbf{x}$   
 $A_c \mathbf{e}_c = 0$   
 $\mathbf{x}_{i+1} = P \mathbf{e}_c$ 



# We Need 'Smoothed Aggregation'...

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





**Smoothed Aggregation** 

A = D - (L + U)

• smooth the columns of *P* with weighted Jacobi:

 $P_s = (1 - w) \operatorname{diag}(\mathbf{x}_i) Q + w D^{-1} (L + U) \operatorname{diag}(\mathbf{x}_i) Q$ 

• smooth the rows of *R* with weighted Jacobi:

$$R_s = R(1 - w) + Rw(L + U)D^{-1}$$



# **Smoothed Aggregation**

smoothed coarse level operator:

$$\begin{aligned} A_{cs} &= R_s \left( D - (L+U) \right) P_s & \mathbf{1}_c^T A_{cs} = 0 \quad \forall \mathbf{x}_i, \\ &= R_s D P_s - R_s \left( L+U \right) P_s & A_{cs} \mathbf{1}_c = 0 \quad \text{for } \mathbf{x}_i = \mathbf{x} \end{aligned}$$

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

 $\hat{A}_{cs} = \hat{S} - G$ 

• solution: lumping approach on S in

 $A_{cs} = S - G$ 

$$A = \begin{bmatrix} + & - & - & - & - \\ - & + & - & - & - \\ - & - & + & - & - \\ - & - & - & + & - \\ - & - & - & - & + \end{bmatrix}$$



# **Smoothed Aggregation**

$$A_{cs} = S - G \qquad \qquad \hat{A}_{cs} = \hat{S} - G$$

- we want as little lumping as possible
- only lump 'offending' elements (*i*,*j*):

$$A = \begin{bmatrix} + & - & - & - & - \\ - & + & - & - & - \\ - & - & + & - & - \\ - & - & - & + & - \\ - & - & - & - & + \end{bmatrix}$$

$$\mathbf{1}_{c}^{T} \hat{A}_{cs} = 0 \quad \forall \mathbf{x}_{i},$$

$$s_{ij} \neq$$
 0,  $i \neq j$  and  $s_{ij} - g_{ij} \ge$  0

$$\hat{A}_{cs} \mathbf{1}_{c} = 0 \quad \text{for } \mathbf{x}_{i} = \mathbf{x}$$

(we consider both off-diagonal signs and reducibility here!)

• for 'offending' elements (*i*,*j*), add  $S_{\{i,j\}}$  to S:

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

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  $\mathbf{e}_c$  with strictly positive components (up to scaling) on all levels.

THEOREM 4.2 (Fixed-point property of lumped SAM V-cycle). Exact solution  $\mathbf{x}$  is a fixed point of the SAM V-cycle (with lumping).

(De Sterck et al., SISC (accepted, 2009), 'Smoothed aggregation multigrid for Markov chains')



# 5. Algebraic Multigrid for Markov Chains

- scaled problem matrix:  $\bar{A} := A \operatorname{diag}(\mathbf{x}_i)$
- multiplicative error eqaution:  $\bar{A} \mathbf{e}_i = \mathbf{0}$ At convergence, **1** lies in the nullspace of  $\bar{A}$
- we can use 'standard' AMG on  $\bar{A} \, {f e}_i = {f 0}$
- define AMG coarsening and interpolation  $\begin{array}{l} R\,\bar{A}\,P\,\mathbf{e}_c=\mathbf{0} \quad \text{or} \quad \bar{A}_c\,\mathbf{e}_c=\mathbf{0} \\ R=P^T \end{array}$



### AMG (two-pass) Coarsening and Interpolation



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# **AMG Properties**

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

$$A = \begin{bmatrix} + & - & - & - & - \\ - & + & - & - & - \\ - & - & + & - & - \\ - & - & - & + & - \\ - & - & - & - & + \end{bmatrix}$$

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

$$\hat{A}_c = \hat{S} - G$$



# Algebraic Multigrid for Markov Chains (MCAMG)

Algorithm 1: MCAMG(A, x,  $\nu_1$ ,  $\nu_2$ ), AMG for Markov chains (V-cycle)

if not at the coarsest level then  $\mathbf{x} \leftarrow \operatorname{Relax}(A, \mathbf{x}) \nu_1$  times  $\overline{A} \leftarrow A \operatorname{diag}(\mathbf{x})$ Compute the set of coarse-level points CConstruct the interpolation operator  $\overline{A}_c \leftarrow P^T \overline{A} P$ Obtain the lumped coarse-level operator  $\widehat{A}_c \leftarrow \operatorname{Lump}(\overline{A}_c, \eta)$   $\mathbf{e}_c \leftarrow \operatorname{MCAMG}(\widehat{A}_c, \mathbf{1}_c, \nu_1, \nu_2)$  /\* coarse-level solve \*/  $\mathbf{x} \leftarrow \operatorname{diag}(\mathbf{x}) P \mathbf{e}_c$  /\* coarse-level correction \*/  $\mathbf{x} \leftarrow \operatorname{Relax}(A, \mathbf{x}) \nu_2$  times else  $\mathbf{x} \leftarrow \operatorname{direct}$  solve of  $K \mathbf{x} = \mathbf{z}$  /\* 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,  $\mathbf{x}$ , 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





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### Size of Subdominant Eigenvalue



FIG. 5.1. Magnitude of subdominant eigenvalue as a function of problem size.



### 6.5 Tandem Queueing Network





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### 6.6 ATM Queueing Network





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# 7. Numerical Results

# 7.1 Uniform 1D Chain

			MCA	MG		A-SAM [8] distance-two						
n	$\gamma$	it	$C_{op}$	$\gamma_{eff}$	lev	$R_l$	$\gamma$	it	$C_{op}$	$\gamma_{eff}$	lev	$R_l$
2187	0.18	11	1.99	0.43	9	0	0.31	12	1.49	0.46	6	0
6561	0.18	11	2.00	0.43	11	0	0.31	12	1.49	0.46	7	0
19683	0.18	11	2.00	0.43	12	0	0.32	12	1.49	0.47	8	0
59049	0.18	11	2.00	0.43	14	0	0.32	12	1.50	0.47	9	0

TABLE 5.1

 ${\it Uniform \ chain.}$ 





### 7.2 Uniform 2D Lattice

			MCA	MG			A-SAM [8] distance-two						
n	$\gamma$	it	$C_{op}$	$\gamma_{eff}$	lev	$R_l$	$\gamma$	it	$C_{op}$	$\gamma_{eff}$	lev	$R_l$	
1024	0.23	11	2.20	0.51	6	0	0.49	20	1.42	0.60	4	4.5e-3	
4096	0.23	11	2.20	0.52	7	0	0.49	20	1.47	0.62	4	1.7e-3	
16384	0.24	11	2.20	0.52	8	0	0.59	20	1.56	0.72	5	1.4e-3	
65536	0.24	11	2.20	0.52	9	0	0.66	21	1.59	0.77	6	1.3e-3	

TABLE 5.2 Uniform 2D lattice.





### 7.3 Anisotropic 2D Lattice

			MCA	MG			A-SAM [8] distance-two					
n	$\gamma$	it	$C_{op}$	$\gamma_{eff}$	lev	$R_l$	$\gamma$	it	$C_{op}$	$\gamma_{eff}$	lev	$R_l$
1024	0.18	11	2.58	0.52	8	0	0.33	14	2.81	0.68	5	1.6e-3
4096	0.18	11	2.67	0.53	10	0	0.33	14	3.43	0.73	7	4.9e-4
16384	0.18	11	2.73	0.54	12	0	0.33	13	4.17	0.77	7	2.5e-4
65536	0.18	11	2.76	0.54	14	0	0.32	13	4.80	0.79	9	7.6e-5

TABLE 5.3 Anisotropic 2D lattice ( $\varepsilon = 1e - 6$ ).





# 7.4 Unstructured Planar Graph

			MC	CAMG			A-SAM [8] distance-one					
n	$\gamma$	it	$C_{op}$	$\gamma_{eff}$	lev	$R_l$	$\gamma$	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

			MC	CAMG			A-SAM [8] distance-two					
n	$\gamma$	it	$C_{op}$	$\gamma_{eff}$	lev	$R_l$	$\gamma$	it	$C_{op}$	$\gamma_{eff}$	lev	$R_l$
1024	0.33	16	4.41	0.78	7	1.4e-1	0.41	20	2.04	0.64	4	7.6e-2
4096	0.32	15	4.54	0.78	8	1.2e-1	0.45	24	2.12	0.69	5	5.5e-2
16384	0.33	16	4.59	0.78	10	1.6e-1	0.56	30	2.18	0.77	6	5.3e-2
65536	0.33	15	4.61	0.79	11	7.0e-2	0.71	37	2.37	0.86	6	1.3e-1

TABLE 5.5 Tandem queueing network.





FIG. 5.7. Graph for tandem queueing network.





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### 7.6 ATM Queueing Network (MCAMG)

	n	$  \gamma$	it	$C_{op}$	$\gamma_{eff}$	lev	$R_l$
	1940	0.37	19	7.06	0.87	9	3.65e-2
	3060	0.43	19	7.46	0.89	12	3.29e-2
	5220	0.44	21	7.62	0.90	15	3.11e-2
	10100	0.46	20	7.64	0.90	18	2.87e-2
	13796	0.47	21	8.08	0.91	22	2.68e-2
	19620	0.48	21	8.12	0.91	27	2.58e-2
:	32276	0.45	21	8.58	0.91	29	2.35e-2

TABLE 5.7ATM queueing network.







# 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?

