Smoothed Aggregation Multigrid for Slowly Mixing Markov Chains

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1. Simple Markov Chain Example

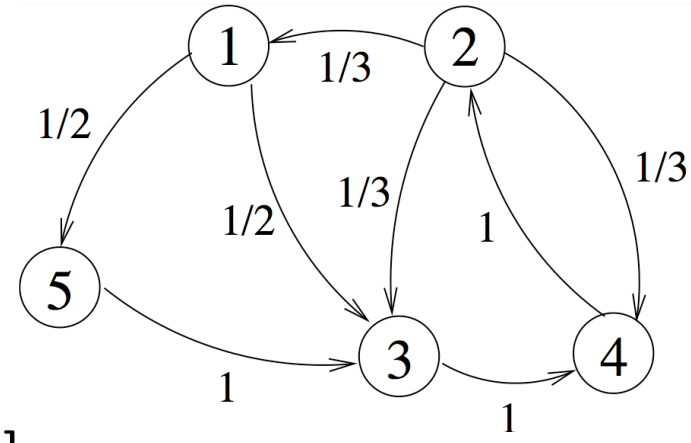
- start in one state with probability 1: what is the stationary probability vector after ∞ number of steps?

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

- stationary probability:

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

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



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

2. Problem Statement

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

- *B* is column-stochastic

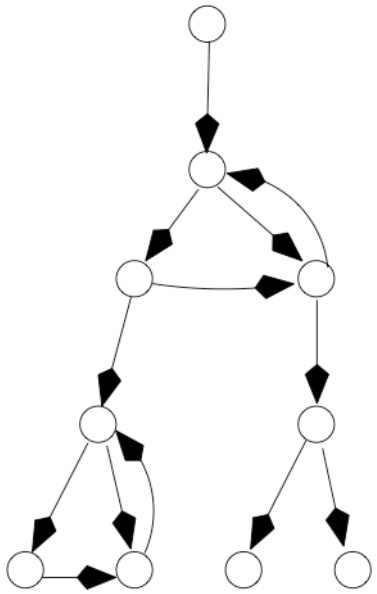
$$0 \leq b_{ij} \leq 1\ \forall i,\ j \qquad \mathbf{1}^T B = \mathbf{1}^T$$

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

$$\Rightarrow$$

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

(no probability sinks!)



3. Power Method

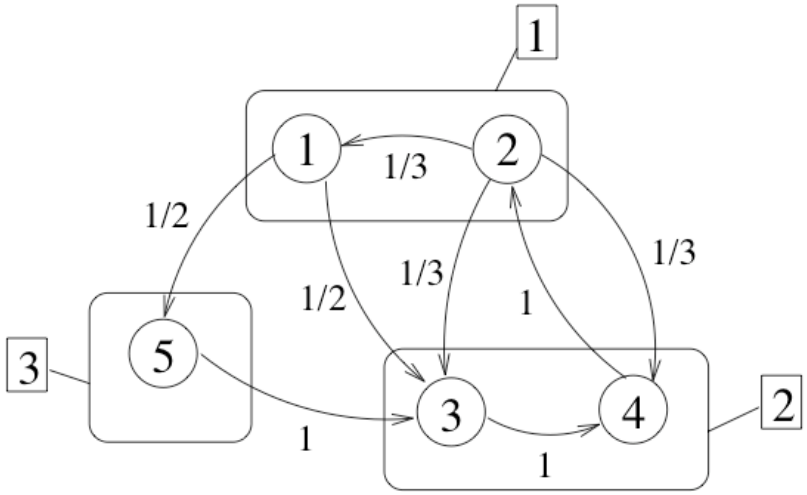
$$B\,\mathbf{x} = \mathbf{x} \quad \text{or} \quad (I - B)\,\mathbf{x} = 0 \quad \text{or} \quad A\,\mathbf{x} = 0$$

- 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)

4. Aggregation for Markov Chains

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

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



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

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

$$\mathbf{x}_c = Q^T \mathbf{x}$$

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

(Krieger, Horton, ... 1990s)

5. Error Equation

- error equation - coarse grid correction:

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

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

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

$$\mathbf{x}_{i+1} = P\,\mathbf{e}_c$$

Error Equation

- important properties of A_c:

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

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

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

(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 $\mathbf{x}_i = \mathbf{x}$

$$A_c\,(\text{diag}(P^T\,\mathbf{1}))^{-1}$$
$$= R\,(I - B)\,P\,(\text{diag}(P^T\,\mathbf{1}))^{-1}$$
$$= I_c - B_c$$

6. Multilevel Aggregation Algorithm

Algorithm: Multilevel Adaptive Aggregation method (V-cycle)

$\mathbf{x} = \text{AM\_V}(A, \mathbf{x}, \nu_1, \nu_2)$

begin

$\mathbf{x} \leftarrow \text{Relax}(A, \mathbf{x})$ ν_1 times

build Q based on $\mathbf{x}$ and A (Q is rebuilt every level and cycle)

$R = Q^T$ and $P = \text{diag}(\mathbf{x})\, Q$

$A_c = R\, A\, P$

$\mathbf{x}_c = \text{AM\_V}(A_c\, \text{diag}(P^T 1)^{-1}, P^T 1, \nu_1, \nu_2)$ (coarse-level solve)

$\mathbf{x} = P\, (\text{diag}(P^T 1))^{-1} \mathbf{x}_c$ (coarse-level correction)

$\mathbf{x} \leftarrow \text{Relax}(A, \mathbf{x})$ ν_2 times

end

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

7. Well-posedness: Singular M-matrices

- singular M-matrix:

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

$$A \in \mathbb{R}^{n \times n} \text{ is a singular M-matrix} \Leftrightarrow$$

$$\exists\, B \in \mathbb{R}^{n \times n},\ b_{ij} \geq 0 \,\forall i,j\ :\ A = \rho(B)\, I - B$$

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

(1) Irreducible singular M-matrices have a unique solution to the problem $A\mathbf{x} = 0$, *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.*

(1) $\mathbf{1}_c^T A_c = 0 \quad \forall\, \mathbf{x}_i$
(since $\mathbf{1}_c^T R = \mathbf{1}^T$ and $\mathbf{1}^T A = 0$)

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

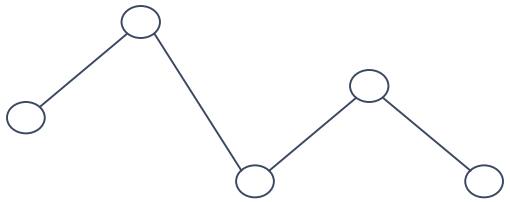
THEOREM 3.2 (Fixed-point property of AM V-cycle). *Exact solution $\mathbf{x}$ is a fixed point of the AM V-cycle.*

(2) $A_c\, \mathbf{1}_c = 0 \quad$ for $\mathbf{x}_i = \mathbf{x}$

$$A_c\, \mathbf{e}_c = 0$$
$$\mathbf{x}_{i+1} = P\, \mathbf{e}_c$$

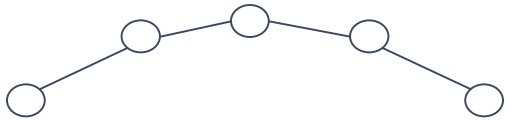
8. We Need 'Smoothed Aggregation'...

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

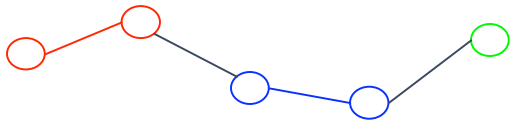


$$Q = \begin{bmatrix} 1 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

after smoothing:

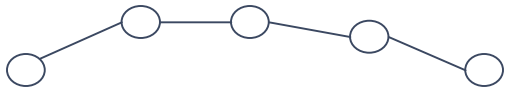


coarse grid correction with Q:



$$Q_s = \begin{bmatrix} \times & 0 & 0 \\ \times & \times & 0 \\ \times & \times & 0 \\ 0 & \times & \times \\ 0 & \times & \times \end{bmatrix}$$

coarse grid correction with Q_s:



Smoothed Aggregation

$$A = D - (L + U)$$

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

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

- 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:

$$A_{cs} = R_s \left(D - (L+U)\right) P_s$$
$$= R_s D P_s - R_s (L+U) P_s$$

$$\mathbf{1}_c^T A_{cs} = 0 \quad \forall \mathbf{x}_i,$$
$$A_{cs} \mathbf{1}_c = 0 \quad \text{for } \mathbf{x}_i = \mathbf{x}$$

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

- solution: lumping approach on S in

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

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

Smoothed Aggregation

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

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

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

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

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

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

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

$$S_{\{i,j\}} = \begin{array}{c} \\ i \\ \\ j \\ \\ \end{array} \begin{array}{c} \begin{array}{ccccc} & i & & j & \end{array} \\ \begin{bmatrix} \ddots & \vdots & & \vdots & \\ \cdots & \beta_{\{i,j\}} & \cdots & -\beta_{\{i,j\}} & \cdots \\ & \vdots & & \vdots & \\ \cdots & -\beta_{\{i,j\}} & \cdots & \beta_{\{i,j\}} & \cdots \\ & \vdots & & \vdots & \end{bmatrix} \end{array}$$

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

conserves both row and column sums

9. Lumped Smoothed Method is Well-posed

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.*

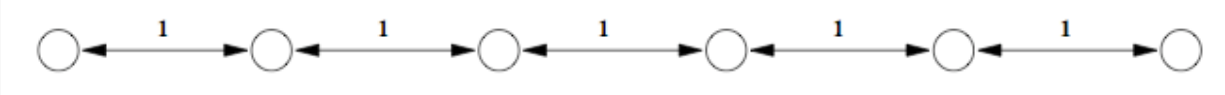
THEOREM 4.2 (Fixed-point property of lumped SAM V-cycle). *Exact solution $\mathbf{x}$ is a fixed point of the SAM V-cycle (with lumping).*

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

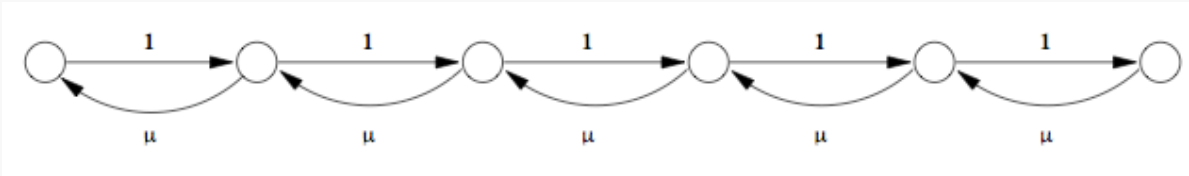
$$A = \begin{bmatrix} + & - & - & - & - \\ - & + & - & - & - \\ - & - & + & - & - \\ - & - & - & + & - \\ - & - & - & - & + \end{bmatrix}$$

10. Numerical Results: Test Problems

- uniform chain

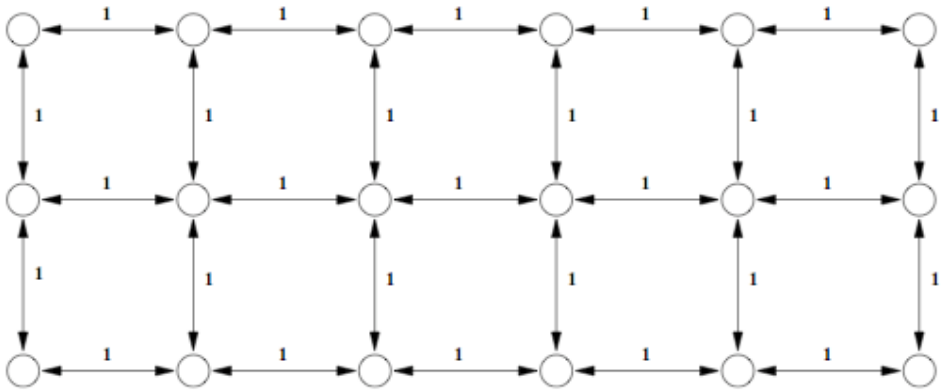


- birth-death chain

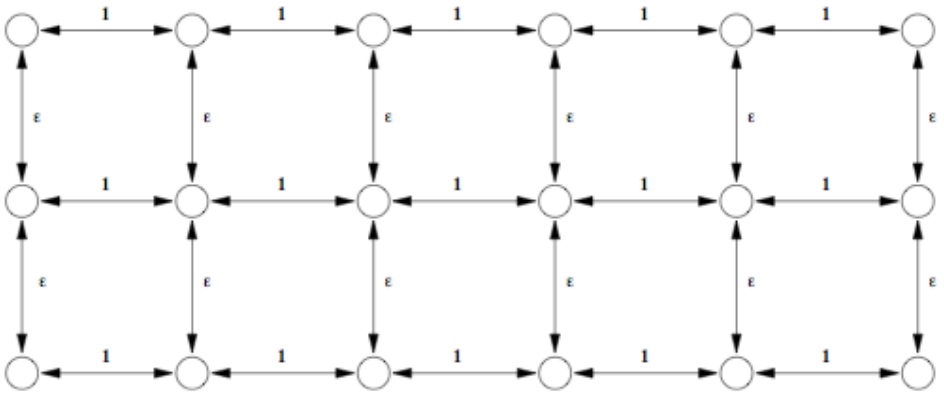


Test Problems

- uniform 2D lattice



- anisotropic 2D lattice



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Test Problems

- tandem queueing network

FIG. 5.6. *Tandem queueing network.*

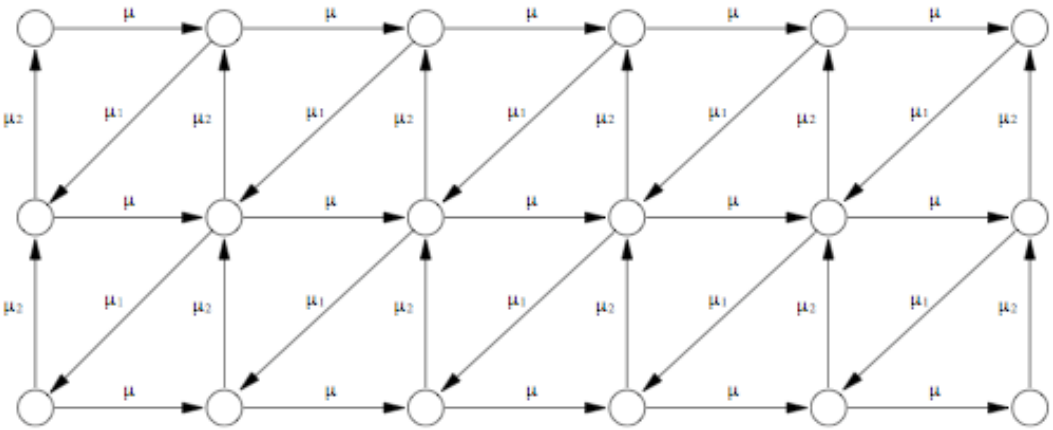
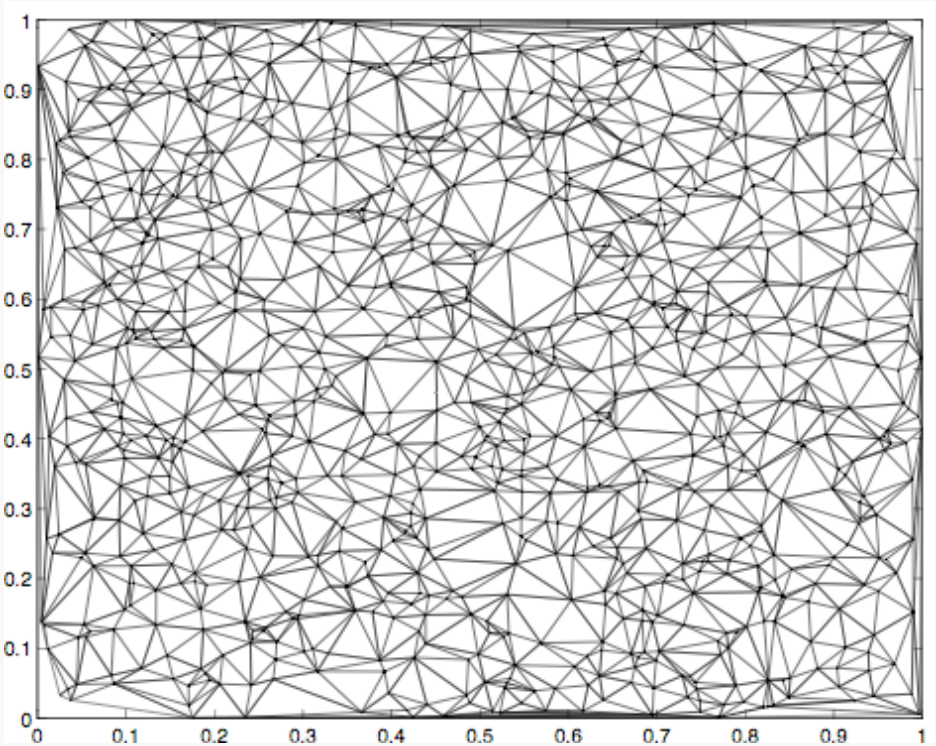


FIG. 5.7. *Graph for tandem queueing network.*

Test Problems

- random walk on triangulation of random points in unit square



11. Numerical Results: Geometric Aggregation (size 3)

n	lev	it	C_{op}	γ	γ_{eff}	it	C_{op}	γ	γ_{eff}
27	2	32	1.32	0.66	0.73	32	1.63	0.66	0.78
81	3	85	1.43	0.87	0.91	52	2.07	0.80	0.90
243	4	>100	1.47	0.95	0.97	73	2.37	0.87	0.94
729	5	>100	1.49	0.98	0.98	>100	2.58	0.92	0.97
2187	6	>100	1.50	0.98	0.98	>100	2.72	0.95	0.98

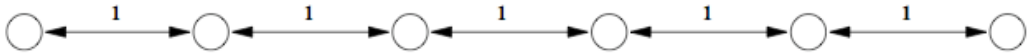
TABLE 5.1

Uniform chain. G-AM with V-cycles (left) and W-cycles (right). (Size-three aggregates, no smoothing.)

n	it	C_{op}	lev	γ	γ_{eff}	R_{lump}
27	13	1.32	2	0.27	0.37	0
81	13	1.43	3	0.27	0.40	0
243	13	1.47	4	0.27	0.41	0
729	13	1.49	5	0.27	0.41	0
2187	13	1.50	6	0.27	0.42	0
6561	13	1.50	7	0.27	0.42	0
19683	13	1.50	8	0.27	0.42	0
59049	13	1.50	9	0.27	0.42	0

TABLE 5.2

Uniform chain. G-SAM with V-cycles and size-three aggregates. (Smoothing with lumping.)

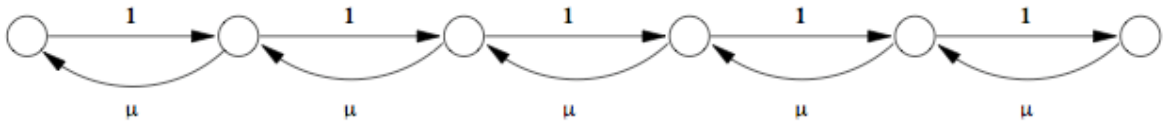


Numerical Results: Geometric Aggregation (size 3)

n	C_{op}	lev	it	γ	γ_{eff}	it	γ	γ_{eff}	R_{lump}
27	1.32	2	33	0.66	0.73	13	0.27	0.37	0
81	1.43	3	95	0.88	0.92	12	0.27	0.40	0
243	1.47	4	>100	0.95	0.97	13	0.26	0.40	0
729	1.49	5	>100	0.97	0.98	12	0.24	0.38	0

TABLE 5.4

Birth-death chain ($\mu = 0.96$). (left) G-AM (no smoothing) and (right) G-SAM (smoothing with lumping). (V-cycles and size-three aggregates.)



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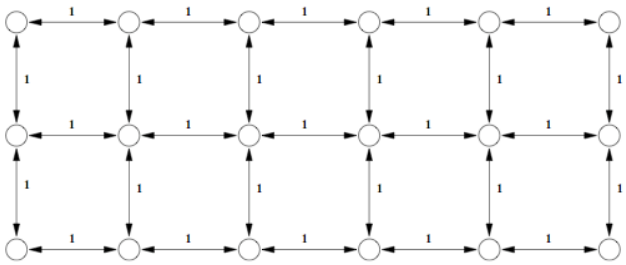
Numerical Results: Geometric Aggregation (3x3)



n	γ_{res}	iter	C_{op}	levels
64	0.71	43	1.11	2
100	0.85	72	1.17	3
169	0.86	85	1.15	3
400	0.89	>100	1.13	3
900	0.95	>100	1.12	4

TABLE 5.9

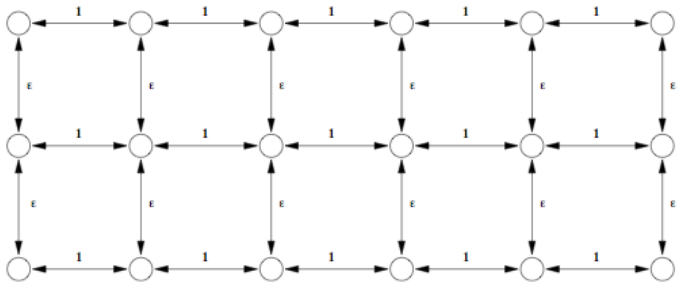
Uniform 2D lattice. G-AM with V-cycles and size-three aggregates. (No smoothing.)

n	lev	it	C_{op}	γ	γ_{eff}	R_{lump}	it	C_{op}	γ	γ_{eff}	R_{lump}
64	2	22	1.17	0.49	0.55	0	17	1.34	0.39	0.49	0
256	3	24	1.22	0.54	0.61	0	17	1.47	0.42	0.55	0
1024	4	25	1.22	0.57	0.63	6.6e-4	18	1.49	0.44	0.58	4.3e-3
4096	4	26	1.23	0.58	0.64	9.7e-4	19	1.52	0.45	0.59	3.6e-3
16384	5	27	1.22	0.61	0.67	4.0e-5	19	1.51	0.45	0.59	1.3e-4
65536	6	27	1.23	0.62	0.67	1.5e-5	19	1.52	0.45	0.59	2.6e-4

TABLE 5.8

Uniform 2D lattice. G-SAM with V-cycles (left) and W-cycles (right), using three-by-three aggregates. (Smoothing with lumping.)

Numerical Results: Geometric Aggregation (3x3)

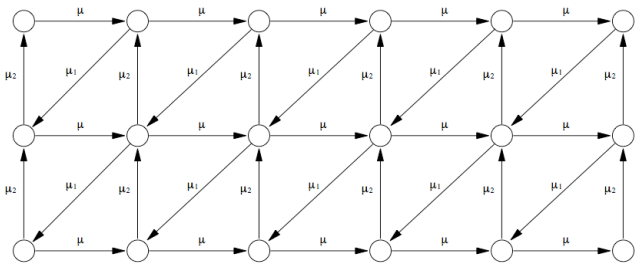


n	lev	it	C_{op}	γ	γ_{eff}	it	C_{op}	γ	γ_{eff}	R_{lump}
64	2	>100	1.11	1.00	1.00	>100	1.17	1.00	1.00	0
256	3	>100	1.14	0.97	0.97	>100	1.22	0.95	0.96	0
1024	4	>100	1.13	0.99	0.99	>100	1.22	0.99	0.99	0
4096	4	>100	1.13	0.99	0.99	>100	1.23	0.99	0.99	0

TABLE 5.9

Anisotropic 2D lattice ($\epsilon = 1e{-}6$). (left) G-AM (no smoothing) and (right) G-SAM (smoothing with lumping) with V-cycles and three-by-three aggregates.

Numerical Results: Geometric Aggregation (3x3)



n	it	C_{op}	lev	γ	γ_{eff}
256	>100	1.19	3	0.91	0.93
1024	>100	1.19	4	0.96	0.97
4096	>100	1.19	4	0.96	0.97

TABLE 5.10

Tandem queueing network. G-AM with V-cycles and three-by-three aggregates. (No smoothing.)

n	lev	it	C_{op}	γ	γ_{eff}	R_{lump}	it	C_{op}	γ	γ_{eff}	R_{lump}
256	3	19	1.28	0.44	0.52	2.4e-2	14	1.60	0.33	0.50	3.9e-2
1024	4	19	1.27	0.46	0.55	2.0e-3	14	1.62	0.32	0.50	5.9e-3
4096	4	20	1.29	0.49	0.57	7.4e-3	14	1.65	0.33	0.51	1.4e-2
16384	5	21	1.28	0.56	0.63	8.1e-4	14	1.63	0.33	0.51	2.0e-3
65536	6	21	1.28	0.51	0.59	1.6e-3	14	1.64	0.33	0.51	3.8e-3

TABLE 5.11

Tandem queueing network. G-SAM with V-cycles (left) and W-cycles (right), using three-by-three aggregates. (Smoothing with lumping.)

12. Numerical Results: Algebraic Aggregation

- error equation: $A\,\mathrm{diag}(\mathbf{x}_i)\,\mathbf{e}_i = 0$
- use strength of connection in $A\,\mathrm{diag}(\mathbf{x}_i)$
- define row-based strength (determine all states that strongly influence a row's state, similar to AMG)
- state that has largest value in $\mathbf{x}_i$ is seed point for new aggregate, and all unassigned states influenced by it join its aggregate
- repeat

(our paper on PageRank in SISC, 2008)

Numerical Results: Algebraic Aggregation

n	it	C_{op}	lev	γ	γ_{eff}
27	39	1.71	3	0.74	0.84
81	83	1.85	4	0.87	0.93
243	>100	1.96	6	0.96	0.98
729	>100	1.98	7	1.00	1.00

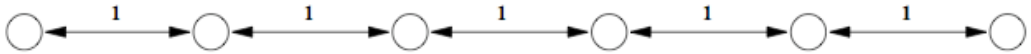
TABLE 6.1

Uniform chain. A-AM with V-cycles and distance-one aggregation. (No smoothing.)

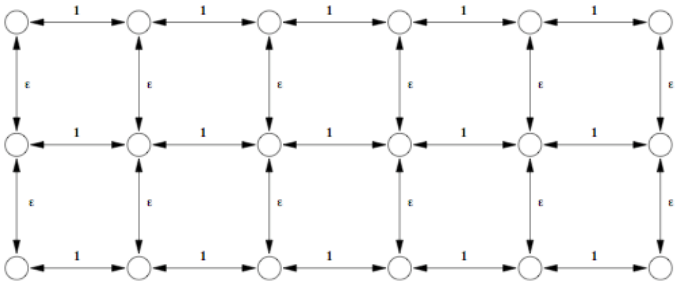
n	it	C_{op}	lev	γ	γ_{eff}	R_{lump}	it	C_{op}	lev	γ	γ_{eff}	R_{lump}
27	10	2.09	3	0.20	0.46	2.4e-2	13	1.33	2	0.32	0.43	0
81	10	2.09	4	0.18	0.44	0.0e-0	13	1.44	3	0.32	0.45	0
243	10	2.20	5	0.21	0.49	1.3e-3	12	1.46	4	0.32	0.46	0
729	11	2.23	6	0.21	0.50	3.3e-3	12	1.49	5	0.31	0.45	0
2187	11	2.24	6	0.23	0.52	2.5e-3	12	1.49	6	0.31	0.46	0
6561	11	2.24	8	0.24	0.53	1.4e-3	12	1.49	7	0.31	0.46	0
19683	11	2.25	8	0.26	0.55	1.4e-3	12	1.49	8	0.32	0.47	0
59049	12	2.25	9	0.30	0.59	1.0e-3	12	1.50	9	0.32	0.47	0

TABLE 6.2

Uniform chain. A-SAM with V-cycles using distance-one aggregation (left) and distance-two aggregation (right). (Smoothing with lumping.)



Numerical Results: Algebraic Aggregation

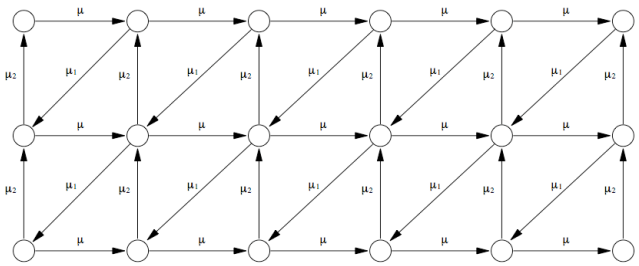


n	it	C_{op}	lev	γ	γ_{eff}	it	C_{op}	lev	γ	γ_{eff}	R_{lump}
64	27	1.78	4	0.55	0.72	17	1.76	3	0.40	0.59	0.0e-0
256	45	1.93	6	0.74	0.86	15	2.23	4	0.33	0.61	7.4e-4
1024	80	2.01	8	0.86	0.93	14	2.81	5	0.33	0.68	1.6e-3
4096	>100	2.04	10	0.93	0.96	14	3.43	7	0.33	0.73	4.9e-4
16384	>100	2.06	11	0.96	0.98	13	4.17	7	0.33	0.77	2.5e-4
65536	>100	2.16	13	0.97	0.99	13	4.80	9	0.32	0.79	7.6e-5

TABLE 6.7

Anisotropic 2D lattice ($\epsilon = 1e-6$). (left) A-AM (no smoothing, distance-one aggregation) and (right) A-SAM (smoothing with lumping, distance-two aggregation) with V-cycles.

Numerical Results: Algebraic Aggregation



n	it	C_{op}	lev	γ	γ_{eff}
256	>100	1.86	5	0.92	0.96
1024	>100	1.96	6	0.91	0.95
4096	>100	2.03	7	0.98	0.99
16384	>100	2.09	9	0.98	0.99

TABLE 6.8

Tandem queueing network. A-AM with V-cycles and distance-one aggregation. (No smoothing.)

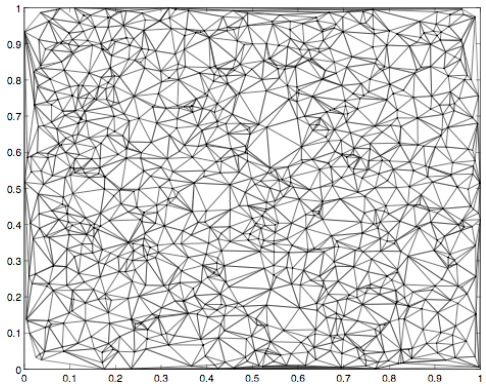
n	it	C_{op}	lev	γ	γ_{eff}	R_{lump}
256	18	1.94	4	0.39	0.61	1.1e-1
1024	20	2.04	4	0.41	0.64	7.6e-2
4096	24	2.12	5	0.45	0.69	5.5e-2
16384	30	2.18	6	0.56	0.77	5.3e-2
65536	37	2.37	6	0.71	0.86	1.3e-1

TABLE 6.9

Tandem queueing network. A-SAM with V-cycles and distance-two aggregation. (Smoothing with lumping.)

University of Waterloo

Numerical Results: Algebraic Aggregation



$n = 32768$	it	C_{op}	lev	γ	γ_{eff}
multilevel A-AM	>100	1.26	8	0.9827	0.9862
two-level A-AM	>100	1.20	2	0.9833	0.9861
one-level method	>100	1.00	1	0.9846	0.9846

TABLE 6.11

Unstructured planar graph with $n = 32768$ nodes. Comparison of multilevel A-AM, two-level A-AM (aggregation-disaggregation), and one-level relaxation. (V-cycles and distance-one aggregation, no smoothing. The V(1,1)-cycles have two relaxations per level per cycle.))

n	it	C_{op}	lev	γ	γ_{eff}	R_{lump}
1024	20	1.69	5	0.5265	0.6848	2.6e-02
2048	19	1.68	5	0.5200	0.6779	2.1e-02
4096	21	1.80	5	0.6069	0.7578	2.4e-02
8192	22	1.92	7	0.6360	0.7904	2.5e-02
16384	30	2.03	7	0.7610	0.8744	2.4e-02
32768	28	2.08	7	0.7399	0.8649	2.4e-02

TABLE 6.10

Unstructured planar graph. A-SAM with V-cycles and distance-one aggregation. (Smoothing with lumping.))

13. AMG version of algorithm also works

$$\mathbf{v} \leftarrow V(A, \mathbf{x})$$

1. Relax a_1 times on $A\mathbf{u} = \mathbf{0}$ with initial guess $\mathbf{x}$.
2. If you have reached the coarsest level, then go to step 4.
   Else

   Set $\bar{A} \leftarrow A\,\mathrm{diag}(\mathbf{x})$.
   Compute the set of coarse grid points C.
   Construct the interpolation operator P.
   Construct the coarse grid operator $\bar{A}_c \leftarrow P^T \bar{A} P$.
   Obtain lumped coarse grid operator $\hat{A}_c \leftarrow Lump(\bar{A}_c, \eta)$.
   Recursively call the algorithm $\mathbf{e}_c \leftarrow V(\hat{A}_c, \mathbf{1}_c)$.
3. Correct $\mathbf{x} \leftarrow \mathrm{diag}(\mathbf{x}) P \mathbf{e}_c$.
4. Relax a_2 times on $A\mathbf{u} = \mathbf{0}$ with initial guess $\mathbf{x}$.

14. Conclusions

- SAM (Smoothed Aggregation for Markov Chains): algorithm for stationary vector of slowly mixing Markov chains with near-optimal complexity
- smoothing is essential for aggregation for many problems
- pretty good convergence results, operator complexity may grow
- AMG works too
- appropriate theoretical framework (well-posedness)
- are there other ways for choosing R, P, lumping?
- no theory yet on optimal convergence (non-symmetric matrices)

- Questions?

Smoothed Aggregation

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

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

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

- for 'offending' elements *(i,j)*, choose $\eta \in (0,1]$ s.t.

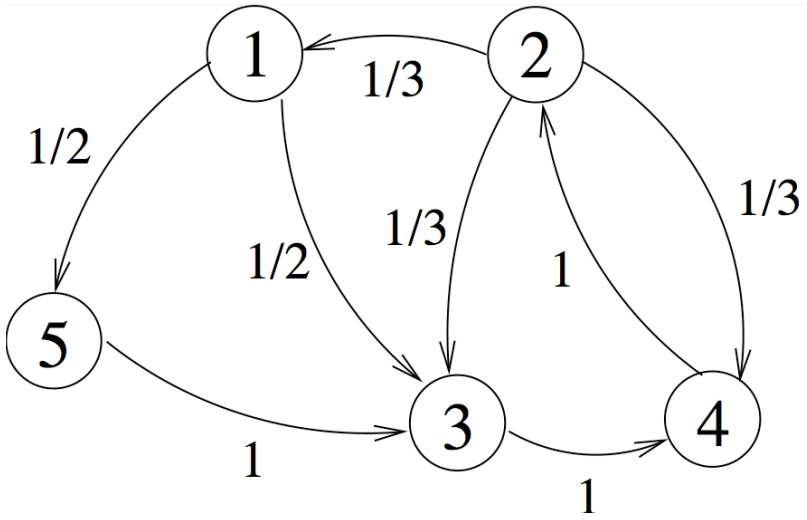
$$s_{ij} - g_{ij} - \beta^{(1)}_{\{i,j\}} = -\eta\, g_{ij}$$
$$s_{ji} - g_{ji} - \beta^{(2)}_{\{i,j\}} = -\eta\, g_{ji}$$

with $\beta_{\{i,j\}} = \max(\beta^{(1)}_{\{i,j\}}, \beta^{(2)}_{\{i,j\}})$

- η=1 means lump full value of offending elements of *S* ($\hat{s}_{ij}$ = 0)

1. Simple Markov Chain Example

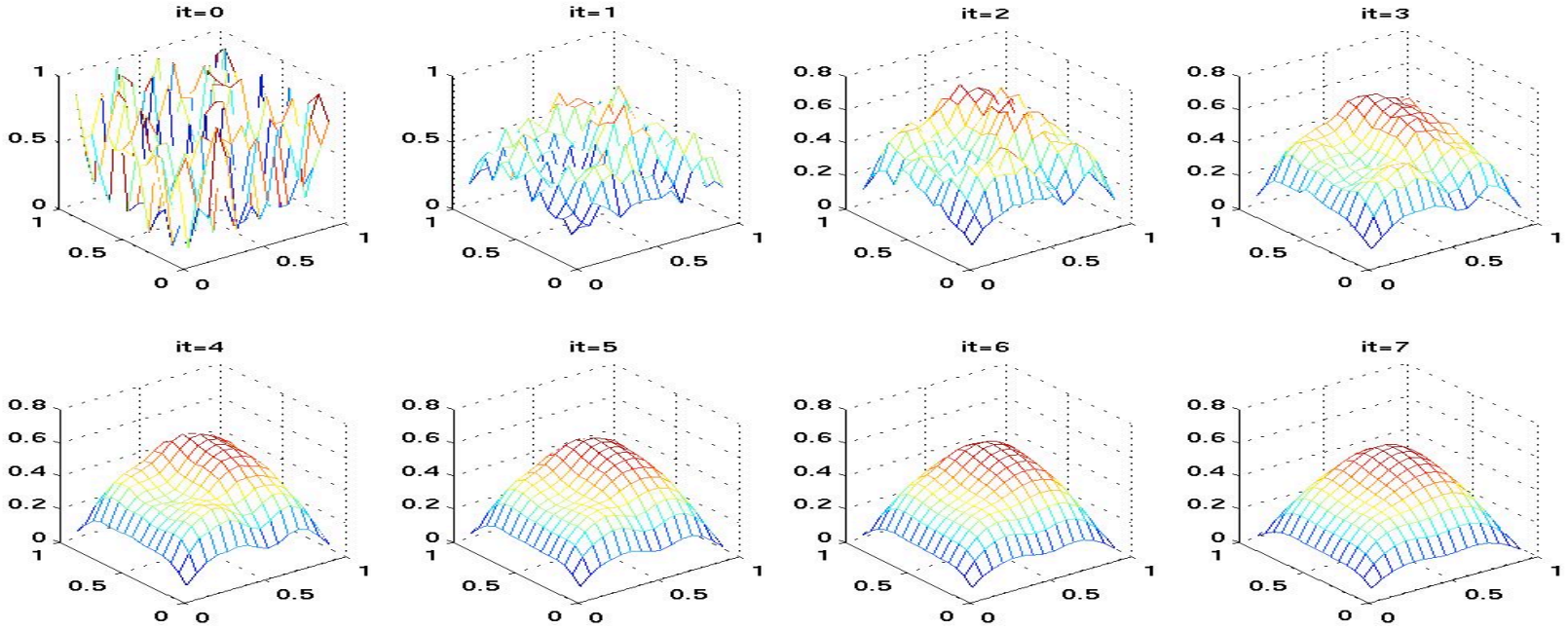
- 5 states
- each outgoing edge same probability (random walk on directed graph)



EMG 2008
hdesterck@uwaterloo.ca

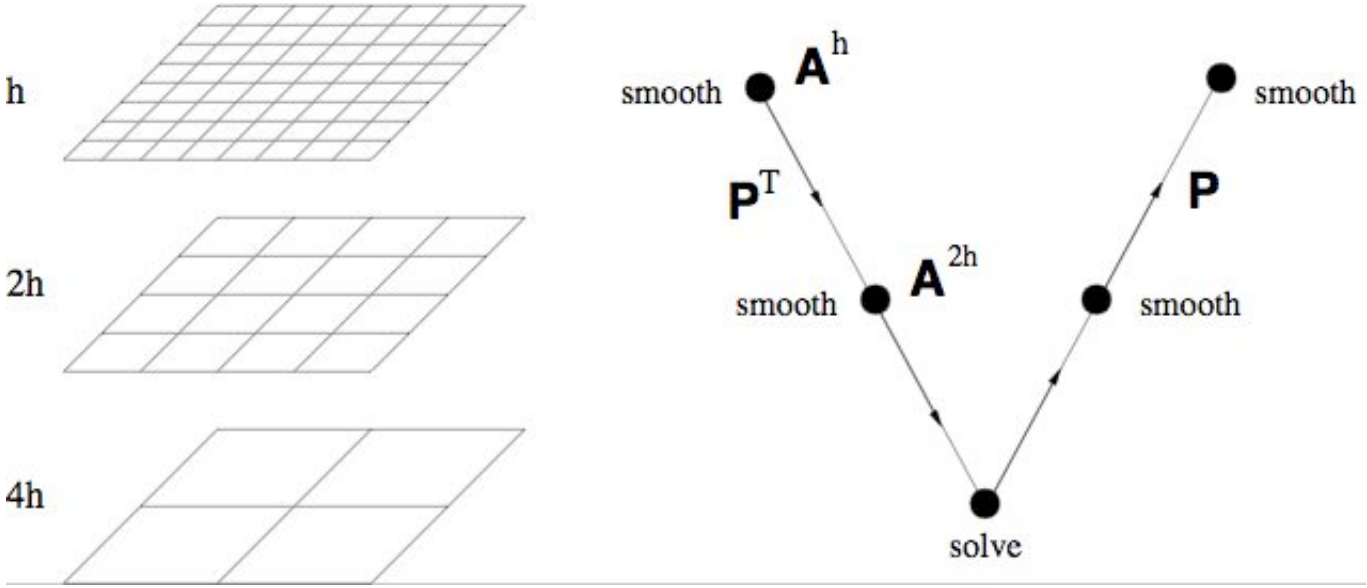
Principle of Multigrid (for PDEs)

$$-u_{xx} - u_{yy} = f(x,y) \qquad Ax = b$$



- high-frequency error is removed by relaxation (weighted Jacobi, Gauss-Seidel, ...)
- 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)

Smoothed Aggregation

$$A_{cs} = R_s \left(D - (L+U)\right) P_s$$
$$= R_s D P_s - R_s (L+U) P_s$$

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

$$A_{cs} = S - G$$

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

- we want to retain crucial properties

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

- we can lump to diagonal in symmetric way, conserving both row and column sums

Numerical Results: Geometric Aggregation (size 3)

n	γ_{res}	iter	C_{op}	levels
54	0.86	75	1.43	3
162	0.95	>100	1.47	4
486	0.97	>100	1.49	5
1458	0.98	>100	1.50	6

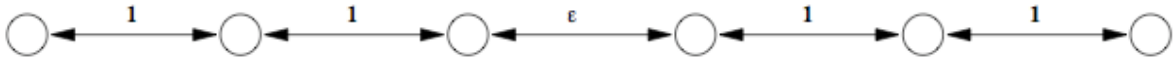
TABLE 5.5

Uniform chain with two weak links ($\epsilon = 0.001$). G-AM with V-cycles and size-three aggregates. The two weak links occur between aggregates at all levels. (No smoothing.)

n	γ_{res}	iter	C_{op}	levels	R_{lump}
54	0.26	12	1.43	3	0
162	0.27	13	1.47	4	0
486	0.27	13	1.49	5	0
1458	0.27	13	1.50	6	0
4374	0.27	13	1.50	7	0

TABLE 5.6

Uniform chain with two weak links ($\epsilon = 0.001$). G-SAM with V-cycles and size-three aggregates. The two weak links occur between aggregates at all levels. (Smoothing with lumping.)



Numerical Results: Geometric Aggregation (size 3)

n	γ_{res}	iter	C_{op}	levels
27	1.00	>100	1.32	2
81	1.00	>100	1.43	3
243	0.98	>100	1.47	4
729	0.98	>100	1.49	5

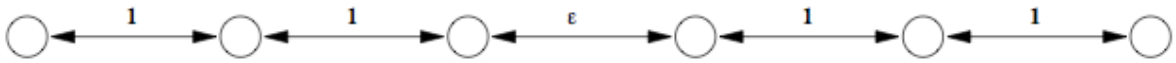
TABLE 5.7

Uniform chain with two weak links ($\epsilon = 0.001$). G-AM with V-cycles and size-three aggregates. The two weak links occur inside an aggregate on the finest level. (No smoothing.)

n	γ_{res}	iter	C_{op}	levels	R_{lump}
27	1.00	>100	1.32	2	0
81	1.00	>100	1.43	3	0
243	1.00	>100	1.47	4	0
729	1.00	>100	1.49	5	0

TABLE 5.8

Uniform chain with two weak links ($\epsilon = 0.001$). G-SAM with V-cycles and size-three aggregates. The two weak links occur inside an aggregate on the finest level. (Smoothing with lumping.)



Numerical Results: effect of η

n	γ_{res}	iter	C_{op}	levels
27	0.75	43	1.71	3
81	0.87	87	1.85	4
243	0.96	>100	1.96	6
729	0.99	>100	1.98	7

TABLE 6.1

Uniform chain. A-AM with V-cycles and distance-one aggregation. (No smoothing.)

n	γ_{res}	iter	C_{op}	levels	γ_{res}	iter	C_{op}	levels
27	0.20	10	2.03	3	0.19	10	2.03	3
81	0.27	11	2.69	4	0.25	11	2.59	4
243	0.32	12	3.33	6	0.32	12	3.33	6
729	0.51	14	3.73	8	0.64	17	3.75	8
2187	0.75	21	3.95	9	0.77	24	3.94	9

TABLE 6.3

Uniform chain. A-SAM with V-cycles using distance-one aggregation, lumping only the off-diagonal elements of $R_s\, D\, P_s$ that cause nonnegative off-diagonal elements of A_{cs}. Lumping their full value ($\eta = 1$, left), and part of their value ($\eta = 0.75$, right).

Numerical Results: effect of η

n	γ_{res}	iter	C_{op}	levels	γ_{res}	iter	C_{op}	levels
27	0.19	10	2.03	3	0.19	10	1.96	3
81	0.19	10	2.51	4	0.20	10	2.61	4
243	0.24	11	2.96	5	0.22	11	3.20	5
729	0.37	12	3.63	7	0.29	12	3.29	6
2187	0.44	14	3.84	8	0.28	12	3.35	7

TABLE 6.4

Uniform chain. A-SAM with V-cycles using distance-one aggregation, lumping part of the value of the off-diagonal elements of $R_s\, D\, P_s$ that cause nonnegative off-diagonal elements of A_{cs}: $\eta = 0.25$, left, and, $\eta = 0.1$, right.

n	γ_{res}	iter	C_{op}	levels	γ_{res}	iter	C_{op}	levels
27	0.20	10	2.03	3	0.20	10	2.03	3
81	0.18	10	2.68	4	0.18	10	2.71	4
243	0.19	10	2.78	5	0.20	10	3.03	5
729	0.24	11	3.41	7	0.24	11	3.50	7
2187	0.27	11	3.75	8	0.26	11	3.81	8

TABLE 6.5

Uniform chain. A-SAM with V-cycles using distance-one aggregation, lumping part of the value of the off-diagonal elements of $R_s\, D\, P_s$ that cause nonnegative off-diagonal elements of A_{cs}: $\eta = 0.01$, left, and, $\eta = 1e-6$, right.

Numerical Results: Algebraic Aggregation

n	γ_{res}	iter	C_{op}	levels
27	0.75	50	1.71	3
81	0.87	92	1.85	4
243	0.96	>100	1.96	6
729	0.97	>100	1.99	8

TABLE 6.6

Birth-death chain ($\mu = 0.96$). A-AM with V-cycles and distance-one aggregation. (No smoothing.)

n	γ_{res}	iter	C_{op}	levels	R_{lump}
27	0.27	12	1.32	2	0
81	0.35	15	1.43	3	0
243	0.35	15	1.47	4	0
729	0.35	15	1.49	5	0

TABLE 6.7

Birth-death chain ($\mu = 0.96$). A-SAM with V-cycles and distance-two aggregation. (Smoothing with lumping.)

Numerical Results: Algebraic Aggregation

n	γ_{res}	iter	C_{op}	levels
64	0.73	41	1.73	3
100	0.80	56	1.83	4
169	0.85	77	1.85	4
400	0.89	>100	1.96	6
900	0.96	>100	1.96	6

TABLE 6.10

Uniform 2D lattice. A-AM with V-cycles and distance-one aggregation. (No smoothing.)

n	γ_{res}	iter	C_{op}	levels	R_{lump}
64	0.42	18	1.30	3	0
100	0.45	19	1.26	3	3.46e-03
169	0.44	18	1.33	3	9.47e-03
400	0.47	20	1.46	4	9.27e-03
900	0.46	18	1.59	4	1.72e-02
1600	0.48	19	1.60	4	1.16e-02
2500	0.48	19	1.67	5	1.44e-02
4900	0.48	18	1.75	5	1.21e-02
6724	0.49	18	1.76	5	1.36e-02

TABLE 6.11

Uniform 2D lattice. A-SAM with V-cycles and distance-two aggregation. (Smoothing with lumping.)

4. Aggregation for Markov Chains

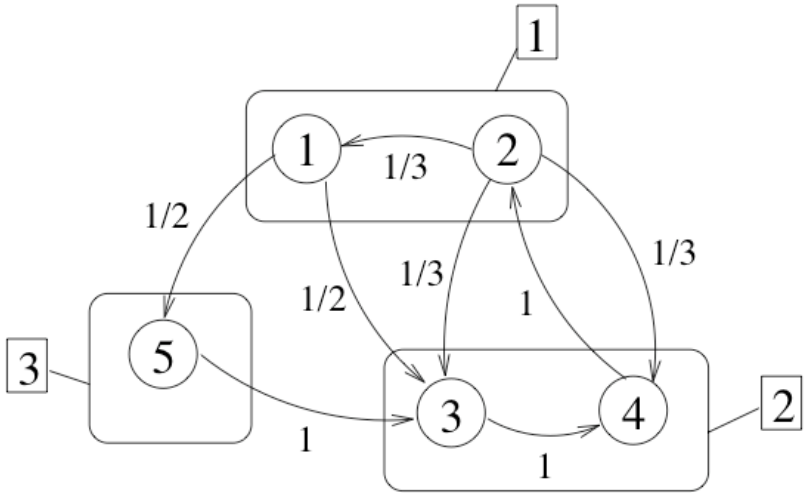
- form three coarse, aggregated states

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

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

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

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



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

(Simon and Ando, 1961)

5. Error Equation

- multiplicative correction: error equation, coarse level error equation, and coarse grid correction

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

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

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

5. Error Equation

- error equation - coarse grid correction:

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

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

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

$$\mathbf{x}_{i+1} = P\,\mathbf{e}_c$$

$$\mathbf{x}_c = \mathrm{diag}(P^T\,\mathbf{1})\,\mathbf{e}_c$$

$$A_c\,(\mathrm{diag}(P^T\,\mathbf{1}))^{-1}\,\mathbf{x}_c = 0$$

$$\mathbf{x}_{i+1} = P\,(\mathrm{diag}(P^T\,\mathbf{1}))^{-1}\mathbf{x}_c$$

Numerical Results: Algebraic Aggregation

n	γ_{res}	iter	C_{op}	levels
54	0.83	67	1.86	4
162	0.93	>100	1.91	5
486	0.96	>100	1.98	7
1458	0.97	>100	1.99	9

TABLE 6.8

Uniform chain with two weak links ($\epsilon = 0.001$). A-AM with V-cycles and distance-one aggregation. (No smoothing.)

n	γ_{res}	iter	C_{op}	levels	R_{lump}
54	0.33	14	1.51	3	0
162	0.33	13	1.50	4	5.51e-03
486	0.34	13	1.50	5	0
1458	0.29	12	1.49	6	3.07e-04
4374	0.27	11	1.50	7	3.05e-04

TABLE 6.9

Uniform chain with two weak links ($\epsilon = 0.001$). A-SAM with V-cycles and distance-two aggregation. (Smoothing with lumping.)