Fast Multilevel Numerical Methods for Random Walks on Directed Graphs

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collaborators

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  Department of Applied Mathematics, University of Colorado at Boulder
- our area of research is numerical linear algebra methods for PDEs, in particular so-called algebraic multigrid methods, and we have recently started to apply these techniques to numerical linear algebra methods for Markov chains

1. problem formulation and example

- develop efficient numerical method for calculating stationary distributions of Markov chains:
  - finite-state (n states)
  - irreducible
  - large
  - sparse
  - slowly mixing
- goal: O(n) method

$\Rightarrow$ approach: use iterative method with multilevel aggregation to distribute probability on all scales quickly

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problem formulation

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

- *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)

$$\Longrightarrow$$

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

- singular M-matrix formulation

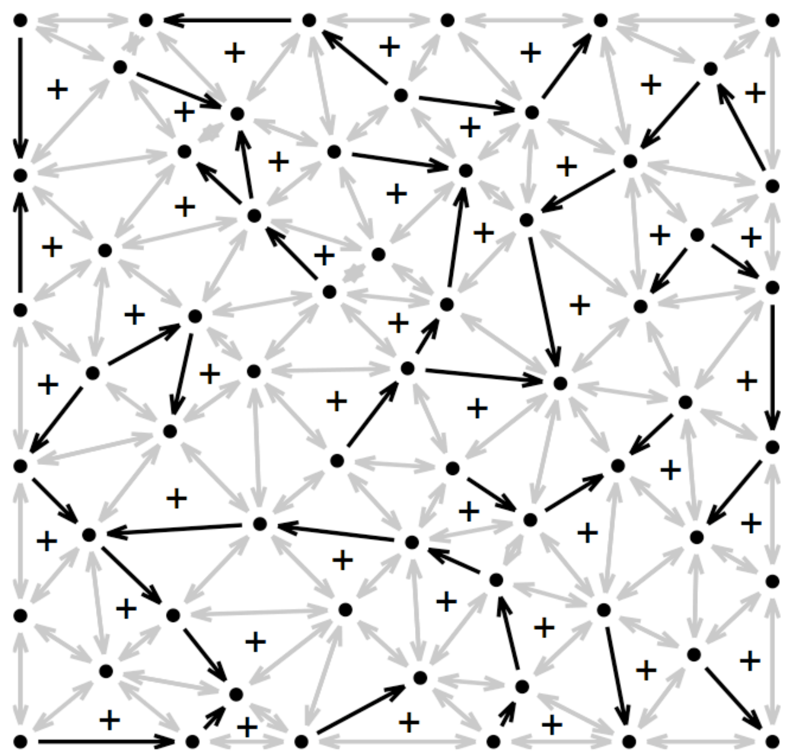
$$A = \begin{bmatrix} + & - & - & - & - \\ - & + & - & - & - \\ - & - & + & - & - \\ - & - & - & + & - \\ - & - & - & - & + \end{bmatrix}$$

$$A\,\mathbf{x} = 0 \qquad A = I - B$$

example

- example: random walk on directed planar graph
- choose n uniformly distributed random points in the unit square
- perform Delaunay triangulation on points
- choose a maximal subset of triangles that are not neighbours
- randomly delete one directed edge from each triangle in this subset

⇒ find stationary distribution of random walk



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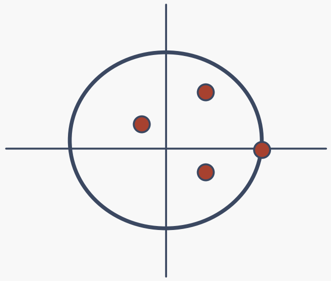
2. power method convergence

- power method: $\mathbf{x}_{i+1} = B\,\mathbf{x}_i$
- largest eigenvalue of *B*: $\lambda_1 = 1$
- power method (nonperiodic *B*):
  - convergence rate: 1-$|\lambda_2|$
  - convergence is slow when 1-$|\lambda_2|$ $\rightarrow$ 0 for increasing n

    (we call this a slowly mixing Markov chain)
  - every power iteration is O(n) work



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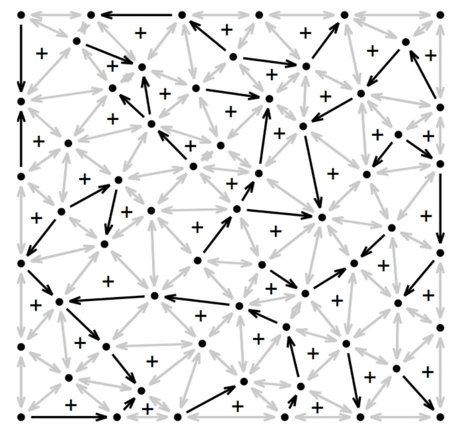
numerical results: one-level iteration for random graph problem

- start from random intial guess $\mathbf{x}_0$
- let $A = D - (L + U)$
- iterate on $\mathbf{x}_{i+1} = (I + w\, D^{-1}\, A)\, \mathbf{x}_i$

  with $w = 0.7$

  until

$$\frac{\|A\,\mathbf{x}_i\|_1}{\|A\,\mathbf{x}_0\|_1} < 10^{-8}$$



n	it
128	322
256	494
512	1010
1024	1768

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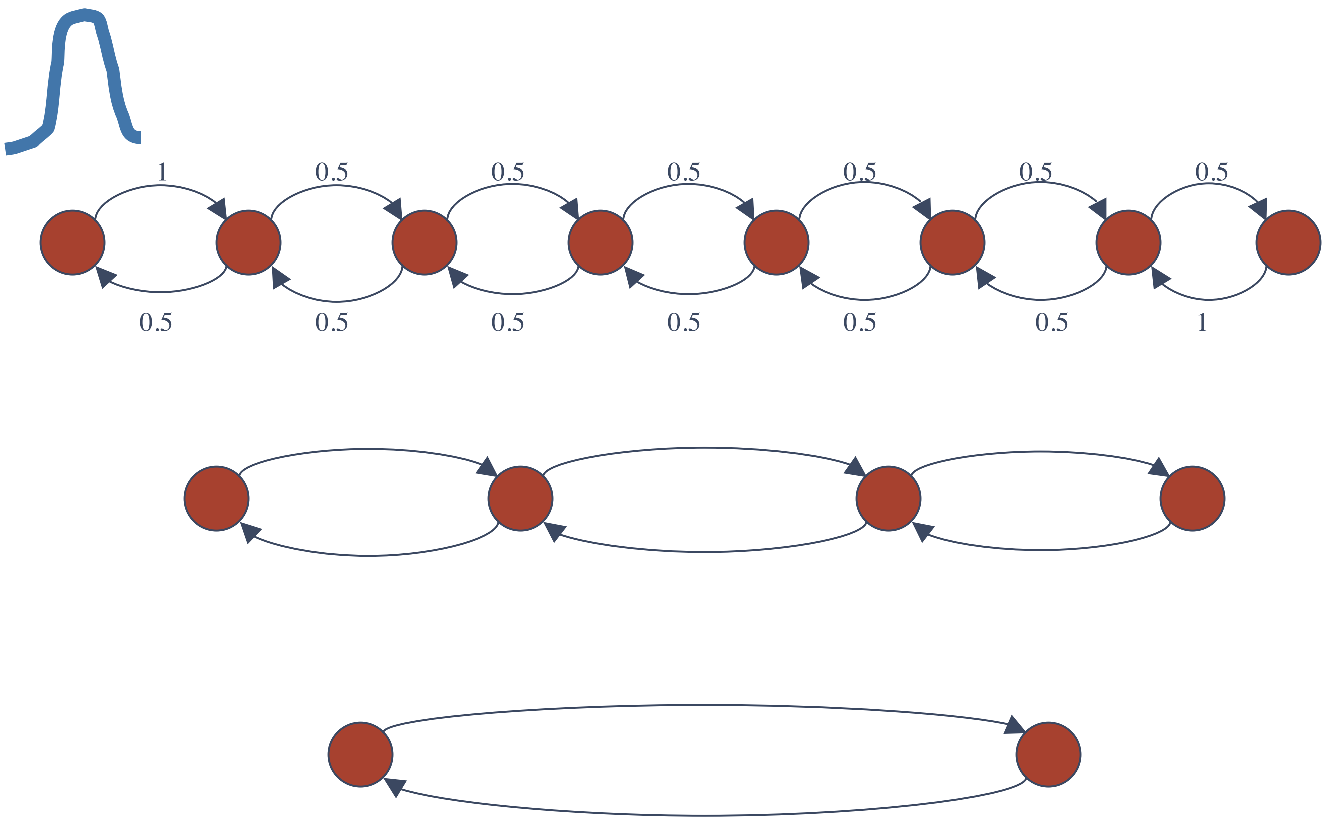
why/when is power method slow?
why multilevel methods?



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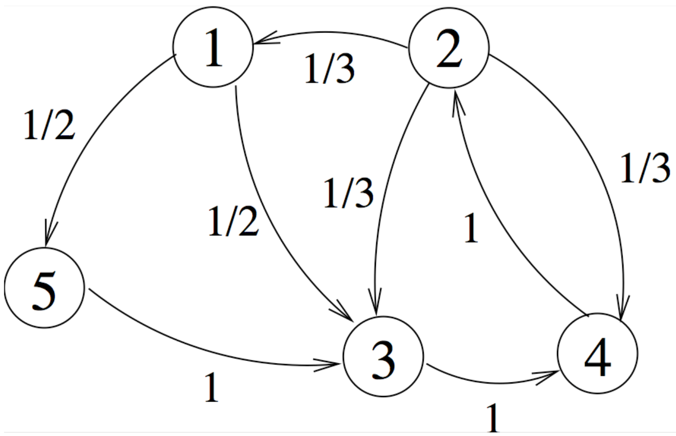
3. multilevel aggregation



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

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

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

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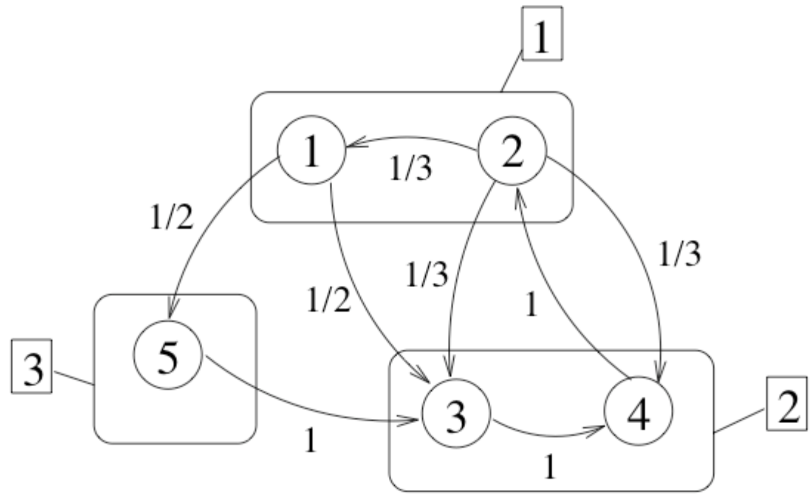
aggregation

- form three coarse, aggregated states

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

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

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



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

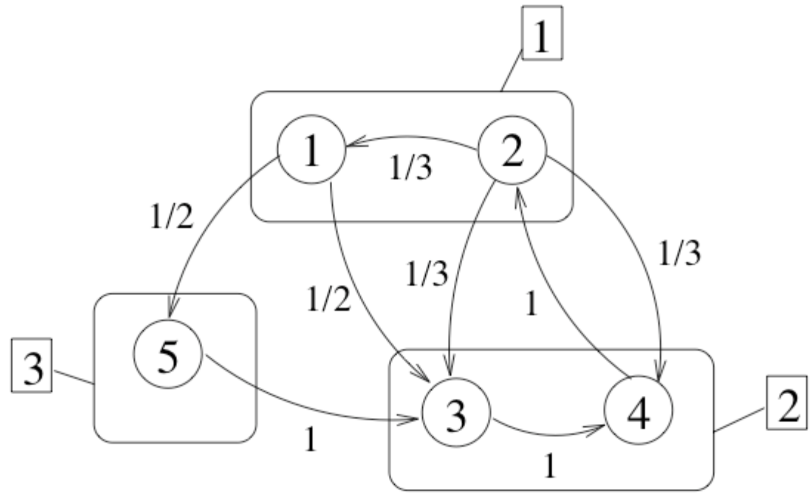
$$\mathbf{x}_c^T = [8/19\;\; 10/19\;\; 1/19]$$

(Simon and Ando, 1961)

matrix form of aggregation

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

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



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

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

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

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

(Krieger, Horton, ... 1990s)

two-level aggregation method

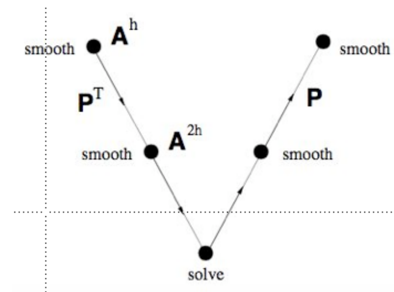
repeat

fine-level relaxation: $\mathbf{x}^* = B\,\mathbf{x}_i$
build Q
build $B_c = Q^T B \,\mathrm{diag}(\mathbf{x}^*)\, Q\, (\mathrm{diag}(Q^T\,\mathbf{x}^*))^{-1}$
coarse-level solve: $B_c\,\mathbf{x}_c = \mathbf{x}_c$
fine-level update: $\mathbf{x}_{i+1} = \mathrm{diag}(\mathbf{x}^*)\, Q\, (\mathrm{diag}(Q^T\,\mathbf{x}^*))^{-1}\mathbf{x}_c$

(note: there is a convergence proof for this two-level method, Marek and Mayer 1998, 2003)

multilevel aggregation method

Algorithm: Multilevel Adaptive Aggregation method (V-cycle)



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

begin

$\mathbf{x} \leftarrow \mathsf{Relax}(A, \mathbf{x}) \quad \nu_1$ times

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

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

$A_c = R\, A\, P$

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

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

$\mathbf{x} \leftarrow \mathsf{Relax}(A, \mathbf{x}) \quad \nu_2$ times

end

(Krieger, Horton 1994)

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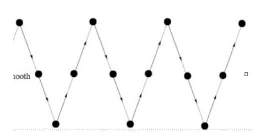
(note: O(n) work per cycle:
n + n/2 + n/4 + n/8 + ... < 2 n)



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aggregation strategy

- fine-level relaxation should efficiently distribute probability within aggregates (smooth out local, high-frequency errors)

- coarse-level update will efficiently distribute probability between aggregates (smooth out global, low-frequency errors)

- base aggregates on 'strong connections' in $A \, \mathrm{diag}(\mathbf{x}_i)$

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aggregation strategy

scaled problem matrix:

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

strong connection: coefficient is large in either of rows *i* or *j*

$$-\hat{a}_{ij} \geq \theta \max_{k \neq i}\{-\hat{a}_{ik}\} \quad \text{or} \quad -\hat{a}_{ji} \geq \theta \max_{k \neq j}\{-\hat{a}_{jk}\}$$

($\theta \in (0,1)$, $\theta=0.25$)

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‘neighbourhood’ aggregation strategy

Algorithm 2: neighborhood-based aggregation, $\{Q_J\}_{J=1}^m \longleftarrow$ **Neighbourhood-hoodAgg** $(A\,\mathrm{diag}(\mathbf{x}),\ \theta)$

For all points i, build strong neighbourhoods $\mathcal{N}_i$ based on $A\,\mathrm{diag}(\mathbf{x})$ and θ.
Set $\mathcal{R} \leftarrow \{1, ..., n\}$ and $J \leftarrow 0$.

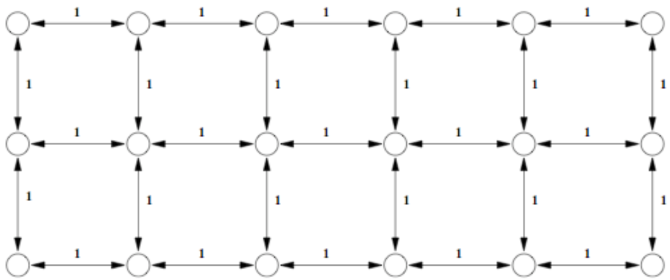
```
/* 1st pass:  assign entire neighborhoods to aggregates */
```

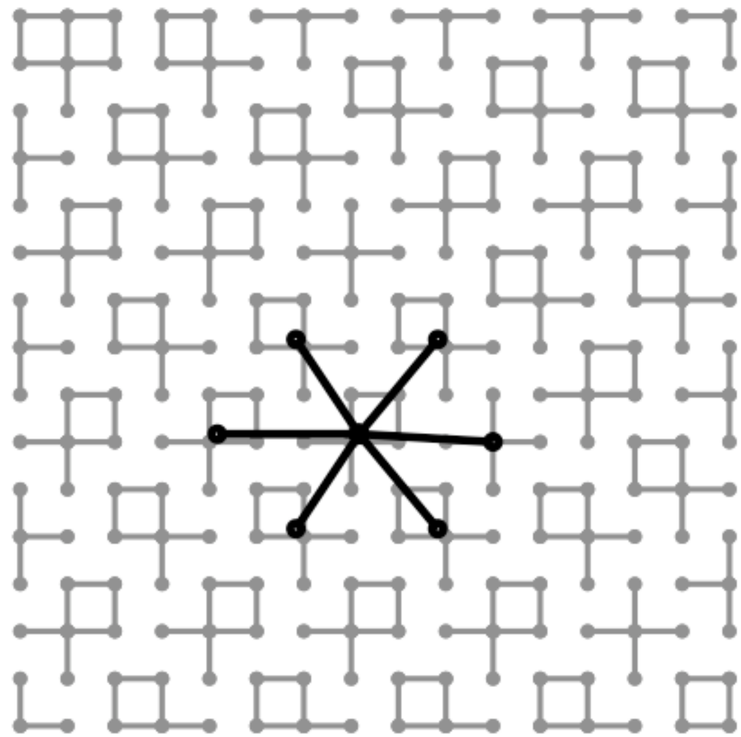
for $i \in \{1, ..., n\}$ **do**
    if $(\mathcal{R} \cap \mathcal{N}_i) = \mathcal{N}_i$ **then**
        $J \leftarrow J + 1$.
        $Q_J \leftarrow \mathcal{N}_i,\ \hat{Q}_J \leftarrow \mathcal{N}_i$.
        $\mathcal{R} \leftarrow \mathcal{R} \setminus \mathcal{N}_i$.
    end
end
$m \leftarrow J$.

```
/* 2nd pass:  put remaining points in aggregates they are most
   connected to */
```

while $\mathcal{R} \neq \emptyset$ **do**
    Pick $i \in \mathcal{R}$ and set $J \leftarrow \mathrm{argmax}_{K=1,...,m}\ \mathrm{card}\,(\mathcal{N}_i \cap Q_K)$.
    Set $\hat{Q}_J \leftarrow Q_J \cup \{i\}$ and $\mathcal{R} \leftarrow \mathcal{R} \setminus \{i\}$.
end
for $J \in \{1, ..., m\}$ **do** $Q_J \leftarrow \hat{Q}_J$.

aggregation: periodic 2D lattice





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

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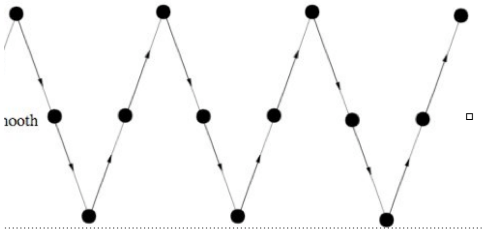
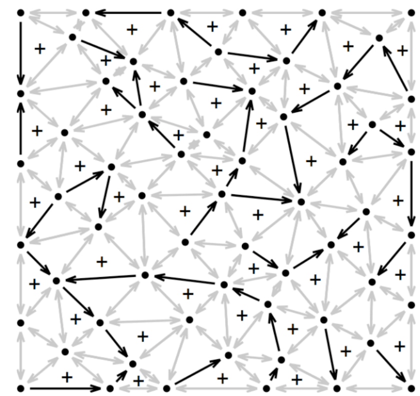
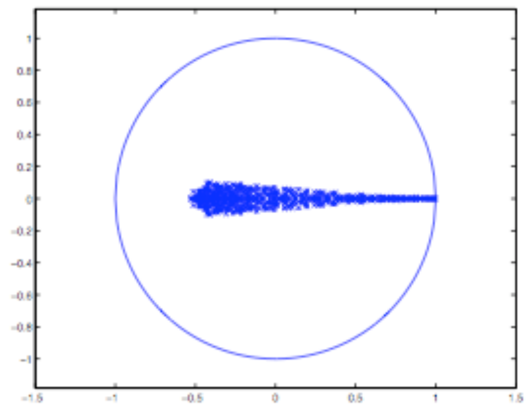
numerical results: aggregation multigrid for random walk problem



	1-level	aggregation		
n	iterations	iterations	C_{op}	levels
128	322	95	1.12	3
256	494	107	1.13	3
512	1010	156	1.14	3
1024	1768	220	1.15	4
2048		352	1.15	4

$$C_{op} = \frac{\sum_{l=0} \mathrm{nonzeros}(A_l)}{nonzeros(A_0)}$$





does not work as well as we would like!

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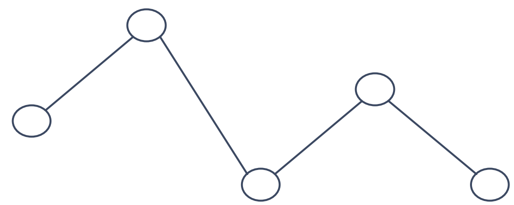
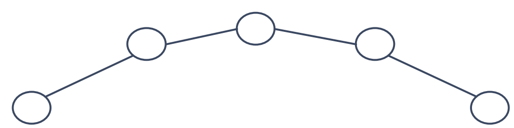
4. overlapping aggregates: we need 'smoothed aggregation'...

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

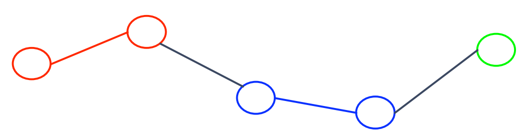


$$Q = \begin{bmatrix} 1 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

after smoothing:

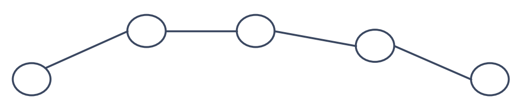


coarse grid correction with Q:



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

coarse grid correction with Q_s:



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smoothed aggregation

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

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

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

$$w = 0.7$$

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

$$R_s = Q^T\, (I + w\, A\, D^{-1})$$

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smoothed aggregation: a problem with signs

- smoothed coarse level operator:

$$\begin{aligned} A_{cs} &= R_s\,(D-(L+U))\,P_s \\ &= R_s\,D\,P_s - R_s\,(L+U)\,P_s \end{aligned}$$

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

- problem: A_{cs} is not a singular M-matrix (signs wrong)
- solution:
  lumping approach
- well-posedness of this approach shown in *De Sterck et al., SIAM J. Sci. Comp., 2009*

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

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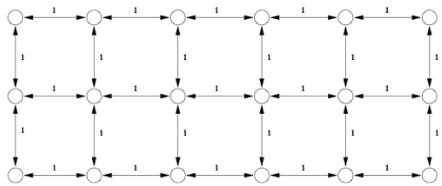
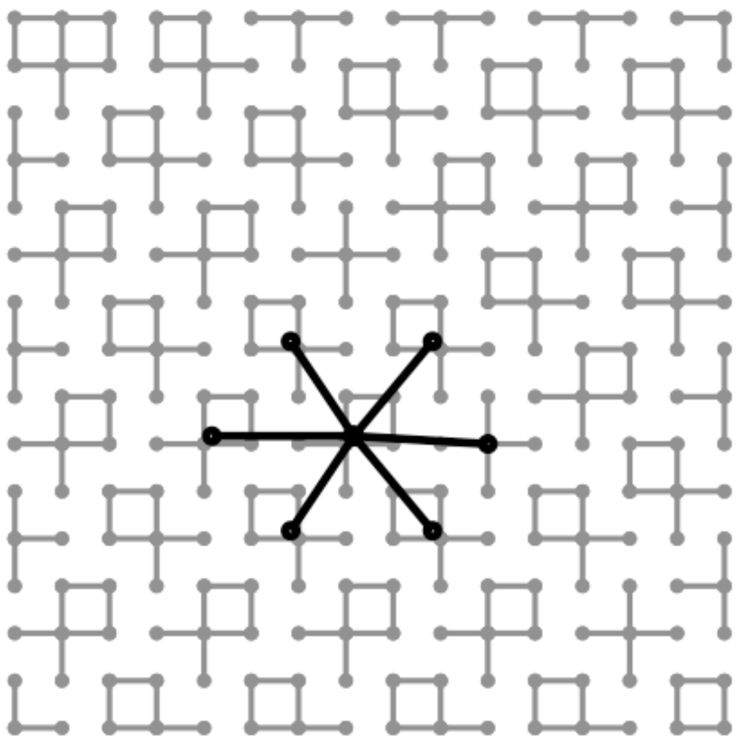
smoothed aggregation: periodic 2D lattice

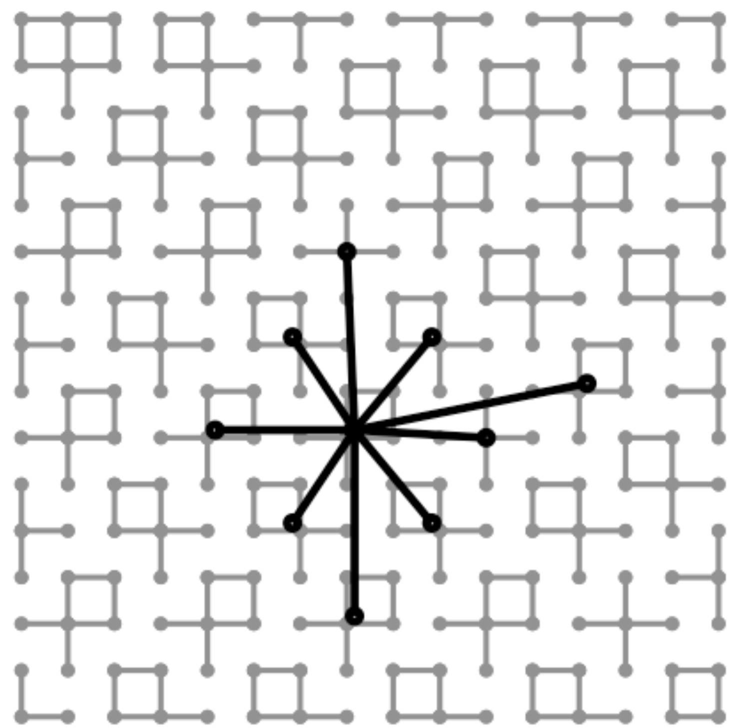


$$A_c = R_s \, A \, P_s$$

unsmoothed

smoothed





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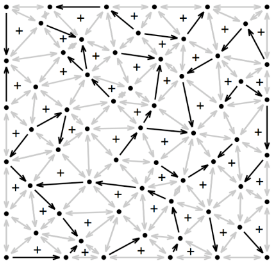
numerical results: smoothed aggregation multigrid for random graph problem



	1-level	aggregation			smoothed aggregation			
n	iterations	iterations	C_{op}	levels	iterations	C_{op}	levels	R_{lump}
128	322	95	1.12	3				
256	494	107	1.13	3				
512	1010	156	1.14	3	36	1.28	3	2.5e-4
1024	1768	220	1.15	4	39	1.31	4	1.2e-4
2048		352	1.15	4	33	1.31	4	6.0e-5
4096					46	1.35	4	2.3e-4
8192					35	1.37	4	2.0e-4
16384					51	1.36	5	9.4e-5
32768					43	1.38	5	1.6e-4

$$C_{op} = \frac{\sum_{l=0} \text{nonzeros}(A_l)}{nonzeros(A_0)}$$

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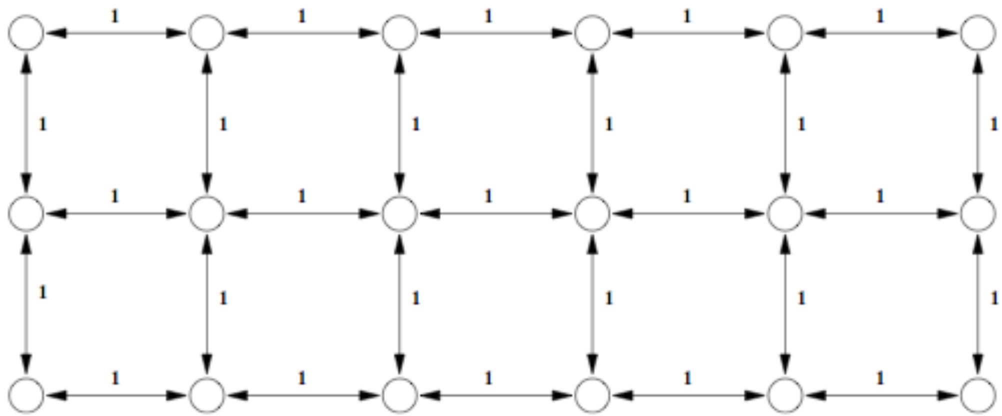
numerical results: smoothed aggregation multigrid for periodic 2D lattice problem



	1-level	aggregation			smoothed aggregation			
n	iterations	iterations	C_{op}	levels	iterations	C_{op}	levels	R_{lump}
64	197	47	1.23	3	16	1.26	3	0
256	760	96	1.26	3	17	1.34	3	0
1024	2411	242	1.25	4	17	1.32	4	0
4096		328	1.26	5	18	1.34	5	0
16384					18	1.33	5	0
32768					19	1.34	6	0

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numerical results: smoothed aggregation multigrid for tandem queueing network problem

FIG. 5.6. *Tandem queueing network.*

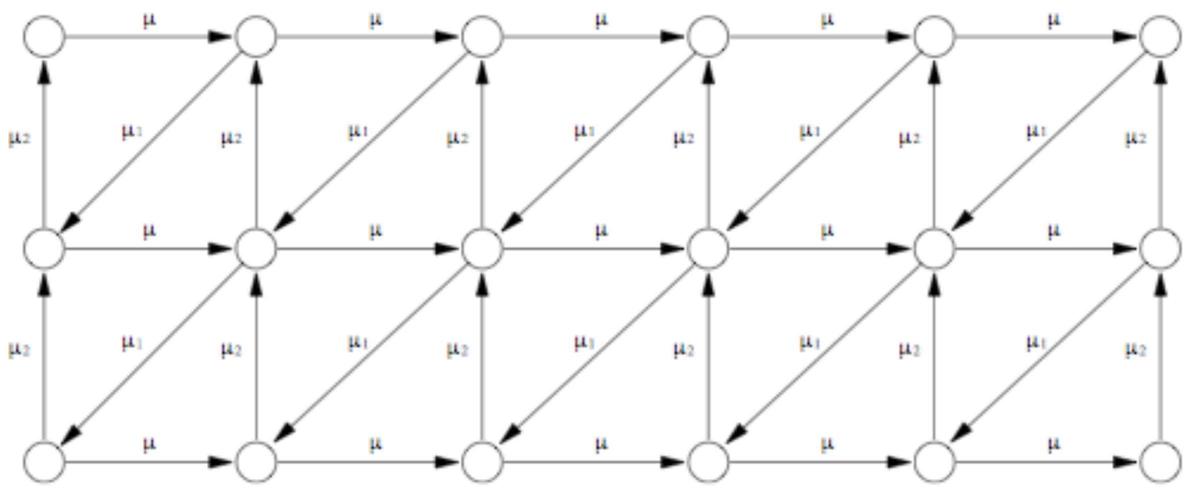

FIG. 5.7. *Graph for tandem queueing network.*

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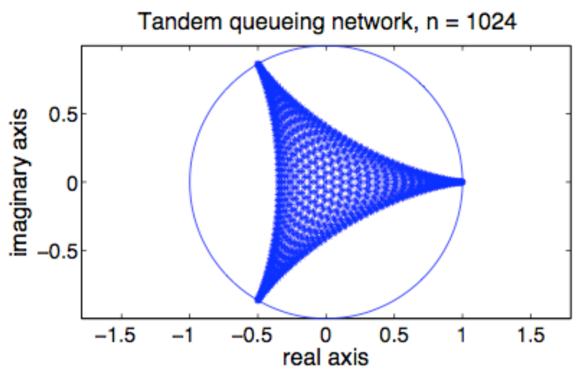
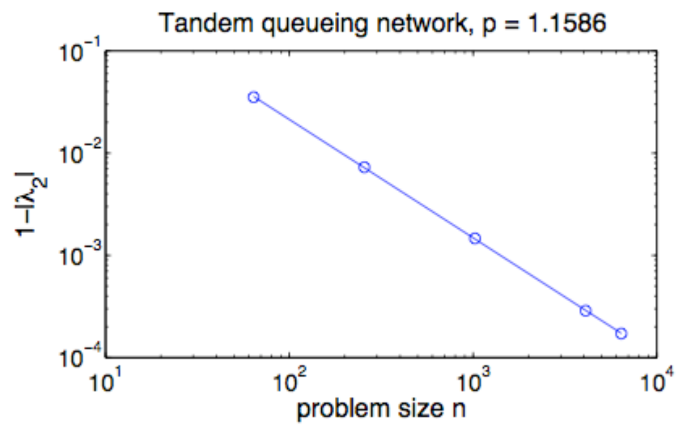
numerical results: smoothed aggregation for tandem queueing network problem





	1-level	aggregation			smoothed aggregation			
n	iterations	iterations	C_{op}	levels	iterations	C_{op}	levels	R_{lump}
256	967	103	1.23	3	17	1.25	3	1.7e-3
1024	4004	256	1.21	4	20	1.25	4	1.4e-3
4096		425	1.22	4	19	1.24	4	9.5e-4
16384					22	1.24	5	5.1e-4
65536					18	1.25	6	3.5e-4

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6. discussion

- multilevel smoothed aggregation gets us close to O(n) algorithm for some slowly mixing Markov chains
- slowly mixing Markov chains are OK (their stationary distribution can be calculated efficiently)

- very little theory exists for these methods
  - convergence
  - optimal convergence (O(n))
- there is optimal convergence theory for SPD matrix discretizations of some elliptic PDEs (Brandt, Stueben, ...)

discussion

- we have several variants of these algorithms that also work well

- we are working on similar multilevel aggregation approach to speed up Markov Chain Monte Carlo methods for lattice spin systems (make groups of groups ... of spins and flip them together)

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7. questions

- any suggestions for further test problems for our algorithms? (large, sparse, irreducible, slowly mixing)
  - real-life problems
  - theoretical models that people care about
- any suggestions for 'pathological' chains that will 'break' our algorithm?
- which classes of Markov chains will this work well for, and which classes not? (how can these classes be characterized?)
- (optimal) convergence proof?

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thanks!

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