Algebraic Multigrid for the Singular Value Problem

UNIVERSITY OF WATERLOO

uwaterloo.ca

Hans De Sterck

Department of Applied Mathematics
University of Waterloo

1. introduction

goal:

compute a few of the largest or smallest singular values of a rectangular matrix $A \in I\!R^{m \times n}$ and their associated singular vectors

introduction

- SVD of $A \in \mathbb{R}^{m \times n}$

$$A = U \Sigma V^t \qquad\qquad m \geq n$$

$$U \in \mathbb{R}^{m \times m} \qquad U^t U = I_m$$
$$V \in \mathbb{R}^{n \times n} \qquad V^t V = I_n$$

$$\sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_l \geq 0 \qquad l = \min(m, n)$$

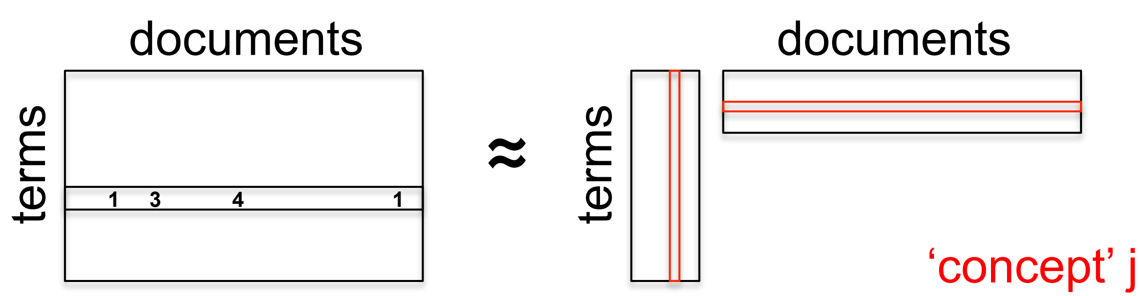
- for definiteness: we seek n_b dominant singular triplets (σ_j, u_j, v_j)

$$A v_j = \sigma_j u_j,$$
$$A^t u_j = \sigma_j v_j.$$

UNIVERSITY OF
WATERLOO

introduction

- why interest in dominant singular triplets?
  - the *k* dominant triplets give the best rank-*k* approximation to *A*
  - applications: principal component analysis
  - applications: term-document matrices



$$A \approx U_k \Sigma_k V_k^t$$

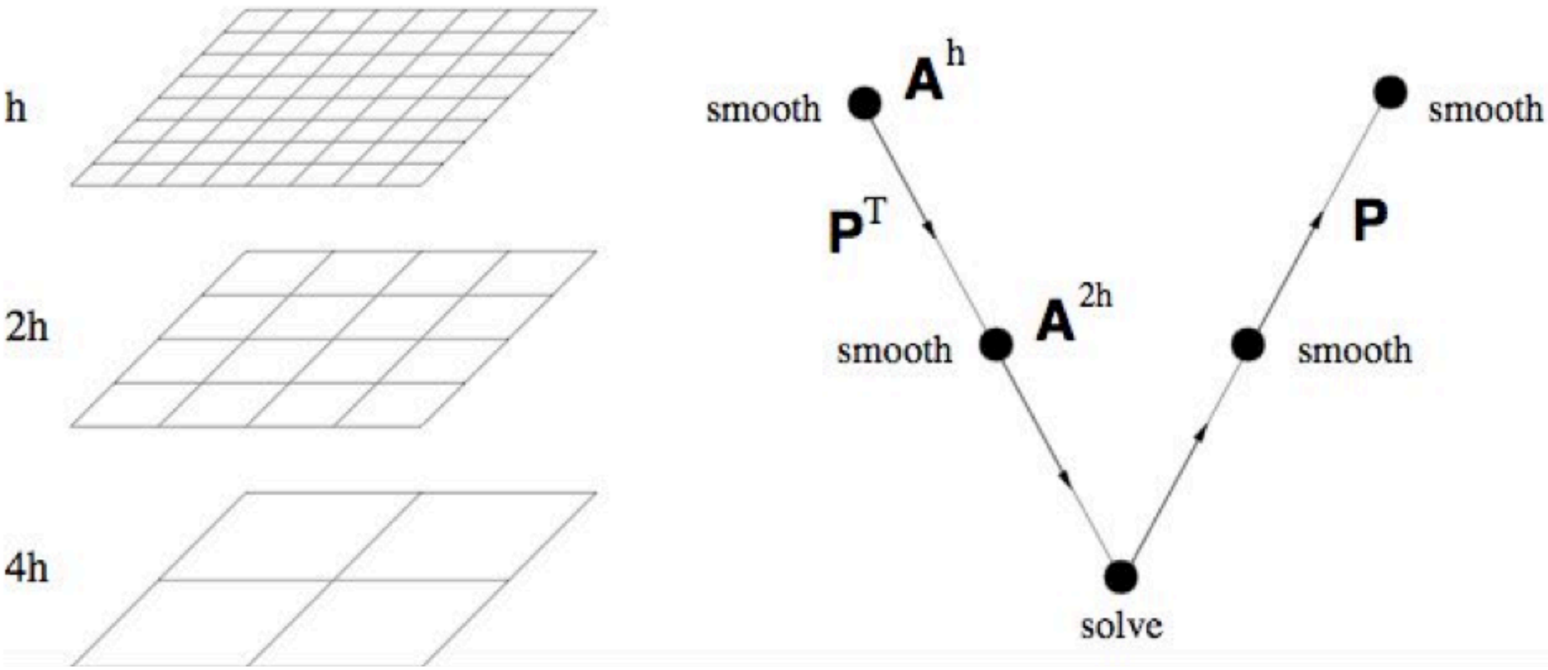
(note: nonnegative factorization is better)

introduction

- why consider (algebraic) multigrid (AMG) for dominant singular triplets?
  - for certain types of problems, multigrid may outperform other methods
  - because we can! ;-)

introduction

- algebraic multigrid V-cycle



UNIVERSITY OF WATERLOO

introduction

$$A = U \Sigma V^t$$

- special case:
  A symmetric positive definite (SPD)

$$A = V \Lambda V^t$$

$$A v_j = \lambda_j v_j$$

- our SVD approach will be applicable to SPD eigenproblem as a special case (or the other way around)

UNIVERSITY OF WATERLOO

2. AMG for SPD eigenproblems

1) AMG for minimal eigenpairs by Borzi and Borzi

INTERNATIONAL JOURNAL FOR NUMERICAL METHODS IN ENGINEERING
Int. J. Numer. Meth. Engng 2006; **65**:1186–1196
Published online 19 September 2005 in Wiley InterScience (www.interscience.wiley.com). DOI: 10.1002/nme.1478

Algebraic multigrid methods for solving generalized eigenvalue problems

Alfio Borzì[1,‡] and Giuseppe Borzì[2,*,†]

- use standard AMG interpolation to build *P* (for elliptic PDE)

- *P* contains slow-to-converge near-nullspace components in its range (including 'small' eigenvectors)

- additive correction formula: $$v_j^{(i+1)} = v_j^{(i)} + P\, e_c$$

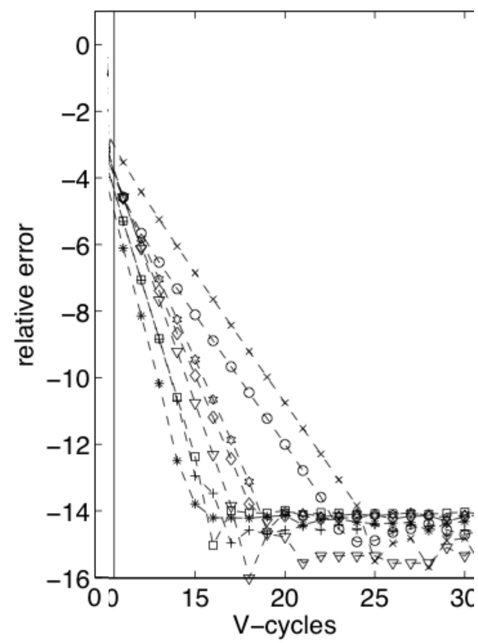
UNIVERSITY OF WATERLOO

AMG for SPD eigenproblems

AMG for minimal eigenpairs by Borzi and Borzi

- use standard AMG interpolation to build *P* (for elliptic PDE)
- *P* contains slow-to-converge near-nullspace components in its range (including ‘small’ eigenvectors)
- additive correction formula:

$$v_j^{(i+1)} = v_j^{(i)} + P\, e_c$$



- plus: converges with high accuracy
- minus: not flexible, only works for small eigenvectors for ‘easy’ elliptic PDEs

UNIVERSITY OF WATERLOO

AMG for SPD eigenproblems

2) adaptive AMG for minimal eigenpairs by Kushnir, Galun and Brandt

IEEE TRANSACTIONS ON PATTERN ANALYSIS AND MACHINE INTELLIGENCE, VOL. 32, NO. XX, XXXXXXX 2010

Efficient Multilevel Eigensolvers with Applications to Data Analysis Tasks

Dan Kushnir, Meirav Galun, and Achi Brandt

(and related work by Brannick, Kahl, Livshits, and others)

- build *P* via bootstrap AMG (BAMG) approach
- *P* approximately fits all desired eigenvectors in its range
- multiplicative update formula: $v_j^{(i+1)} = P\, v_{c,j}$

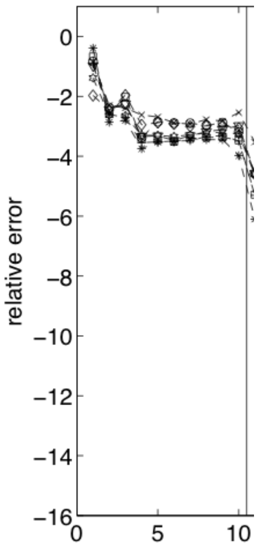
UNIVERSITY OF WATERLOO

AMG for SPD eigenproblems

adaptive AMG for minimal eigenpairs by Kushnir, Galun and Brandt

- build *P* via bootstrap AMG (BAMG) approach
- *P* approximately fits <u>all</u> desired eigenvectors in its range
- multiplicative update formula:

$$v_j^{(i+1)} = P\, v_{c,j}$$

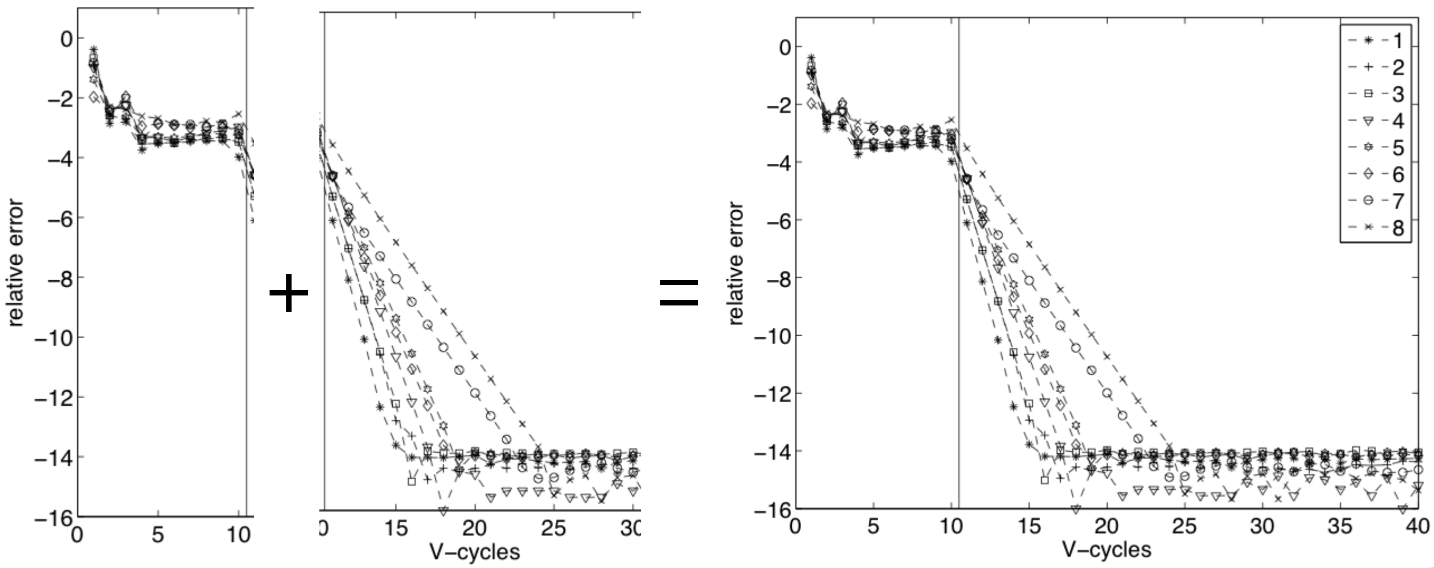


- plus: flexible, adapts to eigenvectors sought
- minus: accuracy limited by accuracy by which the desired eigenvectors are collectively fitted by P

UNIVERSITY OF WATERLOO

our approach

- combine 2) with 1): combine multiplicative (setup) phase (build *P*) with additive (solve) phase (like adaptive AMG for linear equation systems)
- extend to SVD computation



UNIVERSITY OF WATERLOO

3. multiplicative phase: coarse-level equations

- goals of the multiplicative (setup) phase:
  - find n_b tentative dominant triplets (σ_j, u_j, v_j)
  - determine interpolation operators P and Q that approximately contain the tentative singular vectors in their ranges collectively, on all levels

UNIVERSITY OF WATERLOO

multiplicative phase: coarse-level equations

- assume we know triplet (σ, u, v) satisfying

$$A\,v = \sigma\,u,$$
$$A^t\,u = \sigma\,v.$$

$$A \in \mathbb{R}^{m\times n}$$

- assume *P* and *Q* have *u* and *v* exactly in their ranges:

$$u = P\,u_c,$$
$$v = Q\,v_c,$$

$\boxed{P}$

$$P \in \mathbb{R}^{m\times m_c}$$
$$Q \in \mathbb{R}^{n\times n_c}$$

- coarse equations:

$$P^t\,A\,Q\,v_c = \sigma\,P^t\,B\,P\,u_c,$$
$$Q^t\,A^t\,P\,u_c = \sigma\,Q^t\,C\,Q\,v_c,$$

$B = I_m \quad C = I_n$

multiplicative phase: coarse-level equations

- assume we know triplet (σ, u, v)

$$A\,v = \sigma\,u, \qquad u = P\,u_c, \qquad P^t\,A\,Q\,v_c = \sigma\,P^t\,B\,P\,u_c,$$

$$A^t\,u = \sigma\,v. \qquad v = Q\,v_c, \qquad Q^t\,A^t\,P\,u_c = \sigma\,Q^t\,C\,Q\,v_c,$$

- define coarse-level operators and equations

$$A_c = P^t\,A\,Q,$$
$$B_c = P^t\,B\,P,$$
$$C_c = Q^t\,C\,Q,$$

$$A_c\,v_c = \sigma\,B_c\,u_c,$$
$$A_c^t\,u_c = \sigma\,C_c\,v_c.$$

- coarse level will help: solving coarse equations (cheaper) gives exact answer in one step!
- do this approximately, and recursively (V-cycle)

UNIVERSITY OF WATERLOO

4. an uncommon (new?) generalized SVD

- recall generalized symmetric eigenvalue problem for

$$A,\, B \in \mathbb{R}^{m\times m} \;\; (B \text{ SPD})$$

$$A\,v = \lambda\,B\,v \qquad A = B\,V\,\Lambda\,V^t \qquad V^t\,B\,V = I_m$$

- we have to solve coarse-grid problem

$$A\,v = \sigma\,B\,u, \qquad A \in \mathbb{R}^{m\times n}$$

$$A^t\,u = \sigma\,C\,v, \qquad B \in \mathbb{R}^{m\times m} \;\; C \in \mathbb{R}^{n\times n}\,(B,\, C \text{ SPD})$$

- we have to generalize the SVD problem

$$A\,v = \sigma\,u, \qquad A = U\,\Sigma\,V^t$$

$$A^t\,u = \sigma\,v.$$

UNIVERSITY OF
WATERLOO

an uncommon (new?) generalized SVD

$$A \in \mathbb{R}^{m \times n} \qquad\qquad \begin{aligned} A\,v &= \sigma\,B\,u, \\ A^t\,u &= \sigma\,C\,v, \quad (3.6) \end{aligned}$$

DEFINITION 3.1 (Generalized singular value decomposition). *The generalized singular value decomposition of* $A \in \mathbb{R}^{m\times n}$ *with respect to* $B \in \mathbb{R}^{m\times m}$ *and* $C \in \mathbb{R}^{n\times n}$, *with* B *and* C *SPD, is given by*

$$A = B\,U\,\Sigma\,V^t\,C, \tag{3.7}$$

with $U \in \mathbb{R}^{m\times m}$, $V \in \mathbb{R}^{n\times n}$ *and* $\Sigma \in \mathbb{R}^{m\times n}$. *The columns of* U *are called the left generalized singular vectors, and the columns of* V *are called the right generalized singular vectors. They satisfy the orthogonality relations* $U^t\,B\,U = I_m = U\,B\,U^t$ *and* $V^t\,C\,V = I_n = V\,C\,V^t$. *Matrix* Σ *has the* $l = \min(m,n)$ *real nonnegative generalized singular values* $\sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_l \geq 0$ *on its diagonal. Eqs. (3.6) are called the generalized singular value problem for matrix* A *with respect to matrices* B *and* C.

- this appears to be uncommon in the literature

UNIVERSITY OF WATERLOO

first way to compute the generalized SVD $A = B\,U\,\Sigma\,V^t\,C,$

THEOREM 3.2. *Generalized SVD (3.7) has the same existence and uniqueness properties as the standard SVD.*

Proof. This follows from a simple change of variables: with

$$\begin{aligned} T &= B^{1/2}\,U, \\ W &= C^{1/2}\,V, \\ D &= B^{-1/2}\,A\,C^{-1/2}, \end{aligned} \tag{3.8}$$

generalized SVD (3.7) can be rewritten as a standard SVD

$$D = T\,\Sigma\,W^t. \tag{3.9}$$

UNIVERSITY OF WATERLOO

second way to compute the generalized SVD $A = B\,U\,\Sigma\,V^t\,C$,

THEOREM 3.3. *Let $A \in \mathbb{R}^{m\times n}$, $B \in \mathbb{R}^{m\times m}$ and $C \in \mathbb{R}^{n\times n}$, with B and C SPD. Let $l = \min(m,n)$. Then generalized eigenvalue problem*

$$\left(\begin{bmatrix} 0 & A \\ A^t & 0 \end{bmatrix} - \sigma \begin{bmatrix} B & 0 \\ 0 & C \end{bmatrix} \right) \begin{bmatrix} u \\ v \end{bmatrix} = 0, \tag{3.13}$$

has $m+n$ solution triplets (σ, u, v) with linearly independent eigenvectors $[u^t\, v^t]^t \neq 0$. There are l independent solutions with $\sigma_j \geq 0$ and vectors u_j and v_j satisfying orthogonality relations $u_j^t\, B\, u_i = \delta_{i,j}$ and $v_j^t\, C\, v_i = \delta_{i,j}$ $(j = 1, \ldots, l)$. The triplets (σ_j, u_j, v_j) are the generalized singular triplets of A with respect to B and C. Furthermore, there are l independent solutions $(-\sigma_j, u_j, -v_j)$. Finally, there are $\mathrm{abs}(m-n) = m+n-2\,l$ independent solutions with $\sigma = 0$ and either $u = 0$ or $v = 0$.

UNIVERSITY OF WATERLOO

third way to compute the generalized SVD $A = B\,U\,\Sigma\,V^t\,C$,

$$(A^t\,B^{-1}\,A)\,v = \sigma^2\,C\,v,$$
$$(A\,C^{-1}\,A^t)\,u = \sigma^2\,B\,u.$$

UNIVERSITY OF WATERLOO

5. multiplicative phase: BAMG V-cycles

- find n_b tentative dominant triplets (σ_j, u_j, v_j)
- start from n_t random fine-level test vectors
- do relaxation on test vectors using the power method, to obtain first approximations for 'large' singular vectors:
  - start from random v
  - compute new u, σ via $A\,v = \sigma\,u,$
  - compute new v, σ via $A^t\,u = \sigma\,v.$
  - repeat
- determine P and Q to fit the n_t test vectors u and v collectively

$$u = P\,u_c,$$
$$v = Q\,v_c,$$

multiplicative phase: V-cycles

- downwards sweep of first V-cycle: create coarse grids and coarse-level operators P, Q, A_c, B_c, C_c for all levels, using relaxation on n_t initially random test vectors

n_t random test vectors

relax:
$$A_c\, v_c = \sigma\, B_c\, u_c,$$
$$A_c^t\, u_c = \sigma\, C_c\, v_c.$$

build A_c, B_c, C_c:
$$A_c = P^t\, A\, Q,$$
$$B_c = P^t\, B\, P,$$
$$C_c = Q^t\, C\, Q,$$

relax test vectors, coarsen, build P, Q, A_c, B_c, C_c

inject test vectors

relax test vectors, coarsen, build P, Q, A_c, B_c, C_c

inject test vectors

relax test vectors, coarsen, build P, Q, A_c, B_c, C_c

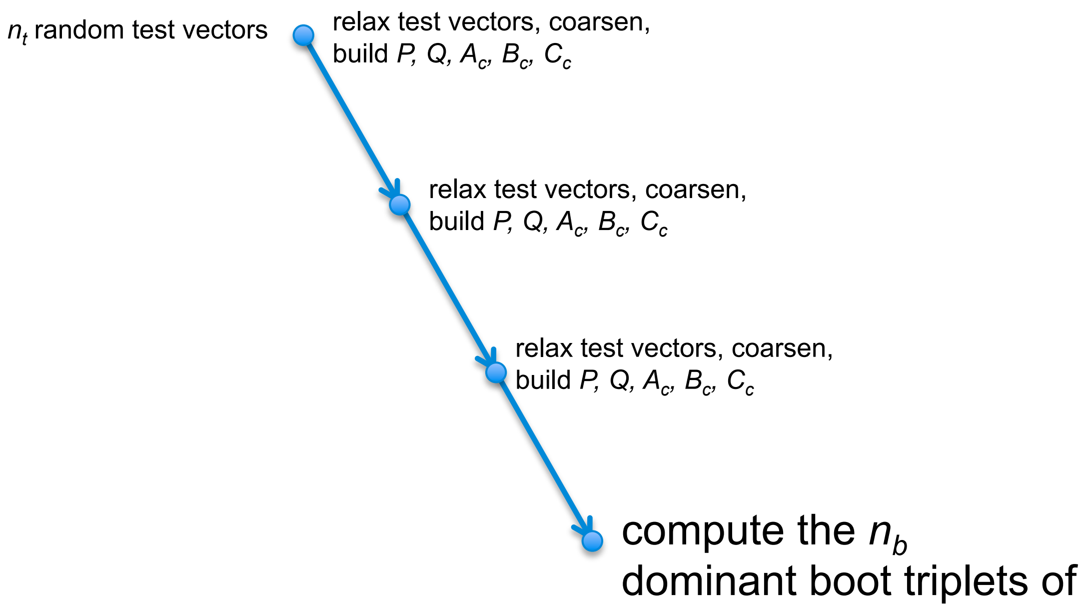
inject test vectors

$$A_c\, v_c = \sigma\, B_c\, u_c,$$
$$A_c^t\, u_c = \sigma\, C_c\, v_c.$$

UNIVERSITY OF WATERLOO

multiplicative phase: V-cycles

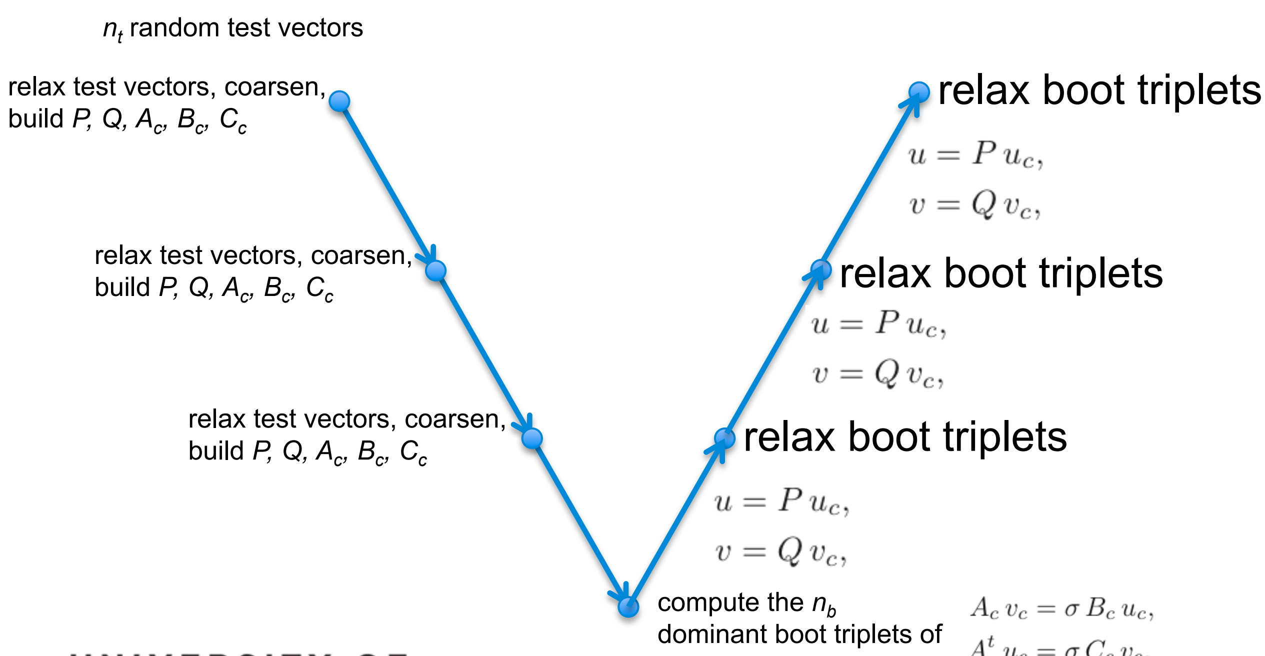
- on the coarsest level: solve the generalized SVD problem, and select the n_b dominant triplets (σ_j, u_j, v_j) as the first (coarse) approximations of the dominant triplets sought (we call these 'boot triplets')



$$A_c\, v_c = \sigma\, B_c\, u_c,$$
$$A_c^t\, u_c = \sigma\, C_c\, v_c.$$

multiplicative phase: V-cycles

- upward sweep of first V-cycle: interpolate the n_b boot triplets up to finer levels, and relax (first fix σ and find u or v, then update σ via Rayleigh quotient formula), on each level



interpolate: $u = P\, u_c,$

$v = Q\, v_c,$

relax: $A_c\, v_c = \sigma\, B_c\, u_c,$

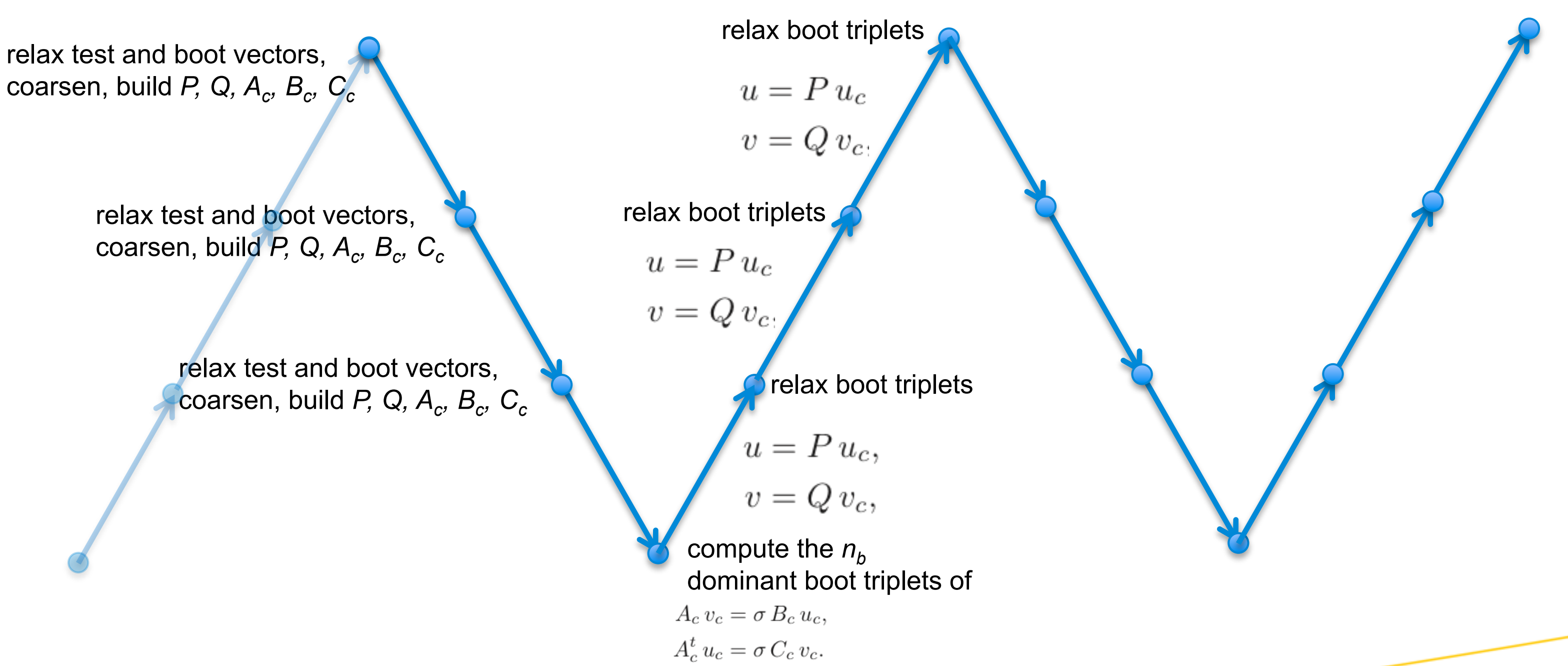
$A_c^t\, u_c = \sigma\, C_c\, v_c.$

$$\sigma = \frac{u^t A v}{(u^t B u)^{1/2}\, (v^t C v)^{1/2}}$$

UNIVERSITY OF WATERLOO

multiplicative phase: V-cycles

- repeat V-cycles until convergence stagnates (*P* and *Q* represent the boot vectors *u* and *v* collectively up to some accuracy)



UNIVERSITY OF WATERLOO

6. multiplicative phase: relaxation

- test vectors: power method on

$$A\,v = \sigma\,B\,u,$$

$$A^t\,u = \sigma\,C\,v,$$

with inexact inversion of *B* and *C* (weighted Jacobi):

$$A^t\,u_j = C\,\bar{v}_j\,, \qquad A\,v_j = B\,\bar{u}_j\,,$$

$$v_j = \bar{v}_j/(\bar{v}_j^t C \bar{v}_j)^{1/2} \qquad u_j = \bar{u}_j/(\bar{u}_j^t B \bar{u}_j)^{1/2}$$

$$\bar{v}_j^{(i+1)} = \bar{v}_j^{(i)} - \omega_J\,D_C^{-1}\,(C\,\bar{v}_j^{(i)} - A^t\,u_j)$$

UNIVERSITY OF WATERLOO

multiplicative phase: relaxation

- boot vectors: block Gauss-Seidel (fix σ) on

$$A\,v = \sigma\,B\,u + \kappa,$$
$$A^t\,u = \sigma\,C\,v + \tau.$$

with inexact inversion of *B* and *C* (weighted Jacobi):

$$u_j^{(i+1)} = u_j^{(i)} - \omega_J\,D_B^{-1}\,(B\,u_j^{(i)} - (A\,v_j - \kappa)/\sigma_j).$$

- update σ using Rayleigh quotient formula

$$\sigma = \frac{u^t A v}{(u^t B u)^{1/2}\,(v^t C v)^{1/2}}$$

UNIVERSITY OF
WATERLOO

7. multiplicative phase: building *P* and *Q*

- coarsening: use standard (one-pass) AMG coarsening on AA^t for the *u*-variables, and on A^tA for the *v*-variables (correlations ...)
- in the future: coarsen directly using *A*
- try 'general' strength of connection formula

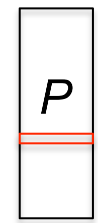
$$\text{variable } i \text{ is strongly influenced by variable } j$$
$$\Updownarrow$$
$$|n_{i,j}| \geq \theta \sum_k |n_{i,k}|$$

- interpolation stencils for F-points are formed by strongly influencing C-points (sparsity of *P* and *Q*)

UNIVERSITY OF WATERLOO

multiplicative phase: building *P* and *Q*

- determine the weights in *P* and *Q* via least-squares fitting of the test (and boot) vectors (injected to the C-points)
- (for *P*) for each F-point *i*:



$$u_k^i = \sum_{j \in C_u^i} p_{i,j} u_{k,c}^j \quad (k = 1, \ldots, n_f)$$

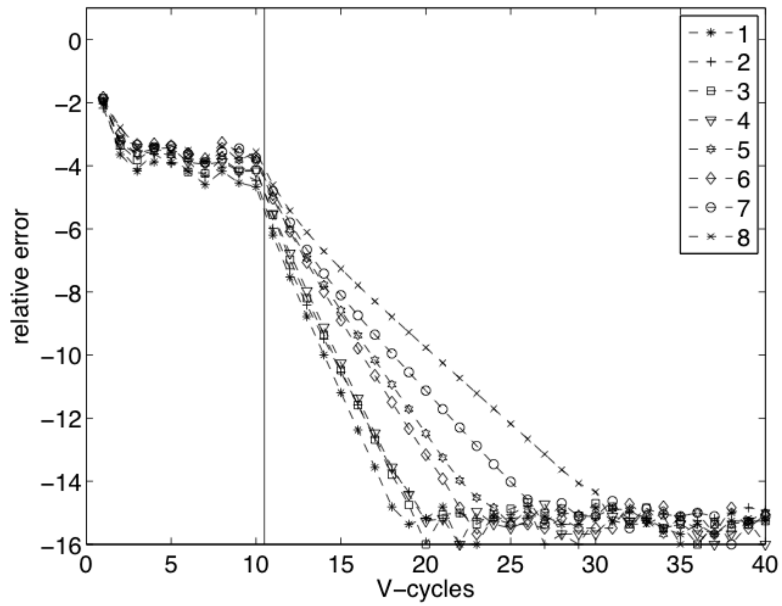
(one equation per test or booth vector *k*)

(over-determined LS system: more test+boot vectors than size of largest stencil)

- larger weight for boot vectors than for test vectors (proportional to σ)

OK, where are we...

- I have discussed how to do the first phase of the algorithm (multiplicative, find tentative triplets starting from random test vectors, build *P* and *Q*, bootstrap AMG)
- I will now discuss the second phase (additive V-cycles, use ‘frozen’ *P* and *Q*)



UNIVERSITY OF WATERLOO

8. additive phase: V-cycles

- for each tentative boot triplet, keep *σ* fixed, improve *u* and *v* in additive-correction V-cycle
- coarse-level equations:

$$\begin{aligned} A\,v_j - \sigma_j\,B\,u_j &= \kappa_j, \\ A^t\,u_j - \sigma_j\,C\,v_j &= \tau_j, \end{aligned} \quad \Longrightarrow \quad \begin{aligned} A_c\,v_{j,c} - \sigma_j\,B_c\,u_{j,c} &= P^t\,r_j, \\ A_c^t\,u_{j,c} - \sigma_j\,C_c\,v_{j,c} &= Q^t\,s_j, \end{aligned}$$

- correction formula: $$\begin{aligned} u_j^{(i+1)} &= u_j^{(i)} + P\,u_{j,c}, \\ v_j^{(i+1)} &= v_j^{(i)} + Q\,v_{j,c}, \end{aligned}$$
- *P* and *Q* from setup phase can be used: additive errors lie approximately in their ranges

9. additive phase: Ritz projection

- on the finest level, all boot triplets (including the σs) are updated after each set of V-cycles
- seek new $u_j \in \mathcal{U},\ v_j \in \mathcal{V}$ s.t

$$\langle u, A\, v_j - \sigma_j\, B\, u_j \rangle_B = 0 \qquad \forall u \in \mathcal{U},$$
$$\langle v, A^t\, u_j - \sigma_j\, C\, v_j \rangle_C = 0 \quad \forall v \in \mathcal{V}.$$

- leads to very small generalized singular value problem

$$\left\langle y, \hat{U}^t\, A\, \hat{V}\, z_j - \sigma_j\, \hat{U}^t\, B\, \hat{U}\, y_j \right\rangle = 0 \quad \forall y \in \mathbb{R}^{m_c},$$
$$\left\langle z, \hat{V}^t\, A^t\, \hat{U}\, y_j - \sigma_j\, \hat{V}^t\, C\, \hat{V}\, z_j \right\rangle = 0 \quad \forall z \in \mathbb{R}^{n_c}.$$

UNIVERSITY OF WATERLOO

10. specializations and extensions

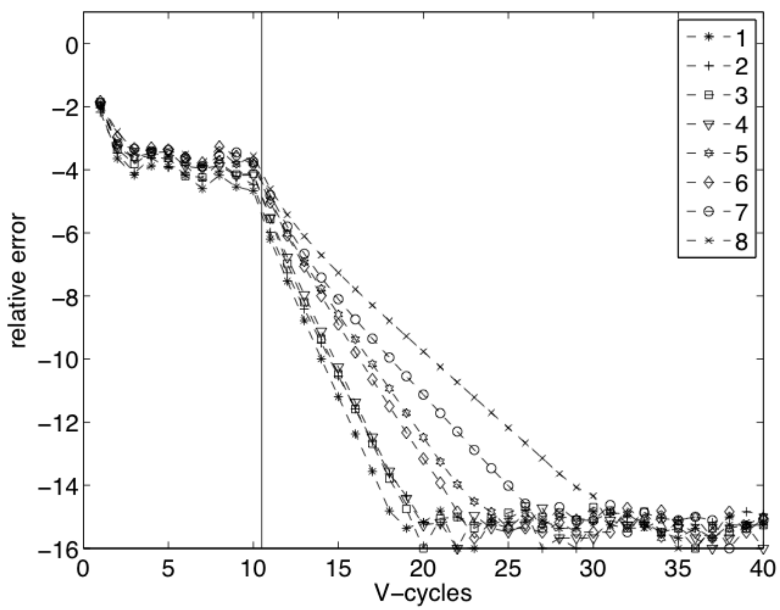
- square matrices (use A or A^t for coarsening)
- SPD matrices: only need A, B, P
- minimal singular triplets and eigenpairs:
  - algorithm is self-learning (adaptive), so we only need to change the relaxation and the coarsest-level solves of the multiplicative phase
  - use Kaczmarz relaxation on blocks of

$$A\,v = \sigma\,B\,u + \kappa,$$
$$A^t\,u = \sigma\,C\,v + \tau.$$

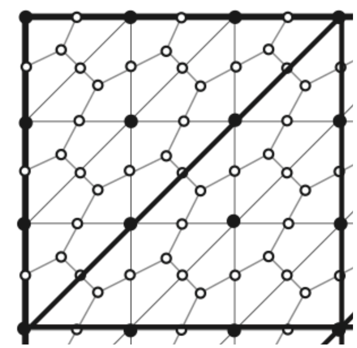
UNIVERSITY OF WATERLOO

11. numerical results

1) high-order finite volume element Laplacian on unit square (square, nonsymmetric, 961x961)



largest singular values



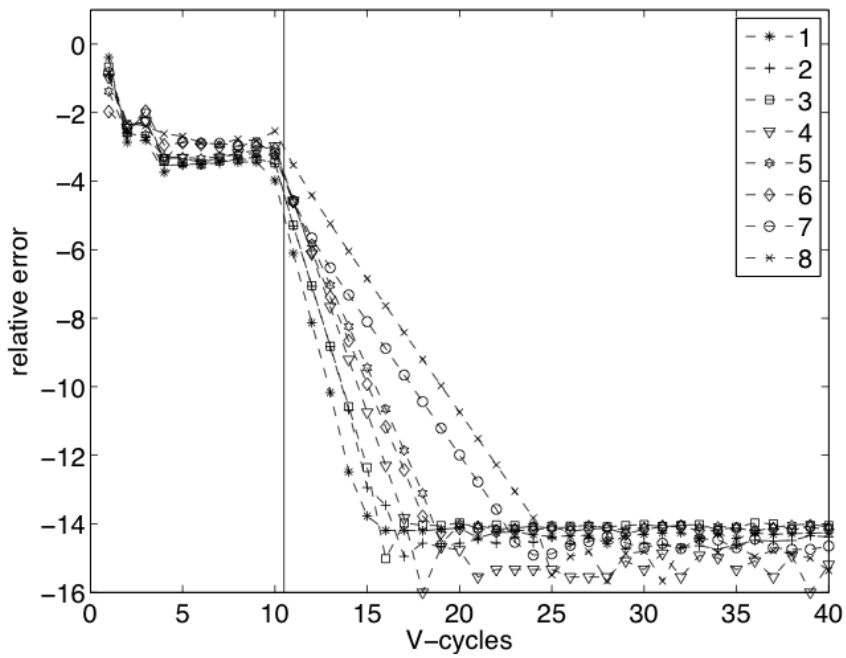
$$error = \frac{|\sigma_{exact} - \sigma_{approx}|}{\sigma_{exact}}$$

(5 test vectors, V(4,4), θ=0.05, 4 levels, 45x45 coarsest)

UNIVERSITY OF WATERLOO

numerical results

high-order finite volume element Laplacian on unit square (square, nonsymmetric, 961x961)



smallest singular values

(5 test vectors, V(4,4), θ=0.05, 5 levels, 51x51 coarsest)

UNIVERSITY OF WATERLOO

numerical results

FVE lge	FVE sm	FD lge	FD sm	Graph lge	Graph sm	Term-Doc
7.9791546	0.01924183	7.9818877	0.01811231	13.509036	0.01000000	84.148337
7.9491729	0.04794913	7.9548012	0.04519876	13.352613	0.03456116	64.707532
7.9468326	0.04801773	7.9548012	0.04519876	13.350454	0.03901593	55.976437
7.9172573	0.07655365	7.9277148	0.07228521	12.472837	0.07966567	50.265499
7.8965349	0.09557904	7.9099298	0.09007021	12.416200	0.09490793	49.265360
7.8960066	0.09558103	7.9099298	0.09007021	11.874669	0.09918138	45.242034
7.8692955	0.12359047	7.8828433	0.11715666			44.400811
7.8616683	0.12415144	7.8828433	0.11715666			41.772394

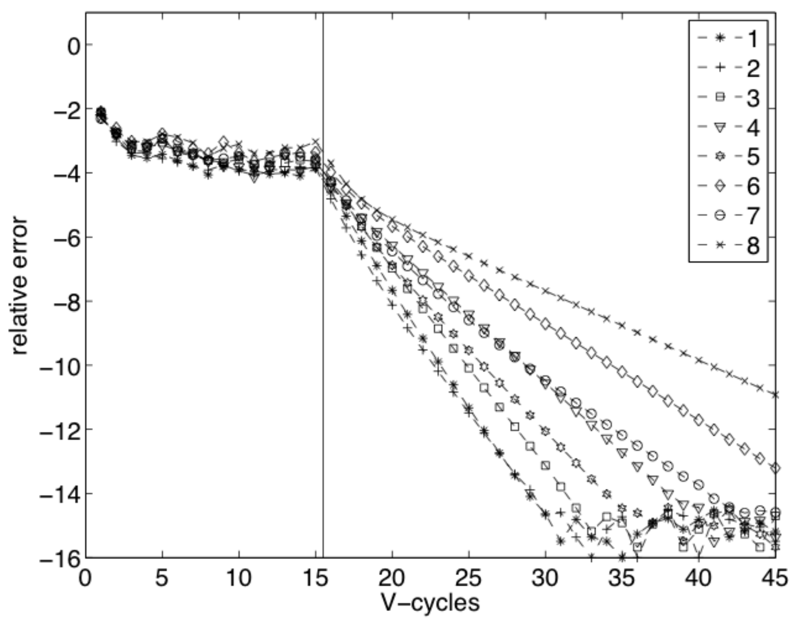
TABLE 6.1

Singular values and eigenvalues sought for each problem (high-accuracy approximations).

UNIVERSITY OF
WATERLOO

numerical results

2) finite difference Laplacian on unit square (square, symmetric, 1024x1024)



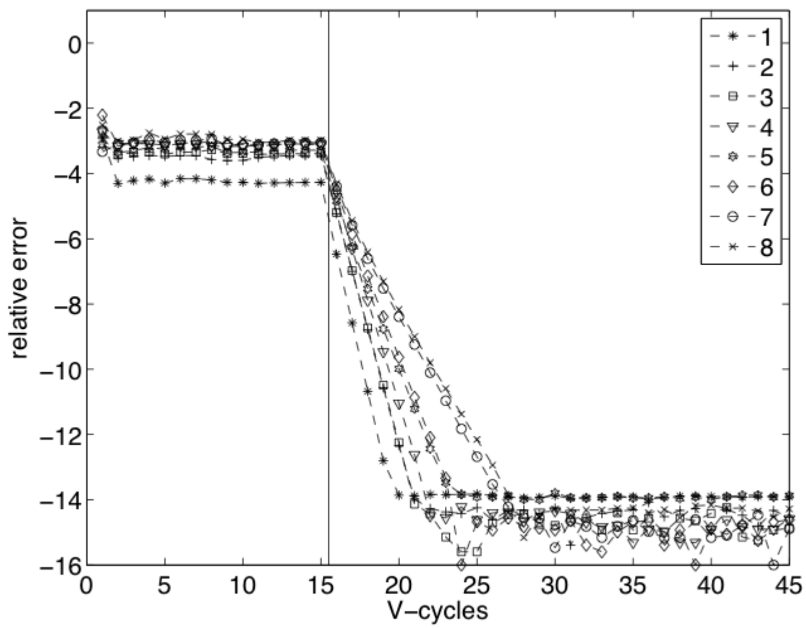
largest
eigenvalues

(6 test vectors, V(8,8) test and V(4,4) boot, θ=0.06,
4 levels, 52x52 coarsest)

UNIVERSITY OF
WATERLOO

numerical results

finite difference Laplacian on unit square (square, symmetric, 1024x1024)



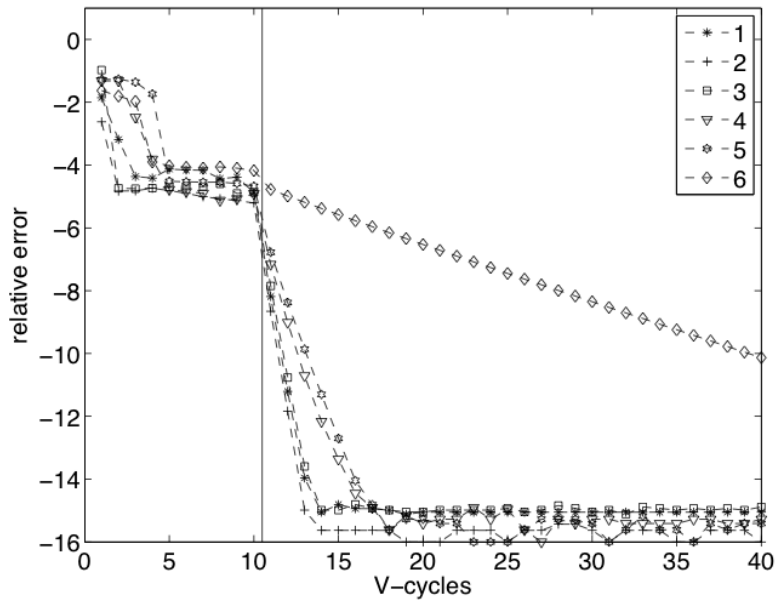
smallest eigenvalues

(6 test vectors, V(8,8) test and V(4,4) boot, θ=0.06, 5 levels, 64x64 coarsest)

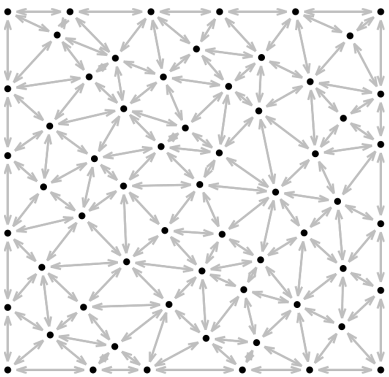
UNIVERSITY OF WATERLOO

numerical results

3) graph Laplacian on random triangular graph in unit square (square, symmetric, 1024x1024)



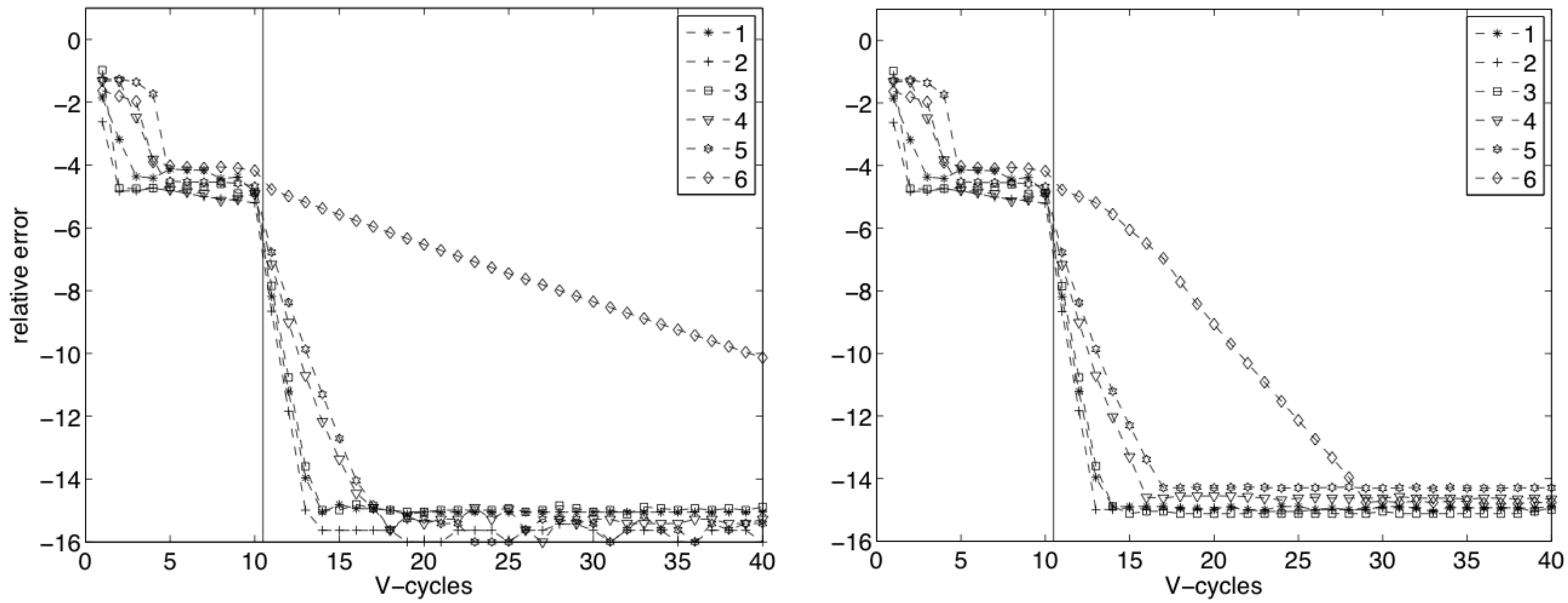
largest eigenvalues



(6 test vectors, V(1,1) test and V(8,8) boot, θ=0.05, 3 levels, 77x77 coarsest)

numerical results

graph Laplacian on random triangular graph in unit square (square, symmetric, 1024x1024)

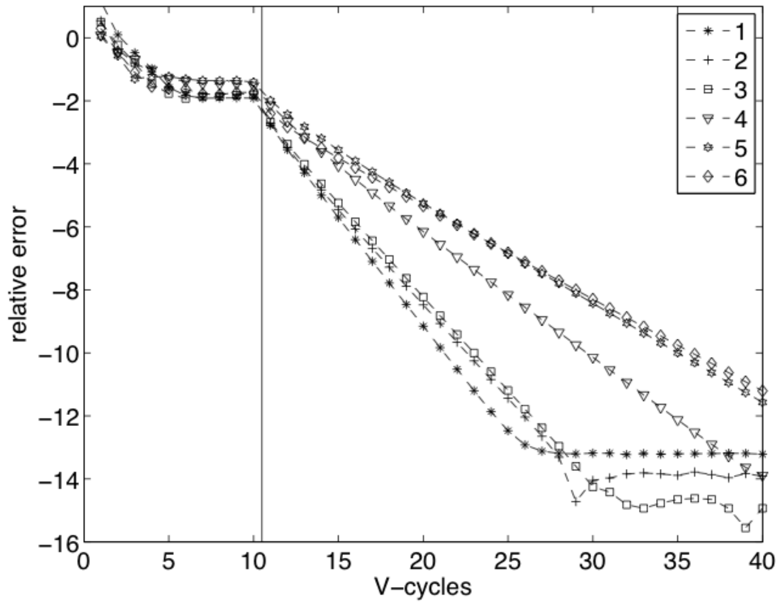


(6 test vectors, V(1,1) test and V(8,8) boot, θ=0.05, 3 levels, 77x77 coarsest)

UNIVERSITY OF WATERLOO

numerical results

graph Laplacian on random triangular graph in unit square (square, symmetric, 1024x1024)



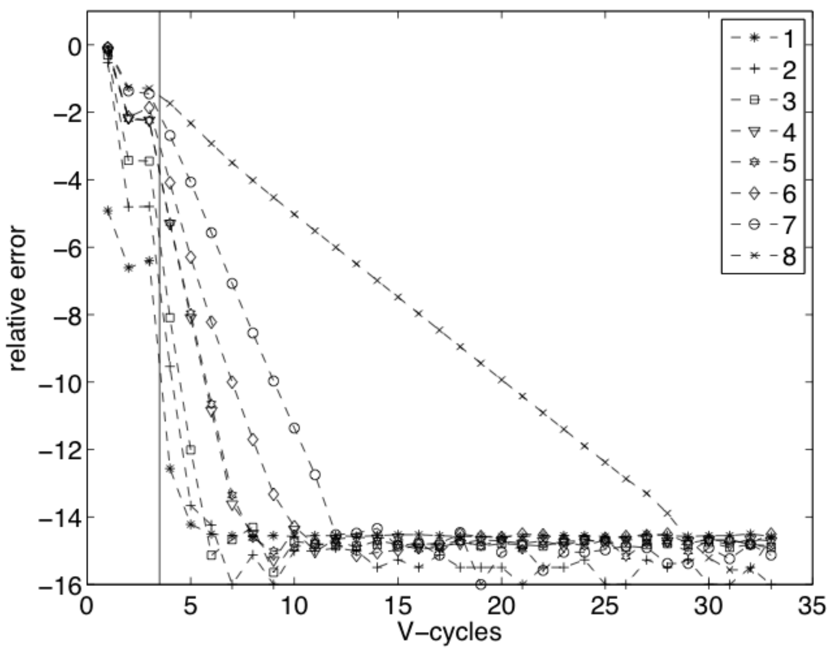
smallest eigenvalues

(6 test vectors, V(1,1) test and V(8,8) boot, θ=0.05, 3 levels, 59x59 coarsest)

UNIVERSITY OF WATERLOO

numerical results

4) Medline tem-document matrix (rectangular, 5735x1033)



largest
singular values

(14 test vectors, V(1,1) test and V(4,4) boot, θ=0.03,
5 levels, 415x198 coarsest)

12. conclusions

- self-learning, collective AMG algorithm to compute a few dominant or minimal singular triplets (or eigenpairs)
- multiplicative setup phase, additive solve phase
- seems to work pretty well
- there are many parameters, and robustness needs to be improved (how many test vectors, relaxations, ...)

conclusions

- improve coarsening (on *A*, compatible relaxation, general graph coarsening, small-world, others ...)
- improve multiplicative phase (‘adaptive’ approach instead of bootstrap?)
- improve additive phase (for example, use LOBPCG or RQMG instead of V-cycle+Ritz)
- parallel?
- approach is quite general (self-learning), high accuracy, so seems promising

UNIVERSITY OF WATERLOO

thank you

questions?