Adaptive Aggregation on Graphs

Wenfang Xu
Department of Mathematics, The Pennsylvania State University, University Park, PA 16802, USA Email: wxx107@psu.edu

Ludmil T. Zikatanov
Department of Mathematics, The Pennsylvania State University, University Park, PA 16802, USA Email: ludmil@psu.edu
Institute for Mathematics and Informatics, Bulgarian Academy of Sciences, Sofia, Bulgaria

Abstract
We generalize some of the functional (hypercircle) a posteriori estimates from finite element settings to general graphs or Hilbert space settings. Several theoretical results in regard to the generalized a posteriori error estimators are provided. We use these estimates to construct aggregation based coarse spaces for graph Laplacians. The estimator is used to assess the quality of an aggregation adaptively. Furthermore, a reshaping based algorithm is tested on several numerical examples.

Keywords: graph Laplacian, graph aggregation, multilevel hierarchy, hypercircle error estimates, matching

1. Introduction
The hypercircle identity was first introduced in [21] to study approximations to elastic problems. Then the so-called hypercircle methods are established and studied in a posteriori error estimates for finite element methods (see, for example, [20], for a comprehensive survey of the main results). Some pioneering works on the hypercircle methods are [14, 6].

The functional a posteriori error estimates are established in [22] for general elliptic problems defined from dual operators between Banach and Hilbert spaces. The estimation is used, for example, in [24] to bound the conforming error in discontinuous Galerkin approximations of elliptic problems (see also [15, 23]). In [1] the hypercircle method is used to construct a posteriori error estimates for the obstacle problem (see also [18]). The formulation of the hypercircle identity and error estimates, however, arises naturally in Hilbert space settings and can be applied to graph Laplacians, a fact which we exploit in what follows.

A multilevel graph coarsening scheme based on matching (that is, collapsing adjacent vertices into aggregates) is studied in [11] and later used in several AMG methods. For example, the multigrid method proposed in [12] uses matching on the graph of the stiffness matrix to solve convection–diffusion equations. The AGMG method (AGgregation-based algebraic MultiGrid) in [17] employs a pairwise aggregation algorithm by matching which minimizes a strength function. In [5] matching techniques which optimize matrix invariants were studied. In our work we use matching to generate multilevel hierarchies for solving the graph Laplacian. We point out that other coarsening techniques exist in the literature, for example the compatible relaxation algorithm [2, 16, 10, 3].

In this paper combinatorial graphs are considered and we are interested in approximations of the associated graph Laplacian matrix from coarse subspaces. We propose Raviart-Thomas-like coarsening schemes for both the vertex and edge spaces defined on graph aggregations. It can be shown that the functional a posteriori error estimates naturally apply to this setting and we provide a short proof of the estimation, inspired by the works in [14, 6, 21, 22]. The estimator is minimized by an inter-leaved method to achieve reliable bound of the error [13]. Lastly we propose a reshaping algorithm that generates aggregations adaptively. This algorithm can be used together with aggregation coarsening methods [11] to form multilevel hierarchies for graph Laplacians.

This work is supported in part by NSF through grants DMS-1522615, DMS-1720114, and by Lawrence Livermore National Lab through subcontract B614127.
the graph Laplacian (see [25] for an analysis on the convergence of an algebraic multigrid method based on smoothed aggregation). We point out that this is the first multilevel hierarchy that we know of that is dependent on the right-hand side of the system. Several numerical experiments are given at the end.

2. Preliminaries and notation

In this section we introduce the notations and preliminaries. Consider a combinatorial graph \( G = (V, E) \), where \( V = \{1, 2, \cdots, n\} \) is the set of vertices and \( E \) is the set of edges containing pairs of the form \((i, j)\), where \( i, j \in \{1, \cdots, n\} \). Let \( V = \mathbb{R}^{|V|} \) be the vertex space of \( G \) and \( W = \mathbb{R}^{|E|} \) be the edge space. We consider \( A \in \mathbb{R}^{n \times n} \) defined via the bilinear form

\[
(Au, v) = \sum_{(i,j) \in E} -a_{ij}(u_i - u_j)(v_i - v_j), \quad \forall u, v \in V.
\]

Here the sum runs over all edges \( e = (i, j) \in E \). The resulting matrix is known as the (weighted) Graph Laplacian of \( G \). Such bilinear forms correspond to the continuous (conforming) finite element as well as the mixed finite element discretizations with lumped mass of a scalar elliptic equation. In our work, we generalize some of the results from finite element a posteriori analysis to the case of general graphs. In particular, we are interested in good approximations of the above bilinear form on a smaller subspace, that is, good approximations to the solution of the problem

\[ Au = f. \quad (2.1) \]

We define operators \( G: V \to W \) and \( D: W \to W \) as follows.

\[
(Gv)_e = v_{\text{head}} - v_{\text{tail}}, \quad \forall v \in V;
\]

\[
(D\tau)_e = a_e \tau_e, \quad a_e = -a_{ij}, \quad \forall \tau \in W;
\]

where \( e = (i, j) \) is any edge of the graph. Here the “head” and “tail” are predetermined for each edge. Given \( G \) and \( D \) we can rewrite the graph Laplacian as \( (Au, v) = (DGu, Gv) \). If \( D \) is chosen to be the identity map we obtain the so called standard graph Laplacian. We further denote by \( G^* \) the adjoint of \( G \) with respect to the \( \ell^2 \)-inner products on \( V \) and \( W \), that is,

\[
(Gu, \tau)_W = (u, G^*\tau)_V, \quad \forall u \in V, \forall \tau \in W.
\]

Some examples from finite element methods naturally arise in the form of graph Laplacian.

2.1. Example I: standard finite elements

Let \( \Omega \) be a domain in \( \mathbb{R}^n \). We consider Poisson’s equation with Neumann boundary condition.

\[-\text{div}(a\nabla u) = f, \quad \text{in } \Omega;\]

\[\nabla u \cdot n = 0, \quad \text{on } \partial \Omega.\]

The weak formulation of the problem is then to find \( u \in H^1(\Omega) \) such that

\[
(Au, v) = (f, v), \quad \forall v \in H^1(\Omega),
\]

where

\[
(Au, v) = \int_{\Omega} a\nabla u \nabla v \, dx.
\]

If the discretization by continuous piecewise linear elements is considered, \( A \) has a matrix representation

\[
(Au, v) = \sum_{(i,j) \in E} -a_{ij}(u_i - u_j)(v_i - v_j).
\]

Clearly the above bilinear form is a weighted graph Laplacian.
2.2. **Example II: mixed finite elements with lumped mass**

We consider again Poisson’s equation, but in mixed formulation.

\[
(a^{-1}\sigma, \tau) + (\text{div} \tau, u) = 0, \quad \forall \tau \in H(\text{div}, \Omega);
\]

\[
(\text{div} \sigma, v) = -(f, v), \quad \forall v \in L^2(\Omega).
\]

Define the operator \( A \) on \( L^2(\Omega) \) as

\[
(Au, v) = (\text{div} \sigma, v).
\]

For discretization let \( W_h \subset H(\text{div}, \Omega) \) be the space of piecewise first order polynomials with continuous normal components across the edges, and \( S_h \subset L^2(\Omega) \) be the space of piecewise constant functions. If we use “mass lumping” for the term \( (a^{-1}\sigma, \tau) \) then we get the discretized \( A \):

\[
(Au, v) = \sum_{\varepsilon = T_e \cap T_2} a_{\varepsilon}(u_{T_e} - u_{T_2})(v_{T_e} - v_{T_2}),
\]

which again is a graph Laplacian.

3. **Generalized functional (hypercircle) a posteriori error estimates**

Here we present two lemmata in general settings that can be used in functional a posteriori estimates. We provide abstract formulations and proofs of the two results so that they can be used on graphs, and even in more general Hilbert space settings.

Let \( V \) and \( W \) be Hilbert spaces and suppose \( G: V \rightarrow W \) is an injective operator. We assume that the Hilbert adjoint of \( G \), \( G^* : W \rightarrow V \) defined via

\[
(G^* \tau, v)_V = (\tau, Gv)_W, \quad \forall v \in V, \ \forall \tau \in W
\]

is surjective with closed range. Note that for finite dimensional cases, the closed range assumption is automatically true.

Let \( D: W \rightarrow W \) be an operator that is symmetric positive definite on \( W \). Define \( A := G^*DG \) which is positive definite.

The problem we are interested in is to find \( u \in V \), such that

\[
(Au, v)_V = f(v), \quad \forall v \in V.
\]

Here \( f \in V' \), the dual space of \( V \). Since \( A \) is positive definite, there exists some \( C_p \), the Poincaré’s constant, such that

\[
C_p \|v\|_V \leq \|v\|_A, \quad \forall v \in V.
\]

In what follows, we will need the space \( W(g) \), which for a fixed \( g \in V' \) is defined to be

\[
W(g) = \{ \tau \in W \mid (\tau, Gv)_W = g(v), \forall v \in V \}.
\]

The first result is the following lemma.

**Lemma 3.1** (Prager and Synge [21]). Let \( u \) be the solution to (3.1). Then for any \( \tau \in W(f) \) and any \( v \in V \), the following identity holds.

\[
\|u - v\|_A^2 + \|DGu - \tau\|_{D^{-1}}^2 = \|DGv - \tau\|_{D^{-1}}^2 - (DGv - \tau)_W - (\tau, \tau)_W
\]

\[
= \|v\|_A^2 - 2(f(v) - \|u\|_A^2 - 2f(u) = \|v\|_A^2 - 2(Au, v)_V - \|u\|_A^2 + 2(Au, u)_V
\]

\[
= \|v\|_A^2 - 2(Au, v)_V - \|u\|_A^2 + 2\|u\|_A^2 = \|u - v\|_A^2.
\]

\[\square\]
We may take \( v \in V \) to be an approximation to the solution \( u \) in (3.1). Using the identity from lemma 3.1 we can obtain the following important result (S. Repin [22], Ladevèze [14] and Destuynder and Métiév [6]).

**Lemma 3.2.** Let \( u \) be the solution to the variational problem (3.1). Assume that \( \phi \in W \) is arbitrary. Then the following inequality holds for all \( v \in V \).

\[
\|u - v\|_A \leq \|DGv - \phi\|_{D^{-1}} + C_P^{-1}\|G^*\phi - f\|_V.
\] (3.4)

**Proof.** By lemma 3.1 for any \( \tau \in W(f) \) we have that

\[
\|u - v\|^2_A \leq \|u - v\|^2_A + \|DGv - \tau\|^2_{D^{-1}} = \|DGv - \tau\|^2_{D^{-1}}.
\]

The triangle inequality then gives, for any \( \phi \in W \),

\[
\|u - v\|_A \leq \|DGv - \phi\|_{D^{-1}} + \|\phi - \tau\|_{D^{-1}}.
\]

Because the inequality holds for all \( \tau \in W(f) \), we can take the infimum with respect to \( \phi \) and get

\[
\|u - v\|_A \leq \|DGv - \phi\|_{D^{-1}} + \inf_{\tau \in W(f)} \|\phi - \tau\|_{D^{-1}}.
\]

We now estimate the last term on the right hand side. Let \( z \in V \) be such that

\[
(\tau, w) = (DGz, w) + (\phi, Gw) = (A_z, w) + (\phi, Gw) = f(w).
\]

This proves that \( \tau \in W(f) \). Hence

\[
\inf_{\tau \in W(f)} \|\phi - \tau\|_{D^{-1}} \leq \|\phi - \tau\|_{D^{-1}} = \|DGz\|_{D^{-1}} = \|z\|_A.
\]

On the other hand, we apply (3.5) again to obtain

\[
\|z\|_A = \frac{\|z\|^2_A}{\|z\|_A} = \frac{(A_z, z)_V}{\|z\|_A} = \frac{(f - G^*\phi, z)_V}{\|z\|_A}
\]

\[
\leq \|f - G^*\phi\|_V \frac{\|z\|_V}{\|z\|_A} \leq C_P^{-1}\|G^*\phi - f\|_V,
\]

which concludes the proof. \( \square \)

**Remark.** Although the original proof was found in the aforementioned papers, the anonymous referee provided a shorter and inspiring proof. We present it here. Since \( A \) is symmetric positive definite, \((\cdot, \cdot)_A\) defines an inner product. We get

\[
\|u - v\|_A = \sup_{\|z\|_A = 1} (u - v, z)_A = \sup_{\|z\|_A = 1} (A(u - v), z)_V = \sup_{\|z\|_A = 1} (f - G^*DGv, z)_V = \sup_{\|z\|_A = 1} \{ (f - G^*\phi, z)_V + (G^*(\phi - DGv), z)_V \}.
\]

We have for the first term

\[
(f - G^*\phi, z)_V \leq \|f - G^*\phi\|_V \|z\|_V \leq \|f - G^*\phi\|_V C_P^{-1}\|z\|_A = C_P^{-1}\|G^*\phi - f\|_V,
\]

and for the second term

\[
(G^*(\phi - DGv), z)_V = (\phi - DGv, Gz)_W = (D^{-1}(\phi - DGv), Gz)_D
\]

\[
\leq \|D^{-1}(\phi - DGv)\|_D \|Gz\|_D = \|\phi - DGv\|_{D^{-1}} \|z\|_A.
\]

This proves the result.
Then $E$ are nonzero. Then an inter-leaved process \cite{13} can be applied to handle the minimization of $\eta$, with respect to $\phi$ and $\beta$. Setting this to be zero we get equation (3.6).

We can minimize the right-hand side of (3.4) with respect to $\phi$ to get an estimate of the error. (See \cite{8} for a treatment of the continuous version of the minimization problem via $H(\text{div})$-liftings.) Denote the right-hand side of (3.4) by

$$\eta(\phi) = \|DGv - \phi\|_{D^{-1}} + C_P^{-1}\|G^*\phi - f\|_V.$$  

Then the minimization process of $\eta(\phi)$ is described as follows.

Using the inequality $(a + b)^2 \leq (1 + \beta)a^2 + (1 + 1/\beta)b^2$ for any positive $\beta$ one obtains

$$\eta^2(\phi) \leq E(\beta, \phi),$$

where

$$E(\beta, \phi) := (1 + \beta)\|DGv - \phi\|^2_{D^{-1}} + (1 + 1/\beta)C_P^{-2}\|G^*\phi - f\|^2_V.$$  

An inter-leaved process \cite{13} can be applied to handle the minimization of $E$, with respect to $\phi$ and $\beta$ repeatedly. We present the following lemmata that are used for minimization.

**Lemma 3.3.** Let $\beta > 0$ be fixed and let

$$a_1 = 1 + \beta, \quad a_2 = (1 + 1/\beta)C_P^{-2}.$$  

Then $E(\beta, \phi)$ attains a unique minimum when $\phi$ is the solution to

$$(a_1D^{-1} + a_2GG^*)\phi = G(a_1v + a_2f).$$  

(3.6)

**Proof.** We have that

$$E(\beta, \phi) = a_1\|\phi - DGv\|^2_{D^{-1}} + a_2\|G^*\phi - f\|^2_V.$$  

Since $E$ is convex in $\phi$, $E$ attains minimum if and only if the directional derivative of $E$ with respect to $\phi$ is zero at some point. For any fixed $\phi$, take a small variation in the direction of $\chi$ we get the directional derivative

$$\chi \mapsto \frac{d}{d\varepsilon}\big|_{\varepsilon=0} E(\beta, \phi + \varepsilon\chi),$$

where

$$\frac{d}{d\varepsilon}\big|_{\varepsilon=0} E(\beta, \phi + \varepsilon\chi) = \frac{d}{d\varepsilon}\big|_{\varepsilon=0} \left[ a_1(\phi + \varepsilon\chi - DGv, \phi + \varepsilon\chi - DGv)_{D^{-1}} 
+ a_2(G^*(\phi + \varepsilon\chi) - f, G^*(\phi + \varepsilon\chi) - f)_V \right]$$

$$= \frac{d}{d\varepsilon}\big|_{\varepsilon=0} \left[ a_1(\varepsilon^2(\chi, \chi)_{D^{-1}} + 2\varepsilon(\chi, \phi - DGv)_{D^{-1}} + (\phi - DGv, \phi - DGv)_{D^{-1}}) 
+ a_2(\varepsilon^2(G^*\chi, G^*\chi)_V + 2\varepsilon(G^*\chi, G^*\phi - f)_V + (G^*\phi - f, G^*\phi - f)_V) \right]$$

$$= 2a_1(\chi, \phi - DGv)_{D^{-1}} + 2a_2(G^*\chi, G^*\phi - f)_V$$

$$= 2a_1(\chi, D^{-1}\phi - Gv)_W + 2a_2(\chi, GG^*\phi - Gf)_W$$

$$= 2(\chi, (a_1D^{-1} + a_2GG^*)\phi - G(a_1v + a_2f))_W.$$  

Setting this to be zero we get equation (3.6). \hfill \square

**Lemma 3.4.** Let $\phi$ be fixed such that

$$b_1 = \|DGv - \phi\|_{D^{-1}} \quad \text{and} \quad b_2 = C_P^{-1}\|G^*\phi - f\|_V$$

are nonzero. Then

$$\arg\min_\beta E(\beta, \phi) = \frac{b_2}{b_1}.$$  

(3.7)
Proof. We have that
\[
E(\beta, \phi) = (1 + \beta)b_1^2 + (1 + 1/\beta)b_2^2 = b_1^2 + b_2^2 + b_1\beta + \frac{b_2^2}{\beta}
\]
where the equal sign holds if and only if \(\beta = \frac{b_2}{b_1}\), giving equation \(3.7\).

The minimization of \(E\) is done by repeatedly minimizing \(E(\beta, \phi)\) with respect to \(\phi\) and \(\beta\) until \(E\) converges. In fact, this process also gives the global minimum of \(\eta(\phi)\). We have the following lemma.

**Lemma 3.5.** If \(E(\beta, \phi)\) attains a local minimum at \((\beta_0, \phi_0)\), then \(\eta(\phi)\) attains a global minimum at \(\phi_0\).

**Proof.** Since \(\eta(\phi)\) is also a convex function, \(\eta(\phi)\) attains a global minimum if its directional derivative is zero at some \(\phi\). The directional derivative of \(\eta(\phi)\) at \(\phi_0\) is
\[
\frac{d}{d\varepsilon} \bigg|_{\varepsilon=0} \eta(\phi_0 + \varepsilon\chi) = \frac{d}{d\varepsilon} \bigg|_{\varepsilon=0} \left[ (\phi_0 + \varepsilon\chi - DGv, \phi_0 + \varepsilon\chi - DGv)\right]_{D-1}^\frac{1}{2} + C_P^{-1}(G^*(\phi_0 + \varepsilon\chi) - f, G^*(\phi_0 + \varepsilon\chi) - f)_V
\]

\[
= \frac{1}{2\|DGv - \phi_0\|_{D-1}} \left( \phi_0 + \varepsilon\chi - DGv, \phi_0 + \varepsilon\chi - DGv \right)_{D-1}^\frac{1}{2} + \frac{1}{2C_P\|G^*\phi_0 - f\|_V} \left( G^*(\phi_0 + \varepsilon\chi) - f, G^*(\phi_0 + \varepsilon\chi) - f \right)_V
\]

\[
= \frac{1}{\|DGv - \phi_0\|_{D-1}} (\chi, D^{-1}\phi_0 - Gv)_W + \frac{1}{C_P\|G^*\phi_0 - f\|_V} (\chi, GG^*\phi_0 - Gf)_W.
\]

Let \(b_1 = \|DGv - \phi_0\|_{D-1}\) and \(b_2 = C_P^{-1}\|G^*\phi_0 - f\|_V\), then
\[
\frac{d}{d\varepsilon} \bigg|_{\varepsilon=0} \eta(\phi_0 + \varepsilon\chi) = \frac{1}{b_1} (\chi, D^{-1}\phi_0 - Gv)_W + \frac{1}{C_Pb_2} (\chi, GG^*\phi_0 - Gf)_W
\]

\[
= \left( \chi, \left( \frac{1}{b_1}D^{-1} + \frac{1}{C_Pb_2}GG^* \right)\phi_0 - G\left( \frac{1}{b_1}v + \frac{1}{C_Pb_2}f \right) \right)_W. \tag{3.8}
\]

Since \(\beta_0\) minimizes \(E(\beta, \phi_0)\), by lemma 3.4 it must be that \(\beta_0 = \frac{b_2}{b_1}\). By lemma 3.3 and the fact that \(\phi_0\) minimizes \(E(\beta_0, \phi)\), we have
\[
(a_1D^{-1} + a_2GG^*)\phi_0 = G(a_1v + a_2f), \tag{3.9}
\]

where \(a_1 = 1 + \beta_0 = \frac{b_1 + b_2}{b_1}\), and \(a_2 = (1 + 1/\beta_0)C_P^{-2} = \frac{b_1 + b_2}{C_Pb_2}\). Thus \(3.9\) becomes
\[
\left( \frac{1}{b_1}D^{-1} + \frac{1}{C_Pb_2}GG^* \right)\phi_0 = G\left( \frac{1}{b_1}v + \frac{1}{C_Pb_2}f \right).
\]

Comparing this with \(3.8\), we get \(\frac{d}{d\varepsilon} \bigg|_{\varepsilon=0} \eta(\phi_0 + \varepsilon\chi) = 0\), which completes the proof. \(\square\)

When \(W\) is of very high dimension, for example in our application, where \(W\) is the edge space of a large graph, the minimization becomes time consuming. We handle this by varying \(\phi\) over only a subspace of \(W\) (say, the subspaces \(W_H\) defined in section 4). It is not hard to show that the above minimization results also hold when \(\phi\) is chosen from a subspace of \(W\).
4. Coarsening through aggregation

In this section we introduce the constructions of coarse subspaces of the vertex space $V$ and edge space $W$ in which approximations of the Laplacian are considered. In what follows we omit the subscripts on the inner products as it will always be clear from the context in which spaces the inner products are taken. An aggregation on a graph $G = (V, E)$ is a splitting of the vertex set $V$ into non-overlapping subsets, each of which is connected in $G$ and called an aggregate:

$$V = \bigcup_{k=1}^{n_c} V_{A_k} = \bigcup_{A} V_{A}.$$ 

Here an aggregate is denoted by $A$ and $V_{A}$ is its set of vertices. This splitting naturally splits the set of edges into interior and interface edges. For each aggregate $A$, we denote by $E_A$ the set of interior edges of $A$:

$$E_A = \{(i,j) \in E | i,j \in V_A\}.$$ 

For any two aggregates $A$ and $A'$, denote by $I_{AA'}$ the set of interface edges between them, that is, the set of edges which connect $A$ and $A'$:

$$I_{AA'} = \{(i,j) \in E | i \in V_A, j \in V_{A'}\}.$$ 

Note edges in the graph are undirected and $\{(i,j) \text{ and } (j,i)\}$ are considered to be the same in $E$. We denote by $\Gamma$ the set of all interfaces in the aggregation.

An aggregation of $G$ is completely characterized by the subspace of $V$ consisting of vectors taking one and the same value at all vertices in an aggregate. We denote this subspace by $V_{H}$ as follows.

$$V_{H} = \{u \in V | u_i = u_j \text{ whenever } i,j \in V_A \text{ for some } A\}.$$ 

This admits a two-level hierarchy. The solution of the variational problem $Au = f$ can be approximated by (for instance) some $u_H \in V_{H}$ by solving:

$$(Au_H, v_H) = (f, v_H), \quad \forall v_H \in V_{H}. \quad (4.1)$$

The results in the previous section can be used to establish a posteriori error estimates for the approximate solution $u_H$. In order to get computable error estimates we also need coarse subspaces of the edge space $W$, from which the $\phi$ in (3.2) will be chosen. We point out that in the context of a posteriori estimates for finite element methods, $\phi$ is sometimes chosen to be the equilibrated flux to make the second term $\|G^*\phi - f\|$ small or zero [9]. Below we present two constructions of coarse edge spaces in an aggregation, which are both Raviart-Thomas-like.

4.1. Coarse edge space via saddle point problem

We introduce for each interface $\mathcal{I} = \mathcal{I}_{AA'} \in \Gamma$ the vector $\sigma_{\mathcal{I}} = \mathcal{E}_{\mathcal{I}} Q_{\mathcal{I}} G_1$, where $\mathcal{E}_{\mathcal{I}} = \pm 1$ is predetermined for the interface and $Q_{\mathcal{I}}$ is the orthogonal projection onto $\mathcal{I}$. For a given $\psi \in W$ define the averaging operator

$$\langle \psi, \sigma_{\mathcal{I}} \rangle_{\mathcal{I}} = \frac{\langle \psi, \sigma_{\mathcal{I}} \rangle}{\|\sigma_{\mathcal{I}}\|^2}.$$ 

In the context of standard finite element methods, this can be viewed as an analogue of Raviart-Thomas degree of freedom on a coarser grid, namely, an analogue of averaging the normal trace of a vector field. The basis for the coarse edge space $W_{H}$ is constructed via solving the following local saddle point problem: find $\varphi_{\mathcal{I},A} \in W_{E_A}$ and $u_{\mathcal{I},A} \in V_{A}$, $(u_{\mathcal{I},A},1) = 0$, such that

$$B(\varphi_{\mathcal{I},A}, \psi) + (u_{\mathcal{I},A}, G^* \psi) = -B(\sigma_{\mathcal{I}}, \psi), \quad \forall \psi \in W_{E_A};$$

$$(G^* \varphi_{\mathcal{I},A}, v) = -(G^* \sigma_{\mathcal{I}}, v), \quad \forall v \in V_{A}, (v,1) = 0.$$
An example of a bilinear form $B(\cdot, \cdot) : W \times W \to \mathbb{R}$ is the $\ell^2$-inner product on $W$, i.e., $B(\varphi, \psi) = \sum_{e \in E} \varphi_e \psi_e$. One can also use a different bilinear form for this. The above saddle problem is the Lagrange multiplier formulation of the following constraint minimization problem [3].

$$\varphi_{I,A} = \arg \min_{\varphi \in W_{I,A}} \{ B(\varphi + \sigma_I, \psi + \sigma_I) \},$$

subject to $$(G^* \psi, v) = -(G^* \sigma_I, v), \ \forall v \in V_A, (v, 1) = 0.$$ 

We then have the following theorem.

**Theorem 4.1** ([Theorem 5.3, [26]]. Let $Q_H$ be the $\ell^2$-based projection on the space $V_H$, that is, averaging on every aggregate. Then for all $\psi \in W$ and all $v \in V$ we have

$$(G^* \pi_H \psi, v) = (Q_H G^* \psi, v).$$

The theorem says that the following diagram commutes.

$$\begin{array}{ccc}
W & \xrightarrow{G^*} & V \\
\pi_H \downarrow & & \downarrow Q_H \\
W_H & \xrightarrow{G^*} & V_H
\end{array}$$

4.2. Coarse edge space via spanning tree

Another way of constructing $W_H$ and $\pi_H$ such that the above diagram commutes is via the spanning trees of the aggregates. For each interface edge $e = (i, j)$ between aggregates $A$ and $B$ ($i \in A, j \in B$), fix a spanning tree of $A$ rooted at $i$ (note $A$ can be viewed a subgraph of $G$), see figure [4]. For an edge $e'$ in the tree and the corresponding child node $i'$, denote by $m_{e'}$ the size of the subrooted at $i'$. Define $\varphi_{A} \in W_{E_A}$ by

$$(\varphi_A)_{e'} = \begin{cases} \pm \frac{m_{e'}}{|V_A|}, & \text{if } e' \text{ is an edge of the tree;} \\ 0, & \text{otherwise.} \end{cases}$$

Here the “$\pm$” takes “+” sign if the vertex $i'$ is the head of $e'$ according to the predetermined orientation on the edges of the graph, and “$-$” otherwise.

Similarly we define $\varphi_{B} \in W_{E_A}$ via a spanning tree of $B$ rooted at $j$. Then let $\varphi^e \in W$ be such that

$$(\varphi^e)_{e'} = \begin{cases} (\varphi_A)_{e'}, & \text{if } e' \in E_A; \\ 1, & \text{if } e' = e; \\ -(\varphi_B)_{e'}, & \text{if } e' \in E_B; \\ 0, & \text{otherwise.} \end{cases}$$

We now define $\pi_H : W \to W_H$ in the following way.

$$\pi_H 1_e = \begin{cases} \varphi^e, & \text{if } e \text{ is an interface edge;} \\ 0, & \text{otherwise.} \end{cases}$$

Then theorem [11] holds for the $\pi_H$ as defined above as well.
Proof. Note that we want
\[(G^* \pi_H \psi, v) = (Q_H G^* \psi, v), \quad \forall \psi \in W, \forall v \in V.\] (4.3)

For any edge \(e\) interior to an aggregate and for \(1_e \in W\), we have \(Q_H G^* 1_e = 0\). On the other hand, \(\pi_H 1_e = 0\) by definition. In this case (4.3) holds.

For an interface edge \(e = (i, j), i \in A, j \in B\), to show (4.3) we observe the left-hand side is \((\pi_H 1_e, G v)\) and the right-hand side is
\[(1_e, G Q_H v) = \frac{1}{|V_A|} \sum_{k \in V_A} v_k - \frac{1}{|V_A'|} \sum_{l \in V_B} v_l.\] (4.4)

For \(v = 1_k\) where \(k\) is any vertex not in \(A\) or \(B\), (4.4) takes value 0. By definition \(\pi_H 1_e\) vanishes on edges that are neither interior to \(A\) or \(B\) nor in the interface \(I_{AB}\), so \((\pi_H 1_e, G 1_k) = 0\). The left-hand side is equal to the right-hand side. For \(v = 1_k\) where \(k\) is any vertex in \(A\), (4.4) becomes \(1/|V_A|\). Thus we need to verify
\[(\pi_H 1_e, G 1_k) = \frac{1}{|V_A|} \quad \text{or} \quad (\varphi_e, G 1_k) = \frac{1}{|V_A'|}.\]

This is immediate from the construction of \(\varphi_e\). The same argument applies if \(k\) is in \(B\).

A basis for \(W_H\) is then constructed in the similar fashion as in the previous subsection, specifically, for \(I = I_{AB}\),
\[\varphi_I := \sum_{e \in I} \delta_e \varphi_e, \quad \text{where} \quad e = (i, j), \quad \delta_e = \begin{cases} 1, & \text{if } i \in A; \\ -1, & \text{if } i \in B. \end{cases}\]

5. Applications to aggregation in graphs

We apply the error estimator in lemma 3.2 to the graph Laplacian problem (2.1), where \(V\) and \(W\) are just the vertex and edge spaces of a graph. The standard graph Laplacian \(A\) takes the form \(A = G^* 1_W G\), and the norms \(\|\cdot\|_V\) and \(\|\cdot\|_W\) are \(l^2\)-norms. We get the following estimate for the error of the approximate solution \(u_H\).
\[\|u - u_H\|_A \leq \|Gu_H - \phi\| + C_P^{-1}\|G^* \phi - f\|.\] (5.1)

Note the graph Laplacian \(A\) is only positive semidefinite. However if we replace \(V\) with the hyperplane in the vertex space that is orthogonal to the first eigenvector \([1 \ 1 \ \cdots \ 1]^T\) of \(A\) then \(A\) becomes positive definite. In this case \(C_P\) is the smallest positive (second) eigenvalue of \(A\).
We use the error estimate (5.1) to devise an algorithm that generates aggregations adaptive to not only $A$, but also the right-hand side $f$. For given $f$ and any aggregation we can minimize the right-hand side of (5.1) over a coarse edge space $W_H$. We denote this minimum by

$$\eta(f, A) = \inf_{\phi \in W_H} \| Gu_H - \phi \| + C_P^{-1} \| G^* \phi - f \|.$$

We then devise a reshaping algorithm that finds a new aggregation, aiming to reduce the this estimator. To do this we first localize our estimator. Note

$$\tilde{\eta} := \| Gu_H - \phi \|^2 + C_P^{-2} \| G^* \phi - f \|^2$$

$$= \sum_{I} \sum_{e \in I} \| Gu_H - \phi \|_e^2 + \sum_{A} \left[ \sum_{e \in \mathcal{E}_A} \| Gu_H - \phi \|_e^2 + C_P^{-2} \| G^* \phi - f \|_{V_A}^2 \right]$$

$$= \sum_{A} \left[ \frac{1}{2} \sum_{A'} \sum_{e \in \mathcal{I}_{A,A'}} \| Gu_H - \phi \|_e^2 + \sum_{e \in \mathcal{E}_A} \| Gu_H - \phi \|_e^2 + C_P^{-2} \| G^* \phi - f \|_{V_A}^2 \right]$$

$$= \sum_{A} \tilde{\eta}_A.$$

The reshaping algorithm 5.1 then iteratively splits the aggregates on which $\tilde{\eta}_A$ is large, until some stopping criterion is met. The stop criterion can be, e.g., the number of aggregates $n_c$ becomes larger than a given threshold $N$, or the error estimate $\eta(f, A)$ drops below some preset value.

**Algorithm 5.1 Reshaping of aggregation**

1. Suppose a graph $G$ and an aggregation $\{A_k\}_{k=1}^{n_c}$ are given.
2. Compute the approximate solution $u_H$. Then find $\phi$ that minimizes $\eta(f, A)$.
3. Split all $A_k$ for which

$$\tilde{\eta}_A > \frac{\sum_{i=1}^{n_c} \tilde{\eta}_A}{n_c}.$$

4. Check if the stopping criterion is met, if not go to step 2.

To mark aggregates for refinement (splitting) we have used an analogue of the equidistribution marking well known in adaptive finite element methods. Other strategies for marking, such as maximum and Dörfler type marking [19, 7] are subject of future research. All aggregates marked for refinement are split using the hierarchy already available via matching described in the next section, since this can be done at virtually zero computational cost.

6. Numerical examples: matching, un-matching and reshaping

In this section we perform several numerical experiments on the error estimates and reshaping algorithm proposed above.

6.1. Experiment I: guided reshaping starting from a coarse aggregation

We test the reshaping algorithm using matching on graphs. By matching we mean an algorithm that aggregates a graph by grouping two vertices together at a time [11]. To be exact, the matching algorithm works as follows.
1. Choose a vertex of smaller degree and group it with one of its unmatched neighbors, if such neighbor exists. The degree of a vertex is defined to be the number of edges attached to this vertex.

2. Repeat this until there are only isolated vertices which have no unmatched neighbors. Then group each isolated vertex with a neighbor with which it has the most connections.

The matching algorithm can be performed repeatedly to generate a hierarchy of coarse aggregates.

Figure 2 then shows a guideline of the experiment. We start from $V$, the finest (original) vertex space, and iteratively apply the matching algorithm. Let $V_{\tilde{H}}$ be the subspace of $V$ obtained after $k_0$ iterations of matching, and $V_J$ be after $k_1$ iterations, where $k_0 < k_1$ so that $V_J$ is coarser than $V_{\tilde{H}}$. We solve for $u_{\tilde{H}}$ on $V_{\tilde{H}}$ and get the error $e_{\tilde{H}} = \|u - u_{\tilde{H}}\|_A$, with the right-hand side $f$ of (2.1) being a “smooth” vector (smoothed by Gauss-Seidel iterations). The reshaping algorithm is then performed on $V_J$ iteratively, where the chosen aggregates are split in the same way they were grouped during matching. The newly generated aggregations are represented by nodes on the oblique line in Figure 2. We do this iteratively until the error $e_H$ on $V_H$ becomes smaller than $e_{\tilde{H}}$. We then compare $V_{\tilde{H}}$ and $V_H$ to see if the algorithm reduces the number of aggregates when achieving the same error. All graphs in the following examples are taken from the SuiteSparse Matrix Collection.

**Example 1**

The first example is the graph barth5. barth5 has 15606 vertices and 45878 edges. The second eigenvalue of its standard graph Laplacian matrix is $\lambda_2 = 0.02776$, and on average each vertex has 5.9 neighbors. The results are shown in Table 1. We see that in achieving the same error, reshaping significantly reduces the number of aggregates compared to matching. Note although the estimation via spanning tree does not give as low efficiency, it results in more reduction of $n_c$ in many cases. Figure 3 plots the aggregations obtained using matching with $k_0 = 6$ and reshaping started from $k_1 = 7$. Note that with reshaping (Figure 3b), fewer aggregates are generated and aggregates close to the “boundary” are more likely to be grouped together.

**Table 1:** Comparison of direct matching and reshaping on the graph barth5, at different levels of coarsening. We show results obtained for both constructions of $W_H$ introduced in section 4. Here $e_{\tilde{H}} := \eta/\|u - u_{\tilde{H}}\|_A$ represents the efficiency of the operator.

| Aggregation | $W_H$ via saddle point problem | $W_H$ via spanning trees |
|-------------|-------------------------------|--------------------------|
| $k_0 = 3$   | $n_c = 1798$ | $e_{\tilde{H}} = 1.9465$ | $\|u - u_{\tilde{H}}\|_A/\|u\|_A = 0.8456$ | $n_c = 1798$ | $e_{\tilde{H}} = 1.4298$ | $\|u - u_{\tilde{H}}\|_A/\|u\|_A = 0.8456$ |
| $k_0 = 4$   | $n_c = 937$  | $e_{\tilde{H}} = 1.7117$ | $\|u - u_{\tilde{H}}\|_A/\|u\|_A = 0.9020$ | $n_c = 837$  | $e_{\tilde{H}} = 1.4897$ | $\|u - u_{\tilde{H}}\|_A/\|u\|_A = 0.9020$ |
| $k_0 = 5$   | $n_c = 395$  | $e_{\tilde{H}} = 1.5754$ | $\|u - u_{\tilde{H}}\|_A/\|u\|_A = 0.9335$ | $n_c = 395$  | $e_{\tilde{H}} = 1.4731$ | $\|u - u_{\tilde{H}}\|_A/\|u\|_A = 0.9335$ |
| $k_0 = 6$   | $n_c = 190$  | $e_{\tilde{H}} = 1.4575$ | $\|u - u_{\tilde{H}}\|_A/\|u\|_A = 0.9586$ | $n_c = 190$  | $e_{\tilde{H}} = 1.4091$ | $\|u - u_{\tilde{H}}\|_A/\|u\|_A = 0.9586$ |
| $k_0 = 7$   | $n_c = 143$  | $e_{\tilde{H}} = 1.1468$ | $\|u - u_{\tilde{H}}\|_A/\|u\|_A = 0.9499$ | $n_c = 143$  | $e_{\tilde{H}} = 1.4574$ | $\|u - u_{\tilde{H}}\|_A/\|u\|_A = 0.9446$ |
Example 2

The second graph we test is the graph power. The second eigenvalue of its Laplacian matrix is $C_P = 0.02755$. The vertices have an average degree of 2.7. Table 2 and figure 4 show the numerical results. Same as in example 1, the reshaping algorithm is able to achieve smaller approximation error with fewer aggregates. Again the method using $W_H$ via spanning trees is more selective in choosing the aggregates to split and thus results in fewer aggregates at the same level.

Example 3

Table 3 shows the numerical results on the graph vsp_vibrobox_scagr7-2c_rlfdd, using the $W_H$ constructed via spanning trees. This is a larger graph with 77328 vertices and 435586 edges. The second eigenvalue of the standard graph Laplacian is $C_P = 0.3033$, and on average each vertex has 11.3 neighbors. We can also see huge reduction in the number of aggregates for achieving the same approximation error. We point out that for all cases, the effect of reduction becomes more significant when it comes to the finer levels (top of the tables), since this allows for more space for improvement.

6.2. Experiment II: point source example

We further test the reshaping algorithm with the exact solution $u$ chosen to be the indicator function of some vertex (and the right-hand side $f$ is set accordingly), and see if the aggregates can be adapted to the solution. In figure 5, the chosen vertex is marked by a red dot. The reshaping algorithm starts with a coarse aggregation with number of aggregates $n_c = 2$ (figure 5a) and ends at $n_c = 15$ (figure 5b). We can see that the algorithm is adaptive to the solution in the sense that it only selects those aggregates around the chosen vertex to split, thus approximating the “point source” solution using very few aggregates.
Table 3: Comparison of direct matching and reshaping on the graph vsp, vibrobox, scag7-2c, rlfd, at different levels of coarsening. The method using $W_H$ via spanning trees is reported here.

| Aggregation | $n_c$ | $\eta/\|u_h - u\|_A$ | $\|u_h - u\|_{A/\|u\|_A}$ |
|-------------|-------|---------------------|--------------------------|
| $k_0 = 3$    | 3582  | 1.1339              | 0.8463                   |
| $k_1 = 7$ then reshape | 611   | 1.3409              | 0.8144                   |
| $k_0 = 4$    | 1784  | 1.1466              | 0.8926                   |
| $k_1 = 7$ then reshape | 400   | 1.3013              | 0.8833                   |
| $k_0 = 5$    | 890   | 1.1934              | 0.9187                   |
| $k_1 = 7$ then reshape | 341   | 1.2858              | 0.9076                   |
| $k_0 = 6$    | 444   | 1.2514              | 0.9438                   |
| $k_1 = 7$ then reshape | 298   | 1.2754              | 0.9235                   |

Figure 4: Plots of aggregations constructed with and without reshaping on the graph power

(a) $k_0 = 5$, $n_c = 86$
(b) $k_1 = 7$ with reshaping, $n_c = 55$

Figure 5: Reshaping algorithm adapted to a $u$ chosen to be the indicator function of a vertex.
7. Conclusions and outlook

In this paper we proposed an aggregation based multilevel hierarchy on graphs for coarsening both the vertex and edge spaces. This hierarchy is used together with the hypercircle a posteriori error estimates to give a reliable bound on the error of approximate solutions to the graph Laplacian equation. We introduced the practical algorithm for reshaping of a given aggregation based on the hypercircle error estimates, and the generated aggregations were compared with a matching algorithm. We observed improvements in the quality of aggregations using our reshaping algorithm.

Some further work may be done on studying how different subspaces $W_H$ can be chosen for right-hand side $f$ of various properties, as well as other mechanisms for splitting the aggregates chosen in the reshaping algorithm.

References

[1] Dietrich Braess, Ronald H. W. Hoppe, and Joachim Schöberl. A posteriori estimators for obstacle problems by the hypercircle method. Comput. Vis. Sci., 11(4-6):351–362, 2008.

[2] Achi Brandt. General highly accurate algebraic coarsening. Electron. Trans. Numer. Anal., 10:1–20, 2000. Multilevel methods (Copper Mountain, CO, 1999).

[3] James J. Brannick and Robert D. Falgout. Compatible relaxation and coarsening in algebraic multigrid. SIAM J. Sci. Comput., 32(3):1393–1416, 2010.

[4] F. Brezzi. On the existence, uniqueness and approximation of saddle-point problems arising from Lagrangian multipliers. Rev. Française Automat. Informat. Recherche Opérationnelle Sér. Rouge, 8(R-2):129–151, 1974.

[5] Pasqua D’Ambra and Panayot S. Vassilevski. Adaptive AMG with coarsening based on compatible weighted matching. Comput. Vis. Sci., 16(2):59–76, 2013.

[6] Philippe Destuynder and Brigitte Métivet. Explicit error bounds in a conforming finite element method. Math. Comp., 68(228):1379–1396, 1999.

[7] Willy Dörfler. A convergent adaptive algorithm for Poisson’s equation. SIAM J. Numer. Anal., 33(3):1106–1124, 1996.

[8] Alexandre Ern, Iain Smears, and Martin Vohralík. Discrete $p$-robust $H(div)$-liftings and a posteriori estimates for elliptic problems with $H^{-1}$ source terms. Calcolo, January 2017.

[9] Alexandre Ern and Martin Vohralík. Polynomial-degree-robust a posteriori estimates in a unified setting for conforming, nonconforming, discontinuous Galerkin, and mixed discretizations. SIAM J. Numer. Anal., 53(2):1058–1081, 2015.

[10] Robert D. Falgout and Panayot S. Vassilevski. On generalizing the algebraic multigrid framework. SIAM J. Numer. Anal., 42(4):1669–1693, 2004.

[11] George Karypis and Vipin Kumar. A fast and high quality multilevel scheme for partitioning irregular graphs. SIAM J. Sci. Comput., 20(1):359–392, 1998.

[12] HwanHo Kim, Jinchao Xu, and Ludmil Zikatanov. A multigrid method based on graph matching for convection-diffusion equations. Numer. Linear Algebra Appl., 10(1-2):181–195, 2003. Dedicated to the 60th birthday of Raytcho Lazarov.

[13] J. K. Kraus and S. K. Tomar. Algebraic multilevel iteration method for lowest order Raviart-Thomas space and applications. Internat. J. Numer. Methods Engrg., 86(10):1175–1196, 2011.

[14] P. Ladevèze. Comparaison de modèles de milieux continus. Université Pierre et Marie Curie, Paris, 1975. PhD Thesis.
[15] Raytcho Lazarov, Sergey Repin, and Satyendra K. Tomar. Functional a posteriori error estimates for discontinuous Galerkin approximations of elliptic problems. *Numer. Methods Partial Differential Equations*, 25(4):952–971, 2009.

[16] O. E. Livne. Coarsening by compatible relaxation. *Numer. Linear Algebra Appl.*, 11(2-3):205–227, 2004.

[17] Artem Napov and Yvan Notay. An algebraic multigrid method with guaranteed convergence rate. *SIAM J. Sci. Comput.*, 34(2):A1079–A1109, 2012.

[18] P. Neittaanmäki and S. Repin. *Reliable methods for computer simulation*, volume 33 of *Studies in Mathematics and its Applications*. Elsevier Science B.V., Amsterdam, 2004. Error control and a posteriori estimates.

[19] Ricardo H. Nochetto, Kunibert G. Siebert, and Andreas Veeser. Theory of adaptive finite element methods: an introduction. In *Multiscale, nonlinear and adaptive approximation*, pages 409–542. Springer, Berlin, 2009.

[20] Ricardo H. Nochetto and Andreas Veeser. Primer of adaptive finite element methods. In *Multiscale and adaptivity: modeling, numerics and applications*, volume 2040 of *Lecture Notes in Math.*, pages 125–225. Springer, Heidelberg, 2012.

[21] W. Prager and J. L. Synge. Approximations in elasticity based on the concept of function space. *Quart. Appl. Math.*, 5:241–269, 1947.

[22] Sergey Repin. *A posteriori estimates for partial differential equations*, volume 4 of *Radon Series on Computational and Applied Mathematics*. Walter de Gruyter GmbH & Co. KG, Berlin, 2008.

[23] Sergey I. Repin and Satyendra K. Tomar. Guaranteed and robust error bounds for nonconforming approximations of elliptic problems. *IMA J. Numer. Anal.*, 31(2):597–615, 2011.

[24] S. K. Tomar and S. I. Repin. Efficient computable error bounds for discontinuous Galerkin approximations of elliptic problems. *J. Comput. Appl. Math.*, 226(2):358–369, 2009.

[25] Petr Vaněk, Marian Brezina, and Jan Mandel. Convergence of algebraic multigrid based on smoothed aggregation. *Numer. Math.*, 88(3):559–579, 2001.

[26] Panayot S. Vassilevski and Ludmil T. Zikatanov. Commuting projections on graphs. *Numer. Linear Algebra Appl.*, 21(3):297–315, 2014.