Numerical Methods for Hodge Decomposition

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Applied Hodge Theory Minisymposium ICIAM 2011, Vancouver Tuesday, July 19, 2011 Triangle meshes: 1-cochains

Tetrahedral meshes: 1- and 2-cochains

Manifolds: Differential forms and vector fields

Graphs: 1-cochains

 $\mathsf{gradients} \oplus \mathsf{curls} \oplus \mathsf{harmonics}$

Computing Hodge Decomposition:

Find two and infer third by subtraction Curl and harmonic part are harder Find gradient part, and curl OR harmonic part

Elementary in principle, but in practice:

Functional Analysis Numerical Linear Algebra Computational Geometry Computational Topology are all connected to the problem.

Functional Analysis :

Convergence and stability

Numerical Linear Algebra :

Least squares for theory and practice On graphs conjugate gradient beats multigrid

Computational Geometry :

Meshing affects choice of method Mesh properties for near-optimal solve time

Computational Topology :

Use (co)homology basis for harmonics Experiments on clique complexes

1-norm and linear programming

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Only the highlighted topics will be discussed

Hodge Decomposition in Finite Dimensions

A pattern that appears in Hodge decomposition on graphs and meshes

U, V, W finite-dimensional inner product spaces

$$V = \operatorname{im} A \oplus \operatorname{im} A^{\perp} = \operatorname{im} A \oplus \operatorname{ker} A^{T}$$
$$V = \operatorname{im} A \oplus \operatorname{im} B^{T} \oplus (\operatorname{ker} B \cap \operatorname{ker} A^{T})$$
$$V = \operatorname{im} A \oplus \operatorname{im} B^{T} \oplus \operatorname{ker} \Delta$$
$$\Delta = A A^{T} + B^{T} B$$

Laplace-deRham Operators on Graphs

Chain and cochain complexes on 2-dimensional clique complex of graph G

$$\begin{split} \Delta_0 &= \partial_1 \, \partial_1^T \\ \Delta_1 &= \partial_1^T \, \partial_1 + \partial_2 \, \partial_2^T \\ \Delta_2 &= \partial_2^T \, \partial_2 \end{split}$$

Hodge Decomposition on Graphs

Useful for least squares ranking on graphs

$$\omega = \partial_1^T \, \alpha + \partial_2 \, \beta + h$$

$$\partial_1 \partial_1^T \mathbf{a} = \partial_1 \omega \qquad \partial_2^T \partial_2 \mathbf{b} = \partial_2^T \omega$$

$$\partial_1^T a \simeq \omega$$

 $\partial_2 b \simeq \omega$

$$\min_{a} ||r||_{2} \text{ such that } r = \omega - \partial_{1}^{T} a$$
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$$(\Delta u, v) = (\mathsf{d} u, \mathsf{d} v) + (\delta u, \delta v)$$

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$$C^{0} \xrightarrow{d_{0}} C^{1} \xrightarrow{d_{1}} C^{2}$$

$$\downarrow^{*_{0}} \qquad \downarrow^{*_{1}} \qquad \downarrow^{*_{2}}$$

$$D^{2} \xleftarrow{d_{0}^{T}} D^{1} \xleftarrow{d_{1}^{T}} D^{0}$$

$$\begin{split} \Delta_0 &= d_0^{\mathcal{T}} *_1 d_0 \\ \Delta_1 &= d_1^{\mathcal{T}} *_2 d_1 + *_1 d_0 *_0^{-1} d_0^{\mathcal{T}} *_1 \\ \Delta_2 &= - *_2 d_1 *_1^{-1} d_1^{\mathcal{T}} *_2 \end{split}$$

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Highlighted part problematic unless inverse Hodge star can be handled easily

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Naive Hodge Decomposition on Meshes

Linear system for curl (β) part has inverse Hodge star

$$\omega = \mathsf{d}\,\alpha + \delta\,\beta + \mathsf{h}$$

$$\delta \omega = \delta d \alpha$$
$$*^{-1} d^{T} * d \alpha = *^{-1} d^{T} * \omega$$
$$d^{T} * d \alpha = d^{T} * \omega$$

$$d \omega = d \delta \beta$$
$$d *^{-1} d^{T} * \beta = d \omega$$

Strategy for Computing Hodge Decomposition Different for graphs and meshes

Graphs (no metric involved – Hodge star is Identity):

- Use least squares for gradient and curl
- Find harmonic component by subtraction

Manifold simplicial complexes (Hodge star is not Identity):

- Use weighted least squares for gradient part. In addition:
- Find harmonic basis as eigenvectors and project OR
- Find harmonic basis by discrete Hodge-deRham and project

Eigenvector Method for Harmonic Basis

Use of weak form to avoid inverse Hodge stars

Consider the linear system for σ and u :

$$(\sigma, \tau) - (d_{\rho-1} \tau, u) = 0,$$

 $(d_{\rho-1} \sigma, v) + (d_{\rho} u, d_{\rho} v) = 0,$

for all τ and v. Then (σ, u) is a solution if and only if $\sigma = 0$ and u is a harmonic *p*-form.

$$\begin{bmatrix} *_{p-1} & -\mathsf{d}_{p-1}^{\mathsf{T}} *_p \\ *_p \mathsf{d}_{p-1} & \mathsf{d}_p^{\mathsf{T}} *_{p+1} \mathsf{d}_p \end{bmatrix}$$

Eigenvectors of 0 eigenvalue are harmonic cochains.

Harmonic cochains using eigenvector method



Discrete Hodge-deRham Method for Harmonic Basis

Avoids inverse Hodge stars and in addition provides topological control

- Find a homology basis and its dual cohomology basis
- Find harmonic cochains cohomologous to cohomology basis



Chain a homologous to b if $a - b \in \operatorname{im} \partial$



Cochain *h* cohomologous to ω if $h - \omega \in \operatorname{im} d$



Poincaré-Lefschetz duality:

M manifold of dimension n

If
$$\partial M = \emptyset$$
, then $H^p(M; \mathbb{R}) \cong H_{n-p}(M; \mathbb{R})$
If $\partial M \neq \emptyset$, then $H^p(M; \mathbb{R}) \cong H_{n-p}(M, \partial M; \mathbb{R})$

Naive Cohomologous Harmonic Cochain

Given $[\omega] \in H^p(M; \mathbb{R})$. Find α such that

 $\Delta (\omega + d \alpha) = 0$

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Given $[\omega] \in H^p(M; \mathbb{R})$. Find α such that

$$\Delta \left(\omega + \mathsf{d} \ \alpha \right) = \mathsf{0}$$

Since $\omega \in \ker d$, above is equivalent to

$$\label{eq:deltadd} \begin{array}{l} \mathsf{d} \ \mathsf{\delta} \ \mathsf{d} \ \alpha = - \ \mathsf{d} \ \delta \ \omega \\ \\ \mathsf{d} \ \ast^{-1} \ \mathsf{d}^{\mathsf{T}} \ast \ \mathsf{d} \ \alpha = - \ \mathsf{d} \ \ast^{-1} \ \mathsf{d}^{\mathsf{T}} \ast \ \omega \end{array}$$

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$$\mathsf{d} \ \delta \ \mathsf{d} \ \alpha = - \mathsf{d} \ \delta \ \omega$$
$$\mathsf{d} \ *^{-1} \mathsf{d}^{\mathsf{T}} * \mathsf{d} \ \alpha = - \mathsf{d} \ *^{-1} \mathsf{d}^{\mathsf{T}} * \omega$$

Again, the inverse Hodge stars could be a problem

Discrete Hodge-deRham Method

Smallest cochain in each cohomology class is harmonic

Given $[\omega] \in H^p(M; \mathbb{R})$. Find α such that

$$\min_{\alpha \in C^{p-1}} (\omega + \mathsf{d}\,\alpha\,,\,\omega + \mathsf{d}\,\alpha)$$

$$\min_{\alpha \in C^{p-1}} (\omega + \mathsf{d}\,\alpha)^T * (\omega + \mathsf{d}\,\alpha)$$

$$\mathsf{d}_{p-1}^{\mathcal{T}} \ast_p \mathsf{d}_{p-1} \alpha = -\,\mathsf{d}_{p-1}^{\mathcal{T}} \ast_p \omega$$

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Note : no inverse Hodge stars

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Inspired by a result in the smooth case that smallest differential form cohomologous to a given form is harmonic. Precise statement of theorem in discrete case given later.

Sample Code for Harmonic Cochain Computation

Using discrete Hodge-deRham method

```
from numpy import zeros, loadtxt
from numpy.linalg import inv
from scipy.sparse import csr_matrix
from scipy.sparse.linalg import cg
from dlnyhdg.simplicial_complex import simplicial_complex
from pydec import whitney_innerproduct
tol = 1e-8; scale = 5; width = 0.001
vertices = loadtxt('vertices.txt')
triangles = loadtxt('triangles.txt', dtype=int)
sc = simplicial_complex((vertices, triangles))
edge_list, edge_orientation = loadtxt('12cocycle.txt', dtype=int)
omega = zeros(sc[1].num_simplices)
for i, e in enumerate(edge_list):
    omega[e] += edge_orientation[i]
d0 = sc[0].d
hodge1 = whitney_innerproduct(sc, 1)
A = d0.T * hodge1 * d0; b = -d0.T * hodge1 * omega
alpha = cg(A, b, tol=tol)[0]
harmonic = omega + d0 * alpha
```







Compare with harmonic cochains using eigenvector method





Isomorphism Theorem in Smooth Case

Inspiration for the discrete Hodge-deRham method

Theorem (Hodge-deRham Isomorphism)

For a boundaryless manifold M ($\partial M = \emptyset$), $H^p(M; \mathbb{R}) \cong \mathcal{H}^p(M) = \ker \Delta_p$. For manifolds with boundary, $H^p(M; \mathbb{R}) \cong \mathcal{H}^p_N(M)$ and $H^p(M, \partial M; \mathbb{R}) \cong \mathcal{H}^p_D(M)$.

Harmonic forms : ker Δ Harmonic fields : $\mathcal{H}(M) = \ker d \cap \ker \delta$ Harmonic Neumann fields : $\mathcal{H}_N(M)$ normal component 0 Harmonic Dirichlet fields : $\mathcal{H}_D(M)$ tangential component 0

Isomorphism Theorem in Discrete Case

Theorem (Discrete Hodge-deRham Isomorphism, H-K-W-W) Let $[\omega] \in H^p(K; \mathbb{R})$. Then

- 1. There exists a cochain $\alpha \in C^{p-1}(K; \mathbb{R})$, not necessarily unique, such that $\delta_p(\omega + d_{p-1}\alpha) = 0$;
- 2. There is a unique cochain $d_{p-1} \alpha$ satisfying $\delta_p (\omega + d_{p-1} \alpha) = 0$; and

3.
$$\delta_{p}(\omega + \mathsf{d}_{p-1}\alpha) = 0 \Rightarrow \Delta_{p}(\omega + \mathsf{d}_{p-1}\alpha) = 0.$$

Theorem (H-Demlow)

Let $[\omega] \in H^{p}(\mathcal{T}_{h}; \mathbb{R})$ and let $\alpha \in C^{p-1}$ be such that $(\omega + d_{p-1}\alpha, d_{p-1}\tau) = 0$ for all $\tau \in C^{p-1}$. Then $W(\omega + d_{p-1}\alpha) \in \mathfrak{H}_{h}^{p}$.

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If Whitney Hodge star is used, the method produces a solution to the finite element exterior calculus equations for harmonic cochains.

Back to Graphs

Comparison of algebraic multigrid and conjugate gradient

- Results from experiments on graphs will be shown next
- 2-dimensional clique complexes for Erdős-Rényi random graphs and Barabási-Albert scale-free graphs were used
- ► *N_p* is number of *p*-simplices
- Conjugate gradient easily beats algebraic multigrid in these experiments
- Smoothed aggregation and Lloyd aggregation were used
- Entries for algebraic multigrid show setup time, solve time, and total time
- Pictures of system matrices hint at reason for poor performance of multigrid

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Case	N ₀	<i>N</i> ₁	<i>N</i> ₂	Edge	Triangle
				Density	Density
а	100	1212	2359	2.45e-01	1.46e-02
b	100	2530	21494	5.11e-01	1.33e-01
с	100	3706	67865	7.49e-01	4.20e-01
d	500	1290	21	1.03e-02	1.01e-06
e	500	12394	20315	9.94e-02	9.81e-04

Numerical experiments on Erdős-Rényi graphs

Casa	Algebraic	: Multigrid	Conjugate Gradient	
Case	α	β	α	β
	0.0001	0.5708		
a	0.0078	0.0551	0.0023	0.0191
	0.0079	0.6259		
	0.0030	0.866		
b	0.0111	1.236	0.0017	0.1033
	0.0141	2.102		
	0.0303	5.66		
с	0.0386	11.08	0.0015	0.4759
	0.0689	16.74		
d	0.1353	0.0071		
	0.5760	0.0289	0.0072	0.0007
	0.7113	0.0360		
e	0.0001	0.49		
	0.3303	2.22	0.0030	0.2155
	0.3305	2.71		

Case	N ₀	<i>N</i> ₁	<i>N</i> ₂	Edge	Triangle
				Density	Density
а	100	900	1701	1.82e-01	1.05e-02
b	100	1600	8105	3.23e-01	5.01e-02
с	100	2400	24497	4.85e-01	1.51e-01
d	500	9600	25016	7.70e-02	1.21e-03
e	1000	19600	37365	3.92e-02	2.25e-04

Numerical experiments on Barabási-Albert graphs

Case	Algebraic	: Multigrid	Conjugate Gradient	
	α	β	α	β
а	0.0005	0.0242		
	0.0012	0.0753	0.0033	0.0281
	0.0017	0.0995		
	0.0001	0.1842		
b	0.0008	0.1720	0.0032	0.0967
	0.0009	0.3562		
	0.0005	1.111		
с	0.0012	1.521	0.0030	0.2435
	0.0017	2.632		
d	0.0002	1.018		
	0.0140	3.608	0.0056	1.043
	0.0142	4.626		
e	0.0174	2.40		
	0.0219	8.21	0.0088	2.521
	0.0393	10.61		

Pictures of system matrices for graph experiments



Meshes versus Graphs

A mesh, its Δ_0 , and Δ_0 for a graph with same number of vertices and same edge density







Experiments with Random Clique Complexes

Graph Hodge decomposition code can be used to formulate conjectures



Dashed lines are Kahle's bounds [Kahle, Discrete Math., Vol. 309, pp. 1658–1671]. Betti number is almost always zero before the first bound and after third bound. It is almost always nonzero between first and second bounds. Theory is silent about the region between second and third bounds and about harmonic norm.

Optimal (Co)homologous (Co)chains

Common threads

Cohomologous harmonic cochains:

$$\begin{split} & \min_{\alpha \,\in\, C^{p-1}} (\omega + \mathsf{d}\,\alpha\,,\,\omega + \mathsf{d}\,\alpha) \\ & \min_{\alpha} \,\|h\|_{*_p} \quad \text{subject to} \quad h = \omega + \mathsf{d}\,\alpha \quad (\text{all vectors real}) \end{split}$$

Least squares ranking on graphs:

$$\begin{split} \min_{\alpha} & \|r\|_2 \quad \text{subject to} \quad r = \omega - \partial_1^T \alpha \quad \text{(all vectors real)} \\ \min_{\beta} & \|s\|_2 \quad \text{subject to} \quad s = \omega - \partial_2 \beta \quad \text{(all vectors real)} \end{split}$$

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Optimal homologous chains: [See Dey-Hirani-Krishnamoorthy and Dunfield-Hirani]

 $\min_{x,y} \|x\|_1 \quad \text{subject to} \quad x = c + \partial y \quad \text{(all vectors integer)}$

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