The Combinatorics of Finite Element Methods

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Outline

1. What is the finite element method?
   - A method for numerically solving partial differential equations.
2. Why am I talking about PDEs / applied math at a combinatorics / number theory conference?
   - Euler characteristic / simplicial cohomology naturally arises in the study of finite elements.
   - Finite element exterior calculus (Arnold, Falk, Winther, 2006).
3. That's a cool connection, but does understanding cohomology actually improve numerical methods?
   - Yes.
4. Has anything interesting happened since then?
   - Yes.

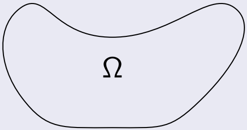
Numerically solving PDEs

Sample Problem

- Given $f\colon \Omega \to \mathbb{R}$, find $u\colon \Omega \to \mathbb{R}$ such that

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = f$$

and u vanishes on the boundary.

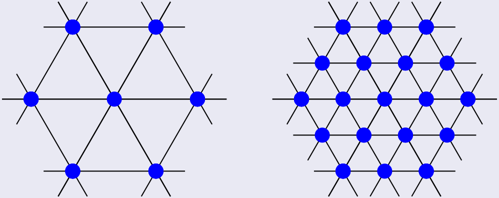


Discretization

- To solve numerically, we must discretize.
- We need a finite-dimensional space of functions that "approximates" the full infinite-dimensional space of possible u.

Finite-dimensional function spaces

Continuous piecewise linear functions to $\mathbb{R}$



Continuous piecewise polynomial functions to $\mathbb{R}$

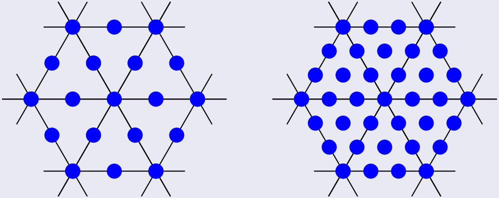
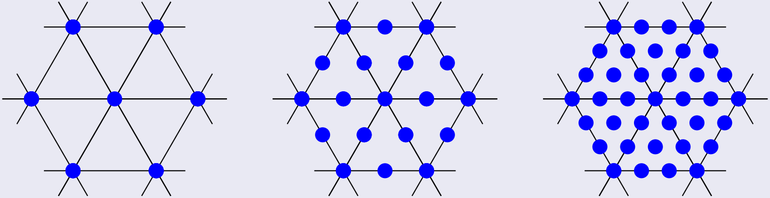


Figure: Piecewise quadratic (left) and piecewise cubic (right)

Degrees of freedom

Piecewise linear/quadratic/cubic continuous scalar-valued functions



Degrees of freedom (DOFs)

- One value per degree of freedom (blue dot)
  - yields a unique function on each triangle, and
  - enforces continuity between adjacent triangles.

Piecewise linear	$\mathbb{R}^{V}$
Piecewise quadratic	$\mathbb{R}^{V+E}$
Piecewise cubic	$\mathbb{R}^{V+2E+F}$

Finite-dimensional spaces of vector fields

Continuity conditions

- If we view a vector field as a tuple of scalar fields, we can use the above finite-dimensional spaces of scalar-valued functions.
    - Doing so yields continous piecewise polynomial vector fields.
- But we want only tangential continuity, not full continuity.

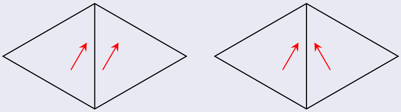


Figure: Full continuity (left) vs. tangential continuity (right)

- Why do we only want tangential continuity?
    - Gradients of continuous piecewise smooth scalar fields only have tangential continuity.
        - Gradients of "valid objects" should be "valid objects".
    - Having well-defined line integrals requires only tangential continuity.

Gradients of piecewise smooth scalar fields

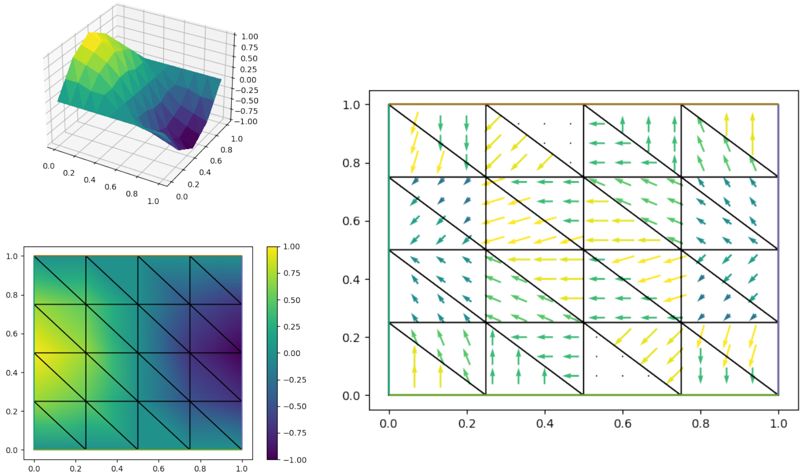
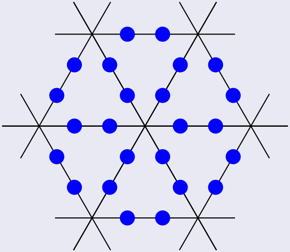


Figure: A piecewise linear function (left) and its gradient (right)

Degrees of freedom (DOFs)

DOFs of piecewise linear vector fields with tangential continuity?

- Values should
  - uniquely specify a linear vector field on each triangle, and
  - enforce tangential continuity between adjacent triangles.



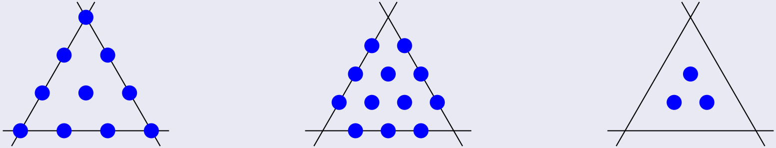
Higher degree?

Periodic Table of the Finite Elements

Complexes and cohomology

A discrete subcomplex of the de Rham complex

continuous piecewise cubic scalar fields $\xrightarrow{\text{grad}}$ tangentially continuous piecewise quadratic vector fields $\xrightarrow{\text{curl}}$ discontinuous piecewise linear scalar fields



$$\mathbb{R}^{V+2E+F} \longrightarrow \mathbb{R}^{3E+3F} \longrightarrow \mathbb{R}^{3F}$$

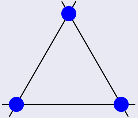
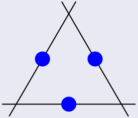
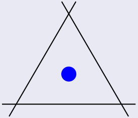
Euler characteristic and cohomology of triangulated surfaces

- This complex has the right Euler characteristic:
$$(V + 2E + F) - (3E + 3F) + 3F = V - E + F.$$
- The cohomology agrees with simplicial/de Rham cohomology.
  - (Arnold, Falk, Winther, 2010).

Whitney forms (Whitney, 1957)

Can we get simplicial cochains?

$$\mathbb{R}^V \longrightarrow \mathbb{R}^E \longrightarrow \mathbb{R}^F$$

continuous piecewise linear scalar fields $\xrightarrow{\text{grad}}$ span of Whitney forms $\xrightarrow{\text{curl}}$ discontinuous piecewise constant scalar fields

Barycentric coordinates (the standard simplex)

$$\{(\lambda_1, \lambda_2, \lambda_3) \in \mathbb{R}^3_{\geq 0} \mid \lambda_1 + \lambda_2 + \lambda_3 = 1\}$$

Whitney one-forms:

$$\lambda_1 \, d\lambda_2 - \lambda_2 \, d\lambda_1,$$
$$\lambda_2 \, d\lambda_3 - \lambda_3 \, d\lambda_2,$$
$$\lambda_3 \, d\lambda_1 - \lambda_1 \, d\lambda_3.$$

Definition (the $\mathcal{P}_r\Lambda^k$ spaces)

- Let $\mathcal{T}$ be a triangulation of a manifold of dimension n.
- Let $\mathcal{P}_r\Lambda^k(\mathcal{T})$ be the space of k-forms that
  - are piecewise polynomial of degree at most r, and
  - are tangentially continuous.

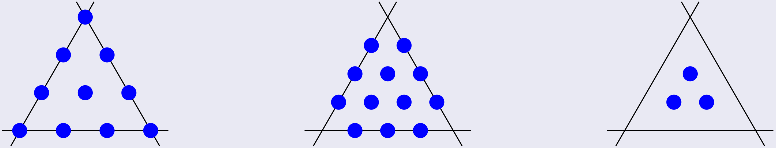
Example

$\mathcal{P}_r\Lambda^0(\mathcal{T})$	continuous piecewise polynomial scalar fields
$\mathcal{P}_r\Lambda^1(\mathcal{T})$	tangentially continuous piecewise polynomial vector fields
$\mathcal{P}_r\Lambda^{n-1}(\mathcal{T})$	normally continuous piecewise polynomial vector fields
$\mathcal{P}_r\Lambda^n(\mathcal{T})$	discontinuous piecewise polynomial scalar fields

Complexes revisited

We've seen

continuous piecewise cubic scalar fields $\xrightarrow{\text{grad}}$ tangentially continuous piecewise quadratic vector fields $\xrightarrow{\text{curl}}$ discontinuous piecewise linear scalar fields



$$\mathcal{P}_3\Lambda^0(\mathcal{T}) \xrightarrow{\quad d \quad} \mathcal{P}_2\Lambda^1(\mathcal{T}) \xrightarrow{\quad d \quad} \mathcal{P}_1\Lambda^2(\mathcal{T})$$

On a single simplex T

- The Whitney k-forms have one DOF per k-dimensional face.
- Call their span $\mathcal{P}_1^-\Lambda^k(T)$.
  - Note: $\mathcal{P}_0\Lambda^k(T) \subseteq \mathcal{P}_1^-\Lambda^k(T) \subseteq \mathcal{P}_1\Lambda^k(T)$.
- Multiply Whitney forms by arbitrary scalar-valued polynomials of degree at most $r-1$. Call the span of these $\mathcal{P}_r^-\Lambda^k(T)$.
  - So, $\mathcal{P}_{r-1}\Lambda^k(T) \subseteq \mathcal{P}_r^-\Lambda^k(T) \subseteq \mathcal{P}_r\Lambda^k(T)$.

Definition (the $\mathcal{P}_r^-\Lambda^k$ spaces on a triangulation)

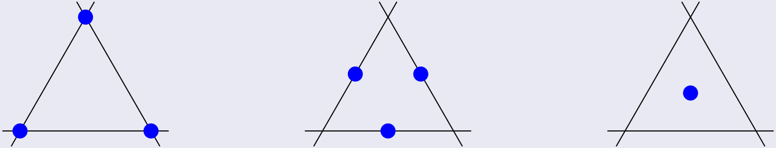
- Let $\mathcal{T}$ be a triangulation of a manifold of dimension n.
- Let $\mathcal{P}_r^-\Lambda^k(\mathcal{T})$ be the space of k-forms that
  - are in $\mathcal{P}_r^-\Lambda^k(T)$ for each element T of the triangulation, and
  - are tangentially continuous.

Duality between $\mathcal{P}$ and $\mathcal{P}^-$

Complexes revisited

We've also seen

continuous piecewise linear scalar fields $\xrightarrow{\text{grad}}$ Whitney forms $\xrightarrow{\text{curl}}$ discontinuous piecewise constant scalar fields



$$\mathcal{P}_1^-\Lambda^0(\mathcal{T}) \xrightarrow{\quad d \quad} \mathcal{P}_1^-\Lambda^1(\mathcal{T}) \xrightarrow{\quad d \quad} \mathcal{P}_1^-\Lambda^2(\mathcal{T})$$

More complexes

Theorem (Arnold, Falk, Winther, 2006)

For a triangulation $\mathcal{T}$, the cohomology of the complexes

$$\mathcal{P}_r\Lambda^0(\mathcal{T}) \xrightarrow{d} \mathcal{P}_{r-1}\Lambda^1(\mathcal{T}) \xrightarrow{d} \cdots \xrightarrow{d} \mathcal{P}_{r-n}\Lambda^n(\mathcal{T})$$

$$\mathcal{P}_r^-\Lambda^0(\mathcal{T}) \xrightarrow{d} \mathcal{P}_r^-\Lambda^1(\mathcal{T}) \xrightarrow{d} \cdots \xrightarrow{d} \mathcal{P}_r^-\Lambda^n(\mathcal{T})$$

agrees with de Rham cohomology (provided $r \geq n$ in the first line).

Remark

The second line with $r = 1$ is isomorphic to simplicial cochains.

Theorem (Arnold, Falk, Winther, 2006)

We can "mix and match" using any of the maps

$$\mathcal{P}_r\Lambda^k(\mathcal{T}) \xrightarrow{d} \mathcal{P}_{r-1}\Lambda^{k+1}(\mathcal{T}), \qquad \mathcal{P}_r\Lambda^k(\mathcal{T}) \xrightarrow{d} \mathcal{P}_r^-\Lambda^{k+1}(\mathcal{T})$$

$$\mathcal{P}_r^-\Lambda^k(\mathcal{T}) \xrightarrow{d} \mathcal{P}_r^-\Lambda^{k+1}(\mathcal{T}), \qquad \mathcal{P}_r^-\Lambda^k(\mathcal{T}) \xrightarrow{d} \mathcal{P}_{r-1}\Lambda^{k+1}(\mathcal{T})$$

References

Douglas N. Arnold, Richard S. Falk, and Ragnar Winther.
Finite element exterior calculus, homological techniques, and applications.
Acta Numer., 15:1–155, 2006.

Douglas N. Arnold, Richard S. Falk, and Ragnar Winther.
Finite element exterior calculus: from Hodge theory to numerical stability.
Bull. Amer. Math. Soc. (N.S.), 47(2):281–354, 2010.

How do finite element spaces yield numerical methods?

Recall our sample problem

- Given $f\colon \Omega \to \mathbb{R}$, find $u\colon \Omega \to \mathbb{R}$ vanishing on $\partial\Omega$ such that

$$\Delta u = f.$$

- Equivalently,

$$\int_\Omega (\Delta u) v = \int_\Omega fv \qquad \forall\, v \text{ vanishing on } \partial\Omega.$$

- Intergating by parts,

$$-\int_\Omega \operatorname{grad} u \cdot \operatorname{grad} v = \int_\Omega fv \quad \forall\, v \text{ vanishing on } \partial\Omega. \tag{1}$$

Galerkin method

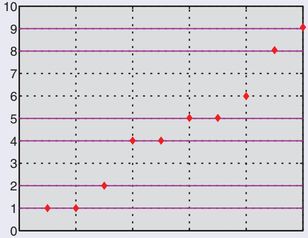
- Given f, solve (1) for u, where u and v are restricted to be in the finite element space.
- Get a finite-dimensional linear system of equations.

Why do numerical analysts care about cohomology?

Eigenvalues of the curl curl operator

On a square domain, find a vector field u (with appropriate boundary conditions) such that $\operatorname{curl}\operatorname{curl} u = \lambda u$.

Bad things happen if we do not respect cohomology (AFW, 2010)



- Using vector fields with full continuity yields false eigenvalue $\lambda = 6$.
- In contrast, using the spaces we've discussed yields the correct spectrum.

How does cohomology play a role?

- $\dim(\ker\operatorname{curl}) = \infty$, so zero eigenspace hard to control.
- Can control if $\ker\operatorname{curl} = \operatorname{im}\operatorname{grad}$ holds on the discrete level.

Why do numerical analysts care about cohomology?

Noether's Theorem, conservation laws, and discretization

- Noether's theorem: a system that is invariant under a transformation has a corresponding conservation law:
  - translation invariance $\Rightarrow$ conservation of momentum
  - rotation invariance $\Rightarrow$ conservation of angular momentum
  - time-translation invariance $\Rightarrow$ conservation of energy
- Discretizations that respect Noether's theorem will conserve these quantities exactly.
  - Otherwise, the quantities will be conserved only approximately and may drift over time.

Charge conservation in electromagnetism / Yang-Mills

- $\operatorname{curl} u$ invariant under $u \mapsto u + \operatorname{grad} f$
- $\Rightarrow$ weighted average $\int \rho f$ conserved (ρ is charge).
  - continuous setting: all f allowed $\Rightarrow$ ρ conserved.
  - discrete setting: only f in finite element space (Nédélec, 1980).
- can conserve ρ even in discrete setting (—, Stern, 2021).

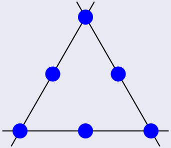
Bases for scalar fields

- Recall barycentric coordinates:

$$\left\{(\lambda_1, \lambda_2, \lambda_3) \in \mathbb{R}^3_{\geq 0} \mid \lambda_1 + \lambda_2 + \lambda_3 = 1\right\}.$$

- Quadratic scalar fields have *monomial basis*

$$\lambda_1^2, \quad \lambda_2^2, \quad \lambda_3^2, \quad \lambda_1\lambda_2, \quad \lambda_2\lambda_3, \quad \lambda_3\lambda_1.$$



Symmetry

- For scalar fields, the monomial basis is invariant under permuting $\lambda_1, \lambda_2, \lambda_3$.
- For vector fields, such an invariant basis may or may not exist, even up to sign.
  - In 2D and 3D, depends on the type of finite element space (e.g. $\mathcal{P}\Lambda^1$, $\mathcal{P}^-\Lambda^2$), and the polynomial degree modulo 3 (Licht, 2019; —, 2023).

Further directions

Riemannian geometry

So far we've discussed

- discretizing differential forms:
  - differential topology / smooth manifolds.

Riemannian geometry / Riemannian manifolds

- Must discretize the Riemannian metric:
  - Lowest order is just specifying the length of every edge of the triangulation (Regge, 1961).
  - Higher polynomial degree (Li, 2018).
- Must understand curvature:
  - Lowest order scalar curvature is just angle defect.
    - 2D: Gauss–Bonnett. General dimension: Regge, 1961.
  - Several papers towards full Riemann curvature tensor in general piecewise polynomial/smooth setting:
    - various combinations of —, Gawlik, Neunteufel, and others; 2019–2023 and in preparation.

Thank you