Chapter 1

Course Overview

We had a stance that our workflow in numerical analysis goes in the following way.

1. We are given either a mathematical definition, or a theorem stating the existence.
   (a) Example: The definition of *rank* of a matrix.
   (b) Example: For an equation $u'(t) = f(t, u(t))$, $u(0) = \alpha$ with f smooth, there exists $T_{max} > 0$ and a solution in $[0, T_{max}]$.
2. Not all of them come with *methodology* to capture them.
3. If one comes with a methodology, we specify the algorithm and implement it.
4. If an implementation comes as an *approximation*, we should be able to estimate the size of error.

We will keep the same stance in the course.

Based on what we have learned, we could apply our study to two major fields of mathematics

1. many notions, definitions, and theorems in Linear Algebra,
2. existence theorem of a certain partial differential equation.

1. Each of the two would take one or two semesters.
2. So that students who studies PDE course along with this course can benefit from here,
3. We set our objective to be to implement what are studied in Chapter 6 and 7 in Evans textbook.
4. This means two things:
   (a) We work with a pde that is either elliptic or parabolic, and the method we employ is the Galerkin method.
   (b) The important class of pde of hyperbolic type will not be studied. Hyperbolic pde solver has to be implemented differently, where one needs to reflect knowledge of theory of hyperbolic pdes.

The objective of our course is from the following theorem.

We consider the Initial Boundary Value Problem of the following pde:

$$\begin{aligned} -\sum_{i,j=1}^{n} \partial_{x_i}\big(a^{ij}(x)\partial_{x_j}u(x)\big) &= \varphi(x), \quad x \in \Omega, \\ -\sum_{i,j=1}^{n} \big(a^{ij}(x)\partial_{x_j}u(x)\big)\nu_i &= \psi(x), \quad x \in \partial\Omega \end{aligned} \tag{P}$$

with constraint $\displaystyle\int_{\partial\Omega} \psi = \int_{\Omega} \varphi$.

We will specify assumptions on Ω, coefficients $a^{ij}(x)$, and (r-h-s) $\varphi(x)$ and $\psi(x)$.

Theorem 1. *There exists a solution of the boundary value problem* (P).

We will make the course as parallel as possible to the previous one.

1. The problem, taken as a root-finding problem for an equation
$$F(x) = y \quad \text{for given } y,$$
is tackled in 2nd half of the course.
2. The first half of the course is to extend our knowledge on piecewise polynomial functions to the multi-dimensional settings.

The first half: pp functions in $\Omega \subset \mathbb{R}^n$.

In this course, unless otherwise specified, $\Omega \subset \mathbb{R}^n$ is a bounded open set with smooth boundary, that is simply connected. Also $n = 3$ in most cases.

This is to extend our far reaching 1d remainder theorem into multi-dimensional setting. Recall

Theorem 2 (1d remainder theorem)**.** *Let $f \in C^{n+1}([a, b])$ and $x_0,\ x_1,\ \cdots,\ x_n \in [a, b]$. Then, for $x \in [a, b]$,*

$$\begin{aligned} R(x) &= f[x_0, x_1, x_2, \cdots, x_n, x](x - x_0)(x - x_1)\cdots(x - x_{n-1})(x - x_n) \\ &= f(x) - \Big(f[x_0] + f[x_0, x_1](x - x_0) + f[x_0, x_1, x_2](x - x_0)(x - x_1) + \cdots \\ &\quad + f[x_0, x_1, \cdots, x_n](x - x_0)(x - x_1)(x - x_2)\cdots(x - x_{n-1})\Big). \end{aligned}$$

The extension to multi-dimensional setting is not at all trivial.

Partitioning of Ω

To partition Ω into small pieces is not trivial. We will be speaking of the *Simplicial complex*, tetrahedrons in $\mathbb{R}^3$ for example, borrowing language of *Combinatorial Algebraic Topology.*

Kinds of functions on Ω

In $\mathbb{R}^3$, not only the function $f : \Omega \subset \mathbb{R}^3 \to \mathbb{R}$ but also for instance the vector field
$$E : \Omega \subset \mathbb{R}^3 \to \mathbb{R}^3,$$
is relevant. We will be speaking of k-covector fields, for $k = 0, 1, 2, 3$, borrowing language of *Differential Geometry.*

Remainder formula or remainder estimates

We present Poincare inequality, Bramble-Hilbert inequality, etc.

The second half: a rootfinding problem framework

We recall the set up for a rootfinding problem for $F : X \to Y$, solving for a given $y \in Y$ such that

$$F(x) = y.$$

1. We will specify X and Y for the pde.
2. We will recall the design of the solver. This includes
3. Consistency of the parametrized approximation $(\tilde{F}_h)$.
4. Consistency of the parametrized approximate solver $(\tilde{R}_h)$.
5. Continuity properties of solver.
6. A priori error estimate.
7. A posteriari error estimate.

Chapter 2

Partitioning of Domain

- In 1-d, the domain $[a, b]$ is partitioned simply by specifying points in ascending order

$$a = x_0 < x_1 < x_2 < \cdots < x_n = b,$$

  producing n small intervals

$$I_j = [x_{j-1}, x_j] \quad j = 1, 2, \cdots, n.$$

- The role of the interval in 1-d is taken by the oriented triangle in 2-d, by the oriented tetrahedron in 3-d, and by the oriented n-simplex in n-d.

- We first introduce a few notions to speak of partitioning a domain.

k-cells

- A polyhedral convex set is a finite intersection of closed half spaces of $\mathbb{R}^n$.
- A nonempty polyhedral convex set that is k-dimensional and compact is called a k-cell.
  1. We make use of the fact that the dimension of any convex set is well-defined.
  2. The k-dimensional area of k-cell τ is thus
  $$0 < \mathcal{H}^k(\tau) < \infty.$$

An open set $\Omega \subset \mathbb{R}^n$ equipped with the partition by n-cells

We say $(\Omega, \mathcal{P})$ of an open set $\Omega \subset \mathbb{R}^n$ and a set of n-cells $\mathcal{P}$ is an n-cell partition of Ω if

1. If $K_1, K_2 \in \mathcal{P}$ and $K_1 \neq K_2$ then $\operatorname{int}(K_1) \cap \operatorname{int}(K_2) = \emptyset$.
2. $\bar{\Omega} = \bigcup_{K \in \mathcal{P}} K$.

Examples of n-cell partition

CF. For an open set with smooth curved boundary, we in general consider a partition of Ω by a homeomorphic image of n-cell, not n-cell itself. For simplicity, we assume Ω is just a union of n-cells, omitting the flattening procedure.

1. A partition of Ω by n-cells works fine. But we may want more structured partitioning of Ω.
2. $(\Omega, \mathcal{P})$ may be said to be inconvenient in the following sense.
   (a) n-cells in $\mathcal{P}$ are not conformal to each other. For example in 3-d, some may be tetrahedrons, some may be cubes, octahedrons, and so on.
   (b) It is not suitable to define the boundary faces.

Examples of n-cell partition

In our course, we work with n-simplices. We consider $(\Omega, \mathcal{S})$ an open set $\Omega \subset \mathbb{R}^n$ equipped with *a simplicial complex*. We borrow terminology from combinatorial topology, which describes every (topological) detail of Ω in precise manner.

k-simplex

1. As a generalization of an interval in 1-d, we define the oriented k-simplex.
2. (Warning: Let us not bother too much about definitions arising one after another here.)
3. Let $k \in \{0, 1, \cdots, n\}$. A k-simplex is a juxtaposition of $k+1$ points
$$[x_0 x_1 x_2 \cdots x_k],$$
where $x_0, x_1, \cdots, x_k$ are affine independent.
4. $x_0, x_1, \cdots, x_k$ are affine independent if
$$\lambda_0 + \lambda_1 + \cdots + \lambda_k = 0 \quad \text{and} \quad \lambda_0 x_0 + \lambda_1 x_1 + \cdots \lambda_k x_k = 0 \quad \Longrightarrow \lambda_0 = \lambda_1 = \cdots = \lambda_k = 0.$$
This notion is to say that any point of them are not lied in the plane that rest make up.
5. For a $\tau = [x_0 x_1 x_2 \cdots x_k]$, we define its closed point set
$$\overline{\mathsf{pts}}\,(\tau) = \overline{\mathsf{conv}}\,\{x_0, x_1, \cdots, x_k\}.$$
1d example, 2d example

We can consider a partition whose n-cells are all the closed point sets of n-simplices.

- But we can simply do better by storing all the information by the notion of simplicial complex we soon introduce, and more importantly
- n-simplices partitioning still does not resolve the problem of defining the boundary face.

A simplicial complex S satisfying further assumptions.

We consider a set S of closed point sets of k-simplices for $k \in \{0, 1, 2, \cdots, n\}$ that satisfies the following conditions:

1. If $A, B \in S$ then either $A \cap B = \emptyset$ or the intersection is a common face of both A and B.
2. If $A \in S$ then every face of A is also included in S.
3. Every $A \in S$ whose dimension is less than n is a face of some $\sigma \in S$ of dimension n.

We observe from the definition following:

1. Up to item 1, the hanging node problem is resolved.
2. We are able to speak of boundary faces now, which are all stored in S by the condition item 2. A set S satisfying item 1 and 2 are called a simplicial complex.

   Example

3. S satisfying further the item 3 is suitable for our purpose.

   Example

Eventually, we consider $(\Omega, \mathcal{S})$ where $\mathcal{S}$ is a simplicial complex satisfying additionally the condition item 3, such that

$$
\begin{aligned}
\bar{\Omega} &= |\mathcal{S}| \quad \text{that is} \\
&= \bigcup_{A \in S} A \\
&= \bigcup_{\sigma \in S_n} \sigma, \quad S_k = \{A \in S \mid \dim(A) = k\} \quad \text{for } k = 0, 1, 2, \cdots, n.
\end{aligned}
$$

Inspite of all efforts borrowing terminology from the combinatorial topology, from now on we assume $(\Omega, \mathcal{S})$ is given such that Ω is simply connected and bounded.

Implementing $\mathcal{S}$

We can store simplices of $\mathcal{S}$ in the following manner.

- We store $\mathcal{S}_0$ and $\mathcal{S}_n$ legitimately.
- We identify the set S_0 as the set of coordinates $x = (x^0, x^1, x^2, \cdots, x^n)$ and store it.
    1. Let n_0 = number of elements in $\mathcal{S}_0$.
    2. Consider enumeration of $\mathcal{S}_0$ by $i = 1, 2, \cdots, n_0$.
- We identify the set S_n as the $(n+1)$-tuples

$$[i_0 i_1 i_2 \cdots i_n], \quad i_0, i_1, \cdots, i_n \in \{1, 2, \cdots, n_0\}.$$

- Now from $k = n-1$ to $k = 1$ we can store S_k by the following manner.

$$S_{k-1} = \{\text{boundary faces of } a \mid a \in S_k\}.$$

- Along with this, one can store for each $f \in S_{k-1}$

$$\{a \in S_k \mid f \text{ is a boundary face of } a.\}$$

Chapter 3

Polynomials on n-simplex

- Started from the preceding chapter, we are in the program of implementing an approxmation of a given function v defined in Ω.
- On Ω, one thinks of real-valued functions, vector fields, and so on.
- For a while, we first consider a set of smooth real-valued functions defined on Ω,

$$\Lambda_0(\Omega) = C^\infty(\bar{\Omega}).$$

- We recall the thumb rules in making approximation from data:
  1. Under the limited number of available (sampling) data, do the piecewise low order polynomial approximation rather than one high order polynomial approximation.
  2. If we go for the piecewise approximaion, in one such a small domain, choose the preferable sampling points and the preferable basis whenever possible.
- Following the thumb rule, we did the partitioning of Ω into small nice n-simplices.
- Now we discuss polynomials on a n-simplex.

- We consider an n-simplex $\sigma = [x_0 x_1 x_2 \cdots x_n]$ and its point set

$$M = \overline{\mathsf{pts}}\,(\sigma).$$

- We first consider real-valued functions defined on M,

$$v \in \Lambda_0(M) = C^\infty(M).$$

- We consider the subspace of Λ_0 that consists of polynomials of order at most m,

$$\mathbb{P}_m(M) \subset \Lambda_0(M).$$

- We consider a problem of choosing an element $p \in \mathbb{P}_m(M)$ for an approximation of $v \in \Lambda_0(M)$, out of suitable number of sampling data

$$(x_i, v(x_i)), \quad x_i \in M, \quad i = 1, 2, \cdots d.$$

Polynomials in M and Multi index notation

As an example, let us consider a second order polynomial in $\mathbb{R}^2$ that is written as

$$p(x, y) = ax^2 + bxy + cy^2 + dx + ey + f, \quad a, b, c, d, e, f \in \mathbb{R}$$

of three quadratic terms, two linear terms, and one constant term.

To study polynomials in $\mathbb{R}^n$ in a systemtic way, we introduce the multi index.

Multi Index

We introduce a convenient notation for a polynomial in multi dimensions.

- A multi index α is an n-tuple of nonnegative integers $\alpha_1, \alpha_2, \cdots, \alpha_n$,

$$\alpha = (\alpha_1, \alpha_2, \cdots, \alpha_n) \in \big(\mathbb{N} \cup \{0\}\big)^n.$$

- We let

$$x^\alpha = (x_1, x_2, \cdots, x_n)^{(\alpha_1, \alpha_2, \cdots, \alpha_n)} = x_1^{\alpha_1} x_2^{\alpha_2} x_3^{\alpha_3} \cdots x_n^{\alpha_n} \in \mathbb{R}.$$

- The degree or the order of α is

$$|\alpha| = \alpha_1 + \alpha_2 + \cdots \alpha_n \in \mathbb{N} \cup \{0\}.$$

- A homogeneous r-th order polynomial is thus a linear combination of

$$\{x^\alpha \mid |\alpha| = r\}.$$

- For a fixed $r \in \mathbb{N} \cup \{0\}$, how many distinct multi indices with degree r are there ? This is to choose r numbers out of $\{1, 2, \cdots, n\}$ with repeatition allowed,

$$d_{n,r} = \binom{n + r - 1}{r}.$$

- An element $p \in \mathbb{P}_m(M)$ of polynomials of order at most m is thus written as

$$p(x) = \sum_{0 \le |\alpha| \le m} c_\alpha x^\alpha, \quad c_\alpha \in \mathbb{R} \text{ is a coefficient.}$$

- We note that

$$\mathbb{P}_m(M) \simeq \mathbb{R}^d, \quad d = \sum_{r=0}^{m} d_{n,r}.$$

  In fact, d is to choose m numbers for the exponents of $\{1, x_1, x_2, \cdots, x_n\}$ of $n+1$ elements with repeatition allowed, and thus

$$d = \sum_{r=0}^{m} d_{n,r} = \binom{n+m}{m}.$$

- For later purposes, we also define the factorial

$$\alpha! = \alpha_1! \alpha_2! \cdots \alpha_n! \in \mathbb{R}, \quad \text{having in mind that } 0! = 1.$$

Examples: $n = 2$.

- $\mathbb{P}_0(M)$ is of dimension 1,
$$d_{2,0} = 1.$$
- $\mathbb{P}_1(M)$ is of dimensions
$$1 + d_{2,1} = 1 + 2 = 3.$$
- $\mathbb{P}_2(M)$ is of dimensions
$$1 + 2 + d_{2,2} = 1 + 2 + 3 = 6.$$

Examples: $n = 3$.

- $\mathbb{P}_0(M)$ is of dimension 1,
$$d_{3,0} = 1.$$
- $\mathbb{P}_1(M)$ is of dimensions
$$1 + d_{3,1} = 1 + 3 = 4.$$
- $\mathbb{P}_2(M)$ is of dimensions
$$1 + 3 + d_{3,2} = 1 + 3 + 6 = 10.$$

Hence, for $M \subset \mathbb{R}^2$, to fix an element in $\mathbb{P}_0(M)$, $\mathbb{P}_1(M)$, and $\mathbb{P}_2(M)$, we need to provide sampling data $(x_i, v(x_i))$ respectively as many as 1, 3, and 6.

Hence, for $M \subset \mathbb{R}^3$, to fix an element in $\mathbb{P}_0(M)$, $\mathbb{P}_1(M)$, and $\mathbb{P}_2(M)$, we need to provide sampling data $(x_i, v(x_i))$ respectively as many as 1, 4, and 10.

Choosing a Basis of $\mathbb{P}_m(M)$

- We do not use *power basis*

$$\{x^\alpha \mid 0 \le |\alpha| \le m.\}$$

- We use *Lagrange basis* (nodal basis): for each $i = 1, 2, \cdots, d$, we choose sampling points $(x_i)_{i=1}^d$ and basis functions $\theta_i \in \mathbb{P}_m(M)$ so that

$$\theta_i(x_j) = \begin{cases} 0 & \text{if } i \neq j \\ 1 & \text{if } i = j. \end{cases}$$

  1. This is because, of course, if we are given sampling data $(x_i, v(x_i))$, $i = 1, 2, \cdots, d$, we immediately pick up an element in $\mathbb{P}_m(M)$ that is

$$x \mapsto \sum_{i=1}^{d} v(x_i)\theta_i(x),$$

     compatible with the sampling data.
  2. Then it matters that how we choose the sampling points x_i, $i = 1, 2, \cdots, d$. In our course, we will not be bothered too much on the choice of preferable sampling points unlike in 1-d.

Examples of sampling points in triangle and in tetrahedron

$$\mathbb{P}_0(M), \quad \mathbb{P}_0(M), \quad \mathbb{P}_2(M).$$

- Such nodal basis, as well as other basis in many cases, are better expressed in the *barycentric coordinate system* rather than the given $\mathbb{R}^n$-coordinate system. We specify the barycentric coordinate system for a given k-simplex now.

Barycentric coordinate system for k-simplex

Example: line passing x_0 and x_1

$$\ell : \{(1-\lambda)x_0 + \lambda x_1 \mid \lambda \in \mathbb{R}\}.$$

For a given k-simplex $\tau = [x_0 x_1 x_2 \cdots x_k]$, there is the unique k-dimensional plane where τ is lied. It is a set of points expressed by a combination

$$\mathrm{P}(\tau) = \{\lambda_0 x_0 + \lambda_1 x_1 + \lambda_2 x_2 + \cdots + \lambda_k x_k \in \mathbb{R}^n \bigm| \lambda_i \in \mathbb{R}, \quad \lambda_0 + \lambda_1 + \lambda_2 + \cdots \lambda_k = 1.\}$$

Now,

1. Consider a hyperplane $\hat{\mathrm{P}}_k$ in $\mathbb{R}^{k+1}$ constrained by one equation:

$$\hat{\mathrm{P}}_k = \{\lambda \in \mathbb{R}^{k+1} \mid \lambda_0 + \lambda_1 + \lambda_2 + \cdots \lambda_k = 1\} \subset \mathbb{R}^{k+1}$$

2. The barycentric coordinate system is a parametrization from $\hat{\mathrm{P}}_k$ to $\mathrm{P}(\tau)$:

$$\chi : \hat{\mathrm{P}}_k \to \mathrm{P}(\tau), \quad \lambda \mapsto \lambda_0 x_0 + \lambda_1 x_1 + \lambda_2 x_2 + \cdots + \lambda_k x_k.$$

3. In particular, the parametrization of $\overline{\mathsf{pts}}\,(\sigma)$ is from the set

$$\chi^{-1}(\overline{\mathsf{pts}}\,(\sigma)) = \{(\lambda_0, \lambda_1, \cdots, \lambda_k) \in \hat{\mathrm{P}}_k \mid \forall i \quad \lambda_i \geq 0\} =: L_k \subset \hat{\mathrm{P}}_k.$$

Before we specify basis functions in barycentric coordinate system, we get familiar with them by a few observations:

We let $n = 3$ and consider a tetrahedron $\sigma = [x_0 x_1 x_2 x_3]$.

1. Faces parametrized by $\lambda = (\lambda_0, \lambda_1, \lambda_2, \lambda_3) \in L_3$.

2. Level sets of λ_e, $e = 0, 1, 2, 3$.

3. The point $x_c = \frac{1}{4}(x_0 + x_1 + x_2 + x_3)$ corresponds to $\lambda = \left(\frac{1}{4}, \frac{1}{4}, \frac{1}{4}, \frac{1}{4}\right)$. We will show that x_c is the center of mass.

The map from x to λ.

1. We should be able to obtain for a given $x \in \overline{\mathsf{pts}}\,(\tau)$ the $(\lambda_0, \lambda_1, \cdots, \lambda_k)$.
2. This can be simply done as below, which is numerically not preferable.
   For a given $(\lambda_0, \lambda_1, \cdots, \lambda_k) \in L_k$,
$$\begin{aligned} x(\lambda) &= \lambda_0 x_0 + \lambda_1 x_1 + \cdots \lambda_k x_k \\ &= x_0 + \lambda_1(x_1 - x_0) + \lambda_2(x_2 - x_0) + \cdots \lambda x_k(x_k - x_0) \\ &= x_0 + \begin{pmatrix} | & | & \cdots & | \\ x_1 - x_0 & x_2 - x_0 & \cdots & x_k - x_0 \\ | & | & \cdots & | \end{pmatrix} \begin{pmatrix} \lambda_1 \\ \lambda_2 \\ \vdots \\ \lambda_k \end{pmatrix} \end{aligned}$$
   By the affine independence assumption, the matrix must be invertible. This gives that
$$\begin{aligned} \begin{pmatrix} \lambda_1 \\ \lambda_2 \\ \vdots \\ \lambda_k \end{pmatrix} &= \begin{pmatrix} | & | & \cdots & | \\ x_1 - x_0 & x_2 - x_0 & \cdots & x_k - x_0 \\ | & | & \cdots & | \end{pmatrix}^{-1} \big(x(\lambda) - x_0\big)\,, \\ \lambda_0 &= 1 - \lambda_1 - \lambda_2 - \cdots - \lambda_k. \end{aligned}$$
3. Importantly, we record here that $x \mapsto \lambda$ map is just linear.
4. The inverse map as generalization of internal dividing point in a line segment.
   (a) We denote the k-volume of $[x_0 x_1 x_2 \cdots x_k]$ by
$$\big|[x_0 x_1 x_2 \cdots x_k]\big| = \mathcal{H}^k\big(\overline{\mathsf{pts}}\,([x_0 x_1 x_2 \cdots x_k])\big)$$
   (b) Then, the i-th barycentric coordinate is computed by the volume ratio
$$\lambda_i = \frac{\big|[x_0 x_1 \cdots x_{i-1}\ x\ x_{i+1} x_{i+2} \cdots x_k]\big|}{\big|[x_0 x_1 x_2 \cdots x_k]\big|}.$$
   We will prove this in the next lecture.

Nodal basis functions for $\mathbb{P}_0(M)$, $\mathbb{P}_1(M)$, $\mathbb{P}_2(M)$

- Here, we make use of $x \mapsto \lambda_e(x)$ for $e = 0, 1, 2, \cdots, n$, the barycentric coordinates, to express the nodal basis functions.
- It is nice to know that, for given degree m, there are exactly d elements in the set

  $$\left\{\lambda_0(x)^{m_0}\lambda_1(x)^{m_1}\cdots\lambda_n(x)^{m_n} \mid m_0 + m_1 + \cdots m_n = m\right\}$$

  and that each of $x \mapsto \lambda_e(x)$ is linear in x.
- We proceed with $n = 3$ for $\mathbb{P}_0(M)$, $\mathbb{P}_1(M)$, and $\mathbb{P}_2(M)$.

$\mathbb{P}_0(M)$

The only basis function of $\mathbb{P}_0(M)$ is simply a constant function

$$\theta(x) \equiv 1.$$

$\mathbb{P}_1(M)$

For $\mathbb{P}_1(M)$, we define 4 basis functions to be

$$\theta_e(\lambda) = \lambda_e, \quad e = 0, 1, 2, 3.$$

- Note that

  $$\theta_e(\hat{e}') = \begin{cases} 0 & \text{if } e \neq e' \\ 1 & \text{if } e = e'. \end{cases}$$

  where $\hat{e}$ is the e-th coordinate basis.

$\mathbb{P}_2(M)$

For $\mathbb{P}_2(M)$, we define the 10 basis functions to be

$$\begin{array}{l} \lambda_e(2\lambda_e - 1), \quad e = 0, 1, 2, 3, \\ 4\lambda_e\lambda_{e'}, \quad e, e' = 0, 1, 2, 3, \quad e \neq e'. \end{array}$$

Summary up to now

1. We are given
$$\bar{\Omega} = |\mathcal{S}| = \bigcup_{M \in S_n} M, \quad \text{interiors of elements in } S_n \text{ are pairwise disjoint.}$$
2. The objective is to be able to implement an approximation of a function
$$v : \bar{\Omega} \to \mathbb{R},$$
where $v \in C^\infty(\bar{\Omega})$.
3. To ends this, we first consider a local objective to be able to implement an approximation of a function
$$v : M \to \mathbb{R}, \quad v \in C^\infty(M), \quad M \in S_n.$$
4. For each $v \in C^\infty(M)$, the sampling procedure is
$$v \mapsto (x_i, v(x_i))_{i=1}^d, \quad (x_i)_{i=1}^d \text{ of points in } M \text{ are sampling points.}$$
5. A polynomial of order at most m is a linear combination
$$\sum_{0 \le |\alpha| \le m} c_\alpha x^\alpha$$
and $\mathsf{span}\left\langle x^\alpha \right\rangle_{0 \le |\alpha| \le m}$ is a vector space of dimensions
$$d = \binom{n+m}{m}.$$
6. For given sample data, we pick up an element in $\mathbb{P}_m(M)$. This will be done by selecting basis functions $\theta_i(x)$ as we want so that the element is
$$x \mapsto \sum_{i=1}^d v(x_i)\theta_i(x).$$
The sampling procedure and picking up procedure are combined:
$$I : C^\infty(M) \to \mathbb{P}_m(M) \subset C^\infty(M).$$
7. Selecting d basis of $\mathbb{P}_m(M)$ we want:
Let $n = 3$ and fix M.
Below, λ will be composited with the linear bijective map $x \mapsto \lambda$.
   (a) Let $m = 0$. Then
   $$\mathbb{P}_0(M) = \mathsf{span}\left\langle \mathbf{1} \right\rangle.$$
   (b) Let $m = 1$. Then $\mathbb{P}_1(M)$ is spanned by four functions
   $$(\lambda_0, \lambda_1, \lambda_2, \lambda_3) \mapsto \lambda_e, \quad e = 0, 1, 2, 3.$$
   (c) Let $m = 2$. Then $\mathbb{P}_2(M)$ is spanned by ten functions
   $$\begin{aligned}(\lambda_0, \lambda_1, \lambda_2, \lambda_3) \mapsto & \lambda_e(2\lambda_e - 1), \quad e = 0, 1, 2, 3 \quad \text{and} \\ (\lambda_0, \lambda_1, \lambda_2, \lambda_3) \mapsto & 4\lambda_e\lambda_{e'}, \quad e, e' = 0, 1, 2, 3 \quad e \ne e'\end{aligned}$$

Chapter 4

Vector fields and etc.

Let $n = 3$.

- Unlike in 1-d case, where the approximation target was a function

  $$f : [a, b] \subset \mathbb{R} \to \mathbb{R},$$

  the approximation targets defined on Ω include not only $\mathbb{R}$-valued functions but include also vector fields, and so on.

- This time, we borrow language from *Differential Geometry*, to identify the target objectives of

  $$\Lambda_0(\Omega), \quad \Lambda_1(\Omega), \quad \Lambda_2(\Omega), \quad \Lambda_3(\Omega)$$

  that are the vector spaces of k-covector fields.

- We introduce what are the k-covectors and what are the k-covector fields below, which is very crude explanation in the Euclidean space.

k-vectors

We let the vector space V to be $\mathbb{R}^3$.

- A real number $a \in \mathbb{R}$ is called a 0-vector.

- An element of V is called a 1-vector.
- The space V of 1-vectors is equipped with the inner product
$$v_1^T v_2.$$

- The space of 2-vectors is
$$\mathsf{span}\left\langle e_1 \wedge e_2, e_1 \wedge e_3, e_2 \wedge e_3 \right\rangle.$$
- For two 1-vectors v_1 and v_2, the notation
$$v_1 \wedge v_2$$
denotes an element of space of 2-vectors in the following sense.
- $(av_1 \wedge bv_2) = ab\ v_1 \wedge v_2$, and distribution law works for two linear combinations of vectors in V.
- The notation $v_2 \wedge v_1$ is identified by
$$-v_1 \wedge v_2$$
in the space of 2-vectors.
- Calculus:
If $v_1 \wedge v_2$ and $w_1 \wedge w_2$ are given, where $v_1, v_2, w_1, w_2 \in V$, we define the inner product
$$\left\langle v_1 \wedge v_2, w_1 \wedge w_2 \right\rangle = \det \left(\begin{pmatrix} - & v_1^T & - \\ - & v_2^T & - \end{pmatrix} \begin{pmatrix} | & | \\ w_1 & w_2 \\ | & | \end{pmatrix} \right)$$
- Inner product of two linear combinations of such forms are then computed following distribution law.

- The space of 3-vectors is
$$\mathsf{span}\left\langle e_1 \wedge e_2 \wedge e_3 \right\rangle.$$
- Calculus works in the same principle.

- If $v_1 \wedge v_2 \wedge v_3$ and $w_1 \wedge w_2 \wedge w_3$ are given, where $v_1, v_2, v_3, w_1, w_2, w_3 \in V$, we define the inner product

$$\langle v_1 \wedge v_2 \wedge v_3, w_1 \wedge w_2 \wedge w_3 \rangle = \det \left(\begin{pmatrix} - & v_1^T & - \\ - & v_2^T & - \\ - & v_3^T & - \end{pmatrix} \begin{pmatrix} | & | & | \\ w_1 & w_2 & w_3 \\ | & | & | \end{pmatrix} \right)$$

k-covectors

- In the flat Euclidean geometry, a dual element is essentially the same object to the k-vector.

  (A k-vector is identified by the corresponding k-covector by the inner product.)

- We will work with k-covectors for our purposes.

k-covector fields

- A k-covector field on Ω is a k-covector-valued function defined on Ω.
- Here, the role of the vector space V is taken by $T_x\Omega$ of tangent space at $x \in \Omega$, but every $T_x\Omega$ is identified by the same space $\mathbb{R}^3$.
- Unless otherwise specified, we restrict ourselves in the C^∞ (up to boundary) fields. The space of such smooth k-covector fields are denoted by

$$\Lambda_0(\Omega), \quad \Lambda_1(\Omega), \quad \Lambda_2(\Omega), \quad \Lambda_3(\Omega)$$

- We already discussed about $\Lambda_0(\Omega)$.
- Elements of them are our targets of approximation in our course.

Local polynomial spaces suitable for $\big(\Lambda_0, \Lambda_1, \Lambda_2, \Lambda_3\big)$

Let $n = 3$ and fix M an n-simplex.

- The easiest choice for $\big(\Lambda_0(M), \Lambda_1(M), \Lambda_2(M), \Lambda_3(M)\big)$ is the following.

$$
\begin{aligned}
\mathbb{P}_1(M) &\subset \Lambda_0, \\
\mathbb{E}_1(M) &\subset \Lambda_1, \\
\mathbb{J}_1(M) &\subset \Lambda_2, \\
\mathbb{P}_0(M) &\subset \Lambda_3,
\end{aligned}
$$

- $\mathbb{E}_1(M)$ is the *Nedelec polynomial space* of lowest order, restricted in M.
- $\mathbb{J}_1(M)$ is the *Raviart-Thomas polynomial space* of lowest order, restricted in M.

We will delve into them one-by-one: Definition, Basis.

$k = 3$: constant approximation

- A function in $\Lambda_3(M)$ typically represents a *density* of chemical concentraion, population, mass, etc.
- In the sense that we require mere integrability of them, $\mathbb{P}_0(M)$ works fine for $\Lambda_3(M)$.

Sampling Data

- For a given function $x \mapsto \rho(x)\ e_1 \wedge e_2 \wedge e_3$, we store the value

$$L = \frac{1}{|M|} \int_M \rho(x)\, dx.$$

Basis functions

- We just recall the basis function is the constant function

$$\theta : x \mapsto 1\ e_1 \wedge e_2 \wedge e_3.$$

The Projector (approximation)

- For a given $x \mapsto \rho(x)\ e_1 \wedge e_2 \wedge e_3$ in $\Lambda_3(M)$, we let its approximation

$$\left(\frac{1}{|M|} \int_M \rho(x)\, dx \right) e_1 \wedge e_2 \wedge e_3 \quad \in \quad \mathbb{P}_0(M).$$

  This defines the projector

$$I : \Lambda_3(M) \to \mathbb{P}_0(M).$$

$k = 2$: constant outward normals

Let M be the point set of 3-simplex $[x_0x_1x_2x_3]$.

- Here, we may assume that the center of mass of M is at origin, or
- if $x_c = \frac{1}{4}(x_0 + x_1 + x_2 + x_3)$, we let $z = x - x_c$ and use z coordinates.

Writing an element $J \in \Lambda_2(M)$

- We write an element in $\Lambda_2(M)$ in the following way:

$$\begin{aligned} J : x &\mapsto J_1(x)e_2 \wedge e_3 + J_2(x)e_3 \wedge e_1 + J_3(x)e_1 \wedge e_2, \\ &= J_1(x)\check{e}_1 + J_2(x)\check{e}_2 + J_3(x)\check{e}_3. \end{aligned}$$

- This arrangement is because we want to interprete d operator for J-field as div operator:
$$dJ(x) = \Big(\frac{\partial J_1}{\partial x_1}(x) + \frac{\partial J_2}{\partial x_2}(x) + \frac{\partial J_3}{\partial x_3}(x)\Big)e_1 \wedge e_2 \wedge e_3.$$
- $\big(\mathbb{P}_1(M)\big)^n$, the space of first order 1-vector fields (2-vector fields as well), has the degrees of freedom $(n+1)n$. Indeed,
$$x \mapsto J_0 + A(x - x_c), \quad J_0 \text{ a constant vector, and } A \text{ an } n \times n \text{ matrix.}$$
In 3-d, in total 12 freedoms.

Definition of $\mathbb{J}_1(M)$

- We define $\mathbb{RT}(M)$ to be
$$\Big\{J_0 + c_0(x - x_c) \;\Big|\; J_0 \text{ is a constant 1-vector and } c_0 \in \mathbb{R}\Big\}$$
restricted in M.
- Replacing $e_i \to \check{e}_i$ in $\mathbb{RT}(M)$ let the element be in $\mathbb{J}_1(M) \subset \Lambda_2(M)$.
- For notational clarification, we let $\mathbb{RT}(M)$ to be of 1-vector fields, and let $\mathbb{J}_1(M)$ of 2-vector fields after the replacement $e_i \to \check{e}_i$.

- Observations:
  1. $\mathbb{J}_1(M)$ is a 4-dimensional subspace $\mathbb{J}_1(M) \subset \big(\mathbb{P}_1(M)\big)^3 \subset \Lambda_2(M)$.
  2. dJ for $J = J_0 + c_0(x - x_c)$, (after replacement), in the interior of M, is simply a constant $3c_0$.
  3. $\mathbb{J}_1(M)$: A minimal requirement so that J itself and dJ both are nontrivial and in control.

Sampling Data

- For a given function $J : x \mapsto J_1(x)e_2 \wedge e_3 + J_2(x)e_3 \wedge e_1 + J_3(x)e_1 \wedge e_2$, we store four values.
- We store for $e = 0, 1, 2, 3$

$$L_e = \frac{1}{|f_{\check{e}}|} \int_{\overline{\mathsf{pts}}\,(f_{\check{e}})} J^{RT}(x) \cdot \nu_{\check{e}} \, d\mathcal{H}^2 :$$

  where
- For given J, let J^{RT} be the 1-vector field where $\check{e}_i$ is replaced by e_i.
- $\nu_{\check{e}}$ is the outward unit normal vector seen from M on $f_{\check{e}}$.
- There are four boundaries:

$$[x_1 x_2 x_3], \quad -[x_0 x_2 x_3], \quad [x_0 x_1 x_3], \quad -[x_0 x_1 x_2].$$

  denoted by $f_{\check{e}}$, with x_e missing.

Basis functions of $\mathbb{RT}(M)$

- Nodal basis: We look for a vector field $\theta_{\check{e}}$ of the form $J_0 + c_0(x - x_c)$ such that

$$\theta_{\check{e}}(x) \cdot \nu_{\check{e}'} = \begin{cases} \mathsf{Const.}, & e = e' \quad \text{and} \quad x \in f_{\check{e}} \\ 0, & e \neq e' \quad \text{and} \quad x \in f_{\check{e'}}. \end{cases}$$

- We show that

$$\theta_{\check{e}} : x \mapsto \mathsf{Const.}(x - x_e)$$

  do the job.

  1. If $e \neq e'$ and x is on the face $f_{\check{e'}}$, then $x - x_e$ is a tangent vector of the face $f_{\check{e'}}$.
     Therefore, the inner product with the normal must be 0.
  2. Let x be on the face $f_{\check{e}}$. Let $e = 3$ for example.

     The outward normal $\quad \nu_{\check{3}} \quad \| \quad (x_1 - x_0) \times (x_2 - x_0).$

     x is a combination $\quad x = \lambda_0 x_0 + \lambda_1 x_1 + \lambda_2 x_2, \quad \lambda_0 + \lambda_1 + \lambda_2 = 1,$

     $\quad = x_0 + \lambda_1(x_1 - x_0) + \lambda_2(x_2 - x_0).$

     Hence, $\quad x - x_3 = x_0 - x_3 + \lambda_1(x_1 - x_0) + \lambda_2(x_2 - x_0)$

     and $\quad (x - x_3) \cdot \nu_{\check{3}} = (x_0 - x_3) \cdot \nu_{\check{3}}$

     and this must be a nonzero constant.

- The normalizing constant can be computed. We present the result:

$$\theta^{RT}_{\check{e}}(x) = \frac{|f_{\check{e}}|}{3|M|}(x - x_e).$$

The projector (approximation)

We define an approximation, the projector $I : \Lambda_2(M) \to \mathbb{J}_1(M)$ that is

$$J \quad \mapsto \quad \sum_{e=0}^{3} L_e \theta_{\check{e}}^{RT} \quad \text{with } \check{e}_i \text{ in place of } e_i.$$

$k = 1$: constant tangentials on edges

Let M be the point set of 3-simplex $[x_0x_1x_2x_3]$.

- Here, we may assume that the center of mass of M is at origin, or
- if $x_c = \frac{1}{4}(x_0 + x_1 + x_2 + x_3)$, we let $z = x - x_c$ and use z coordinates.
- As same as in the $k = 2$ case, $\big(\mathbb{P}_1(M)\big)^n$, the space of first order 1-vector fields has the degrees of freedom $(n+1)n$. Indeed,

  $$z \mapsto E_0 + Az, \quad E_0 \text{ a constant vector, and } A \text{ an } n \times n \text{ matrix.}$$

  In 3-d, in total 12 freedoms.
- We look for a simpler subspace with 6 degrees of freedom.

Definition of $\mathbb{E}_1(M)$

- We define $\mathbb{E}_1(M)$ to be

  $$\Big\{E_0 + (c_1, c_2, c_3) \times (z_1, z_2, z_3) \;\Big|\; E_0 \text{ is a constant 1-vector and } c_1, c_2, c_3 \in \mathbb{R}\Big\}$$

  restricted in M.

- Observations:
  1. $\mathbb{E}_1(M)$ is a 6-dimensional subspace $\mathbb{E}_1(M) \subset \big(\mathbb{P}_1(M)\big)^3 \subset \Lambda_1(M)$.
  2. dE for $E = E_0 + (c_1, c_2, c_3) \times (z_1, z_2, z_3)$, in the interior of M, is simply a constant vector $2(c_1, c_2, c_3)$.
  3. $\mathbb{E}_1(M)$: A minimal requirement so that E itself and dE both are nontrivial and in control.

Sampling Data

- For a given function $E : x \mapsto E_1(x)e_1 + E_2(x)e_2 + E_3(x)e_3$, we store six values.
- We store for each edges, designated by $[ee']$ in the set
$$\{[01], [02], [03], [12], [13], [23]\} = Key_1,$$
the line integrals
$$L_{[ee']} = \frac{1}{|[ee']|} \int_{\mathsf{pts}([ee'])} E(x) \cdot \frac{x_{e'} - x_e}{|x_{e'} - x_e|} \, d\mathcal{H}^1.$$

Basis functions of $\mathbb{E}_1(M)$

- Nodal basis: We look for a vector field $\theta_{[ee']}$ of the form $E_0 + (c_1, c_2, c_3) \times (z_1, z_2, z_3)$ such that for $[\alpha\alpha'] \in Key_1$
$$\theta_{[ee']}(x) \cdot \frac{x_{\alpha'} - x_\alpha}{|x_{\alpha'} - x_\alpha|} = \begin{cases} \mathsf{Const.}, & [ee'] = [\alpha\alpha'] \quad \text{and} \quad x \in [\alpha\alpha'] \\ 0, & [ee'] \neq [\alpha\alpha'] \quad \text{and} \quad x \in [\alpha\alpha'] \end{cases}$$

- We show that
$$\theta_{[ee']} : x \mapsto \mathsf{Const.}(x - x_\gamma) \times (x - x_{\gamma'})$$
do the job, where we let (e, e', γ, γ') is an even permutation of (0123).

  1. First, note that $\theta_{[ee']}(x)$ is of 1st order in x, not of 2nd order:
  $$(x - x_\gamma) \times (x - x_{\gamma'}) = x \times x - x \times x_{\gamma'} - x_\gamma \times x + x_\gamma \times x_{\gamma'},$$
  but the quadratic term is 0.
  2. Also, it is in the form of $E_0 + (c_1, c_2, c_3) \times (x - x_c)$ because
  $$x \times (x_\gamma - x_{\gamma'}) + x_\gamma \times x_{\gamma'} = (x - x_c) \times (x_\gamma - x_{\gamma'}) + x_c \times (x_\gamma - x_{\gamma'}) + x_\gamma \times x_{\gamma'}.$$

3. Now, among Key_1 elements, if $[ee'] \neq [\alpha\alpha']$ and x is on the face $[\alpha\alpha']$, then $\{\alpha, \alpha'\}$ and $\{\gamma, \gamma'\}$ has at least one element in common.
   In other words, the tangent vector on $[\alpha\alpha']$ is proportional to either $x - x_\gamma$ or $x - x_{\gamma'}$.
   Therefore, the inner product of $(x - x_\gamma) \times (x - x_{\gamma'})$ with the tangent must be 0.
4. Let x be on the face $[ee']$. Let $[ee'] = [01]$ for example. Then $[\gamma\gamma'] = [23]$.

   The tangent $\quad \dfrac{x_1 - x_0}{|x_1 - x_0|}$

   $x \in [01]$

$$
\begin{aligned}
x &= \lambda_0 x_0 + \lambda_1 x_1, \quad \lambda_0 + \lambda_1 = 1, \\
&= x_0 + \lambda_1(x_1 - x_0). \\
x - x_2 &= x_0 - x_2 + \lambda_1(x_1 - x_0), \\
x - x_3 &= x_0 - x_3 + \lambda_1(x_1 - x_0), \\
(x - x_2) \times (x - x_3) &= (x_0 - x_2) \times (x_0 - x_3) + \lambda_1(x_1 - x_0) \times (x_2 - x_3),
\end{aligned}
$$

   Hence $\quad \dfrac{x_1 - x_0}{|x_1 - x_0|} \cdot (x - x_2) \times (x - x_3) = \dfrac{x_1 - x_0}{|x_1 - x_0|} \cdot (x_0 - x_2) \times (x_0 - x_3)$

   and this must be a nonzero constant.

- The normalizing constant can be computed. We present the result:

$$
\theta_{[ee']} = \frac{s|[ee']|}{3!|M|}(x - x_\gamma) \times (x - x_{\gamma'}),
$$

  where s appears as a sign factor: $+1$ if $[x_0x_1x_2x_3]$ is positively oriented, and -1 if $[x_0x_1x_2x_3]$ is negatively oriented.

The projector (approximation)

We define an approximation, the projector $I : \Lambda_1(M) \to \mathbb{E}_1(M)$ that is

$$
E \quad \mapsto \quad \sum_{[ee'] \in Key_1} L_{[ee']}\theta_{[ee']}.
$$

$k = 0$

- We did this before.

Sampling Data

- For a given function $x \mapsto v(x)$, we store the values

$$v(x_0), v(x_1), v(x_2), v(x_3).$$

Basis functions

- We just recall the four basis functions in barycentric coordinate are

$$\theta_e(\lambda) = \lambda_e, \quad e = 0, 1, 2, 3.$$

- This time, we prove that

$$\lambda_e(x) = \frac{\big|[x_0 x_1 \cdots x_{e-1}\ x\ x_{e+1} x_{e+2} \cdots x_n]\big|}{\big|[x_0 x_1 x_2 \cdots x_n]\big|}.$$

  Note that this is a $\mathsf{Const.}$ multiple of the determinant of matrix with columns $x_i - x$, with e-th column missing.

The Projector (approximation)

- For a given $x \mapsto v(x)$ in $\Lambda_3(M)$, we let its approximation

$$\sum_{e=0}^{3} v(x_e)\lambda_e(x).$$

  This defines the projector

$$I : \Lambda_0(M) \to \mathbb{P}_1(M).$$

Proposition 1. *Let $[x_0x_1\cdots x_n]$ be an n-simplex. Then the 0-th barycentric coordinate*

$$\lambda_0(x) = \frac{\big|[xx_1x_2\cdots x_n]\big|}{\big|[x_0x_1x_2\cdots x_n]\big|}.$$

Proof. .

1. For the case x is on the face $[x_1x_2\cdots x_n]$, then $\lambda_0(x) = 0$ and the numerator in the volume ratio is also 0. Thus equality holds for this case.

2. Now we assume x is not on the face $[x_1x_2\cdots x_n]$.

   - We know that

   $$\begin{aligned}\begin{pmatrix}\lambda_1(x)\\ \lambda_2(x)\\ \vdots\\ \lambda_n(x)\end{pmatrix} &= \begin{pmatrix} | & | & \cdots & | \\ x_1-x_0 & x_2-x_0 & \cdots & x_n-x_0 \\ | & | & \cdots & | \end{pmatrix}^{-1} \begin{pmatrix} | \\ x-x_0 \\ | \end{pmatrix} \\ &= M_0^{-1}(x-x_0).\end{aligned}$$

   - For each $e \neq 0$, we can write

   $$\begin{pmatrix}\lambda_1(x)\\ \lambda_2(x)\\ \vdots\\ \lambda_n(x)\end{pmatrix} = M_0^{-1}(x_e - x_0) + M_0^{-1}(x - x_e) \quad\Longleftrightarrow\quad M_0^{-1}(x_e - x) = M_0^{-1}(x_e - x_0) - \begin{pmatrix}\lambda_1(x)\\ \lambda_2(x)\\ \vdots\\ \lambda_n(x)\end{pmatrix}.$$

   - Listing aboves in the columns of matrix, we write

   $$\begin{aligned}&M_0^{-1}\begin{pmatrix} | & | & \cdots & | \\ x_1-x & x_2-x & \cdots & x_n-x \\ | & | & \cdots & | \end{pmatrix} \\ =&M_0^{-1}\begin{pmatrix} | & | & \cdots & | \\ x_1-x_0 & x_2-x_0 & \cdots & x_n-x_0 \\ | & | & \cdots & | \end{pmatrix} - \begin{pmatrix}\lambda_1(x) & \lambda_1(x) & \cdots & \lambda_1(x)\\ \lambda_2(x) & \lambda_2(x) & \cdots & \lambda_2(x)\\ \vdots & \vdots & \vdots & \vdots\\ \lambda_n(x) & \lambda_n(x) & \cdots & \lambda_n(x)\end{pmatrix} \\ =&I - \begin{pmatrix}\lambda_1(x)\\ \lambda_2(x)\\ \vdots\\ \lambda_n(x)\end{pmatrix}\begin{pmatrix}1 & 1 & \cdots 1\end{pmatrix}.\end{aligned}$$

   - The determinant of (RHS), which is of identity matrix + rank one matrix, is computed by

   $$1 - \lambda_1(x) - \lambda_2(x) - \cdots - \lambda_n(x).$$

   - The determinant of (LHS) is the signed volume ratio of $[xx_1x_2\cdots x_n]$ and $[x_0x_1\cdots x_n]$. We make use of the fact that x and x_0 are in the same side of $\mathbb{R}^n$ divided by the hyperplane specified by $[x_1x_2\cdots x_n]$. Thus, the sign factor must be same. The proof is done.

$\square$