

PDE Constrained Optimization: Implementation Aspects

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PDE Constrained Optimization – Overview

Derivative Computation

Application of Abstract Approach

Finite Element Method

Matlab Code: Newton CG, L-BFGS, Semismooth Newton

PDE Constrained Optimization (PDECO) Overview

Literature: [Lions, 1971, Tröltzsch, 2010, Ito and Kunisch, 2008, Antil et al., 2018, Hinze et al., 2009, Ulbrich, 2011, Attouch et al., 2006, Ekeland and Témam, 1999]

PDE constrained optimization has 4-5 major components:

- ▶ **control** z
- ▶ **state** u
- ▶ **state equation** (i.e., PDE) which associates with every control z a state u .
- ▶ **cost functional** J which depends on z and u , to be minimized;
- ▶ constraints obeyed by z (**control constraints**) and u (**state constraints**);

In the most abstract form this problem can be written as

$$\min J(u, z)$$

$$\text{s.t. } e(u, z) = 0,$$

$$z \in Z_{ad},$$

$$u \in U_{ad},$$

PDE

control constraints

state constraints

Abstract PDECO Problem

$$\begin{array}{ll}\min J(u, z) & \\ \text{s.t. } e(u, z) = 0, & \text{PDE} \\ z \in Z_{ad}, & \text{control constraints} \\ u \in U_{ad}, & \text{state constraints}\end{array}$$

where u : states, z : controls,

- ▶ $(U, \|\cdot\|_U)$, $(Y, \|\cdot\|_Y)$ Banach spaces, $(Z, \|\cdot\|_Z)$ is a reflexive Banach space.
- ▶ $Z_{ad} \subset Z$ and $U_{ad} \subset U$ are nonempty, closed convex set.
- ▶ $J : U \times Z \rightarrow \mathbb{R}$, $e : U \times Z_{ad} \rightarrow Y$ are sufficiently smooth mappings.
- ▶ Can think $(U, \|\cdot\|_U) = (\mathbb{R}^n, \|\cdot\|_2)$, $(Y, \|\cdot\|_Y) = (\mathbb{R}^n, \|\cdot\|_2)$, $(Z, \|\cdot\|_Z) = (\mathbb{R}^m, \|\cdot\|_2)$.

For simplicity we shall focus on the control constrained case, i.e., $U_{ad} = U$.

Three different formulations

► Full space form

$$\begin{aligned} \min J(u, z) \\ \text{s.t. } e(u, z) &= 0, && \text{PDE} \\ z &\in Z_{ad}, && \text{control constraints} \end{aligned}$$

► Let $x = (u, z)$, $X = U \times Z$, $X_{ad} = U \times Z_{ad}$ then we arrive at the following abstract problem

$$\begin{aligned} \min J(x) \\ \text{s.t. } e(x) &= 0, && \text{PDE} \\ x &\in X_{ad}. && \text{constraints} \end{aligned}$$

► Reduced form. Let us consider a map

$$S : \mathcal{Z} \rightarrow U, \quad z \mapsto S(z) = u \text{ with } e(S(z), z) = 0.$$

Here $\mathcal{Z}$ is open such that $Z_{ad} \subset \mathcal{Z} \subset Z$. We assume that for $z \in \mathcal{Z}$ there is a unique $u = S(z) \in U$. Then we can write

$$\min_{z \in Z_{ad}} \mathcal{J}(z) := J(S(z), z)$$

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Derivative Computation

Compute gradient and Hessian information for

$$\mathcal{J}(z) = J(S(z), z), \quad \text{where } S(z) = u \text{ solves } e(u, z) = 0$$

Assumption

- ▶ J and e are twice continuously differentiable,
- ▶ $e_u(u, z)$ is continuously invertible.

Use adjoint equation approach for derivative computation.

See, e.g., Chapter 1 in [Hinze et al., 2009], Chapter 1 in [Antil et al., 2018] or [Heinkenschloss, 2008].

Gradient Computation: Reduced Form

► Derivative

$$\langle \mathcal{J}'(z), h \rangle_{Z^*, Z} = \langle J_u(S(z), z), S'(z)h \rangle_{U^*, U} + \langle J_z(S(z), z), h \rangle_{Z^*, Z}$$

► Implicit function theorem applied to $e(S(z), z) = 0$ gives

$$\begin{aligned} e_u(S(z), z) (S'(z)h) + e_z(S(z), z)h &= 0 \\ \implies S'(z)h &= -e_u^{-1}(S(z), z)e_z(S(z), z). \end{aligned}$$

► Derivative ($u = S(z)$)

$$\begin{aligned} \langle \mathcal{J}'(z), h \rangle_{Z^*, Z} &= \langle J_u(u, z), -e_u(u, z)^{-1}e_z(u, z)h \rangle_{U^*, U} + \langle J_z(u, z), h \rangle_{Z^*, Z} \\ &= \underbrace{\langle e_u(u, z)^{-*}J_u(u, z), -e_z(u, z)h \rangle_{Y^*, Y}}_{=:p} + \langle J_z(u, z), h \rangle_{Z^*, Z} \\ &= \langle -e_z(u, z)^*p + J_z(u, z), h \rangle_{Z^*, Z} \end{aligned}$$

- ▶ Connection with Lagrangian $L(u, z, p) = J(u, z) - \langle p, e(u, z) \rangle_{Y^*, Y}$:
 - ▶ The adjoint variable p solves $e_u^*(u, z)p = J_u(u, z)$,
which is equivalent to $L_u(u, z, p) = 0$.
 - ▶ Derivative

$$\begin{aligned}\langle \mathcal{J}'(z), h \rangle_{Z^*, Z} &= \langle -e_z(u, z)^* p + J_z(u, z), h \rangle_{Z^*, Z} \\ &= \langle L_z(u, z, p), h \rangle_{Z^*, Z}\end{aligned}$$

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- Assuming that Z is a Hilbert space the **gradient** $\nabla \mathcal{J}(z)$ is such that

$$\begin{aligned}(\nabla \mathcal{J}(z), h)_Z &= \langle \mathcal{J}'(z), h \rangle_{Z^*, Z} \\ &= \langle -e_z(u, z)^* p + J_z(u, z), h \rangle_{Z^*, Z} \quad \forall h \in Z\end{aligned}$$

(Riesz representation Theorem)

► Connection with Lagrangian $L(u, z, p) = J(u, z) - \langle p, e(u, z) \rangle_{Y^*, Y}$:

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► Assuming that Z is a Hilbert space the **gradient** $\nabla \mathcal{J}(z)$ is such that

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(Riesz representation Theorem)

Derivative Computation Using Adjoint

1. Given z , solve $e(u, z) = 0$ for u (if not done already).
2. Solve the adjoint equation $e_u(u(z), z)^* p = J_u(u(z), z)$ for p . Denote the solution by $p(z)$.
3. Compute $\mathcal{J}'(z) = J_z(u(z), z) - e_z(u(z), z)^* p(z)$.

Two PDE solves (possibly nonlinear in step 1, linear PDE in step 2)

Hessian Computation

- Apply **implicit differentiation** to

$$\mathcal{J}'(z) = J_z(u(z), z) - e_z(u(z), z)^* p(z)$$

to compute Hessian information.

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to compute Hessian information.

- This leads to

$$\mathcal{J}''(z) = T(S(z), z)^* H(S(z), z, p) T(S(z), z)$$

where

$$T(u, z) = \begin{pmatrix} -e_u(u, z)^{-1} e_z(u, z) \\ I_Z \end{pmatrix}$$

and $H(u, z, p)$ is given by

$$H(u, z, p) = \begin{pmatrix} L_{uu}(u, z, p) & L_{uz}(u, z, p) \\ L_{zu}(u, z, p) & L_{zz}(u, z, p) \end{pmatrix}$$

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- In practice we are interested in computing **Hessian times vector**. For instance in the absence of control constraints we need to solve

$$\mathcal{J}'(z) = 0$$

which we can do so by solving Newton's equation for s_z in an iterative fashion

$$\mathcal{J}''(z)s_z = -\nabla \mathcal{J}(z).$$

Hessian-Times-Vector Computation

► Hessian-Times-Vector Computation

1. Given z , solve $e(u, z) = 0$ for u (if not done already).
2. Solve adjoint equation: $e_u(u, z)^* p = J_u(u, z)$ for p (if not done already).
3. Solve $e_u(u, z)w = -e_z(u, z)v$.
4. Solve $e_u(u, z)^* q = D_{uu}L(u, z, p)w + D_{uz}L(u, z, p)v$.
5. Compute

$$\mathcal{J}''(z)v = -e_z(u, z)^* q + L_{uz}(u, z, p)w + L_{zz}(u, z, p)v.$$

Two linear PDE solves in steps 3+4 per direction v .

- Vector s_z solves Newton equation $\mathcal{J}''(z)s_z = -\mathcal{J}'(z)$ if and only if (s_u, s_z) solves the quadratic program

$$\begin{aligned} \min \quad & \left\langle \begin{bmatrix} J_u(\cdot) \\ J_z(\cdot) \end{bmatrix}, \begin{bmatrix} s_u(\cdot) \\ s_z(\cdot) \end{bmatrix} \right\rangle + \frac{1}{2} \left\langle \begin{bmatrix} s_u(\cdot) \\ s_z(\cdot) \end{bmatrix}, \begin{bmatrix} L_{uu}(\cdot) & L_{uz}(\cdot) \\ L_{zu}(\cdot) & L_{zz}(\cdot) \end{bmatrix} \begin{bmatrix} s_u(\cdot) \\ s_z(\cdot) \end{bmatrix} \right\rangle \\ \text{s.t.} \quad & e_u(\cdot)s_u + e_z(\cdot)s_z = 0, \end{aligned}$$

where $(\cdot) = (u(z), z)$ and $(\cdot\cdot) = (u(z), z, p(z))$.

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Semilinear Elliptic PDECO Problem

► Problem:

$$\text{Minimize } J(u, z) = \frac{1}{2} \int_{\Omega} |u(x) - u_d(x)|^2 dx + \frac{\lambda}{2} \int_{\Omega} |z(x)|^2 dx$$

s.t.

$$\begin{aligned} -\operatorname{div}(A \nabla u) + f(\cdot, u) &= z && \text{in } \Omega \\ u &= 0 && \text{on } \partial\Omega \end{aligned}$$

$$z \in Z_{ad} := \{z \in L^\infty(\Omega) : z_a(x) \leq z(x) \leq z_b(x) \text{ a.e. in } \Omega\}$$

with $z_a, z_b \in L^\infty(\Omega)$ and $z_a < z_b$ a.e. in Ω .

- **Control space:** $L^\infty(\Omega)$. For existence we use $L^p(\Omega)$ with $N/2 < p < \infty$. Notice that $Z_{ad} \subset L^\infty(\Omega) \subset L^p(\Omega)$.

Semilinear Elliptic PDECO Problem

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► **Control space:** $L^\infty(\Omega)$. For existence we use $L^p(\Omega)$ with $N/2 < p < \infty$. Notice that $Z_{ad} \subset L^\infty(\Omega) \subset L^p(\Omega)$.

State space: $U = L^\infty(\Omega) \cap H_0^1(\Omega)$. [Antil et al., 2017, Antil and Warma, 2020].

Semilinear Elliptic PDECO Problem

► Problem:

$$\text{Minimize } J(u, z) = \frac{1}{2} \int_{\Omega} |u(x) - u_d(x)|^2 dx + \frac{\lambda}{2} \int_{\Omega} |z(x)|^2 dx$$

s.t.

$$-\operatorname{div}(A \nabla u) + f(\cdot, u) = z \quad \text{in } \Omega$$

$$u = 0 \quad \text{on } \partial\Omega$$

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State space: $U = L^\infty(\Omega) \cap H_0^1(\Omega)$. [Antil et al., 2017, Antil and Warma, 2020].

- Notice that $Z \subset L^\infty(\Omega)$. This is a sufficient condition for the differentiability of S , a Nemytskii (superposition) operator.

► Lagrangian:

$$L(y, u, p) = \frac{1}{2} \int_{\Omega} |u(x) - u_d(x)|^2 dx + \frac{\lambda}{2} \int_{\Omega} |z(x)|^2 dx \\ - \int_{\Omega} (A \nabla u \cdot \nabla p + f(x, u)p - zp) dx.$$

► Adjoint equation:

$$-\operatorname{div}(A^T \nabla p) + f_u(\cdot, u)p = (u - u_d) \quad \text{in } \Omega \\ p = 0 \quad \text{on } \partial\Omega$$

► Derivative

$$\langle \mathcal{J}'(z), h \rangle_{Z^*, Z} = \langle \lambda z + p, h \rangle_{Z^*, Z}.$$

► Gradient: $\nabla \mathcal{J}$ is computed as follows:

$$(\nabla \mathcal{J}(z), h)_Z = \langle \mathcal{J}'(z), h \rangle_{Z^*, Z}, \quad \forall h \in Z.$$

► Hessian: $L_{uz} = L_{zu} = 0$. Then use the approach described before.

Linear Parabolic PDECO Problem

► Problem:

$$\text{Minimize } \frac{1}{2} \int_0^T \int_{\Omega} |u(x, t) - u_d(x, t)|^2 \, dx \, dt + \frac{\lambda}{2} \int_0^T \int_{\Omega} |z(x, t)|^2 \, dx \, dt$$

where u solves

$$\begin{aligned} \partial_t u(x, t) - \operatorname{div} (A \nabla u) + \mathbf{b} \cdot \nabla u &= z \quad \text{in } \Omega \times (0, T) \\ u &= 0, \quad \text{on } \Gamma_D \times (0, T), \\ A \nabla u \cdot \boldsymbol{\nu} &= 0 \quad \text{on } \Gamma_N \times (0, T) \\ u(x, 0) &= 0 \quad \text{in } \Omega. \end{aligned}$$

► Lagrangian (formally)

$$\begin{aligned} L(u, z, p) &= \frac{1}{2} \int_0^T \int_{\Omega} |u(x, t) - u_d(x, t)|^2 \, dx \, dt + \frac{\lambda}{2} \int_0^T \int_{\Omega} |z(x, t)|^2 \, dx \, dt \\ &\quad \int_0^T \int_{\Omega} (\partial_t u(x, t)p - \operatorname{div} (A \nabla u)p + \mathbf{b} \cdot \nabla up - zp) \, dx \, dt \end{aligned}$$

► Adjoint equation

$$\begin{aligned} -\partial_t p(x, t) - \operatorname{div} (A^T \nabla p) - \operatorname{div}(\mathbf{b}p) &= (u - u_d) \quad \text{in } \Omega \times (0, T) \\ p &= 0, \quad \text{on } \Gamma_D \times (0, T), \\ (A \nabla p + \mathbf{b}p) \cdot \boldsymbol{\nu} &= 0 \quad \text{on } \Gamma_N \times (0, T) \\ p(x, T) &= 0 \quad \text{in } \Omega. \end{aligned}$$

► Gradient

$$(\nabla \mathcal{J}(z), h)_Z = \langle \mathcal{J}'(z), h \rangle_{Z^*, Z} = \langle p + \lambda z, h \rangle_{Z^*, Z} \quad h \in Z.$$

where $Z = L^2(0, T; L^2(\Omega))$.

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Linear elliptic PDE and Weak Form

Literature: [Braess, 1997, Ciarlet, 2002, Brenner and Scott, 2008, Ern and Guermond, 2004]

Poisson's equation. Let Ω be a bounded open Lipschitz domain with boundary $\partial\Omega$. Consider the following elliptic boundary value problem where given f we seek u solving

$$\begin{aligned} -\operatorname{div}(A\nabla u) &= f && \text{in } \Omega \\ u &= g_D && \text{on } \partial\Omega_D \\ A\nabla u \cdot \boldsymbol{\nu} &= g_N && \text{on } \partial\Omega_N. \end{aligned}$$

Linear elliptic PDE and Weak Form

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Weak solution. We define

$$V := \{v \in H^1(\Omega) : v|_{\partial\Omega_D} = g_D\}, \quad V_0 := \{v \in H^1(\Omega) : v|_{\partial\Omega_D} = 0\}.$$

We seek $u \in V$ such that

$$\int_{\Omega} A\nabla u \cdot \nabla v dx = \int_{\Omega} f v dx + \int_{\partial\Omega_N} g_N v ds, \quad \forall v \in V_0.$$

Assume that there exist $w \in H^1(\Omega)$ such that $w|_{\partial\Omega_D} = g_D$. Then we write $u = u_0 + w$ with $u_0|_{\partial\Omega_D} = 0$.

Thus we are reduced to finding $u_0 \in V_0$ solving:

$$\int_{\Omega} A \nabla u_0 \cdot \nabla v dx = \int_{\Omega} f v dx + \int_{\partial\Omega_N} g_N v ds - \int_{\Omega} A \nabla w \cdot \nabla v dx, \quad \forall v \in V_0.$$

Then $u = u_0 + w$.

Galerkin Approximation

- **Weak form.** Find $u_0 \in V_0$ solving:

$$\int_{\Omega} A \nabla u_0 \cdot \nabla v dx = \int_{\Omega} f v dx + \int_{\partial \Omega_N} g_N v ds - \int_{\Omega} A \nabla w \cdot \nabla v dx, \quad \forall v \in V_0.$$

- **Galerkin approximation.** Find subspace $V_h \subset V_0$ with basis $\{v_1, \dots, v_n\}$. Approximate u_0 by $u_h = \sum_{j=1}^n u_j v_j$.

Find $u_h \in V_h$ such that $u_h \in V_h$ solves

$$\int_{\Omega} A \nabla u_h \cdot \nabla v dx = \int_{\Omega} f v dx + \int_{\partial \Omega_N} g_N v ds - \int_{\Omega} A \nabla w \cdot \nabla v dx, \quad \forall v \in V_h$$

or equivalently

$$\int_{\Omega} A \nabla u_h \cdot \nabla v_i dx = \int_{\Omega} f v_i dx + \int_{\partial \Omega_N} g_N v_i ds - \int_{\Omega} A \nabla w \cdot \nabla v_i dx, \quad i = \overline{1, n}.$$

Galerkin Approximation

Find $u_h \in V_h$ solving:

$$\int_{\Omega} A \nabla u_h \cdot \nabla v_i dx = \int_{\Omega} f v_i dx + \int_{\partial\Omega_N} g_N v_i ds - \int_{\Omega} A \nabla w \cdot \nabla v_i dx, \quad i = \overline{1, n}.$$

Equivalently we can write a matrix vector system:

$$\mathbf{A} \mathbf{u} = \mathbf{b}$$

where $\mathbf{u} = (u_1, \dots, u_n)^T$, $\mathbf{A} \in \mathbb{R}^{n \times n}$, $\mathbf{b} \in \mathbb{R}^n$ with entries

$$\begin{aligned} \mathbf{A}_{ij} &= \int_{\Omega} A \nabla v_j \cdot \nabla v_i \\ \mathbf{b}_i &= \int_{\Omega} f v_i dx + \int_{\partial\Omega_N} g_N v_i ds - \int_{\Omega} A \nabla w \cdot \nabla v_i dx, \quad i = \overline{1, n}. \end{aligned}$$

Piecewise linear basis functions on triangles

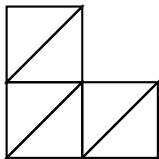
- ▶ We haven't specified V_h or basis functions $v_1, \dots, v_n$ yet.
- ▶ We will define V_h as a subspace with piecewise polynomials.
- ▶ For simplicity let us consider $\Omega \subset \mathbb{R}^2$, and consider the subspace V_h of functions that are continuous on $\overline{\Omega}$ and piecewise linear basis functions on triangles.

Assume polygonal domain Ω and subdivide into open triangles $K_1, \dots, K_{\text{elem}}$ such that

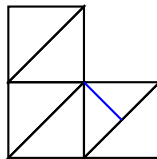
$$\overline{\Omega} = \cup_i \overline{K}_i,$$

$$K_i \cap K_j = \emptyset, \quad i \neq j,$$

$$\overline{K}_i \cap \overline{K}_j = \emptyset, \text{ or } = \text{a vertex, or } = \text{an edge of both } K_i \text{ and } K_j.$$



Admissible triangulation



Inadmissible triangulation

- ▶ Subspace V_h consists of functions that are globally continuous on $\overline{\Omega}$ and piecewise linear on the triangles.
- ▶ Let $\mathbf{n}_1, \dots, \mathbf{n}_{n_n} \in \overline{\Omega}$ are the nodes (same as vertices for piecewise linear elements). Here n_n is the number of nodes in the mesh.
- ▶ Basis functions $N_1, \dots, N_{n_n}$ are piecewise linear on triangles and satisfy

$$N_i(\mathbf{n}_j) = \delta_{ij}.$$

(refer to as *nodal basis*).

- ▶ Notice that $N_i(x)$ is nonzero only if x is contained in a element K that contains the node $\mathbf{n}_i$, i.e.,

$$N_i(x) = 0 \quad \text{for } x \notin \cup_{\mathbf{n}_i \in \overline{K}} \overline{K}.$$

- For notation simplicity we assume that $\mathbf{n}_{n+1}, \dots, \mathbf{n}_{n_n}$ are the nodes corresponding to the Dirichlet boundary conditions, i.e.,
 $\mathbf{n}_1, \dots, \mathbf{n}_n \notin \partial\Omega_D$,
 $\mathbf{n}_{n+1}, \dots, \mathbf{n}_{n_n} \in \partial\Omega_D$.
- The subspace V_h has basis $\{N_1, \dots, N_n\}$.
- Thus the Galerkin approximation now reads

$$\mathbf{A}\mathbf{u} = \mathbf{b},$$

where

$$\begin{aligned} \mathbf{A}_{ij} &= \int_{\Omega} A \nabla N_j \cdot \nabla N_i \\ \mathbf{b}_i &= \int_{\Omega} f N_i dx + \int_{\partial\Omega_N} g_N N_i ds - \int_{\Omega} A \nabla w \cdot \nabla N_i dx, \quad i = \overline{1, n}. \end{aligned}$$

- We will incorporate the Dirichlet boundary conditions later.
- Let us first compute $\mathbf{A} \in \mathbb{R}^{n_n, n_n}$ with entries

$$\mathbf{A}_{ij} = \int_{\Omega} A \nabla N_j \cdot \nabla N_i$$

$$\mathbf{b}_i = \int_{\Omega} f N_i dx + \int_{\partial\Omega_N} g_N N_i ds.$$

- We notice that

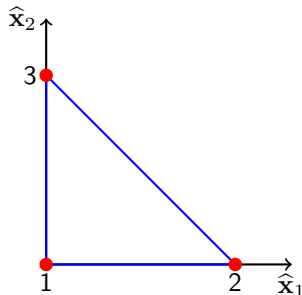
$$\int_{\Omega} A \nabla N_j \cdot \nabla N_i = \sum_{\ell=1}^{n_{\text{elem}}} \int_{K_{\ell}} A \nabla N_j \cdot \nabla N_i$$

and

$$\int_{K_{\ell}} A \nabla N_j \cdot \nabla N_i = 0$$

if node $\mathbf{n}_i$ or $\mathbf{n}_j$ is not in $\overline{K_{\ell}}$.

- For piecewise linear basis functions there are $n_{\text{basis}} = 3$ nodes per element. For each element K_ℓ compute $n_{\text{basis}} \times n_{\text{basis}}$ integrals. The resulting matrices are called *local*.
- Compute these integrals by transforming onto a reference element $\hat{K}$ with vertices $(0,0)$, $(1,0)$, $(1,1)$.
- The linear basis on the reference triangle are given by

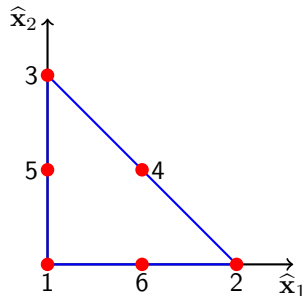


$$\hat{N}_1(\hat{x}) = 1 - \hat{x}_1 - \hat{x}_2$$

$$\hat{N}_2(\hat{x}) = \hat{x}_1$$

$$\hat{N}_3(\hat{x}) = \hat{x}_2$$

Quadratic Basis Functions on Reference Triangle



$$\hat{N}_1(\hat{x}) = (1 - \hat{x}_1 - \hat{x}_2)(1 - 2\hat{x}_1 - 2\hat{x}_2)$$

$$\hat{N}_2(\hat{x}) = \hat{x}_1(2\hat{x}_1 - 1)$$

$$\hat{N}_3(\hat{x}) = \hat{x}_2(2\hat{x}_2 - 1)$$

$$\hat{N}_4(\hat{x}) = 4\hat{x}_1\hat{x}_2$$

$$\hat{N}_5(\hat{x}) = 4\hat{x}_2(1 - \hat{x}_1 - \hat{x}_2)$$

$$\hat{N}_6(\hat{x}) = 4\hat{x}_1(1 - \hat{x}_1 - \hat{x}_2)$$

- **Element transformation.** The map

$$F_E : \hat{K} \rightarrow K,$$
$$\hat{x} \mapsto F_K(x) = \mathbf{v}_{k_1} + B\hat{x}$$

where $B = (\mathbf{v}_{k_2} - \mathbf{v}_{k_1}, \mathbf{v}_{k_3} - \mathbf{v}_{k_1}) \in \mathbb{R}^{2 \times 2}$ is bijective and maps vertex $\hat{\mathbf{v}}_i$ to $\mathbf{v}_{k_i}$, $i = 1, 2, 3$.

- The basis function on element K is given by

$$N_{k_i}(x) = \hat{N}_i(F_K^{-1}(x)), \quad i = 1, \dots, n_{\text{basis}}.$$

- Derivative. $\nabla N_{k_i}(x) = B^{-T} \nabla \hat{N}_i(\hat{x})$.

- ▶ Let K be an element with nodes $\mathbf{n}_{k_1}, \dots, \mathbf{n}_{k_{n_{\text{basis}}}}$.

- ▶ The integral

$$\int_K A(x) \nabla N_j(x) \cdot \nabla N_i(x) \, dx$$

is only nonzero if $i, j \in \{k_1, \dots, k_{n_{\text{basis}}}\}$.

- ▶ If $i = k_\ell$ and $j = k_m$ then

$$\begin{aligned} \int_K A(x) \nabla N_j(x) \cdot \nabla N_i(x) \, dx &= \int_K A(x) \nabla N_{k_m}(x) \cdot \nabla N_{k_\ell}(x) \, dx \\ &= |\det(B)| \int_{\hat{K}} A(F_K(\hat{x})) \left(B^{-T} \nabla \hat{N}_m \right) \left(B^{-T} \nabla \hat{N}_\ell \right) \end{aligned}$$

Dirichlet Boundary Conditions

- ▶ Let n_n be the number of nodes in the mesh.
- ▶ $\mathbf{n}_{n+1}, \dots, \mathbf{n}_{n_n}$ be the Dirichlet nodes. The subspace V_h has basis $\{N_1, \dots, N_n\}$.
- ▶ So far we have assembled $\mathbf{A} \in \mathbb{R}^{n_n \times n_n}$ and $\mathbf{b} \in \mathbb{R}^{n_n}$.
- ▶ Approximate w by

$$w(x) \approx \sum_{j=n+1}^{n_n} d(\mathbf{n}_j) N_j(x)$$

(Interpolation at nodes).

- ▶ We then modify $\mathbf{b}$ to incorporate nonzero boundary conditions as

$$\mathbf{b}_i = \int_{\Omega} f N_i + \int_{\partial\Omega} g_N N_i ds - \sum_{j=n+1}^{n_n} \mathbf{A}_{ij} d(\mathbf{n}_j).$$

- ▶ Then we need to solve

$$\mathbf{A}(1:n, 1:n) \mathbf{u}(1:n) = \mathbf{b}(1:n),$$

where $1:n$ corresponds to the free nodes (nodes at which no Dirichlet conditions are given).

PDE Constrained Optimization – Overview

Derivative Computation

Application of Abstract Approach

Finite Element Method

Matlab Code: Newton CG, L-BFGS, Semismooth Newton

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