Least-Squares Finite Element Methods for Optimal Control Problems

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The Abstract Problem

The optimal control problems we consider consist of the following ingredients:

- State variables → describe the system being modeled
- Control variables → can be used to affect the state variables
- State system → PDE relating the state and control variables
- Cost functional → a function of the state and control variables

We restrict attention to

- Linear, elliptic state systems
- Quadratic functionals

Find state and control variables that minimize the given functional, subject to the state system being satisfied

Hilbert spaces

$\Theta \rightarrow$ control space

$\Phi \rightarrow$ state space

$\hat{\Phi} \rightarrow$ data space

$\tilde{\Phi} \rightarrow$ pivot space

$$\Phi \subseteq \hat{\Phi} \subseteq \tilde{\Phi} \subseteq \hat{\Phi}^* \subseteq \Phi^*$$

$$\langle \psi, \phi \rangle_{\Phi^*,\Phi} = \langle \psi, \phi \rangle_{\hat{\Phi}^*,\hat{\Phi}} = (\psi, \phi)$$

$$\forall \psi \in \hat{\Phi}^* \subseteq \Phi^* \quad \forall \phi \in \Phi \subseteq \hat{\Phi}$$

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Objective Functional

$$J(\phi,\theta) = \frac{1}{2} a_1(\phi - \hat{\phi}, \phi - \hat{\phi}) + \frac{1}{2} a_2(\theta,\theta)$$

$a_1(\cdot,\cdot) \leftarrow$ symmetric bilinear on $\hat{\Phi} \times \hat{\Phi}$

$a_2(\cdot,\cdot) \leftarrow$ symmetric bilinear on $\Theta \times \Theta$

Assumptions

$$\begin{cases} a_1(\phi,\mu) \le C_1 \|\phi\|_{\hat{\Phi}} \|\mu\|_{\hat{\Phi}} & \leftarrow \text{continuity} \\ a_2(\theta,\nu) \le C_2 \|\theta\|_{\Theta} \|\nu\|_{\Theta} & \leftarrow \text{continuity} \\ a_1(\phi,\phi) \ge 0 & \leftarrow \text{non-negativity} \\ a_2(\theta,\theta) \ge K_2 \|\theta\|_{\Theta} & \leftarrow \text{coercivity} \end{cases}$$

$$\begin{cases} \phi \in \Phi & \leftarrow \text{state} \\ \theta \in \Theta & \leftarrow \text{control} \\ \hat{\phi} \in \hat{\Phi} & \leftarrow \text{given} \end{cases}$$

- Often Θ is finite dimensional. Then θ is referred to as the vector of design variables
- The second term is penalty that limits the size of the control θ

Linear Constraint Equation

$$b_1(\phi,\psi) + b_2(\theta,\psi) = \langle g,\psi \rangle_{\Lambda^*,\Lambda}$$

$b_1(\cdot,\cdot)$ ← bilinear form on $\Phi \times \Lambda$

$b_2(\cdot,\cdot)$ ← bilinear form on $\Theta \times \Lambda$

Λ ← another Hilbert space

g∈Λ* ← a given function

Assumptions

$$\begin{cases} b_1(\phi,\psi) \le c_1 \|\phi\|_\Phi \|\psi\|_\Lambda & \leftarrow \text{continuity} \\ b_2(\theta,\psi) \le c_2 \|\theta\|_\Theta \|\psi\|_\Phi & \leftarrow \text{continuity} \\ \sup_{\psi\in\Lambda} \dfrac{b_1(\phi,\psi)}{\|\psi\|_\Lambda} \ge k_1 \|\phi\|_\Phi & \leftarrow \text{weak coercivity} \\ \sup_{\phi\in\Phi} \dfrac{b_1(\phi,\psi)}{\|\phi\|_\Phi} > 0 & \leftarrow \text{weak coercivity} \end{cases}$$

These assumptions are sufficient to guarantee that given any control θ the constraint equation is uniquely solvable for the state ϕ.

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The Optimal Control Problem

$$\min_{\phi,\theta} J(\phi,\theta) \quad \text{subject to} \quad b_1(\phi,\psi) + b_2(\theta,\psi) = \langle g,\psi \rangle_{\Lambda^*,\Lambda}$$

Operator notation

$$a_1(\cdot,\cdot) \to A_1 : \hat{\Phi} \mapsto \hat{\Phi}^*$$

$$a_2(\cdot,\cdot) \to A_2 : \Theta \mapsto \Theta^*$$

$$\Rightarrow \quad J(\phi,\theta) = \frac{1}{2}\left\langle A_1(\phi-\hat{\phi}),(\phi-\hat{\phi})\right\rangle_{\hat{\Phi}^*,\hat{\Phi}} + \frac{1}{2}\left\langle A_2\theta,\theta\right\rangle_{\Theta^*,\Theta}$$

$$b_1(\cdot,\cdot) \to B_1 : \Phi \mapsto \Lambda^*$$

$$b_2(\cdot,\cdot) \to B_2 : \Lambda \mapsto \Theta^*$$

$$\Rightarrow \quad B_1\phi + B_2\theta = g$$

$$\min_{\phi,\theta} J(\phi,\theta) \quad \text{subject to} \quad B_1\phi + B_2\theta = g \ \text{ in } \ \Lambda^*$$

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Lagrange Multiplier Solution

Saddle point optimality system

$$\begin{cases} a_1(\phi,\mu) \qquad\qquad + b_1(\mu,\lambda) = a_1(\hat{\phi},\mu) & \forall \mu \in \Phi \\ \qquad a_2(\theta,\nu) + b_2(\nu,\lambda) = 0 & \forall \nu \in \Theta \\ b_1(\phi,\psi) + b_2(\theta,\psi) \qquad = \langle g,\psi \rangle_{\Lambda^*,\Lambda} & \forall \psi \in \Lambda \end{cases}$$

$$\begin{cases} A_1\phi \qquad + B_1^*\lambda = A_1\hat{\phi} & \text{in} \quad \Phi^* \\ \qquad A_2\theta + B_2^*\lambda = 0 & \text{in} \quad \Theta^* \\ B_1\phi + B_2\theta \qquad = g & \text{in} \quad \Lambda^* \end{cases}$$

Assumptions imply that (using the Brezzi theory)

– The optimal control problem has a unique solution $(\phi,\theta) \in \Phi \times \Theta$

– That solution can be determined by solving the saddle point optimality system

– The optimality system has a unique solution $(\phi,\theta,\lambda) \in \Phi \times \Theta \times \Lambda$

– That solution depends continuously on the data

$$\|\phi\|_{\Phi} + \|\theta\|_{\Theta} + \|\lambda\|_{\Lambda} \le C\left(\|g\|_{\Lambda^*} + \|\hat{\phi}\|_{\hat{\Phi}}\right)$$

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Galerkin approximation of the optimality system

Approximation spaces $\Phi^h \subset \Phi \quad \Theta^h \subset \Theta \quad \Lambda^h \subset \Lambda$

Discrete problem

$$\begin{cases} a_1(\phi^h,\mu^h) \qquad\qquad + b_1(\mu^h,\lambda^h) = a_1(\hat{\phi},\mu^h) & \forall \mu^h \in \Phi^h \\ \qquad a_2(\theta^h,\nu^h) + b_2(\nu^h,\lambda^h) = 0 & \forall \nu^h \in \Theta^h \\ b_1(\phi^h,\psi^h) + b_2(\theta^h,\psi^h) \qquad = \langle g,\psi\rangle_{\Lambda^*,\Lambda} & \forall \psi^h \in \Lambda^h \end{cases}$$

Weak coercivity not inherited on subspaces ⇒ Discrete inf-sup conditions

$$\sup_{\psi^h\in\Lambda^h} \frac{b_1(\phi^h,\psi^h)}{\|\psi^h\|_\Lambda} \ge k_i^h \|\phi^h\|_\Phi \quad \text{and} \quad \sup_{\phi^h\in\Phi^h} \frac{b_1(\phi^h,\psi^h)}{\|\phi^h\|_\Phi} > 0$$

$$\|\phi^h\|_\Phi + \|\theta^h\|_\Theta + \|\lambda^h\|_\Lambda \le C\left(\|g\|_{\Lambda^*} + \|\hat{\phi}\|_{\hat{\Phi}}\right)$$

$$\|\phi-\phi^h\|_\Phi + \|\theta-\theta^h\|_\Theta + \|\lambda-\lambda^h\|_\Lambda \le C\inf\left(\|\phi-\mu^h\|_\Phi + \|\theta-\zeta^h\|_\Theta + \|\lambda-\psi^h\|_\Lambda\right)$$

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The Algebraic Problem

- The discrete optimality system is equivalent to the linear system

$$\begin{pmatrix} \mathbf{A}_1 & & \mathbf{B}_1^T \\ & \mathbf{A}_2 & \mathbf{B}_2^T \\ \mathbf{B}_1 & \mathbf{B}_2 & \end{pmatrix} \begin{pmatrix} \phi \\ \theta \\ \lambda \end{pmatrix} = \begin{pmatrix} \mathbf{f} \\ 0 \\ \mathbf{g} \end{pmatrix}$$

- The saddle point nature of optimality system **cannot be avoided**
  - It occurs even when the state system is strongly coercive, i.e., **even if the form** $b_1(.,.)$ is coercive

The Galerkin approach will always yield indefinite matrix problems

- The discretized optimality system is **formidable**
  - At least **twice the size** of the state system
  - One shot solution is often **impractical**
  - Many strategies for **uncoupling** the equations have been proposed

Necessitates an iterative approach to solving the system

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Least-Squares Methods I: Application to the Optimality System

Starting point

$$\begin{cases} A_1\phi \qquad\qquad + B_1^*\lambda = A_1\hat{\phi} & \text{in} \quad \Phi^* \\ \qquad\quad A_2\theta + B_2^*\lambda = 0 & \text{in} \quad \Theta^* \\ B_1\phi + B_2\theta \qquad\quad = g & \text{in} \quad \Lambda^* \end{cases}$$

Well-posed in

$\Phi \times \Theta \times \Lambda$ ← data space

$\Phi^* \times \Theta^* \times \Lambda^*$ ← solution space

Least-squares functional

$$K\left(\phi,\theta,\lambda;\hat{\phi},g\right) = \frac{1}{2}\left(\left\|A_1\phi + B_1^*\lambda - A_1\hat{\phi}\right\|_{\Phi^*}^2 + \left\|A_2\theta + B_2^*\lambda\right\|_{\Theta^*}^2 + \left\|B_1\phi + B_2\theta - g\right\|_{\Lambda^*}^2\right)$$

Minimization problem

$$\min_{\phi,\theta,\lambda} K\left(\phi,\theta,\lambda;\hat{\phi},g\right)$$

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Optimality condition $B(\{\phi,\theta,\lambda\},\{\mu,\nu,\psi\}) = F\left(\{\mu,\nu,\psi\},\left\{A_1\hat{\phi},0,g\right\}\right)$

$$B(\{\phi,\theta,\lambda\},\{\mu,\nu,\psi\}) = \left(A_1\phi + B_1^*\lambda, A_1\mu + B_1^*\psi\right)_{\Phi^*} + \left(A_2\theta + B_2^*\lambda, A_2\nu + B_2^*\psi\right)_{\Theta^*} + \left(B_1\phi + B_2\theta, B_1\mu + B_2\nu\right)_{\Lambda^*}$$

$$F\left(\{\mu,\nu,\psi\},\left\{A_1\hat{\phi},0,g\right\}\right) = \left(A_1\hat{\phi}, A_1\mu + B_1^*\psi\right)_{\Phi^*} + \left(g, B_1\mu + B_2\nu\right)_{\Lambda^*}$$

Our assumptions imply that

- *B(.,.)* is symmetric, continuous and coercive: $B(\{\phi,\theta,\lambda\},\{\phi,\theta,\lambda\}) \geq C\left(\|\phi\|_\Phi^2 + \|\theta\|_\Theta^2 + \|\lambda\|_\Lambda^2\right)$
- *F(.)* is continuous

And since $K(\phi,\theta,\lambda;0,0) \equiv B(\{\phi,\theta,\lambda\},\{\phi,\theta,\lambda\})$ the least-squares functional is norm-equivalent

$$C_1\left(\|\phi\|_\Phi^2 + \|\theta\|_\Theta^2 + \|\lambda\|_\Lambda^2\right) \leq K(\phi,\theta,\lambda;0,0) \leq C_2\left(\|\phi\|_\Phi^2 + \|\theta\|_\Theta^2 + \|\lambda\|_\Lambda^2\right)$$

The least-squares minimization problem has a unique minimizer and

$$\|\phi\|_\Phi + \|\theta\|_\Theta + \|\lambda\|_\Lambda \leq C\left(\|g\|_{\Lambda^*} + \left\|\hat{\phi}\right\|_{\hat{\Phi}}\right)$$

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Least-Squares Finite Element Method

Approximation spaces

$$\Phi^h \subset \Phi \quad \Theta^h \subset \Theta \quad \Lambda^h \subset \Lambda$$

Discrete problem

$$B\left(\left\{\phi^h,\theta^h,\lambda^h\right\},\left\{\mu^h,\nu^h,\psi^h\right\}\right) = F\left(\left\{\mu^h,\nu^h,\psi^h\right\},\left\{A_1\hat{\phi},0,g\right\}\right)$$

Coercivity is inherited on subspaces ⇒ no inf-sup conditions are needed!

$$B\left(\left\{\phi^h,\theta^h,\lambda^h\right\},\left\{\phi^h,\theta^h,\lambda^h\right\}\right) \ge C\left(\left\|\phi^h\right\|_\Phi^2 + \left\|\theta^h\right\|_\Theta^2 + \left\|\lambda^h\right\|_\Lambda^2\right)$$

$$\Downarrow$$

$$\left\|\phi^h\right\|_\Phi + \left\|\theta^h\right\|_\Theta + \left\|\lambda^h\right\|_\Lambda \le C\left(\left\|g\right\|_{\Lambda^*} + \left\|\hat{\phi}\right\|_{\hat{\Phi}}\right)$$

$$\left\|\phi-\phi^h\right\|_\Phi + \left\|\theta-\theta^h\right\|_\Theta + \left\|\lambda-\lambda^h\right\|_\Lambda \le C\inf\left(\left\|\phi-\mu^h\right\|_\Phi + \left\|\theta-\zeta^h\right\|_\Theta + \left\|\lambda-\psi^h\right\|_\Lambda\right)$$

Practicality of this approach requires one to cast the constraint equations as first-order systems

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The Algebraic Problem

The discrete least-squares optimality system is equivalent to a linear system

$$\begin{pmatrix} \mathbf{K}_1 & \mathbf{C}_1^T & \mathbf{C}_2^T \\ \mathbf{C}_1 & \mathbf{K}_2 & \mathbf{C}_3^T \\ \mathbf{C}_2 & \mathbf{C}_3 & \mathbf{K}_3 \end{pmatrix} \begin{pmatrix} \phi \\ \theta \\ \lambda \end{pmatrix} = \begin{pmatrix} \mathbf{f} \\ \mathbf{h} \\ \mathbf{g} \end{pmatrix}$$

- The coefficient matrix of this system is **symmetric and positive definite**
  - this should be compared to the Galerkin linear system for which the coefficient matrix is **symmetric and indefinite**
- This system is also formidable and calls for uncoupling strategies for its solution

Uncoupling strategies

$$\begin{pmatrix} \mathbf{A}_1 & & \mathbf{B}_1^T \\ & \mathbf{A}_2 & \mathbf{B}_2^T \\ \mathbf{B}_1 & \mathbf{B}_2 & \end{pmatrix} \begin{pmatrix} \phi \\ \theta \\ \lambda \end{pmatrix} = \begin{pmatrix} \mathbf{f} \\ 0 \\ \mathbf{g} \end{pmatrix}$$

- Rely on invertibility of $\mathbf{B}_1$ and $\mathbf{A}_2$
- $\mathbf{B}_1$ is, in general, non-symmetric and indefinite

$$\begin{pmatrix} \mathbf{K}_1 & \mathbf{C}_1^T & \mathbf{C}_2^T \\ \mathbf{C}_1 & \mathbf{K}_2 & \mathbf{C}_3^T \\ \mathbf{C}_2 & \mathbf{C}_3 & \mathbf{K}_3 \end{pmatrix} \begin{pmatrix} \phi \\ \theta \\ \lambda \end{pmatrix} = \begin{pmatrix} \mathbf{f} \\ \mathbf{h} \\ \mathbf{g} \end{pmatrix}$$

- Rely on invertibility of $\mathbf{K}_1$, $\mathbf{K}_2$ and $\mathbf{K}_2$
- all are symmetric and positive definite
- true even if discrete inf-sup for b_1 *does not hold*

A Simple Uncoupling Strategy

An example of a simple uncoupling strategy is to apply block-Gauss Seidel method

Start with initial guesses $\phi^{(0)}$ and $\theta^{(0)}$ for the discretized state and control; then, for k=1,2…successively solve the linear systems

$$\mathbf{K}_3\lambda^{(k+1)} = \mathbf{g} - \mathbf{C}_2\phi^{(k)} - \mathbf{C}_3\theta^{(k)}$$

$$\mathbf{K}_1\phi^{(k+1)} = \mathbf{f} - \mathbf{C}_1^T\theta^{(k)} - \mathbf{C}_2^T\lambda^{(k+1)}$$

$$\mathbf{K}_2\theta^{(k+1)} = \mathbf{h} - \mathbf{C}_1\phi^{(k+1)} - \mathbf{C}_3^T\lambda^{(k+1)}$$

until satisfactory convergence is achieved

– The matrices $\mathbf{K}_1$, $\mathbf{K}_2$ and $\mathbf{K}_3$ are all symmetric positive definite so that efficient solution strategies are available

– of course, more sophisticated uncoupling strategies can also be defined

Least-Squares Methods II: Bi-level Minimization Problem

Least-squares form of the constraint

$B_1\phi + B_2\theta = g$ Treat the control θ as being a given function

Define the least-squares functional $H(\phi;\theta,g) = \frac{1}{2}\|B_1\phi + B_2\theta - g\|^2_{\Lambda^*}$

Consider the minimization problem $\min_{\phi} H(\phi;\theta,g)$

Euler-Lagrange equation

$$\tilde{b}_1(\phi,\mu) = (g, B_1\mu)_{\Lambda^*} - \tilde{b}_2(\theta,\mu) \quad \forall \mu \in \Phi$$

$$\tilde{b}_1(\phi,\mu) = (B_1\phi, B_1\mu)_{\Lambda^*}$$

$$\tilde{b}_2(\theta,\nu) = (B_2\theta, B_2\nu)_{\Lambda^*}$$

Norm-equivalence: $\tilde{b}_1(\phi,\phi) \geq C\|\phi\|^2_{\Phi} \quad \Longrightarrow \quad C_2\|\phi\|^2_{\Phi} \leq H(\phi;0,0) \leq C_2\|\phi\|^2_{\Phi}$

- The least-squares form of the constraint is a well-posed problem for all θ
- Its approximation does not require inf-sup conditions
- The discrete problem leads to symmetric and positive definite systems

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Bi-level Minimization problem

Instead of considering the optimal control problem

$$\min_{\phi,\theta} J(\phi,\theta) \quad \text{subject to} \quad B_1\phi + B_2\theta = g \quad \text{in} \quad \Lambda^*$$

we consider the equivalent problem

$$\min_{\phi,\theta} J(\phi,\theta) \quad \text{subject to} \quad \min_{\phi} H(\phi;\theta,g)$$

- This is a bi-level optimization problem
- There are, of course, many ways to address such problems
- We will describe two possible approaches

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Direct Penalization

Form the penalized functional

$$J_\varepsilon(\phi,\theta) = J(\phi,\theta) + \frac{1}{\varepsilon} H\left(\phi;\theta,g\right)$$

Unfortunately, this approach does not take full advantage of the least-squares formulation of the constraint equation:

– in particular, the discrete inf-sup condition on the bilinear form $b_1(.,.)$ cannot be circumvented;

– one also has to worry about choosing a “good” value for the penalty parameter ε.

Constraining by Least-Squares First Order Necessary Conditions

The bi-level optimization problem is

$$\min_{\phi,\theta} J(\phi,\theta) \quad \text{subject to} \quad \min_{\phi} H(\phi;\theta,g)$$

And the first-order necessary condition for the least-squares principle in operator form is:

$$B_1^* B_1 \phi + B_1^* B_2 \theta = B_1^* g \quad \text{in} \quad \Phi^*$$

Therefore,

$$\min_{\phi,\theta} J(\phi,\theta) \quad \text{subject to} \quad B_1^* B_1 \phi + B_1^* B_2 \theta = B_1^* g \quad \text{in} \quad \Phi^*$$

is an equivalent reformulation of our optimal control problem

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Lagrange Multiplier Solution

The Euler-Lagrange equations corresponding to the reformulated bi-level optimization

$$\begin{cases} A_1\phi \qquad\qquad + B_1^*B_1\lambda = A_1\hat{\phi} & \text{in} \quad \Phi^* \\ \qquad A_2\theta + B_2^*B_1\lambda = 0 & \text{in} \quad \Theta^* \\ B_1^*B_1\phi + B_1^*B_2\theta \qquad = B_1^*g & \text{in} \quad \Lambda^* \end{cases}$$

– This is a saddle-point problem and so the resulting matrix problem is indefinite

– The only advantage over Galerkin is that $B_1^*B_1$ is positive definite even when B_1 is not

There are several effective means for discretizing the new optimality system

– Penalty methods are one approach

– One also has the choice of discretize-then-optimize and optimize-then-discretize

A Taxonomy of Optimization Approaches

1.	LM	FE			
2.	LM	PEN	FE	ELIM	
3.	LM	LS	FE		
4.	LS-PEN	OPTIM	FE		
5.	LS-CON	LM	FE		
6.	LS-CON	LM	PEN	FE	ELIM
7.	LS-CON	PEN	OPTIM	FE	

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The score card

Criteria	Method						
	1	2	3	4	5	6	7
Discrete inf-sup not required	✗	✗	✓	✓	✓	✓	✓
Locking impossible	✓	✓	✓	✗	✓	✓	✗
Optimal error estimate	✓	✓	✓	✗	✓	✓	✗
Symmetric matrix system	✓	✓	✓	✓	✓	✓	✓
Reduced number of unknowns	✗	✓	✗	✓	✗	✓	✓
Positive definite linear system	✗	✓	✓	✓	✗	✓	✓

From the table we see that only Method 6

LS-CON LM PEN FE ELIM

has all its boxes checked ⇒ it seems to be the preferred method

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But…

There are additional issues that arise in practice and must also be considered:

- Use standard finite elements
- Ease of asembly of the discrete system
- Manageable conditioning of the discrete system

When these are added to the mix, it seems that method 3 wins out:

LM | LS | FE

For further details see:

P. Bochev and M. Gunzburger, *Least-squares finite element methods for optimization and control problems for the Stokes equations*. Comp. Math. Appl., Vol. 48, No.7, 2004, pp. 1035-1057.

P. Bochev and M. Gunzburger, *Least-squares finite element methods for optimality systems arising in optimization and control problems*. Accepted in SIAM J. Num. Anal.

P. Bochev and M. Gunzburger, *Least-squares/penalty finite element methods for optimization and control problems*. To appear in "Proceeding of Santa Fe workshop on PDE constrained optimization".