PDE - constraint optimization

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Forward and Inverse Problem

Forward problem

$$\mathscr{F}(c;\alpha) = 0$$

$\mathscr{F}(c;\alpha)$ represents a PDE operator acting on c
α is a coefficient

Inverse problem

$$\text{find } \alpha, \min_{\alpha} f(c(\alpha))$$
$$\text{s.t. } \mathscr{F}(c;\alpha) = 0$$

f : objective function ($ie.\, |c - c_o|^2$)
α : design variable
c : state variable

https://www.cs.cmu.edu/~ateh/presentations/slides-pde-constrained-optimization.html

https://kailaix.github.io/ADCME.jl/stable/tu_optimization/

Find adjoint variable

$$\text{find } \alpha, \min_{\alpha} f(c(\alpha))$$

$$\text{s.t. } \mathscr{F}(c;\alpha) = 0$$

f : objective function, $(ie. |c - c_o|^2)$

α : design variable

c : state variable

we want to use gradeint based optimization,

we need, $\partial_\alpha f(c(\alpha))$

$$\partial_\alpha f = \partial_c f \, \boxed{\partial_\alpha c}$$

Obtain by using PDE

from $\mathscr{F}(\mathrm{c}(\alpha);\alpha) = 0$,

we have $\mathrm{d}_\alpha \mathscr{F} = \partial_\mathrm{c} \mathscr{F} \, \partial_\alpha \mathrm{c} + \partial_\alpha \mathscr{F} = 0$

$$\rightarrow \partial_\alpha c = -(\partial_c \mathscr{F})^{-1} \, \partial_\alpha \mathscr{F}$$

$$\partial_\alpha f = \lambda^\mathrm{T} \, \partial_c f, \quad \text{where } \lambda^T = -(\partial_c \mathscr{F})^{-1} \, \partial_\alpha \mathscr{F}$$

Link to Lagrange function

$$\text{find } \alpha, \min_{\alpha} f(c(\alpha))$$
$$\text{s.t. } \mathcal{F}(c;\alpha) = 0$$

$f:$ objective function, $(ie. |c - c_o|^2)$

$\alpha:$ design variable

$c:$ state variable

we want to use gradeint based optimization,

we need, $\partial_\alpha f(c(\alpha))$

$$\partial_\alpha f = \partial_c f \, \partial_\alpha c$$

Obtain by using PDE

from $\mathcal{F}(\mathrm{x}(\alpha);\alpha) = 0$,

we have $\mathrm{d}_\alpha \mathcal{F} = \partial_\mathrm{c} \mathcal{F} \, \partial_\alpha \mathrm{c} + \partial_\alpha \mathcal{F} = 0$

$$\rightarrow \partial_\alpha c = -(\partial_c \mathcal{F})^{-1} \, \partial_\alpha \mathcal{F}$$

$\partial_\alpha f = \lambda^\mathrm{T} \, \partial_c f$, where $\lambda^T = -(\partial_c \mathcal{F})^{-1} \, \partial_\alpha \mathcal{F}$, is adjoint variable

langrange function, $L(c, \alpha, \lambda) = f(c(\alpha)) + \lambda^T \, \mathcal{F}(c;\alpha)$

KKT conditions :

(1) $\partial_\lambda L(c, \alpha, \lambda) = \mathcal{F}(c;\alpha) = 0$

(2) $\partial_c L(c, \alpha, \lambda) = \partial_c f(c) + \lambda^T \, \partial_c \mathcal{F}(c;\alpha) = 0$

(3) $\partial_\alpha L(c, \alpha, \lambda) = \partial_\alpha f(c) + \lambda^T \, \partial_\alpha \mathcal{F}(c;\alpha) = 0$

for a given α, solve for c, λ, from(1), (2),

$$\rightarrow \partial_\alpha L(c, \alpha, \lambda) = \partial_\alpha f - \partial_c f (\partial_c \mathcal{F})^{-1} \, \partial_\alpha \mathcal{F}$$

When alpha is optimal, this expression is equal to zero, i.e., all the KKT conditions are satisfied.

https://en.wikipedia.org/wiki/Karush–Kuhn–Tucker_conditions#:~:text=In