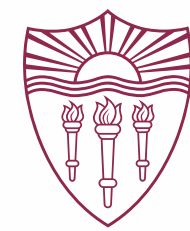


# PDE - constraint optimization

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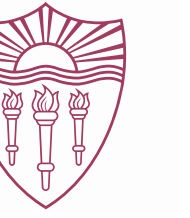
University of Southern California



Kanso's Bio-inspired Lab

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# Forward and Inverse Problem



## Forward problem

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

$\mathcal{F}(c; \alpha)$  represents a PDE operator acting on  $c$ ,  
with coefficient  $\alpha$

## Inverse problem

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

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

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

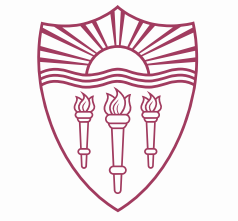
$\alpha$ : design variable

$c$ : state variable

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

[https://kailaix.github.io/ADCME.jl/stable/tu\\_optimization/](https://kailaix.github.io/ADCME.jl/stable/tu_optimization/)

# Find adjoint variable



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

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

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

$\alpha$ : design variable

$c$ : state variable

we want to use gradient based optimization,

we need,  $\nabla_{\alpha} f(c(\alpha))$

$$\nabla_{\alpha} f = \nabla_c f \boxed{\nabla_{\alpha} c}$$

Obtain by using PDE

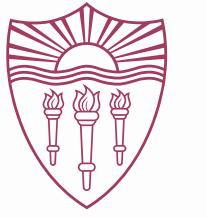
from  $\mathcal{F}(c(\alpha); \alpha) = 0$  holds for any  $\alpha$ ,

$$\text{we have } d_{\alpha} \mathcal{F} = \partial_c \mathcal{F} \partial_{\alpha} c + \partial_{\alpha} \mathcal{F} = 0$$

$$\rightarrow \nabla_{\alpha} c = - (\nabla_c \mathcal{F})^{-1} \nabla_{\alpha} \mathcal{F}$$

$$\nabla_{\alpha} f = \lambda^T \nabla_c f, \quad \text{where } \lambda^T = - (\nabla_c \mathcal{F})^{-1} \nabla_{\alpha} \mathcal{F}$$

# Link to Lagrange multiplier



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

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 gradient based optimization,  
we need,  $\partial_{\alpha} f(c(\alpha))$

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

KKT conditions :

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

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

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

$$\nabla_{\alpha} f = \nabla_c f \nabla_{\alpha} c$$

Obtain by using PDE

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

$$\text{we have } d_{\alpha} \mathcal{F} = \partial_c \mathcal{F} \partial_{\alpha} c + \partial_{\alpha} \mathcal{F} = 0$$

$$\rightarrow \nabla_{\alpha} c = - (\nabla_c \mathcal{F})^{-1} \nabla_{\alpha} \mathcal{F}$$

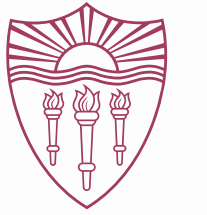
$$\nabla_{\alpha} f = \lambda^T \nabla_c f, \text{ where } \lambda^T = - (\nabla_c \mathcal{F})^{-1} \nabla_{\alpha} \mathcal{F}, \text{ is adjoint variable}$$

for a given  $\alpha$ , solve for  $c, \lambda$ , from(1), (2),

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

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

# Apply adjoint method



$$\text{find } \boldsymbol{\beta}, \max_{\boldsymbol{\beta}} \text{Sh}(c(\boldsymbol{\beta}))$$

$$\text{s.t. } \mathcal{F}(c; \boldsymbol{\beta}) = \text{Pe } \mathbf{u}(\boldsymbol{\beta}) \cdot \nabla c - \Delta c = 0,$$

$$||\boldsymbol{\beta}^2|| = 1$$

where  $Sh = \int_S \nabla c \cdot \hat{\mathbf{n}} dS$ , represents flux,

$c(r, \theta, \phi)$  represents concentration field in spherical coordinates

$\mathcal{F}$  represents advection – diffusion equation

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$$\mathcal{L} = \text{Sh}(c(\boldsymbol{\beta})) + \int g(\text{Pe } \mathbf{u}(\boldsymbol{\beta}) \cdot \nabla c - \Delta c) dV = 0,$$

See details in: <https://arxiv.org/abs/2404.13467>

# Automatic differentiation in computation graph



$$\text{find } \alpha, \min_{\alpha, \mathbf{c}_1} J = f(\mathbf{c}_1, \mathbf{c}_2, \mathbf{c}_3, \mathbf{c}_4)$$

$$\text{s.t. } \mathbf{c}_2 = \mathcal{F}_1(\mathbf{c}_1; \alpha)$$

$$\mathbf{c}_3 = \mathcal{F}_2(\mathbf{c}_2; \alpha)$$

$$\mathbf{c}_4 = \mathcal{F}_3(\mathbf{c}_3; \alpha)$$

$f$  is loss function

$$\begin{aligned} \text{adjoint variables : } \lambda_4^T &= \frac{\partial f}{\partial \mathbf{c}_4} \\ \lambda_3^T &= \frac{\partial f}{\partial \mathbf{c}_3} + \lambda_4^T \frac{\partial \mathcal{F}_3}{\partial \mathbf{c}_3} \\ \lambda_2^T &= \frac{\partial f}{\partial \mathbf{c}_2} + \lambda_3^T \frac{\partial \mathcal{F}_2}{\partial \mathbf{c}_2} \end{aligned}$$

$$\text{langrange function, } L = f + \lambda_2^T (\mathcal{F}_1(\mathbf{c}_1; \alpha) - \mathbf{c}_2) + \lambda_3^T (\mathcal{F}_2(\mathbf{c}_2; \alpha) - \mathbf{c}_3) + \lambda_4^T (\mathcal{F}_3(\mathbf{c}_3; \alpha) - \mathbf{c}_4)$$

$$\text{gradient of objective function, } \frac{\partial L}{\partial \alpha} = \lambda_2^T \frac{\partial \mathcal{F}_1}{\partial \alpha} + \lambda_3^T \frac{\partial \mathcal{F}_2}{\partial \alpha} + \lambda_4^T \frac{\partial \mathcal{F}_3}{\partial \alpha}$$

$$\text{relations : } \frac{\partial f}{\partial \mathbf{c}_2} = \frac{\partial J_{\text{total}}}{\partial \mathbf{c}_3} \frac{\partial \mathcal{F}_2}{\partial \mathbf{c}_2}, \quad \frac{\partial f}{\partial \alpha} = \frac{\partial J_{\text{total}}}{\partial \mathbf{c}_3} \frac{\partial \mathcal{F}_2}{\partial \alpha}$$

$$\text{total gradient of } \mathbf{c}_2 : \frac{\partial J_{\text{total}}}{\partial \mathbf{c}_2} = \frac{\partial f}{\partial \mathbf{c}_2} + \frac{\partial J_{\text{total}}}{\partial \mathbf{c}_3} \frac{\partial \mathcal{F}_2}{\partial \mathbf{c}_2} \quad \rightarrow \lambda_i^T = \frac{\partial J_{\text{total}}}{\partial \mathbf{c}_i}$$

# Thank you!

[https://kailaix.github.io/ADCME.jl/stable/tu\\_optimization/](https://kailaix.github.io/ADCME.jl/stable/tu_optimization/)

<https://www.cs.cmu.edu/~ateh/presentations/slides-pde-constrained-optimization.html#/4>

