The Adjoint method in design

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Discrete Adjoint method

- Primal

$$\begin{aligned} \text{min/max/find} \quad & \mathbf{h}^T\mathbf{u} \\ \text{s.t.} \quad & \mathbf{A}\mathbf{u} = \mathbf{f} \end{aligned}$$

- Dual (Adjoint)

$$\begin{aligned} \text{min/max/find} \quad & \mathbf{f}^T\mathbf{v} \\ \text{s.t.} \quad & \mathbf{A}^T\mathbf{v} = \mathbf{h} \end{aligned}$$

- If $\mathbf{f} \in \{\mathbf{f}_i | i = 1 \ldots p\}$ and $\mathbf{h} \in \{\mathbf{h}_j | j = 1 \ldots m\}$, dual is cheaper when $m \ll p$

Green's function interpretation

- The Green's functions $\mathbf{g}_A^{(k)}$ of $\mathbf{A}$ are given by

$$\mathbf{A}\ \mathbf{g}_A^{(k)} = \boldsymbol{\delta}^{(k)} \quad k = 1 \dots N$$

- Given the adjoint form

$$\mathbf{A}^T \mathbf{v} = \mathbf{h}$$

by strong duality,

$$\mathbf{v}^T \boldsymbol{\delta}^{(k)} = v_k = \mathbf{h}^T \mathbf{g}_A^{(k)}$$

Discretized design problem

- Consider the following setting

$$\min_{\alpha} \quad J(\mathbf{U}, \boldsymbol{\alpha})$$
$$\text{s.t.} \quad \mathbf{N}(\mathbf{U}, \boldsymbol{\alpha}) = 0$$

where

$\boldsymbol{\alpha}$: Design Variables

$\mathbf{U}$: Flow variables at discrete grid points (implicit $\boldsymbol{\alpha}$ dep)

$\mathbf{N}(\mathbf{U}, \boldsymbol{\alpha}) = 0$: Discrete flow equations

Linearized form

- Linearize w.r.t $\boldsymbol{\alpha}$

$$\frac{dJ}{d\alpha} = \frac{\partial J}{\partial U}\frac{dU}{d\alpha} + \frac{\partial J}{\partial \alpha}$$

$$\text{s.t.} \quad \frac{\partial N}{\partial U}\frac{dU}{d\alpha} + \frac{\partial N}{\partial \alpha} = 0$$

- Defining $\mathbf{u} := \frac{dU}{d\alpha} \quad \mathbf{A} := \frac{\partial N}{\partial U} \quad \mathbf{f} := -\frac{\partial N}{\partial \alpha} \quad \mathbf{h}^T := \frac{\partial J}{\partial U}$, primal form is

$$\mathbf{h}^T\mathbf{u} + \frac{\partial J}{\partial \alpha}$$
$$\text{s.t.} \quad \mathbf{Au} = \mathbf{f}(\alpha)$$

Discrete adjoint form

- The dual form is hence given by

$$\mathbf{f}^T \boldsymbol{\lambda} + \frac{\partial J}{\partial \alpha}$$
$$\text{s.t.} \quad \mathbf{A}^T \boldsymbol{\lambda} = \mathbf{h}$$

- $\mathbf{h}^T = \frac{\partial J}{\partial U}$ does not depend on design variables!
- Exploited in 2D and 3D aircraft wing optimization by Elliot and Peraire [1]

Lagrange Viewpoint

- Augmented objective function

$$I(U,\alpha) = J(U,\alpha) - \boldsymbol{\lambda}^T N(U,\alpha)$$

- Linearizing it recovers the same dual form as earlier

$$\frac{dI}{d\alpha} = \frac{\partial J}{\partial \alpha} - \boldsymbol{\lambda}^T \frac{\partial N}{\partial \alpha} = \frac{\partial J}{\partial \alpha} + \mathbf{f}^T \boldsymbol{\lambda}$$

$$\left(\frac{\partial N}{\partial U}\right)^T \boldsymbol{\lambda} = \left(\frac{\partial J}{\partial U}\right)^T \Rightarrow \mathbf{A}^T \boldsymbol{\lambda} = \mathbf{h}$$

Continuous adjoint approach

- PDE $\iff$ Adjoint PDE. Inner product convention

$$< v, u >_\Omega \; := \int_\Omega v(x)u(x)dx$$

- Primal

$$\begin{aligned} &< h, u >_\Omega \\ \text{s.t.} \quad & Lu = f \\ & \text{HBC on } \partial\Omega \end{aligned}$$

- Dual

$$\begin{aligned} &< v, f >_\Omega \\ \text{s.t.} \quad & L^* v = h \\ & \text{HBC on } \partial\Omega \end{aligned}$$

Adjoint Operator

- For HBCs, the adjoint L^* of an operator L is defined by

$$< v, Lu > \quad = \quad < L^* v, u >$$

- Eg. If $Lu = \left(\frac{d}{dx} - \epsilon \frac{d^2}{dx^2}\right) u, \quad 0 < x < 1, \quad u(0) = u(1) = 0$

$$\begin{aligned} < v, Lu > &= \int_0^1 v \left(\frac{du}{dx} - \epsilon \frac{d^2 u}{dx^2} \right) dx \\ &= \int_0^1 u \left(-\frac{dv}{dx} - \epsilon \frac{d^2 v}{dx^2} \right) + \left[-\epsilon v \frac{du}{dx} \right]_0^1 \quad = \quad < L^* v, u > \end{aligned}$$

$$\Rightarrow L^* = \left(-\frac{d}{dx} - \epsilon \frac{d^2}{dx^2} \right) \quad v(0) = v(1) = 0$$

Green's function interpretation of the continuous adjoint approach

- $Lu = f \Rightarrow Lg_L(x, x') = \delta(x, x')$
- Given $L^*v = h$,

$$\begin{aligned} < v, \delta(x, x') > &= < h, g(x, x') > \\ &\Rightarrow v(x) = \int_\Omega h(x')g_L(x, x')dx' \end{aligned}$$

Generalized Adjoint Identity

- If the primal objective includes a boundary integral, for eg

$$\begin{aligned} &< h, u >_\Omega + < h_2, Cu >_{\partial\Omega} \\ \text{s.t.} \quad & Lu = f \text{ in } \Omega \\ & Bu = f_2 \text{ on } \partial\Omega \end{aligned}$$

- The adjoint identity is modified to

$$< v, Lu >_\Omega + < C^* v, Bu >_{\partial\Omega} \quad = \quad < L^* v, u >_\Omega + < B^* v, Cu >_{\partial\Omega}$$

- This gives the dual form

$$\begin{aligned} &< v, f >_\Omega + < C^* v, f_2 >_{\partial\Omega} \\ \text{s.t.} \quad & L^* v = h \text{ in } \Omega \\ & B^* v = h_2 \text{ on } \partial\Omega \end{aligned}$$

Main conceptual difference between the discrete and continuous approach

- Discrete approach : Discretize, Linearize, Adjoint
- Continuous approach : Linearize, Adjoint, Discretize

Applications of the Adjoint method

- Aircraft design (eg. Optimal shape for drag and lift)
- Electromagnetic Shape Optimization (eg. Photonic components)

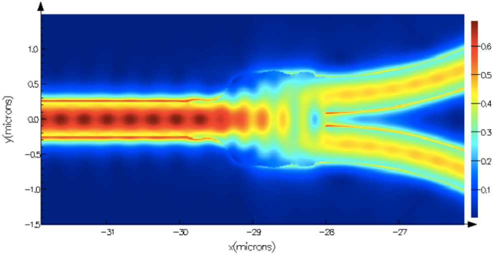

Fig. 5. Simulated field intensity $|E|^2$ for the optimized structure at λ = 1550nm for a slice in the middle of the device.

Optimal Y-beam splitter, Lalau-Keraly *et. al.* [2]

Authors

- Giles and Pierce (2000) [3]

Michael Giles (Oxford)

Niles Pierce (Caltech)

(Images: Google)

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Jonathan Elliott and Jaime Peraire. "Aerodynamic design using unstructured meshes". In: *Fluid Dynamics Conference*. 1996, p. 1941.

Christopher M Lalau-Keraly et al. "Adjoint shape optimization applied to electromagnetic design". In: *Optics express* 21.18 (2013), pp. 21693–21701.

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Thank You