A Review of the Adjoint Method: Continuous and Discrete approaches

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December 20, 2010

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Lagrange multipliers

Original problem	Modified problem
$\min\{f(x) : h(x) = 0\}$	$\min\{f(x) : h(x) = \vec{\delta}\}$
x^* solution	$x^* + \Delta x$ solution

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Lagrange multipliers

Using Karush-Kuhn-Tucker necessary conditions:

$$\nabla f(x^*) = -\nabla h(x^*)\lambda$$

we have:

$$\begin{aligned}
\Delta f &= f(x^* + \Delta x) - f(x^*) \\
&= \nabla f(x^*)^T \Delta x + o(\|\Delta x\|) \\
&= (-\nabla h(x^*)\lambda)^T \Delta x + o(\|\Delta x\|) \\
&= -\lambda^T \nabla h(x^*)^T \Delta x + o(\|\Delta x\|)
\end{aligned}$$

and also:

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Lagrange multipliers

Formally:

Theorem (Sensitivity with equality constraints)

Let (x^*, λ^*) local minimum and associated Lagrange multiplier. Also assume that the second order sufficiency conditions holds for (x^*, λ^*). Consider the family of problems:

$$\min\{f(x) : h(x) = u\}$$

where u is a parameter.
Then, for all u exists $(x(u), \lambda(u))$ local minimum and associated Lagrange multiplier of the problem $\min\{f(x) : h(x) = u\}$, $x^* = x(0)$, $\lambda^* = \lambda(0)$ and

$$\nabla_u f(x(u)) = -\lambda(u)$$

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- **Objective**:
  - We want to solve optimal control problems associated with numerical simulations governed by a partial differential equation:

$$\min\{J(\gamma, s) : C(\gamma, s) = 0, (\gamma, s) \in D \times S\} \tag{1}$$

  - Using gradient-based optimization methods for design variables γ:

$$\gamma_{k+1} = \gamma_k - \alpha_k \frac{\partial J}{\partial \gamma}(\gamma_k)$$

- **Central idea**:
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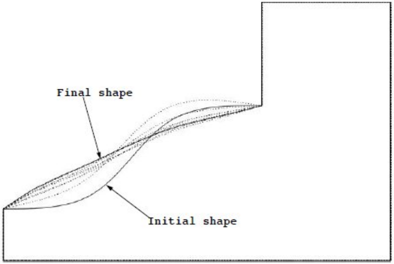
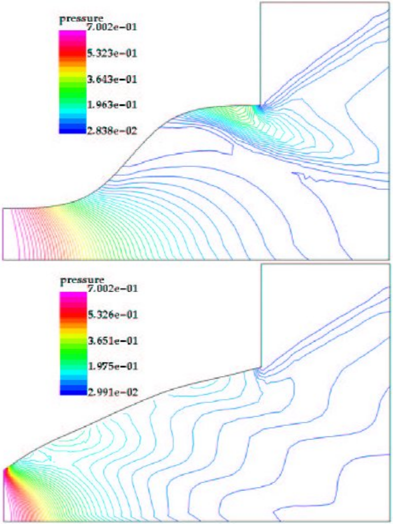
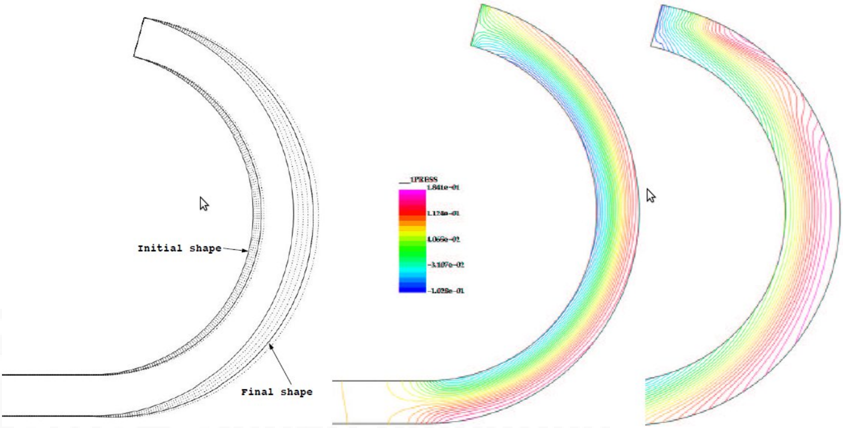




Overview: examples (Air duct)



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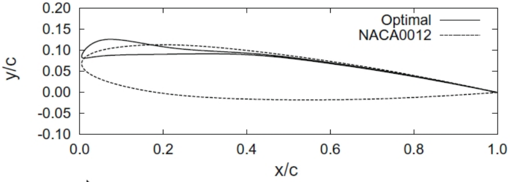

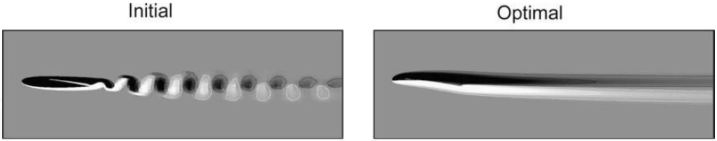

Overview: approaches

- **Continuous approach**:
  - First differentiate, then discretize.
- **Discrete approach**:
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Summary:

- Differentiate the continuous original system with respect to the design variables.
- Formulate the adjoint system.
- Solve the adjoint system (discrete).
- Use the adjoint solution to calculate derivatives of the cost function $J(\gamma, s)$ with respect to design variables.

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Example: Wave equation with homogeneous b.c.

- State equations:

$$
\begin{aligned}
\underbrace{\rho(x)\partial_t^2 u - \nabla\cdot(\mu(x)\nabla u)}_{Lu} &= g, & \Omega\times[0,T] \qquad (2a)\\
u &= 0, & \partial\Omega_1\times[0,T] \qquad (2b)\\
\nabla u\cdot n &= 0, & \partial\Omega_2\times[0,T] \qquad (2c)\\
u(x,0)=\partial_t u(x,0) &= 0, & \Omega\times\{0\} \qquad (2d)
\end{aligned}
$$

- Cost functional:

$$
J(u) = \int_\Omega\int_0^T \underbrace{\frac{1}{2}[u(x,t)-u_0(x,t)]^2\delta(x-\xi)\,dtdV}_{f(u)} \qquad (3)
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- Adjoint equations:

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\underbrace{\rho(x)\partial_t^2\lambda - \nabla\cdot(\mu(x)\nabla\lambda)}_{L^*\lambda} &= -D_u f(u), && \Omega\times[0,T] && \text{(4a)}\\
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- Differentiated cost functional:

$$
D_{(\rho,\mu)}J(u) = \int_\Omega\int_0^T \mu'\nabla u\cdot\nabla\lambda\, dt dV - \int_\Omega\int_0^T \rho'\partial_t u\partial_t\lambda\, dt dV \qquad (5)
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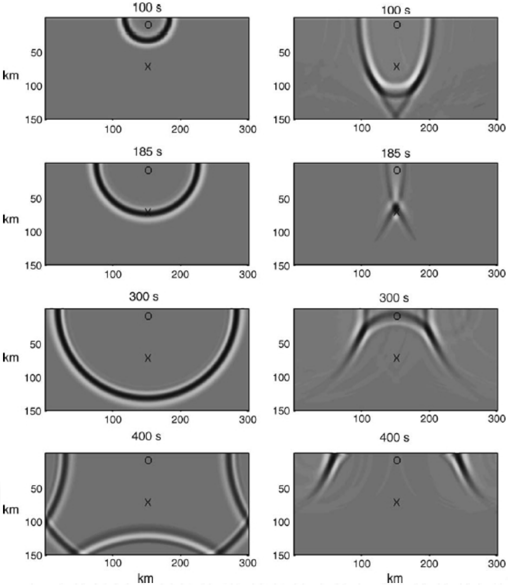

Continuous approach: reviewed applications

- Aerodynamics
  - Transonic small disturbances
  - 2D Euler equations using conformal mapping
  - 3D Euler equations
- Meteorology
  - Parameter estimation
  - Athmosphere-Ocean interaction
- Seismology
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Example: Data assimilation in Geophysics

- State equations:

$$\frac{d\theta(t)}{dt} = \frac{1}{h(t)} C_T V (1+K)(T(t)-\theta(t)) \quad (6a)$$

$$\frac{dh(t)}{dt} = K C_T V \frac{T(t)-\theta(t)}{\sigma(t)} + W \quad (6b)$$

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$$J(\theta, h, \sigma) = \sum_{i=0}^{n} \left[\frac{(\theta_i - \tilde{\theta}_i)^2}{\delta_\theta^2} + \frac{(h_i - \tilde{h}_i)^2}{\delta_h^2} + \frac{(\sigma_i - \tilde{\sigma}_i)^2}{\delta_\sigma^2} \right] \quad (7)$$

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Example: Data assimilation in Geophysics

- State equations:

$$\frac{d\theta(t)}{dt} = \frac{1}{h(t)} C_T V(1+K)(T(t)-\theta(t)) \tag{6a}$$

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  - Each problem has its own adjoint (some are very complex).
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- Powerful tool to calculate derivatives in complex systems.
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Thanks for your attention!

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Continuous approach: calculating the adjoint

First step: differentiate equation (2a) with respect to $\gamma = (\rho, \mu)$:

$$\begin{aligned} D_\gamma Lu &= D_\rho Lu + D_\mu Lu \\ &= 0 \qquad (D_\gamma g = 0) \end{aligned}$$

$$\begin{aligned} D_\rho Lu &= \rho' \frac{\partial^2 u}{\partial t^2} + \rho \frac{\partial^2}{\partial t^2}(D_\rho u) \\ &\quad - \nabla \cdot (\mu \nabla (D_\rho u)) \end{aligned}$$

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Continuous approach: calculating the adjoint

Second step: multiply (11) by a test function v and integrate over $\Omega \times [0, T]$.

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\begin{aligned}
\int_\Omega \int_0^T v D_\gamma(Lu)\,dtdV = & \\
& \int_\Omega \int_0^T v\rho(x)' \frac{\partial^2 u}{\partial t^2} dtdV && (12)\\
& - \int_\Omega \int_0^T v\nabla \cdot (\mu'(x)\nabla u) dtdV && (13)\\
& + \int_\Omega \int_0^T v\rho(x) \frac{\partial^2}{\partial t^2}(D_\gamma u) dtdV && (14)\\
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Continuous approach: calculating the adjoint

Applying integration by parts to each term and fixing boundary and initial conditions to the test function v, gives us:

$$\begin{aligned}
\int_\Omega \int_0^T D_\gamma u \cdot (\rho \frac{\partial^2 v}{\partial t^2} - \nabla \cdot (\mu \nabla v)) dtdV \\
- \int_\Omega \int_0^T \rho' \frac{\partial u}{\partial t} \frac{\partial v}{\partial t} dtdV \\
+ \int_\Omega \int_0^T \mu' \nabla u \cdot \nabla v dtdV &= 0 \\
v &= 0, \qquad \partial\Omega_1 \times [0, T] \\
\frac{\partial v}{\partial n} &= 0, \qquad \partial\Omega_2 \times [0, T] \\
v(x, T) = \frac{\partial v}{\partial t}(x, T) &= 0, \qquad \Omega \times T
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Discrete approach: calculating λ

Relative to the problem (1), we define the Lagrangian as:

$$L(\gamma, s) = J(\gamma, s) - \lambda^T C(\gamma, s) \tag{16}$$

If appropriate conditions are met (continuity and differentiability), we can discretize $J(\gamma, s)$ and $C(\gamma, s)$, and write the Karush-Kuhn-Tucker conditions for the discretized problem:

$$\begin{aligned} \nabla L(\gamma, s) &= 0 \qquad (17) \\ C(\gamma, s) &= 0 \qquad (18) \end{aligned}$$

or equivalently:

$$\begin{aligned} \nabla_\gamma J(\gamma, s) - (\lambda_\gamma)^T \nabla_\gamma C(\gamma, s) &= 0 \qquad (19) \\ \nabla_s J(\gamma, s) - (\lambda_s)^T \nabla_s C(\gamma, s) &= 0 \qquad (20) \\ C(\gamma, s) &= 0 \qquad (21) \end{aligned}$$

Discrete approach: calculating λ

Let's consider that the state variables s depend on the design variables γ, ie, $s(\gamma) : D \subset \mathbb{R}^{d_\gamma} \rightarrow \mathbb{R}^{d_s}$, then, the cost function J can be written:

$$j(\gamma) = J(\gamma, s(\gamma)) \tag{22}$$

and the derivative of the state equation with respect of γ is:

$$\underbrace{\nabla_\gamma C(\gamma, s(\gamma))}_{d_C \times d_\gamma} + \underbrace{\nabla_s C(\gamma, s(\gamma))}_{d_C \times d_s} \underbrace{\nabla_\gamma s(\gamma)}_{d_s \times d_\gamma} = 0 \tag{23}$$

If $d_C = d_s$ holds (number of state equations equal to the number of state variables) and assuming that $\nabla_s C(\gamma, s(\gamma))$ is invertible, it follows that:

$$\nabla_\gamma s(\gamma) = -\left(\nabla_s C(\gamma, s(\gamma))\right)^{-1} \nabla_\gamma C(\gamma, s(\gamma)) \tag{24}$$

Discrete approach: calculating λ

Derivating j we get:

$$D_\gamma j(\gamma) \quad = \quad \nabla_\gamma J(\gamma, s(\gamma)) + \nabla_s J(\gamma, s(\gamma)) \nabla_\gamma s(\gamma) \qquad (25)$$

and replacing (24) into (25), and using the equation (20) from the KKT system in order to define $\nabla_s J$, it follows:

$$\begin{aligned} D_\gamma j(\gamma) &= \nabla_\gamma J(\gamma, s(\gamma)) - \nabla_s J(\gamma, s(\gamma)) \left(\nabla_s C(\gamma, s(\gamma))\right)^{-1} \nabla_\gamma C(\gamma, s(\gamma)) \\ &= \nabla_\gamma J(\gamma, s(\gamma)) - \lambda_s^T \nabla_s C(\gamma, s(\gamma)) \left(\nabla_s C(\gamma, s(\gamma))\right)^{-1} \nabla_\gamma C(\gamma, s(\gamma) \\ &= \nabla_\gamma J(\gamma, s(\gamma)) - \lambda_s^T \nabla_\gamma C(\gamma, s(\gamma)) \end{aligned} \qquad (26)$$

[GP97],[Pir84],[Bre92],[Eva10],[Jam88],[HVKD08], [Fie98],[FBI06]