Calculating Derivatives (§8 in part)

Finite difference approximation
(Automatic differentiation) (e.g. ADIFOR)
Adjoint state method (not in book, see "Computational methods for inverse problems", Vogel)

Finite difference approx

$g : \mathbb{R} \to \mathbb{R}$ want $g'(x) = \lim_{h \to 0} \dfrac{g(x+h) - g(x)}{h}$

For small h:

$$g'(x) \approx \frac{g(x+h) - g(x)}{h}$$

Taylor:

$$g(x+h) - g(x) - g'(x)h = \frac{1}{2} h^2 g''(x+th) \quad \text{for some } t \in (0,1)$$

$$\to \left| \frac{g(x+h) - g(x)}{h} - g'(x) \right| \le \frac{L}{2} |h|$$

if $g''(x)$ is bounded in a neighborhood of x.

So in principle: smaller $h \Rightarrow$ better approx.
However this changes when we have error in function eval.

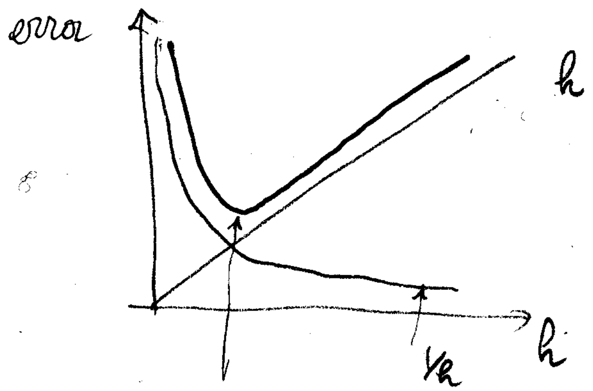
$g(x) \rightsquigarrow g_\varepsilon(x)$, where $|g(x) - g_\varepsilon(x)| < \varepsilon$ (ε = floating pt error for example)

$$\Rightarrow \left| g'(x) - \frac{g_\varepsilon(x+h) - g_\varepsilon(x)}{h} \right|$$

$$\le \left| g'(x) - \frac{g(x+h) - g(x)}{h} \right| + \left| \frac{(g_\varepsilon(x+h) - g(x+h)) - (g_\varepsilon(x) - g(x))}{h} \right|$$

$$\le \frac{Lh}{2} + \frac{2\varepsilon}{h}$$

Typical behavior



$h^* = O(\sqrt{\varepsilon})$

This gives a constant error term. $\delta_k \sim \sqrt{\varepsilon}$ in inexact Newton's method theory.

$\rightsquigarrow$ The best precision we can get is $O(\sqrt{\varepsilon})$

(so if ε = machine precision $\approx 10^{-16}$, $\sqrt{\varepsilon} = 10^{-8}$)

Approximating the gradient: Forward difference.

$$\nabla f(x) = \begin{bmatrix} \frac{\partial f}{\partial x_1}(x) \\ \frac{\partial f}{\partial x_2}(x) \\ \vdots \\ \frac{\partial f}{\partial x_n}(x) \end{bmatrix} \qquad \frac{\partial f}{\partial x_i}(x) = \frac{f(x+he_i) - f(x)}{h} + O(h)$$

cost: n function evaluations.

Central differences:

$$\frac{\partial f}{\partial x_i}(x) = \frac{f(x+he_i) - f(x-he_i)}{2h} + O(h^2)$$

cost: $2n$ function eval

proof:

$$f(x+he_i) = f(x) + h\frac{\partial f}{\partial x_i}(x) + \frac{1}{2}h^2\frac{\partial^2 f}{\partial x_i^2} + O(h^3)$$

$$f(x-he_i) = f(x) - h\frac{\partial f}{\partial x_i}(x) + \frac{1}{2}h^2\frac{\partial^2 f}{\partial x_i^2} + O(h^3)$$

Similarly Hessian can be approximated as:

$$\nabla^2 f(x)\, p = \frac{\nabla f(x+hp) - \nabla f(x)}{h} + O(h)$$ FWD differences (cost: 1 grad eval)

$$= \frac{\nabla f(x+hp) - \nabla f(x-hp)}{h} + O(h^2)$$ Central differences (cost: 2 grad eval)

Adjoint state method (abstract formulation) (a.k.a. Costate method)

$$A(q)\, u = f$$

$A(q)$ = lin operator depending on q, $\in \mathcal{L}(\mathcal{U}, \mathcal{U})$

u = state variable $\in \mathcal{U}$

q = parameter $\in \mathcal{Q}$

Observations (data) $d = Cu + \eta$, C = linear state-to-observation map

$d \in \mathcal{Y}$ = observation space

η = noise

we would like to compute derivatives for the NL least squares problem:

$$\min_{u \in \mathcal{U},\, q \in \mathcal{Q}} \frac{1}{2} \| Cu - d \|^2_{\mathcal{Y}} + \dots$$

s.t. $A(q)u = f$

$\Longleftrightarrow$ if $A(q)u = f$ is a well-posed problem

$$\min_{q \in \mathcal{Q}} \underbrace{\frac{1}{2} \| F(q) - d \|^2_{\mathcal{Y}} + \dots}_{J(q)}$$

where $F : \mathcal{Q} \to \mathcal{Y}$ is the parameter-to-data map.

$$F(q) = C A(q)^{-1} f$$

First notice that:

$$A(q)\, A(q)^{-1} = I$$

$$\frac{d}{dq}\left(A(q)\, A(q)^{-1} \right) = 0$$

$$\frac{dA}{dq} A(q)^{-1} + A(q)\, \frac{d A(q)^{-1}}{dq} \quad \Rightarrow \quad \boxed{\frac{dA(q)^{-1}}{dq} = -A(q)^{-1} \frac{dA}{dq} A(q)^{-1}}$$

$\frac{dA(q)}{dq}$ (or also denoted $D_q A[q]$) $\in \mathcal{L}(Q, \mathcal{L}(\mathcal{U}, \mathcal{U}))$

= linear operator approximating $A(\cdot)$ i.e.

$$A(q + \delta q) = A(q) + D_q A[q]\, \delta q + o(\delta q).$$

= Fréchet derivative of $A(q)$ w.r.t. q.

let $J(q) = \frac{1}{2} \| \underbrace{F(q) - d}_{r(q)} \|_{\mathcal{Y}}^2$

$$\left(\nabla J(q), \delta q \right)_Q = \left(\frac{dF}{dq} \delta q, r(q) \right)_{\mathcal{Y}} \quad]^{(*)}$$

$$= \left(-C\, A(q)^{-1} \left(\frac{dA}{dq} \delta q \right) A(q)^{-1} f, r(q) \right)_{\mathcal{Y}}$$

$$= -\left(\left(\frac{dA}{dq} \delta q \right) \underbrace{A(q)^{-1} f}_{\text{fwd problem}}, \underbrace{A^*(q)^{-1} C^* r(q)}_{\text{adjoint problem}} \right)_{\mathcal{U}}$$

If $A(q) u = f$ FWD
$A^*(q) z = -C^* r(q)$ adjoint

The bulk of the cost: do 2 solves.
Typically adjoint problem cost ~ FWD problem cost

$$\boxed{\Rightarrow \quad \left(\nabla J(q), \delta q \right)_Q = \left(\left(\frac{dA}{dq} \delta q \right) u, z \right)_{\mathcal{U}}}$$

((*) $F(q) = C\, A(q)^{-1} f \qquad \frac{dF}{dq} \delta q = C \left[\frac{d A(q)^{-1}\delta q}{dq} \right] f$)

Why is the Adjoint state computation cheaper?

Imagine we have discretized our problem and $q \in Q = \mathbb{R}^n$ is the parameter space.

Then

$$\left(\nabla J(q), \underset{\substack{i\text{th-canonical}\\ \text{basis vector}}}{e_i}\right) = \left(\underbrace{\left(\frac{dA}{dq} e_i\right)}_{\substack{\text{Can be computed}\\ \text{ahead of time}}} \overset{\text{FWD solve}}{u}, \overset{\text{Adjoint solve.}}{z}\right)_u$$

Fréchet derivative supplement

Def: $f: \mathcal{X} \to \mathcal{Y}$, ($\mathcal{X}, \mathcal{Y}$ = Banach spaces) is Fréchet differentiable iff there is a bounded linear operator:

$$Df[x]: \mathcal{X} \to \mathcal{Y} \text{ s.t.}$$

$$\lim_{h \to 0} \frac{\| f(x+h) - f(x) - Df[x]h \|}{\| h \|} = 0$$

or in other words:

$$f(x+h) = f(x) + Df[x]h + o(h)$$

Useful properties:

- Fréchet derivative of a linear functional:

  If $f \in \mathcal{L}(\mathcal{X}, \mathcal{Y})$ (i.e. $f: \mathcal{X} \to \mathcal{Y}$ is a bounded lin. op.)

  then $Df[x] = f$ (derivative is function itself)

  proof: $f(x+h) = f(x) + f(h)$
  $= f(x) + Df[x]h$

- Chain rule

  If $f: \mathcal{U} \to \mathcal{Y}$, $g: \mathcal{X} \to \mathcal{U}$ are Fréchet differentiable then so is $f \circ g: \mathcal{X} \to \mathcal{Y}$, $x \to f(g(x))$ and $\boxed{D(f \circ g)[x] = Df[g(x)]\, Dg[x]}$

Electrical Impedance Tomography (EIT: project problem)

PDE modeling DC conduction of electricity is:

$$(*)\quad \boxed{\begin{cases} \nabla\cdot[\sigma\nabla u]=0 & x\in\Omega \\ -\sigma n(x)\cdot\nabla u = I(x) & x\in\partial\Omega \end{cases}}$$

here:

$u(x)$ = potential inside Ω

$\sigma(x)$ = electric conductivity in Ω

$\sigma\nabla u$ = current distribution in Ω (so $\nabla\cdot[\sigma\nabla u]=0$ means no sources or sinks of currents inside Ω)

$\sigma n\cdot\nabla u$ = current density exiting Ω.

In order for $(*)$ to make sense physically, we must require that all currents that enter Ω must leave Ω:

$$\boxed{\int_{\partial\Omega} I(x)\, dS_x = 0}$$

There are infinitely many solutions to $(*)$: if u solves $(*)$ then $u+c$ ______, $\forall c\in\mathbb{R}$.

We choose solution for which:

$$\boxed{\int_{\partial\Omega} u(x)\, dS_x = 0} \quad \text{(grounding condition)}$$

Project problem:

Given $u^{(1)}, u^{(2)}, \dots, u^{(n_{exp})}$ on $\partial\Omega$ = measured voltages arising from $I_1, I_2, \dots, I_{n_{exp}}$ known currents, estimate σ.

Non Linear Least Squares formulation: Find σ that solves

$$\min_{\sigma} \frac{1}{2}\sum_{k=1}^{n_{exp}} \int_{\partial\Omega} \left| u(x;\sigma,I_k) - u^{(k)}_{(x)}\right|^2 + J_{reg}(\sigma)$$

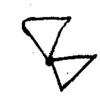
Here $J_{reg}(\sigma)$ is a regularization term that ensures the minimization can be solved. Example:

$$J_{reg}(\sigma) = \alpha \, \frac{1}{2} \int_{\Omega} |\sigma(x)|^2 \, dx .$$

where α is a parameter that weights how much importance we give to the regularization.
(α large: smoother more regularized solution
α small: trust more the data fit term)

Finite Element discretization

Divide Ω into n_t triangles T_k



where: $T_j \cap T_k$ = one point $\Rightarrow$ common vertex

$T_j \cap T_k$ = one edge $\Rightarrow$ common edge

Let x_j = the vertices of the triangles
n_v = # vertices

Define function $\varphi_j(x)$ which are linear on each triangle s.t.

$$\varphi_j(x_i) = \delta_{ij} = \begin{cases} 1 & i = j \\ 0 & i \neq j \end{cases} \qquad j = 1 \dots n_v$$

Define

$$\psi_j(x) = \chi_{T_j}(x) = \begin{cases} 1 & \text{if } x \in T_j \\ 0 & \text{otherwise} \end{cases} \qquad j = 1 \dots n_t .$$

We approximate potential by

$$u_h(x) = \sum_{j=1}^{n_v} u_j \varphi_j(x) \rightarrow \underline{u} = (u_1, \dots, u_{n_v}) \in \mathbb{R}^{n_v}$$

And conductivity by

$$\sigma_h(x) = \sum_{j=1}^{n_t} \sigma_j \psi_j(x) \rightarrow \underline{\sigma} = (\sigma_1, \dots, \sigma_{n_t}) \in \mathbb{R}^{n_t}$$

Multiply (*) on both sides by φ_i and integrate over Ω:

$$\int_\Omega \nabla\cdot[\sigma\nabla u]\,\varphi_i\,dx = 0$$

|| Green's theorem (~ IBP)

$$\int_{\partial\Omega} \sigma\nabla u\cdot\underline{n}\,\varphi_i - \int_\Omega \sigma(x)\,\nabla u\cdot\nabla\varphi_i\,dx$$

$$= \int_{\partial\Omega} -I(x)\,\varphi_i(x)\,dx - \int_\Omega \sigma\,\nabla u\cdot\nabla\varphi_i\,dx$$

Since $u(x)\simeq u_h(x) = \sum_{j=1}^{n_v} u_j\varphi_j(x)$

$$\sum_{j=1}^{n_v} u_j \int_\Omega \sigma\,\nabla\varphi_j\cdot\nabla\varphi_i\,dx = -\int_{\partial\Omega} I(x)\,\varphi_i(x)\,dx \;, \quad i=1\dots n_v.$$

$\Leftrightarrow$ linear system

(1) $$\boxed{A(\underline{\sigma})\,\underline{u} = \underline{I}}$$ where:

$$A(\underline{\sigma})\in\mathbb{R}^{n_v\times n_v},\quad (A(\underline{\sigma}))_{ij} = \int_\Omega \sigma\,\nabla\varphi_i\cdot\nabla\varphi_j\,dx$$

$$\underline{u} = (u_1,\dots,u_{n_v})$$

$$\underline{I} = -\left(\int_{\partial\Omega} I(x)\,\varphi_1(x)\,dx,\dots,\int_{\partial\Omega} I(x)\,\varphi_{n_v}(x)\,dx\right)$$

System (1) is singular:

$$A(\underline{\sigma})\,\underline{e} = \underline{0}\,,\quad \underline{e} = (1,\dots,1).$$

since:

$$(A(\underline{\sigma})\,\underline{e})_i = \sum_{j=1}^{n_v}\int_\Omega \sigma(x)\,\nabla\varphi_j(x)\cdot\nabla\varphi_i(x)\,dx$$

$$= \int_\Omega \sigma(x)\,\nabla\Big(\underbrace{\cancel{\sum_{j=1}^{n_v}\varphi_j(x)}}_{=1}\Big)\cdot\nabla\varphi_i(x)\,dx = 0.$$

$\Rightarrow$ $\ker A(\sigma) = \operatorname{span}\{e\}$

But system (1) has infinitely many solutions because:

$$\underline{I} \in \text{range } A(\sigma) = \text{null}(A(\sigma)^T)^\perp = \{\underline{e}\}^\perp$$

Indeed:

$$\underline{I}^T \underline{e} = \sum_{j=1}^{m_N} \int_{\partial\Omega} I(x)\,\varphi_j(x)\,dx = \int_{\partial\Omega} I(x) \underbrace{\Big(\sum_{j=1}^{m_N} \varphi_j(x)\Big)}_{=1} dx$$
$$= 0.$$

We pick solution for which:

$$(2) \quad \int_{\partial\Omega} \Big(\sum_{j=1}^{m_N} \varphi_j(x)\, u_j\Big) dx = \sum_{j=1}^{m_N} \int_{\partial\Omega} \varphi_j(x)\,dx\; u_j = 0$$

Since $A(\underline{\sigma})\,\underline{e} = 0$, we can eliminate one equation (say last one) and replace it by (2):

we get $\mathbb{L}(\underline{\sigma})\,\underline{u} = \underline{I}$, which is invertible

<u>Discretization of obj. function</u>: (misfit part only)

$$J_{LS}(\sigma) = \frac{1}{2}\int_{\partial\Omega} \left(u(x;\sigma,I^k) - u^{(k)}(x)\right)^2 = \sum_{i,j=1}^{m_N} (u_i - u_i^{(k)})\, Q_{ij}\, (u_j - u_j^{(k)})$$

using discretization

$$= (\underline{u} - \underline{u}^{(k)})^T Q\, (\underline{u} - \underline{u}^{(k)})$$

where $Q_{ij} = \int_{\partial\Omega} \varphi_i(x)\,\varphi_j(x)\,dx$ (mass matrix)

$$\Rightarrow \quad J_{LS}(\sigma) = \frac{1}{2}\left\| Q^{1/2}(\underline{u} - \underline{u}^{(k)}) \right\|_2^2$$

as Q is positive definite

proof:

$$v^T Q v = \int_{\partial\Omega} \sum_{j=1}^{m_N} v_j\,\varphi_j(x) \sum_{i=1}^{m_N} v_i\,\varphi_i(x)\,dx$$
$$= \int_{\partial\Omega} \Big(\sum_{j=1}^{m_N} v_j\,\varphi_j(x)\Big)^2 dx \geq 0$$

$\Rightarrow Q$ pos semi def

and

$$v^T Q v = 0 \Rightarrow \int_\Omega \left(\sum_{j=1}^{n_v} v_j \varphi_j(x) \right)^2 dx = 0$$

$$\Rightarrow \sum_{j=1}^{n_v} v_j \varphi_j(x) = 0 \Rightarrow v_j = 0, \; j = 1 \ldots n_v$$

Gradient computation with the Adjoint state method

CONTINUUM | **DISCRETE**

Objective function (one experiment only for simplicity)

CONTINUUM:

$$J(\sigma) = \frac{1}{2} \| F(\sigma) - V \|^2_{L^2(\partial\Omega)}$$

where V = measured voltages

$F(\sigma) = u|_{\partial\Omega}$ where u solves FORWARD problem

$$\begin{cases} \nabla \cdot [\sigma \nabla u] = 0 \\ -\sigma \nabla u \cdot n = I \end{cases}$$

DISCRETE:

$$J(\sigma) = \frac{1}{2} \| Q^{\frac{1}{2}} (F(\sigma) - V) \|^2$$

where $F(\sigma) = Cu$ where u solves FORWARD problem:

$$L[\sigma] u = I$$

and C is the measurements operator:

$$C = \underbrace{\left[\; \overset{\text{identity}}{I} \;\middle|\; 0 \; \right]}_{n_v} \updownarrow n_v \text{ on } \partial\Omega$$

(if boundary nodes are the first ones in the numbering of vertices)

Linearization of $F(\sigma)$:

CONTINUUM:

If δu solves:

$$\begin{cases} \nabla \cdot [\sigma \nabla \delta u] = -\nabla \cdot [\delta\sigma \nabla u] \\ \sigma \nabla u \cdot n = 0 \end{cases}$$

then

$$\delta u|_{\partial\Omega} = DF[\sigma] \delta\sigma$$

(assuming $\delta\sigma|_{\partial\Omega} = 0$)

DISCRETE:

If δu solves:

$$L[\sigma] \delta u = -L[\delta\sigma] u$$

$$\delta u = -L[\sigma]^{-1} L[\delta\sigma] L[\sigma]^{-1} I$$

then

$$C \delta u = DF[\sigma] \delta\sigma$$

(assuming $C\delta\sigma = 0$)

CONTINUUM	DISCRETE

Adjoint problem

Continuum:

$$\begin{cases} \nabla \cdot [\sigma \nabla \Psi] = 0 \\ -\sigma \nabla \Psi \cdot n = r(\sigma) \end{cases}$$

where $r(\sigma) = F(\sigma) - V$
$= u_{|\partial\Omega} - V$

Discrete:

$$L[\sigma]^T \Psi = C^T Q\, r(\sigma)$$

where $r(\sigma) = F(\sigma) - V$
$= Cu - V$

Calculation of $\nabla J(\sigma)$

Continuum:

$(\nabla J(\sigma), \delta\sigma)$

$= (DF^T[\sigma]\underbrace{(F(\sigma)-V)}_{r(\sigma)}, \delta\sigma)$

$= (DF[\sigma]\delta\sigma, r(\sigma))$

$= -\int_{\partial\Omega} \delta u\, \underbrace{\sigma \nabla\Psi\cdot n}_{=0}\, dS$

$= \int_{\partial\Omega} \Psi \sigma \nabla \delta u \cdot n - \underbrace{\delta u\, \sigma \nabla\Psi \cdot n}_{=0}\, dS$

GREEN ↓

$= \int_{\Omega} \Psi \nabla\cdot[\sigma\nabla\delta u] - \delta u \nabla\cdot[\sigma\nabla\Psi]\, dx$

$= \int_{\Omega} \Psi \nabla\cdot[\sigma\nabla\delta u]\, dx$

using lin prob ↓

$= -\int_{\Omega} \Psi \nabla\cdot[\delta\sigma \nabla u]\, dx$

$= \int_{\Omega} \delta\sigma\, \nabla\Psi\cdot\nabla u\, dx \quad - \int_{\partial\Omega} \Psi\, \underbrace{\delta\sigma}_{0}\, \nabla u\cdot n\, dS$

↑ GREEN

By identification:

$$\nabla J(\sigma) = \nabla\Psi \cdot \nabla u$$

Discrete:

$(\nabla J(\sigma), \delta\sigma)$

$= (DF^T[\sigma]\underbrace{Q^{1/2}Q^{1/2}}_{=Q}(F(\sigma)-V), \delta\sigma)$

$= (DF[\sigma]\delta\sigma, Q r(\sigma))$

$= (-C L[\sigma]^{-1} L[\delta\sigma] u, Q r(\sigma))$

$= -(L[\delta\sigma]u, L[\sigma]^{-T} C^T Q r(\sigma))$

$= (-L[\delta\sigma]u, \Psi)$

compare

Now if it is possible to write:

$$-L[\delta\sigma] = B^T \operatorname{diag}(\delta\sigma) B$$

$\Rightarrow$

$(\nabla J(\sigma), \delta\sigma) = (B^T \operatorname{diag}(\delta\sigma) B u, \Psi)$

$= (\operatorname{diag}(\delta\sigma) Bu, B\Psi)$

$= (\delta\sigma, (Bu).*(B\Psi))$

element by element mu[ltiplication]

By identification Gradient is

$$\nabla J(\delta\sigma) = (Bu).*(B\Psi)$$

Note for the continuum problem I used Green's identities:

$$\int_\Omega \nabla\cdot[\sigma u \nabla v]\,dx = \int_\Omega u\, \nabla\cdot[\sigma \nabla v] + \sigma \nabla u\cdot\nabla v \, dx$$

$$\| $$

$$\int_{\partial\Omega} \sigma u \nabla v\cdot n \, dS$$

or equivalently:

$$\int_\Omega u\, \nabla\cdot[\sigma\nabla v] - v\, \nabla\cdot[\sigma \nabla u]\,dx = \int_{\partial\Omega} \sigma u \nabla v\cdot n - \sigma v \nabla u\cdot n \, dS$$

Note 2: A summary of the adjoint computation of the gradient in the NLLSQ formulation of EIT will be posted with the project.