Recall

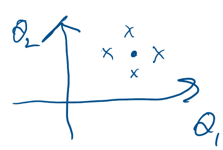
$$\frac{d\vec{s}}{dt} = \frac{\partial g}{\partial \vec{u}} \cdot \frac{\partial \vec{u}}{\partial \vec{\alpha}} + \frac{\partial g}{\partial \vec{\alpha}}, \quad \vec{s}(t_0) = \frac{\partial \vec{u}_0}{\partial \vec{\alpha}}$$

$$\frac{d\vec{s}_0}{dt} = \frac{\partial g}{\partial \vec{u}} \cdot \vec{s}_0(t), \quad \vec{s}(t_0) = 1$$

- Full System for Calculating ODE Sensitivity

$$\boxed{\begin{aligned}
&\frac{d\vec{u}}{dt} = g(t, \vec{u}, \vec{\alpha}), && \vec{u}(t_0) = \vec{u}_0 \\
&\frac{d\vec{s}}{dt} = \frac{\partial g}{\partial \vec{u}} \cdot \vec{s}(t) + \frac{\partial g}{\partial \vec{\alpha}}, && \vec{s}(t_0) = \left.\frac{\partial g}{\partial u}\right|_{t=t_0}, \quad \vec{s}(t) = \frac{\partial \vec{u}}{\partial \vec{\alpha}} \\
&\frac{d\vec{s}_0}{dt} = \frac{\partial g}{\partial \vec{u}} \vec{s}_0(t), && \vec{s}_0(t_0) = \vec{1}, \quad \vec{s}_0(t) = \frac{\partial \vec{u}}{\partial \vec{u}_0}
\end{aligned}}$$

Finite differences



- Two common approaches

FWD

$$\left.\frac{\partial f}{\partial \theta_j}\right|_{\vec{\theta}^*} \approx \frac{f(\vec{\theta}^* + \vec{e}_j h_j) - f(\vec{\theta}^*)}{h_j},$$

Cent

$$\left.\frac{\partial f}{\partial \theta_j}\right|_{\vec{\theta}^*} \approx \frac{f(\vec{\theta}^* + \vec{e}_j h_j) - f(\vec{\theta}^* - \vec{e}_j h_j)}{2h_j}$$

where $\vec{e}_j$ is a unit vector in j-th direction, $\vec{e}_j = [0 \dots 0\ 1\ 0 \dots 0]$

Complex Step Method

- Consider a complex variable $z = x + iy$, $i = \sqrt{-1}$.
  - The Cauchy-Riemann equations satisfy:

$$f(x+iy) = u(x,y) + iv(x,y) \Rightarrow \begin{cases} \frac{\partial u}{\partial x} = \frac{\partial v}{\partial y} \\ \frac{\partial u}{\partial y} = -\frac{\partial v}{\partial x} \end{cases}$$

- Note:

$$\frac{\partial u}{\partial x} = \frac{\partial v}{\partial y} = \lim_{h \to 0} \frac{v(x,y+h) - v(x,y)}{h} = \lim_{h \to 0} \frac{\mathrm{Im}[f(x+i(y+h))] - \mathrm{Im}[f(x+iy)]}{h}$$

- Now assume f is strictly real-valued, for $x \in \mathbb{R}$ so that $y=0$ & $f(x) = u(x,0)$
  - So $\mathrm{Im}[f(x)] = v(x,0) = 0$

- So, if we perturb x by ih, $x \to x+ih$

$$\Rightarrow \frac{\partial f}{\partial x} = \lim_{h \to 0} \frac{\mathrm{Im}[f(x+ih)] - \mathrm{Im}[f(x)]}{h} = \lim_{h \to 0} \frac{\mathrm{Im}[f(x+ih)]}{h}$$

* This is no longer a finite difference. *

$\boxed{\text{Notes}}$

- FD methods $\Rightarrow$ Possible cancellation errors when h is small.
- Comp. step $\Rightarrow$ No issue
- Issues Comp. Step
  - Coding complex values can be a bottleneck
  - This only holds when f is "analytic", i.e. f can be represented by a convergent power series

- ... issues | ... different magnitudes

Scaling issues

- In some applications, $\vec{y}$ or $\vec{\theta}$, have significantly different magnitudes + units.

- Two approaches

i) Unitless scaling: $\vec{S}_j^s = \dfrac{\theta_j^*}{\vec{y}|_{\vec{\theta}^*}} \dfrac{\partial f}{\partial \theta_j}\Big|_{\vec{\theta}^*}$

ii) log-scaling: if $\vec{\theta}^* > 0$, let $\vec{\theta}^*_{log} = \ln(\vec{\theta}^*)$

$$\Rightarrow \frac{\partial f}{\partial \vec{\theta}^*_{log}} = \frac{\partial f}{\partial \ln(\vec{\theta}^*)} = \theta_j^* \cdot \frac{\partial f}{\partial \theta_j}\Big|_{\vec{\theta}^*}$$

$\boxed{\text{Parameter Subset Selection}}$

- Given $\vec{S}_j = \dfrac{\partial f}{\partial \theta_j}$, we know that given $J(\theta)$ to be minimized

$$\Rightarrow J(\theta) = \frac{1}{n} \sum (y - f)^2 \Rightarrow J(\vec{\theta} + \Delta\theta) \approx \frac{1}{n}\left[\underset{\sim}{S}\Delta\vec{\theta}\right]^T\left[\underset{\sim}{S}\Delta\vec{\theta}\right]$$