

Push forward / Jvp rule of nonlinear system solve

$$f(\underline{\theta}) = \left\{ \text{solve } g(\underline{x}, \underline{\theta}) = \underline{0} \text{ for } \underline{x} \right\} =: \underline{x}$$

$$\underline{\theta} \in \mathbb{R}^p$$

$$\underline{x} \in \mathbb{R}^n$$

$$g: \mathbb{R}^n \times \mathbb{R}^p \rightarrow \mathbb{R}^n$$

$$f: \mathbb{R}^p \rightarrow \mathbb{R}^n$$

e.g. Newton-Raphson scheme

→ assume it always converges

task: forward propagate tangent information on the input $\dot{\underline{\theta}} \in \mathbb{R}^p$ to the output $\dot{\underline{x}} \in \mathbb{R}^n$

without forward-mode AD through the solver

(= unrolling / piggybacking)

in general

$$\dot{\underline{x}} = \underbrace{\frac{\partial f}{\partial \underline{\theta}}}_{\substack{\text{Jacobian} \\ \text{Jacobian-vector product}}} \dot{\underline{\theta}}$$

more precisely $\left. \frac{\partial f}{\partial \underline{\theta}} \right|_{\underline{\theta} = \underline{\theta}^*}$

$\in \mathbb{R}^{n \times p}$

because we first solved the forward / primal problem $\underline{x}^* = f(\underline{\theta}^*)$

→ total derivative of the optimality criterion

$$\frac{dg}{d\underline{\theta}} = \frac{\partial g}{\partial \underline{x}} \underbrace{\frac{\partial \underline{x}}{\partial \underline{\theta}}}_{\hat{=} \frac{\partial f}{\partial \underline{\theta}}} + \frac{\partial g}{\partial \underline{\theta}} \stackrel{!}{=} \underline{0}$$

$$\Leftrightarrow \frac{\partial f}{\partial \underline{\theta}} \hat{=} \frac{\partial \underline{x}}{\partial \underline{\theta}} = - \left(\frac{\partial g}{\partial \underline{x}} \right)^{-1} \frac{\partial g}{\partial \underline{\theta}}$$

plug back in

$$\dot{\underline{x}} = - \left(\frac{\partial g}{\partial \underline{x}} \right)^{-1} \frac{\partial g}{\partial \underline{\theta}} \dot{\underline{\theta}}$$

$\underline{d} = \frac{\partial g}{\partial \underline{\theta}} \dot{\underline{\theta}}$

$$\frac{\partial g}{\partial \underline{x}} \dot{\underline{x}} = - \underline{d}$$

$$\Leftrightarrow \dot{\underline{x}} = \left\{ \begin{array}{l} \text{solve } \frac{\partial g}{\partial \underline{x}} \dot{\underline{x}} = - \underline{d} \text{ for } \dot{\underline{x}} \\ \text{with } \underline{d} = \frac{\partial g}{\partial \underline{\theta}} \dot{\underline{\theta}} \end{array} \right\}$$

Full push forward rule

$$\tilde{f}(f_1(\underline{\theta}_1), (\dot{\underline{\theta}}_1)) = ((f(\underline{\theta}),), (\dots,))$$

given the optimality criterion is differential

$$\underline{d} = \frac{\partial g}{\partial \underline{\theta}} \dot{\underline{\theta}} \quad \text{is just forward-mode AD}$$

The solution to the linear system

$$\frac{\partial g}{\partial \underline{x}} \dot{\underline{x}} = - \underline{d}$$

Can be solved with an iterative

which just needs matrix-vector products

(= matrix-free solver)

→ these can be expressed using forward-mode AD as Jacobian-vector products