Adjoint state Method for an ODE

ODE with initial value

$$\begin{cases} \frac{d\underline{u}}{dt} = \underline{f}(\underline{u}, t, \underline{\theta}) \\ \underline{u}(t=0) = \underline{u}_0 \end{cases}$$

RK 4(5)

$\underline{u}(t)$ → loss functional $J(\underline{u}; \underline{\theta})$ → Sensitivities $\frac{dJ}{d\underline{\theta}}$

implicit problem

- optimization
- local sensitivity analysis

- Dynamics & Control
- transient PDEs by method of lines
- Neural ODEs

$\underline{u}(t) \in \mathbb{R}^N$ ... solution function – time dependent

$\underline{f} \in \mathbb{R}^N$ ... right-hand side

t ... time

$\underline{\theta} \in \mathbb{R}^P$ ... collection of parameters

difference to linear / non-linear due to the time causality

loss functional

$$J(\underline{u}; \underline{\theta}) = \int_0^T g(\underline{u}; \underline{\theta})\, dt$$

e.g. quadratic loss $\underline{u}^T \underline{\underline{Q}}\, \underline{u}$

maps the entire solution function $\underline{u}(t)$ to a scalar

---

total derivative

$$\underbrace{\frac{dJ}{d\underline{\theta}}}_{\in \mathbb{R}^{1\times P}} = \int_0^T \frac{d}{d\underline{\theta}} g(\underline{u}; \underline{\theta})\, dt$$

$$= \int_0^T \underbrace{\frac{\partial g}{\partial \underline{\theta}}}_{\mathbb{R}^{1\times P}} + \underbrace{\frac{\partial g}{\partial \underline{u}}}_{\mathbb{R}^{1\times N}} \underbrace{\frac{d\underline{u}}{d\underline{\theta}}}_{\in \mathbb{R}^{N\times P}}\, dt$$

difficult → how?

→ forward

→ adjoint/backward

here: gradient is a row vector

A) Forward Sensitivity

$$\frac{d\underline{u}}{d\underline{\theta}} = \underbrace{\begin{bmatrix} \frac{d\underline{u}}{d\theta_0} & \frac{d\underline{u}}{d\theta_1} & \frac{d\underline{u}}{d\theta_2} & \cdots \end{bmatrix}}_{P \text{ columns}} \Big\} N \text{ rows}$$

take IVP: $\begin{cases} \frac{d\underline{u}}{dt} = \underline{f} \\ \underline{u}(0) = \underline{u}_0 \end{cases}$

implicitly derive wrt. $\frac{d}{d\theta_i}$

swap

$$\begin{cases} \frac{d}{d\theta_i} \frac{d\underline{u}}{dt} = \frac{d}{d\theta_i} \underline{f} \\ \frac{d\underline{u}}{d\theta_i}(0) = \frac{d\underline{u}_0}{d\theta_i} \end{cases}$$

← apply total derivative

$$\begin{cases} \frac{d}{dt} \frac{d\underline{u}}{d\theta_i} = \frac{\partial \underline{f}}{\partial \underline{u}} \frac{d\underline{u}}{d\theta_i} + \frac{\partial \underline{f}}{\partial \theta_i} \\ \frac{d\underline{u}}{d\theta_i}(0) = \frac{d\underline{u}_0}{d\theta_i} \end{cases}$$

a new system of ODEs

define $\underline{s}_i = \frac{d\underline{u}}{d\theta_i}$

$$\begin{cases} \frac{d}{dt} \underline{s}_i = \frac{\partial \underline{f}}{\partial \underline{u}} \underline{s}_i + \frac{\partial \underline{f}}{\partial \theta_i} \\ \underline{s}_i(0) = \frac{d\underline{u}_0}{d\theta_i} \end{cases}$$

solve jointly with original IVP

↳ build Jacobian $\frac{d\underline{u}}{d\underline{\theta}}$

↳ plug into integral & solve by quadrature

but we get P such systems

hence we have to solve (P+1) ODE systems

with N variables each

:(scales linearly with P

Remedy: B) Adjoint sensitivities

frame as optimization

$$\min_{\underline{\theta}} \; J(\underline{u}; \underline{\theta})$$

$$\text{s.t.} \; \frac{d\underline{u}}{dt} = \underline{f}(\underline{u}, t, \underline{\theta}) \qquad \left(\text{or } \underline{0} = \underline{f} - \frac{d\underline{u}}{dt}\right)$$

equality-constrained optimization → Lagrangian

$$\mathcal{L}(\underline{u}, \underline{\lambda}; \underline{\theta}) = J(\underline{u}; \underline{\theta}) + \int_0^T \underline{\lambda}(t)^T \left(\underline{f} - \frac{d\underline{u}}{dt}\right) dt$$

→ continuous Lagrange Multiplier $\underline{\lambda}(t) \in \mathbb{R}^N$

$$\mathcal{L} = \int_0^T g(\underline{u}; \underline{\theta}) + \underline{\lambda}(t)^T \left(\underline{f} - \frac{d\underline{u}}{dt}\right) dt$$

difficult

$$\frac{d\mathcal{L}}{d\underline{\theta}} = \int_0^T \frac{\partial g}{\partial \underline{\theta}} + \frac{\partial g}{\partial \underline{u}} \frac{d\underline{u}}{d\underline{\theta}} + \underline{\lambda}(t)^T \left(\frac{\partial \underline{f}}{\partial \underline{\theta}} + \frac{\partial \underline{f}}{\partial \underline{u}} \frac{d\underline{u}}{d\underline{\theta}} - \frac{d}{dt} \frac{d\underline{u}}{d\underline{\theta}} \right) dt$$

rearrange

integration by parts

$$\frac{d\mathcal{L}}{d\underline{\theta}} = \int_0^T \frac{\partial g}{\partial \underline{\theta}} + \underline{\lambda}(t)^T \frac{\partial \underline{f}}{\partial \underline{\theta}} + \underbrace{\left(\frac{\partial g}{\partial \underline{u}} + \underline{\lambda}(t)^T \frac{\partial \underline{f}}{\partial \underline{u}} - \underline{\lambda}(t)^T \frac{d}{dt} \right)}_{\text{make zero}} \frac{d\underline{u}}{d\underline{\theta}}\, dt$$

$$\int_0^T -\underline{\lambda}(t)^T \frac{d}{dt} \frac{d\underline{u}}{d\underline{\theta}}\, dt = \left[-\underline{\lambda}(t)^T \frac{d\underline{u}}{d\underline{\theta}}\right]_0^T + \int_0^T \left(\frac{d\underline{\lambda}}{dt}\right)^T \frac{d\underline{u}}{d\underline{\theta}}\, dt$$

$$= \underline{\lambda}(0)^T \frac{d\underline{u}}{d\underline{\theta}}(0) - \underline{\lambda}(T)^T \frac{d\underline{u}}{d\underline{\theta}}(T) + \int_0^T \left(\frac{d\underline{\lambda}}{dt}\right)^T \frac{d\underline{u}}{d\underline{\theta}}\, dt$$

plug back in

$$\frac{d\mathcal{L}}{d\underline{\theta}} = \int_0^T \frac{\partial g}{\partial \underline{\theta}} + \underline{\lambda}^T \frac{\partial \underline{f}}{\partial \underline{\theta}} + \left(\frac{\partial g}{\partial \underline{u}} + \underline{\lambda}^T \frac{\partial \underline{f}}{\partial \underline{u}} + \left(\frac{d\underline{\lambda}}{dt}\right)^T \right) \frac{d\underline{u}}{d\underline{\theta}}\, dt$$

$$+ \underline{\lambda}(0)^T \underbrace{\frac{d\underline{u}}{d\underline{\theta}}(0)}_{= \frac{d\underline{u}_0}{d\underline{\theta}}} - \underline{\lambda}(T)^T \frac{d\underline{u}}{d\underline{\theta}}(T)$$

make zero

$$\begin{cases} \frac{\partial g}{\partial \underline{u}} + \underline{\lambda}^T \frac{\partial \underline{f}}{\partial \underline{u}} + \left(\frac{d\underline{\lambda}}{dt}\right)^T = \underline{0}^T \\ \underline{\lambda}(T) = \underline{0} \end{cases}$$

apply transpose

$$\begin{cases} \left(\frac{\partial g}{\partial \underline{u}}\right)^T + \left(\frac{\partial \underline{f}}{\partial \underline{u}}\right)^T \underline{\lambda} + \frac{d\underline{\lambda}}{dt} = \underline{0} \\ \underline{\lambda}(T) = 0 \end{cases}$$

rearrange

$$\begin{cases} \frac{d\underline{\lambda}}{dt} = -\left(\frac{\partial \underline{f}}{\partial \underline{u}}\right)^T \underline{\lambda} - \left(\frac{\partial g}{\partial \underline{u}}\right)^T \\ \underline{\lambda}(T) = \underline{0} \end{cases}$$

! A terminal value problem

→ solve backwards in time

a linear system of ODEs

↳ though inhomogeneous

now we have $\frac{d\mathcal{L}}{d\underline{\theta}}$, but we wanted $\frac{dJ}{d\underline{\theta}}$

↳ they are identical

$$\mathcal{L} = J + \int_0^T \underline{\lambda}^T \underbrace{\left(\underline{f} - \frac{d\underline{u}}{dt}\right)}_{\text{always zero } \forall \underline{\theta}} dt$$

then $\frac{d}{d\underline{\theta}}$ of it is $\underline{0}^T$

$$\frac{d\mathcal{L}}{d\underline{\theta}} = \frac{dJ}{d\underline{\theta}}$$

Strategy for $\frac{dJ}{d\underline{\theta}}$

① Solve forward $\begin{cases} \frac{d\underline{u}}{dt} = \underline{f}(\underline{u}, t, \underline{\theta}) \\ \underline{u}(t=0) = \underline{u}_0 \end{cases}$

for $\underline{u}(t)$ (e.g. by RK 4(5))

② Solve backward $\begin{cases} \frac{d\underline{\lambda}}{dt} = -\left(\frac{\partial \underline{f}}{\partial \underline{u}}\right)^T \underline{\lambda} - \left(\frac{\partial g}{\partial \underline{u}}\right) \\ \underline{\lambda}(t=T) = \underline{0} \end{cases}$

for $\underline{\lambda}(t)$ (e.g. by RK 4(5))

③ Evaluate: $\frac{dJ}{d\underline{\theta}} = \int_0^T \frac{\partial g}{\partial \underline{\theta}} + \underline{\lambda}^T \frac{\partial \underline{f}}{\partial \underline{\theta}}\, dt + \underline{\lambda}(0)^T \frac{d\underline{u}_0}{d\underline{\theta}}$

(by quadrature e.g. trapezoidal rule)

→ only solve 2 ODEs

↳ scales constantly in number of parameters $\underline{\theta} \in \mathbb{R}^P$

other derivatives:

$$\frac{\partial \underline{f}}{\partial \underline{u}}, \quad \frac{\partial g}{\partial \underline{u}}, \quad \frac{\partial g}{\partial \underline{\theta}}, \quad \frac{\partial \underline{f}}{\partial \underline{\theta}}, \quad \frac{d\underline{u}_0}{d\underline{\theta}}$$

How? → Automatic Differentiation

↳ analytically