"First slides"

- Accurately calculating sensitivities of a time dependent system with regard to its initial conditions, in a computationally efficient way, requires a symplectic integrator (in our case a Runge-Kutta (RK) integrator) to find the gradient of the forward model with respect to its initial conditions.
- Bonus: If automatic differentiation is used to compute this gradient then symplectic integration is implicitly supplied

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Set up

System of ODES:

$$\dot{u} = f(u,t)$$

maybe they model some physical phenomena directly or maybe they come from a spatial discretization of a PDE: L is a differential operator:

$$L(u) = 0 \underset{\substack{\text{FEM,}\\ \text{FD,}\\ \text{etc.}}}{\Longrightarrow} \dot{u} = f(u,t)$$

Goal:

- Integrate forward in time
- Find sensitives of solutions with respect to initial conditions $u(t_0) = \Omega$

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with this as the goal we now examine 3 different topics and connect them into our orginal statement:

- Rk methods
- Symplectic integrators
- Adjoint methods

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RK 2nd order accuracy conditions

Take the taylor expansion (TE) of $u(t+h)$:

$$u(t+h) = u(t) + hf + \frac{h^2}{2}\left[f_t + f_y f\right] + O(h^3)$$

Take the TE of the numerical method plugged into the solution.

Assume derivative evaluation for RK scheme is:

$$F(u, t, a, b, c) = b_1 f + b_2 f(a_{21} h_n f u, \; t + c_2 h)$$

then:

$$\bar{u}(t+h) = u(t) + (b_1 + b_2) h f + b_2 h^2 \left[c_2 f_t + a_{21} f_y f\right] + O(h^3)$$

- subtract the two:

$$u(t+h) - \bar{u}(t+h) = h(1 - b_1 - b_2) + h^2\left[(\tfrac{1}{2} - c_2 b_2) f_t + (\tfrac{1}{2} - a_{21} b_2) f_y f\right] + O(h^3)$$

zeroing out as much as we can in truncation error:

$$1 - b_1 - b_2 = 0 \Rightarrow b_1 + b_2 = 1$$

$$\frac{1}{2} - c_2 b_2 = 0 \Rightarrow c_2 b_2 = \frac{1}{2}$$

$$\frac{1}{2} - a_{21} b_2 = 0 \Rightarrow a_{21} b_2 = \frac{1}{2}$$

Under determined non-linear system. This is important because...

"back to slides"

How to find $Q(u)$, called the first integral:

From the slides the point is Q is invarient in time so: in the 2D case, now x and y are the solution:

$$\dot{Q}(x,y) = 0 \Rightarrow \frac{\partial Q}{\partial x}\underbrace{\boxed{\dot{x}}}_{\text{know}} + \frac{\partial Q}{\partial y}\underbrace{\boxed{\dot{y}}}_{\text{known}} = 0$$

↑

non-linear PDE, this is hard...

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3 important examples:

1. Linear 2D orbitals

There are only 6 qualitatively different phase portraits for 2D linear systems and only 1 is conservative, when

$$\dot{x} = A x \qquad \text{where } a_{ij} = -a_{ji} \text{ (skew-symmetric)}$$

if A isn't skew symmetric it could be converted to a skew-symmetric matrix with the transformation:
→ canonical form

$$x = S y$$

So that the system is:

$$\dot{y} = S^{-1} A S y \quad \text{whe } S^{-1}AS \text{ is skew symmetric.}$$

Now to show conservation:

$$(y^T y)_t = \dot{y}^T y + y^T \dot{y} = y^T (S^{-1}AS)^T y + y^T(S^{-1}AS)y =$$

$$-y^T A y + y^T A y = 0$$

Since $x = Sy$ then $(y^T y) = (S^{-1}x)^T S^{-1}x)$ $\cancel{x}S^{-1T}S^{-1}x = C = Q(x)$

2. Non-linear example: (Purely constructed for example)

$$\dot{x} = -y(1-x^2-y^2)$$
$$\dot{y} = x(1-x^2-y^2)$$

"show slide"

NL PDE for this:

$$\frac{\partial Q}{\partial x}\left(-y\,(1-x^2-y^2)\right) + \frac{\partial Q}{\partial y}\left(x(1-x^2+y^2)\right) = 0$$

looks like harmonic oscillator so guess a invariant that looks like kinetic plus potential energy:

$$Q(x,y) = ax^2 + by^2 + Cxy$$

Plugging into PDE we get:

$$2\boxed{a}xy(1-x^2-y^2) - \boxed{c}y^2(1-x^2-y^2) + 2\boxed{b}xy(1-x^2-y^2) + \boxed{c}x^2((1-x^2-y^2)$$

so $a=b$ and $c=0$ and $Q(x,y) = x^2+y^2$

3. predator prey model (Lotka-volterra)

$$\dot{x} = x(1-y)$$
$$\dot{y} = y(x-1)$$

seperation of variables:

look at variation of x interms of y:

$$\frac{\partial x}{\partial y} = \frac{x(1-y)}{y(x-1)} \Rightarrow \frac{(x-1)}{x}\partial x = \frac{(1-y)}{y}dy \Rightarrow \int \frac{x-1}{x}dx = \int \frac{(1-y)}{y}\partial y \Rightarrow$$

$$x - \log x + c_1 = \log(y) - y + c_2 \Rightarrow Q(x,y) = x - \log x - \log y + y = C$$

"show slide"

This is not quadratic and is non-linear

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now understand conservation, back to symplecticness:

Symplectic integrators conserve quadratic invariants.

Example - Forward-Euler isn't symplectic:

$$u_{n+1} = u_n + h f(u_n, t_n)$$

a, b, c coefficients are, $b_1 = 1$

So "see slides": $-1(0) + -1(0) - 1 \neq 0$

Additionally we can check that it doesn't conserve $Q(x,y)$ for the harmonic oscillator: Euler for HO:

$$x_{n+1} = x_n - h y_n$$
$$y_{n+1} = y_n + h x_n$$

Compute the difference of Q between timesteps:

$$Q(x_{n+1}, y_{n+1}) - Q(x_n, y_n) =$$

$$(x_n - h y_n)^2 + (y_n + h x_n)^2 - (x_n^2 + y_n^2) = h^2 (x_n^2 + y_n^2)$$

So energy grows with h^2.

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is symplectic - leap frog method:

$c_1 = \frac{1}{2}$, $a_{11} = \frac{1}{2}$, $b_2 = 1$

Part 3: Adjoint methods

Goal: Find sensativities of u in direction ω with respect to η

where $\dot{u} = f(u,t)$

Method 1: sensativity equations

let:

$\bar{u}(t_0) = \alpha + \eta$ be the perturbed initial condition

$\bar{u}(t) \approx u(t) + \delta(t)$ be the perturbed solution

linear perturbation

linearize the ode's and solve for the perturbation with:

$$\dot{\delta} = \left(\frac{\partial f}{\partial u}\bigg|_{u=u(t)} \right) \delta = J(u(t))\,\delta$$

$$\delta(t_0) = \eta$$

Solve this system along with $\dot{u} = f(u,t)$ and look at $\omega^T \delta(t_0 + T)$ for different η. Needs new integration each time.

Method 2: Adjoint equations

without motivation define: Hold on with me, this is one of those math tricks...

$$\dot{\lambda} = -\left(\frac{\partial f}{\partial u}\Big|_{u=u(t)}\right)^T \lambda = -J(u(t))^T \lambda$$

we define λ this way specifically because

$$(\lambda^T \delta)_t = \dot{\lambda}^T \delta + \lambda^T \dot{\delta} = (-J^T \lambda)^T \delta + \lambda^T J \delta =$$
$$-\lambda^T J \delta + \lambda^T J \delta = 0$$

so $\lambda^T \delta$ is conserved in time that is:

$$\lambda(t_0+T)^T \delta(t_0+T) = \lambda(t_0)^T \delta(t_0)$$

Now here is the trick to evalutate $w^T \delta(t_0+T)$:

set $\lambda(t_0+T) = w$ as a final condition, because of the conservation property we can also evaluate this as:

$$w^T \delta(t_0+T) = \lambda(t_0+T)^T \delta(t_0+T) = \lambda(t_0)^T \delta(t_0) = \lambda(t_0)^T \eta$$

This means we want to solve the adjoint equation with final condition $\lambda(t_0+T) = w$ backwards in time to eval $\lambda(t_0)^T \eta$.

Now consider all together:

$$\begin{bmatrix} u \\ \delta \\ \lambda \end{bmatrix}_t = \begin{bmatrix} f(u,t) \\ J\delta \\ -(J)^T \lambda \end{bmatrix}$$

Since $(\lambda^T \delta)_T = 0$ this is a quadratic invariant and should by integrated with a SRK