Notes

Solving Nonlinear Systems

- Most thoroughly explored in the context of optimization
- For systems arising in implicit time integration of stiff problems:
  - Must be more efficient than taking k substeps of an explicit method ruling out e.g. fixed point iteration
  - But if we have difficulties converging (a solution might not even exist!) we can always reduce time step and try again
- Thus Newton's method is usually chosen

Newton's method

- Start with initial guess y_0 at solution (e.g. current y) of F(y)=0
- Loop until converged:
  - Linearize around current guess: $F(y_k+\Delta y) \approx F(y_k) + dF/dy\ \Delta y$
  - Solve linear equations: $dF/dy\ \Delta y = -F(y_k)$
  - Line search along direction Δy with initial step size of 1

Variations

- Just taking a single step of Newton corresponds to "freezing" the coefficients in time: sometimes called "semi-implicit"
  - Just a linear solve, but same stability according to linear analysis
  - However, usually nonlinear effects cause worse problems than for fully implicit methods
- In between: keep Jacobian dF/dy constant but iterate as in Newton
- And endless variations on inexact Newton

Second order systems

- One of the most important time differential equations is F=ma, 2nd order in time
- Reduction to first order often throws out useful structure of the problem
- In particular, F(x,v) often has special properties that may be useful to exploit
  - E.g. nonlinear in x, but linear in v: mixed implicit/explicit methods are natural
- We'll look at Hamiltonian systems in particular

Hamiltonian Systems

- For a Hamiltonian function H(p,q), the system:

$$\frac{dp}{dt} = \frac{\partial H}{\partial q}$$

$$\frac{dq}{dt} = -\frac{\partial H}{\partial p}$$

- Think q=positions, p=momentum (mass times velocity), and H=total energy (kinetic plus potential) for a conservative mechanical system

Conservation

- Take time derivative of Hamiltonian:

$$\frac{dH}{dt} = \frac{\partial H}{\partial p}\frac{dp}{dt} + \frac{\partial H}{\partial q}\frac{dq}{dt}$$
$$= -\frac{\partial H}{\partial p}\frac{\partial H}{\partial q} + \frac{\partial H}{\partial q}\frac{\partial H}{\partial p} = 0$$

- Note H is generally like a norm of p and q, so we're on the edge of stability: solutions neither decay nor grow
  - Eigenvalues are pure imaginary!

The Flow

- For any initial condition (p,q) and any later time t, can solve to get p(t), q(t)
- Call the map $\Phi_t(p,q) = (p(t),q(t))$ the "flow" of the system
- Hamiltonian dynamics possess flows with special properties

Area in 2D

- What is the area of a parallelogram with vector edges (u_1,u_2) and (v_1,v_2)?

$$\begin{aligned}\text{area}(u,v) &= u \times v \\ &= u_1 v_2 - u_2 v_1 \\ &= \begin{pmatrix} u_1 & u_2 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} \\ &= u^T J v\end{aligned}$$

Area-preserving linear maps

- Let A be a linear map in 2D: x'=Ax
  - A is a 2x2 matrix
- Then A is area-preserving if the area of any parallelogram is equal to the area of the transformed parallelogram:

$$u'^T J v' = u^T J v$$
$$u^T A^T J A v = u^T J v$$
$$A^T J A = J$$

Symplectic Matrices

- We can generalize this to any even dimension
- Let

$$J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}$$

- Then matrix A is symplectic if $A^T J A = J$
- Note that $u^T J v$ is just the sum of the projected areas

Symplectic Maps

- Consider a nonlinear map $y' = \Phi(y)$
- Assume it's adequately smooth
- At a given point, infinitesimal areas are transformed by Jacobian matrix:

$$A(y) = \frac{\partial \Phi}{\partial y}$$

- Map is symplectic if its Jacobian is everywhere a symplectic matrix
  - Area (or summed projected area) is preserved

Hamiltonian Flows

- Let's look at Jacobian of a Hamiltonian flow

$$y = \begin{pmatrix} p \\ q \end{pmatrix} \qquad \Phi_t(y_0) = y(t)$$

$$\frac{dy}{dt} = J^{-1}\frac{\partial H}{\partial y} \qquad \frac{\partial \Phi_t}{\partial t}(y_0) = \frac{dy}{dt}(t) = J^{-1}\nabla H\left(\Phi_t(y_0)\right)$$

$$\frac{\partial}{\partial t}\nabla\Phi_t(y_0) = J^{-1}\,\nabla\nabla H\left(\Phi_t(y_0)\right)\nabla\Phi_t(y_0)$$

$$\frac{\partial A}{\partial t} = J^{-1}\,\nabla\nabla H\;A$$

- Important point: ∇∇H, the Hessian, is symmetric.

Hamiltonian Flows are Symplectic

- Theorem: for any fixed time t, the flow of a Hamiltonian system is symplectic
  - Note at time 0, the flow map is the identity (which is definitely symplectic)
  - Differentiate A^TJA:

$$\frac{\partial}{\partial t}\left(A^T JA\right) = \frac{\partial A^T}{\partial t}JA + A^T J\frac{\partial A}{\partial t} = \ldots = 0 = \frac{\partial J}{\partial t}$$

Trajectories

- Volume preservation:
  - if you start off a set of trajectories occupying some region, that region may get distorted but it will maintain its volume
- General ODE's usually have sources/sinks
  - Trajectories expand away or converge towards a point or a manifold
  - Obviously not area preserving
- General ODE methods don't respect symplecticity: area not preserved
  - In long term, the trajectories have the wrong behaviour

Symplectic Methods

- A symplectic method is a numerical method whose map is symplectic
  - Note if map from any t_n to t_{n+1} is symplectic, then composition of maps is symplectic, so full method is symplectic
- Example: symplectic Euler
  - Goes by many names, e.g. velocity Verlet
- Also implicit midpoint
  - Not quite trapezoidal rule, but the two are essentially equivalent…

Modified Equations

- Backwards error analysis for differential equations
- Say we are solving

$$\frac{dy}{dt} = f(y)$$

- Goal: show that numerical solution $\{y_n\}$ is actually the solution to a modified equation:

$$y_n = \bar{y}(t_n), \quad \frac{d\bar{y}}{dt} = f(\bar{y}) + hf_2(\bar{y}) + h^2 f_3(\bar{y}) + \ldots$$

Symplectic Euler

- Look at simple example: H=T(p)+V(q)
- Symplectic Euler is essentially

$$p_{n+1} = p_n - \Delta t H_q\left(p_n, q_n\right)$$
$$q_{n+1} = q_n + \Delta t H_p\left(p_{n+1}, q_n\right)$$

- Do some Taylor series expansions to find first term in modified equations…

Modified Equations are Hamiltonian!

- The first expansion is:

$$\frac{dp}{dt} = -\frac{\partial}{\partial q}\left(H - \frac{\Delta t}{2} H_p \cdot H_q\right) + O(\Delta t^2)$$
$$\frac{dq}{dt} = \frac{\partial}{\partial p}\left(H - \frac{\Delta t}{2} H_p \cdot H_q\right) + O(\Delta t^2)$$

- So numerical solution is, to high order, solving a Hamiltonian system (but with a perturbed H)
  - So to high order has the same structure

Modified equations in general

- Under some assumptions, any symplectic method is solving a nearby Hamiltonian system exactly
- Aside: this modified Hamiltonian depends on step size h
  - If you use a variable time step, modified Hamiltonian is changing every time step
  - Numerical flow is still symplectic, but no strong guarantees on what it represents
  - As a result - may very well see much worse long-time behaviour with a variable step size than with a fixed step size!