A Study on

Numerical Algorithms as Dynamical Systems

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What This Study Is About?

- To recast many numerical algorithms as special dynamical systems, whence to derive new understandings and insights.
- To exploit the notion of dynamical systems as a special realization process for problems arising from the field of numerical analysis, whence to develop possible new schemes.
- To forge the idea that, while these “things" have been differentiated from each other, they can also be integrated together.

Topics of Lessons

1. Numerical Analysis versus Dynamical Systems
2. Dynamics and Controls in Solving Algebraic Equations
3. Lax Evolution and Its Equivalents
4. Lotka-Volterra Equations and Singular Values
5. Dynamics via Group Actions
6. Structure-preserving Dynamical Systems and Applications

Lecture 1
Numerical Analysis versus Dynamical Systems
An Overview

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June 14, 2009 @ MCM, CAS

Outline

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Realization Process

- A logical procedure used to reason or to infer.
- Usually done deductively or inductively.
- Aim to draw conclusion or make decision.

Dynamical System

- A realization process in the recursive form.
- One state develops into another state by following a certain specific rule.
- Often appears in the form of an iterative procedure or a differential equation.

Basic Components

- Two abstract problems:
  - One is a make-up and is easy.
  - The other is the real problem and is difficult.
- A bridge:
  - A continuous path connecting the two problems.
  - A path that is easy to follow.
- A numerical method:
  - A method for moving along the bridge.
  - A method that is readily available.

Building the Bridge

- Specified guidance is available.
  - The bridge is constructed by monitoring the values of certain specified functions.
  - The path is guaranteed to work.
  - e.g. The projected gradient method.
- Only some general guidance is available.
  - A bridge is built in a straightforward way.
  - No guarantee the path will be complete.
  - e.g. The homotopy method.
- No guidance at all.
  - A bridge is built seemingly by accident.
  - Usually deeper mathematical theory is involved.
  - e.g. The isospectral flows.

Characteristics of a Bridge

- A bridge, if it exists, usually is characterized by an ordinary differential equation.
- The discretization of a bridge, or a numerical method in traveling along a bridge, usually produces an iterative scheme.

Symmetric Eigenvalue Problem

- The mathematical problem:
  - A symmetric matrix A_0 is given.
  - Solve the equation
    $$A_0\mathbf{x} = \lambda\mathbf{x}$$
    for a nonzero vector **x** and a scalar λ.

An Iterative Realization

- The QR decomposition:
$$A = QR$$
where Q is orthogonal and R is upper triangular.
- The QR algorithm (Francis'61):
$$\begin{aligned} A_k &= Q_k R_k, \\ A_{k+1} &= R_k Q_k. \end{aligned}$$
- Theory:
  - Every matrix A_k has the same eigenvalues of A_0.
  - The sequence $\{A_k\}$ converges to a diagonal matrix.

A Continuous Realization

- Lie algebra decomposition:

$$X = X^o + X^+ + X^-$$

  where X^o is the diagonal, X^+ the strictly upper triangular, and X^- the strictly lower triangular part of X.

- Toda lattice (Symes'82, Deift el al'83):

$$\begin{aligned} \frac{dX}{dt} &= [X, X^- - X^{-^T}] \\ X(0) &= X_0. \end{aligned}$$

- Theory:
  - Sampled at integer times, $\{X(k)\}$ gives the same sequence as does the QR algorithm applied to the matrix $A_0 = exp(X_0)$.

How Is the Bridge Built?

- The bridge between X_0 and the limit point of Toda flow is built on the basis of maintaining isospectrum.
- Points to ponder:
  - What motivates the construction of the Toda lattice?
  - Why is convergence guaranteed?
  - What is the advantage of one approach over the other?

Nonlinear Algebraic Equations

- The mathematical problem:
  - A sufficiently smooth function $\mathbf{f} : \mathbb{R}^n \to \mathbb{R}^n$ is given.
  - Solve the equation

$$\mathbf{f}(\mathbf{x}) = 0.$$

An Iterative Realization

- The Newton method:

$$\mathbf{x}_{k+1} = \mathbf{x}_k - \alpha_k (\mathbf{f}'(\mathbf{x}_k))^{-1} \mathbf{f}(\mathbf{x}_k).$$

- Theory:
  - The sequence $\{\mathbf{x}_k\}$ converges quadratically to a solution, if $\mathbf{x}_0$ is sufficiently close to that solution.

A Continuous Realization

- The Newton homotopy (Smale '76, Keller '78, etc.):

$$H(\mathbf{x}, t) = \mathbf{f}(\mathbf{x}) - t\mathbf{f}(\mathbf{x}_0).$$

  - The zero set $\{(\mathbf{x}, t) \in \mathbb{R}^{n+1} \mid H(\mathbf{x}, t) = 0\}$ forms a smooth curve.
  - The homotopy curve:

$$\mathbf{f}'(\mathbf{x})\frac{d\mathbf{x}}{ds} - \frac{1}{t}\mathbf{f}(\mathbf{x})\frac{dt}{ds} = 0, \quad \mathbf{x}(0) = \mathbf{x}_0, \quad t(0) = 1,$$

  where s is the arc length.

- Suppose $f'(\mathbf{x})$ is nonsingular. Then written as

$$\frac{d\mathbf{x}}{ds} = \frac{dt}{ds}\frac{1}{t}(\mathbf{f}'(\mathbf{x}))^{-1}\mathbf{f}(\mathbf{x}).$$

- Theory:
  - With appropriate step size chosen, an Euler step is equivalent to a regular Newton method.

How Is the Bridge Built?

- The bridge is built upon the hope that the obvious solution will be deformed mathematically into the solution that we are seeking for.
- Points to ponder:
  - Will this idea always work?
  - How to mathematically design an appropriate homotopy?

Least Squares Matrix Approximation

- The mathematical problem:
  - A symmetric matrix N and a set of real values $\{\lambda_1, \ldots, \lambda_n\}$ are given.
  - Find a least squares approximation of N that has the prescribed eigenvalues.

A Standard Formulation

$$\begin{aligned} \text{Minimize } F(Q) &:= \frac{1}{2}||Q^T \Lambda Q - N||^2 \\ \text{Subject to } Q^T Q &= I \end{aligned}$$

- Equality Constrained Optimization:
  - Augmented Lagrangian methods.
  - Sequential quadratic programming methods.
  - Interior point method.
- All these techniques employ iterative realization.
  - Linearize the Lagrangian.
  - Sequential quadratic approximation.
  - Follow the central path.

A Continuous Realization

- The projection of the gradient of F can easily be calculated.
- Projected gradient flow (Chu&Driessel'90):

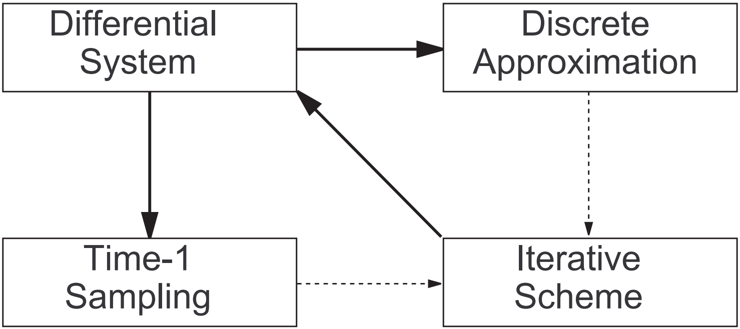
$$\begin{aligned} \frac{dX}{dt} &= [X, [X, N]] \\ X(0) &= \Lambda \end{aligned}$$

  - $X := Q^T \Lambda Q$.
  - Flow $X(t)$ moves in a descent direction to reduce $||X - N||^2$.
- Theory:
  - The optimal solution X can be fully characterized by the spectral decomposition of N and is unique.

How Is the Bridge Built?

- The bridge between a starting point and the optimal point is built on the basis of systematically reducing the difference between the current position and the target position.
- Points to ponder:
  - How to get to the limit point of the gradient flow efficiently?

Mutual Implications



Technology Limitations

- Floating-point arithmetic is the most common and effective way for computation.
- Almost a mandate to discretize a continuous problem.
- A majority of numerical algorithms in practice are iterative in nature.

Iterative Scheme

$$\mathbf{x}_{k+1} = G_k(\mathbf{x}_k, \ldots, \mathbf{x}_{k-p+1}), \quad k = 0, 1, \ldots,$$

- A p-step sequential process (Ortega&Rheinboldt'00),:
- $G_k : D_k \subset V^p \to V$ is a predetermined map.
  - Could be stationary.
  - A bridge intends to achieve a certain goal.
  - V is a designated set of states. Could be a manifold.
- Need initial values $\mathbf{x}_0, \mathbf{x}_{-1}, \ldots, \mathbf{x}_{-p+1}$.

Initial Value Problem

$$\frac{d\mathbf{x}}{dt} = \mathbf{f}(t, \mathbf{x}), \quad \mathbf{x}(0) = \mathbf{x}_0,$$

- $\mathbf{f}$ defines a flow moving in a specific direction.
- In many applications, $\mathbf{x}(t)$ is supposed to preserve certain quantities, such as mass, volume, or stay on a certain manifold.
  - Challenging to realize this conservation law.

Numerical ODE Techniques

- Conventional Runge-Kutta method:

$$\mathbf{x}_{n+1} = \underbrace{\mathbf{x}_n + h\sum_{r=1}^{R} c_r \mathbf{k}_r}_{G_n(\mathbf{x}_n)}, \quad \sum_{r=1}^{R} c_r = 1.$$

  - $\mathbf{k}_r := \mathbf{f}(t_n + a_r h, \mathbf{x}_n + h\sum_{s=1}^{R} b_{rs}\mathbf{k}_s), \quad \sum_{s=1}^{R} b_{rs} = a_r.$
- Conventional linear multi-step method:

$$\mathbf{x}_{n+1} := \underbrace{\sum_{i=0}^{p}(\alpha_i \mathbf{x}_{n-i} + h\beta_i \mathbf{f}_{n-i})}_{G(\mathbf{x}_n,\ldots,\mathbf{x}_{n-p})} + h\beta_{-1}\mathbf{f}_{n+1}.$$

- Special purpose geometric integrator .....

Sarkovskii's Theorem

- Consider the iteration

$$x_{k+1} = f(x_k),$$

  where $f : \mathbb{R} \to \mathbb{R}$ is continuous.
- A number x_0 is of period m if $x_m = x_0$ and having least period m if $x_k \neq x_0$ for all $0 < k < m$.
- Arrange positive integers in the following ordering:

$$3, 5, 7, 9, \ldots, 2 \cdot 3, 2 \cdot 5, 2 \cdot 7, \ldots, 2^2 \cdot 3, 2^2 \cdot 5, \ldots, 2^4, 2^3, 2^2, 2, 1.$$

- Sharkovskii's theorem:
  - If f has a periodic point of least period m and $m \leq n$ in the above ordering, then f has also a periodic point of least period n.
- Remarkable for its lack of hypotheses and its qualitative universality.

Two Different Views

Numerical Analysis	Dynamical System
Consider systems with only trivial asymptotic behavior.	Interested in systems with more complicated behavior.
Concerned about convergence and stability.	Study overall trajectories.
Meant to trace the flow of ODEs with reliable and reasonable accuracy — local behavior of the trajectory.	Want to differentiate the intrinsic geometric structure — long-term behavior of the trajectory.
Meant to converge to a unique equilibrium point.	Search for limit cycles, bifurcations, or strange attractors.

Logistic Equation

$$\frac{dx}{dt} = x(1-x), \quad x(0) = x_0.$$

- Exact solution:

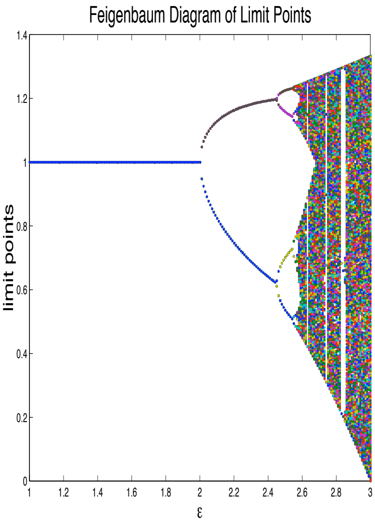
$$x(t) = \frac{x_0}{x_0 + e^{-t}(1-x_0)},$$

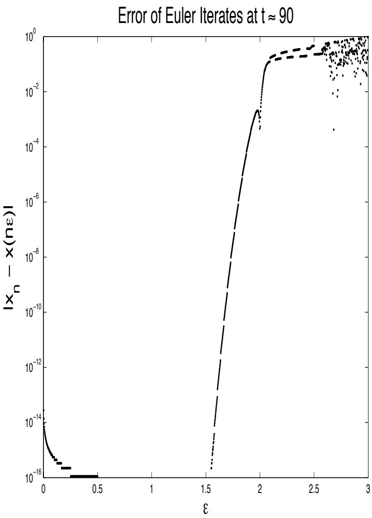
  - Converge to the equilibrium $x(\infty) = 1$ for any initial value $x_0 \neq 0$.

Explicit Euler Iteration

$$x_{k+1} = x_k + \epsilon x_k(1 - x_k), \quad \epsilon = \text{step size}.$$

- Fix t, $x_n \to x(t)$ as $n \to \infty$ in the sense of $\epsilon = \frac{t}{n}$.
- With $n = \lceil \frac{90}{\epsilon} \rceil$ and $0 < \epsilon \leq 3$, plot the absolute error $|x_n - x(n\epsilon)|$.
  - Theoretic error estimate $O(\epsilon)$.
- Fix ϵ, iterate the Euler step 5000 times to see the limit points.
  - A cascade of period doubling as ϵ increases.
  - The equilibrium $x(\infty) = 1$ is not even an attractor for large ϵ.


Feigenbaum Diagram of Limit Points
limit points
ε
1
1.2
1.4
1.6
1.8
2
2.2
2.4
2.6
2.8
3
0
0.2
0.4
0.6
0.8
1
1.2
1.4


Error of Euler Iterates at t ≈ 90
$|x_n - x(n\varepsilon)|$
ε
0
0.5
1
1.5
2
2.5
3
10^{-16}
10^{-14}
10^{-12}
10^{-10}
10^{-8}
10^{-6}
10^{-4}
10^{-2}
10^{0}

Implicit Euler Iterations

$$
\begin{aligned}
x_{k+1} &= x_k + \epsilon x_{k+1}(1 - x_{k+1}), \\
x_{k+1} &= x_k + \epsilon x_k(1 - x_{k+1}).
\end{aligned}
$$

- Converge to the equilibrium $x(\infty) = 1$ for any step size ϵ.
- Points to ponder:
    - Distinguish limiting behavior between an iterative algorithm designed originally to solve a specific problem and a discrete approximation of a differential system formulated to mimic an existing iterative algorithm.
    - Distinguish asymptotic behavior between a differential system developed originally from a specific realization process and its discrete approximation which becomes an iterative scheme.

Gradient Flow

$$\frac{d\mathbf{x}}{dt} = -\nabla F(\mathbf{x}), \quad \mathbf{x}(0) = \mathbf{x}_0,$$

- $F : \mathbb{R}^n \to \mathbb{R}$ is a specified smooth objective function.
- Goal: Find the limit point $\mathbf{x}^* = \lim_{t\to\infty} \mathbf{x}(t)$ of the gradient flow $\mathbf{x}(t)$.
- Wish list:
  - Do not want to solve the equation $\nabla F(\mathbf{x}) = 0$ by Newton-like methods.
    - Ignore the gradient property.
    - Might locate undesirable, dynamically unstable critical points.
  - Do not want to follow the solution curve $\mathbf{x}(t)$ closely.
    - Too expensive computation at the transient state.

Pseudo-transient Continuation

- Idea: Stay near the true trajectory, but not strive for accuracy.
- Employ one implicit Euler step with step size ϵ_k:

$$\mathbf{x}_{k+1} = \mathbf{x}_k - \epsilon_k \nabla F(\mathbf{x}_{k+1}).$$

- Perform only one correction using one Newton iteration starting at $\mathbf{x}_k$ and accept the outcome as $\mathbf{x}_{k+1}$.

$$\mathbf{x}_{k+1} = \mathbf{x}_k - \left(\frac{1}{\epsilon_k} I_n + \nabla^2 F(\mathbf{x}_k) \right)^{-1} \nabla F(\mathbf{x}_k).$$

- The step size changes the nature of iterations.
  - Small values of $\epsilon_k \Rightarrow$ Scheme behaves like a steepest descent method.
  - Large values of $\epsilon_k \Rightarrow$ Scheme behaves like a Newton iteration.

Hamiltonian Flow

$$\begin{cases} \frac{dp_i}{dt} = \{p_i, H\}, \\ \frac{dq_i}{dt} = \{q_i, H\}, \end{cases} \quad i = 1, \ldots, n,$$

with Poisson bracket

$$\{f, g\} := \sum_{i=1}^{n} \left(\frac{\partial f}{\partial q_i} \frac{\partial g}{\partial p_i} - \frac{\partial f}{\partial p_i} \frac{\partial g}{\partial q_i} \right).$$

- Goal: Find the long-term evolution behavior.
- Wish list:
  - Want to keep the simplectic form $d\mathbf{p} \wedge d\mathbf{q}$ invariant $\Rightarrow$ Preserving qualitative properties of phase space trajectories.

Runge-Kutta Methods

$$\begin{array}{c|c} \mathbf{a} & B \\ \hline & \mathbf{c}^\top \end{array}$$

- If $m_{ij} := c_i b_{ij} + c_j b_{ji} - c_i c_j = 0$ for all $1 \le i, j \le R$, then the RK method is simplectic. (Sanz-Serna'88).
- Gauss-Legengre RK methods are simplectic.

$$\begin{array}{c|cc} \frac{1}{2} - \frac{\sqrt{3}}{6} & \frac{1}{4} & \frac{1}{4} - \frac{\sqrt{3}}{6} \\ \frac{1}{2} + \frac{\sqrt{3}}{6} & \frac{1}{4} + \frac{\sqrt{3}}{6} & \frac{1}{4} \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}$$