Lecture 2
Dynamics and Controls in Solving Algebraic Equations
Oldies and New

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June 15, 2009 @ MCM, CAS
Outline

**Linear Systems**
- History
- Stationary Iteration
- Krylov Subspace Methods

**Nonlinear Systems**
- Continuous Control
- Discrete Control
Outline

Linear Systems
- History
- Stationary Iteration
- Krylov Subspace Methods

Nonlinear Systems
- Continuous Control
- Discrete Control
Linear System

- The problem:
  \[ Ax = b. \]

  - Fundamental in scientific computation.

- Two basic approaches:
  - Direct methods:
    - Decompose \( A \) as the product of some easier factors.
    - \( LU, \ QR, \ SVD \) and so on.
    - Though called a direct method, the series of steps taken to achieve the factorization is itself an iterative process.
  - Iterative methods:
    - Repeat some recursive schemes until convergence.
A Long Way of Developments

Some popular techniques:
- Acceleration of classical iterative schemes (Hageman & Young’81).
- Krylov subspace approximation (van der Vorst ’03).
- Multi-grid (Briggs ’87, Bramble ’93).
- Domain decomposition (Toselli & Widlund ’05).

Some favorite methods:
- ITPACK (Grimes, Kincaid, Macgregor, & Young ’78)
- PCG (Hestenes & Stiefel ’52).
- GMRES (Saad & Schultz ’86).
- QMR (Freund & Nachtigal’91),
One-step Stationary Sequential Process

- The scheme:
  \[ x_{k+1} = Gx_k + c, \quad k = 0, 1, 2, \ldots. \]

- The iteration matrix \( G \in \mathbb{R}^{n \times n} \) plays a crucial role.
  - Want convergence of \( \{x_k\} \).
  - The spectral radius \( \rho(G) \) should be strictly less than one (Varga’90).
  - Extensive efforts have been made to construct \( G \).
Splitting and Preconditioning

- One possible way of writing $G$:
  \[
  G = I - K^{-1}A,
  \]
  \[
  c = K^{-1}b,
  \]
  for some nonsingular matrix $K$.
- $A$ is “split’ by $K$ in the sense that
  \[
  A = K - KG.
  \]
- Choose a splitting matrix $K$ of $A$ such that
  - $\rho(I - K^{-1}A) < 1$.
  - $K^{-1}$ is relatively easy to compute.
Continuous Generalization

- **Iterative scheme:**
  \[ x_{k+1} = x_k - K^{-1}(Ax_k - b). \]

- **An Euler step with step size** \( h = 1 \):
  \[ \frac{dx}{dt} = f(x; K) := -K^{-1}(Ax - b). \]

- **Analytic solution:**
  \[ x(t) = e^{-K^{-1}At}(x_0 - A^{-1}b) + A^{-1}b. \]
Fundamental Difference in $K$

- By iteration,
  - $|1 - \lambda(K^{-1}A)| < 1 \Rightarrow$ convergence.
  - $\lambda(K^{-1}A)$ clustered near 1 $\Rightarrow$ faster convergence.

- By continuation,
  - $\Re(\lambda(K^{-1}A)) > 0 \Rightarrow$ convergence.
  - $\Re(\lambda(K^{-1}A)) >> 1 \Rightarrow$ faster convergence.
  - $\Im(\lambda(K^{-1}A))$ clustered near 0 $\Rightarrow$ avoid high oscillation.
  - $\lambda(K^{-1}A)$ clustered $\Rightarrow$ avoid stiffness.

- Continuous methods are much more relaxed than iterative methods.
  - Can a discretization of the continuous system gives rise to a better iterative scheme?
Trapezoidal Rule

With step size $h$,

$$\mathbf{x}_{k+1} = \left( I + \frac{h}{2} K^{-1} A \right)^{-1} \left( I - \frac{h}{2} K^{-1} A \right) \mathbf{x}_k + h \left( I + \frac{h}{2} K^{-1} A \right)^{-1} K^{-1} \mathbf{b},$$

$(1,1)$-pair Padé

$2$nd order Taylor

Comparing with the analytic solution,

$$\mathbf{x}(t + h) = e^{-hK^{-1}A} \mathbf{x}(t) + \int_t^{t+h} e^{-(t+h-s)K^{-1}A} (K^{-1} \mathbf{b}) ~ ds.$$ 

$$\mathbf{x}(t_{k+1}) - \mathbf{x}_{k+1} = (I + \frac{h}{2} K^{-1} A)^{-1} (I - \frac{h}{2} K^{-1} A) \left( \mathbf{x}(t_k) - \mathbf{x}_k \right) + O(h^3).$$

- An $A$-stable method.
- Not practical, but better convergence.
Polynomial Acceleration

- Three-term recurrence:

\[ x_1 = \epsilon_1 (Gx_0 + c) + (1 - \epsilon_1)x_0, \]
\[ x_{k+1} = \alpha_{k+1} [\epsilon_{k+1}(Gx_k + c) + (1 - \epsilon_{k+1})x_k] + (1 - \alpha_{k+1})x_{k-1}, \]

with some properly defined real numbers $\alpha_k$ and $\epsilon_k$ (Hageman & Young '81).

- Rewrite as

\[ x_1 = x_0 + \epsilon_1 f_0, \]
\[ x_{k+1} = \alpha_{k+1} x_k + (1 - \alpha_{k+1})x_{k-1} + \epsilon_{k+1} \alpha_{k+1} f_k, \]

with $f_k := f(x_k; K)$. 
Two-step Stationary Sequential Process

- General explicit, linear two-step method (for ODEs):
  - Of order 2:
    \[
    x_{k+1} = \alpha x_k + (1 - \alpha) x_{k-1} + h \left( (2 - \frac{\alpha}{2}) f_k - \frac{\alpha}{2} f_{k-1} \right).
    \]
  - Of order 1:
    \[
    x_{k+1} = \alpha x_k + (1 - \alpha) x_{k-1} + h (2 - \alpha) f_k.
    \]

- Acceleration from ODE point of view:
  - Low order of accuracy, but has a faster rate of convergence.
  - Non-stationary sequential process — More than just variable step sizes.
Line Search

- Rewrite the ODE as
  \[
  \frac{dx}{dt} = K^{-1}r,
  \]
  with a state feedback (residual) \( r := b - Ax \).

- Interpret the Euler step with variable step size \( h_k \)
  \[
  x_{k+1} = x_k + h_k K^{-1}r_k,
  \]
  as a line search in the \( K^{-1}r_k \) direction for a given \( K^{-1} \).

- Not immediately concern about convergence to an equilibrium, but control the flow via some objective values.
Step Size Selection

- Minimize \( r_{k+1}^T r_{k+1} \) \( \Rightarrow \)
  \[
h_k = \frac{\langle AK^{-1} r_k, r_k \rangle}{\langle AK^{-1} r_k, AK^{-1} r_k \rangle}.
  \]

- Minimize \( r_{k+1} A^{-1} r_{k+1} \) with \( A \succ 0 \) \( \Rightarrow \)
  \[
h_k = \frac{\langle K^{-1} r_k, r_k \rangle}{\langle AK^{-1} r_k, K^{-1} r_k \rangle}.
  \]
Two Steps Again!

- Rewrite the explicit, linear two-step method of order 1

\[
x_{k+1} = \alpha x_k + (1 - \alpha)x_{k-1} + h(2 - \alpha)f_k,
\]

as

\[
x_{k+1} = x_k + \epsilon_k \left[ K^{-1}r_k + \gamma_k (x_k - x_{k-1}) \right].
\]

- Starting with \( p_0 = K^{-1}r_0 \), define

\[
p_k := K^{-1}r_k + \gamma_k (x_k - x_{k-1}) = K^{-1}r_k + \beta_k p_{k-1},
\]

\[
\beta_k := \epsilon_{k-1} \gamma_k.
\]

- Rewrite

\[
x_{k+1} = x_k + \epsilon_k p_k,
\]

\[
r_{k+1} = r_k - \epsilon_k A p_k,
\]
Suppose $A \succ 0$,

\[
\epsilon_k = \frac{\langle p_k, r_k \rangle}{\langle Ap_k, p_k \rangle},
\]

\[
\beta_{k+1} = -\frac{\langle K^{-1}r_{k+1}, Ap_k \rangle}{\langle Ap_k, p_k \rangle}, \quad k = 0, 1, \ldots,
\]

- $K$ is a symmetric preconditioner.
- Laughable accuracy, but $\{x_k\}$ converges in at most $n$ iterations.
Lessons We Have Learned

- A very basic discrete dynamical system $\Rightarrow$ A very general continuous dynamical system.
- Use the system as a guide to draw up some general procedures that roughly solve the continuous system, but not with great accuracy.
- Aptly tune the parameters which masquerade as the step sizes in the procedures $\Rightarrow$ Achieve fast convergence to the equilibrium point of the continuous system.
- Eventually accomplish the goal of the original basic discrete dynamical system.
Mutual Implications

- Differential System
- Time-1 Sampling
- Iterative Scheme
- Discrete Approximation
Nonlinear System

The problem:

\[ g(x) = 0, \]

- \( g : \mathbb{R}^n \rightarrow \mathbb{R}^n \) is nonlinear.

Various numerical techniques can be cast in an input-output control framework with different control strategies.
Continuous Control

- Basic model:

\[
\frac{dx(t)}{dt} = u(t),
\]

\[
y(t) = -r(t),
\]

- State variable \(x(t)\).
- Controller \(u(t)\).
- Output variable \(y(t)\) observed from the residue function

\[
r(t) = -g(x(t)).
\]

- Use both the state and the output as feedback to estimate the control strategy,

\[
u = \phi(x, r).
\]
Control Strategies  
(Bhaya & Kaszkurewicz '06)

<table>
<thead>
<tr>
<th>( \phi(x, r) )</th>
<th>( \frac{dV}{dt} )</th>
<th>( \frac{dx}{dt} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( g'(x)^{-1}r )</td>
<td>(-|r|^2)</td>
<td>(-g'(x)^{-1}g(x))</td>
</tr>
<tr>
<td>( g'(x)^\top r )</td>
<td>(-|g'(x)^\top r|^2)</td>
<td>(-g'(x)^\top g(x))</td>
</tr>
<tr>
<td>( g'(x)^{-1}sgn(r) )</td>
<td>(-|r|_1)</td>
<td>(-g'(x)^{-1}sgn(g(x)))</td>
</tr>
<tr>
<td>( sgn(g'(x)^\top r) )</td>
<td>(-|g'(x)^\top r|_1)</td>
<td>(-sgn(g'(x)^\top g(r)))</td>
</tr>
<tr>
<td>( g'(x)^\top sgn(r) )</td>
<td>(-|g'(x)^\top sgn(r)|^2)</td>
<td>(-g'(x)^\top sgn(g(x)))</td>
</tr>
</tbody>
</table>

▶ Lyapunov function

\[
V(t) = \begin{cases} 
\frac{1}{2} \|r(t)\|^2, & \text{first four cases,} \\
\|r(t)\|_1, & \text{last case.}
\end{cases}
\]
Continuous Newton

- Closed-loop dynamics for the state variable:

\[
\frac{dx}{dt} = u = -g'(x)^{-1}g(x).
\]

- Sure-fire method ⇒ Would fail, only if \( g'(x) \) becomes singular (Smale '76).

- Dynamics for the residual:

\[
\frac{dr}{dt} = -g'(x)\frac{dx}{dt} = -r.
\]

- Dynamics for the cost function:

\[
V(t) := \frac{1}{2}\langle r(t), r(t) \rangle,
\]

\[
\frac{dV}{dt} = -\|r\|_2^2.
\]
Discretization

- Only the continuous Newton method has been extensively studied.
  - An Euler step ⇒ Classical Newton iteration scheme.
- Some of the vector fields for $\mathbf{x}(t)$ are only piecewise continuous.
- A discretization of the differential system may not be trivial.
  - Scheme?
  - Convergence analysis?
Discrete Control

- **Basic model:**
  \[ x_{k+1} = x_k + u_k. \]

- **Controller:**
  - Follow the feedback law:
    \[ u_k = \epsilon_k \phi(x_k, r_k). \]
  - Also control the step size \( \epsilon_k \).
Informal Inquiries

- Assume $\phi(x, r)$ is fixed,

$$r_{k+1} \approx r_k - \epsilon_k g'(x_k) \phi(x_k, r_k).$$

- Line search,

$$\epsilon_k = \frac{\langle g'(x_k) \phi(x_k, r_k), r_k \rangle}{\langle g'(x_k) \phi(x_k, r_k), g'(x_k) \phi(x_k, r_k) \rangle}.$$

- Some special cases:
  - $\phi(x, r) = g'(x)^{-1} r \Rightarrow \epsilon_k = 1 \Rightarrow$ Classical Newton iteration.
  - $g(x) = Ax - b$ and $\phi(x, r) = K^{-1} r \Rightarrow$ ORTHOMIN(1) method.
Limiting Behavior of the Residual

- \( \{ r_k \} \) may not be a decreasing sequence.
  - \( x_{k+1} - x_k \) may not be small enough to warrant the Taylor series expansion.
  - The Newton iteration with \( \epsilon_k \equiv 1 \) does not necessarily give rise to a descent step.
- A dividing line between a discrete dynamical system and a continuous dynamical system is at the behavior of \( r \) before reaching convergence.
Continuity versus Discreteness
(Hauser & Nedić ’07)

Compare the dynamical systems:

\[
x_{k+1} = x_k + \nu(x_k).
\]

\[
\frac{dx}{dt} = \nu(x).
\]

\(\nu'(x)\) is continuous at \(x^*\).

Superlinear Convergence

\[ \{x_k\} \text{ converges } Q\text{-superlinearly} \]
\[ \iff \lim_{x \to x^*} \frac{\|x + \nu(x) - x^*\|}{\|x - x^*\|} = 0. \]
\[ \iff \begin{cases} 
\nu(x^*) = 0, \\
\nu'(x^*) = -I.
\end{cases} \]

\[ x(t) \text{ converges exponentially} \]
\[ \iff \left\{ \begin{array}{l}
e^{-(1+\epsilon)t} \leq \frac{\|x(t)-x^*\|}{\|x_0-x^*\|} \leq e^{-(1-\epsilon)t}, \\
\| \frac{\partial}{\partial t} \left( \frac{x(t)-x^*}{\|x(t)-x^*\|} \right) \| \leq \epsilon.
\end{array} \right. \]

\[ Q\text{-superlinear convergence} \iff \text{Exponential convergence}. \]
Higher Order Q-convergence

- \( \{x_k\} \) Q-converges at rate \( p + 1 \)

\[ \Leftrightarrow \| x + \nu(x) - x^* \| \leq \beta \| x - x^* \|^{p+1}. \]

\[ \Leftrightarrow \begin{cases} 
\nu(x^*) = 0, \\
\nu'(x^*) = -I, \\
\| \nu'(x) - \nu'(x^*) \| \leq \alpha \| x - x^* \|^p.
\end{cases} \]

- \( x(t) \) converges \( p \)-exponentially

\[ \Leftrightarrow \begin{cases} 
e^{-\left(1+\epsilon\right)t} \leq \frac{\| x(t)-x^* \|}{\| x_0-x^* \|} \leq e^{-\left(1-\epsilon\right)t}, \\
\| \frac{\partial}{\partial t} \left( \frac{x(t)-x^*}{\| x(t)-x^* \|} \right) \| \leq \gamma e^{-\left(1-\epsilon\right)p t} \| x_0 - x^* \|^p.
\end{cases} \]

- Q-convergence at rate \( p + 1 \) \( \Leftrightarrow \) \( p \)-exponential convergence.