Lecture 2
Dynamics and Controls in Solving Algebraic Equations

Oldies and New

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Outline

Linear Systems

- History
- Stationary Iteration
- Krylov Subspace Methods

Nonlinear Systems

- Continuous Control
- Discrete Control

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Linear Systems
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- Stationary Iteration
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Nonlinear Systems
- Continuous Control
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Linear System

- The problem:

$$A\mathbf{x} = \mathbf{b}.$$

  - 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 (Toseli & 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:

$$\mathbf{x}_{k+1} = G\mathbf{x}_k + \mathbf{c}, \quad k = 0, 1, 2, \ldots.$$

- The *iteration matrix* $G \in \mathbb{R}^{n \times n}$ plays a crucial role.
  - Want convergence of $\{\mathbf{x}_k\}$.
  - 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:

$$\begin{aligned} G &= I - K^{-1}A, \\ \mathbf{c} &= K^{-1}\mathbf{b}, \end{aligned}$$

  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:

$$\mathbf{x}_{k+1} = \mathbf{x}_k - K^{-1}(A\mathbf{x}_k - \mathbf{b}).$$

- An Euler step wit step size $h = 1$:

$$\frac{d\mathbf{x}}{dt} = \mathbf{f}(\mathbf{x}; K) := -K^{-1}(A\mathbf{x} - \mathbf{b}).$$

- Analytic solution:

$$\mathbf{x}(t) = e^{-K^{-1}At}(\mathbf{x}_0 - A^{-1}\mathbf{b}) + A^{-1}\mathbf{b}.$$

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,

$$\mathbf{x}_{k+1} = \underbrace{\left(I + \frac{h}{2}K^{-1}A\right)^{-1}\left(I - \frac{h}{2}K^{-1}A\right)}_{\text{(1,1)-pair Padè}}\mathbf{x}_k + h\underbrace{\left(I + \frac{h}{2}K^{-1}A\right)^{-1}}_{\text{2nd order Taylor}}K^{-1}\mathbf{b},$$

- Comparing with the analytic solution,

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

- $\mathbf{x}(t_{k+1}) - \mathbf{x}_{k+1} = \left(I + \frac{h}{2}K^{-1}A\right)^{-1}\left(I - \frac{h}{2}K^{-1}A\right)(\mathbf{x}(t_k) - \mathbf{x}_k) + O(h^3).$
  - An A-stable method.
  - Not practical, but better convergence.

Polynomial Acceleration

- Three-term recurrence:

$$\begin{aligned} \mathbf{x}_1 &= \epsilon_1(G\mathbf{x}_0 + \mathbf{c}) + (1-\epsilon_1)\mathbf{x}_0, \\ \mathbf{x}_{k+1} &= \alpha_{k+1}\left[\epsilon_{k+1}(G\mathbf{x}_k + \mathbf{c}) + (1-\epsilon_{k+1})\mathbf{x}_k\right] + (1-\alpha_{k+1})\mathbf{x}_{k-1}, \end{aligned}$$

  with some properly defined real numbers α_k and ϵ_k (Hageman & Young '81).

- Rewrite as

$$\begin{aligned} \mathbf{x}_1 &= \mathbf{x}_0 + \epsilon_1\mathbf{f}_0, \\ \mathbf{x}_{k+1} &= \alpha_{k+1}\mathbf{x}_k + (1-\alpha_{k+1})\mathbf{x}_{k-1} + \epsilon_{k+1}\alpha_{k+1}\mathbf{f}_k, \end{aligned}$$

  with $\mathbf{f}_k := \mathbf{f}(\mathbf{x}_k; K)$.

Two-step Stationary Sequential Process

- General explicit, linear two-step method (for ODEs):
  - Of order 2:

$$\mathbf{x}_{k+1} = \alpha \mathbf{x}_k + (1-\alpha)\mathbf{x}_{k-1} + h\left((2-\frac{\alpha}{2})\mathbf{f}_k - \frac{\alpha}{2}\mathbf{f}_{k-1}\right).$$

  - Of order 1:

$$\mathbf{x}_{k+1} = \alpha \mathbf{x}_k + (1-\alpha)\mathbf{x}_{k-1} + h(2-\alpha)\mathbf{f}_k.$$

- 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
$$\frac{d\mathbf{x}}{dt} = K^{-1}\mathbf{r},$$
with a state feedback (residual) $\mathbf{r} := \mathbf{b} - A\mathbf{x}$.
- Interpret the Euler step with variable step size h_k
$$\mathbf{x}_{k+1} = \mathbf{x}_k + h_k K^{-1}\mathbf{r}_k,$$
as a line search in the $K^{-1}\mathbf{r}_k$ 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 $\mathbf{r}_{k+1}^\top \mathbf{r}_{k+1} \Rightarrow$

$$h_k = \frac{\langle AK^{-1}\mathbf{r}_k, \mathbf{r}_k \rangle}{\langle AK^{-1}\mathbf{r}_k, AK^{-1}\mathbf{r}_k \rangle}.$$

- Minimize $\mathbf{r}_{k+1} A^{-1} \mathbf{r}_{k+1}$ with $A \succ 0 \Rightarrow$

$$h_k = \frac{\langle K^{-1}\mathbf{r}_k, \mathbf{r}_k \rangle}{\langle AK^{-1}\mathbf{r}_k, K^{-1}\mathbf{r}_k \rangle}.$$

Two Steps Again!

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

$$\mathbf{x}_{k+1} = \alpha \mathbf{x}_k + \underbrace{(1-\alpha)}_{-\epsilon_k \gamma_k} \mathbf{x}_{k-1} + \underbrace{h(2-\alpha)}_{\epsilon_k} \mathbf{f}_k,$$

  as

$$\mathbf{x}_{k+1} = \mathbf{x}_k + \epsilon_k \left[K^{-1}\mathbf{r}_k + \gamma_k(\mathbf{x}_k - \mathbf{x}_{k-1}) \right].$$

- Starting with $\mathbf{p}_0 = K^{-1}\mathbf{r}_0$, define

$$\begin{aligned} \mathbf{p}_k &:= K^{-1}\mathbf{r}_k + \gamma_k(\mathbf{x}_k - \mathbf{x}_{k-1}) = K^{-1}\mathbf{r}_k + \beta_k \mathbf{p}_{k-1}, \\ \beta_k &:= \epsilon_{k-1}\gamma_k. \end{aligned}$$

- Rewrite

$$\begin{aligned} \mathbf{x}_{k+1} &= \mathbf{x}_k + \epsilon_k \mathbf{p}_k, \\ \mathbf{r}_{k+1} &= \mathbf{r}_k - \epsilon_k A \mathbf{p}_k, \end{aligned}$$

PCG

- Suppose $A \succ 0$,

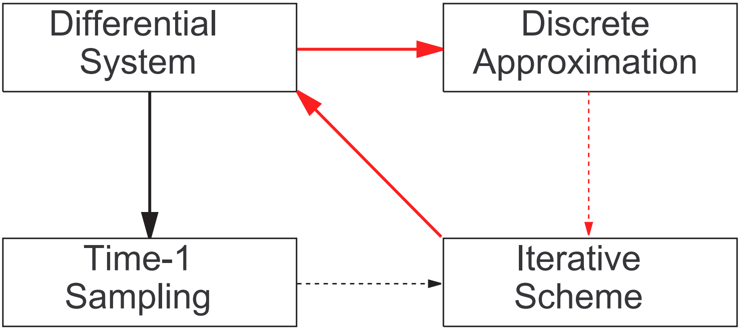
$$\begin{aligned}\epsilon_k &= \frac{\langle \mathbf{p}_k, \mathbf{r}_k \rangle}{\langle A\mathbf{p}_k, \mathbf{p}_k \rangle},\\ \beta_{k+1} &= -\frac{\langle K^{-1}\mathbf{r}_{k+1}, A\mathbf{p}_k \rangle}{\langle A\mathbf{p}_k, \mathbf{p}_k \rangle}, \quad k = 0, 1, \ldots,\end{aligned}$$

- K is a symmetric preconditioner.
- Laughable accuracy, but $\{\mathbf{x}_k\}$ 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



Nonlinear System

- The problem:

$$\mathbf{g}(\mathbf{x}) = 0,$$

  - $\mathbf{g} : \mathbb{R}^n \to \mathbb{R}^n$ is nonlinear.
- Various numerical techniques can be cast in an input-output control framework with different control strategies.

Continuous Control

- Basic model:

$$\begin{aligned} \frac{d\mathbf{x}(t)}{dt} &= \mathbf{u}(t), \\ \mathbf{y}(t) &= -\mathbf{r}(t), \end{aligned}$$

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

$$\mathbf{r}(t) = -\mathbf{g}(\mathbf{x}(t)).$$

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

$$\mathbf{u} = \phi(\mathbf{x}, \mathbf{r}).$$

Control Strategies
(Bhaya & Kaszkurewicz '06)

$\phi(\mathbf{x},\mathbf{r})$	$\frac{dV}{dt}$	$\frac{d\mathbf{x}}{dt}$
$\mathbf{g}'(\mathbf{x})^{-1}\mathbf{r}$	$-\lVert\mathbf{r}\rVert_2^2$	$-\mathbf{g}'(\mathbf{x})^{-1}\mathbf{g}(\mathbf{x})$
$\mathbf{g}'(\mathbf{x})^\top\mathbf{r}$	$-\lVert\mathbf{g}'(\mathbf{x})^\top\mathbf{r}\rVert_2^2$	$-\mathbf{g}'(\mathbf{x})^\top\mathbf{g}(\mathbf{x})$
$\mathbf{g}'(\mathbf{x})^{-1}\mathrm{sgn}(\mathbf{r})$	$-\lVert\mathbf{r}\rVert_1$	$-\mathbf{g}'(\mathbf{x})^{-1}\mathrm{sgn}(\mathbf{g}(\mathbf{x}))$
$\mathrm{sgn}(\mathbf{g}'(\mathbf{x})^\top\mathbf{r})$	$-\lVert\mathbf{g}'(\mathbf{x})^\top\mathbf{r}\rVert_1$	$-\mathrm{sgn}(\mathbf{g}'(\mathbf{x})^\top\mathbf{g}(\mathbf{r}))$
$\mathbf{g}'(\mathbf{x})^\top\mathrm{sgn}(\mathbf{r})$	$-\lVert\mathbf{g}'(\mathbf{x})^\top\mathrm{sgn}(\mathbf{r})\rVert_2^2$	$-\mathbf{g}'(\mathbf{x})^\top\mathrm{sgn}(\mathbf{g}(\mathbf{x}))$

- Lyapunov function

$$V(t) = \begin{cases} \frac{1}{2}\lVert\mathbf{r}(t)\rVert_2^2, & \text{first four cases,} \\ \lVert\mathbf{r}(t)\rVert_1, & \text{last case.} \end{cases}$$

Continuous Newton

- Closed-loop dynamics for the state variable:

$$\frac{d\mathbf{x}}{dt} = \mathbf{u} = -\mathbf{g}'(\mathbf{x})^{-1}\mathbf{g}(\mathbf{x}).$$

  - Sure-fire method $\Rightarrow$ Would fail, only if $\mathbf{g}'(\mathbf{x})$ becomes singular (Smale '76).

- Dynamics for the residual:

$$\frac{d\mathbf{r}}{dt} = -\mathbf{g}'(\mathbf{x})\frac{d\mathbf{x}}{dt} = -\mathbf{r}.$$

- Dynamics for the cost function:

$$\begin{aligned} V(t) &:= \frac{1}{2}\langle \mathbf{r}(t), \mathbf{r}(t)\rangle, \\ \frac{dV}{dt} &= -\|\mathbf{r}\|_2^2. \end{aligned}$$

Discretization

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

Discrete Control

- Basic model:

$$\mathbf{x}_{k+1} = \mathbf{x}_k + \mathbf{u}_k.$$

- Controller:
  - Follow the feedback law:

$$\mathbf{u}_k = \epsilon_k \phi(\mathbf{x}_k, \mathbf{r}_k).$$

  - Also control the step size ϵ_k.

Informal Inquiries

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

$$\mathbf{r}_{k+1} \approx \mathbf{r}_k - \epsilon_k \mathbf{g}'(\mathbf{x}_k)\phi(\mathbf{x}_k, \mathbf{r}_k).$$

  - Line search,

$$\epsilon_k = \frac{\langle \mathbf{g}'(\mathbf{x}_k)\phi(\mathbf{x}_k, \mathbf{r}_k), \mathbf{r}_k \rangle}{\langle \mathbf{g}'(\mathbf{x}_k)\phi(\mathbf{x}_k, \mathbf{r}_k), \mathbf{g}'(\mathbf{x}_k)\phi(\mathbf{x}_k, \mathbf{r}_k) \rangle}.$$

- Some special cases:
  - $\phi(\mathbf{x}, \mathbf{r}) = \mathbf{g}'(\mathbf{x})^{-1}\mathbf{r} \Rightarrow \epsilon_k = 1 \Rightarrow$ Classical Newton iteration.
  - $\mathbf{g}(\mathbf{x}) = A\mathbf{x} - \mathbf{b}$ and $\phi(\mathbf{x}, \mathbf{r}) = K^{-1}\mathbf{r} \Rightarrow$ ORTHOMIN(1) method.

Limiting Behavior of the Residual

- $\{\mathbf{r}_k\}$ may not be a decreasing sequence.
  - $\mathbf{x}_{k+1} - \mathbf{x}_k$ 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 $\mathbf{r}$ before reaching convergence.

Continuity versus Discreteness

(Hauser & Nedić '07)

- Compare the dynamical systems:

$$\begin{aligned} \mathbf{x}_{k+1} &= \mathbf{x}_k + \nu(\mathbf{x}_k). \\ \frac{d\mathbf{x}}{dt} &= \nu(\mathbf{x}). \end{aligned}$$

- $\nu'(\mathbf{x})$ is continuous at $\mathbf{x}^*$.

Superlinear Convergence

- $\{\mathbf{x}_k\}$ converges Q-superlinearly

$$\Leftrightarrow \quad \lim_{\mathbf{x}\to\mathbf{x}^*} \frac{\|\mathbf{x}+\nu(\mathbf{x})-\mathbf{x}^*\|}{\|\mathbf{x}-\mathbf{x}^*\|} = 0.$$

$$\Leftrightarrow \quad \begin{cases} \nu(\mathbf{x}^*) = 0, \\ \nu'(\mathbf{x}^*) = -I. \end{cases}$$

- $\mathbf{x}(t)$ converges exponentially

$$\Leftrightarrow \quad \begin{cases} e^{-(1+\epsilon)t} \le \frac{\|\mathbf{x}(t)-\mathbf{x}^*\|}{\|\mathbf{x}_0-\mathbf{x}^*\|} \le e^{-(1-\epsilon)t}, \\ \left\| \frac{\partial}{\partial t}\left(\frac{\mathbf{x}(t)-\mathbf{x}^*}{\|\mathbf{x}(t)-\mathbf{x}^*\|}\right) \right\| \le \epsilon. \end{cases}$$

- Q-superlinear convergence $\Leftrightarrow$ Exponential convergence.

Higher Order Q-convergence

- $\{\mathbf{x}_k\}$ Q-converges at rate $p+1$

$$\Leftrightarrow \quad \|\mathbf{x}+\nu(\mathbf{x})-\mathbf{x}^*\| \leq \beta\|\mathbf{x}-\mathbf{x}^*\|^{p+1}.$$

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

- $\mathbf{x}(t)$ converges p-exponentially

$$\Leftrightarrow \quad \begin{cases} e^{-(1+\epsilon)t} \leq \frac{\|\mathbf{x}(t)-\mathbf{x}^*\|}{\|\mathbf{x}_0-\mathbf{x}^*\|} \leq e^{-(1-\epsilon)t}, \\ \left\|\frac{\partial}{\partial t}\left(\frac{\mathbf{x}(t)-\mathbf{x}^*}{\|\mathbf{x}(t)-\mathbf{x}^*\|}\right)\right\| \leq \gamma e^{-(1-\epsilon)pt}\|\mathbf{x}_0-\mathbf{x}^*\|^p. \end{cases}$$

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