Continuous Realization Methods and Their Applications

Moody T. Chu

Department of Mathematics
North Carolina State University

About these notes:

Realization process, in a sense, means any deducible procedure that we use to rationalize and solve problems. In mathematics, especially for existence questions, a realization process often appears in the form of an iterative procedure or a differential equation. For years researchers have taken great effort to describe, analyze, and modify realization processes. Nowadays the success is especially evident in discrete numerical algorithms. On the other hand, the use of differential equations to issues in computation has been found recently to afford fundamental insights into the structure and behavior of existing discrete methods and, sometimes, to suggest new and improved numerical methods. In some cases, there are remarkable connections between smooth flows and discrete numerical algorithms. In other cases, the flow approach seems advantageous in tackling very difficult problems.

These notes, summarizing my limited understanding and ongoing research on the subject of *continuous realization methods*, were prepared for lecture presentations at the Academia Sinica in Taiwan, the Australian National University in Canberra, and various other universities during my sabbatical leave in 1996.

In this expository series the emphasis is on using differential equation techniques as a special continuous realization process for problems arising from the field of linear algebra. The matrix differential equations are cast in fairly general frameworks of which special cases have been found to be closely related to important numerical algorithms. The main thrust is to study the dynamics of various isospectral flows. This approach has potential applications ranging from new development of numerical algorithms, including VLSI implementation, to theoretical solution of open problems. Various aspects of the recent development and application in this direction will be discussed in the sequel.

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Moody T. Chu

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Contents

Lecture 1

Introduction

- Basic component
- Building the bridge
- Characteristic of a bridge
- Examples

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. Projected gradient methods.
- Only some general guidance is available.
  - ◇ A bridge is built in a straightforward way.
  - ◇ No guarantee the path will be complete.
  - ◇ e.g. Homotopy methods.
- 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 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.

Examples

- The eigenvalue problem
- The nonlinear algebraic equation
- The least squares matrix approximation
- List of other applications

The Eigenvalue Problem

- The mathematical problem:
  - ◇ A symmetric matrix A_0 is given.
  - ◇ Solve the equation

$$A_0 x = \lambda x$$

for a nonzero vector x and a scalar λ.

- An iterative method :
  - ◇ The QR decomposition:

$$A = QR$$

where Q is orthogonal and R is upper triangular.

  - ◇ The QR algorithm (Francis '61):

$$\begin{aligned} A_k &= Q_k R_k \\ A_{k+1} &= R_k Q_k. \end{aligned}$$

  - ◇ The sequence $\{A_k\}$ converges to a diagonal matrix.
  - ◇ Every matrix A_k has the same eigenvalues of A_0.

- A continuous method:
  - ◇ 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):

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

  - ◇ Sampled at integer times, $\{X(k)\}$ gives the same sequence as does the QR algorithm applied to the matrix $A_0 = exp(X_0)$.
- The bridge between X_0 and the limit point of Toda flow is built on the basis of maintaining isospectrum.
  - ◇ What motivates the construction of Toda lattice?
  - ◇ Why is convergence guaranteed?

Nonlinear algebraic equations

- The mathematical problem:
  - ◇ A sufficiently smooth function $f : R^n \rightarrow R^n$ is given.
  - ◇ Solve the equation

$$f(x) = 0.$$

- An iterative method:
  - ◇ The Newton method:

$$x_{k+1} = x_k - \alpha_k (f'(x_k))^{-1} f(x_k).$$

  - ◇ The sequence $\{x_k\}$ converges quadratically to a solution, if x_0 is sufficiently close to that solution.

- A continuous method (Smale '76, Keller '78, etc.):
  - ◇ The Newton homotopy:
  $$H(x,t) = f(x) - tf(x_0).$$
  - ◇ The zero set $\{(x,t) \in R^{n+1} | H(x,t) = 0\}$ is a smooth curve.
  - ◇ The homotopy curve:
  $$\begin{aligned} f'(x)\frac{dx}{ds} - \frac{1}{t}f(x)\frac{dt}{ds} &= 0 \\ x(0) &= x_0 \\ t(0) &= 1 \end{aligned}$$
  where s is the arc length.
  - ◇ Suppose $f'(x)$ is nonsingular. Then written as
  $$\frac{dx}{ds} = \frac{dt}{ds}\frac{1}{t}(f'(x))^{-1}f(x).$$
  - ◇ With appropriate step size chosen, an Euler step is equivalent to a regular Newton method.

- The bridge is built upon the hope that the obvious solution will be deformed mathematically into the solution that we are seeking for.
  - ◇ 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.
  - ◇ None of these techniques is easy.

- A continuous approach (Brockett '88, Chu & Driessel '90):
  - ◇ The projection of the gradient of F can easily be calculated.
  - ◇ Projected gradient flow:

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

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

Isospectral Flows

- QR flow for normal matrices (Chu '84).
- Generalized Toda flow (Chu '84, Watkins '84).
- QZ flow (Chu '86).
- Continuous Rayleigh quotient flow (Chu '86).
- SVD flow (Chu '86).
- Abstract QR-type flow (Chu '88).
- Scaled Toda-like flow (Chu '95).

Projected Gradient Flows

- Brockett's double bracket flow (Brockett '88).
- Least squares approximation with spectral constraints (Chu & Driessel '90).
- Simultaneous reduction problem (Chu '91).
- Nearest normal matrix problem (Chu '91).
- Inverse eigenvalue problem for nonnegative matrices (Chu & Driessel '91).
- Inverse singular value problem (Chu '92).

Generalized Flows

- Matrix differential equations (Chu '92).
- Schur-Horn theorem (Chu '95).
- Least squares inverse eigenvalue problem (Chu & Chen '96).
- Inverse generalized eigenvalue problem (Chu & Guo '??).
- Inverse stochastic eigenvalue problem (Chu & Guo '??).

Lecture 2

QR-Type Flows

- Overview
- Basic form
- General framework
- Governing flows
- Basic theorems
- Abstract QR decompositions
- Abstract QR-type algorithms
- Relation to classical algorithms
- Nonclassical examples

Overview

- Construct a flow in the space of all $n \times n$ real matrices.
- Every element in the flow has the same eigenvalues.
- The flow converges to a limit point which has a specified structure.

Notations

$$\begin{aligned}
Gl(n) &:= \{n \times n \text{ real nonsingular matrices}\} \\
gl(n) &:= \{n \times n \text{ real matrices}\} \\
X_0 &:= \text{A given matrix in} gl(n) \\
M(X_0) &:= \{g^{-1} X_0 g | g \in Gl(n)\} \\
[A, B] &:= AB - BA \text{ (Lie bracket)} \\
T &:= \text{Subspace of } gl(n) \\
P_T &:= \text{Projection mapping from } gl(n) \text{ to } T
\end{aligned}$$

Basic Form

- Generic flow:

$$\frac{dX}{dt} = [X, k(X)].$$

- Basic relationship:
  - ◇
  $$\begin{aligned} \frac{dg(t)}{dt} &= g(t)k(t) \\ g(0) &= I \end{aligned}$$
  - ◇
  $$\begin{aligned} \frac{dX(t)}{dt} &= [X(t), k(t)] \\ X(0) &= X_0 \end{aligned}$$
  - ◇
  $$X(t) = g(t)^{-1} X_0 g(t).$$

General Framework

- Subspace splitting of $gl(n)$:

$$gl(n) = T_1 + T_2.$$

  - ◇ T_1 and T_2 are subspaces of $gl(n)$.
  - ◇ This is a subspace decomposition only, not necessarily a subalgebra decomposition of $gl(n)$.
  - ◇ Given T_1, one may choose $T_2 = gl(n) - T_1$. This is not necessarily a direct sum decomposition.

Examples

- Toda flow:
  - ◇ T_1 = Subspace of skew symmetric matrices.
  - ◇ $$k(X) := (X^-) - (X^-)^T.$$
- General flow:
  - ◇ T_1 = Arbitrary linear subspace.
  - ◇ $$k(X) := \text{Projection of } X \text{ onto subspace } T_1.$$
  - ◇ Time-1 mapping of the solution still enjoys a QR-type algorithm.
- Application to structured eigenvalue problems:
  - ◇ A QR-type algorithm preserving the Hamiltonian structure exists for the Hamiltonian eigenvalue problem.

Governing Flows

- The governing flow:

$$\begin{aligned} \frac{dX(t)}{dt} &:= [X(t), P_1(X(t))] \\ X(0) &:= X_0 \end{aligned}$$

  - ◇ P_1 := Projection onto T_1.
- The associated flows:

$$\begin{aligned} \frac{dg_1(t)}{dt} &:= g_1(t)P_1(X(t)) \\ g_1(0) &:= I \end{aligned}$$

and

$$\begin{aligned} \frac{dg_2(t)}{dt} &:= P_2(X(t))g_2(t) \\ g_2(0) &:= I \end{aligned}$$

  - ◇ P_2 := Projection onto T_2.

Basic Theorems

All flows enjoys three basic properties:

- Similarity Property
- Decomposition Property
- Reverse Property

Similarity Property

$$X(t) = g_1(t)^{-1} X_0 g_1(t) = g_2(t) X_0 g_2(t)^{-1}.$$

- Define $Z(t) = g_1(t) X(t) g_1(t)^{-1}$.
- Check

$$\begin{aligned}\frac{dZ}{dt} &= \frac{dg_1}{dt} X g_1^{-1} + g_1 \frac{dX}{dt} g_1^{-1} + g_1 X \frac{dg_1^{-1}}{dt} \\ &= (g_1 P_1(X)) X g_1^{-1} \\ &\quad + g_1 (X P_1(X) - P_1(X) X) g_1^{-1} \\ &\quad + g_1 X (-P_1(X) g_1^{-1}) \\ &= 0.\end{aligned}$$

- Thus $Z(t) = Z(0) = X(0) = X_0$.

Decomposition Property

$$exp(tX_0) = g_1(t)g_2(t).$$

- Trivially $exp(X_0 t)$ satisfies the IVP
$$\frac{dY}{dt} = X_0 Y, Y(0) = I.$$
- Define $Z(t) = g_1(t)g_2(t)$.
- Then $Z(0) = I$ and
$$\begin{aligned} \frac{dZ}{dt} &= \frac{dg_1}{dt} g_2 + g_1 \frac{dg_2}{dt} \\ &= (g_1 P_1(X))g_2 + g_1(P_2(X)g_2) \\ &= g_1 X g_2 \\ &= X_0 Z \quad \text{(by Similarity Property).} \end{aligned}$$
- By the uniqueness theorem in the theory of ordinary differential equations, $Z(t) = exp(X_0 t)$.

Reverse Property

$$exp(tX(t)) = g_2(t)g_1(t).$$

- By Decomposition Property,
$$\begin{aligned} g_2(t)g_1(t) &= g_1(t)^{-1} exp(X_0 t) g_1(t) \\ &= exp(g_1(t)^{-1} X_0 g_1(t) t) \\ &= exp(X(t)t). \end{aligned}$$

Abstract QR-type Decomposition

- In Lie theory, corresponding to a Lie algebra decomposition of $gl(n)$, there is a Lie group decomposition of $Gl(n)$ in the neighborhood of I.
- We have shown, corresponding to a subspace decomposition $gl(n) = T_1 + T_2$, every matrix in the neighborhood of I can still be written as the product of two nonsingular matrices, i.e.,

$$exp(X_0 t) = g_1(t) g_2(t).$$

- The product $g_1(t)g_2(t)$ will be called the abstract $g_1 g_2$ decomposition of $exp(X_0 t)$.

Abstract QR-type Algorithm

- By setting $t = 1$ in Theorems 2 and 3, we have

$$\begin{aligned} exp(X(0)) &= g_1(1)g_2(1) \\ exp(X(1)) &= g_2(1)g_1(1). \end{aligned}$$

- Since the differential equation for $X(t)$ is autonomous, the above phenomenon will occur at every feasible integer time.
- Corresponding to the abstract $g_1 g_2$ decomposition, the above iterative process for all feasible integers will be called the abstract $g_1 g_2$ algorithm.

Relation to Classical Algorithms

	Case 1	Case 2	Case 3
T_1	$o(n)$	$l(n)$	$l(n)+d(n)/2$
T_2	$r(n)+d(n)$	$r(n)+d(n)$	$r(n)+d(n)/2$
$k(t)=P_1(X(t))$	$X^- - X^{-T}$	X^-	$X^- + X^0/2$
$P_2(X(t))$	$X^+ + X^0 + X^{-T}$	$X^+ + X^0$	$X^+ + X^0/2$
$g_1(t)$	$\mathrm{Q}(t)\in O(n)$	$\mathrm{L}(t)\in L(n)$	$\mathrm{G}(t)\in L(n)$
$g_2(t)$	$\mathrm{R}(t)\in R(n)$	$\mathrm{U}(t)\in R(n)$	$\mathrm{H}(t)\in R(n)$
Algorithm	QR	LU	Cholesky

$$
\begin{aligned}
o(n) &:= \{\text{Skew-symmetric matrices in } gl(n)\}\\
O(n) &:= \{\text{Orthogonal matrices in } Gl(n)\}\\
r(n) &:= \{\text{Strictly upper triangular matrices in } gl(n)\}\\
R(n) &:= \{\text{Upper triangular matrices in } Gl(n)\}\\
l(n) &:= \{\text{Strictly lower triangular matrices in } gl(n)\}\\
L(n) &:= \{\text{Lower triangular matrices in } Gl(n)\}\\
d(n) &:= \{\text{Diagonal matrices in } Gl(n)\}
\end{aligned}
$$

$$
\begin{aligned}
X^+ &:= \text{The strictly upper triangular matrix of } X\\
X^o &:= \text{The diagonal matrix of } X\\
X^- &:= \text{The strictly lower triangular matrix of } X
\end{aligned}
$$

Nonclassical Examples

- Assume:

$$
\begin{aligned}
X_0 &:= \text{symmetric}\\
\Delta &:= \text{Active index subset}\\
\hat{X}(t) &:= \text{Portion of } X(t) \text{ conforming to } \Delta\\
P_1(X(t)) &:= \hat{X}(t) - (\hat{X}(t))^T\\
P_2(X(t)) &:= X(t) - P_1(X(t))
\end{aligned}
$$

Then:

For all $(i,j)\in\Delta,\ x_{ij}(t)\longrightarrow 0$ as $t\longrightarrow\infty$.

- ◇ The above result suggests a way to produce (or knock out) any prescribed pattern that is symmetric to the diagonal of a symmetric matrix.
- ◇ The above result may be interpreted as a generalization of the Schur decomposition theorem (which knocks out the entire off-diagonal elements) for symmetric matrices.
- ◇ When $\Delta = \{(i,j)|1\le j < i-1 \le n-1\}$, the dynamical system represents a continuous tridiagonalization process.

- Assume

$$
\begin{aligned}
X_0 &:= \text{general (distinct eigenvalues)} \\
\Delta &\subset \{(i,j) | 1 \le j < i \le n\} \\
&:= \text{a } \textit{rectangular} \text{ index subset} \\
\hat{X}(t) &:= \text{Portion of } X(t) \text{ conforming to } \Delta \\
P_1(X(t)) &:= \hat{X}(t) - (\hat{X}(t))^T \\
P_2(X(t)) &:= X(t) - P_1(X(t))
\end{aligned}
$$

Then

For all $(i,j) \in \Delta$, $x_{ij}(t) \longrightarrow 0$ as $t \longrightarrow \infty$.

◇ The above result remains true if Δ is such that its complement represents a block upper triangular matrix. In this case, we have a continuous realization of the so called treppeniteration.

- Assume

$$
\begin{aligned}
X_0 &:= \text{Hamiltonian } \in gl(2n) \\
&:= \begin{bmatrix} A_0, & N_0 \\ K_0, & -A_0^T \end{bmatrix} \\
K, N &:= \text{symmetric } \in gl(n) \\
P_1(X(t)) &:= \begin{bmatrix} 0, & -K(t) \\ K(t), & 0 \end{bmatrix}
\end{aligned}
$$

Then

a) $[X, P_1(X)]$ is Hamiltonian

b) g_1 is both orthogonal and sympletic

c) $X(t)$ remains Hamiltonian

d) $K(t) \longrightarrow 0$ as $t \longrightarrow \infty$.

◇ The Hamiltonian eigenvalue problem for X_0 practically becomes the eigenvalue problem for

$$\lim_{t\to\infty} A(t).$$

◇ No explicit iterative scheme is known for the Hamiltonian eigenvalue problem due to the lack of knowledge of the structure of $g_2(t)$ in the abstract decomposition of $exp(X_0 t)$.

Lecture 3

Homotopy Method for λ-Matrix Problem

- Overview
- Basic ideas
- Preliminary facts
- Homotopy method
- Numerical experiment

Overview

- The problem:
  - ◇ Given $A_0, A_1, \ldots, A_k \in C^{n\times n}$, define
    $P(\lambda) := A_k\lambda^k + A_{k-1}\lambda^{k-1} + \ldots + A_1\lambda + A_0.$
  - ◇ Find $\lambda \in C$ and $x \in C^n$ such that
    $$P(\lambda)x = 0.$$
- Special cases:
  - ◇ Regular eigenvalue problem:
    $$\lambda x = Ax.$$
  - ◇ Generalized eigenvalue problem:
    $$\lambda Bx = Ax.$$

Numerical Methods

- Solving the linearized problem:
  - ◇ Can make use of existing software.
  - ◇ Increase the size considerably.
- Direct iteration:
  - ◇ Subspace iteration — global but slow
  - ◇ Newton-type iteration — fast but local
- Reducing to the canonical form:
  - ◇ Need polynomial root solver.
  - ◇ Ill-conditioned.
- Homotopy method:
  - ◇ Maybe costly in tracing curves.
  - ◇ Can follow curves simultaneously.
  - ◇ Guarantee to reach all isolated eigenpairs.
  - ◇ Matrix structure is respected.

Basic Ideas

- Homotopy equation:

$$H(x,t) = (1-t)g(x) + tf(x) = 0.$$

- Zero set:

$$H^{-1}(0) = \{(x,t) | H(x,t) = 0\}.$$

- Practical concerns:
  - ◇ Need to ensure $H^{-1}(0)$ is a 1-dimensional manifold.
  - ◇ Need to ensure the curve extens from $t = 0$ to $t = 1$.
- Curve tracing:

$$\begin{aligned} \left[\, D_x H \;\; D_t H \,\right] \begin{bmatrix} \frac{dx}{ds} \\ \frac{dt}{ds} \end{bmatrix} &= 0 \\ x(0) &= \text{zero(s) of } g(x) \\ t(0) &= 0. \end{aligned}$$

A Simple Example

- The problem:

$$\begin{aligned} \lambda x &= Ax \\ x^T x &= 1 \\ A &:= \text{real, symmetric and tridiagonal.} \end{aligned}$$

  - ◇ A nonlinear (polynomial) system in $n+1$ unknowns x and λ.
  - ◇ # of solutions $\leq$ Bezout number $= 2^{n+1}$.
- The homotopy:

$$\begin{aligned} H &: R^n \times R \times R \longrightarrow R^n \times R \\ H(x,\lambda,t) &:= \left([D + t(A-D)]x - \lambda x, \frac{1 - x^T x}{2} \right) \\ D &:= \text{diagonal with distinct elements.} \end{aligned}$$

- Existence of the curve:
  - ◇ Rank of

$$D_{(x,\lambda)} = \begin{bmatrix} D + t(A-D) - \lambda, & -x \\ -x^T, & 0 \end{bmatrix}$$

    is of rank $n+1$.
  - ◇ Implicit function theorem $\Rightarrow (x, \lambda)$ is a function of t.
- Extension of the curve:
  - ◇ Gershgorin's theorem $\Rightarrow$ Boundedness of the curves.
  - ◇ Curves must extend to $t = 1$.

Preliminary Facts

- Regularity and canonical form
- Resultant theorem
- Perturbation theorem
- Rank property

Regularity and Canonical Form

- A_k is nonsingular $\Rightarrow$ $P(\lambda)$ is regular, i.e., has nk eigenvalues.
- $P(\lambda)$ is regular $\Rightarrow$ There exist $E(\lambda)$ and $F(\lambda)$ such that

$$E(\lambda)P(\lambda)F(\lambda) = \mathrm{diag}(a_1(\lambda), \ldots, a_n(\lambda)).$$

  - ◇ $\det(E(\lambda)), \det(F(\lambda))$ = nonzero constants.
  - ◇ $a_i(\lambda)$ is a monic polynomial.
  - ◇ $a_i(\lambda)$ is unique.
  - ◇ $a_i(\lambda) | a_{i+1}(\lambda)$.

Resultant Theorem

- Resultant of two polynomials:

$$\begin{aligned} R &= R(a_0, \ldots, a_n, b_0, \ldots, b_m) \\ &= \det \begin{bmatrix} a_0 & a_1 & & \ldots & a_n & 0 & \ldots & 0 \\ 0 & a_0 & a_1 & & & a_n & \ldots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots & & \ddots & \\ & & & & a_1 & & & \\ 0 & \ldots & & & a_0 & a_1 & \ldots & a_n \\ b_0 & b_1 & \ldots & & 0 & \ldots & & \\ 0 & b_0 & b_1 & \ldots & & & & 0 \\ \vdots & \ddots & \ddots & & \vdots & & & \\ 0 & \ldots & & b_0 & b_1 & \ldots & & b_m \end{bmatrix}. \end{aligned}$$

  - ◇ $f(x) = a_0 + a_1 x + \ldots\ldots + a_n x^n$.
  - ◇ $g(x) = b_0 + b_1 x + \ldots + b_m x^m$.
- f and g have common non-constant factor $\Leftrightarrow$ $R = 0$.

Perturbation Theorem

- There exist real numbers $d_1, \ldots, d_n$ such that $p(\lambda) := \det(P(\lambda) - D)$ has no multiple roots.
  - ◇ $D := \mathrm{diag}(d_1, \ldots, d_n)$.
- The set

  $$\{(d_1, \ldots, d_n) | P(\lambda) - D \text{ has multiple eigenvalues}\}$$

  is of complex codimension 1.
- With probability one the matrix $P(\lambda) - D$ has distinct eigenvalues.

Rank Property

- $P(\lambda)$ has nk distinct eigenvalues and $P(\lambda_j)x_j = 0 \Rightarrow$

  $$Q(x_j, \lambda_j) := [P(\lambda_j), P'(\lambda_j)x_j]$$

  is of complex rank n.
- Identify a linear transformation $C^{n+1} \longrightarrow C^n$ as a transformation $R^{2n+2} \longrightarrow R^{2n}$:
  - ◇ Replace each component, say $x_j = a_j + ib_j$, of the vector by $[a_1, b_1]^T$.
  - ◇ Replace each component, say $z = a + ib$, of the transformation matrix by $\begin{bmatrix} a, & -b \\ b, & a \end{bmatrix}$.

  $$Q \in C^{n \times (n+1)} \hookrightarrow \hat{Q} \in R^{2n \times (2n+2)}.$$

- If $P(\lambda)x = 0$, then

  $$M(x, \lambda) := \begin{bmatrix} \hat{Q}(x_j, \lambda_j) \\ a_1, b_1, a_2, \ldots, a_n, b_n, 0, 0 \end{bmatrix}$$

  is of real rank $2n + 1$ in $R^{(2n+1) \times (2n+2)}$.

Homotopy Method

- Notation:

$$\begin{aligned} P(\lambda) &= A_k\lambda^k + A_{k-1}\lambda^{k-1} + \ldots + A_0 \\ Q(\lambda) &= cI\lambda^k - D \\ R(\lambda, t, c, D) &= (1-t)Q(\lambda) + tP(\lambda) \\ D &= \mathrm{diag}(d_1, \ldots, d_n) \\ c, d_1, \ldots, d_n &= \text{ complex numbers} \end{aligned}$$

- Control of regularity:

$$R(\lambda, t, c, D) = [(1-t)cI + tA_k]\lambda^k + \ldots$$

◇ Choose d from an open dense set such that $[(1-t)cI + tA_k]$ is nonsingular for $0 \leq t < 1$.

- The homotopy:

$$\begin{aligned} H &: C^n \times C \times [0,1) \longrightarrow C^n \times C \\ H(x, \lambda, t) &:= \begin{bmatrix} R(\lambda, t, c, D)x \\ \frac{x^*x-1}{2} \end{bmatrix}. \end{aligned}$$

- Initial values:

$$\begin{aligned} e_i &= \text{ The standard } i\text{-th unit vector,} \\ \lambda_{ij} &= \text{ The } j\text{-th complex root of } (\frac{d_i}{d})^{1/k}. \end{aligned}$$

◇ $i = 1, \ldots, n$ and $j = 1, \ldots, k$.

◇ $H(e_i, \lambda_{ij}, 0) = 0$.

Major Theorem

There exists an open, dense, full measure subset $U \subset C^n$ such that, for $(d_1, \ldots, d_n) \in U$ and each initial point $y_{ij} := (e_i, \lambda_{ij}, 0)$, the connected component $C(y_{ij})$ of y_{ij} in $H^{-1}(0)$, when identified as a subset in $R^{2n} \times R^2 \times R$, has the following properties:

- $C(y_{ij})$ is a real analytic submanifold with real dimension 2.
- The intersection of $C(y_{ij})$ with each hyperplane $t \equiv$ constant $\in [0, 1)$ is a unit circle centered $(0, \lambda) \in R^{2n} \times R$ for some λ.
- Manifolds $C(y_{ij})$ corresponding to different initial points do not intersect for $t \in [0, 1)$.
- Each manifold $C(y_{ij})$ is bounded for $t \in [0, 1)$.

Computation

- It is a tube:

$$H : R^{2n} \times R^2 \times R \longrightarrow R^{2n} \times R.$$

  - ◇ $C(y_{ij})$ is a 2-dimensional tube with unit radius at each cross-section $t \equiv$ constant.

- Need a vector field on the tube:
  - ◇ The path can be parametrized by the variable t.
  - ◇ Define vector field $(\dot{x}, \dot{\lambda}, 1)$ on $H^{-1}(0)$ by

$$M(x, \lambda, t) \begin{bmatrix} \dot{x} \\ \dot{\lambda} \end{bmatrix} = \begin{bmatrix} (Q(\lambda) - P(\lambda))x \\ 0 \end{bmatrix},$$

$$[ix^T, 0] \begin{bmatrix} \dot{x} \\ \dot{\lambda} \end{bmatrix} = 0.$$

    - ▷ First equation is necessary for being tangent.
    - ▷ Second equation means the vector field is perpendicular to the circle of intersection.

- Observe:

$$\begin{bmatrix} M(x,\lambda,t) \\ ix^T, 0 \end{bmatrix} = \begin{bmatrix} & \hat{Q}(x,\lambda,t) & \\ a_1, & b_1, \ldots, a_n, & b_n, \ 0, \ 0 \\ -b_1, & a_1, \ldots, -b_n, & a_n, \ 0, \ 0 \end{bmatrix}$$
$$\hookrightarrow \begin{bmatrix} R(\lambda,t,c,D), & R'(\lambda,t,c,D)x \\ x^*, & 0 \end{bmatrix}.$$

- The initial value problem in $C^n \times C$:

$$\begin{bmatrix} R(\lambda,t,c,D), & R'(\lambda,t,c,D)x \\ x^*, & 0 \end{bmatrix} \begin{bmatrix} \frac{dx}{dt} \\ \frac{d\lambda}{dt} \end{bmatrix} = \begin{bmatrix} (Q(\lambda)-P(\lambda))x \\ 0 \end{bmatrix},$$
$$x(0)=e_i$$
$$\lambda(0)=\lambda_{ij}$$

  ◇ $i = 1, \ldots, n$ and $j = 1, \ldots, k$.

- Parallel computation:
  ◇ Homotopy curves are independent of each other.
  ◇ Can integrate simultaneously.
- Sparsity preservation: $R(\lambda, t, c, D)$ does not destroy the matrix structure of the coefficients in $P(\lambda)$.

Lecture 4

Spectrally Constrained Problems

- Overview
- General framework
- Special cases
- Reformulation
- Geometry of $\mathcal{O}(n)$
- Projected gradient
- Isospectral descent flow
- Second order condition
- Least squares matrix approximation
- Inverse eigenvalue problem
- Symmetric eigenvalue problem

Overview

- Least squares approximations for various types of real and symmetric matrices subject to spectral constraints share a common structure.
- The projected gradient can be formulated explicitly.
- A descent flow can be followed numerically.
- The procedure can be extended to general matrices subject to singular value constraints.

General Framework

$$\begin{aligned} \text{Minimize } F(X) &:= \frac{1}{2}||X - P(X)||^2 \\ \text{Subject to } X &\in M(\Lambda) \end{aligned}$$

$$\begin{aligned} S(n) &:= \{\text{All real symmetric matrices}\} \\ O(n) &:= \{\text{All real orthogonal matrices}\} \\ ||X|| &:= \text{ Frobenius matrix norm of } X \\ \Lambda &:= \text{ A given matrix in } S(n) \\ M(\Lambda) &:= \{Q^T \Lambda Q | Q \in O(n)\} \\ V &:= \text{ A single matrix or a subspace in } S(n) \\ P(X) &:= \text{ The projection of } X \text{ into } V \end{aligned}$$

Special Cases

- Problem A:
  - ◇ Find the least squares approximation of a given symmetric matrix subject to a prescribed set of eigenvalues.
- Problem B:
  - ◇ Construct a symmetric Toeplitz matrix that has a prescribed set of eigenvalues.
- Problem C:
  - ◇ Calculate the eigenvalue of a given symmetric matrix.

Reformulation

- Rewrite the problem in terms of the coordinate variable Q:

$$\begin{aligned}\text{Minimize } F(Q) &:= \frac{1}{2}\langle Q^T\Lambda Q - P(Q^T\Lambda Q), \\ &\qquad Q^T\Lambda Q - P(Q^T\Lambda Q)\rangle \\ \text{Subject to } Q^TQ &= I\end{aligned}$$

  - ◇ $\langle A, B\rangle = \text{trace}(AB^T)$ is the Frobenius inner product.

Geometry of $\mathcal{O}(n)$

- The set $O(n)$ is a regular surface.
- The tangent space of $O(n)$ at any orthogonal matrix Q is given by
$$T_Q O(n) = QK(n)$$
  ◇
$$K(n) = \{\text{All skew-symmetric matrices}\}.$$
- The normal space of $O(n)$ at any orthogonal matrix Q is given by
$$N_Q O(n) = QS(n).$$

Projected Gradient

- The Fréchet Derivative of F at a general matrix A acting on B:
$$F'(A)B = 2\langle \Lambda A(A^T \Lambda A - P(A^T \Lambda A)), B\rangle.$$
- The gradient of F at a general matrix A:
$$\nabla F(A) = 2\Lambda A(A^T \Lambda A - P(A^T \Lambda A)).$$

The Projected Gradient

- A splitting of $R^{n\times n}$:

$$\begin{aligned} R^{n\times n} &= T_Q O(n) + N_Q O(n) \\ &= QK(n) + QS(n). \end{aligned}$$

- Any $X \in R^{n\times n}$ has a unique orthogonal splitting:

$$X = Q\left\{\frac{1}{2}(Q^T X - X^T Q) + \frac{1}{2}(Q^T X + X^T Q)\right\}.$$

- The gradient $\nabla F(Q)$ can be projected into the tangent space easily:

$$\begin{aligned} g(Q) &= Q\left\{\frac{1}{2}(Q^T \nabla F(Q) - \nabla F(Q)^T Q)\right\} \\ &= Q[P(Q^T \Lambda Q), Q^T \Lambda Q]. \end{aligned}$$

Isospectral Descent Flow

- A descent flow on the manifold $O(n)$:

$$\frac{dQ}{dt} = Q[Q^T \Lambda Q, P(Q^T \Lambda Q)].$$

- A descent flow on the manifold $M(\Lambda)$:

$$\begin{aligned} \frac{dX}{dt} &= \frac{dQ^T}{dt}\Lambda Q + Q^T \Lambda \frac{dQ}{dt} \\ &= [X, [X, P(X)]]. \end{aligned}$$

Second Order Derivative

- Extend the projected gradient g to the function
$$G(Z) := Z[P(Z^T\Lambda Z), Z^T\Lambda Z]$$
for general matrix Z.
- The Fréchet derivative of G:
$$\begin{aligned} G'(Z)H &= H[P(Z^T\Lambda Z), Z^T\Lambda Z] \\ &+ Z[P(Z^T\Lambda Z), Z^T\Lambda H + H^T\Lambda Z] \\ &+ Z[P'(Z^T\Lambda Z)(Z^T\Lambda H + H^T\Lambda Z), Z^T\Lambda Z]. \end{aligned}$$
- The projected Hessian at a critical point $X = Q^T\Lambda Q$ for the tangent vector QK with $K \in K(n)$ is described explicitly by the quadratic form:
$$\begin{aligned} &\langle G'(Q)QK, QK\rangle = \\ &\langle [P(X), K] - P'(X)[X, K], [X, K]\rangle. \end{aligned}$$

Least Squares Matrix Approximation

- Given a symmetric matrix N, find its least squares approximation whose eigenvalues are $\{\lambda_1, \ldots, \lambda_n\}$.
- Setup:
  - ⋄ $\Lambda := \mathrm{diag}\{\lambda_1, \ldots, \lambda_n\}$.
  - ⋄ The projection is $P(X) = N$.
- The projected gradient:
$$g(Q) = Q[N, Q^T\Lambda Q].$$
- The descent flow:
$$\begin{aligned} \frac{dX}{dt} &= [X, [X, N]] \\ X(0) &= \Lambda. \end{aligned}$$

Second Order Condition

- Assume
  - ◇ The given eigenvalues are $\lambda_1 > \ldots > \lambda_n$.
  - ◇ The eigenvalues of N are $\mu_1 > \ldots > \mu_n$.
  - ◇ Q is a critical point on $O(n)$ and define

$$\begin{aligned} X &:= Q^T \Lambda Q \\ E &:= Q N Q^T. \end{aligned}$$

- The first order condition:

$$[N, X] = 0$$

  - ◇ E must be a diagonal matrix.
  - ◇ E must be a permutation of $\mu_1, \ldots, \mu_n$.
- The projected Hessian:

$$\begin{aligned} \langle G'(Q)QK, QK \rangle &= \langle [N, K], [X, K] \rangle \\ &= \langle E\hat{K} - \hat{K}E, \Lambda\hat{K} - \hat{K}\Lambda \rangle \\ &= 2 \sum_{i<j} (\lambda_i - \lambda_j)(e_i - e_j)\hat{k}_{ij}^2. \end{aligned}$$

Significance

- If a matrix Q is optimal, then:
  - ◇ Columns of $Q^T = [q_1, \ldots, q_n]$ must be the normalized eigenvectors of N corresponding in the order to $\mu_1, \ldots, \mu_n$.
  - ◇ The solution is unique.
  - ◇ The solution is given by

$$X = \lambda_1 q_1 {q_1}^T + \ldots + \lambda_n q_n {q_n}^T.$$

- We have reproved the Wielandt-Hoffman theorem.
- The dynamics in the problem enjoys a special sorting property.
  - ◇ Can be applied to data matching and a variety of combinatorial optimization problems, including the LP problem.

Inverse Toeplitz Eigenvalue Problem

- Construct a symmetric Toeplitz matrix whose eigenvalues are $\{\lambda_1, \ldots, \lambda_n\}$
- Setup:
  - ⋄ The set $\mathcal{T}$ of all symmetric Toeplitz matrices forms a linear subspace with a natural basis $E_1, \ldots, E_n$.
  - ⋄ $\Lambda := \mathrm{diag}\{\lambda_1, \ldots, \lambda_n\}$.
  - ⋄ The projection of any matrix X is easy:

$$P(X) = \sum_{i=1}^{n} \langle X, E_i \rangle E_i.$$

- The projected gradient:

$$g(Q) = Q[P(Q^T \Lambda Q), Q^T \Lambda Q].$$

- The descent flow:

$$\begin{aligned} \frac{dX}{dt} &= [X, [X, P(X)]] \\ X(0) &= \text{Anything but diagonals in } M(\Lambda). \end{aligned}$$

Significance

- The descent flow approach offers a globally convergent method for solving the inverse Toeplitz eigenvalue problem.
- A stable critical point may not be Toeplitz.
- The second order condition has not be analyzed yet. Further work is needed.

Symmetric Eigenvalue Problem

- Setup:
  - ◇ $\Lambda = X_0$, the matrix whose eigenvalues are to be found.
  - ◇ V = the subspace of all diagonal matrices.
  - ◇ $P(X) = \mathrm{diag}(X)$.
- The objective is the same as that of the Jacobi method, i.e., to minimize the off-diagonal elements.
- The descent flow:

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

- Let X be a critical point. Then
  - ◇ If X is a diagonal matrix, then X is a global minimizer.
  - ◇ If X is not a diagonal matrix but $\mathrm{diag}(X)$ is a scalar matrix, then X is a global maximizer.
  - ◇ If X is not a diagonal matrix and $\mathrm{diag}(X)$ is not a scalar matrix, then X is a saddle point.

Lecture 5

Simultaneous Reduction Problems

- Overview
- Reduction by orthogonal similarity
- Gradient flow for orthogonal similarity
- Nearest commuting pair problem
- Reduction by orthogonal equivalence
- Descent flow for orthogonal equivalence
- Nearest normal matrix problem

Overview

What is the simplest form to which a family of matrices depending smoothly on the parameters can be reduced by a change of coordinates depending smoothly on the parameters?

- Arnold '88

- Two types of transformations:
  - ◇ Similarity transformation $Q^T AQ$.
  - ◇ Equivalence transformation $Q^T AZ$.

- Applications:
  - ◇ Computation of eigenvalues, generalized eigenvalues and singular values.
  - ◇ Simultaneous reduction of more than one matrices:
    - ▷ System identification in control.
    - ▷ Multibody oscillations in mechanics.
  - ◇ Matrix canonical forms.
- Significance:
  - ◇ Very few theories or numerical methods are available.
  - ◇ Projected gradient method offers an easy but versatile reduction procedure.

Reduction by Orthogonal Similarity

- The problem:
  - ◇ Matrices A_i and subspaces V_i in $R^{n\times n}$, $i = 1,\ldots,p$, are given.
  - ◇ Find the best reduction of A_i to an element in V_i through orthogonal similarity transformation.
- The idea:
  - ◇ $P_i(X) =$ projection of X onto V_i.
  - ◇ Simultaneously reduce the norm of all residuals:

$$\alpha_i(Q) := Q^T A_i Q - P_i(Q^T A_i Q).$$

- Formulation:

$$\begin{array}{rll} \text{Minimize} & F(Q) & := \frac{1}{2}\sum_{i=1}^{k} \|\alpha_i(Q)\|^2 \\ \text{Subject to} & Q & \in \mathcal{O}(n). \end{array}$$

Gradient Flow under Similarity

- The gradient:

$$\nabla F(X) = \sum_{i=1}^{k} (A_i^T X \alpha_i(X) + A_i X \alpha_i^T(X)).$$

- The projected gradient on $\mathcal{O}(n)$:

$$\begin{aligned} g(Q) &= \frac{Q}{2}\{Q^T \nabla F(X) - \nabla F(X)^T Q\} \\ &= \frac{Q}{2}\sum_{i=1}^{k} \left([Q^T A_i^T Q, \alpha_i(Q)] + [Q^T A_i Q, \alpha_i^T(Q)]\right). \end{aligned}$$

- The descent flow:

$$\begin{aligned} \frac{dX_i}{dt} &= \left[X_i, \sum_{j=1}^{p} \frac{[X_j, P_j^T(X_j)] - [X_j, P_j^T(X_j)]^T}{2}\right] \\ X_i(0) &= A_i \end{aligned}$$

  - ◇ $X_i := Q^T A Q$.

Examples

- A continuous Jacobi algorithm for symmetric eigenvalue problem:

$$\begin{aligned}\frac{dX}{dt} &= [X,[X,diag(X)]] \\ X(0) &= A_1 \text{ (symmetric)}\end{aligned}$$

  ◇ V_1 = subspace of all diagonal matrices.

  ◇ Diagonal matrices are the only stable equilibrium points for the system.

  ◇ Any of these isospectral diagonal matrices is a global minimizer.

- A similar idea for general eigenvalue problem?

$$\begin{aligned}\frac{dX}{dt} &= \left[X, \frac{[X,P_1^T(X)]-[X,P_1^T(X)]^T}{2}\right] \\ X(0) &= A_1 \text{ (general).}\end{aligned}$$

  ◇ V_1 = subspace of upper triangular matrices.

$$\begin{bmatrix} 1.0000 & 3.0000 & 5.0000 & 7.0000 \\ -3.0000 & 1.0000 & 2.0000 & 4.0000 \\ 0.0000 & 0.0000 & 3.0000 & 5.0000 \\ 0.0000 & 0.0000 & 0.0000 & 4.0000 \end{bmatrix}$$

$$\downarrow$$

$$\begin{bmatrix} 2.2500 & 3.3497 & 3.1713 & 2.8209 \\ -0.3506 & 2.2500 & 8.0562 & 6.1551 \\ 0.6247 & -0.8432 & 2.2500 & 3.2105 \\ -0.0846 & 0.2727 & -0.3360 & 2.2500 \end{bmatrix}$$

    ▷ Upper quasi-triangular matrices are not necessarily stable.

  ◇ V_1 = subspace of structure B matrices, i.e., block upper triangular matrices with all diagonal blocks 2×2 except possibly the last one, which is 1×1.

    ▷ ω-limit set contains only a singleton.

The Nearest Commuting-Pair Problem

- The problem:
  - ⋄ Given a pair of symmetric matrices (A_1, A_2).
  - ⋄ Determine how far (A_1, A_2) is away from a symmetric pair (E_1, E_2) satisfying $E_1E_2 = E_2E_1$.
- Symmetric and commuting pairs can be simultaneously diagonalized by orthogonal similarity transformation.
- Reformulation:

$$\sum_{i=1}^{2} \|E_i - A_i\|^2 = \sum_{i=1}^{2} \|D_i - Q^T A_i Q\|^2$$

  - ⋄ $D_i = Q^T E_i Q$ is diagonal.
- The descent flow:

$$\begin{aligned} \frac{dX_i}{dt} &= \left[X_i, \sum_{j=1}^{2} [X_j, diag(X_j)]\right] \\ X_i(0) &= A_i, \quad i = 1, 2 \end{aligned}$$

Reduction by Orthogonal Equivalence

- The problem:
  - ⋄ Matrices A_i and subspaces V_i in $R^{m\times n}$, $i = 1, \ldots, p$, are given.
  - ⋄ Find the best reduction of A_i to an element in V_i through orthogonal equivalence transformation .
- Formulation:

$$\begin{array}{ll} \text{Minimize} & F(Q, Z) := \frac{1}{2} \sum_{i=1}^{k} \|\beta_i(Q, Z)\|^2 \\ \text{Subject to} & Q \in O(m) \\ & Z \in O(n). \end{array}$$

  - ⋄ Residuals:

$$\beta_i(Q, Z) := Q^T A_i Z - P(Q^t A_i Z).$$

Gradient Flow under Equivalence

- Frobenius inner product in product topology $R^{m\times m} \times R^{n\times n}$:

$$\langle (X_1, Y_1), (X_2, Y_2)\rangle_P := \langle X_1, X_2\rangle + \langle Y_1, Y_2\rangle.$$

- The gradient:

$$\nabla F(X,Y) = \left(\sum_{i=1}^{k} A_i Y \alpha_i^T(X,Y), \sum_{i=1}^{k} A_i^T X \alpha_i(X,Y)\right).$$

- The projected gradient on $\mathcal{O}(m) \times \mathcal{O}(n)$:

$$g(Q,Z) = \left(\frac{Q}{2}\sum_{i=1}^{k}(Q^T A_i Z \alpha_i^T(Q,Z) - \alpha_i(Q,Z) Z^T A_i^T Q), \right.$$
$$\left. \frac{Z}{2}\sum_{i=1}^{k}(Z^T A_i^T Q \alpha_i(Q,Z) - \alpha_i^T(Q,Z) Q^T A_i Z)\right).$$

- The decent flow:

$$\begin{aligned}\frac{dX_i}{dt} &= \sum_{j=1}^{p}\left\{X_i \frac{X_j^T P_j(X_j) - P_j^T(X_j) X_j}{2}\right. \\ &\qquad \left. + \frac{P_j(X_j) X_j^T - X_j P_j^T(X_j)}{2} X_i\right\} \\ X_i(0) &= A_i\end{aligned}$$

$\diamond$ $X_i := Q^T A_i Z$.

Example

- A continuous Jacobi algorithm for the singular value problem:

$$\begin{aligned}\frac{dX}{dt} &= \frac{1}{2}\{X\left(X^T(diagX)-(diagX)^TX\right)\\ &+ \left((diagX)X^T - X(diagX)^T\right)X.\}\end{aligned}$$

  - ◇ V_1 = subspace of diagonal matrices in $R^{m\times n}$.
  - ◇ Diagonal matrices (of the singular values) are the only stable equilibrium points.

Nearest Normal Matrix Problem

- The problem:
  - ◇ Determine the closest normal matrix to a given square complex matrix A.
  - ◇ Normal matrices can be diagonalized by unitary similarity transformation. Thus

$$\begin{aligned}\text{Minimize} \quad & F(U,D) := \frac{1}{2}\|A-UDU^*\|^2\\ \text{Subject to} \quad & U \in \mathcal{U}(n)\\ & D \in \mathcal{D}(n).\end{aligned}$$

- Reformulation:
  - ◇ Consider U and D as independent variables:

$$\|A-Z\|^2 = \|U^*AU - D\|^2.$$

  - ◇ At global minimum,

$$\begin{aligned}\text{Minimize} \quad & F(U) = \frac{1}{2}\|U^*AU - diag(U^*AU)\|^2\\ \text{Subject to} \quad & U^*U = I.\end{aligned}$$

- Identify $C^{n\times n} \equiv R^{n\times n} \times R^{n\times n}$ to take advantage of earlier techniques:
  - ◇ $Z = (\Re Z, \Im Z)$.
  - ◇ Inner product:
  $$\langle X, Y\rangle_C := \langle \Re X, \Re Y\rangle + \langle \Im X, \Im Y\rangle.$$
  - ◇ The project gradient of F onto the manifold $\mathcal{U}(n)$ is given by:
  $$\begin{aligned} g(U) \;=\; & \frac{U}{2}\{[diag(U^*AU), U^*A^*U] \\ & - [diag(U^*AU), U^*A^*U]^*\}. \end{aligned}$$
- New characterization: Let $W := U^*AU$. Then necessary (sufficient) conditions for $U \in \mathcal{U}(n)$ to be a local minimizer are that:
  - ◇ The matrix $[diag(W), W^*]$ is Hermitian.
  - ◇ The quadratic form
  $$\langle [diag(W), K] - diag([W, K]), [W, K]\rangle_C$$
  is nonnegative (positive) for every skew Hermitian matrix K.

- The descent flow:
$$\begin{aligned} \frac{dU}{dt} &= Uk(W) \\ \frac{dW}{dt} &= [W, k(W)] \end{aligned}$$
  - ◇ $k(W) := \frac{1}{2}[W, diag(W^*)] - [W, diag(W^*)]^*$.
  - ◇ $W(t) := U(t)^*AU(t)$.
  - ◇ $Z := \tilde{U} diag(\tilde{W})\tilde{U}^*$ (where $\tilde{}$ denotes a limit point of the flow) is a putative nearest normal matrix.
- Advantages:
  - ◇ The necessary conditions are derived without reference to Lagrange multipliers.
  - ◇ Computation is easier. No shift, phase, or rotation angles are needed as in the Jacobi algorithm. (Goldstine et al. '59, Ruhe '87).

Lecture 6

Inverse Problem in the Schur-Horn Theorem

- Overview
- Schur-Horn theorem
- Lift and projection
- A projected gradient method
- Convergence
- Numerical experiment

Overview

- Given vectors $a = [a_i], \lambda = [\lambda_i] \in R^n$, a majorizes λ if and only if
  - ◇ Arranged in increasing order:
$$\begin{aligned} a_{j_1} &\leq \ldots \leq a_{j_n}, \\ \lambda_{m_1} &\leq \ldots \leq \lambda_{m_n}; \end{aligned}$$
  - ◇ For all $k = 1, 2, \ldots, n$
$$\sum_{i=1}^{k} a_{j_i} \geq \sum_{i=1}^{k} \lambda_{m_i};$$
  - ◇ Equality holds for $k = n$.
- Majororization theory has important applications (Marshall el al., 79, Arnold '87).
- Would like to construct a Hermitian matrix with specified diagonal entries and eigenvalues.
  - ◇ Can this be done?
  - ◇ How to do it?

- Two methods are proposed:
  - ◇ Lift and projection method
    - ▷ Iterative approach
    - ▷ Linear convergence
    - ▷ Connects to the Wielandt-Hoffman theorem.
  - ◇ Projected gradient method
    - ▷ Continuous approach
    - ▷ Easy to implement
    - ▷ Offers a new proof of existence.

Schur-Horn Theorem

- The Theorem: Hermitian matrix H with eigenvalues λ and diagonal entries a if and only if a majorizes λ.
  - ◇ The known proof is not constructive.
- An inverse eigenvalue problem (SHIEP): Construct a Hermitian matrix with given eigenvalues and diagonal entries.
  - ◇ Known as the harder part of the Schur-Horn Theorem.
  - ◇ Far more variable in the SHIEP than constraints $\Rightarrow$ Solution is far from unique.

Notion

- Notation:

$$\begin{aligned} \mathrm{diag}(M) &= \text{Diagonal matrix from matrix } M \\ \mathrm{diag}(v) &= \text{Diagonal matrix from vector } v \\ \mathcal{T}(a) &:= \{T \in R^{n\times n} | \mathrm{diag}(T) = \mathrm{diag}(a)\} \\ \mathcal{M}(\Lambda) &:= \{Q^T \Lambda Q | Q \in \mathcal{O}(n)\} \\ \Lambda &:= \mathrm{diag}(\lambda) \\ \mathcal{O}(n) &= \text{Orthogonal matrices in } R^{n\times n}. \end{aligned}$$

- Idea:

$$\min_{T\in\mathcal{T}(a), Z\in\mathcal{M}(\Lambda)} \|T - Z\|$$

  - ◇ Find the shortest distance between $\mathcal{T}(a)$ and $\mathcal{M}(\Lambda)$.
  - ◇ Schur-Horn Theorem $\Rightarrow \mathcal{T}(a) \cap \mathcal{M}(\Lambda) \neq \emptyset$.
  - ◇ SHIEP $\equiv$ Find the intersection.

SHIEP versus PIEP

- PIEP:
  - ◇ Given symmetric matrices $A_0, A_1, \ldots, A_n \in R^{n\times n}$ and $\lambda \in R^n$,
  - ◇ Find values of $c := (c_1, \ldots, c_n)^T \in R^n$ such that eigenvalues of
  $$A(c) := A_0 + c_1A_1 + \ldots + c_nA_n$$
  are precisely λ.
- SHIEP in terms of PIEP?
  - ◇ Needs to specify A_i a priori so that a SHIEP solution may be written in the form of a PIEP.
  - ◇ Not easy because off-diagonal elements are free and too many.
  - ◇ Numerical techniques proposed for PIEP are not directly applicable for SHIEP unless A_i are properly selected.

Structure SHIEP

- Totally $2n-1$ given data elements — a and λ.
- Sensible to restrict the structure of the matrix, say a Jacobi matrix?
  - ◇ Interesting, but
  - ◇ An example: No real numbers b_1, b_2 such that
  $$\begin{bmatrix} 1 & b_1 & 0 \\ b_1 & 2 & b_2 \\ 0 & b_2 & 3 \end{bmatrix}$$
  has eigenvalues $\{-5, -4, 15\}$.

Lift and Projection

- Alternate between $\mathcal{T}$ and $\mathcal{M}(\Lambda)$ in the following way:
  - ◇ A lift: From $T^{(k)} \in \mathcal{T}$, find $Z^{(k)} \in \mathcal{M}(\Lambda)$ such that
  $$\|T^{(k)} - Z^{(k)}\| = \mathrm{dist}(T^{(k)}, \mathcal{M}(\Lambda)).$$
  - ◇ A projection: Find $T^{(k+1)} \in \mathcal{T}$ such that
  $$\|T^{(k+1)} - Z^{(k)}\| = \mathrm{dist}(\mathcal{T}, Z^{(k)}).$$

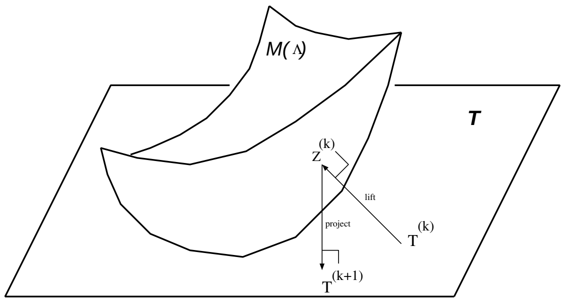

Figure 6.1: Geometric sketch of lifting and projection.

Calculation

- Projection is easy.
  - ◇ If $T = [t_{ij}] = P(Z = [z_{ij}])$ onto $\mathcal{T}$, then
  $$t_{ij} := \begin{cases} z_{ij}, & \text{if } i \neq j \\ a_i, & \text{if } i = j. \end{cases}$$
- Lifting is by Wielandt-Hoffman theorem.
  - ◇ Assume Λ and $T \in \mathcal{T}$ have simple spectrum.
    - ▷ Multiple eigenvalues needs only a slight modification.
  - ◇ Spectral decomposition $T = Q^T D Q$.
  - ◇ π = permutation so that $\lambda_{\pi_1}, \ldots, \lambda_{\pi_n}$ and D are in the same algebraic ordering.
  - ◇ Then the lift of T onto $\mathcal{M}(\Lambda)$ is
  $$Z := Q^T \mathrm{diag}(\lambda_{\pi_1}, \ldots, \lambda_{\pi_n}) Q$$

- Both lifting or projection minimize the distance between a point and a set:

$$\|T^{(k+1)}-Z^{(k+1)}\|^2 \leq \|T^{(k+1)}-Z^{(k)}\|^2 \leq \|T^{(k)}-Z^{(k)}\|^2.$$

- The lift and projection is a descent method.
- The method is essentially the same as Von Neumann's alternating projection method for convex sets (Cheney '59, Deutsch '83, Boyle et al. '89).
  - ⋄ $\mathcal{M}(\Lambda)$ is not convex.
  - ⋄ A stationary point is not necessarily in the intersection $\mathcal{T} \cap \mathcal{M}(\Lambda)$.
  - ⋄ The proximity map is defined by applying the Wielandt-Hoffman theorem.
  - ⋄ Linear convergence.

Gradient Flow

- Solve the problem:

$$\min_{Q \in \mathcal{O}(n)} F(Q) := \frac{1}{2}\|\mathrm{diag}(Q^T \Lambda Q) - \mathrm{diag}(a)\|^2.$$

- Schur-Horn theorem $\Rightarrow$ Existence of a Q at which F vanishes.
- Fréchet derivative of F:

$$\begin{aligned} F'(Q)U &= 2\langle \mathrm{diag}(Q^T\Lambda Q) - \mathrm{diag}(a), \mathrm{diag}(Q^T\Lambda U)\rangle \\ &= 2\langle \mathrm{diag}(Q^T\Lambda Q) - \mathrm{diag}(a), Q^T\Lambda U\rangle \\ &= 2\langle \Lambda Q(\mathrm{diag}(Q^T\Lambda Q) - \mathrm{diag}(a)), U\rangle. \end{aligned}$$

  - ⋄ Diagonal matrix in the first entry of the inner product $\Rightarrow$ The second equality.
  - ⋄ Adjoint property $\Rightarrow$ The third equality.
- Gradient ∇F can be interpreted as:

$$\nabla F(Q) = 2\Lambda Q \beta(Q)$$

  - ⋄ $\beta(Q) := \mathrm{diag}(Q^T\Lambda Q) - \mathrm{diag}(a)$.

- The projected gradient of $\nabla F(Q)$ onto $\mathcal{O}(n)$:

$$g(Q) = Q[Q^T \Lambda Q, \beta(Q)]$$

- The projected Hessian:

$$\langle g'(Q)QK, QK\rangle = \langle \mathrm{diag}[Q^T\Lambda Q, K] - [\beta(Q), K], [Q^T \Lambda Q, K]\rangle.$$

- The steepest descent flow on $\mathcal{O}(n)$:

$$\dot{Q} = -g(Q).$$

- An isospectral flow on $\mathcal{M}(\Lambda)$:

$$\dot{X} = [X, [\alpha(X), X]]$$

  - ◇ $X := Q^T \Lambda Q$.
  - ◇ $\alpha(X) := \beta(Q) = \mathrm{diag}(X) - \mathrm{diag}(a)$.
  - ◇ Reducing the distance between $\mathrm{diag}(X)$ and $\mathrm{diag}(a)$.

- The SHIEP can be solved by integrating the differential equation.

Convergence

- First order necessary condition:

$$[\alpha(X), X] = 0.$$

- Second order necessary condition if $\beta(Q) = 0$:

$$\langle g'(Q)QK, QK\rangle = \|\mathrm{diag}[Q^T\Lambda Q, K]\|q^2 \geq 0$$

  for all skew-symmetric matrices K.

- The strict inequality is not true in general.
  - ◇ Denote $\Omega := \mathrm{diag}[X, K] = \mathrm{diag}\{\omega_1, \ldots, \omega_n\}$.
  - ◇ Then

$$\omega_i = \sum_{s=1}^{i-1} x_{si}k_{si} - \sum_{t=i+1}^{n} x_{it}k_{it}.$$

  - ◇ The system $\omega_i = 0$ for $i = 1, \ldots, n$ contains only $n-1$ independent equations in the $\frac{n(n-1)}{2}$ unknowns k_{ij}.
  - ◇ Can find a non-trivial skew symmetric matrix K that makes $\Omega = 0$.

Asymptotically Stable Equilibrium

- If $\beta(Q) \neq 0$ at a stationary point Q, then there exists a skew-symmetric matrix K such that $\langle g'(Q)QK, QK\rangle < 0$.
- If $\beta(Q) \neq 0$ at a stationary point Q, there exists an unstable direction along which F is increasing.
- Converge to an unstable equilibrium point is numerically impossible.
- Only X's such that $\beta(Q) = 0$ are the possible *asymptotically stable* equilibrium points.

Proof of Unstable Manifold

- Assume $\beta(Q) = \mathrm{diag}\{\beta_1 I_{n_1}, \ldots, \beta_k I_{n_k}\}$.
- $[Q^T \Lambda Q, \beta(Q)] = 0 \Rightarrow$

$$X = Q^T \Lambda Q = \mathrm{diag}\{X_{11}, \ldots, X_{kk}\}.$$

  - ⋄ $X_{ii} = n_i \times n_i$ real symmetric matrix.
- Define $E := Q\beta(Q)Q^T$.
- $[\Lambda, E] = 0 \Rightarrow$
  - ⋄ $E = \mathrm{diag}(e_1, \ldots, e_n)$.
  - ⋄ $\{e_1, \ldots, e_n =$ a permutation of elements of $\beta(Q)$.
- $Q^T =$ Matrix of eigenvectors of $X \Rightarrow Q$ has the same block structure as X.

- Consider a skew-symmetric matrix $K = [K_{ij}]$ such that,
  - $\diamond$ Partitioned in the same way as X
  - $\diamond$ $K_{ii} = 0$ for all $i = 1, \ldots, k$.
- Observe
  - $\diamond$ $\mathrm{diag}[Q^T \Lambda Q, K] = 0$.
  - $\diamond$ The projected Hessian:

$$\begin{aligned} & \langle g'(Q)QK, QK\rangle \\ = & -\langle[\beta(Q), K], [Q^T\Lambda Q, K]\rangle \\ = & -\langle E\tilde{K} - \tilde{K}E, \Lambda\tilde{K} - \tilde{K}\Lambda\rangle \\ = & -2\sum_{i<j}(\lambda_i - \lambda_j)(e_i - e_j)\tilde{k}_{ij}^2 \end{aligned}$$

  - $\diamond$ Easy to pick up values of $\tilde{k}_{ij}$ so that

$$\langle g'(Q)QK, QK\rangle < 0.$$

Numerical Experiment

- Initial value:
  - $\diamond$ Cannot use Λ as the initial value.
  - $\diamond$ $X_0 := Q^T \Lambda Q$ with Q a random orthogonal matrix.
- Integrator:
  - $\diamond$ Subroutine ODE
  - $\diamond$ $RELERR = ABSERR = 10^{-12}$.
  - $\diamond$ Check output values at interval of 1.

Example 1

- Test data:

$$a=[4.3792\times10^{-1}, 1.0388\times10^{+0}, 1.5396\times10^{-2}, 1.8609\times10^{+0}, 1.4024\times10^{+0}]$$

$$\lambda=[-1.4169\times10^{+0}, -5.6698\times10^{-1}, 4.3890\times10^{-1}, 1.4162\times10^{+0}, 4.8842\times10^{+0}]$$

- Random orthogonal matrix:

$$\begin{bmatrix} -6.4009\times10^{-1} & -5.3594\times10^{-1} & -1.8454\times10^{-1} & -3.3375\times10^{-2} & -5.1757\times10^{-1} \\ 2.1804\times10^{-1} & -1.2359\times10^{-1} & -5.0336\times10^{-1} & -8.2193\times10^{-1} & 9.0802\times10^{-2} \\ -7.2099\times10^{-1} & 5.6072\times10^{-1} & 1.4302\times10^{-2} & -2.4876\times10^{-1} & 3.2199\times10^{-1} \\ 2.8417\times10^{-3} & -1.9828\times10^{-1} & 8.4401\times10^{-1} & -4.9375\times10^{-1} & -6.7297\times10^{-2} \\ -1.5134\times10^{-1} & -5.8632\times10^{-1} & 3.0406\times10^{-3} & 1.3284\times10^{-1} & 7.8464\times10^{-1} \end{bmatrix}$$

- Limit point: At $t \approx 11$, the gradient flow converges to:

$$\begin{bmatrix} 4.3792\times10^{-1} & 2.6691\times10^{-1} & -1.9178\times10^{-1} & -6.1356\times10^{-1} & -1.5920\times10^{+0} \\ 2.6691\times10^{-1} & 1.0388\times10^{+0} & -7.2845\times10^{-1} & -8.6726\times10^{-1} & -1.9618\times10^{+0} \\ -1.9178\times10^{-1} & -7.2845\times10^{-1} & 1.5396\times10^{-2} & -6.3601\times10^{-1} & 1.6256\times10^{-1} \\ -6.1356\times10^{-1} & -8.6726\times10^{-1} & -6.3601\times10^{-1} & 1.8609\times10^{+0} & 1.5032\times10^{+0} \\ -1.5920\times10^{+0} & -1.9618\times10^{+0} & 1.6256\times10^{-1} & 1.5032\times10^{+0} & 1.4024\times10^{+0} \end{bmatrix}$$

- Different random orthogonal matrix $\Rightarrow$ Different limit point.

Example 2

- Repeat the experiment with $2,000$ test data.
  - ◇ Entries in a and λ are from random symmetric matrices with distribution $\mathcal{N}(0,1)$.
  - ◇ Orthogonal matrices Q are from the QR decomposition of non-symmetric random matrices (Stewart ,80).
- Collect the length of integration required for reaching convergence in each case.
  - ◇ Inherent only to the individual problem data (and the stopping criterion).
  - ◇ Independent of the machine used.
- Histogram:
  - ◇ $\approx 77\%$ of the cases converge with the length of integration less than 7.
  - ◇ $\approx 93\%$ converge with length less than 17.
  - ◇ Maximal length of integration $= 296$.
  - ◇ All $2,000$ cases converge.

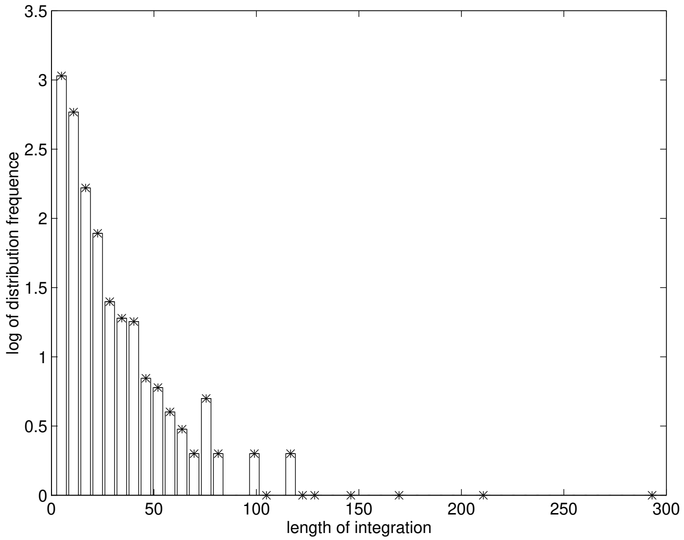

Figure 6.2: Histogram on the length of integration required for convergence.

Conclusion

- The lift-and-project method makes a connection with the Wielandt-Hoffman theorem.
- The gradient flow method can be integrated by any available ordinary differential equation solver.
- Numerical methods for general PIEP will not work.
- The gradient flow method always converges.
- A constructive proof of the Schur-Horn theorem.

Lecture 7

Stochastic Inverse Eigenvalue Problem

- Overview
- Relation to nonnegative matrices
- Basic formulation
- ASVD flow
- Convergence
- Numerical Experiment

Overview

- Inverse Eigenvalue Problem (IEP):
  - ◇ Reconstruction of matrices from prescribed spectral data.
  - ◇ Spectral data may involve complete or partial information of eigenvalues or eigenvectors.
  - ◇ Often necessary to restrict the construction to special classes of matrices.
- Fundamental questions:
  - ◇ Solvability: Determine a necessary or a sufficient condition under which an IEP has a solution.
  - ◇ Computability: Develop a scheme through which, knowing a priori that the given spectral data are feasible, a matrix can be constructed numerically.

An Example: Parametrized IEP

- Given
  - ◇ Symmetric matrices $A_0, A_1, \ldots, A_n \in R^{n\times n}$;
  - ◇ Real numbers $\lambda_1^* \geq \ldots \geq \lambda_n^*$,
- Find
  - ◇ Values of $c := (c_1, \ldots, c_n)^T \in R^n$
  - ◇ Eigenvalues of the matrix

$$A(c) := A_0 + c_1 A_1 + \ldots + c_n A_n$$

  are precisely $\lambda_1^*, \ldots, \lambda_n^*$.
- Not always does the PIEP has a solution.
- Iterative and continuous methods exist (Friedland et al. '87, Chu et al., '90).

Inverse Stochastic Spectrum Problem

- Construct a stochastic matrix with prescribed spectrum.
  - ◇ Stochastic structure.
  - ◇ No strings of symmetry.
  - ◇ Eigenvalues can appear in complex conjugate pairs.
- A hard problem (Karpelevič '51, Minc '88).
  - ◇ The set Θ_n of points in the complex plane that are eigenvalues of stochastic $n \times n$ matrices is completely characterized.
  - ◇ The Karpelevič theorem characterizes only one complex value a time and does not provide further insights into when two or more points in Θ_n are eigenvalues of the *same* stochastic matrix.

Karpelevič's Theorem

- A number λ is an eigenvalue for a stochastic matrix if and only if it belongs to a region Θ_n such as the one shown below for $n = 4$.

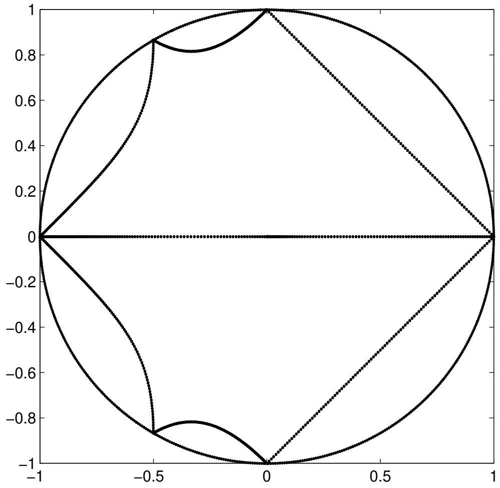

Figure 7.1: Θ_4 by the Karpelevič Theorem.

- ◇ Region is symmetric about the real axis.
- ◇ The points on the unit circles are given by $e^{2\pi a/b}$ where a and b range over all integers such that $0 \leq a < b \leq n$.
- ◇ The boundary of Θ_n consists of curvilinear arcs connecting these points in circular order. These arcs are characterized by specific parametric equations (Minc, '88).

Relation to Nonnegative Matrices

- A complex nonzero number α is an eigenvalue of a nonnegative matrix with a positive maximal eigenvalue r if and only if α/r is an eigenvalue of a stochastic matrix.
- If A is a nonnegative matrix with positive maximal eigenvalue r and a positive maximal eigenvector x, then $D^{-1}r^{-1}AD$ is a stochastic matrix where $D := \mathrm{diag}\{x_1, \ldots, x_n\}$.
  - ◇ The IEP for nonnegative matrices (NIEP) has received considerable interest in the literature (Berman et al., 94).
  - ◇ Some necessary and a few sufficient conditions for the NIEP are available.
- A continuous method for the NIEP of *symmetric* matrices has been studied (Chu, '91).

Basic Formulation

- Notation:

$$\mathcal{M}(\Lambda) := \{P\Lambda P^{-1} | P \in R^{n\times n} \text{ is nonsingular}\}$$
$$\pi(R^n_+) := \{B \circ B | B \in R^{n\times n}\}$$

  - ◇ Λ = real-valued matrix carrying the spectrum information.
  - ◇ $\circ$ = Hadamard product.

- Idea:
  - ◇ Find the intersection of $\mathcal{M}(\Lambda)$ and $\pi(R^n+)$.
  - ◇ The intersection, if exists, results in a nonnegative matrix isospectral to Λ.
  - ◇ Reduce the nonnegative matrix, if its maximal eigenvector is positive, to a stochastic matrix by diagonal similarity transformation.

Reformulation

$$\begin{array}{ll} \text{Minimize} & F(P,R) := \frac{1}{2}||PJP^{-1} - R \circ R||^2 \\ \text{Subject to} & P \in Gl(n), \; R \in gl(n) \end{array}$$

- P and R are used as coordinates to maneuver elements in $\mathcal{M}(\Lambda)$ and $\pi(R^n_+)$ to reduce the objective value.
- Feasible domains are open sets.
- A minimum may not exist.

Gradient of F

- Inner product in the product topology:

$$\langle (X_1, Y_1), (X_2, Y_2) \rangle := \langle X_1, X_2 \rangle + \langle Y_1, Y_2 \rangle.$$

- With respect to the product topology:

$$\nabla F(P, R) = \left((\Delta(P,R) M(P)^T - M(P)^T \Delta(P,R)) P^{-T}, \right.$$
$$\left. -2\Delta(P,R) \circ R \right).$$

  ◇ Abbreviation:

$$\begin{aligned} M(P) &:= PJP^{-1} \\ \Delta(P,R) &:= M(P) - R \circ R. \end{aligned}$$

Steepest Descent Flow

- Steepest descent flow:

$$\begin{aligned} \frac{dP}{dt} &= [M(P)^T, \Delta(P,R)] P^{-T} \\ \frac{dR}{dt} &= 2\Delta(P,R) \circ R. \end{aligned}$$

- Advantages:
  - ◇ No longer need the projection of $\nabla F(P, R)$ as does in the symmetric case.
  - ◇ The zero structure in the original matrix $R(0)$ is preserved throughout the integration — may be used to explore the possibility of constructing a Markov chain with prescribed linkages and spectrum.
- Disadvantage:
  - ◇ The solution flow $P(t)$ is susceptible to becoming unbounded — a possible frailty.
  - ◇ The involvement of P^{-1} is somewhat worrisome.

ASVD flow

- An analytic singular value decomposition of the path of matrices $P(t)$ is an analytic path of factorizations
$$P(t) = X(t)S(t)Y(t)^T$$
where $X(t)$ and $Y(t)$ are orthogonal and $S(t)$ is diagonal.
- An ASVD exists if $P(t)$ is analytic (Bunse-Gerstner et al., '91).
- The $P(t)$ defined by the differential system is analytic follows from the Cauchy-Kovalevskaya theorem since the coefficients of the vector field are analytic.

New Coordinate System

- The two matrices P and R are used, respectively, as *coordinates* to describe the isospectral matrices and nonnegative matrices.
  - ◇ May have used more dimensions of variables than necessary — does no harm.
  - ◇ When flows $P(t)$ and $R(t)$ are introduced, in a sense a flow in $\mathcal{M}(\Lambda)$ and a flow in $\pi(R_+^n)$ are also introduced.
- The motion of the coordinate P is further described by three other variables X, S, and Y according to the ASVD.
- To produce the steepest descent flow, a coordinate system $(X(t), S(t), Y(t), R(t))$ is eventually imposed on matrices in $\mathcal{M}(\Lambda) \times \pi(R_+^n)$.

Calculating the ASVD

- Differentiate $P(t) = X(t)S(t)Y(t)^T$: (Wright '92):

$$\begin{aligned} \dot{P} &= \dot{X}SY^T + X\dot{S}Y^T + XS\dot{Y}^T \\ X^T\dot{P}Y &= \underbrace{X^T\dot{X}}_{Z}S + \dot{S} + S\underbrace{\dot{Y}^TY}_{W} \end{aligned}$$

  - ◇ Z, W are skew-symmetric matrices.
- Define $Q := X^T\dot{P}Y$.
  - ◇ Q is known since $\dot{P}$ is already specified.
  - ◇ The inverse of $P(t)$ is calculated from

$$P^{-1} = YS^{-1}X^T.$$

  - ◇ The diagonal entries of $S = \mathrm{diag}\{s_1, \ldots, s_n\}$ provide us with information about the proximity of $P(t)$ to singularity.

- Flow for $S(t)$:

$$\frac{dS}{dt} = \mathrm{diag}(Q).$$

- Obtain $W(t)$ and $Z(t)$:

$$\begin{aligned} q_{jk} &= z_{jk}s_k + s_j w_{jk}, \\ -q_{kj} &= z_{jk}s_j + s_k w_{jk}. \end{aligned}$$

  - ◇ If $s_k^2 \neq s_j^2$, then

$$z_{jk} = \frac{s_k q_{jk} + s_j q_{kj}}{s_k^2 - s_j^2},$$
$$w_{jk} = \frac{s_j q_{jk} + s_k q_{kj}}{s_j^2 - s_k^2}$$

  for all $j > k$.
- Flow for $X(t)$ and $Y(t)$:

$$\begin{aligned} \frac{dX}{dt} &= XZ. \\ \frac{dY}{dt} &= YW. \end{aligned}$$

- The flow is now ready to be integrated by any IVP solvers.

Convergence

- The approach fails only when:
  - ◇ $P(t)$ becomes singular in finite time — requires a restart.
  - ◇ $F(P(t), R(t))$ converges to a nonzero constant — a LS local solution is found.
- Gradient flows enjoy global convergence:
  - ◇ $G(t) := F(P(t), R(t))$ enjoys the property:

    $$\frac{dG}{dt} = -\|\nabla F(P(t), R(t))\|^2 \leq 0$$

    along any solution curve $(P(t), R(t))$.
  - ◇ Suppose $P(t)$ remains nonsingular. Then $G(t)$ converges.

Numerical Experiment

- Integrator: MATLAB ODE SUITE
  - ◇ **ode113** = ABM, PECE, non-stiff system.
  - ◇ **ode15s** = Klopfenstein-Shampine, quasi-constant step size, stiff system.
- Stopping criteria:
  - ◇ ABSERR = RELERR = 10^{-12}.
  - ◇ $\|\Delta(P, R)\| \leq 10^{-9} \Rightarrow$ a stochastic matrix has been found.
  - ◇ Relative improvement of $\Delta(P, R)$ between two consecutive output points $\leq 10^{-9} \Rightarrow$ a LS solution is found.

Example 1

- Spectrum:

$$\{1.0000, -0.2403, 0.1186 \pm 0.1805i, -0.1018\}$$

- Initial values:

$$P_0 = \begin{bmatrix} 0.2002 & 0.4213 & 0.9229 & 0.7243 & 0.4548 \\ 0.6964 & 0.0752 & 0.9361 & 0.2235 & 0.0981 \\ 0.7538 & 0.3620 & 0.2157 & 0.5272 & 0.2637 \\ 0.4366 & 0.3220 & 0.8688 & 0.1729 & 0.8697 \\ 0.8897 & 0.1436 & 0.7097 & 0.5343 & 0.7837 \end{bmatrix}$$

$$R_0 = .8328\mathbf{1}$$

- Limit point:

$$B = \begin{bmatrix} 0.1679 & 0.0522 & 0.4721 & 0.0000 & 0.3078 \\ 0.1436 & 0.1779 & 0.4186 & 0.1901 & 0.0698 \\ 0.0000 & 0.1377 & 0.5291 & 0.3034 & 0.0299 \\ 0.0560 & 0.4690 & 0.2404 & 0.0038 & 0.2309 \\ 0.1931 & 0.1011 & 0.5339 & 0.1553 & 0.0165 \end{bmatrix}.$$

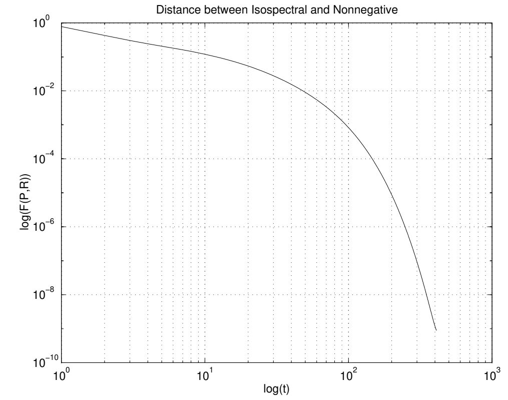

Figure 7.2: A log-log plot of $F(P(t), R(t))$ versus t for Example 1.

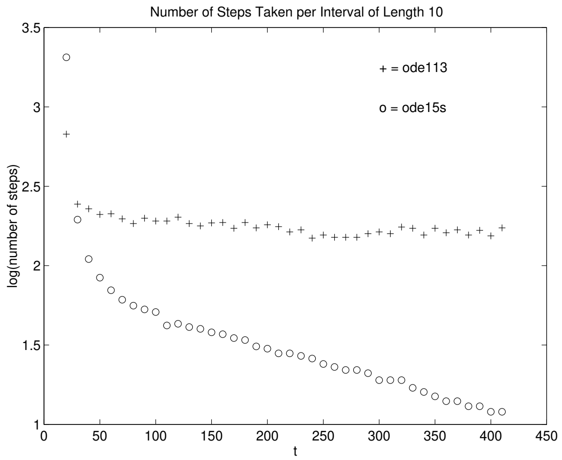

Figure 7.3: A comparison of steps taken by **ode113** and **ode15s** for Example 1.

- Both solvers work reasonably.
  - ◇ **ode15s** advances with larger step sizes at the cost of solving implicit algebraic equations.
  - ◇ Jacobians are calculated by finite difference. Function calls could be reduced by fewer output points.
- Different initial values lead to different stochastic matrices.

Example 2

- Spectrum:

$$\{1.0000, -0.2608, 0.5046, 0.6438, -0.4483\}$$

- Looking for a Markov chain with ring linkage, i.e., each state is linked at most to its two immediate neighbors.

- Initial values:

$$P_0 = \begin{bmatrix} 0.1825 & 0.7922 & 0.2567 & 0.9260 & 0.9063 \\ 0.1967 & 0.5737 & 0.7206 & 0.5153 & 0.0186 \\ 0.5281 & 0.2994 & 0.9550 & 0.6994 & 0.1383 \\ 0.7948 & 0.6379 & 0.5787 & 0.1005 & 0.9024 \\ 0.5094 & 0.8956 & 0.3954 & 0.6125 & 0.4410 \end{bmatrix}$$

$$R_0 = 0.9210 \begin{bmatrix} 1 & 1 & 0 & 0 & 1 \\ 1 & 1 & 1 & 0 & 0 \\ 0 & 1 & 1 & 1 & 0 \\ 0 & 0 & 1 & 1 & 1 \\ 1 & 0 & 0 & 1 & 1 \end{bmatrix}.$$

- Limit point:

$$D = \begin{bmatrix} 0.0000 & 0.3094 & 0 & 0 & 0.6906 \\ 0.0040 & 0.5063 & 0.4896 & 0 & 0 \\ 0 & 0.0000 & 0.5134 & 0.4866 & 0 \\ 0 & 0 & 0.7733 & 0.2246 & 0.0021 \\ 0.4149 & 0 & 0 & 0.3900 & 0.1951 \end{bmatrix}$$

Example 3

- Spectrum

$$\{1.0000, -0.2403, 0.3090 \pm 0.5000i, -0.1018\}$$

- Initial values: same as Example 1 (or modify R_0).
- Slow convergence:

$$E = \begin{bmatrix} 0.3818 & 0.0000 & 0.4568 & 0.0000 & 0.1614 \\ 0.5082 & 0.3314 & 0.0871 & 0.0049 & 0.0684 \\ 0.0000 & 0.0000 & 0.5288 & 0.4712 & 0.0000 \\ 0.0266 & 0.7634 & 0.0292 & 0.0310 & 0.1498 \\ 0.5416 & 0.0524 & 0.3835 & 0.0196 & 0.0029 \end{bmatrix}$$

$$F = \begin{bmatrix} 0.3237 & 0 & 0.4684 & 0 & 0.2079 \\ 0.4742 & 0.3184 & 0.1303 & 0.0007 & 0.0764 \\ 0 & 0.0000 & 0.5231 & 0.4769 & 0 \\ 0.0066 & 0.7536 & 0.0372 & 0.0958 & 0.1068 \\ 0.5441 & 0.0429 & 0.3959 & 0.0022 & 0.0149 \end{bmatrix}$$

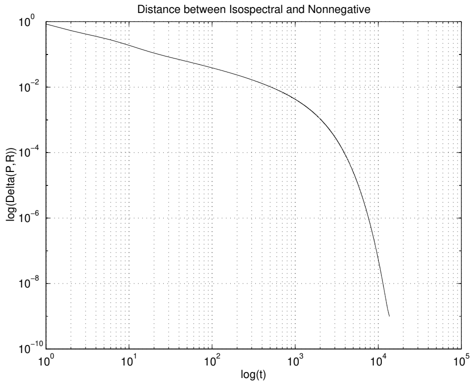

Figure 7.4: A log-log plot of $F(P(t), R(t))$ versus t for Example 3.

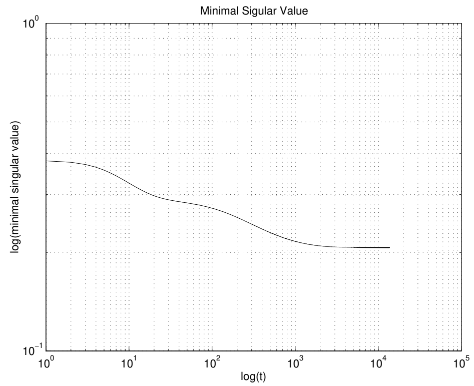

Figure 7.5: History of the smallest singular value for Example 3.

Conclusion

- The theory of solvability on the StIEP or the NIEP is yet to be developed.
- An ODE approach capable of solving the StIEP or the NIEP numerically, if the prescribed spectrum is feasible, is proposed.
- The method is easy to implement by existing ODE solvers.
- The method can also be used to approximate least squares solutions or linearly structured matrices.

Lecture 8

Inverse Singular Value Problems

- IEP versus ISVP
- Existence question
- A continuous approach
- An iterative method for the IEP
- An iterative method for the ISVP

IEP versus ISVP

- Inverse Eigenvalue Problem (IEP):
  - ◇ Given
    - ▷ Symmetric matrices $A_0, A_1, \ldots, A_n \in R^{n\times n}$;
    - ▷ Real numbers $\lambda_1^* \geq \ldots \geq \lambda_n^*$,
  - ◇ Find
    - ▷ Values of $c := (c_1, \ldots, c_n)^T \in R^n$
    - ▷ Eigenvalues of the matrix

$$A(c) := A_0 + c_1 A_1 + \ldots + c_n A_n$$

are precisely $\lambda_1^*, \ldots, \lambda_n^*$.

- Inverse Singular Value Problem ISVP:
  - ◇ Given
    - ▷ General matrices $B_0, B_1, \ldots, B_n \in R^{m\times n}$, $m \geq n$;
    - ▷ Nonnegative real numbers $\sigma_1^* \geq \ldots \geq \sigma_n^*$,
  - ◇ Find
    - ▷ Values of $c := (c_1, \ldots, c_n)^T \in R^n$
    - ▷ Singular values of the matrix

$$B(c) := B_0 + c_1 B_1 + \ldots + c_n B_n$$

are precisely $\sigma_1^*, \ldots, \sigma_n^*$.

Existence Question

- Not always does the IEP have a solution.
- Inverse Toeplitz Eigenvalue Problem (ITEP)
  - ◇ A special case of the (IEP) where $A_0 = 0$ and $A_k := (A_{ij}^{(k)})$ with
$$A_{ij}^{(k)} := \begin{cases} 1, & \text{if } |i-j| = k-1; \\ 0, & \text{otherwise.} \end{cases}$$
  - ◇ Symmetric Toeplitz matrices can have *arbitrary* real spectra. (Landau '94, nonconstructive proof by topological degree argument).
- Not aware of any result concerning the existence question for ISVP.

Notation

- $\mathcal{O}(n) :=$ All orthogonal matrices in $R^{n\times n}$;
- $\Sigma = (\Sigma_{ij}) :=$ A "diagonal" matrix in $R^{m\times n}$
$$\Sigma_{ij} := \begin{cases} \sigma_i^*, & \text{if } 1 \le i = j \le n; \\ 0, & \text{otherwise.} \end{cases}$$
- $\mathcal{M}_s(\Sigma) := \{U\Sigma V^T | U \in \mathcal{O}(m), V \in \mathcal{O}(n)\}$
  - ◇ Contains all matrices in $R^{m\times n}$ whose singular values are precisely $\sigma_1^*, \ldots, \sigma_n^*$.
- $\mathcal{B} := \{B(c) | c \in R^n\}$.
- Solving the ISVP $\equiv$ Finding an intersection of the two sets $\mathcal{M}_s(\Sigma)$ and $\mathcal{B}$.

A Continuous Approach

- Assume
  - ⋄ $\langle B_i, B_j\rangle = \delta_{ij}$ for $1 \le i \le j \le n$.
  - ⋄ $\langle B_0, B_k\rangle = 0$ for $1 \le k \le n$.
- The projection of X onto the linear subspace spanned by $B_1, \ldots, B_n$:

$$P(X) = \sum_{k=1}^{n} \langle X, B_k\rangle B_k.$$

- The distance from X to the affine subspace $\mathcal{B}$:

$$dist(X, \mathcal{B}) = \|X - (B_0 + P(X))\|.$$

- Define, for any $U \in R^{m\times m}$ and $V \in R^{n\times n}$, a residual matrix:

$$R(U,V) := U\Sigma V^T - (B_0 + P(U\Sigma V^T)).$$

- Consider the optimization problem:

$$\begin{array}{rl} \text{Minimize} & F(U,V) := \dfrac{1}{2}\|R(U,V)\|^2 \\ \text{Subject to} & (U,V) \in \mathcal{O}(m) \times \mathcal{O}(n). \end{array}$$

Compute the Projected Gradient

- Frobenius inner product on $R^{m\times m} \times R^{n\times n}$:

$$\langle (A_1, B_1), (A_2, B_2)\rangle := \langle A_1, A_2\rangle + \langle B_1, B_2\rangle.$$

- The gradient ∇F may be interpreted as the pair of matrices:

$$\nabla F(U,V) = (R(U,V)V\Sigma^T, R(U,V)^T U\Sigma).$$

- Tangent space can be split:

$$\mathcal{T}_{(U,V)}(\mathcal{O}(m) \times \mathcal{O}(n)) = \mathcal{T}_U\mathcal{O}(m) \times \mathcal{T}_V\mathcal{O}(n).$$

- Projection is easy because:

$$\begin{aligned} R^{n\times n} &= T_V\mathcal{O}(n) \oplus T_V\mathcal{O}(n)^{\perp} \\ &= V\mathcal{S}(n)^{\perp} \oplus V\mathcal{S}(n) \end{aligned}$$

- Project the gradient $\nabla F(U,V)$ onto the tangent space $\mathcal{T}_{(U,V)}(\mathcal{O}(m)\times\mathcal{O}(n))$:

$$g(U,V) = \left(\frac{R(U,V)V\Sigma^T U^T - U\Sigma V^T R(U,V)^T}{2}U, \frac{R(U,V)^T U\Sigma V^T - V\Sigma^T U^T R(U,V)}{2}V\right).$$

- Descent vector field:

$$\frac{d(U,V)}{dt} = -g(U,V)$$

defines a steepest descent flow on the manifold $\mathcal{O}(m)\times\mathcal{O}(n)$ for the objective function $F(U,V)$.

The Differential Equation on $\mathcal{M}_s(\Sigma)$

- Define

$$X(t) := U(t)\Sigma V(t)^T.$$

- $X(t)$ satisfies the differential system:

$$\frac{dX}{dt} = X\frac{X^T(B_0+P(X)) - (B_0+P(X))^T X}{2} - \frac{X(B_0+P(X))^T - (B_0+P(X))^T X}{2}X.$$

- $X(t)$ moves on the surface $\mathcal{M}_s(\Sigma)$ in the steepest descent direction to minimize $dist(X(t),\mathcal{B})$.
- This is a continuous method for the ISVP.

Remarks

- No assumption on the multiplicity of singular values is needed.
- Any tangent vector $T(X)$ to $\mathcal{M}_s(\Sigma)$ at a point $X \in \mathcal{M}_s(\Sigma)$ about which a local chart can be defined must be of the form
$$T(X) = XK - HX$$
for some skew symmetric matrices $H \in R^{m\times m}$ and $K \in R^{n\times n}$.

An Iterative Method for IEP

- Assume all eigenvalues $\lambda_1^*, \ldots, \lambda_n^*$ are distinct.
- Consider:
  - ◇ The affine subspace
$$\mathcal{A} := \{A(c)|c \in R^n\}.$$
  - ◇ The isospectral surface
$$\mathcal{M}_e(\Lambda) := \{Q\Lambda Q^T|Q \in \mathcal{O}(n)\}$$
where
$$\Lambda := diag\{\lambda_1^*, \ldots, \lambda_n^*\}.$$
- Any tangent vector $T(X)$ to $\mathcal{M}_e(\Lambda)$ at a point $X \in \mathcal{M}_e(\Lambda)$ must be of the form
$$T(X) = XK - KX$$
for some skew-symmetric matrix $K \in R^{n\times n}$.

A Classical Newton Method

- A function $f : R \longrightarrow R$.
- The scheme:

$$x^{(\nu+1)} = x^{(\nu)} - (f'(x^{(\nu)}))^{-1} f(x^{(\nu)})$$

- The intercept:
  - ◇ The new iterate $x^{(\nu+1)}$ = The x-intercept of the tangent line of the graph of f from $(x^{(\nu)}, f(x^{(\nu)}))$.
- The lifting:
  - ◇ $(x^{(\nu+1)}, f(x^{(\nu+1)}))$ = The natural "lift" of the intercept along the y-axis to the graph of f from which the next tangent line will begin.

An Analogy of the Newton Method

- Think of:
  - ◇ The surface $\mathcal{M}_e(\Lambda)$ as playing the role of the graph of f.
  - ◇ The affine subspace $\mathcal{A}$ as playing the role of the x-axis.
- Given $X^{(\nu)} \in \mathcal{M}_e(\Lambda)$,
  - ◇ There exist a $Q^{(\nu)} \in \mathcal{O}(n)$ such that

$$Q^{(\nu)^T} X^{(\nu)} Q^{(\nu)} = \Lambda.$$

  - ◇ The matrix $X^{(\nu)} + X^{(\nu)}K - KX^{(\nu)}$ with any skew-symmetric matrix K represents a tangent vector to $\mathcal{M}_e(\Lambda)$ emanating from $X^{(\nu)}$.
- Seek an $\mathcal{A}$-intercept $A(c^{(\nu+1)})$ of such a vector with the affine subspace $\mathcal{A}$.
- Lift up the point $A(c^{(\nu+1)}) \in \mathcal{A}$ to a point $X^{(\nu+1)} \in \mathcal{M}_e(\Lambda)$.

Find the Intercept

- Find a skew-symmetric matrix $K^{(\nu)}$ and a vector $c^{(\nu+1)}$ such that

$$X^{(\nu)} + X^{(\nu)}K^{(\nu)} - K^{(\nu)}X^{(\nu)} = A(c^{(\nu+1)}).$$

- Equivalently, find $\tilde{K}^{(\nu)}$ such that

$$\Lambda + \Lambda\tilde{K}^{(\nu)} - \tilde{K}^{(\nu)}\Lambda = {Q^{(\nu)}}^T A(c^{(\nu+1)})Q^{(\nu)}.$$

◇ $\tilde{K}^{(\nu)} := {Q^{(\nu)}}^T K^{(\nu)}Q^{(\nu)}$ is skew-symmetric.

- Can find $c^{(\nu)}$ and $K^{(\nu)}$ separately.

- Diagonal elements in the system $\Rightarrow$

$$J^{(\nu)}c^{(\nu+1)} = \lambda^* - b^{(\nu)}.$$

◇ Known quantities:

$$\begin{aligned} J_{ij}^{(\nu)} &:= {q_i^{(\nu)}}^T A_j q_i^{(\nu)}, \text{ for } i,j = 1,\ldots,n \\ \lambda^* &:= (\lambda_1^*,\ldots,\lambda_n^*)^T \\ b_i^{(\nu)} &:= {q_i^{(\nu)}}^T A_0 q_i^{(\nu)}, \text{ for } i = 1,\ldots,n \\ q_i^{(\nu)} &= \text{the } i\text{-th column of the matrix } Q^{(\nu)}. \end{aligned}$$

- The vector $c^{(\nu+1)}$ can be solved.
- Off-diagonal elements in the system together with $c^{(\nu+1)} \Rightarrow \tilde{K}^{(\nu)}$ (and, hence, $K^{(\nu)}$):

$$\tilde{K}_{ij}^{(\nu)} = \frac{{q_i^{(\nu)}}^T A(c^{(\nu+1)})q_j^{(\nu)}}{\lambda_i^* - \lambda_j^*}, \text{ for } 1 \le i < j \le n.$$

Find the Lift-up

- No obvious coordinate axis to follow.
- Solving the IEP $\equiv$ Finding $\mathcal{M}_e(\Lambda) \cap \mathcal{A}$.
- Suppose all the iterations are taking place near a point of intersection. Then

$$X^{(\nu+1)} \approx A(c^{(\nu+1)}).$$

- Also should have

$$A(c^{(\nu+1)}) \approx e^{-K^{(\nu)}} X^{(\nu)} e^{K^{(\nu)}}.$$

- Replace $e^{K^{(\nu)}}$ by the Cayley transform:

$$R := (I + \frac{K^{(\nu)}}{2})(I - \frac{K^{(\nu)}}{2})^{-1} \approx e^{K^{(\nu)}}.$$

- Define

$$X^{(\nu+1)} := R^T X^{(\nu)} R \in \mathcal{M}_e(\Lambda).$$

- The next iteration is ready to begin.

Remarks

- Note that

$$X^{(\nu+1)} \approx R^T e^{K^{(\nu)}} A(c^{(\nu+1)}) e^{-K^{(\nu)}} R \approx A(c^{(\nu+1)})$$

  represents a lifting of the matrix $A(c^{(\nu+1)})$ from the affine subspace $\mathcal{A}$ to the surface $\mathcal{M}_e(\Lambda)$.
- The above offers a geometrical interpretation of Method III developed by Friedland, Nocedal and Overton (SINUM, 1987).
- Quadratic convergence even for multiple eigenvalues case.

An Iterative Approach for ISVP

- Assume
  - ◇ Matrices $B_0, B_1, \ldots, B_n$ are arbitrary.
  - ◇ All singular values $\sigma_1^*, \ldots, \sigma_n^*$ are positive and distinct.
- Given $X^{(\nu)} \in \mathcal{M}_s(\Sigma)$
  - ◇ There exist $U^{(\nu)} \in \mathcal{O}(m)$ and $V^{(\nu)} \in \mathcal{O}(n)$ such that
$$U^{(\nu)^T} X^{(\nu)} V^{(\nu)} = \Sigma.$$
  - ◇ Seek a $\mathcal{B}$-intercept $B(c^{(\nu+1)})$ of a line that is tangent to the manifold $\mathcal{M}_s(\Sigma)$ at $X^{(\nu)}$.
  - ◇ Lift the matrix $B(c^{(\nu+1)}) \in \mathcal{B}$ to a point $X^{(\nu+1)} \in \mathcal{M}_s(\Sigma)$.

Find the Intercept

- Find skew-symmetric matrices $H^{(\nu)} \in R^{m\times m}$ and $K^{(\nu)} \in R^{n\times n}$, and a vector $c^{(\nu+1)} \in R^n$ such that
$$X^{(\nu)} + X^{(\nu)}K^{(\nu)} - H^{(\nu)}X^{(\nu)} = B(c^{(\nu+1)})$$
- Equivalently,
$$\Sigma + \Sigma\tilde{K}^{(\nu)} - \tilde{H}^{(\nu)}\Sigma = U^{(\nu)^T} B(c^{(\nu+1)}) V^{(\nu)}$$
  - ◇ Underdetermined skew-symmetric matrices:
$$\begin{aligned}\tilde{H}^{(\nu)} &:= U^{(\nu)^T} H^{(\nu)} U^{(\nu)},\\ \tilde{K}^{(\nu)} &:= V^{(\nu)^T} K^{(\nu)} V^{(\nu)}.\end{aligned}$$
- Can determine $c^{(\nu+1)}$, $H^{(\nu)}$ and $K^{(\nu)}$ separately.

- Totally $\frac{m(m-1)}{2} + \frac{n(n-1)}{2} + n$ unknowns — the vector $c^{(\nu+1)}$ and the skew matrices $\tilde{H}^{(\nu)}$ and $\tilde{K}^{(\nu)}$.
- Only mn equations.
- Observe: $\tilde{H}_{ij}^{(\nu)}$, $n+1 \leq i \neq j \leq m$,
  - ◇ $\frac{(m-n)(m-n-1)}{2}$ unknowns.
  - ◇ Locate at the lower right corner of $\tilde{H}^{(\nu)}$.
  - ◇ Are not bound to any equations at all.
  - ◇ Set
$$\tilde{H}_{ij}^{(\nu)} = 0 \text{ for } n+1 \leq i \neq j \leq m.$$
- Denote
$$W^{(\nu)} := {U^{(\nu)}}^T B(c^{(\nu+1)}) V^{(\nu)}.$$

Then
$$W_{ij}^{(\nu)} = \Sigma_{ij} + \Sigma_{ii}\tilde{K}_{ij}^{(\nu)} - \tilde{H}_{ij}^{(\nu)}\Sigma_{jj},$$

Determine $c^{(\nu+1)}$

- For $1 \leq i = j \leq n$,
$$J^{(\nu)} c^{(\nu+1)} = \sigma^* - b^{(\nu)}$$
  - ◇ Know quantities:
$$\begin{aligned} J_{st}^{(\nu)} &:= {u_s^{(\nu)}}^T B_t v_s^{(\nu)}, \text{ for } 1 \leq s,t \leq n, \\ \sigma^* &:= (\sigma_1^*, \ldots, \sigma_n^*)^T, \\ b_s^{(\nu)} &:= {u_s^{(\nu)}}^T B_0 v_s^{(\nu)}, \text{ for } 1 \leq s \leq n. \\ u_s^{(\nu)} &= \text{column vectors of } U^{(\nu)}, \\ v_s^{(\nu)} &= \text{column vectors of } V^{(\nu)}. \end{aligned}$$
- The vector $c^{(\nu+1)}$ is obtained.
- $c^{(\nu+1)} \Rightarrow W^{(\nu)}$.

Determine $H^{(\nu)}$ and $K^{(\nu)}$

- For $n+1 \le i \le m$ and $1 \le j \le n$,

$$\tilde{H}_{ij}^{(\nu)} = -\tilde{H}_{ji}^{(\nu)} = -\frac{W_{ij}^{(\nu)}}{\sigma_j^*}.$$

- For $1 \le i < j \le n$,

$$\begin{aligned} W_{ij}^{(\nu)} &= \Sigma_{ii}\tilde{K}_{ij}^{(\nu)} - \tilde{H}_{ij}^{(\nu)}\Sigma_{jj}, \\ W_{ji}^{(\nu)} &= \Sigma_{jj}\tilde{K}_{ji}^{(\nu)} - \tilde{H}_{ji}^{(\nu)}\Sigma_{ii} \\ &= -\Sigma_{jj}\tilde{K}_{ij}^{(\nu)} + \tilde{H}_{ij}^{(\nu)}\Sigma_{ii}. \end{aligned}$$

Solving for $\tilde{H}_{ij}^{(\nu)}$ and $\tilde{K}_{ij}^{(\nu)}$ $\Rightarrow$

$$\begin{aligned} \tilde{H}_{ij}^{(\nu)} = -\tilde{H}_{ji}^{(\nu)} &= \frac{\sigma_i^* W_{ji}^{(\nu)} + \sigma_j^* W_{ij}^{(\nu)}}{(\sigma_i^*)^2 - (\sigma_j^*)^2}, \\ \tilde{K}_{ij}^{(\nu)} = -\tilde{K}_{ji}^{(\nu)} &= \frac{\sigma_i^* W_{ij}^{(\nu)} + \sigma_j^* W_{ji}^{(\nu)}}{(\sigma_i^*)^2 - (\sigma_j^*)^2}. \end{aligned}$$

- The intercept is now completely found.

Find the Lift-Up

- Define orthogonal matrices

$$\begin{aligned} R &:= (I + \frac{H^{(\nu)}}{2})(I - \frac{H^{(\nu)}}{2})^{-1}, \\ S &:= (I + \frac{K^{(\nu)}}{2})((I - \frac{K^{(\nu)}}{2})^{-1}. \end{aligned}$$

- Define the lifted matrix on $\mathcal{M}_s(\Sigma)$:

$$X^{(\nu+1)} := R^T X^{(\nu)} S.$$

- Observe

$$X^{(\nu+1)} \approx R^T(e^{H^{(\nu)}} B(c^{(\nu+1)}) e^{-K^{(\nu)}}) S$$

and

$$\begin{aligned} R^T e^{H^{(\nu)}} &\approx I_m \\ e^{-K^{(\nu)}} S &\approx I_n, \end{aligned}$$

if $\|H^{(\nu)}\|$ and $\|K^{(\nu)}\|$ are small.

- For computation,
  - ◇ Only need orthogonal matrices

$$\begin{aligned} U^{(\nu+1)} &:= R^T U^{(\nu)} \\ V^{(\nu+1)} &:= S^T V^{(\nu)}. \end{aligned}$$

  - ◇ Does not need to form $X^{(\nu+1)}$ explicitly.

Quadratic Convergence

- Measure the discrepancy between $(U^{(\nu)}, V^{(\nu)}) \in R^{m\times m} \times R^{n\times n}$ in the induced Frobenius norm.
- Observe:
  - ◇ Suppose:
    - ▷ The ISVP has an exact solution at c^*.
    - ▷ SVD of $B(c^*) = \hat{U}\Sigma\hat{V}^T$.
  - ◇ Define error matrix::

$$E := (E_1, E_2) := (U - \hat{U}, V - \hat{V}).$$

  - ◇ If $U\hat{U}^T = e^H$ and $V\hat{V}^T = e^K$, then

$$\begin{aligned} U\hat{U}^T &= (E_1 + \hat{U})\hat{U}^T \\ &= I_m + E_1\hat{U}^T \\ &= e^H = I_m + H + O(||H||^2). \end{aligned}$$

    and a similar expression for $V\hat{V}^T$.
  - ◇ Thus,

$$||(H, K)|| = O(||E||).$$

- At the ν-th stage, define

$$E^{(\nu)} := (E_1^{(\nu)}, E_2^{(\nu)}) = (U^{(\nu)} - \hat{U}, V^{(\nu)} - \hat{V}).$$

- How far is ${U^{(\nu)}}^T B(c^*) V^{(\nu)}$ away from Σ?
  - ◇ Write

$$\begin{aligned} {U^{(\nu)}}^T B(c^*) V^{(\nu)} &:= e^{-\hat{H}^{(\nu)}} \Sigma e^{\hat{K}^{(\nu)}} \\ &:= ({U^{(\nu)}}^T e^{-H_*^{(\nu)}} U^{(\nu)}) \Sigma ({V^{(\nu)}}^T e^{K_*^{(\nu)}} V^{(\nu)}) \end{aligned}$$

  with

$$\begin{aligned} H_*^{(\nu)} &:= U^{(\nu)} \hat{H}^{(\nu)} {U^{(\nu)}}^T, \\ K_*^{(\nu)} &:= V^{(\nu)} \hat{K}^{(\nu)} {V^{(\nu)}}^T, \end{aligned}$$

  - ◇ Then

$$e^{H_*^{(\nu)}} = U^{(\nu)} \hat{U}^T, e^{K_*^{(\nu)}} = V^{(\nu)} \hat{V}^T.$$

  - ◇ So

$$||(H_*^{(\nu)}, K_*^{(\nu)})|| = O(||E^{(\nu)}||).$$

  - ◇ Norm invariance under orthogonal transformations $\Rightarrow$

$$||(\hat{H}^{(\nu)}, \hat{K}^{(\nu)})|| = O(||E^{(\nu)}||).$$

- Rewrite

$${U^{(\nu)}}^T B(c^*) V^{(\nu)} = \Sigma + \Sigma \hat{K}^{(\nu)} - \hat{H}^{(\nu)} \Sigma + O(\|E^{(\nu)}\|^2).$$

- Compare:

$$\begin{aligned} & {U^{(\nu)}}^T (B(c^*) - B(c^{(\nu+1)})) V^{(\nu)} \\ = \ & \Sigma(\hat{K}^{(\nu)} - \tilde{K}^{(\nu)}) - (\hat{H}^{(\nu)} - \tilde{H}^{(\nu)}) \Sigma \\ + \ & O(||E^{(\nu)}||^2). \end{aligned}$$

- Diagonal elements $\Rightarrow$

$$J^{(\nu)}(c^* - c^{(\nu+1)}) = O(||E^{(\nu)}||^2).$$

  - ◇ Thus

$$||c^* - c^{(\nu+1)}|| = O(||E^{(\nu)}||^2).$$

- Off-diagonal elements $\Rightarrow$

$$\begin{aligned} ||\hat{H}^{(\nu)} - \tilde{H}^{(\nu)}|| &= O(||E^{(\nu)}||^2), \\ ||\hat{K}^{(\nu)} - \tilde{K}^{(\nu)}|| &= O(||E^{(\nu)}||^2). \end{aligned}$$

  - ◇ Therefore,

$$||(\tilde{H}^{(\nu)}, \tilde{K}^{(\nu)})|| = O(||E^{(\nu)}||).$$

- Together,

$$\begin{aligned} ||H^{(\nu)} - H_*^{(\nu)}|| &= O(||E^{(\nu)}||^2), \\ ||K^{(\nu)} - K_*^{(\nu)}|| &= O(||E^{(\nu)}||^2). \end{aligned}$$

- Observe:

$$
\begin{aligned}
E_1^{(\nu+1)} &:= U^{(\nu+1)} - \hat{U} = R^T U^{(\nu)} - e^{-H_*^{(\nu)}} U^{(\nu)} \\
&= \left[(I - \frac{H^{(\nu)}}{2}) - (I - H_*^{(\nu)} + O(||H_*^{(\nu)}||^2) \right. \\
&\quad \left. (I + \frac{H^{(\nu)}}{2}) \right] (I + \frac{H^{(\nu)}}{2})^{-1} U^{(\nu)} \\
&= \left[H_*^{(\nu)} - H^{(\nu)} + O(||H_*^{(\nu)} H^{(\nu)}|| \right. \\
&\quad \left. + ||H^{(\nu)}||^2) \right] (I + \frac{H^{(\nu)}}{2})^{-1} U^{(\nu)}.
\end{aligned}
$$

  ◇ It is clear now that

$$
||E_1^{(\nu+1)}|| = O(||E^{(\nu)}||^2).
$$

- A similar argument works for $E_2^{(\nu+1)}$.
- We have proved that

$$
||E^{(\nu+1)}|| = O(||E^{(\nu)}||^2).
$$

Multiple Singular Values

- Previous definition in finding the $\mathcal{B}$-intercept of a tangent line of $\mathcal{M}_s(\Sigma)$ allows
  - ◇ No zero singular values.
  - ◇ No multiple singular values.
- Now assume
  - ◇ All singular values are positive.
  - ◇ Only the first singular value σ_1^* is multiple, with multiplicity p.

- Observe:
  - ◇ All formulas work, except
    - ▷ For $1 \leq i < j \leq p$, only know
    $$W_{ij}^{(\nu)} + W_{ji}^{(\nu)} = 0.$$
    - ▷ No values for $\tilde{H}_{ij}^{(\nu)}$ and $\tilde{K}_{ij}^{(\nu)}$ can be determined.
    - ▷ Additional $q := \frac{p(p-1)}{2}$ equations for the vector $c^{(\nu+1)}$ arise.
- Multiple singular values gives rise to an overdetermined system for $c^{(\nu+1)}$.
  - ◇ Tangent lines from $\mathcal{M}_s(\Sigma)$ may not intercept the affine subspace $\mathcal{B}$ at all.
  - ◇ The ISVP needs to be modified.

Modified ISVP

- Given
  - ◇ Positive values $\sigma_1^* = \ldots = \sigma_p^* > \sigma_{p+1}^* > \ldots > \sigma_{n-q}^*$,
- Find
  - ◇ Real values of $c_1, \ldots, c_n$,
  - ◇ The $n-q$ largest singular values of the matrix matrix $B(c)$ are $\sigma_1^*, \ldots, \sigma_{n-q}^*$.

Find the Intercept

- Use the equation

$$\hat{\Sigma} + \hat{\Sigma}\tilde{K}^{(\nu)} - \tilde{H}^{(\nu)}\hat{\Sigma} = {U^{(\nu)}}^T B(c^{(\nu+1)})V^{(\nu)}$$

to find the $\mathcal{B}$-intercept where

◇ The diagonal matrix

$$\hat{\Sigma} := diag\{\sigma_1^*, \ldots, \sigma_{n-q}^*, \hat{\sigma}_{n-q+1}, \ldots, \hat{\sigma}_n\}$$

◇ Additional singular values $\hat{\sigma}_{n-q+1}, \ldots, \hat{\sigma}_n$ are free parameters.

The Algorithm

Given $U^{(\nu)} \in \mathcal{O}(m)$ and $V^{(\nu)} \in \mathcal{O}(n)$,

- Solve for $c^{(\nu+1)}$ from the system of equations:

$$\sum_{k=1}^{n} \left({u_i^{(\nu)}}^T B_k v_i^{(\nu)}\right) c_k^{(\nu+1} = \sigma_i^* - {u_i^{(\nu)}}^T B_0 v_i^{(\nu)},$$

for $i = 1, \ldots, n-q$

$$\sum_{k=1}^{n} \left({u_s^{(\nu)}}^T B_k v_t^{(\nu)} + {u_t^{(\nu)}}^T B_k v_s^{(\nu)}\right) c_k^{(\nu+1)} =$$

$$-{u_s^{(\nu)}}^T B_0 v_t^{(\nu)} - {u_t^{(\nu)}}^T B_0 v_s^{(\nu)},$$

for $1 \leq s < t \leq p$.

- Define $\hat{\sigma}_k^{(\nu)}$ by

$$\hat{\sigma}_k^{(\nu)} := \begin{cases} \sigma_k^*, & \text{if } 1 \leq k \leq n-q; \\ {u_k^{(\nu)}}^T B(c^{(\nu+1)}) v_k^{(\nu)}, & \text{if } n-q < k \leq n \end{cases}$$

- Once $c^{(\nu+1)}$ is determined, calculate $W^{(\nu)}$.

- Define skew symmetric matrices $\tilde{K}^{(\nu)}$ and $\tilde{H}^{(\nu)}$:
  - ⋄ For $1 \le i < j \le p$, the equation to be satisfied is

$$W_{ij}^{(\nu)} = \hat{\sigma}_i^{(\nu)} \tilde{K}_{ij}^{(\nu)} - \tilde{H}_{ij}^{(\nu)} \hat{\sigma}_j^{(\nu)}.$$

    - ▷ Many ways to define $\tilde{K}_{ij}^{(\nu)}$ and $\tilde{H}_{ij}^{(\nu)}$.
    - ▷ Set $\tilde{K}_{ij}^{(\nu)} \equiv 0$ for $1 \le i < j \le p$.
  - ⋄ $\tilde{K}^{(\nu)}$ is defined by

$$\tilde{K}_{ij}^{(\nu)} := \begin{cases} \frac{\hat{\sigma}_i^{(\nu)} W_{ij}^{(\nu)} + \hat{\sigma}_j^{(\nu)} W_{ji}^{(\nu)}}{(\hat{\sigma}_i^{(\nu)})^2 - (\hat{\sigma}_j^{(\nu)})^2}, & \text{if } 1 \le i < j \le n;\ p < j; \\ 0, & \text{if } 1 \le i < j \le p \end{cases}$$

  - ⋄ $\tilde{H}^{(\nu)}$ is defined by

$$\tilde{H}_{ij}^{(\nu)} := \begin{cases} -\frac{W_{ij}^{(\nu)}}{\hat{\sigma}_j^{(\nu)}}, & \text{if } 1 \le i < j \le p; \\ -\frac{W_{ij}^{(\nu)}}{\hat{\sigma}_j^{(\nu)}}, & \text{if } n+1 \le i \le m;\ 1 \le j \le n; \\ \frac{\hat{\sigma}_i^{(\nu)} W_{ji}^{(\nu)} + \hat{\sigma}_j^{(\nu)} W_{ij}^{(\nu)}}{(\hat{\sigma}_i^{(\nu)})^2 - (\hat{\sigma}_j^{(\nu)})^2}, & \text{if } 1 \le i < j \le n;\ p < j; \\ 0, & \text{if } n+1 \le i \ne j \le m. \end{cases}$$

- Once $\tilde{H}^{(\nu)}$ and $\tilde{K}^{(\nu)}$ are determined, proceed the lifting in the same way as for the ISVP.

Remarks

- No longer on a fixed manifold $\mathcal{M}_s(\Sigma)$ since $\hat{\Sigma}$ is changed per step.
- The algorithm for multiple singular value case converges quadratically.

Zero Singular Value

- Zero singular value $\Rightarrow$ rank deficiency.
- Finding a lower rank matrix in a generic affine subspace $\mathcal{B}$ is intuitively a more difficult problem.
- More likely the ISVP does not have a solution.
- Consider the simplest case where $\sigma_1^* > \ldots > \sigma_{n-1}^* > \sigma_n^* = 0$.
  - ◇ Except for $\tilde{H}_{in}$ (and $\tilde{H}_{ni}$), $i = n+1, \ldots, m$, all other quantities including $c^{(\nu+1)}$ are well-defined.
  - ◇ It is necessary that
    $$W_{in}^{(\nu)} = 0 \text{ for } i = n+1, \ldots, m.$$
  - ◇ If the necessary condition fails, then no tangent line of $\mathcal{M}_s(\Sigma)$ from the current iterate $X^{(\nu)}$ will intersect the affine subspace $\mathcal{B}$.

Example of the Continuous Approach

- Integrator — Subroutine ODE (Shampine et al, '75).
  - ◇ ABSERR and RELERR $= 10^{-12}$.
  - ◇ Output values examined at interval of 10.
- Two consecutive output points differ by less than 10^{-10} $\Rightarrow$ Convergence.
- Stable equilibrium point is not necessarily a solution to the ISVP.
- Change to different initial value $X(0)$ if necessary.

Example of the Iterative Approach

- Easy implementation by MATLAB.
  - ◇ Consider the case when $m = 5$ and $n = 4$.
  - ◇ Randomly generated basis matrices by the Gaussian distribution.
- Numerical experiment meant solely to examine the quadratic convergence.
  - ◇ Randomly generate a vector $c^{\#} \in R^4$.
  - ◇ Singular values of $B(c^{\#})$ used as the prescribed singular values.
  - ◇ Perturb each entry of $c^{\#}$ by a uniform distribution between -1 and 1.
  - ◇ Use the perturbed vector as the initial guess.

Observations

- The limit point c^* is not necessary the same as the original vector $c^{\#}$.
- Singular values of $B(c^*)$ do agree with those of $B(c^{\#})$.
- Differences between singular values of $B(c^{(\nu)})$ and $B(c^*)$ are measured in the 2-norm.
- Quadratic convergence is observed.

Example of Multiple Singular Values

- Construction of an example is not trivial.
  - ◇ Same basis matrices as before.
  - ◇ Assume $p = 2$.
  - ◇ Prescribed singular values $\sigma^* = (5, 5, 2)^T$.
  - ◇ Initial guess of $c^{(0)}$ is searched by trials
- The order of singular values could be altered.
  - ◇ The value 5 is no longer the largest singular value.
  - ◇ Unless the initial guess $c^{(0)}$ is close enough to an exact solution c^*, no reason to expect that the algorithm will preserve the ordering.
  - ◇ Once convergence occurs, then σ^* must be part of the singular values of the final matrix.
- At the initial stage the convergence is slow, but eventually the rate is picked up and becomes quadratic.

Lecture 9

Toeplitz Inverse Eigenvalue Problem

- Overview
- Spectral properties of $\mathcal{C}(n)$
- An example on the effect of parity assignment
- A Newton method in $\mathcal{C}(n)$
- Numerical experiment

Overview

- Symmetric Toeplitz Matrix $T(r)$:

$$t_{ij} = r_{|i-j|+1}.$$

e.g.

$$T(r) := \begin{bmatrix} r_1 & r_2 & \dots & r_{n-1} & r_n \\ r_2 & r_1 & & r_{n-2} & r_{n-1} \\ \vdots & \ddots & \ddots & & \vdots \\ r_{n-1} & & & r_1 & r_2 \\ r_n & r_{n-1} & & r_2 & r_1 \end{bmatrix}.$$

- Unit perdiagonal matrix J:

$$j_{ij} = \delta_{i,n-j+1}.$$

  - ◇ Symmetric vector, if $Jv = v$.
  - ◇ Skew-symmetric vector, if $Jv = -v$.

- Centrosymmetric matrix M:

$$m_{ij} = m_{n-i+1,n-j+1}.$$

- $\mathcal{C}(n) := \{M | M = M^T, M = JMJ\}$.

Questions & Known Results

- ToIEP: *Find $r \in R^n$ such that $T(r)$ has a prescribed set of real numbers $\{\lambda_1, \dots, \lambda_n\}$ as its spectrum.*
- Solvability has been a challenge.
  - ◇ $n \geq 5$ is analytically intractable.
  - ◇ Symmetric Toeplitz matrices can have *arbitrary* real spectra. (Landau '94, nonconstructive proof by topological degree argument).
  - ◇ Eigenvalues *cannot* have arbitrary parity.
- Numerical calculation is possible.
  - ◇ n equations in n unknowns.
    - ▷ Newton's methods.
    - ▷ Continuation methods.
  - ◇ Mostly done in $\mathcal{S}(n)$.
- *Can the calculation be done in $\mathcal{C}(n)$? What are the advantages?*

Spectral Properties of $\mathcal{C}(n)$

- (Cantoni & Butler, '76) Any $M \in \mathcal{C}(n)$:

n	even	odd
M	$\begin{bmatrix} A & C^T \\ C & JAJ \end{bmatrix}$	$\begin{bmatrix} A & x & C^T \\ x^T & q & x^TJ \\ C & Jx & JAJ \end{bmatrix}$
$\sqrt{2}K$	$\begin{bmatrix} I & -J \\ I & J \end{bmatrix}$	$\begin{bmatrix} I & 0 & -J \\ 0 & \sqrt{2} & 0 \\ I & 0 & J \end{bmatrix}$
KMK^T	$\begin{bmatrix} A-JC & 0 \\ 0 & A+JC \end{bmatrix}$	$\begin{bmatrix} A-JC & 0 & 0 \\ 0 & q & \sqrt{2}x^T \\ 0 & \sqrt{2}x & A+JC \end{bmatrix}$

  - ◇ $A, C, J \in R^{\lfloor \frac{n}{2} \times \frac{n}{2} \rfloor}$.
  - ◇ $x \in R^{\lfloor \frac{n}{2} \rfloor}$.
  - ◇ $q \in R$.
  - ◇ $A = A^T$.

- Orthonormal basis of eigenvectors:

$$Q = K^T Z$$

  - ◇ $Z := Z := \begin{bmatrix} Z_1 & 0 \\ 0 & Z_2 \end{bmatrix}$.
    - ▷ $Z_1 :=$ Eigenvectors of $A - JC$.
    - ▷ $Z_2 :=$ Eigenvectors of $\begin{bmatrix} q & \sqrt{2}x^T \\ \sqrt{2}x & A+JC \end{bmatrix}$ or $A + JC$.

- Parity of eigenvectors:
  - ◇ $K^T \begin{bmatrix} Z_1 \\ 0 \end{bmatrix} = \lfloor \frac{n}{2} \rfloor$ skew-symmetric eigenvectors ⇒ "Odd" eigenvalues.
  - ◇ $K^T \begin{bmatrix} 0 \\ Z_2 \end{bmatrix} = \lceil \frac{n}{2} \rceil$ symmetric eigenvectors ⇒ "Even" eigenvalues.

- *For an ToIEP to be solvable, each given eigenvalue must carry a specific parity.*

Inverse Problem for Centrosymmetric Matrices

- Given *arbitrary*:
  - ⋄ Diagonal matrix $\Lambda := \mathrm{diag}\{\lambda_1, \ldots, \lambda_n\}$.
  - ⋄ Orthogonal matrix $Z_1 \in R^{\lfloor \frac{n}{2} \rfloor \times \lfloor \frac{n}{2} \rfloor}$.
  - ⋄ Orthogonal matrix $Z_2 \in R^{\lceil \frac{n}{2} \rceil \times \lceil \frac{n}{2} \rceil}$.
- Then:
  - ⋄ Centrosymmetric matrix:

$$M := K^T \begin{bmatrix} Z_1 & 0 \\ 0 & Z_2 \end{bmatrix} \Lambda \begin{bmatrix} Z_1 & 0 \\ 0 & Z_2 \end{bmatrix}^T K.$$

  - ⋄ $\{\lambda_1, \ldots, \lambda_{\lfloor \frac{n}{2} \rfloor}\}$ = Odd eigenvalues of M.
  - ⋄ $\{\lambda_{\lfloor \frac{n}{2} \rfloor + 1}, \ldots, \lambda_n\}$ = Even eigenvalues of M.
- Isospectral surface $\mathcal{M}_{\mathcal{C}}(\lambda_1, \ldots, \lambda_n)$:

$$\mathcal{M}_{\mathcal{C}} := \{M \in \mathcal{C}(n) |\ \text{eigenvalues} = \lambda_1, \ldots, \lambda_n\}.$$

- M may not be Toeplitz.

An Example of $n = 3$

- $M \in \mathcal{C}(3)$:

$$M = \begin{bmatrix} m_{11} & m_{12} & m_{13} \\ \times & m_{22} & \times \\ \times & \times & \times \end{bmatrix}.$$

  - ⋄ $\mathrm{trace}(M) = 0 \Longrightarrow$ Three free parameters in $\mathcal{C}(3)$.
- Isospectral subset $\mathcal{M}_{\mathcal{C}}(\lambda_1, \lambda_2, \lambda_3)$:

$$\begin{aligned} (m_{11} - \frac{\lambda_{\sigma_1}}{4})^2 + \frac{1}{2} m_{12}^2 &= \frac{(\lambda_{\sigma_2} - \lambda_{\sigma_3})^2}{16}, \\ m_{13} &= m_{11} - \lambda_{\sigma_1}. \end{aligned}$$

  - ⋄ σ = A permutation of integers $\{1, 2, 3\}$.
- $\mathcal{M}_{\mathcal{C}}$ = Three ellipses.
  - ⋄ One circumscribes the other two.
- Check # of m_{12}-intercepts $\Rightarrow$

$$\#\ \text{of solutions} = \begin{cases} 4, & \text{if distinct eigenvalues;} \\ 2, & \text{if multiplicity 2.} \end{cases}$$

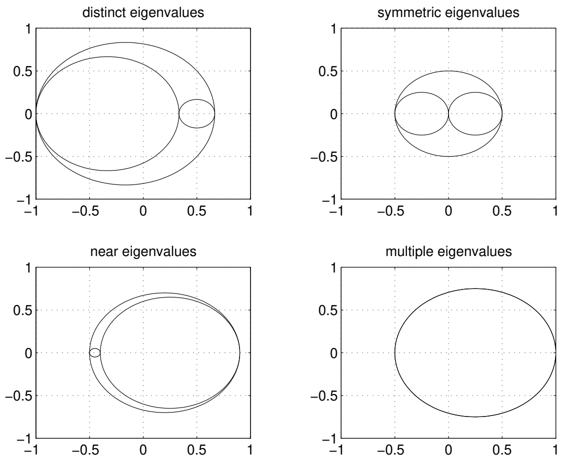

Figure 9.1: Plots of m_{11} versus m_{12} for $\mathcal{M}_{\mathcal{C}}$ in $\mathcal{C}(3)$.

- Each ellipse = One parity assignment among eigenvalues.
- Wrong assignment $\Rightarrow$ No Toeplitz.
- Magnitude of eigenvalues $\rightarrow$ Solvability.
- Ordered eigenvalues alternate in parity $\stackrel{?}{\Rightarrow}$ Safeguard.

A Newton Method in $\mathcal{C}(n)$

- A tangent step
- Lift by approximation
- Lift by global ordering
- Lift by local ordering

A Classical Newton Method

- A function:
$$f : R \longrightarrow R.$$
- The scheme:
$$x^{(\nu+1)} = x^{(\nu)} - (f'(x^{(\nu)}))^{-1} f(x^{(\nu)}).$$
- The intercept:
  - ⋄ $x^{(\nu+1)} =$ The x-intercept of the tangent line of the graph of f from $(x^{(\nu)}, f(x^{(\nu)}))$.
- The lifting:
  - ⋄ $(x^{(\nu+1)}, f(x^{(\nu+1)})) =$ The natural "lift" of the intercept along the y-axis to the the graph of f.

An Analogy of the Newton Method

- Think of
  - ⋄ $\mathcal{M}_{\mathcal{C}}(\Lambda) =$ The graph of f.
  - ⋄ $\mathcal{T}(n) := \{$Toeplitz matrices$\} =$ The x-axis.
  - ⋄ Limit the iteration to $\mathcal{C}(n)$.
- Manifold $\mathcal{M}_{\mathcal{C}}(\Lambda)$:
  - ⋄ Parametrization:
$$\begin{aligned} M &= Q\Lambda Q^T, \\ Q &= K^T Z, \\ Z &\in \mathcal{O}(\lfloor\frac{n}{2}\rfloor) \times \mathcal{O}(\lceil\frac{n}{2}\rceil). \end{aligned}$$
  - ⋄ Tangent vector:
$$\begin{aligned} T_M(\mathcal{M}_{\mathcal{C}}) &= \tilde{S}M - M\tilde{S}, \\ \tilde{S} &:= Q\begin{bmatrix} S_1 & 0 \\ 0 & S_2 \end{bmatrix} Q^T. \end{aligned}$$
    - ▷ $S_1 =$ skew-symmetric in $R^{\lfloor\frac{n}{2}\rfloor\times\lfloor\frac{n}{2}\rfloor}$.
      $S_2 =$ skew-symmetric in $R^{\lceil\frac{n}{2}\rceil\times\lceil\frac{n}{2}\rceil}$

A Tangent Step

- Given $M^{(\nu)} \in \mathcal{M}_{\mathcal{C}}(\Lambda)$ (*Parity fixed*),
  - ◇ Find $\tilde{S}^{(\nu)}$ and $r^{(\nu+1)}$ for
$$M^{(\nu)} + \tilde{S}^{(\nu)} M^{(\nu)} - M^{(\nu)} \tilde{S}^{(\nu)} = T(r^{(\nu+1)}).$$
- Equivalently:
$$\begin{aligned} \Lambda + S^{(\nu)}\Lambda - \Lambda S^{(\nu)} &= {Q^{(\nu)}}^T T(r^{(\nu+1)}) Q^{(\nu)} \\ &= {Z^{(\nu)}}^T K T(r^{(\nu+1)}) K^T Z^{(\nu)}. \end{aligned}$$
  - ◇ Spectral decomposition:
$$\begin{aligned} {Q^{(\nu)}}^T M^{(\nu)} Q^{(\nu)} &= \Lambda, \\ Q^{(\nu)} &= K^T Z^{(\nu)}. \end{aligned}$$
- Key observation:
$$KT(r^{(\nu+1)})K^T = \begin{bmatrix} T_1^{(\nu+1)} & 0 \\ 0 & T_2^{(\nu+1)} \end{bmatrix}.$$

$\Rightarrow$ The system is split in half.

Find the Intercept

- The right-hand side of the system is linear in $r^{(\nu+1)}$.
- Diagonal elements in the system $\Rightarrow$ A linear system for $r^{(\nu+1)}$ without reference to $S^{(\nu)}$:
$$J^{(\nu)} r^{(\nu+1)} = \lambda.$$
  - ◇ $\lambda := [\phi_1, \ldots, \phi_{\lfloor \frac{n}{2} \rfloor}, \psi_1, \ldots \psi_{\lceil \frac{n}{2} \rceil}]^T$ (*Fixed parity*).
  - ◇
$$J_{ij}^{(\nu)} := \begin{cases} (Z_1^{(\nu)})_{*i}^T E_1^{[j]} (Z_1^{(\nu)})_{*i}, & \text{if } 1 \le i \le \lfloor \frac{n}{2} \rfloor; \\ (Z_2^{(\nu)})_{*i}^T E_2^{[j]} (Z_2^{(\nu)})_{*i}, & \text{if } \lfloor \frac{n}{2} \rfloor < i \le n. \end{cases}$$
    - ▷
$$\begin{bmatrix} E_1^{[j]} & 0 \\ 0 & E_2^{[j]} \end{bmatrix} = KT(e_j)K^T.$$
    - ▷ $(Z_k^{(\nu)})_{*i}$:= the i^{th} column of the matrix $Z_k^{(\nu)}$.
- Only length of $\approx \frac{n}{2}$ in all vector-matrix-vector multiplications.

Compute $S^{(\nu)}$

- Once $T(r^{(\nu+1)})$ is determined, off-diagonal elements in the system $\Rightarrow S^{(\nu)}$:

$$(S_1^{(\nu)})_{ij} = \frac{(Z_1^{(\nu)})_{*i}^T T_1^{(\nu+1)} (Z_1^{(\nu)})_{*j}}{\phi_i - \phi_j}, \; 1 \le i < j \le \lfloor \frac{n}{2} \rfloor,$$

$$(S_2^{(\nu)})_{ij} = \frac{(Z_2^{(\nu)})_{*i}^T T_2^{(\nu+1)} (Z_2^{(\nu)})_{*j}}{\psi_i - \psi_j}, \; 1 \le i < j \le \lceil \frac{n}{2} \rceil.$$

  - ◇ Eigenvalues within each parity group must be distinct.
  - ◇ $\lambda_1, \ldots, \lambda_n$ need not be totally distinct.
- Multiple eigenvalues $\Longrightarrow$ Basis of eigenspace splits as evenly as possible between symmetric and skew-symmetric eigenvectors. (Delsarte & Genin, '83)
- Multiplicity of each eigenvalue $\le 2 \Longrightarrow S^{(\nu)}$ can be formulated.

Find the Lift

- Coordinate-free lift (Friedland, '87; Chu, '92):

$$M^{(\nu+1)} := Q^{(\nu)} {R^{(\nu)}}^T {Q^{(\nu)}}^T M^{(\nu)} Q^{(\nu)} R^{(\nu)} {Q^{(\nu)}}^T.$$

  - ◇ Lift by approximation:

$$R^{(\nu)} := \left(I + \frac{S^{(\nu)}}{2}\right)\left(I - \frac{S^{(\nu)}}{2}\right)^{-1}.$$

- In calculation, only need

$$Z^{(\nu+1)} := Z^{(\nu)} {R^{(\nu)}}^T.$$

  - ◇ All matrices involved are 2-block diagonal.
- Quadratic convergence.
- Multiplicity $> 2 \Rightarrow$ No $S^{(\nu)} \Rightarrow$ No lift.
- *Can we by-pass $S^{(\nu)}$ to perform a lift?*

Lift by Global Ordering

- Idea:
  - ◇ Look for matrix $M^{(\nu+1)} \in \mathcal{M}_{\mathcal{C}}$ that is nearest to $T(r^{(\nu+1)})$.

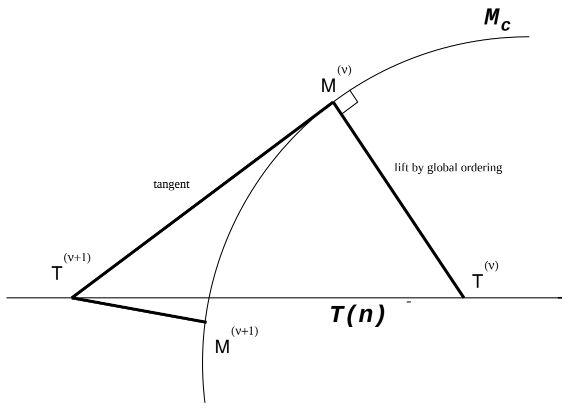

Figure 9.2: Geometry of Lift by Global Ordering.

- Answer: Wielandt-Hoffman theorem.
  - ◇ Spectral decomposition of $T(r^{(\nu+1)})$ is easy:

$$\overline{Z}^{(\nu+1)^T} K T(r^{(\nu+1)}) K^T \overline{Z}^{(\nu+1)} = \begin{bmatrix} \overline{\Lambda}_1^{(\nu+1)} & 0 \\ 0 & \overline{\Lambda}_2^{(\nu+1)} \end{bmatrix}.$$

  - ◇ Rearrange $\{\lambda_1, \ldots, \lambda_n\}$ in the same ordering as in $\overline{\Lambda}_1^{(\nu+1)}$ and $\overline{\Lambda}_2^{(\nu+1)}$ to obtain $\tilde{\Lambda}_1^{(\nu+1)}$ and $\tilde{\Lambda}_2^{(\nu+1)}$.
  - ◇ Define:

$$M^{(\nu+1)} := K^T \overline{Z}^{(\nu+1)} \begin{bmatrix} \tilde{\Lambda}_1^{(\nu+1)} & 0 \\ 0 & \tilde{\Lambda}_2^{(\nu+1)} \end{bmatrix} \overline{Z}^{(\nu+1)^T} K.$$

- New starting point:

$$\Lambda = \Lambda^{(\nu+1)} := \begin{bmatrix} \tilde{\Lambda}_1^{(\nu+1)} & 0 \\ 0 & \tilde{\Lambda}_2^{(\nu+1)} \end{bmatrix},$$
$$Z^{(\nu+1)} := \overline{Z}^{(\nu+1)}.$$

- Significance:
  - ◇ Parity assignment may be changed.
  - ◇ No $S^{(\nu)}$ is needed.
  - ◇ Multiple eigenvalues with same parity can be handled.

Lift by Local Ordering

- Would like to avoid computing $S^{(\nu)}$ as well as parity switching?
- Idea:
  - ◇ Λ is kept fixed.
  - ◇ Reorganize columns of $\overline{Z}_1^{(\nu+1)}$ and $\overline{Z}_2^{(\nu+1)}$.
- Calculation:
  - ◇ Elements in $\overline{\Lambda}_1^{(\nu+1)}, \overline{\Lambda}_2^{(\nu+1)}$ are in the same ordering as those in Λ_1 and Λ_2.
- New starting point:

$$Z^{(\nu+1)} := \text{The reorganized } \overline{Z}^{(\nu+1)}.$$

- Global ordering = Local ordering, when reaching convergence.
- 1st order projection + 2nd order tangent step $\Longrightarrow$ Quadratic convergence. (Traub)

Numerical Experiment

- Example 1: Wrong parity
- Example 2: Quadratic convergence
- Example 3: Multiplicity = 2
- Example 4: Multiplicity = 3
- Example 5: High order case

Example 1: Wrong Parity

- Test data (*Wrong parity*):

$$\left.\begin{array}{rcl}\lambda_1 &=& -2.4128 \times 10^{+0}(E)\\ \lambda_2 &=& -2.6407 \times 10^{-1}(E)\\ \lambda_3 &=& 2.6769 \times 10^{+0}(O)\end{array}\right\} \textit{Wrong parity}$$

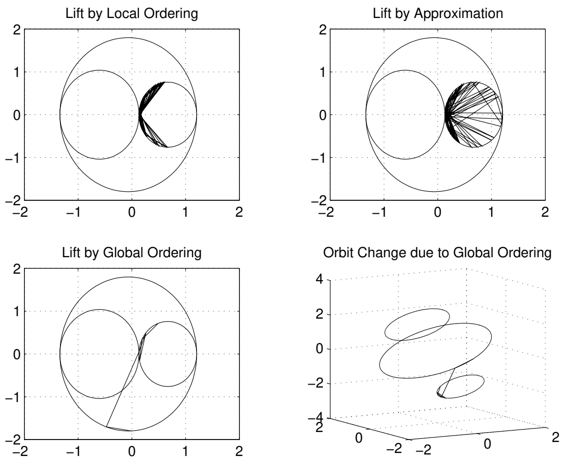

Figure 9.3: Behaviors of Algorithms When Starting with the Wrong Orbit.

- Lift by approximation ⇒ Staying on the *wrong* orbit.
- Local ordering ⇒ Wrong orbit, clustering.
- Global ordering ⇒ Change orbit, convergence.

Example 2: Quadratic Convergence

- Limit point $r^{(*)}$ may be away from original $r^{(\#)}$, even if $r^{(0)} \approx r^{(\#)}$.
- Limit points may be different among methods, even with the same starting $r^{(0)}$.
- Eigenvalues of $T(r^{(*)})$ = those of $T(r^{\#})$, but parity may change in the global ordering case.

Example 3: Multiplicity = 2

- Test data (Random number):

$$\begin{array}{rl} -5.8942 \times 10^{-1} & (E) \\ \left\{\begin{array}{r} -1.8565 \times 10^{-1} \\ -1.8565 \times 10^{-1} \end{array}\right. & \begin{array}{l} (O) \\ (E) \end{array} \\ 3.7508 \times 10^{-1} & (O) \\ 5.8564 \times 10^{-1} & (E) \end{array}$$

- Parity unknown.
  - ◇ Assume the possibly safest assignment.
- Multiply eigenvalues split between parities.
- Quadratic convergence.

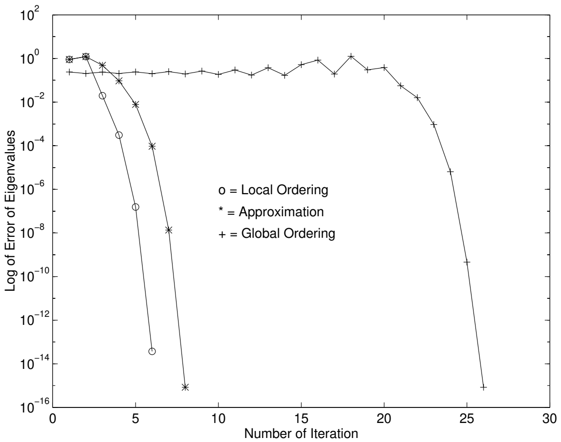

Figure 9.4: Number of Iteration versus Logarithmic Scale of Errors in Example 3.

Example 4: Multiplicity = 3

- Test data:

$$\begin{array}{ll} -8.4328 \times 10^{-1} & (E) \\ \left\{ \begin{array}{l} -1.2863 \times 10^{-1} \\ -1.2863 \times 10^{-1} \\ -1.2863 \times 10^{-1} \end{array} \right. & \begin{array}{l} (O) \\ (E) \\ (O) \end{array} \\ 1.2292 \times 10^{+0} & (E) \end{array}$$

- Lift by approximation fails.
- Methods by local and global ordering converge to

$$\left[.2204 \times 10^{-16}, 4.2222 \times 10^{-1}, 1.2863 \times 10^{-1}, 4.2222 \times 10^{-1}, 1.2863 \times 10^{-1}\right]$$

with error history

$$\begin{array}{l} 2.0327 \times 10^{+0} \\ 4.0355 \times 10^{-2} \\ 1.3903 \times 10^{-4} \\ 3.5477 \times 10^{-9} \\ 7.8896 \times 10^{-16}. \end{array}$$

Example 5: $n = 20$

- Test data:

$-1.0242\times10^{+1}$	$-9.6736\times10^{+0}$	$-5.5608\times10^{+0}$	$-2.2651\times10^{+0}$
5.5692×10^{-1}	$2.1786\times10^{+0}$	$3.3867\times10^{+0}$	$4.0016\times10^{+0}$
$6.3594\times10^{+0}$	$8.7090\times10^{+0}$		

$-1.0416\times10^{+1}$	$-9.4352\times10^{+0}$	$-4.7955\times10^{+0}$	-7.7180×10^{-1}
6.3996×10^{-1}	$2.6374\times10^{+0}$	$4.4879\times10^{+0}$	$4.7572\times10^{+0}$
$6.2222\times10^{+0}$	$9.2230\times10^{+0}$		

  - ◇ Not the safest possible parity assignment, first ten odd, last ten even.
- Method of approximation fails after 100 iterations.
- Method of global ordering performs best.

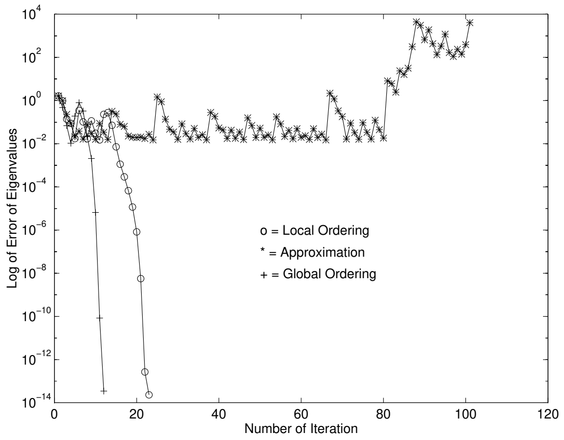

Figure 9.5: Number of Iteration versus Logarithmic Scale of Errors in Example 5.

Conclusion

- Solving the ToIEP within the subspace $\mathcal{C}(n)$ is possible.
    - ◇ Problem size and cost are halved.
    - ◇ Multiple eigenvalue case can be handled.
- Coordinate-free Newton-like methods are available.
    - ◇ Quadratic convergence is observed.
- Parity assignment of eigenvalues plays an important role in whether an ToIEP is solvable.
- Local ordering and global ordering, based on the Wielandt-Hoffman theorem, permit a new way of lifting.
    - ◇ Higher multiplicity eigenvalue case can now be handled.

	Case (a)	Case (b)	Case (c)
$r^{(\#)}$	0	0	0
	-2.0413×10^{-3}	-9.2349×10^{-1}	-3.3671×10^{-1}
	$1.6065\times10^{+0}$	-7.0499×10^{-2}	4.1523×10^{-1}
Original Value	8.4765×10^{-1}	1.4789×10^{-1}	$1.5578\times10^{+0}$
	2.6810×10^{-1}	-5.5709×10^{-1}	$-2.4443\times10^{+0}$
$r^{(0)}$	0	0	0
	-2.8351×10^{-1}	$-1.8024\times10^{+0}$	6.3658×10^{-1}
	9.3953×10^{-1}	7.3881×10^{-1}	4.0318×10^{-1}
Initial Value	8.2068×10^{-1}	1.5694×10^{-1}	$1.0901\times10^{+0}$
	$1.0634\times10^{+0}$	-5.2451×10^{-1}	$-3.2628\times10^{+0}$
$r^{(*)}$	2.0426×10^{-16}	2.2204×10^{-16}	7.4940×10^{-16}
	-2.0413×10^{-3}	-9.2349×10^{-1}	-3.5391×10^{-1}
	$1.6065\times10^{+0}$	-7.0499×10^{-2}	4.3645×10^{-1}
Local Ordering	8.4765×10^{-1}	1.4789×10^{-1}	$1.5244\times10^{+0}$
	2.6810×10^{-1}	-5.5709×10^{-1}	$-2.4655\times10^{+0}$
$r^{(*)}$	8.6831×10^{-16}	0	4.7184×10^{-16}
	-2.0413×10^{-3}	-9.2349×10^{-1}	-3.3671×10^{-1}
	$1.6065\times10^{+0}$	-7.0499×10^{-2}	4.1523×10^{-1}
Approximation	8.4765×10^{-1}	1.4789×10^{-1}	$1.5578\times10^{+0}$
	2.6810×10^{-1}	-5.5709×10^{-1}	$-2.4443\times10^{+0}$
$r^{(*)}$	2.4113×10^{-16}	-1.1102×10^{-16}	6.1062×10^{-16}
	-9.3778×10^{-2}	-9.2646×10^{-1}	3.5391×10^{-1}
	$1.5174\times10^{+0}$	-6.1419×10^{-2}	4.3645×10^{-1}
Global Ordering	9.9597×10^{-1}	1.3518×10^{-1}	$-1.5244\times10^{+0}$
	5.7042×10^{-1}	-5.4694×10^{-1}	$-2.4655\times10^{+0}$

Table 9.1: Initial and Final Values of $r^{(\nu)}$ for Example 2.

Iterations	Local Ordering	Approximation	Global Ordering
0	$1.3847\times10^{+0}$	$1.3847\times10^{+0}$	$1.2194\times10^{+0}$
1	7.1545×10^{-1}	7.1545×10^{-1}	4.2739×10^{-1}
2	2.1982×10^{-2}	6.3866×10^{-2}	1.4179×10^{-2}
3	5.1223×10^{-5}	2.0606×10^{-4}	4.3624×10^{-5}
4	4.4931×10^{-10}	7.1037×10^{-9}	4.7985×10^{-10}
5	1.4729×10^{-15}	2.9671×10^{-15}	1.7659×10^{-15}

Table 9.2: Errors of Eigenvalues for Case (a) in Example 2.

Lecture 10

Miscellaneous Flows

- Flows on S^{n-1}
- Toeplitz annihilator flow
- Linear stationary flow
- SVD flow
- QZ flow
- Scaled Toda flow

Flows on S^{n-1}

- Power method
- Rayleigh quotient method

Power Method

- Iterative method:

$$\begin{aligned} y_{k+1} &= Ax_k \\ x_{k+1} &= \frac{y_{k+1}}{\|y_{k+1}\|}. \end{aligned}$$

  - ◇ Fundamental to the QR algorithm.
  - ◇ $\{x_k\}$ converges to the maximal eigenvector.

- Continuous method:

$$\frac{du}{dt} = Bu - \langle Bu, u\rangle u.$$

  - ◇ Project gradient flow on S^{n-1} for maximizing the Rayleigh quotient

$$\rho(y) := \frac{y^T By}{y^T y}.$$

  - ◇ Closed form solution:

$$u(t) = \frac{e^{tB}u_0}{\|e^{tB}u_0\|}.$$

- Dynamics of $u(t)$:
  - ◇ Maximal eigenvalue is real $\Rightarrow u(t)$ converges to maximal eigenvector.
  - ◇ Maximal eigenvalue is complex $\Rightarrow u(t)$ is attracted to and oscillating around the 2-dim circle ($= S^{n-1} \cap$ subspace spanned by the real and the imaginary parts of maximal eigenvector).
- Choose $B = \ln A$ if A is nonsingular $\Rightarrow$

$$u(t) = \frac{A^t u_0}{\|A^t u_0\|}.$$

  - ◇ Poincaré map $\equiv$ Classical power method.

Rayleigh Quotient Method

- Iterative method:

$$\begin{aligned} \rho_k &= x_k^T A x_k \\ y_{k+1} &= (A - \rho_k I)^{-1} x_k \\ x_{k+1} &= \frac{y_{k+1}}{\|y_{k+1}\|}. \end{aligned}$$

  - ◇ Main objective: Speed up convergence by making $A - \rho_k I$ nearly singular so that $(A - \rho_k I)^{-1}$ has a most dominant eigenvalue.
- Suppose A is normal. Then
  - ◇ $\{\rho_k\}$ converges.
  - ◇ Either $\{(\rho_k, x_k)\}$ converges to an eigenpair cubically,
  - ◇ Or $\{\rho_k\}$ converges linearly to a point equidistant from $s \geq 2$ eigenvalues of A, but $\{x_k\}$, may or may not have a limit cycle, does not converge.

- Can model RQI by continuous power method in the interval $[k, k+1]$:
  - ◇ Choose $x_k = u(k)$ and $B = \ln(A - \rho_k I)^{-1}$.
  $$u(k+1) = \frac{(A-\rho_k I)^{-1} u(k)}{\|(A-\rho_k)^{-1} u(k)\|}.$$
  - ◇ Only piecewise differentiable.
  - ◇ Difficult to analyze asymptotic behavior.

Simulation of RQI

- Behavior of $\ln|z-c|^{-1}$ and $|z-c|^2$ are qualitatively similar near $c \Rightarrow$
$$B = \ln(A - \rho(x_k))^{-1}$$
$$\uparrow$$
$$B = (A - \rho(x_k)I)^{-2}$$
$$\uparrow$$
$$B = B(u) := \left((A - \rho(u)I)^T (A - \rho(u)I)\right)^{-1}.$$
- New differential equation:
$$\frac{du}{dt} = B(u)u - \langle B(u)u, u\rangle u.$$
  - ◇ System becomes singular when reaching the set $\Gamma := \{u \in S^{n-1} | \rho(u) \in \sigma(A)\}$.
- Residue function:
$$r(t) := \|\,(A - \rho(u(t))I)\,u(t)\|.$$

Global Dynamics

- Residue is monotone decreasing:

$$
\begin{aligned}
2r\frac{dr}{dt} &= \frac{d}{dt}\langle u, B^{-1}u\rangle \\
&= \langle \frac{du}{dt}, B^{-1}u\rangle + \langle u, B^{-1}\frac{du}{dt}\rangle \\
&\quad +\langle u, -\frac{d\rho}{dt}\left[(A-\rho)+(A-\rho)^T\right]u\rangle \\
&= 2\langle \frac{du}{dt}, B^{-1}u\rangle \\
&= 2\langle Bu - \rangle Bu, u\rangle u, B^{-1}u\rangle \\
&= 2\left(1-\langle u, Bu\rangle\langle u, B^{-1}u\rangle\right) \\
&\leq 0.(\text{ Kantorovich Inequality})
\end{aligned}
$$

- $u(t)$ can behave as only one of the following three:
  - ⋄ $u(t)$ hits the singular set Γ in finite time.
  - ⋄ $u(t) \to$ an eigenvector of A as $t \to \infty$.
  - ⋄ $u(t)$ has its ω-limit set contained in the set $E = \{u^* | u^* \text{ is an eigenvector of } B(u^*)\}$.
- Dynamics of the DE are parallel to those of the classical RQI (Chu, '86).

Toeplitz Annihilator Flow

- Isospectral flow on $\mathcal{S}(n)$:

$$
\begin{aligned}
\frac{dX}{dt} &= [X, k(X)] \\
k : \mathcal{S}(n) &\to \mathcal{S}(n)^{\perp} \\
&\Updownarrow \\
X(t) &= Q(t)^T X(0) Q(t) \\
&\Updownarrow \\
\frac{dQ}{dt} &= Qk(X),\ Q(0) = I.
\end{aligned}
$$

- Can take k to so that $k(T) = 0$ iff T is symmetric Toeplitz matrices.
- Ideas:
  - ⋄ $X(t)$ stays bounded $\Rightarrow$ Invariant ω-limit set is non-empty.
  - ⋄ Simple spectrum of $X(0)$
    $\Rightarrow [X, k(X)] = 0$ iff $k(X) =$ Polynomial of X
    $\Rightarrow k(X) = 0$
    $\Rightarrow X$ is Toeplitz.

Toeplitz Annihilators

- The simplest annihilator:

$$k_{ij} := \begin{cases} x_{i+1,j} - x_{i,j-1}, & \text{if } 1 \le i < j \le n \\ 0, & \text{if } 1 \le i = j \le n \\ x_{i-1,j} - x_{i,j+1}, & \text{if } 1 \le j < i \le n \end{cases}$$

  ◇ Vector field ⇒ Homogeneous polynomials of degree 2 and norm preserving.

- A more complicated way:

$$k(X) := [L(X), C]$$

  ◇ A constant matrix:

$$C := \begin{bmatrix} 0 & 1 & 0 & \dots & & 0 \\ 1 & 0 & 1 & & & \vdots \\ 0 & 1 & \ddots & & & \\ & & & & & \\ \vdots & & & & 0 & 1 \\ 0 & & \dots & & 1 & 0 \end{bmatrix}.$$

  ◇ $L(X) :=$ Projection of X onto $\mathcal{T}^C$ along $\mathcal{T}$.

  ◇ $\mathcal{T}^C :=$ Any complementary subspace of $\mathcal{T}$ in $\mathcal{S}(n)$.

A Danger

- All annihilators work numerically ⇒ Confirming Landau's result (Landau, '94).
- A similar system (Bender et al., '78):

$$\begin{aligned} \frac{dy_1}{dt} &= y_2y_3 + y_5y_4 - 2\,y_2y_5, \\ \frac{dy_2}{dt} &= y_3y_4 + y_1y_5 - 2y_3y_1, \\ \frac{dy_3}{dt} &= y_5y_4 + y_2y_1 - 2y_2y_4, \\ \frac{dy_4}{dt} &= y_1y_5 + y_2y_3 - 2y_5y_3, \\ \frac{dy_5}{dt} &= y_2y_1 + y_3y_4 - 2y_1y_4, \end{aligned}$$

  ◇ Norm preserving.

  ◇ Random behavior.

- Need to scrutinize the system more!

The System when $n = 3$

- Trace $= 0 \Rightarrow$ Can describe system in terms of $(x_{11}, x_{12}, x_{13}, x_{23}, x_{33})$:

$$
\begin{aligned}
\frac{dx_{11}}{dt} &= 4x_{12}x_{11} + 2x_{12}x_{33} - 2x_{13}x_{23} + 2x_{13}x_{12}, \\
\frac{dx_{12}}{dt} &= -4x_{11}^2 - 4x_{11}x_{33} - 2x_{13}x_{33} - x_{13}x_{11} \\
&\quad -x_{33}^2 - x_{23}^2 + x_{23}x_{12}, \\
\frac{dx_{13}}{dt} &= 3x_{11}x_{23} + 3x_{12}x_{33}, \\
\frac{dx_{23}}{dt} &= x_{23}x_{12} - x_{12}^2 - 4x_{11}x_{33} - x_{11}^2 - 4x_{33}^2 \\
&\quad -2x_{13}x_{11} - x_{13}x_{33}, \\
\frac{dx_{33}}{dt} &= 2x_{13}x_{23} - 2x_{13}x_{12} + 4x_{23}x_{33} + 2x_{11}x_{23}.
\end{aligned}
$$

Invariant Set

- Isospectral surface is invariant.
- Equilibrium points are invariant:
  - ◇ No isolated equilibrium.
  - ◇ $(c_1, 0, -3c_1, 0, c_1)$
    - ▷ Eigenvalues $= 0, \pm 3\sqrt{6}c_1, \pm 6\sqrt{2}|c_1|i$.
    - ▷ Never stable.
    - ▷ Possible periodic solution.
  - ◇ $(0, c_2, c_3, c_2, 0)$
    - ▷ Eigenvalues $= 0, 0, 6c_2, 2(c_2+c_3), 2(c_2-c_3)$.
    - ▷ Stable when $c_2 < 0$ and $|c_2| \geq c_3$.
- $\mathcal{W} = \{(x_{11}, x_{12}, x_{13}, x_{12}, x_{11}) | x_{11}, x_{12}, x_{13} \in R\}$ is invariant.
  - ◇ $\mathcal{T} \subset \mathcal{W}$ with $x_{11} = 0$.
  - ◇ System in $\mathcal{W} \Rightarrow$ Elliptic orbits within $\mathcal{W}$.

$$
\begin{aligned}
\frac{dx_{11}}{dt} &= 6x_{11}x_{12}, \\
\frac{dx_{12}}{dt} &= -9x_{11}^2 - 3x_{11}x_{13}, \\
\frac{dx_{13}}{dt} &= 6x_{11}x_{12}.
\end{aligned}
$$

Orbital Stability

- Numerical integration always solves ITEP.
- Ellipses are orbitally unstable:

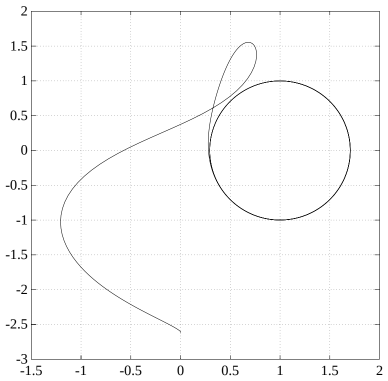

Figure 10.1: Plot of $x_{11}(t)$ versus $x_{12}(t)$.

- Orbital unstability can be confirmed by the *characteristic exponents* at a periodic solution (Coddington et al., '55).

- Orbits stay in isospectral surface $\Rightarrow$ Eigenvalues are not lost.

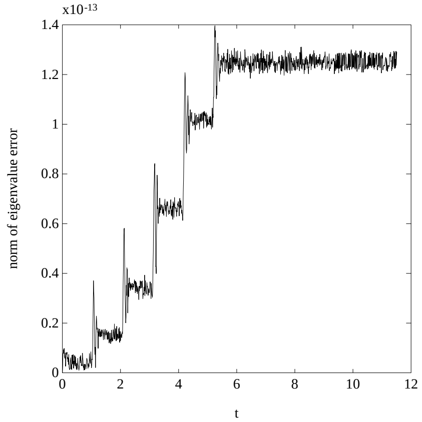

Figure 10.2: Error of eigenvalues between $X(0)$ and $X(t)$.

Linear Stationary Flow

- Stationary iteration for solving $Ax^* = b$:

$$x_{k+1} = Gx_k + c.$$

  - ⋄ $G = I - Q^{-1}A$, $c = Q^{-1}b$.
  - ⋄ Fixed point of iteration $= x^*$.
  - ⋄ Iteration converges $\Leftrightarrow \rho(G) < 1$.

- A differential system:

$$\frac{dx}{dt} = (G - I)x + c = -Q^{-1}Ax + c.$$

  - ⋄ Euler step with unit stepsize $\Rightarrow$ Stationary iteration.
  - ⋄ $\Re\lambda(Q^{-1}A) > 0 \Rightarrow x^* =$ Global attractor.
  - ⋄ The choice of Q exists (Pole assignment).

- Discrete methods for DE $\Rightarrow$ Plenty of new iterative schemes.

- Three-term polynomial acceleration methods $\equiv$ Two-step, explicit, variable coefficient ODE methods.

$$x_1 = \beta_1(Gx_0 + c) + (1 - \beta_1)x_0$$
$$x_{k+1} = \alpha_{k+1}\{\beta_{k+1}(Gx_k + c) + (1 - \beta_{k+1})x_k\} + (1 - \alpha_{k+1})x_{k-1}$$

iff

$$\begin{aligned} x_1 &= x_0 + \beta_1 f_0 \\ x_{k+1} &= \alpha_{k+1}x_k + (1 - \alpha_{k+1})x_{k-1} + \alpha_{k+1}\beta_{k+1}f_k. \end{aligned}$$

  - ⋄ Function evaluation $f_k := (G - I)x_k + c$.

SVD Flow

- Golub and Kahan algorithm:
  - ◇ Use Householder transformations to reduce $A \in R^{m\times n}$ to upper bidiagonal form.
  - ◇ Apply implicit-shift QR steps to the tridiagonal matrix $B^T B$ to compute the SVD of B.
- A one-parameter family of matrices:

$$\begin{aligned} Y(t) &= U(t)BV(t), \\ &\Updownarrow \\ \frac{dY}{dt} &= YN - MY \\ M, N &= \text{skew-symmetric}, \\ &\Updownarrow \\ \frac{dU}{dt} &= -MU, \\ \frac{dV}{dt} &= VN. \end{aligned}$$

- One special choice:

$$\begin{aligned} M(t) &:= \Pi_0\left(Y(t)Y(t)^T\right) \\ N(t) &:= \Pi_0\left(Y(t)^T Y(t)\right). \end{aligned}$$

  - ◇ $Y(t)$ maintains the bidiagonal form.

$$\begin{aligned} \frac{dy_{i,i}}{dt} &= y_{i,i}\left(y_{i,i+1}^2 - y_{i-1,i}^2\right) \\ \frac{dy_{i,i+1}}{dt} &= y_{i,i+1}\left(y_{i+1,i+1}^2 - y_{i,i}^2\right). \end{aligned}$$

  - ◇ Poincaré map $\equiv$ SVD algorithm.

QZ Flow

- Moler and Stewart algorithm:
  - ◇ Simultaneously educe A to upper Hessenberg form and B to upper triangular form.
  - ◇ Apply QR steps to reduce A to upper quasi-triangular form while preserving triangularity of B.
- A one-parameter family of matrices:

$$\begin{aligned}
X(t) &= Q(t)AZ(t), \\
Y(t) &= Q(t)BZ(t), \\
&\Updownarrow \\
\frac{dX}{dt} &= XM - NX \\
\frac{dY}{dt} &= YM - NY \\
M, N &= \text{skew-symmetric}, \\
&\Updownarrow \\
\frac{dQ}{dt} &= -MM, \\
\frac{dZ}{dt} &= ZN.
\end{aligned}$$

- One special choice:

$$\begin{aligned}
M(t) &:= \Pi_0\left(X(t)Y(t)^{-1}\right) \\
N(t) &:= \Pi_0\left(Y(t)^{-1}X(t)\right).
\end{aligned}$$

  - ◇ $X(t)$ maintains upper Hessenberg form.
  - ◇ $Y(t)$ maintains upper triangular form.
  - ◇ Poincaré map $\equiv$ QZ algorithm.

Scaled Toda Flow

- Componentwise scaling:

$$\frac{dX}{dt} = [X, A \circ X].$$

  - ◇ $\circ$ = Hadamard product.

- Isospectral flow:

$$\begin{aligned} X(t) &= L(t)^{-1}X_0L(t) = R(t)X_0R(t)^{-1}, \\ &\Updownarrow \\ \frac{dL}{dt} &= L(A \circ X), \\ \frac{dR}{dt} &= ((\mathbf{1} - A) \circ X)R. \end{aligned}$$

- QR-like iteration:

$$\begin{aligned} e^{X_0t} &= L(t)R(t), \\ e^{X(t)t} &= R(t)L(t). \end{aligned}$$

Choices of A

- Continuous power method:

$$a_{ij} := \begin{cases} 1, & \text{if } j = 1 \text{ and } i > j; \\ -1, & \text{if } i = 1 \text{ and } j > i; \\ 0, & \text{otherwise.} \end{cases}$$

- Toda lattice:

$$a_{ij} := \begin{cases} 1, & \text{if } i > j; \\ -1, & \text{if } j > i; \\ 0, & \text{otherwise.} \end{cases}$$

- Arbitrary patten:

$$a_{ij} := \begin{cases} 1, & \text{if } (i,j) \in \Delta; \\ -1, & \text{if } (j,i) \in \Delta; \\ 0, & \text{otherwise.} \end{cases}.$$

  - ◇ Δ = Arbitrary index subset.

- Brockett's double bracket flow:

$$a_{ij} := d_i - d_j$$

  - ◇ $d_i \geq d_j$ if $i \leq j$.

Convergence

- $X(0)$ symmetric, A skew-symmetric and $\mathrm{tril}(A)$ nonnegative $\Rightarrow$

$$\lim_{t\to\infty} A \circ X(t) = 0.$$

  ◇ $x_{ij}(t) \to 0$ whenever $a_{ij} \neq 0$.

Lecture 11

Numerical Computation

- Continuous versus discrete
- Special features of the ODE's
- Challenges
- New directions.

Continuous versus Discrete

- The DE of a bridge can be integrated by any available ODE solvers.
  - ◇ ODE (Shampine and Gordon, '75).
  - ◇ MATLAB ODE SUITE (Shampine and Reichelt, '95).
  - ◇ RK (Sanz-Serna, '88).
- The discretization of a bridge could lead to a new iterative scheme.

- Sometimes the Poincaré map of the DE solution corresponds to the results of an existing iterative method.
  - ◇ Toda lattice and QR algorithm.
  - ◇ QZ flow and QZ algorithm.
  - ◇ SVD flow and SVD algorithm.
- Sometimes an existing discrete method may be extended directly into a continuous model.
  - ◇ Continuous Newton's method.
- Sometimes the underlying geometry suggests insights into the design of new iterative methods.
  - ◇ Newton's method for the inverse eigenvalue problem.
  - ◇ Newton's method for the inverse singular value problem.

Special Features of the ODE's

- For gradient flows:
  - ◇ Only the asymptotically stable equilibria are needed to answer the original problem.
  - ◇ An explicit Lyapunov function is often available.
- Orbits are required to stay on a certain manifold, such as $\mathcal{O}(n)$.
- Solutions usually preserve isospectrality.

Challenges

- Challenge to current ODE techniques:
  - ◇ The size of the differential system can easily be large.
  - ◇ Classical methods, such as multistep methods or Runge-Kutta methods fail to preserve isospectrality or orthonormality.
- Challenge to new ODE techniques:
  - ◇ Need an ODE solver that can effectively approximate the asymptotically stable equilibrium point.
  - ◇ Need an ODE solver that can trace trajectories on a manifold constraint (DAE).
  - ◇ Parallel computation.
  - ◇ VLSI implementation.

New Directions

- Orthogonal integrators (Sanz-Serna, ’88, Dieci et al., ’94, A. Iserles et al, ’95).
  - ◇ Gauss-Legendre RK methods.
- Projected unitary schemes (Gear, ’88).
  - ◇ Project approximations computed by an arbitrary scheme into $\mathcal{O}(n)$:

$$\left.\begin{array}{r} Z^T Z = I + O(h^p) \\ Z = QR \\ R_{ii} > 0 \end{array}\right\} \Rightarrow R = I + O(h^p).$$

- Systolic implementation (Moonen et al., ’95).
  - ◇ A signal flow graph can be derived for the evaluation involved in the vector field.
  - ◇ Pipelining the signal flow graph $\Rightarrow$ Parallel computation.
- Neural network adaptation.
  - ◇ Neural network $\Rightarrow$ Analog computation $\Rightarrow$ Dynamical systems.
  - ◇ Matrix DE’s $\Rightarrow$ Neural-network-like structures.

Lecture 12

Conclusions

- Area of applications.
- Relation to discrete methods.
- Challenge to ODE techniques.
- More to do.

Area of Applications

- Numerical analysis:
  - ◇ Eigenvalue computation.
  - ◇ Singular value computation.
  - ◇ Construction of balanced realizations.
  - ◇ Inverse spectrum problems.
- Matrix theory:
  - ◇ Existence question.
  - ◇ Nearness problems.
- Mechanics:
  - ◇ Mechanical system simulation.
  - ◇ Structure analysis.
  - ◇ Multibody oscillation.
- Control theory:
  - ◇ State or output feedback pole assignment problem.
  - ◇ Multivariable system identification.

- Signal processing.
  - ◇ Molecular spectroscopy.
  - ◇ Antenna array processing.
  - ◇ Seismic tomography.
- Multivariate statistical analysis:
  - ◇ Principal component analysis.
- Mathematical programming.
  - ◇ Interior point method for linear programming.
  - ◇ Quadratic assignment problem.

Relation to Discrete Methods

- Offer critical insights into the understanding of the dynamics of discrete methods.
  - ◇ QR algorithm.
  - ◇ SVD algorithm.
  - ◇ Jacobi algorithm.
- Unify a variety of discrete methods as special cases of different discretization.
  - ◇ QR-type flow.
  - ◇ Spectrally constrained flow.
- Give rise to the design of new numerical algorithms
  - ◇ Difference methods resulted from discretization of differential systems.
  - ◇ Geometric methods resulted from the underlying topology.

Challenge to ODE Techniques

- May be used as benchmark problems for testing new ODE techniques.
  - ◇ Large scale computation — Size grows as n^2.
- New ODE techniques may further benefit the numerical computation.
  - ◇ Parallel ODE methods (Burrage, '95).

More to Do

- Enable to tackle existence problems that are seemingly impossible to be solved by conventional discrete methods.
  - ◇ Inverse eigenvalue problems.
- Usually offers a global method for solving the underlying problem.
- Analog realization:
  - ◇ Cheap and fast.
  - ◇ Discrete counterparts may not be easy to find.
  - ◇ Suffers from limited accuracy.

Bibliography

[1] J. C. Alexander, The additive inverse eigenvalue problem and topological degree, Proc. Amer. Math. Soc., 70(1978), 5-7.

[2] E. L. Allgower and K. Georg, Simplicial and continuation methods for approximating fixed points and solutions to systems of equations, SIAM Review, 22(1980), 28-85.

[3] T. W. Anderson, I. Olkin and L. G. Underhill, Generation of random orthogonal matrices, SIAM Journal on Sci. and Stat. Comput., 8(1987), 625–629.

[4] B. C. Arnold, Majorization and the Lorenz Order: A Brief Introduction, Lecture Notes in Statistics 43, Springer-Verlag, Berlin, 1987.

[5] W. W. Barrett and C. R. Johnson, Possible spectra of totally positive matrices, Linear Alg. Appl., 62(1984), 231-233.

[6] V. I. Arnold, Geometrical Methods in the Theory of Ordinary Differntial Equations, 2nd ed., Springer-Verlag, New York, 1988.

[7] A. Berman and R. J. Plemmons, Nonnegative Matrices in the Mathematical Sciences, Academic Press, New York, 1979, also Classics in Applied Mathematics 9, SIAM, Philadelphia, 1994.

[8] R. Bhatia, Perturbation Bounds for Matrix Eigenvalues, Longman Scientific & Technical, Wiley, New York, 1987.

[9] F. W. Biegler-König, A Newton iteration process for inverse eigenvalue problems, Numer. Math., 37(1981), 349-354.

[10] F. W. Biegler-König, Construction of band matrices from spectral data, Linear Alg. Appl., 40(1981), 79-84.

[11] A. M. Bloch, R. W. Brockett and T. S Ratiu, A new formulation of the generalized Toda lattice equations and their fixed point analysis via the momentum map, Bull. Amer. Math. Soc. (N.S.) 23(1990), 477-485.

[12] A. M. Bloch, Steepest descent, linear programming, and Hamiltonian flows, Contemporary Math., 114(1990), 77-88.

[13] D. Boley and G. H. Golub, A modified method for reconstructing periodic Jacobi matrices, Math. Comput., 24(1984), 143-150.

[14] D. Boley and G. H. Golub, A survey of matrix inverse eigenvalue problem, Inverse Problems 3(1987), 595-622.

[15] C. de Boor and G. H. Golub, The numerically stable reconstruction of a Jacobi matrix from spectral data, Linear Alg. Appl., 21(1978), 245-260.

[16] S. Boyd, L. E. Ghaoui, E. Feron and V. Balakrishnan, Linear Matrix inequalities in System and Control Theory, 15, Studies in Applied Mathematics, SIAM, Philadelphia, 1994.

[17] J. P. Boyle and R. L. Dykstra, A method for finding projections onto the intersection of convex sets in Hilbert space, in Advances in Order Restricted Statistical Inference, Lecture Notes in Statistics, Vol. 37, ed. R. Dykstra, T. Robertston, and F. Wright, Springer-Verlag, Berlin, 1986, 28-47.

[18] M. Boyle and D. Handelman, The spectra of nonnegative matrices via symbolic dynamics, Ann. Math., 133(1991), 249-316.

[19] F. Brauer and J. A. Hohel, Qualitative Theory of Ordinary Differential Equations, Benjamin, New York, 1969.

[20] R. W. Brockett, Least squares matching problems, Linear Alg. Appl., 122/123/124(1989), 761-777.

[21] R. W. Brockett, Dynamical systems that sort lists, diagonalize matrices and solve linear programming problems, in Proc. 27th IEEE Conf. Decision and Control, (1988), 799-803, and Linear Alg. Appl. 146(91), 79-91.

[22] A. Bunse-Gerstner, R. Byers and V. Mehrmann, A chart of numerical methods for structured eigenvalue problems, Materialien LVII, Universitát Bielefeld, preprint, 1989.

[23] A. Bunse-Gerstner, R. Byers, V. Mehrmann and N. K. Nichols, Numerical computation of an analytic singular value decomposition of a matrix valued function, Numer. Math. 60(1991), 1-40.

[24] R. E. Burkard and U. Derigs, Assignment and Matching Problems: Solution Methods with FORTRAN-Programs, Springer-Verlag, Berlin Heidelberg New York 1980.

[25] R. Byers, A Hamiltonian QR algorithm, SIAM J. Sci. Stat. Comput., 7(1986), 212-229.

[26] M. P. Calvo, A. Iserles and A. Zanna, Numerical solution of isospectral flows, DAMTP 1995/NA03, University of Cambridge, preprint.

[27] A. Cantoni and P. Butler, Eigenvalues and eigenvectors of symmetric centrosymmetric matrices, Linear Alg. Appl., 13(1976), 275-288.

[28] R. L. Causey, On Closest Normal Matrices, Ph.D. Thesis, Department of Computer Science, Stanford University, 1964.

[29] P. J. Channell and C. Scovel, Sympletic integration of Hamiltonian systems, Nonlinearity, 3(1990), 231-259.

[30] X. Chen and M. T. Chu, On the least squares solution of inverse eigenvalue problems, SIAM J. Numer. Anal., to appear.

[31] W. Cheney and A. Goldstein, Proximity maps for convex sets, Proc. Amer. Math. Soc., 10(1959), 448-450

[32] S. N. Chow, J. Mallet-Paret and J. A. Yorke, Finding zeros of maps: Homotopy methods that are constructive with probability one, Math. Comp., 32(1978), 887-899.

[33] M. T. Chu, The generalized Toda flow, the QR algorithm and the center manifold theorem, SIAM J. Alg. Disc. Meth., 5(1984), 187-210.

[34] M. T. Chu, A simple application of the homotopy method to symmetric eigenvalue problems, Linear Alg. Appl., 59(1984), 85-90.

[35] M. T. Chu, A continuous approximation to the generalized Schur decomposition, Linear Alg. Appl., 78(1986), 119-132.

[36] M. T. Chu, Curves on S^{n-1} that lead to eigenvalues or their means of a matrix, SIAM J. Alg. Disc. Meth., 7(1986), 425-432.

[37] M. T. Chu, On a differential equation approach to the singular value decomposition of bidiagonal matrices, Linear Alg. Appl., 80(1986), 71-79.

[38] M. T. Chu, T. Y. Li and T. Sauer, Homotopy method for general λ-matrix problems, SIAM J. Matrix Anal. Appl., 9(1988), 528-536.

[39] M. T. Chu, On the continuous realization of iterative processes, SIAM Review, 30(1988), 375-387.

[40] M. T. Chu and L. K. Norris, Isospectral flows and abstract matrix factorizations, SIAM J. Numer. Anal., 25(1988), 1383-1391.

[41] M. T. Chu, Solving additive inverse eigenvalue program for symmetric matrices by the homotopy method, IMA J. Numer. Anal., 9(1990), 331-342.

[42] M. T. Chu and K. R. Driessel, The projected gradient method for least squares matrix approximations with spectral constraints, SIAM J. Numer. Anal., 27(1990), 1050-1060.

[43] M. T. Chu, A continuous Jacobi-like approach to the simultaneous reduction of real matrices, Linear Alg. Appl., 147(1991), 75-96.

[44] M. T. Chu and K. R. Driessel, Constructing symmetric nonnegative matrices with prescribed eigenvalues by differential equations, SIAM J. Math. Anal., 22(1991), 1372-1387.

[45] M. T. Chu and M. A. Erbrecht, Symmetric Toeplitz matrices with two prescribed eigenpairs, SIAM J. Matrix Anal. Appl., 15(1994), 623-635.

[46] M. T. Chu, Numerical methods for inverse singular value problems, SIAM J. Numer. Anal., 29(1992), 885-903.

[47] M. T. Chu, Matrix differential equations: A continuous realization process for linear algebra problems, Nonlinear Anal., TMA, 18(1992), 1125-1146.

[48] M. T. Chu and J. L. Watterson, Multivariate eigenvalue problem: I. Algebraic Theory and Power method, SIAM J. Sci. Comput., 14(1993), 1089-1106.

[49] M. T. Chu, Constructing a Hermitian matrix from its diagonal entries and eigenvalues, SIAM J. Matrix Anal. Appl., to appear, 1993.

[50] M. T. Chu, On the refinement of a Newton method for the inverse Toeplitz eigenvalue problem, SIAM J. Numer. Anal., under revision.

[51] M. T. Chu, On the Differential Equation $\frac{dX}{dt} = [X, k(X)]$ where k is a Toeplitz annihilator, J. Math. Anal. Appl., submitted.

[52] G. J. Cooper, Stability of Runge-Kutta methods for trajectory problems, IMA J. Numer. Anal., 7(1987), 1-13.

[53] M. L. Curtis, Matrix Groups, Springer-Verlag, New York, 1979.

[54] G. Cybenko, On the eigenstructure of Toeplitz matrices, IEEE Trans. Acoust., Speech, Signal Process., ASSP-32(1984), 918-920.

[55] P. Deift, T. Nanda,and C. Tomei, Differential equations for symmetric eigenvalue eigenvalue problems, SIAM J. Numer. Anal., 20(1983), 1-22.

[56] P. Deift, J. Demmel, L. C. Li and C. Tomei, The bidiagonal singular value decomposition and the Hamiltonian mechanics, LAPACK Working Note #11, Argonne National Laboratory, 1989.

[57] J. Della-Dora, Numerical linear algorithms and group theory, Linear Alg. Appl., 10(1975),267-283.

[58] P. Delsarte and Y. Genin, Spectral properties of finite Toeplitz matrices, Proceedings of the 1983 International Symposium of Mathematical Theory of Networks and Systems, Beer-Sheva, Israel, Lecture Notes in Control and Information Sciences, 58(1984), 194-213.

[59] J. W. Demmel and A. Edelman, The dimension of matrices (matrix pencils) with given Jordan (Kronecker) canonical forms, Linear Alg. Appl., 230(1995), 47-60.

[60] J. E. Dennis, Jr. and R. B. Schnabel, Numerical Methods for Unconstrained Optimization and Nonlinear Equations, Prentice-Hall, Inc., Englewood Cliffs, 1983.

[61] F. Deutsch, Von Neumann's alternating method: the rate of convergence, Approximation Theory IV, C. Chui, L. Schumaker and J. Ward, ed., Academic Press, New York, 1983, 427-434.

[62] L. Dieci, R. D. Russel and E. S. Van Vleck, Unitary integrators and applications to continuous orthonormalisation techniques, SIAM J. Numer. Anal., 31(1994), 261-281.

[63] A. C. Downing and A. S. Householder, Some inverse characteristic value problems, J. Assoc. Comput. Mach., 3(1956), 203-207.

[64] T. Eirola and O. Nevanlinna, What do multistep methods approximate? Numer. Math., 53(1988), 559-569.

[65] T. Eirola and J. M. Sanz-Serna, Conservation of integrals and symplectic structure in the integration of differential equations by multistep method, Numer. Math., 61(1992), 281-290.

[66] L. E. Faibusovich, QR-type factorizations, the Yang-Baxter equations, and an eigenvalue problem of control theory, Linear Alg. Appl., 122/123/124(1989), 943-971.

[67] L. Faybusovich, Hamiltonian structure of dynamical systems which solve linear programming problems, Physics D, 53(1991), 217-232.

[68] L. Faybusovich, Dynamical systems which solve optimization problems with linear constraints, IMA J. Math. Control Inform., 8(1991), 135-149.

[69] M. Fiedler, Eigenvalues of nonnegative symmetric matrices, Linear Algebra and Appl., 9(1974), 119-142.

[70] W. Ferguson, The construction of Jacobi and periodic Jacobi matrices with prescribed spectra, Math. Comput., 35(1980), 79-84.

[71] G. E. Forsythe and E. G. Strauss, On best conditioned matrices, Proc. Amer. Math. Soc., 6(1955), 340-345.

[72] S. Friedland, On inverse multiplicative eigenvalue problems for matrices, Linear Alg. Appl., 12(1975), 127-137.

[73] S. Friedland, Inverse eigenvalue problems, Linear Alg. Appl., 17(1977), 15-71.

[74] S. Friedland, On an inverse problem for nonnegative and eventually nonnegative matrices, Israel J. Math., 29(1978), 43-60.

[75] S. Friedland, The reconstruction of a symmetric matrix from the spectra data, J. Math. Anal. Appl., 71(1979), 412-422.

[76] S. Friedland and A. A. Melkman, On the eigenvalues of nonnegative Jacobi matrices, Linear Algebra and Appl., 25(1979), 239-254.

[77] S. Friedland, J. Nocedal and M. L. Overton, The formulation and analysis of numerical methods for inverse eigenvalue problems, SIAM J. Numer. Anal., 24(1987), 634-667.

[78] S. Friedland, Inverse eigenvalue problems for symmetric Toeplitz matrices, SIAM J. Matrix Anal. Appl., 13(1992), 1142-1153.

[79] R. Gabriel, Matrizen mit maximaler Diagonale bei unitärer Similarität, J. Reine Angew. Math., 307/308(1979), 31-52.

[80] R. Gabriel, The normal ΔH-matrices with connection to some Jacobi-like methods, Linear Alg. Appl., 91(1987), 181-194.

[81] F. R. Gantmacher, The Theory of Matrices, Vols. 1-2, Chelsea, New York, 1959.

[82] C. B. Garcia and T. Y. Li, On the number of solutions to polynomial systems of equations, SIAM J. Numer. Anal., 17(1980), 540-546.

[83] C. W. Gear, Maintaining solution invariants in the numerical solution of ODEs, SIAM J. Sci. Stat. Comput., 7(1986), 734-743.

[84] C. W. Gear, Invariants and methods for ODEs, NEC Research Institute, preprint, 1991.

[85] I. M. Gelfand and V. A. Ponomarev, Remarks on the classification of a pair of commuting linear transformations in a finite dimensional space, Functional Anal. Appl., 3(1969), 325-326.

[86] P. E. Gill, W. Murray and M. H. Wright, Practical Optimization, Academic Press, London, 1981.

[87] G. M. L. Gladwell, The inverse problem for the vibrating beam, Proc. R. Soc., A 393(1984), 277-295.

[88] G. M. L. Gladwell and J. A. Gbadeyan, On the inverse problem of the vibrating string or rod, Q. J. Mech. Appl. Math., 38(1985), 169-174.

[89] G. M. L. Gladwell, The inverse mode problem for lumped-mass systems, Q. J. Mech. Appl. Math., 39(1986), 297-307.

[90] G. M. L. Gladwell, Inverse Problems in Vibration, Martinus Nijhoff, Dordrecht, Netherlands, 1986.

[91] W. K. Glunt, An alternating projections method for certain linear problems in a Hilbert space, preprint, University of Kentucky, 1992.

[92] A. Greenbaum and G. H. Rodrigue, Optimal preconditioners of a given sparsity pattern, BIT, 29(1989), 610-634.

[93] A. Greenbaum, Diagonally scalings of the Laplacian as preconditioners for other elliptic differential operators, SIAM J. Matrix Anal. Appl., 13(1992), 826-846.

[94] G. H. Golub, Some modified matrix eigenvalue problems, SIAM Review, 15(1973), 318-344.

[95] G. H. Golub, and C. F. Van Loan, Matrix Computations, 2nd ed., Johns Hopkins University Press, Baltimore, 1989.

[96] A. Greenbaum and G. H. Rodrigue, Optimal preconditioners of a given sparsity pattern, BIT, 29(1989), 610-634.

[97] A. Greenbaum, Diagonally scalings of the Laplacian as preconditioners for other elliptic differential operators, SIAM J. Matrix Anal. Appl., 13(1992), 826-846.

[98] R. Grone, C. R. Johnson, E. M. Sa and H. Wolkowicz, Normal matrices, Linear Alg. Appl., 87(1987), 213-225.

[99] O. H. Hald, On discrete and numerical inverse Sturm-Liouville problems, Ph. D. Thesis, New York University, 1972.

[100] O. H. Hald, Inverse eigenvalue problems for Jacobi matrices, Linear Alg. Appl., 14(1976), 63-85.

[101] L. A. Hageman and D. M. Young, Applied Iterative Methods, Academic Press, New York, 1981.

[102] S. P. Han, A successive projection method, Math. Programming, 40(1988), 1-14.

[103] U. Helmke and J. B. Moore, Optimization and Dynamical Systems, Springer-Verlag, London, 1994.

[104] Hershkowits, D., Existence of matrices with prescribed eigenvalues and entries, Linear and Multilinear Algebra, 14(1983), 315-342.

[105] N. J. Higham, Matrix nearest problems and applications, Proceedings of the IMA Conference on Applications of Matrix Theory, S. Barnett and M. J. C. Gover, eds., Oxford University Press, 1989, to appear.

[106] R. D. Hill, R. G. Bates and S. R. Waters, On centrohermitian matrices, SIAM J. Matrix Anal. Appl., 11(1990), 128-133.

[107] M. Hirsch and S. Smale, On algorithms for solving $f(x) = 0$, Comm. Pure Appl. Math., 32(1979), 281-312.

[108] H. Hochstadt, On some inverse problems in matrix theory, Arch. Math., 18(1967),201-207.

[109] H. Hochstadt, On construction of a Jacobi matrix from spectral data, Linear Alg. Appl., 8(1974), 435-446.

[110] D. Hershkowits, Existence of matrices with prescribed eigenvalues and entries, Linear and Multilinear Algebra, 14(1983), 315-342.

[111] H. Hochstadt, On the construction of a Jacobi matrix from mixed given data, Linear Alg. Appl., 28(1979), 113-115.

[112] A. J. Hoffman and H. Wielandt, The variation of the spectrum of a normal matrix, Duke Math. J., 20(1953), pp. 37-39.

[113] R. A. Horn and C. A. Johnson, Matrix Analysis, Cambridge University Press, Cambridge, 1985.

[114] P. Horst, Factor Analysis of Data Matrices, Holt, Rinehart and Winston, New York, 1965.

[115] F. I. Karpelevič, On the characteristic roots of matrices with nonnegative elements, Izv. Akad. Nauk SSSR Ser. Mat. 15(1951), 361-383 (in Russian).

[116] H. B. Keller, Global homotopies and Newton methods, in Recent Advances in Numerical Analysis, C. de Boor and G. H. Golub, eds., Academic Press, New York, 1978, 73-94.

[117] P. E. Kloeden and J. Lorenz, A note on multistep methods and attracting sets of dynamical systems, Numer. Math., 56(1990), 667-673

[118] P. Lancaster, On eigenvalues of matrices dependent on a parameter, Numer. Math., 6, pp. 377-387.

[119] H. J. Landau, The inverse eigenvalue problem for real symmetric Toeplitz matrices, J. AMS, 7(1994), 749-767.

[120] D. P. Laurie, A numerical approach to the inverse Toeplitz eigenproblem, SIAM J. Sci. Stat. Comput., 9(1988), 401-405.

[121] C. L. Lawson and R. J. Hanson, Solving Least Squares Problems, Prentice-Hall, New Jersey, 1974.

[122] T. Y. Li, On Chow, Mallet-Paret and Yorke, homotopy for solving systems of polynomials, Bulletin Inst. Math. Acad. Sinica, 11(1983), 433-437.

[123] T. Y. Li and N. H. Rhee, Homotopy algorithms for symmetric eigenvalue problems, Numer. Math., 55(1989), 265-280.

[124] T. Y. Li, H. Z. Sun and X. H. Sun, Parallel homotopy algorithm for symmetric tridiagonal eigenvalue problem, SIAM J. Sci. Stat. Comput., 12(1991), 469-487.

[125] N. G. Lloyd, Degree Theory, Cambridge University Press, New York, 1978.

[126] R. Loewy and D. London, A note on an inverse problems for nonnegative matrices, Linear and Multilinear Algebra, 6(1978), 83-90.

[127] D. G. Luenberger, Introduction to Linear and Nonlinear Programming, Addison-Wesley, Reading, Mass., 1984.

[128] A. W. Marshall and I Olkin , Inequalities: Theory of Majorization and Its Applications, Academic Press, New York, 1979.

[129] V. Mehrmann and W. Rath, Numerical methods for the computation of analytic singular value decompositions, preprint, 1993.

[130] J. Milnor, Singular Points of Complex Hyper surfaces, Annals of Mathematics Studies 61, Princeton University Press, Princeton, New Jersey, 1968.

[131] H. Minc, Nonnegative matrices, Wiley, New York, 1988.

[132] L. Mirsky, Matrices with prescribed characteristic roots and diagonal elements, J. London Math. Soc., 33(1958), 14-21.

[133] J. B. Moore, R. E. Mahony and U. Helmke, Numerical gradient algorithms for eigenvalue and singular value decomposition, SIAM J. Matrix Anal. Appl., 15(1994), 881-902.

[134] A. P. Morgan, A homotopy for solving polynomial systems, Applied Math. Comput., 18(1986), 87-92.

[135] J. Moser, Finitely many mass points on the line under the influence of an exponential potential — An integrable dynamical system, in Dynamical Systems Theory and Application, ed. J. Moser, Springer- Verlag, New York, 1975.

[136] M. Muller, An inverse eigenvalue problem computing B-stable Runge-Kutta methods having real poles, BIT, 32(1992), 676.

[137] Y. Nakamura, Group actions on linear predictors for nonstationary processes, IMA J. Math. Control Inform., 5(1988), 69-75.

[138] J. Nocedal and M. L. Overton, Numerical methods for solving inverse eigenvalue problems, Lect. Notes Math., 1005(1983), 212-226.

[139] G. N. Oliveira, Nonnegative matrices with prescribed spectrum, Linear Algebra Appl., 54(1983), 117-121.

[140] J. Paine, A numerical method for the inverse Sturm-Liouville problem, SIAM J. Sci. Stat. Comput., 5(1984), 149-156.

[141] B. N. Parlett, The Symmetric Eigenvalue Problem, Prentice-Hall, Englewood Cliffs, N.J., 1980.

[142] J. D. Pryce, Numerical Solution of Sturm-Liouville Problems, Oxford University Press, New York, 1993.

[143] R. L. Parker and K. A. Whaler, Numerical methods for establishing solutions to the inverse problem of electromagnetic induction, J. Geophys. Research, 86(1981), 9574-9584.

[144] M. Renardy and R. C. Rogers, An Introduction to Partial Differential Equations, Springer-Verlag, New York, 1993.

[145] A. Ruhe, Closest normal matrix finally found!, BIT, 27(1987), 585-595.

[146] J. M. Sanz-Serna, Runge-Kutta schemes for Hamiltonian systems, BIT, 28(1988), 877-883.

[147] J. M. Sanz-Serna and M. P. Calvo, Numerical Hamiltonian Problems, Chapman and Hall, London, 1994.

[148] L. F. Shampine and M. K. Gordon, Computer Solution of Ordinary Differential Equations: The Initial Value Problem, Freeman, San Francisco, 1975.

[149] L. F. Shampine and M. W. Reichelt, The MATLAB ODE suite, preprint, 1995.

[150] A. Shapiro, On the unsolvability of inverse eigenvalue problems almost everywhere, Linear Alg. Appl., 49(1983), 27-41.

[151] S. Smale, A convergent process of price adjustment and global Newton methods, J. Math. Econ., 3(1976), 107-120.

[152] S. T. Smith, Geometric Optimization Methods for Adaptive Filtering, Ph.D. Thesis, Harvarad University, 1993.

[153] G. W. Soules, Constructing symmetric nonnegative matrices, Linear and Multilinear Algebra, 13(1983), 241-251.

[154] G. W. Stewart, The efficient generation of random orthogonal matrices with an application to condition estimators, SIAM Journal on Numerical Analysis, 17(1980), 403–404.

[155] G. W. Stewart and J. Sun, Matrix Perturbation Theory, Academic Press, Boston, 1990.

[156] J. Sun, Eigenvalues and eigenvectors of a matrix dependent on several parameters, J. Comput. Math., 3(1985), 351-364.

[157] W. W. Symes, The QR algorithm and scattering for the finite nonperiodic Toda lattice, Physica, 4D(1982), 275-280.

[158] J. F. Traub, Iterative Methods for the Solution of Equations, Prentice-Hall, Englewood Cliffs, N.J., 1964.

[159] W. F. Trench, Numerical solution of the eigenvalue problem for Hermitian Toeplitz matrices, SIAM J. Matrix Anal. Appl., 10(1989), 135-146.

[160] A. van der Sluis, Condition numbers and equilibration matrices, Numer. Math., 14(1969), 14-23.

[161] H. J. Wacker, Continuation Methods, Academic, New York, 1978.

[162] J. Y. Wang and B. S Garbow, A numerical method for solving inverse real symmetric eigenvalue problem, SIAM J. Sci. Stat. Comput., 4(1983), 45-51.

[163] D. S. Watkins, Isospectral Flows, SIAM Review, 26(1984), 379-391.

[164] L. T. Watson, S. C. Billups and A. P. Morgan, Algorithm 652: HOMPACK: A suite of codes for globally convergent homotopy algorithms, ACM Trans. Math. Software, 13(1987), 281-310.

[165] W. Wilhelmi, Eig Algorithmus zur Losung eines inversen Eigenwertproblems, ZAMM., 54(1974), 53-55.

[166] J. H. Wilkinson, The Algebraic Eigenvalue Problem, Clarendon Press, Oxford, 1965.

[167] S. S. Wilks, Mathematical Statistics, John Wiley and Sons, New York, 1962.

[168] K. Wright, Differential equations for the analytic singular value decomposition of a matrix, Numer. Math., 3(1992), 283-295.

[169] Z. Y. Zhang, On the perturbation of the eigenvalues of a nondefective matrix, Math. Numer. Sinica, 8(1986), 106-108.