Inverse Eigenvalue Problems: Theory and Applications

A Series of Lectures to be Presented at IRMA, CNR, Bari, Italy

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June 6, 2001

Preface

An inverse eigenvalue problem concerns the reconstruction of a matrix from prescribed spectral data. The spectral data involved may consist of the complete or only partial information of eigenvalues or eigenvectors. The objective of an inverse eigenvalue problem is to construct a matrix that maintains a certain specific structure as well as that given spectral property.

Inverse eigenvalue problems arise in a remarkable variety of applications, including system and control theory, geophysics, molecular spectroscopy, particle physics, structure analysis, and so on. Generally speaking, the basic goal of an inverse eigenvalue problem is to reconstruct the physical parameters of a certain system from the knowledge or desire of its dynamical behavior. Since the dynamical behavior often is governed by the underlying natural frequencies and/or normal modes, the spectral constraints are thus imposed. On the other hand, in order that the resulting model is physically realizable, additional structural constraints must also be imposed upon the matrix. Depending on the application, inverse eigenvalue problems appear in many different forms.

Associated with any inverse eigenvalue problem are two fundamental questions – the theoretic issue on solvability and the practical issue on computability. Solvability concerns obtaining a necessary or a sufficient condition under which an inverse eigenvalue problem has a solution. Computability concerns developing a procedure by which, knowing a priori that the given spectral data are feasible, a matrix can be constructed numerically. Both questions are difficult and challenging.

In this note the emphasis is to provide an overview of the vast scope of this fascinating problem. The fundamental questions, some known results, many applications, mathematical properties, a variety of numerical techniques, as well as several open problems will be discussed.

This research was supported in part by the National Science Foundation under the grants DMS-9803759 and DMS-0073056. The lectures are to be presented at the Istituto per Ricerche di Matematica Applicata (IRMA), Bari, Italy, from June 23 to July 20, 2001, upon the invitation by Fasma Diele. The visit to present this series of lectures is made possible by Professor Roberto Peluso at the IRMA and Professor Dario Bini at the Universita' di Pisa with the support from Il Consiglio Nazionale delle Ricerche (CNR) and the Gruppo Nazionale per il Calcolo Scientifico (GNCS) under the project Lineare con Struttura e Applicazioni. The warm kindness and encouragement received from these colleagues are greatly appreciated.

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Raleigh, North Carolina
May, 2001

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Chapter 1

Introduction

- Overview
- A Brief History
- Classification
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- Conclusion

Overview

- Often a physical process is described by a mathematical model of which parameters represent important physical quantities.
  - ◇ Direct analysis — Analyze or predict the behavior of the underlying physical process from the parameters.
  - ◇ Inverse analysis — Validate, determine, or estimate the parameters adaptively from the behavior of the physical process.

Inverse Eigenvalue Problem (IEP)

- The mathematical model involves matrices whose spectral properties determine the dynamics of the physical system.
- Reconstruct a matrix from prescribed spectral data.
  - ◇ Spectral data may involve a mixture information of eigenvalues or eigenvectors.
  - ◇ Sometimes complete information is difficult to obtain. Only partial information is available.
  - ◇ For feasibility, 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.
- Sensitivity:
  - ◇ Quantify how a solution to an IEP is subject to changes of the spectral data.
- Applicability:
  - ◇ Differentiate whether the given data are exact or approximate, complete or incomplete, and whether only an estimation of the parameters of the system is sufficient.
  - ◇ Decide between physical realizability and physical uncertainty which constraint of the problem should be enforced.

Brief History

- Studies of IEP's have been quite extensive
  - ◇ Engineering application.
  - ◇ Algebraic theorization.
- Mathematical techniques employed in the study are quite sophisticated:
  - ◇ Algebraic curves.
  - ◇ Degree theory.
  - ◇ Differential geometry.
  - ◇ Matrix theory.
  - ◇ Differential equations.
  - ◇ Functional analysis.
  - ◇ ⋮
- Results are quite few and scattered even within the same field of discipline.

Literature Review

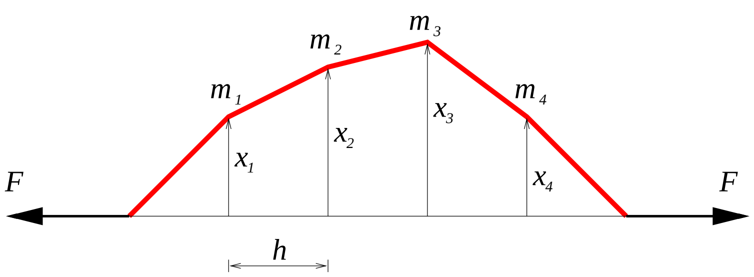
- Inverse Sturm-Liouville problem:
  - ◇ Ambartsumyan'29
  - ◇ Krein'33
  - ◇ Borg'46, Levinson'49
  - ◇ **Gel'fand&Levitan'51**
  - ◇ Kac'66 (Can one hear the shape of a drum?)
  - ◇ Hochstadt'73, Barcilon'74, McLaughlin'76, Hald'78
  - ◇ Zayed'82, Issacson et al'83, **McLaughlin'86**, Andersson'88
  - ◇ Lowe et al'95, **Rundell'97**
- Matrix theory:
  - ◇ Downing&Householder'56, Mirsky'58
  - ◇ Hochstadt'67
  - ◇ de Oliveira'70, Hald'72, Golub'73, Friedland'77, de Boor&Golub'78
  - ◇ Biegler-König'81, Shapiro'83, Barcilon'86, Sun'86, **Boley&Golub'87**
  - ◇ Landau'94, **Chu'98**

- Applied Mechanics:
  - ◇ Barcilon'74
  - ◇ Gottlieb'83, Gladwell'86
  - ◇ Ram'91, **Gladwell'96**, Nylen&Uhlig'97
- Computation:
  - ◇ Morel'76, Boley&Golub'77
  - ◇ Nocedal et al'83, Friedland et al'88, Laurie'88
  - ◇ Chu'90, Zhou&Dai'91, Trench'97, **Xu'98**

Applications

- System identification and control theory.
  - ◇ State/output feedback pole assignment problems.
- Applied mechanics and structure design.
  - ◇ Construct a model of a (damped) mass-spring system with prescribed natural frequencies/modes.
- Applied physics.
  - ◇ Compute the electronic structure of an atom from measured energy levels.
  - ◇ Neutron transport theory.
- Numerical analysis.
  - ◇ Preconditioning.
  - ◇ Computing B-stable RK methods with real poles.
  - ◇ Gaussian quadratures.
- Mathematical analysis.
  - ◇ Inverse Sturm-Liouville problems.

An Example



- Vibration of equally spaced particles (with spacing h and mass m_i) on a string subject to a constant horizontal tension F.
- Equation of motion for 4 particles:

$$\begin{aligned}
m_1\frac{d^2x_1}{dt^2} &= -F\frac{x_1}{h} + F\frac{x_2 - x_1}{h} \\
m_2\frac{d^2x_2}{dt^2} &= -F\frac{x_2 - x_1}{h} + F\frac{x_3 - x_2}{h} \\
m_3\frac{d^2x_3}{dt^2} &= -F\frac{x_3 - x_2}{h} + F\frac{x_4 - x_3}{h} \\
m_4\frac{d^2x_4}{dt^2} &= -F\frac{x_4 - x_3}{h} - F\frac{x_4}{h}
\end{aligned}$$

- In matrix form:

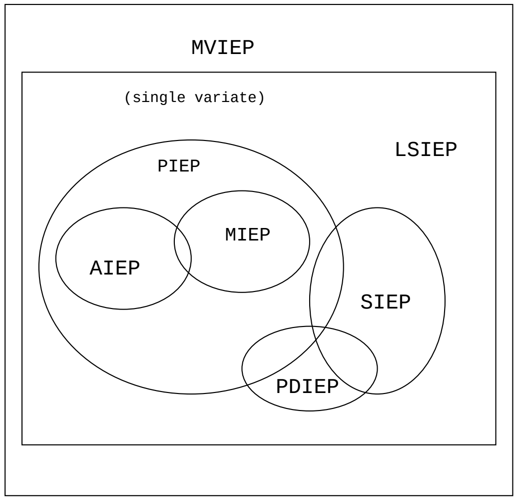
$$\frac{d^2\mathbf{x}}{dt^2} = -DA\mathbf{x}$$

  - ◇ $\mathbf{x} = [x_1, x_2, x_3, x_4]^T$
  - ◇ $A = \begin{bmatrix} 2 & -1 & 0 & 0 \\ -1 & 2 & -1 & 0 \\ 0 & -1 & 2 & -1 \\ 0 & 0 & -1 & 2 \end{bmatrix}$
  - ◇ $D = \mathrm{diag}(d_1, d_2, d_3, d_4)$ with $d_i = \frac{F}{m_i h}$.
- Eigenvalues of DA are the squares of the so called *natural frequencies* of the system.
- Want to place weights m_i so that the system has a prescribed set of natural frequencies.
  - ◇ A is symmetric and tridiagonal.
  - ◇ D is diagonal.
  - ◇ This is a multiplicative inverse eigenvalue problem.
- Open Question: Can such a string have arbitrarily prescribed natrual frequencies by adjusting the diagonal matrix D?

Classification

- Based on constraint.
  - ◇ Spectral constraint.
  - ◇ Structure constraint.
- Based on physical suitability.
  - ◇ Physical realizability.
  - ◇ Physical uncertainty.
- Based on discipline.
  - ◇ Essentially mathematical problem.
  - ◇ Essentially engineering problem.
- Based on expectation.
  - ◇ Determination problem.
  - ◇ Estimation problem.

Via Algebraic Characteristics



MVIEP	=	Multi-Variate IEP
LSIEP	=	Least Squares IEP
PIEP	=	Parameterized IEP
SIEP	=	Structured IEP
PDIEP	=	Partially Described IEP
AIEP	=	Additive IEP
MIEP	=	Multiplicative IEP

PIEP

- Generic form:
  - ◇ Given
    - ▷ A *family* of matrices $A(c) \in \mathcal{M}$ with $c \in \mathbf{F}^m$,
    - ▷ A set of scalars $\Omega \subset \mathbf{F}$,
  - ◇ Find
    - ▷ Values of parameter c such that

$$\sigma(A(c)) \subset \Omega$$

- Remarks:
  - ◇ Not necessarily $m = n$.
  - ◇ Commonly used Ω:
    - ▷ $\Omega = \{\lambda_k^*\}_{k=1}^n$.
    - ▷ $\Omega =$ left-half complex plan.
    - ▷ $\Omega =$ anything but must have a specific number of zeros.

Some Special PIEP's

- $A(c) = A_0 + \sum_{i=1}^n c_i A_i$
  - ◇ $A_i \in \mathcal{R}(n)$, $\mathbf{F} = \mathbb{R}$.
  - ◇ $A_i \in \mathcal{S}(n)$, $\mathbf{F} = \mathbb{R}$.
- **(AIEP)** $A(c) = A(X) = A_0 + X$, $X \in \mathcal{N}$.
  - ◇ $A_0 \in \mathcal{C}(n)$, $\mathbf{F} = \mathbb{C}$, $\mathcal{N} = \mathcal{D}_{\mathcal{C}}(n)$.
- **(MIEP)** $A(c) = A(X) = XA_0$, $X \in \mathcal{N}$.
  - ◇ Preconditioning?
- $A(c) = A(K_1, \ldots, K_q) = A_0 + \sum_{i=1}^q B_i K_i C_i$.
  - ◇ Pole assignment problem.

SIEP

- Generic form:
  - ◇ Given
    - ▷ A set $\mathcal{N}$ of specially structured matrices,
    - ▷ A set of scalars $\{\lambda_k^*\}_{k=1}^n \in \mathbf{F}$,
  - ◇ Find
    - ▷ $X \in \mathcal{N}$ such that

$$\sigma(X) = \{\lambda_k^*\}_{k=1}^n.$$

- Some special cases:
  - ◇ $\mathcal{N} = \{$Toeplitz matrices in $\mathcal{S}(n)\}$.
  - ◇ $\mathcal{N} = \{$Persymmetric Jacobi matrices in $\mathcal{S}(n)\}$.
  - ◇ $\mathcal{N} = \{$Nonnegative matrices in $\mathcal{S}(n)\}$.
  - ◇ $\mathcal{N} = \{$Row-stochastic matrices in $\mathcal{R}(n)\}$.

A Few More Special SIEP's

- Given scalars $\lambda_i^* \leq \mu_i \leq \lambda_{i+1}^*$, $i = 1, \ldots, n-1$, find a Jacobi matrix J such that

$$\begin{aligned} \sigma(J) &= \{\lambda_k^*\}_{k=1}^n \\ \sigma(J(1:n-1, 1:n-1)) &= \{\mu_1, \ldots, \mu_{n-1}\}. \end{aligned}$$

- Given scalars $\{\lambda_1, \ldots, \lambda_{2n}\}$ and $\{\mu_1, \ldots, \mu_{2n-2}\} \in \mathbb{C}$, find tridiagonal symmetric matrices C and K for the λ-matrix $Q(\lambda) = \lambda^2 I + \lambda C + K$ so that

$$\begin{aligned} \sigma(Q) &= \{\lambda_1, \ldots, \lambda_{2n}\}, \\ \sigma(Q(1:n-1, 1:n-1)) &= \{\mu_1, \ldots, \mu_{2n-2}\}. \end{aligned}$$

- Given distinct scalars $\{\lambda_1, \ldots, \lambda_{2n}\} \subset \mathbb{R}$ and a Jacobi matrix $J_n \in \mathcal{R}(n)$, find a Jacobi matrix a Jacobi matrix $J_{2n} \in \mathcal{R}(2n)$ so that

$$\begin{aligned} \sigma(J_{2n}) &= \{\lambda_1, \ldots, \lambda_{2n}\}, \\ J_{2n}(1:n, 1:n) &= J_n. \end{aligned}$$

- Given a family of matrices $A(c) \in \mathbb{R}^{m \times n}$, with $c \in \mathbb{R}^n$, $m \geq n$, find a parameter c such that the singular values of $A(c)$ are precisely the same as a prescribed set of nonnegative real values $\{\sigma_1, \ldots, \sigma_n\}$.

LSIEP

- Maintain the structure, approximate the eigenvalues:
  - ◇ Given
    - ▷ A set of scalars $\{\lambda_1^*, \ldots, \lambda_m^*\} \subset \mathbf{F}$ $(m \leq n)$,
    - ▷ A set $\mathcal{N}$ of specially structured matrices,
  - ◇ Find
    - ▷ A matrix $X \in \mathcal{N}$
    - ▷ An index subset $\sigma = \{\sigma_1 < \ldots < \sigma_m\}$ such that

$$F(X, \sigma) := \frac{1}{2}\sum_{i=1}^{m}(\lambda_{\sigma_i}(X) - \lambda_i^*)^2,$$

is minimized.

- Maintain the spectrum, approximate the structure:
  - ◇ Given
    - ▷ A set $\mathcal{M}$ of spectrally constrained matrices,
    - ▷ A set $\mathcal{N}$ of specially structured matrices,
    - ▷ A projection P from $\mathcal{M}$ onto $\mathcal{N}$,
  - ◇ Find
    - ▷ $X \in \mathcal{M}$ that minimizes

$$F(X) := \frac{1}{2}\|X - P(X)\|^2.$$

Via Physical Characteristics

- By mechanical types:
  - ◇ Continuous vs. discrete.
  - ◇ Damped vs. undamped.
- By data type:
  - ◇ Spectral, modal, or nodal.
  - ◇ Complete vs incomplete.

A Glimpse of Some Major Issues

- Studies on IEP's have been intensive, ranging from acquiring a pragmatic solution to a real-world application dealing the metaphysical theory of an abstract fromulation.
- Results are scattered even within the same field of discipline.
- Only a handful of the problems have been completely understood.
- Many interesting yet challenging questions remain to be answered.

Complex Solvability

- Solving an IEP over complex field amounts to solving a polynomial system with complex coefficients. Generally speaking, the system is generically solvable.
- Given $A_0 \in \mathcal{C}(n)$ and arbitrary $\{\lambda_k^*\}_{k=1}^n \subset \mathbb{C}$,
  - ◇ There exists $D \in \mathcal{D}_{\mathcal{C}}(n)$ such that
  $$\sigma(A_0 + D) = \{\lambda_k^*\}_{k=1}^n$$
  and there are at most $n!$ solutions.
  - ◇ If $\det(A_0(1:j,1:j) \neq 0$, $j = 1,\ldots,n$, then there exists $D \in \mathcal{D}_{\mathcal{C}}(n)$ such that
  $$\sigma(DA_0) = \{\lambda_k^*\}_{k=1}^n$$
  and there are at most $n!$ solutions.

Real Solvability

- Solving an IEP over real field is a much harder problem. Sufficient conditions are generally quite restrictive.
- Assume all matrices involved are real,
  - ◇ If the prescribed *real* eigenvalues are sufficiently different, then there exist $c_1, \ldots, c_n \in \mathbb{R}$ such that
  $$\sigma(A_0 + \sum_{i=1}^n c_i A_i) = \{\lambda_k^*\}_{k=1}^n.$$
  - ◇ The inverse eigenvalue problem associated with
  $$A_0 + \sum_{i=1}^n c_i A_i$$
  is unsolvable almost everywhere if and only if any of the prescribed eigenvalues has multiplicity great than 1.
- Symmetric Toeplitz matrices can have arbitrary spectra.

Numerical Methods

- Direct methods
  - ◇ Lanczos method.
  - ◇ Orthogonal reduction methods.
- Iterative methods
  - ◇ Newton-type iteration.
- Continuous methods:
  - ◇ Homotopy approach.
  - ◇ Projected gradient method.
  - ◇ ASVD approach.

Sensitivity Analysis

- Assume all matrices are symmetric and the PIEP for
$$A(c) = A_0 + \sum_{i=1}^{n} c_i A_i$$
is solvable.
- Assume $A(c) = Q(c)\mathrm{diag}\{\lambda_k^*\}_{k=1}^n Q(c)^T$ and define
$$\begin{aligned} J(c) &= \left[q_i(c)^T A_j q_i(c)\right], \quad i, j = 1, \ldots, n, \\ b &= \left[q_1(c)^T A_0 q_1(c), \ldots, q_n^T A_0 q_n(c)\right]^T. \end{aligned}$$
- If
$$\delta = \|\lambda - \tilde{\lambda}\|_\infty + \sum_{i=0}^{n} \|A_i - \tilde{A}_i\|_2$$
is sufficiently small, then
  - ◇ The PIEP associated with $\tilde{A}_i$, $i = 0, \ldots, n$ and $\{\tilde{\lambda}_1, \ldots, \tilde{\lambda}_n\}$ is solvable.
  - ◇ There is a solution $\tilde{c}$ near to c,

$$\frac{\|c - \tilde{c}\|_\infty}{\|c\|_\infty} \leq \kappa_\infty(J(c)) \left(\frac{\|\lambda - \tilde{\lambda}\|_\infty + \|A_0 - \tilde{A}_0\|_2}{\|\lambda - b\|_\infty} + \frac{\sum_{i=1}^n \|A_i - \tilde{A}_i\|_2}{\|J(c)\|_\infty} \right) + O(\delta^2).$$

Summary

- An IEP concerns the reconstruction of a matrix satisfying two constraints.
  - ◇ *Spectral constraint* – the prescribed spectral data.
  - ◇ *Structural constraint* – the desirable structure.
- Different constraints define a variety of IEP's.
- Studies on IEP's have been intensive, ranging from engineering application to algebraic theorization.
  - ◇ Many unanswered yet interesting questions.
- A common phenomenon in all applications is that the physical parameters of a certain system are to be reconstructed from knowledge of its dynamical behavior, in particular, of its natural frequencies/modes.
  - ◇ Sometimes the constraints can be precisely determined.
  - ◇ Sometimes the constraints are only approximate and often incomplete.

Chapter 2

Applications

- Pole Assignment Problem
- Control of Vibration
- Inverse Strum-Liouville Problem
- Geophysics Application
- Numerical Analysis
- Low Rank Application

Pole Assignment Problem

- Dynamic state equation:

$$\dot{\mathbf{x}}(t) = A\mathbf{x}(t) + B\mathbf{u}(t).$$

  - ◇ $\mathbf{x}$ = state of the system $\in \mathbb{R}^n$.
  - ◇ $\mathbf{u}$ = input to the system $\in \mathbb{R}^m$.
  - ◇ $A \in \mathbb{R}^{n\times n}$, $B \in \mathbb{R}^{n\times m}$.
- Want to select $\mathbf{u}(t)$ so as to control the dynamics of $\mathbf{x}(t)$.
  - ◇ Classical problem in control theory.
  - ◇ Extensively studied and very rich in literature.
  - ◇ Several different types.

State Feedback Control

- Choose input $\mathbf{u}$ as a linear function of current state $\mathbf{x}$,
$$\mathbf{u}(t) = F\mathbf{x}(t).$$
- Closed-loop dynamical system:
$$\dot{\mathbf{x}}(t) = (A + BF)\mathbf{x}(t).$$
- Want to choose the *gain matrix* F so as to
  - ◇ Achieve stability.
  - ◇ Speed up response.
- Choose F so as to reassign eigenvalues of $A + BF$.
  - ◇ Usually F carries no structure at all.
  - ◇ It becomes a much harder IEP if F needs to satisfy a certain structural constraint.

Output Feedback Control

- Often $\mathbf{x}(t)$ is not directly observable. Instead, only output $\mathbf{y}(t)$ where
$$\mathbf{y}(t) = C\mathbf{x}(t)$$
is available.
- Choose input $\mathbf{u}$ as a linear function of current output $\mathbf{y}$,
$$\mathbf{u}(t) = K\mathbf{y}(t).$$
- Closed-loop dynamical system:
$$\dot{\mathbf{x}}(t) = (A + BKC)\mathbf{x}(t).$$
- Want to choose the *output matrix* K so as to reassign the eigenvalues of $A + BKC$.

Control of Vibration

- Area of applications:
  - ◇ Transverse vibrations of masses on a string.
  - ◇ Buckling of structures.
  - ◇ Transient current of electric circuits.
  - ◇ Acoustic vibration in a tube.
- Equation of motion:

$$M\ddot{\mathbf{x}} + C\dot{\mathbf{x}} + K\mathbf{x} = f(\mathbf{x}).$$

  - ◇ $\mathbf{x} \in \mathbb{R}^n$, M, C, $K \in \mathbb{R}^{n\times n}$.
  - ◇ M = diagonal, C, K = symmetric tridiagonal.
- Motion is governed by the homogeneous equation.
  - ◇ Try a solution $\mathbf{x}(t) = \mathbf{v}e^{\lambda t}$.
  - ◇ $\mathbf{v}$ and λ are solutions to the quadratic eigenvalue problem

$$(\lambda^2 M + \lambda C + K)\mathbf{v} = 0.$$

  - ◇ General solution:

$$\mathbf{x}(t) = \sum_{k=1}^{2n} \alpha_k \mathbf{v}_k e^{\lambda_k t}.$$

Undamped System

- $C = 0$, M, K = symmetric and positive definite.
- Try a solution of the form $\mathbf{x}(t) = \mathbf{v}e^{i\omega t}$
- $\mathbf{v}$ and ω solves the generalized eigenvalue problem

$$(K - \omega^2 M)\mathbf{v} = 0$$

  - ◇ ω = the natural frequency.
  - ◇ $\mathbf{v}$ = the natural mode.
- Let $\lambda = \omega^2$, $J := M^{-1/2}KM^{-1/2}$, and $\mathbf{z} = M^{1/2}\mathbf{x}$. Solve the Jacobi eigenvalue problem

$$J\mathbf{z} = \lambda\mathbf{z}.$$

- Two types of inverse eigenvalue problems:
  - ◇ Stiffness matrix K usually is more complicated than the mass matrix M.
    - ▷ Determine K from static constraints, but find M so that some desired natural frequencies are achieved.
    - ▷ This is equivalent to an multiplicative inverse eigenvalue problem.
  - ◇ Construct an unreduced, symmetric, and tridiagonal matrix J from its n eigenvalues and those of its leading principal submatrix of dimension $n-1$.
    - ▷ This IEP can be identified as configuring a spring system from its spectrum and from the spectrum of the same system but the last mass is fixed to have no motion.
    - ▷ This is one kind of Jacobi inverse eigenvalue problems.

Damped System

- Normalize M to identity.
- Define
  - ◇ $Q(\lambda) = \lambda^2 I + \lambda C + K$.
  - ◇ $\tilde{Q}(\lambda)$ = The leading principal submatrix of $Q(\lambda)$ of dimension $n-1$.
- Given scalars
  - ◇ $\{\lambda_1, \ldots, \lambda_{2n}\}$, and
  - ◇ $\{\mu_1, \ldots, \mu_{2n-2}\} \in \mathbb{C}$,
- Find
  - ◇ tridiagonal symmetric matrices C and K, or
  - ◇ real-valued, tridiagonal, symmetric, and weakly diagonally dominant matrices C and K with positive diagonal and negative off-diagonal elements,
- Such that
  - ◇ $\det(Q(\lambda))$ has zeros precisely $\{\lambda_1, \ldots, \lambda_{2n}\}$, and
  - ◇ $\det(\tilde{Q}(\lambda))$ has zeros precisely $\{\mu_1, \ldots, \mu_{2n-2}\}$.

Inverse Sturm-Liouville Problem

- The classical Sturm-Liouville problem:

$$\begin{aligned} \mathcal{L}[u] := -u_n''(x) + p(x)u_n(x) &= \lambda_n u_n(x), \ 0 < x < 1 \\ u_n'(0) - h u_n(0) &= 0 \\ u_n'(1) + H u_n(1) &= 0. \end{aligned}$$

  - ◇ Eigenvalues of $\mathcal{L}$ are real, simple, countable, and tend to infinity.
  - ◇ Increasing q, h, or H increases all eigenvalues of $\mathcal{L}$.
- Can the function $p(x)$ be determined from eigenvalues? (Two data sequences are required [150].)

Matrix Analogue

- Discretize the BVP by the central difference scheme with mesh $h = \frac{1}{n+1}$,

$$\left(\frac{1}{h^2} \begin{bmatrix} 2 & -1 & 0 & & & \\ -1 & 2 & -1 & & & \\ 0 & -1 & 2 & \dots & & 0 \\ \vdots & & & \ddots & & \\ 0 & & & & 2 & -1 \\ 0 & & & & -1 & 2 \end{bmatrix} + X \right) \mathbf{u} = \lambda \mathbf{u}.$$

  - ◇ X = diagonal matrix representing the discretization of $p(x)$.
- Determine X so that the system processes a prescribed spectrum.
  - ◇ This is an additive inverse eigenvalue problem.
- Caution: There is a significant difference in asymptotic behavior between the discrete and continuous cases.

Applied Physics

- Quantum Mechanics
- Geophysics
- Neutron Transport Theory

Quantum Mechanics

- Computing the electronic structure of an atom requires the spectral and diagonal information of a Hamiltonian matrix H.
- Diagonal elements of H cannot be measured accurately.
- Eigenvalues of H correspond to energy levels of an atom that can be measured to a high degree of accuracy.
- Want to use eigenvalues to correct diagonal elements.
- A least squares IEP [110]:
  - ◇ Given
    - ▷ A real symmetric matrix A,
    - ▷ A set of real eigenvalues $\omega = [\omega_1, \ldots, \omega_n]^T$,
  - ◇ Find a real diagonal matrix D such that

$$\|\sigma(A + D) - \omega\|_2$$

is minimized.

Geophysics

- Assuming spherical symmetry, want to infer the internal structure of the Earth from the frequencies of spheroidal and torsional modes of oscillations.
- The model involves the generalized Sturm-Liouville problem, i.e.,

$$u^{(2k)} - (p_1 u^{(k-1)})^{(k-1)} + \ldots + (-1)^k p_k u = \lambda u.$$

  - ◇ For well-posedness, $k+1$ spectra associated with $k+1$ distinct sets of boundary conditions are required to construct the unknown coefficients $p_1, \ldots, p_k$ [14, 15].
  - ◇ Theoretical solution can be constructed iteratively for the cases $k = 1, 2$.
  - ◇ Open Question: What is the matrix analogue of this high order problem and how to solve it numerically?

Neutron Transport Theory

- Dynamics in an additive neural network

$$\frac{du_i}{dt} = -a_i u_i + \sum_{j=1}^{n} \omega_{ij} g_j(u_j) + p_i, \quad , i = 1, \ldots n.$$

  - ◇ ω_{ij} = connection coefficient between the ith and jth neurons.
  - ◇ $g_j' > 0$ and g_j is bounded.
- Want to choose W so that a designated point $\mathbf{u}^*$ is a stable equilibrium.
  - ◇ At the critical point, there is a linear constraint

$$-A\mathbf{u}^* + W\mathbf{g}(\mathbf{u}^*) + \mathbf{p} = 0.$$

  - ◇ The eigenvalues of the Jacobian matrix should be in the left half plane.

- An equality constrained IEP [235]:
  - ◇ Given
    - ▷ Two sets of real vectors $\{\mathbf{x}_i\}_{i=1}^{p}$ and $\{\mathbf{y}_i\}_{i=1}^{p}$ with $p \le n$, and
    - ▷ A set of complex numbers $\mathcal{L} = \{\lambda_1, \ldots, \lambda_n\}$, closed in conjugation,
  - ◇ Find a real matrix A such that

$$\begin{aligned} A\mathbf{x}_i &= \mathbf{y}_i, \\ \sigma(A) &= \mathcal{L} \end{aligned}$$

Numerical Analysis

- Preconditioning
- High Order Stable Runge-Kutta Schemes
- Gauss Quadratures

Preconditioning

- Preconditioning the equation $Ax = b$ is a means of transforming the original system into one that has the same solution, but is easier (quicker) to solve with an iterative scheme.
  - ◇ Preconditioning A can be thought of as implicitly multiplying A by M^{-1}.
    - ▷ M is a matrix for which $Mz = y$ can easily be solved, and
    - ▷ $M^{-1}A$ is not too far from normal and its eigenvalues are clustered.
  - ◇ Many types of unstructured preconditioners have been proposed:
    - ▷ Low-order (Coarse-grid) approximation, SOR, incomplete LU factorization, polynomial, and so on.
    - ▷ Open Question: Given a structure of M, what is the best achievable conditioning [166]?

- Precondition by low rank matrices might have applications in practical optimization.
  - ◇ Open Question: Given a matrix matrix $C \in \mathbb{R}^{m\times n}$ and a constant vector $\mathbf{b} \in \mathbb{R}^m$, find a vector $\mathbf{x} \in \mathbb{R}^n$ such that the rank-one updated matrix $\mathbf{b}\mathbf{x}^T + C$ has a prescribed set of singular values.

High Order Stable Runge-Kutta Schemes

- An s-stage Runge-Kutta method is uniquely determined by the Butcher array

$$\begin{array}{c|cccc} c_1 & a_{11} & a_{12} & \dots & a_{1s} \\ c_2 & a_{21} & a_{22} & \dots & a_{2s} \\ \vdots & \vdots & & & \vdots \\ c_s & a_{s1} & a_{s2} & \dots & a_{ss} \\ \hline & b_1 & b_2 & \dots & b_s \end{array}$$

  - ◇ The stability function is given by

$$R(z) = 1 + z\mathbf{b}^T (I - zA)^{-1}\mathbf{1}.$$

- To attain stability, implicit methods are preferred.
  - ◇ Fully implicit methods are too expensive.
  - ◇ Diagonally implicit methods (DIRK), i.e., A is low triangular with *identical* diagonal entries, is computationally more efficient, but is difficult to construct.
  - ◇ Singly implicit methods (SIRK) requires that the matrix A, though not lower triangular, should have an s-fold eigenvalue.

- An IEP with prescribed entries [269]:
  - ◇ Given
    - ▷ The number s of stages,
    - ▷ The the desired order p,
    - ▷ Define $k = \lfloor (p-1)/2 \rfloor$,
    - ▷ Constants $\xi_j = 0.5(4J^2 - 1)^{-1/2}$, $j = 1, \dots, k$,
  - ◇ Find a real number λ and $Q \in \mathbb{R}^{(s-k)\times(s-k)}$ such that
    - ▷ $Q + Q^T$ is positive semi-definite.
    - ▷ $\sigma(X) = \{\lambda\}$ where $X \in \mathbb{R}^{s\times s}$ is of the form

$$X = \left[\begin{array}{cccc|c} 1/2 & -\xi_1 & & & \\ \xi_1 & 0 & & & \\ 0 & & & & \\ \vdots & & \ddots & & \\ & & & 0 & -\xi_k \\ \hline 0 & & & \xi_k & Q \end{array}\right]$$

    and $q_{11} = 0$ if p is even.

Gauss Quadratures

- With respect to a given a weight function $\omega(x) \geq 0$ on $[a, b]$, one can define a sequence of orthonormal polynomials $\{p_n(x)\}_{n=0}^{\infty}$ satisfying

$$\int_a^b \omega(x) p_i(x) p_j(x) dx = \delta_{ij}.$$

  - ◇ Roots of each $p_n(x)$ are simple, distinct, and lie in the interval $[a, b]$.
  - ◇ The roots $\{\lambda_i\}_{i=1}^{n}$ of a fixed $p_n(x)$ define a Gaussian quadrature

$$\int_a^b \omega(x) f(x) dx = \sum_{i=1}^{n} w_i f(\lambda_i),$$

    that has degree of precision up to $2n-1$.

- With $p_0(x) \equiv 1$ and $p_{-1}(x) \equiv 0$, orthogonal polynomials satisfy a three-term recurrence relationship:

$$p_n(x) = (a_n x + a_n) p_{n-1}(x) - c_n p_{n-2}(x).$$

  - ◇ In matrix form:

$$x \underbrace{\begin{bmatrix} p_0(x) \\ p_1(x) \\ \\ \vdots \\ p_{n-2}(x) \\ p_{n-1}(x) \end{bmatrix}}_{\mathbf{p}(x)} = \underbrace{\begin{bmatrix} \frac{-a_1}{a_1} & \frac{1}{a_1} & 0 & & 0 \\ \frac{c_2}{a_2} & \frac{-a_2}{a_2} & \frac{1}{a_2} & & \\ 0 & & & & \\ \vdots & & & \ddots & \vdots \\ 0 & & & & \frac{1}{a_{n-1}} \\ 0 & & & \dots \frac{c_n}{a_n} & \frac{-a_n}{a_n} \end{bmatrix}}_{\mathbf{T}} \begin{bmatrix} p_0(x) \\ p_1(x) \\ \\ \vdots \\ p_{n-2}(x) \\ p_{n-1}(x) \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ \\ \vdots \\ 0 \\ p_n(x) \end{bmatrix}$$

  - ◇ $p_n(\lambda_j) = 0$ if and only if

$$\lambda_i \mathbf{p}(\lambda_i) = T \mathbf{p}(\lambda_i).$$

  - ◇ T can be symmetrized by diagonal similarity transformation into a Jacobi matrix J.
  - ◇ It can be shown that the weight w_j in the quadrature is given by

$$w_i = q_{1i}^2, \quad i = 1, \dots n$$

    where $\mathbf{q}_i$ is the i-th normalized eigenvector of J.

- The inverse problem:
  - ◇ Given a quadrature, i.e.,
    - ▷ abscissas $\{\lambda_k^*\}_{k=1}^n$, and
    - ▷ weights $\{w_1, \ldots, w_n\}$ with $\sum_{i=1}^n w_i = 1$,
  - ◇ Determine the corresponding orthogonal polynomials.

Low Rank Approximation

- Noise removal in signal/image processing with Toeplitz structure.
  - ◇ rank = noise level where SNR is high.
- Model reduction problem in speech encoding and filter design with Hankel structure.
  - ◇ rank = # of sinusoidal components in the signal.
- GCD approximation for multivariate polynomials with Sylvester structure.
  - ◇ rank = degree of GCD.
- Molecular structure modeling for protein folding with nonnegative matrices.
  - ◇ rank ≤ 5.
- LSI application.
  - ◇ rank = # of factors capturing the random nature of the indexing matrix but structure = ?
- Preconditioning or regularization of ill-posed inverse problems.

Chapter 3

Parameterized Inverse Eigenvalue Problems

- Overview.
- General Results.
- Additive Inverse Eigenvalue Problems.
- Multiplicative Inverse Eigenvalue Problems.

Overview

- The structural constraint is regulated by a set of parameters.
- Most discussion concentrates on linear dependence of the problem on the parameters.

Generic Form

- Given
  - ◇ A *family* of matrices $A(c) \in \mathcal{M}$ with parameters $c \in \mathbf{F}^m$,
  - ◇ A set of scalars $\Omega \subset \mathbf{F}$,
- Find
  - ◇ Values of parameter c such that
$$\sigma(A(c)) \subset \Omega.$$
    - ▷ $\mathcal{M}$ = One particular class of submatrices in $\mathbf{F}^{n\times n}$.
    - ▷ $\mathbf{F}$ = One particular field of scalars.
- Remark:
  - ◇ Degree of free parameters m needs not be the same as the size n of the matrix.
  - ◇ Commonly used Ω:
    - ▷ $\Omega = \{\lambda_k^*\}_{k=1}^n$.
    - ▷ Ω = left-half complex plan.
  - ◇ Depending upon how $A(c)$ is defined, the PIEP can appear in very different form.

Variations

- Linear dependence on parameters (LiPIEP):
$$A(c) = A_0 + \sum_{i=1}^{m} c_i A_i.$$
  - ◇ $A_i \in \mathcal{R}(n)$, $\mathbf{F} = \mathbb{R}$.
  - ◇ $A_i \in \mathcal{S}(n)$, $\mathbf{F} = \mathbb{R}$.
- **(AIEP)** $A(c) = A(X) = A_0 + X$, $X \in \mathcal{N}$.
  - ◇ $\mathcal{N}$ = Some special class of submatrices.
  - ◇ X can be expressed in terms of linear combinations of basis $\{A_{i\}}$ of $\mathcal{N}$.
- **(MIEP)** $A(c) = A(X) = XA_0$, $X \in \mathcal{N}$.
  - ◇ XA_0 can still be expressed as a linear combination of some A_i, $i = 1, \ldots, m$.
  - ◇ If $X = \mathrm{diag}\{c_1, \ldots, c_n\}$, write $A_0 = [a_1^T, \ldots, a_n^T]^T$ in rows. Then
$$XA_0 = \sum_{i=1}^{n} c_i \underbrace{e_i a_i^T}_{A_i}.$$
- **(Generalized Pole Assignment Problem)** $A(c) = A(K_1, \ldots, K_q) = A_0 + \sum_{i=1}^{q} B_i K_i C_i$.

General Results

- Lot of attention has been paid to the theory and numerical method of the LiPIEP.
  - ◇ Finding a solution over real field is more complicated and difficult than over complex field.
- Whatever is known about LiPIEP applies to AIEP and MIEP.
- Pole assignment problem itself stands alone as an important application for decades.
  - ◇ Has been extensively studied already.
  - ◇ Many theoretical results and numerical techniques are available.
  - ◇ Approaches include skills from linear system theory, combinatorics, complex analysis to algebraic geometry.
  - ◇ Will not be discussed in this note.

Existence Theory for Linear PIEP

- Most discussions concentrate on the LiPIEP.

$$A(c) = A_0 + \sum_{i=1}^{m} c_i A_i.$$

- Complex solvability is generally expected by solving polynomial systems.
- Presence of multiple eigenvalues in real case makes a big difference.

Complex Solvability

- Given n complex numbers $\{\lambda_k^*\}_{k=1}^n$,
  - ◇ For almost all $A_i \in \mathbb{C}^{n\times n}$, there exists $c \in \mathbb{C}^n$ such that $A(c) = A_0 + \sum_{k=1}^n c_k A_k$ has eigenvalues $\{\lambda_k^*\}_{k=1}^n$.
  - ◇ There are at most $n!$ distinct solutions.

Real Solvability ($n = m$)

- Notation and Definitions:

$$
\begin{aligned}
A_k &:= \left[a_{ij}^{(k)}\right], \quad k = 0, 1, \ldots, n,\\
E &:= \left[a_{ii}^{(k)}\right], \quad i, k = 1, \ldots, n,\\
S &:= \sum_{i=1}^{m} |A_k|,\\
\pi(M) &:= \|M - \operatorname{diag}(M)\|_\infty,\\
d(\lambda) &:= \min_{i\neq j} |\lambda_i - \lambda_j|
\end{aligned}
$$

- Normalize the diagonals of A_j:
  - ◇ Assume $E^{-1} = [\ell_{ij}]$ exists and $\tilde{c} := Ec$.
  - ◇ Rewrite

$$
\begin{aligned}
A(c) &= A_0 + \sum_{k=1}^n c_k A_k = A_0 + \sum_{k=1}^n \left(\sum_{j=1}^n \ell_{kj}\tilde{c}_j\right) A_k\\
&= A_0 + \sum_{j=1}^n \tilde{c}_j \underbrace{\left(\sum_{k=1}^n \ell_{kj} A_k\right)}_{\tilde{A}_j}.
\end{aligned}
$$

$$\operatorname{diag}(\tilde{A}_j) = e_j, \quad j = 1, \ldots n.$$

- [34] Sufficient condition:
  - ◇ Given
    - ▷ n real numbers $\lambda^* = \{\lambda_k^*\}_{k=1}^n$, and
    - ▷ $n+1$ real $n \times n$ matrices A_i, $i = 0, 1, \ldots, n$,
  - ◇ Assume
    - ▷ $\mathrm{diag}(A_k) = e_k$, $k = 1, \ldots, n$,
    - ▷ $\pi(S) < 1$,
    - ▷ The gap $d(\lambda^*)$ is sufficiently large, i.e.,

$$d(\lambda^*) \geq 4\frac{\pi(S)\|\mathrm{diag}(\lambda^*) - diag(A_0)\|_\infty + \pi(A_0)}{1 - \pi(S)}.$$

  - ◇ Then the LiPIEP (with $m = n$) has a real solution $c \in \mathbb{R}^n$.
  - ◇ Idea of proof:
    - ▷ Prove that Gerschgorin circles of $A(c)$ are disjoint.
    - ▷ Use Brouser fixed-point theorem to find a fixed point for the map $T(c) = \lambda^* + c - \lambda(A(c))$.
- Open Question: What can be said if $m > n$?

Multiple Eigenvalue

- Consider the LiPIEP associated with
  - ◇ Matrices $A_i \in \mathbb{R}^{n\times n}$, $i = 0, 1, \ldots, m$, and
  - ◇ k real eigenvalue $\{\lambda_1^*, \ldots, \lambda_k^*\}$,
    - ▷ λ_i^* has multiplicity $r_i \geq 0$.
    - ▷ $r_1 + \ldots + r_k = n$.
- Let $r = \max\{r_1, \ldots, r_k\}$ = maximal multiplicity.
- [310, 332] The LiPIEP is unsolvable almost everywhere if $n - m + r(r-1) > 1$.
  - ◇ If $n = m$, then the LiPIEP is unsolvalbe almost everywhere if and only if $r > 1$.

Sensitivity Analysis

- The solution to an IEP is generally not unique.
- The IEP is generally ill-posed.
  - ◇ Even if a solution depends continuously upon the problem data, the numerical solution could differ by a great deal with small perturbation.

Forward Problem for General $A(c)$

- Assume
  - ◇ $A(c) \in \mathbb{C}^{n\times n}$ is analytic in $c \in \mathbb{C}^m$ over a neighborhood of 0.
  - ◇ λ_0 is a *simple* eigenvalue of $A(0)$.
  - ◇ $\mathbf{x}_0$ and $\mathbf{y}_0$ are the right and left unit eigenvector, respectively, of $A(0)$ corresponding to λ_0.
- Then
  - ◇ There exists an analytic function $\lambda(c)$ in a neighborhood N of $0 \in \mathbb{C}^m$ such that
    - ▷ $\lambda(c)$ is a simple eigenvalue of $A(c)$.
    - ▷ $\lambda(0) = \lambda_0$.
  - ◇ There exist analytic functions $\mathbf{x}(c)$ and $\mathbf{y}(c)$ in N such that
    - ▷ $\mathbf{x}(c)$ is a right eigenvector corresponding to $\lambda(c)$.
    - ▷ $\mathbf{y}(c)$ is a left eigenvector corresponding to $\lambda(c)$.
    - ▷ $\mathbf{x}(0) = \mathbf{x}_0$, $\mathbf{y}(0) = \mathbf{y}_0$.
- Furthermore,

$$\left(\frac{\partial \lambda(c)}{\partial c_i}\right)_{c=0} = \mathbf{y}_0^T \left(\frac{\partial A(c)}{\partial c}\right)_{c=0} \mathbf{x}_0.$$

Inverse Problem for Linear Symmetric $A(c)$

- Assume all matrices are symmetric and the LiPIEP
$$A(c) = A_0 + \sum_{i=1}^{n} c_i A_i$$
is solvable.
- Assume $A(c) = Q(c)\text{diag}\{\lambda_k^*\}_{k=1}^n Q(c)^T$ and define
$$\begin{aligned} J(c) &= \left[\mathbf{q}_i(c)^T A_j \mathbf{q}_i(c)\right], \quad i, j = 1, \ldots, n, \\ b &= \left[\mathbf{q}_1(c)^T A_0 \mathbf{q}_1(c), \ldots, \mathbf{q}_n^T A_0 \mathbf{q}_n(c)\right]^T. \end{aligned}$$
- [360] If
$$\delta = \|\lambda^* - \tilde{\lambda}\|_\infty + \sum_{i=0}^{n} \|A_i - \tilde{A}_i\|_2$$
is sufficiently small, then
  - ◇ The PIEP associated with $\tilde{A}_i$, $i = 0, \ldots, n$ and $\{\tilde{\lambda}_1, \ldots, \tilde{\lambda}_n\}$ is solvable.
  - ◇ There is a solution $\tilde{c}$ near to c,

$$\frac{\|c - \tilde{c}\|_\infty}{\|c\|_\infty} \leq \kappa_\infty(J(c)) \left(\frac{\|\lambda^* - \tilde{\lambda}\|_\infty + \|A_0 - \tilde{A}_0\|_2}{\|\lambda^* - b\|_\infty} + \frac{\sum_{i=1}^n \|A_i - \tilde{A}_i\|_2}{\|J(c)\|_\infty} \right) + O(\delta^2).$$

Numerical Methods

- Direct methods.
  - ◇ Lanczos method.
- Iterative methods.
  - ◇ Newton's method.
  - ◇ Orthogonal reduction method.
- Continuous Methods.
  - ◇ Homotopy method.
  - ◇ Projected gradient method.
  - ◇ ASVD flow method.

Direct Method

- Solution can be found in finite number of steps.
- Formulation exists for IEP with Jacobi structure.
- Will be discussed in Chapter 4.

Iterative Methods

- Netwon's method.
  - ◇ Applicable to real symmetric LiPIEP.
  - ◇ Fast, but only local convergence.
  - ◇ Multiple eigenvalue case needs to be handled more carefully.
- Orthogonal reduction method.
  - ◇ Employs QR-like decomposition.
  - ◇ Can handle multiple eigenvalues easily.

Newton's Method (for real symmetric LiPIEP)

- Assume:
  - ◇ All matrices in
$$A(c) = A_0 + \sum_{i=1}^{n} c_i A_i$$
are real and symmetric.
  - ◇ 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:

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

- 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, $K^{(\nu)}$):

$$\tilde{K}_{ij}^{(\nu)} = \frac{\mathbf{q}_i^{(\nu)^T} A(c^{(\nu+1)}) \mathbf{q}_j^{(\nu)}}{\lambda_i^* - \lambda_j^*}, \text{ for } 1 \leq i < j \leq n.$$

Find the Lift-up

- No obvious coordinate axis to follow.
- Solving the IEP $\equiv$ Finding $\mathcal{M}_e(\Lambda) \bigcap \mathcal{A}$.
- 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 el al [145].
- Quadratic convergence even for multiple eigenvalues case.

Continuous Methods

- Homotopy method.
  - ◇ Homotopy theory for some AIEP's can be established.
    - ▷ Open Question: Describe a homotopy for general PIEP.
  - ◇ Provides both an existence proof and a numerical method.
  - ◇ See discussion in AIEP.
- Projection gradient method.
  - ◇ General, least squares setting.
  - ◇ Can be generalized to SIEP with any linear structure.
  - ◇ The method enjoys the globally descent property, but slow.
- ASVD flow method.
  - ◇ Provides stable coordinate transformations for nonsymmetric matrices.
  - ◇ Will be discissed in SIEP for stochastic structure.

Projected Gradient Method (for SIEP)

- The idea works for general *symmetric* $A(c)$ so long as the projection $P(X)$ of a matrix X to $\mathcal{A}$ can be calculated.
- The idea applies to SIEP and is described in that setting.
- Idea:
  - ⋄ $X \in \mathcal{M}_e(\Lambda)$ satisfies the spectral constraint.
  - ⋄ $P(X) \in \mathcal{V}$ has the desirable structure in $\mathcal{V}$.
  - ⋄ Minimize the undesirable part $\|X - P(X)\|$.
- Working with the parameter Q is easier:

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

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

Feasible Set $O(n)$ & Gradient of F

- The set $O(n)$ is a regular surface.
- The tangent space of $O(n)$ at any orthogonal matrix Q is given by

$$T_QO(n) = QK(n)$$

  where

$$K(n) = \{\text{All skew-symmetric matrices}\}.$$

- The normal space of $O(n)$ at any orthogonal matrix Q is given by

$$N_QO(n) = QS(n).$$

- 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 $R^{n\times n}$:

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

- A unique orthogonal splitting of $X \in R^{n\times n}$:

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

- The projection of $\nabla F(Q)$ into the tangent space:

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

An 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 $M(\Lambda)$:

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

- The entire concept can be obtained by utilizing the Riemannian geometry on the Lie group $O(n)$.

Additive Inverse Eigenvalue Problems

- Subvariations.
- Solvability Issues.
- Sensitivity Issues.
- Numerical Methods.
- Applications.

Subvariations

- Generic form:
  - ◇ Given
    - ▷ A fixed matrix A and a class of matrices $\mathcal{N}$ in $\mathbf{F}^{n\times n}$,
    - ▷ A subset $\Omega \subset \mathbf{F}$,
  - ◇ Find
    - ▷ $X \in \mathcal{N}$ such that $\sigma(A+X) \subset \Omega$.
- Some special cases:
  - ◇ (AIEP1) A is real, X is real diagonal, and $\mathbf{F}$ is real.
  - ◇ (AIEP2) A is real symmetric, X is real diagonal, and $\mathbf{F}$ is real.
  - ◇ (AIEP3) A is complex general, X is complex diagonal, and $\mathbf{F}$ is complex.
  - ◇ Open Question: $A = 0$, X has prescribed entries at specific location.

Solvability Issues

- If $X = \mathrm{diag}(c_1, \ldots, c_n)$, then consider

$$A + X = A + \sum_{i=1}^{n} c_i \underbrace{e_i e_i^T}_{A_i}.$$

This is a special PIEP.

- Complex solvability [2, 63, 138]:
  - ◇ For any specified $\{\lambda_k^*\}_{k=1}^n \in \mathbb{C}$, the AIEP3 is solvable.
  - ◇ There are at most $n!$ solutions.
  - ◇ For almost all $\{\lambda_k^*\}_{k=1}^n$, there are exactly $n!$ solutions.

- Real solvability
  - ◇ Some sufficient conditions:
    - ▷ If $d(\lambda^*) > 4\pi(A)$, then AIEP1 is solvable [101].
    - ▷ If $d(\lambda^*) > 2\sqrt{3}\,(\pi(A \circ A))^{1/2}$, then AIEP2 is solvable [170].
  - ◇ Some necessary conditions:
    - ▷ If AIEP1 is solvable, then

$$\sum_{i \neq j} (\lambda_i^* - \lambda_j^*)^2 \geq 2n \sum_{i \neq j} a_{ij} a_{ji}.$$

- Unsolvability:
  - ◇ Both AIEP1 and AIEP2 are unsolvable almost everywhere if an multiple eigenvalue is present [332].

Sensitivity Issues (for AIEP2)

- Suppose that the AIEP2 is solvable.
- Assume
  - ◇ $A(X) := A + X = Q(X)^T \Lambda Q(X)$,
    - ▷ Define

$$J(X) := [q_{ji}^2(X)],$$
$$b(X) := [q_1(X)^T A q_1(X), \ldots, q_n(X)^T A q_n(X)]^T.$$

  - ◇ $J(X)$ is nonsingular,
  - ◇ The perturbation

$$\delta = \|\lambda^* - \tilde{\lambda}\|_\infty + \|A - \tilde{A}\|_2$$

  is small enough.
- Then
  - ◇ The AIEP2 associated with $\tilde{A}$ and $\tilde{\lambda}$ is solvable.
  - ◇ There is a solution $\tilde{X}$ near to X, i.e.,

$$\frac{\|X - \tilde{X}\|_\infty}{\|X\|_\infty} \le \kappa_\infty(J(X)) \left(\frac{\|\lambda^* - \tilde{\lambda}\|_\infty + \|A - \tilde{A}\|_2}{\|\lambda * - b\|_\infty} \right) + O(\delta^2).$$

Numerical Methods

- Most methods for symmetric or Hermitian problem depend heavily on the fact that the eigenvalues are real and can be totally ordered.
  - ◇ Can consider each eigenvalue λ_i as piecewise differential function $\lambda_i(X)$.
  - ◇ Newton's iteration for AIEP2 is easy to formulate.
- For general matrices where eigenvalues are complex, tracking each eigenvalue requires some kind of matching mechanism.
  - ◇ Homotopy method naturally track each individual eigenvalue curves as are predetermined by initial values.
  - ◇ Homotopy method for AIEP3 gives rise to both an existence proof and a numerical method for finding all solutions.

Newton's Method (for AIEP2)

- At the ν-th iterate, assume $Z^{(\nu)} \in \mathcal{M}_e(\Lambda)$,

$$\begin{aligned} Z^{(\nu)} &= {Q^{(\nu)}}^T \Lambda Q^{(\nu)}, \\ A(X^{(\nu)}) &:= A + X^{(\nu)}, \\ J^{(\nu)} &:= \left[{q_{ji}^{(\nu)}}^2 \right], \\ b^{(\nu)} &:= \left[{q_1^{(\nu)}}^T A q_1^{(\nu)}, \ldots, {q_n^{(\nu)}}^T A q_n^{(\nu)} \right]^T. \end{aligned}$$

- Solve $J^{(\nu)} X^{(\nu+1)} = \lambda^* - b^{(\nu)}$ for $X^{(\nu+1)}$.
- Define skew-symmetric matrix

$$K^{(\nu)} := Q^{(\nu)} \left[\frac{{q_i^{(\nu)}}^T A(X^{(\nu+1)}) q_j^{(\nu)}}{\lambda_i^* - \lambda_j^*} \right] {Q^{(\nu)}}^T.$$

- Update the lift,

$$\begin{aligned} R^{(\nu)} &:= \left(I + \frac{K^{(\nu)}}{2} \right) \left(I - \frac{K^{(\nu)}}{2} \right)^{-1}, \\ Z^{(\nu+1)} &:= {R^{(\nu)}}^T X^{(\nu)} R^{(\nu)}, \\ Q^{(\nu+1)} &:= {R^{(\nu)}}^T Q^{(\nu)}. \end{aligned}$$

Homotopy Method (for AIEP3)

Multiplicative Inverse Eigenvalue Problems

- Subvariations.
- Solvability Issues.
- Sensitivity Issues.
- Numerical Methods.
- Applications.

Subvariations

- Generic form:
  - ◇ Given
    - ▷ A fixed matrix A and a class of matrices $\mathcal{N}$ in $\mathbf{F}^{n\times n}$,
    - ▷ A subset $\Omega \subset \mathbf{F}$,
  - ◇ Find
    - ▷ $X \in \mathcal{N}$ such that $\sigma(XA) \subset \Omega$.
- Some special cases:
  - ◇ (MIEP1) A is real, X is real diagonal, and $\mathbf{F}$ is real.
  - ◇ (MIEP2) A is real, symmetric, and positive definite, X is nonnegative diagonal, and $\mathbf{F}$ is real.
  - ◇ (MIEP3) A is complex general, X is complex diagonal, and $\mathbf{F}$ is complex.
  - ◇ (MIEP4) A is complex Hermitian, $\mathbf{F}$ is real, want $\sigma(X^{-1}AX^{-1}) = \{\lambda_k^*\}_{k=1}^n$ [120].
  - ◇ (MIEP5) Preconditioning applications.

Solvability Issues

- If $X = \mathrm{diag}(c_1, \ldots, c_n)$ and $A = [\mathbf{a}_1^T, \ldots, \mathbf{a}_n^T]^T$, then write

$$XA = \sum_{i=1}^{n} c_i \underbrace{\mathbf{e}_i \mathbf{a}_i^T}_{A_i}.$$

This is a special PIEP.

- Complex solvability [137]:
  - ◇ Assume that
    - ▷ All principal minors of A are distinct from zero,
  - ◇ Then
    - ▷ For any specified $\{\lambda_k^*\}_{k=1}^n \in \mathbb{C}$, the MIEP3 is solvable.
    - ▷ There are at most $n!$ solutions.

- Real solvability:
  - ◇ Some sufficient conditions:
    - ▷ Suppose
      - · The diagonals of A are normalized to 1, i.e., $a_{ii} = 1$.
      - · $\pi(A) < 1$.
      - · $d(\lambda) \geq \frac{4\pi(A)\|\lambda^*\|_{infty}}{1-\pi(A)}$.
    - ▷ Then the MIEP1 is solvable.
  - ◇ Some necessary conditions:
    - ▷ If MIEP1 is solvable, then

$$\sum_{i=1}^{n} x_i = \sum_{i=1}^{n} \lambda_i^*,$$

$$\det(A) \prod_{i=1}^{n} x_i = \prod_{i=1}^{n} \lambda_i^*.$$

Optimal Conditioning by Diagonal Matrices

- Friedland's result on MIEP1 suggests that a general complex matrix A can be perfectly conditioned.
  - ◇ Lacks an efficient algorithm to implement the result.
- Open question: Want to know the optimal preconditioner of a given sparsity pattern [165].
  - ◇ Suppose
    - ▷ A is symmetric and positive definite.
    - ▷ A has property A, i.e., A can be symmetrically permuted into
$$\begin{bmatrix} D_1 & B \\ B^T & D_2 \end{bmatrix}$$
where D_1 and D_2 are diagonal.
    - ▷ $D = \operatorname{diag}(A)$.
  - ◇ Then [134]
$$\kappa(D^{-1/2}AD^{-1/2}) = \min_{\widehat{D}>0, \widehat{D}=\text{diagonal}} \kappa(\widehat{D}A\widehat{D}).$$

Sensitivity Issues (for MIEP2)

- Suppose that the MIEP2 is solvable.
- MIEP2 is equivalent to the symmetrized problem:
$$X^{-1/2}A(X)X^{1/2} = X^{1/2}AX^{1/2}.$$
- Define
$$\begin{aligned} X^{1/2}AX^{1/2} &= U(X)^T \Lambda U(X), \\ W(X) &:= [u_{ji}^2(X)]. \end{aligned}$$
- Assume
  - ◇ $W(X)$ is nonsingular,
  - ◇ The perturbation
$$\delta = \|\lambda^* - \tilde{\lambda}\|_\infty + \|A - \tilde{A}\|_2$$
is small enough.
- Then
  - ◇ The MIEP2 associated with $\tilde{A}$ and $\tilde{\lambda}$ is solvable.
  - ◇ There is a solution $\tilde{X}$ near to X, i.e.,
$$\frac{\|X - \tilde{X}\|_\infty}{\|X\|_\infty} \le \frac{\lambda_n^*}{\lambda_1^*}\|W(X)^{-1}\|_\infty \left(\frac{\|\lambda^* - \tilde{\lambda}\|_\infty}{\|\lambda^*\|_\infty} + \|A - \tilde{A}\|_2 \right) + O(\delta^2).$$

Numerical Methods

- For preconditioning purpose, no need to solve the MIEP precisely.
  - ◇ There are many techniques for picking up a preconditioner.
  - ◇ Will not be discussed in this note.
- The MIEP is a linear, but not symmetric PIEP even if A is symmetric.
  - ◇ The numerical methods for symmmtric PIEP need to be modified.
  - ◇ If A is a Jacobi matrix, the problem can be solved by direct methods. Will be discussed in Chapter 4.

Reformulate MIEP1 as Nonlinear Equations

- Formulate MIEP1 as solving $f(X) = 0$ for some nonlinear function $f : \mathbb{R}^n \longrightarrow \mathbb{R}^n$.
- Different ways to formulate $f(X)$:
  - ◇ $f_i(X) := \det(XA - \lambda_i^* I)$.
  - ◇ $f_i(X) := \lambda_i(XA) - \lambda_i^*$.
  - ◇ $f_i(X) := \alpha_n(XA - \lambda_i^* I)$, where $\alpha_n(M) =$ the smallest singular values of M.
- Assume that $\lambda_i \neq 0$ and, therefore, $Y = X^{-1}$ exists.
  - ◇ $g_i(Y) := \det(A - \lambda_i^* Y)$.
  - ◇ $g_i(Y) := \lambda_i(A, Y) - \lambda_i^*$.

Newton's Method (for MIEP2)

- Reformulate the MIEP2 as solving equations
$$\lambda_i(A, Y) - \lambda_i^* = 0, \quad i = 1, \dots n$$
to maintain symmetry.
- At the ν-th stage [213],
  - ◇ Solve the generalized eigenvalue problem
$$\left(A - \lambda(\nu) Y^{(\nu)}\right) \mathbf{x}^{(\nu)} = 0.$$
    - ▷ Normalize $\mathbf{x}_i^{(\nu)}$ so that $\mathbf{x}_i^{(\nu)^T} Y^{(\nu)} \mathbf{x}_i^{(\nu)} = 1$.
    - ▷ Denote $Q^{(\nu)} = [\mathbf{x}_1^{(\nu)}, \dots \mathbf{x}_n^{(\nu)}] = [q_{ij}^{(\nu)}]$.
  - ◇ Define (the Jacobian matrix of $\lambda(A, Y)$)
$$J(Y^{(\nu)}) := [-\lambda_i^{(\nu)} q_{ji}^{(\nu)}].$$
  - ◇ Solve $J(Y^{(\nu)}) d^{(\nu)} = \lambda^* - \lambda^{(\nu)}$.
  - ◇ Update $Y^{(\nu+1)} := Y^{(\nu)} + \operatorname{diag}(d^{(\nu)})$.

Numerical Experience

- Open Question: Given the standard Jacobi matrix A with nonzero row entries $[-1, 2, -1]$, what is the set of all reachable spectra of XA via a nonnegative diagonal matrix X?
- Open Question: In structure design, often we are only interested in a few low order natrual frequencies. Indeed, for large structures, it is impractical to calculate all of the frequencies and modes. How should one solve the problem if only a few low order frequencies are given?
- The above Newton method is only a locally convergent method. It appears that in the case of divergence, the Jacobian matrix J becomes highly ill-conditioned and nearly singular.
- To effectively develop an algorithm for controlling the vibration of a string with a specified set of natural frequencies, for example, we need to have another mechanism that can somehow provide a good initial guess before the Newton's method can be employed.

Chapter 4

Structured Inverse Eigenvalue Problems

- Jacobi Inverse Eigenvalue Problems
- Toeplitz Inverse Eigenvalue Problem
- Nonnegative Inverse Eigenvalue Problem
- Stochastic Inverse Eigenvalue Problem
- Unitary Inverse Eigenvalue Problem
- Inverse Eigenvalue Problem with Prescribed Entries
- Inverse Singular Value Problems
- Inverse Singular/Eigenvalue Problem

Jacobi Inverse Eigenvalue Problems

- Overview.
- Subvariations.
- Existence Theory.
- Sensitivity Issues.
- Numerical Methods.

Overview

- Jacobi structure, i.e.,

$$J = \begin{bmatrix} a_1 & b_1 & 0 & & & 0 \\ b_1 & a_2 & b_2 & & & 0 \\ 0 & b_2 & a_3 & & & 0 \\ \vdots & & & \ddots & & \\ & & & & a_{n-1} & b_{n-1} \\ 0 & & & & b_{n-1} & a_n \end{bmatrix}, \quad b_i > 0,$$

appears in many areas of applications.
  - ◇ Oscillatory mass-spring systems.
  - ◇ Composite pendulum.
  - ◇ Sturm-Liouville problems.
- Jacobi IEP often can be solved by direct methods in finitely many steps.
- For symmetric tridiagonal matrices, there are $2n+1$ unknown entries to be determined. Thus there is in need of $2n+1$ pieces of information.
- For convenience, denote the leading principal submatrix of M by $\bar{M}$.

Subvariations

- (SIEP6a) [41, 98, 153, 164, 175, 193, 197]:
  - ◇ Given
    - ▷ Real scalars $\{\lambda_k^*\}_{k=1}^n$ and $\{\mu_1^*, \dots, \mu_{n-1}^*\}$,
    - ▷ Interlacing property:

$$\lambda_i^* \le \mu_i^* \le \lambda_{i+1}^*, \quad i = 1, \dots, n-1,$$

  - ◇ Find a Jacobi matrix J such that

$$\begin{aligned} \sigma(J) &= \{\lambda_k^*\}_{k=1}^n \\ \sigma(\bar{J}) &= \{\mu_1^*, \dots, \mu_{n-1}^*\}. \end{aligned}$$

- (SIEP2) [40, 98, 193].
  - ◇ Given
    - ▷ Real scalars $\{\lambda_k^*\}_{k=1}^n$,
  - ◇ Find a persymmetric Jacobi matrix J such that

$$\begin{aligned} \sigma(J) &= \{\lambda_k^*\}_{k=1}^n \\ a_i &= a_{n+1-i} \\ b_i &= b_{n+2-i}. \end{aligned}$$

- (SIEP6b) [289]:
  - ◇ Given
    - ▷ Complex and distinct scalars $\{\lambda_1^*, \dots, \lambda_{2n}^*\}$ and $\{\mu_1^*, \dots, \mu_{2n-2}^*\} \in \mathbb{C}$,
    - ▷ Closed with complex conjugation.
  - ◇ Find tridiagonal symmetric matrices C and K for the λ-matrix $Q(\lambda) = \lambda^2 I + \lambda C + K$ so that

$$\begin{aligned} \sigma(Q) &= \{\lambda_1^*, \dots, \lambda_{2n}^*\}, \\ \sigma(\bar{Q}) &= \{\mu_1^*, \dots, \mu_{2n-2}^*\}. \end{aligned}$$

    - ▷ Arising from damped oscillatory systems.
    - ▷ Open Question: A practical solution requires additional conditions, i.e., positive diagonal entries, negative off-diagonal entries, and are weakly diagonally dominant.

- (SIEP7) [40, 41, 129]:
  - ◇ Given
    - ▷ Real scalars $\{\lambda_k^*\}_{k=1}^n$ and $\{\mu_1^*, \dots, \mu_{n-1}^*\}$,
    - ▷ Satisfy the interlacing property,
    - ▷ A positive number β,
  - ◇ Find a periodic Jacobi matrix J of the form

$$J = \begin{bmatrix} a_1 & b_1 & & & & b_n \\ b_1 & a_2 & b_2 & & & 0 \\ 0 & b_2 & a_3 & & & 0 \\ \vdots & & & \ddots & & \\ & & & & a_{n-1} & b_{n-1} \\ b_n & & & & b_{n-1} & a_n \end{bmatrix}$$

such that

$$\begin{aligned} \sigma(J) &= \{\lambda_k^*\}_{k=1}^n, \\ \sigma(\bar{J}) &= \{\mu_1^*, \dots, \mu_{n-1}^*\}, \\ \prod_1^n b_i &= \beta. \end{aligned}$$

- (SIEP8) [98]:
  - ◇ Given
    - ▷ Real scalars $\{\lambda_k^*\}_{k=1}^n$ and $\{\mu_1^*, \ldots, \mu_n^*\}$
    - ▷ Satisfy the interlacing property

$$\lambda_i^* \leq \mu_i^* \leq \lambda_{i+1}^*, \quad i = 1, \ldots, n,$$

    with $\lambda_{n+1}^* = \infty$,
  - ◇ Find Jacobi matrices J and $\tilde{J}$ so that

$$\begin{aligned} \sigma(J) &= \{\lambda_k^*\}_{k=1}^n, \\ \sigma(\tilde{J}) &= \{\mu_1^*, \ldots, \mu_n^*\}, \\ J - \tilde{J} &\neq 0, \quad \text{only at the } (n,n) \text{ position.} \end{aligned}$$

- (SIEP9):
  - ◇ Given
    - ▷ Distinct real scalars $\{\lambda_1^*, \ldots, \lambda_{2n}^*\}$,
    - ▷ A Jacobi matrix $J_n \in \mathbb{R}^{n\times n}$,
  - ◇ Find a Jacobi matrix $J_{2n} \in \mathbb{R}^{2n\times 2n}$ so that

$$\begin{aligned} \sigma(J_{2n}) &= \{\lambda_1^*, \ldots, \lambda_{2n}^*\}, \\ J_{2n}(1:n, 1:n) &= J_n. \end{aligned}$$

Physical Interpretations

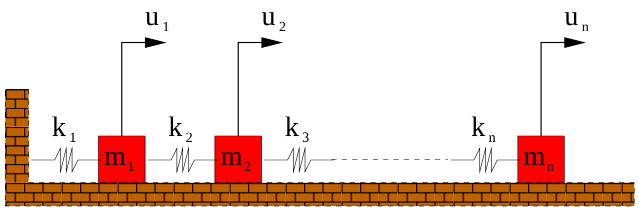


Figure 1: Mass-spring system

- Consider a serially linked mass-spring system with n particles.
  - ◇ m_i = mass of the i-th particle.
  - ◇ k_i = spring constant of the i-th spring.
  - ◇ $u_i(t)$ = displacement of the i-th particle at time t.
- Equation of motion:

$$\begin{aligned} m_1 \frac{d^2 u_1}{dt} &= -k_1 u_1 + k_2(u_2 - u_1), \\ m_i \frac{d^2 u_i}{dt} &= -k_i(u_i - u_{i-1}) + k_{i+1}(u_{i+1} - u_i), \\ & \quad i = 2, \ldots, n-1, \\ m_n \frac{d^2 u_n}{dt} &= -k_n(u_n - u_{n-1}). \end{aligned}$$

- In matrix form:

$$M\frac{d^2\mathbf{u}}{dt} = K\mathbf{u}.$$

  - ◇ $\mathbf{u} = [u_1, \ldots, u_n]^T$.
  - ◇ $M = \mathrm{diag}(m_1, \ldots, m_n)$.
  - ◇ K is the Jacobi matrix given by

$$K = \begin{bmatrix} -(k_1+k_2) & k_2 & 0 & \ldots 0 & 0 \\ k_2 & -(k_2+k_3) & k_3 & & 0 \\ 0 & k_3 & -(k_3+k_4) & & 0 \\ \vdots & & & \ddots & \vdots \\ 0 & & & & k_n \\ 0 & & & k_n & -k_n \end{bmatrix}$$

- Fundamental solutions are of the form $\mathbf{u}(t) = e^{i\omega t}\mathbf{x}$.
  - ◇ Natural frequency/mode equation is governed by

$$K\mathbf{x} = -\omega^2 M\mathbf{x}.$$

  - ◇ Define $J = M^{-1/2}KM^{-1}$ and $\lambda = -\omega^2$. Then

$$J\mathbf{x} = \lambda\mathbf{x}.$$

- Knowing m_i and k_k, we can predict the natural frequencies and modes of the system.
  - ◇ The inverse problem means that we would like to calculate values such as $\frac{-k_i-k_{i+1}}{m_i}$ and $\frac{k_{i+1}}{\sqrt{m_i m_{i+1}}}$ from the spectral data.

- SIEP6a $\Longleftrightarrow$ Identifying the system from its spectrum and the spectrum of the reduced system where the last mass is held to have no motion.
- SIEP2 $\Longleftrightarrow$ Identifying the system from its spectrum if the system is symmetric with respect to its center.
- SIEP6b $\Longleftrightarrow$ Identifying the damped system, including its damper configurations, from its spectrum and the spectrum of the reduced system where the last mass is held immboile.S
- SIEP7 $\Longleftrightarrow$ Same as SIEP6a except that m_1 and m_2 are connected by another spring mechanism to form a loop.
- SIEP8 $\Longleftrightarrow$ Identifying the system from its spectrum and the spectrum of the new system whereas only the last spring constant is changed.
- SIEP9 $\Longleftrightarrow$ Identifying the system from its spectrum and physical paramters m_i, k_i of the first half particles.
- Sometimes it is impossible to gather the entire spectrum information. Partial information of some eigenvalues and some eigenvectors can also be used to determine a Jacobi matrix. See Chapter 6.

Existence Theory

- Very rich and nearly complete theory available.
- Strictly interlacing property, i.e.,

$$\lambda_i^* < \mu_i^* < \lambda_{i+1}^*, \quad i = 1, \ldots, n-1,$$

is a necessary condition unless some subdiagonal (superdiagona) entries are zero.

  - ◇ Jacobi matrices are assumed to have positive b_i for all $i = 1, \ldots, n-1$.
  - ◇ Eigenvalues of a Jacobi matrix are necessarily real and distinct.
  - ◇ Eigenvalues of $\bar{J}$ necessarily separate those of J.
- Most existence proofs are based on the recurrence relationship between characteristic polynomials for Jacobi matrices.

- Assume that the given eigenvalues satisfy the strictly interlacing property. Then
  - ◇ The SIEP6a has a unique solution [175].
  - ◇ The SIEP8 has a unique solution.
- If $\{\lambda_k^*\}_{k=1}^n$ are distinct. Then the SIEP2 has a unique solution.
- Over the complex field $\mathbb{C}$,
  - ◇ If the given eigenvalues are distinct, then the SIEP6b is solvable and has at most $2^n(2n-3)!/(n-2)!$ different solutions [289].
  - ◇ If some eigenvalues are common, then there are infinitely many solutions for the SIEP6b.

- Assume that $\{\mu_1^*, \ldots, \mu_{n-1}^*\}$ are distinct. Then the SIEP7 is solvable if and only if

$$\prod_{k=1}^{n} |\mu_j^* - \lambda_k^*| \geq 2\beta(1 + (-1)^{n-j+1}),$$

for all $j = 1, \ldots, n-1$ [360].

  - ◇ No uniqueness can be assumed.
  - ◇ The eigenvalues of a periodic Jacobi matrix are not necessarily distinct.
  - ◇ The eigenvalues of $\bar{J}$ need not separate those of a periodic Jacobi matrix J.

- Assume that $\{\lambda_1^*, \ldots, \lambda_{2n}^*\}$ are distinct.
  - ◇ Define

$$\Delta_k = \det\left(\begin{bmatrix} 1 & \ldots & 1 & 1 & \ldots & 1 \\ \lambda_1 & \ldots & e_1^T J_n e_1 & \lambda_{k+1} & \ldots & \lambda_{2n} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \lambda_1^{2n-1} & \ldots & e_1^T J_n^{2n-1} e_1 & \lambda_{k+1}^{2n-1} & \ldots & \lambda_{2n}^{2n-1} \end{bmatrix}\right)$$

  - ◇ Then the SIEP9 has a unique solution if and only if

$$\Delta_k > 0$$

for all $k = 1, \ldots, 2n$ [360].

Sensitivity Issues

- The function $F : \mathbb{R}^{2n-1} \longrightarrow \mathbb{R}^{2n-1}$ where

$$F(a_1, \ldots, a_n, b_1, \ldots, b_{n-1}) = (\sigma(J), \sigma(\bar{J}))$$

is differentiable, if $b_i > 0$.

- The solution J to the SIEP6a depends continuously on the given data $\{\lambda_k^*\}_{k=1}^n$ and $\{\mu_1^*, \ldots, \mu_{n-1}^*\}$ [195].
- Let J and $\tilde{J}$ be solutions to the SIEP6a with data

$$\lambda_1^* < \mu_1^* < \lambda_2^* < \ldots < \mu_{n-1}^* < \lambda_n^*,$$
$$\tilde{\lambda}_1^* < \tilde{\mu}_1^* < \tilde{\lambda}_2^* < \ldots < \tilde{\mu}_{n-1}^* < \tilde{\lambda}_n^*$$

Then there exists a constant K such that

$$\|J - \tilde{J}\|_F \leq K \left(\sum_{i=1}^{n} |\lambda_i^* - \tilde{\lambda}_i^*|^2 + \sum_{i=1}^{n-1} |\mu_i^* - \tilde{\mu}_i^*|^2 \right)^{1/2}.$$

  - ◇ K depends on the separation of the given data measured by

$$d = \max\{\lambda_n^*, \tilde{\lambda}_n^*\} - \min\{\lambda_1^*, \tilde{\lambda}_1^*\},$$

$$\epsilon_0 = \frac{\min_{j,k}\{|\lambda_j^* - \mu_k^*|, |\tilde{\lambda}_j^* - \tilde{\mu}_j^*|\}}{d},$$

$$\delta_0 = \frac{\min_{j \neq k}\{|\lambda_j^* - \lambda_k^*|, |\mu_j^* - \mu_k^*|, |\tilde{\lambda}_j^* - \tilde{\lambda}_k^*|, |\tilde{\mu}_j^* - \tilde{\mu}_k^*|, \}}{2d}.$$

Numerical Methods

- Lanczos method.
  - ◇ Given any matrix A, if $Q^T AQ = H$ where Q is orthogonal and H is upper Hessenberg with positive subdiagonal entries, then Q and H are completely determined by A and the first column of Q.
  - ◇ In our application, $J = Q^T \Lambda Q$ in symmetric diagonal.
    1. $a_1 := \mathbf{q}_1^T A \mathbf{q}_1$.
    2. $b_1 := \|\Lambda \mathbf{q}_1 - a_1 \mathbf{q}_1\|$.
    3. $\mathbf{q}_2 = (\Lambda \mathbf{q}_1 - a_1 \mathbf{q}_1)/b_1$.
    4. For $i = 2, \ldots, n-1$,
       (a) $a_i := \mathbf{q}_i^T A \mathbf{q}_i$.
       (b) $b_i := \|\Lambda \mathbf{q}_i - a_i \mathbf{q}_i - b_{i-1}\mathbf{q}_{i-1}\|$.
       (c) $q_{i+1} := (\Lambda \mathbf{q}_i - a_i \mathbf{q}_i - b_{i-1}\mathbf{q}_{i-1})/b_i$.
    5. $a_n := \mathbf{q}_n^T A \mathbf{q}_n$.
- Orthogonal reduction method.
  - ◇ Orthogonal tridiagonalization of a bordered diagonal matrix.

Lanczos Method (for SIEP6a)

- Basic facts:
  - ◇ Given any symmetric matrix A with orthonormal eigenpairs $(\lambda_i, \mathbf{x}_i)$, then

$$\operatorname{adj}(\lambda_i I - A) = \prod_{\substack{k=1\\k\neq i}}^{n} (\lambda_i - \lambda_k)\mathbf{x}_i \mathbf{x}_i^T.$$

  - ◇ Evaluate the above equation at the $(1,1)$ position for each $\mathbf{x}_i$ to obtain

$$x_{1i}^2 = \frac{\prod_{k=1}^{n-1}(\lambda_i - \mu_k)}{\prod_{\substack{k=1\\k\neq i}}^{n}(\lambda_i - \lambda_k)}.$$

- For SIEP6a,
  - ◇ The first column of Q for J can be expressed from the spectral data, i.e., $q_{i1} = x_{1i}$.
  - ◇ The Lanczos algorithm kicks in.
  - ◇ Need reorthogonalization along the way.

Orthogonal Reduction Method (for SIEP6a)

- Construct a bordered diagonal matrix A of the form

$$A = \begin{bmatrix} \alpha & \beta_1 & \dots & \beta_{n-1} \\ \beta_1 & \mu_1^* & & 0 \\ \vdots & & \ddots & \\ \beta_{n-1} & 0 & \dots & \mu_{n-1}^* \end{bmatrix}$$

with specified eigenvalues $\sigma(A) = \{\lambda_k^*\}_{k=1}^n$.

◇ α is trivially determined.

$$\alpha = \sum_{i=1}^{n} \lambda_i^* - \sum_{i=1}^{n-1} \mu_i^*.$$

◇ Characteristic polynomial of A is known.

$$\begin{aligned} \det(\lambda I - A) &= (\lambda - \alpha) \prod_{k=1}^{n-1} (\lambda - \mu_k^*) \\ &\quad - \sum_{i=1}^{n-1} \beta_i^2 \left(\prod_{\substack{k=1 \\ k \neq i}}^{n-1} (\lambda - \mu_k^*) \right). \end{aligned}$$

◇ Border elements β_i can be calculated:

$$\beta_i^2 = -\frac{\prod_{k=1}^{n} (\mu_i^* - \lambda_k^*)}{\prod_{\substack{k=1 \\ k \neq i}}^{n-1} (\mu_i^* - \mu_k^*)}.$$

- Derive orthogonal matrix Q efficiently so that

$$\begin{bmatrix} 1 & \mathbf{0}^T \\ \mathbf{0} & Q^T \end{bmatrix} A \begin{bmatrix} 1 & \mathbf{0}^T \\ 0 & Q \end{bmatrix} = \begin{bmatrix} \alpha & b_1 \mathbf{e}_1^T \\ b_1 \mathbf{e}_1 & \bar{J} \end{bmatrix} = J.$$

◇ $b_1 = \|\beta\|$.

◇ $Q^T \mathrm{diag}(\mu_1^*, \dots, \mu_{n-1}^*) Q = \bar{J}$.

◇ The first column of Q is given by β / b_1.

◇ The Lanczos method can be employed.

- One may also explore the bordered diagonal structure by using Householder transformation, Givens rotations, the Rutishauser method, and so on [41].

Toeplitz Inverse Eigenvalue Problem

- Overview
- Existence Theory
- Numerical Methods

Overview

- Symmetric Toeplitz Matrix $T(r) := t_{ij} = r_{|i-j|+1}$, i.e.,

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

- Is a special case of centrosymmetric matrices

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

  ◇ $\Xi = [\xi_{ij}]$ = unit perdiagonal matrix,

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

  ▷ Symmetric vector, if $\Xi v = v$.

  ▷ Skew-symmetric vector, if $\Xi v = -v$.

- (ToIEP) Find $r \in R^n$ such that $T(r)$ has a prescribed set of real numbers $\{\lambda_k^*\}_{k=1}^n$ as its spectrum.

Spectral Properties of Centrosymmetric Matrices

- Any $M \in \mathcal{C}(n)$ can be decomposed as follows [55]:

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

◇ $A, C, \Xi \in R^{\lfloor \frac{n}{2} \times \frac{n}{2} \rfloor}$.

◇ $x \in R^{\lfloor \frac{n}{2} \rfloor}$.

◇ $q \in R$.

◇ $A = A^T$.

- Orthonormal eigenvectors $Q = K^T Z$ M can be split into two groups based on diagonal block Z.

$$Z = \begin{bmatrix} Z_1 & 0 \\ 0 & Z_2 \end{bmatrix}.$$

◇ $Z_1 :=$ Eigenvectors of $A - \Xi C$.

◇ $Z_2 :=$ Eigenvectors of $\begin{bmatrix} q & \sqrt{2}x^T \\ \sqrt{2}x & A+\Xi C \end{bmatrix}$ or $A+\Xi C$.

- Eigenvectors of M enjoy special parity properties:

◇ $K^T \begin{bmatrix} Z_1 \\ 0 \end{bmatrix} = \lfloor \frac{n}{2} \rfloor$ skew-symmetric eigenvectors $\Rightarrow$ "Odd" eigenvalues.

◇ $K^T \begin{bmatrix} 0 \\ Z_2 \end{bmatrix} = \lceil \frac{n}{2} \rceil$ symmetric eigenvectors $\Rightarrow$ "Even" eigenvalues.

- Open Question: For an ToIEP to be solvable, each given eigenvalue must carry a specific parity. Can this parity be arbitrarily assigned?

A 3×3 Example

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

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

  ⋄ $\mathrm{trace}(M) = 0 \Longrightarrow$ Three free parameters in $\mathcal{C}(3)$.

- Isospectral subset $\mathcal{M}_{\mathcal{C}}(\lambda_1, \lambda_2, \lambda_3)$:

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

  ⋄ $\sigma =$ A permutation of integers $\{1, 2, 3\}$.

- $\mathcal{M}_{\mathcal{C}} =$ Three ellipses.

  ⋄ One circumscribes the other two.

- Check # of m_{12}-intercepts $\Rightarrow$

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

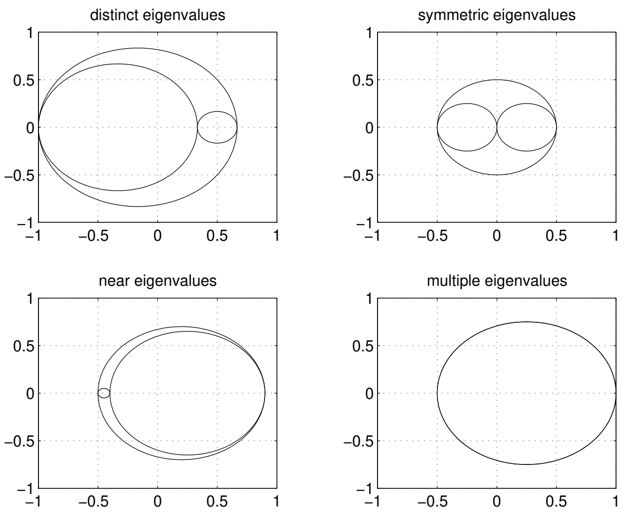


Figure 2: Plots of m_{11} versus m_{12} for $\mathcal{M}_{\mathcal{C}}$ in $\mathcal{C}(3)$.

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

Inverse Problem for Centrosymmetric Matrices

- Close form solution:
  - ◇ Given *arbitrary*
    - ▷ Diagonal matrix $\Lambda := \mathrm{diag}\{\{\lambda_k^*\}_{k=1}^n\}$,
    - ▷ 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 the matrix

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

    - ▷ Is centrosymmetric.
    - ▷ $\{\lambda_1^*, \ldots, \lambda_{\lfloor \frac{n}{2} \rfloor}^*\}$ = Odd eigenvalues of M.
    - ▷ $\{\lambda_{\lfloor \frac{n}{2} \rfloor + 1}^*, \ldots, \lambda_n^*\}$ = Even eigenvalues of M.
    - ▷ M may not be Toeplitz.
- Open Question: Search for a Toeplitz matrix on the isospectral surface $\mathcal{M}_{\mathcal{C}}(\{\lambda_k^*\}_{k=1}^n)$:

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

Existence

- Solvability has been a challenge.
  - ◇ n equations in n unknowns.
  - ◇ $n \geq 5$ is analytically intractable.
  - ◇ Symmetric Toeplitz matrices can have *arbitrary* real spectra [226].
    - ▷ Thus far, it is a nonconstructive proof by topological degree argument.
    - ▷ Open Question: Any algebraic proof of existence?
  - ◇ Eigenvalues *cannot* have arbitrary parity.

Idea in Landau's Proof

- A matrix $T(c_1, \ldots, c_n)$ is *regular* if every principal submatrix $T(c_1, \ldots, c_k)$, $1 \le k \le n$ has the properties:
  - ◇ Distinct eigenvalues.
  - ◇ Alternate parity with the largest one having even parity.
- Assume the given eigenvalues $\lambda_1 \le \ldots \le \lambda_n$ are centered, i.e., $\sum_{i=1}^n \lambda_i = 0$.
  - ◇ Suffices to solve the ToIEP for matrices of the form $T(0, 1, t_3, \ldots, t_n)$.
  - ◇ Necessarily $\lambda_1 < 0$.
- Consider the map

$$\phi(t_3, \ldots, t_n) = (y_2, \ldots, y_{n-1})$$

  - ◇ $y_i = -\frac{\lambda_i}{\lambda_1}$, $i = 2, \ldots, n-1$.
  - ◇ $\sigma(T(0, 1, t_3, \ldots, t_n)) = \{\lambda_1, \ldots, \lambda_n\}$.

- The range of ϕ is the simplex

$$\Delta := \left\{ (y_2, \ldots, y_{n-1}) | \begin{array}{c} -1 \le y_2 \le \ldots \le y_{n-1} \\ y_2 + \ldots + y_{n-2} + 2y_{n-1} \le 1 \end{array} \right\}.$$

- Landau's approach:
  - ◇ The set $\mathcal{F}$ of regular Toeplitz matrices of the form $T(0, 1, t_3, \ldots, t_n)$ is not empty.
  - ◇ The map ϕ restricted to those $(t_3, \ldots, t_n) \in \mathbb{R}^{n-2}$ such that $T(0, 1, t_3, \ldots, t_n) \in \mathcal{F}$ is a surjective map onto Δ.
  - ◇ Any $y_1 \le \ldots \le y_n$ can be *shifted* and *scaled* to a unique point in Δ.

Numerical Methods

- Mostly done in $\mathcal{S}(n)$.
  - ◇ Laurie's Algorithm [227]
  - ◇ Trench's Algorithm [337]
  - ◇ Continuous method
- The calculation could be limited to the smaller space $\mathcal{C}(n)$.
  - ◇ Cayley Transform [119]
  - ◇ Newton's Refinement to Centrosymmetric Structure

Continuous Method

Refined Newton to Centrosymmetric Structure

- 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 elments 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.
- In case of multiple eigenvalues
  - ◇ Basis of eigenspace splits as evenly as possible between symmetric and skew-symmetric eigenvectors [113].
  - ◇ Multiplicity of each eigenvalue ≤ 2 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 $T(r^{(\nu+1)})$.

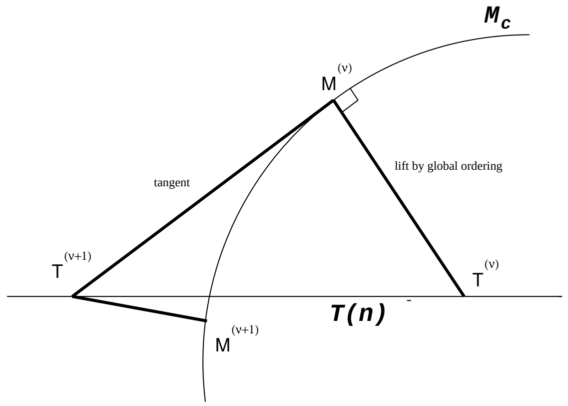


Figure 3: Geometry of Lift by Global Ordering.

- 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:

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

- 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.
- Quadratic convergence:
  - ◇ Order of convergence = (order projection)*(order tangent step). (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*):

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

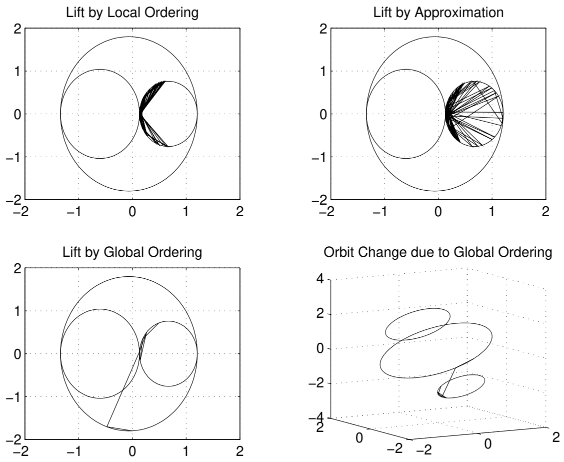


Figure 4: Behaviors of Algorithms When Starting with the Wrong Orbit.

- Lift by approximation $\Rightarrow$ Staying on the *wrong* orbit.
- Local ordering $\Rightarrow$ Wrong orbit, clustering.
- Global ordering $\Rightarrow$ 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.

	Case (a)	Case (b)	Case (c)
$r^{(\#)}$	0	0	0
	-2.0413×10^{-3}	-9.2349×10^{-1}	-3.3671×10^{-1}
	1.6065×10^{+0}	-7.0499×10^{-2}	4.1523×10^{-1}
Original Value	8.4765×10^{-1}	1.4789×10^{-1}	1.5578×10^{+0}
	2.6810×10^{-1}	-5.5709×10^{-1}	-2.4443×10^{+0}
$r^{(0)}$	0	0	0
	-2.8351×10^{-1}	-1.8024×10^{+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}	1.0901×10^{+0}
	1.0634×10^{+0}	-5.2451×10^{-1}	-3.2628×10^{+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}
	1.6065×10^{+0}	-7.0499×10^{-2}	4.3645×10^{-1}
Local Ordering	8.4765×10^{-1}	1.4789×10^{-1}	1.5244×10^{+0}
	2.6810×10^{-1}	-5.5709×10^{-1}	-2.4655×10^{+0}
$r^{(*)}$	8.6831×10^{-16}	0	4.7184×10^{-16}
	-2.0413×10^{-3}	-9.2349×10^{-1}	-3.3671×10^{-1}
	1.6065×10^{+0}	-7.0499×10^{-2}	4.1523×10^{-1}
Approximation	8.4765×10^{-1}	1.4789×10^{-1}	1.5578×10^{+0}
	2.6810×10^{-1}	-5.5709×10^{-1}	-2.4443×10^{+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}
	1.5174×10^{+0}	-6.1419×10^{-2}	4.3645×10^{-1}
Global Ordering	9.9597×10^{-1}	1.3518×10^{-1}	-1.5244×10^{+0}
	5.7042×10^{-1}	-5.4694×10^{-1}	-2.4655×10^{+0}

Table 1: Initial and Final Values of $r^{(\nu)}$ for Example 2.

Iterations	Local Ordering	Approximation	Global Ordering
0	1.3847×10^{+0}	1.3847×10^{+0}	1.2194×10^{+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 2: Errors of Eigenvalues for Case (a) in Example 2.

Example 3: Multiplicity = 2

- Test data (Random number):

$$\begin{array}{ll} & -5.8942\times10^{-1}\ (E) \\ \left\{\begin{array}{l} -1.8565\times10^{-1} \quad (O) \\ -1.8565\times10^{-1} \quad (E) \end{array}\right. & \\ & 3.7508\times10^{-1}\ (O) \\ & 5.8564\times10^{-1}\ (E) \end{array}$$

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

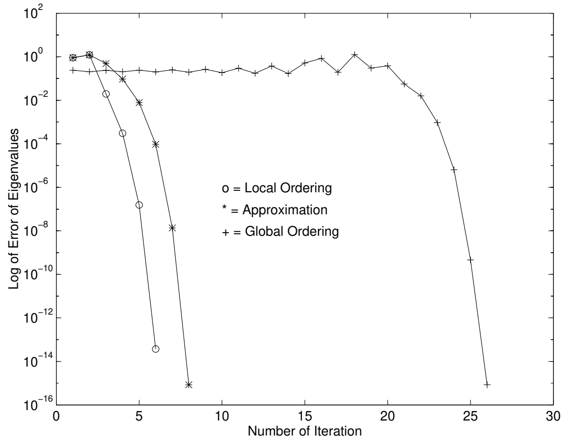


Figure 5: Number of Iteration versus Logarithmic Scale of Errors in Example 3.

Example 4: Multiplicity = 3

- Test data:

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

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

$$[.2204\times10^{-16}, 4.2222\times10^{-1}, 1.2863\times10^{-1}, 4.2222\times10^{-1}, 1.2863\times10^{-1}]$$

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:

$$\begin{array}{rrrr} -1.0242\times10^{+1} & -9.6736\times10^{+0} & -5.5608\times10^{+0} & -2.2651\times10^{+0} \\ 5.5692\times10^{-1} & 2.1786\times10^{+0} & 3.3867\times10^{+0} & 4.0016\times10^{+0} \\ 6.3594\times10^{+0} & 8.7090\times10^{+0} & & \end{array}$$

$$\begin{array}{rrrr} -1.0416\times10^{+1} & -9.4352\times10^{+0} & -4.7955\times10^{+0} & -7.7180\times10^{-1} \\ 6.3996\times10^{-1} & 2.6374\times10^{+0} & 4.4879\times10^{+0} & 4.7572\times10^{+0} \\ 6.2222\times10^{+0} & 9.2230\times10^{+0} & & \end{array}$$

  ◇ 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.

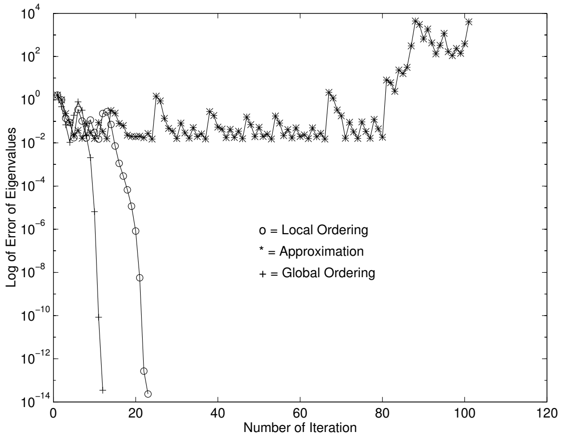


Figure 6: Number of Iteration versus Logarithmic Scale of Errors in Example 5.

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.
- Both local and global ordering, based on the Wielandt-Hoffman theorem, permit a new way of lifting.
  - ◇ Higher multiplicity eigenvalue case can now be handled.

Nonnegative Inverse Eigenvalue Problem

- Overview
- Some Existence Results
- Symmetric Nonnegative Inverse Eigenvalue Problem
- Numerical methods

Overview

- Many discussions in the literature on the subject [26, 30, 45, 130, 140, 143, 245, 262, 109, 318].
- Most discussions center around establishing a sufficient or necessary condition to qualify whether a given set of values is the spectrum of a nonnegative matrix.
- Open Question: Which sets of n real numbers occur as the spectrum of a nonnegative matrix?
- Open Question: Which sets of n real numbers occur as the spectrum of a symmetric nonnegative matrix?
- Open Question: Very few numerical algorithms.

Some Existence Results

- Suppose $\{\lambda_k^*\}_{k=1}^n$ are eigenvalues of an $n \times n$ nonnegative matrix. The the moments

  $$s_k = \sum_{i=1}^{n} (\lambda_i^*)^k$$

  must satisfy

  $$s_k^m \leq n^{m-1} s_{km}$$

  for all $k, m = 1, 2, \ldots$ [245].

- The set $\{\lambda_k^*\}_{k=1}^n \subset \mathbb{C}$ is the nonzero spectrum of a strictly positive matrix of size $m \geq n$ if and only if [45]
  - ⋄ $\lambda_1^* > |\lambda_i^*|$ for all $i > 1$,
  - ⋄ $s_k > 0$ for all $k = 1, 2, \ldots$, and
  - ⋄ The polynomial $\prod_{i=1}^n (t - \lambda_i^*)$ has real coefficients.

Symmetric Nonnegative Inverse Eigenvalue Problem

- There exist real numbers $\{\lambda_k^*\}_{k=1}^n$ that occur as the spectrum of a nonnegative $n \times n$ matrix, but do not occur as the spectrum of a symmetric nonnegative $n \times n$ matrix [212].

- The symmetric nonnegative inverse eigenvalue problem can be formulated as a constrained optimization problem of *minimizing* the objective function

  $$F(Q, R) := \frac{1}{2} \|Q^T \Lambda Q - R \circ R\|^2,$$

  subject to

  $$(Q, R) \in \mathcal{O}(n) \times \mathcal{S}(n).$$

- For nonsymmetric nonnegative inverse eigenvalue problems, see the discussion for the stochastic inverse eigenvalue problems.

Numerical Method

- A dynamical system resulting from projected gradient flow can be formulated as [74]:

$$\begin{aligned}\frac{dX}{dt} &= [X,[X,Y]],\\ \frac{dY}{dt} &= 4Y\circ(X-Y).\end{aligned}$$

  ◇ $X(t) = Q(t)^T\Lambda Q(t)$ is an isospectral matrix.

  ◇ $Y(t) = R(t)\circ R(t)$ is a symmetric nonnegative matrix.

Stochastic Inverse Eigenvalue Problem

- General View
- Karpelevič's Theorem
- Relationship to Nonnegative Matrices
- Basic Formulation
- Steepest Descent Flow
- ASVD Flow
- Convergence
- Numerical Experiment
- Conclusion

General View

- Construct a stochastic matrix with prescribed spectrum.
  - ◇ Stochastic structure.
  - ◇ No strings of symmetry.
  - ◇ Eigenvalues can appear in complex conjugate pairs.
- A hard problem [215, 262].
  - ◇ 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.
  - ◇ Region is symmetric about the real axis.
  - ◇ The points on the unit circles are given by $e^{2\pi i a/b}$ 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

$$\begin{aligned} \lambda^q(\lambda^p - t)^r &= (1-t)^r, \\ (\lambda^b - t)^d &= (1-t)^d \lambda^q, \end{aligned}$$

    where $0 \leq t \leq 1$, and b, d, p, q, r are natural integers determined certain specific rules (explicitly given in [215, 262]).
- The region Θ_4 is shown in Figure 7.

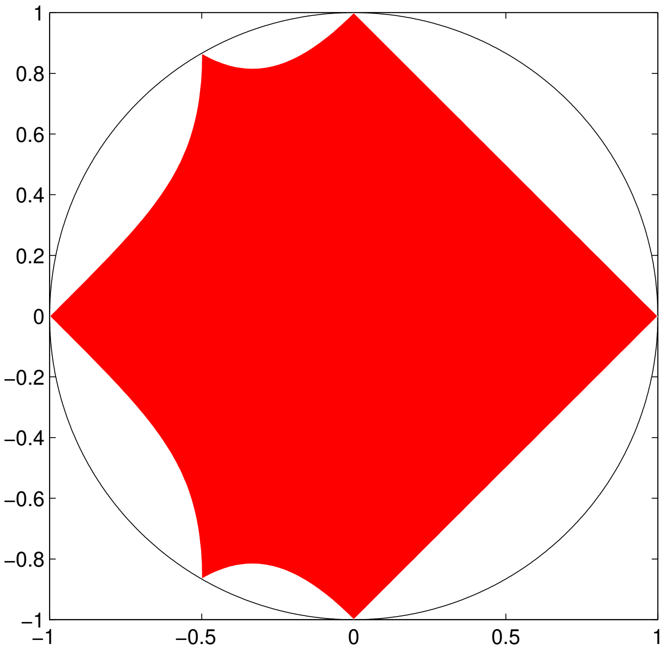


Figure 7: Θ_4 by the Karpelevič Theorem.

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.
- Key transformation:
  - ◇ Suppose 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 nonnegative inverse eigenvalue probelm (NIEP) has been discussed earlier.
  - ◇ Some necessary and a few sufficient conditions for the NIEP are available [30].
  - ◇ A continuous method for the symmetric NIEP can be formulated [74].
  - ◇ Open Question: Need a numerical algorithm for general NIEP.

Basic Formulation

- Notation:

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

  - ◇ 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

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

- 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:

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

  ◇ 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 [48, 345].
- The fact that $P(t)$ 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 $Z(t)$:

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

  - ◇ If $s_k^2 \neq s_j^2$, then

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

  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:

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

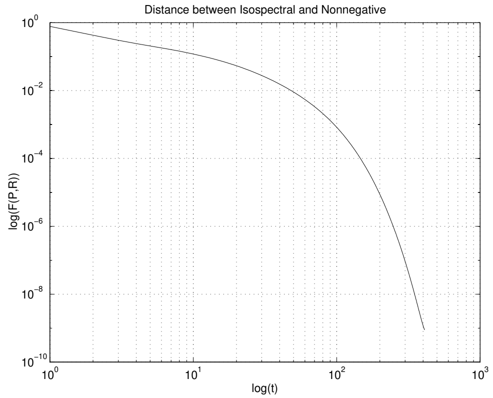


Figure 8: A log-log plot of $F(P(t), R(t))$ versus t for Example 1.

- 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:

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

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

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.

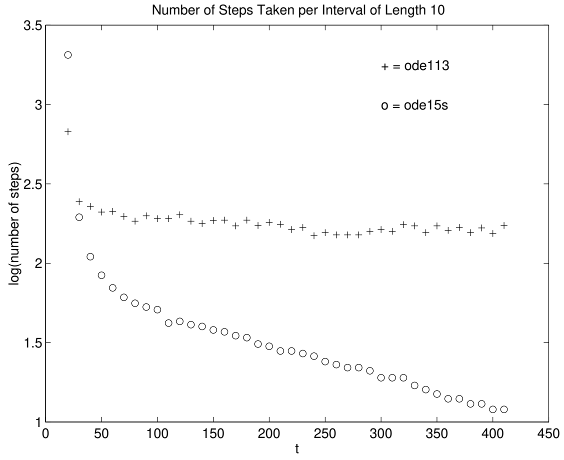


Figure 9: A comparison of steps taken by **ode113** and **ode15s** for Example 1.

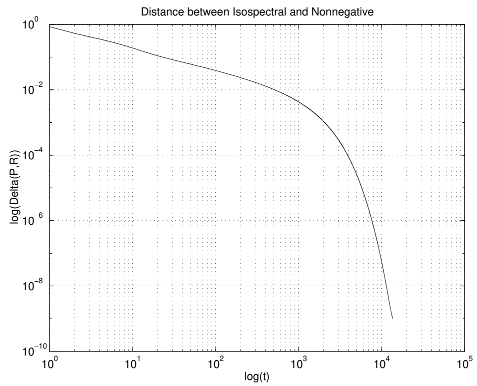


Figure 10: A log-log plot of $F(P(t), R(t))$ versus t for Example 3.

Unitary Inverse Eigenvalue Problem

- Overview
- Formulation
- Existence Theory

Overview

- Eigenvalue of unitary matrices are on the unit circle.
- Suffices to concentrate on unitary Hessenberg matrices.
- Any upper Hessenberg unitary matrix H with positive subdiagonal entries can uniquely expressed as the product
$$H = G_1(\eta_1)\dots G_{n-1}(\eta_{n-1})\tilde{G}_n(\eta_n),$$
  - ◇ $\eta_k \in \mathrm{C}$ with $|\eta_k| < 1$ for $1 \le k < n$ and $|\eta_n| = 1$.
  - ◇ Each $G_k(\eta_k)$, $k = 1, \dots, n-1$ is a Givens rotation,
$$G_k(\eta_k) = \begin{bmatrix} I_{k-1} & & & \\ & -\eta_k & \zeta_k & \\ & \zeta_k & \bar{\eta}_k & \\ & & & I_{n-k+1} \end{bmatrix}$$
with $\zeta_k := \sqrt{1 - |\eta_k|^2}$.
  - ◇ $\tilde{G}_n(\eta_n) = \mathrm{diag}[I_{n-1}, -\eta_n]$.
- Each upper Hessenbergunitary matrix is determined by $2n-1$ *real* parameters.
  - ◇ $\{\eta_k\}_{j=1}^{n}$ are called the Schur parameters.
  - ◇ $H = H(\eta_1, \dots, \eta_n)$.

Formulation

- The Schur parametrization of an upper Hesserberg unitary matrix requies $2n-1$ pieces of information.
  - ◇ The complementary parameters $\{\zeta_k\}_{k=1}^{n-1}$ are the subdiagonal elements of H and cannot be independently given.
- Upper Hessenberg unitary matrices with positive subdiagonal entries are related to orthogonal polynomials on the unit circle.
  - ◇ Jacobi matrices are related to orthogonal polynomials on an interval.
  - ◇ There should considerably similarity between unitary inverse eigenvalue problems the Jacobi inverse eigenvalue problems.
- Need a concept for modified principal submatrices of H.

Existence Theory

- Analogue of SIEP8:
  - ◇ Given
    - ▷ Two sets $\{\lambda_k^*\}_{k=1}^n$ and $\{\mu_k^*\}_{k=1}^n$ strictly interlaced on the unit circle,
  - ◇ Then there exist a unique $H = H(\eta_1, \ldots, \eta_n)$ and a unique $\alpha \in \mathbb{C}$ of unit modulus such that
    - ▷ $\sigma(H) = \{\lambda_k^*\}_{k=1}^n$.
    - ▷ $\sigma(H(\alpha\eta_1, \ldots, \alpha\eta_n)) = \{\mu_k^*\}_{k=1}^n$.
- Analogue of SIEP6a [4]:
  - ◇ Given
    - ▷ Two sets $\{\lambda_k^*\}_{k=1}^n$ and $\{\mu_k^*\}_{k=0}^{n-1}$ strictly interlaced on the unit circle,
  - ◇ Then there exist a unique $H = H(\eta_1, \ldots, \eta_n)$ such that
    - ▷ $\sigma(H) = \{\lambda_k^*\}_{k=1}^n$.
    - ▷ $\sigma(H(\eta_1, \ldots, \eta_{n-2}, \rho_{n-1})) = \{\mu_k^*\}_{k=1}^{n-1}$ with

$$\rho_{n-1} = \frac{\eta_{n-1}\bar{\mu}_0\eta_n}{1 + \bar{\mu}_0\bar{\eta}_{n-1}\eta_n}.$$

Inverse Eigenvalue Problems with Prescribed Entries

- Overview
- Prescribed Entries Along the Diagonal
- Prescribed Entries at Arbitrary Location
- Numerical Methods

Overview

- The PEIEP is a special kind of matrix completion problem [217]:
  - ◇ Given
    - ▷ A certain subset $\mathcal{K} = \{(i_t, j_t\}_{t=1}^{k}$ of pairs of subscripts,
    - ▷ A certain set of values $\{a_1, \ldots, a_k\} \subset \mathbf{F}$,
    - ▷ Another set of n values $\{\lambda_k^*\}_{k=1}^{n}$,
  - ◇ Find a matrix $X \in \mathbf{F}^{n\times n}$ such that
    - ▷ $\sigma(X) = \{\lambda_k^*\}_{k=1}^{n}$.
    - ▷ $X_{i_t,j_t} = a_t$ for $t = 1, \ldots, k$.
- Positions that do not belong to $\mathcal{K}$ are *free*, whose $n^2 - k$ entries are to be determined.
  - ◇ Jacobi structure is a special case.
  - ◇ Sometimes only need to fill $\mathcal{K}$ positions with prescribed values, but not in any specific order.
- What is the minimal/maximal count of k for the problem to make sense?

Prescribed Entries along the Diagonal

- Schur-Horn Theorem (on Hermitain matrices).
- Mirsky Theorem (on general matrices).
- Sing-Thompson Theorem (on singular values).
- de Oliveira Theorem (on general diagonals).

Schur-Horn Theorem

- Concerns with the relationship between diagonal entries and eigenvalues of a Hermitian matrix.
- The vector $a \in \mathbb{R}^n$ is said to majorize $\lambda \in \mathbb{R}^n$ if, assuming the ordering

$$\begin{aligned} a_{j_1} &\leq \ldots \leq a_{j_n}, \\ \lambda_{m_1} &\leq \ldots \leq \lambda_{m_n}, \end{aligned}$$

  the following relationships hold:

$$\begin{aligned} \sum_{i=1}^{k} \lambda_{m_i} &\leq \sum_{i=1}^{k} a_{j_i}, \quad \text{for } k = 1, \ldots n, \\ \sum_{i=1}^{n} \lambda_{m_i} &= \sum_{i=1}^{n} a_{j_i}. \end{aligned}$$

- A Hermitian matrix H with eigenvalues λ and diagonal entries a exists if and only if a *majorizes* λ.
- The proof for the sufficient part is the hard part.
  - ⋄ (SHIEP) Construct such a Hermitian matrix with given diagonals a and eigenvalues λ, if a majorizes λ [78, 379].

Mirsky Theorem

- Is there any similar connection between eigenvalues and diagonal entries of a general matrix?
- A matrix with eigenvalues $\lambda_1, \ldots, \lambda_n$ and main diagonal elements $a_1, \ldots, a_n$ exists if and only if

$$\sum_{i=1}^{n} a_i = \sum_{i=1}^{n} \lambda_i.$$

  ◇ Not an interesting inverse eigenvalue problems.

Sing-Thompson Theorem

- Concerns with the relationship singular values and diagonal entries of a general matrix.
- Given vectors $d, s \in \mathcal{R}^n$,

  ◇ Assume

$$\begin{array}{rll} s_1 & \geq s_2 & \geq \ldots s_n, \\ |d_1| & \geq |d_2| & \geq \ldots |d_n|. \end{array}$$

  ◇ A real matrix with singular values s and main diagonal entries d (possibly in different order) exists if and only if

$$\begin{aligned} \sum_{i=1}^{k} |d_i| &\leq \sum_{i=1}^{k} s_i, \quad \text{for } k = 1, \ldots, n, \\ \left(\sum_{i=1}^{n-1} |d_i|\right) - |d_n| &\leq \left(\sum_{i=1}^{n-1} s_i\right) - s_n. \end{aligned}$$

- (STISVP) Construct such a square matrix with given diagonals and singular values [71].

de Oliveira Theorem

- Corresponding to a given permutation ρ, the set $\mathcal{D} = \{(i, \rho(i))\}_1^n$ is called a ρ-diagonal.
  - ◇ Let $\rho = \rho_1 \dots \rho_s$ be the representation of ρ as the product of disjoint cycles ρ_k.
- A generalizaton of the Mirsky Theorem [105, 106, 107]:
  - ◇ Given
    - ▷ Arbitrary $\{\lambda_k^*\}_{k=1}^n \subset \mathbf{F}$,
    - ▷ Arbitrary numbers $\{a_1, \dots, a_n\} \subset \mathbf{F}$,
    - ▷ Suppose that at least one of the cycles $\rho_1, \dots, \rho_s$ has length > 2.
  - ◇ Then there exists a matrix $X \in \mathbf{F}^{n \times n}$ such that
    - ▷ $\sigma(X) = \{\lambda_k^*\}_{k=1}^n$.
    - ▷ $X_{i,\rho(i)} = a_i$ for $i = 1, \dots n$.

Prescribed Entries at Arbitrary Locations

- London-Minc Theorem [246, 105]:
  - ◇ Given
    - ▷ Arbitrary $\{\lambda_k^*\}_{k=1}^n \subset \mathbf{F}$,
    - ▷ Arbitrary values $a_1, \dots, a_{n-1}$,
    - ▷ Arbitrary but distinct positions $\{(i_t, j_t)\}_{t=1}^{n-1}$,
  - ◇ There exists a matrix $X \in \mathbf{F}^{n \times n}$ such that
    - ▷ $\sigma(X) = \{\lambda_k^*\}_{k=1}^n$.
    - ▷ $X_{i_t, j_t} = a_t$ for $t = 1, \dots, n-1$.
- Can matrices have arbitrary $n-1$ prescribed entries and prescribed characteristic polynomials? (See [116, 217].)
- Open Question: How many more entries of a matrix can be specified with prescribed eigenvalues?

Cardinality and Locations

- Specific locations:
  - ◇ Both the SHIEP and the STISVP have n prescribed entries that are located at the diagonal.
    - ▷ Certain inequalities involving the prescribed eigenvalues and diagonal entries must be satisfied.
  - ◇ The AIEP has $n^2 - n$ prescribed entries that are located at the off-diagonal.
    - ▷ The AIEP is always solvable over an algebraically closed field and there at most $n!$ solutions.
- Arbitrary locations with $|\mathcal{K}| = n$ [217]:
  - ◇ Suppose that
    - ▷ $\mathbf{F}$ is algebraically closed.
    - ▷ The Mirsky condition is satisfied, if $\mathcal{K} = \{(i,i)\}_{i=1}^n$.
    - ▷ $a_i = \lambda_j$ for some j, if $\mathcal{K} = \{(i,j_t)\}_{t=1}^n$ and $a_t = 0$ for all $j_t \neq i$.
  - ◇ Then the PEIPE is solvable via rational algorithm over $\mathbf{F}$.

- Arbitrary location with $|\mathcal{K}| = 2n - 3$ [191]:
  - ◇ Suppose that
    - ▷ $\mathbf{F}$ is algebraically closed.
    - ▷ The Mirsky condition is satisfied, if $\mathcal{K} \supseteq \{(i,i)\}_{i=1}^n$.
    - ▷ $a_i = \lambda_j$ for some j, if $\mathcal{K} \supseteq \{(i,j_t)\}_{t=1}^n$ and $a_t = 0$ for all $j_t \neq i$.
  - ◇ Then the PEIEP is solvable in $\mathbf{F}$.

Numerical Methods

- Projected gradient method can be applied [78].
- An induction proof can be implemented as a recursive algorithm, provided the computer permits a subprogram to invoke itself recursively.
  - ⋄ Fast recursive algorithms have been proposed for inverse problem associated with the SHIEP and the STISVP Theorem.
  - ⋄ Details are similar to discussion for the inverse singular/eigenvalue problem.
- Open Question: Has not seen the numerical implementation of either the de Oliveira Theorem or the London-Minc Theorem, though this could be done in finitely many steps.
- Open Question: Need an algorithm to implement the Hershkowitz results.

Inverse Singular Value Problems

- IEP versus ISVP.
- Existence Question.
- A Continuous Approach.
- An Iterative Method for IEP.
- An Iterative Approach for 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 [226].
- 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:

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

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 iso-singular-value 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 Approach for ISVP

- An analogous Newton iteration for PIEP has been discussed.
- 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: $\tilde{H}_{ij}^{(\nu)}$, $n+1 \le i \ne j \le m$,
  - ◇ $\frac{(m-n)(m-n-1)}{2}$ unknowns.
  - ◇ Locate at the lower right corner of $\tilde{H}^{(\nu)}$.
  - ◇ Are not bound to any equations at all.
  - ◇ Set

$$\tilde{H}_{ij}^{(\nu)} = 0 \text{ for } n+1 \le i \ne j \le m.$$

- 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 $1 \le i = j \le n$,

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

  - ◇ Know quantities:

$$\begin{aligned}
J_{st}^{(\nu)} &:= {u_s^{(\nu)}}^T B_t v_s^{(\nu)}, \text{ for } 1 \le s, t \le n, \\
\sigma^* &:= (\sigma_1^*, \ldots, \sigma_n^*)^T, \\
b_s^{(\nu)} &:= {u_s^{(\nu)}}^T B_0 v_s^{(\nu)}, \text{ for } 1 \le s \le n. \\
u_s^{(\nu)} &= \text{column vectors of } U^{(\nu)}, \\
v_s^{(\nu)} &= \text{column vectors of } V^{(\nu)}.
\end{aligned}$$

- 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

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

  - ◇ 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:
$$\begin{aligned} E_1^{(\nu+1)} &:= U^{(\nu+1)} - \hat{U} = R^T U^{(\nu)} - e^{-H_*^{(\nu)}} U^{(\nu)} \\ &= \left[(I - \frac{H^{(\nu)}}{2}) - (I - H_*^{(\nu)} + O(||H_*^{(\nu)}||^2) \right. \\ & \qquad \left. (I + \frac{H^{(\nu)}}{2}) \right] (I + \frac{H^{(\nu)}}{2})^{-1} U^{(\nu)} \\ &= \left[H_*^{(\nu)} - H^{(\nu)} + O(||H_*^{(\nu)} H^{(\nu)}|| \right. \\ & \qquad \left. + ||H^{(\nu)}||^2) \right] (I + \frac{H^{(\nu)}}{2})^{-1} U^{(\nu)}. \end{aligned}$$
  - ⋄ 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 $1 \leq i < j \leq p$, 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 $1 \leq i < j \leq p$.
  - ◇ $\tilde{K}^{(\nu)}$ is defined by

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

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

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

- 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 behavior of 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.

Inverse Singualar/Eigenvalue Problem

- Overview
- A Recursive Algorithm
- The Matrix Structure
- Numerical Experiment

Overview

- The Schur-Horn Theorem gives the connection between diagonal entries and eigenvalues of a Hermitian matrix.
- The Mirsky Theorem gives a connection between diagonal entries and eigenvalues of a general matrix.
- The Sing-Thompson Theorem gives the connection between diagonal entries and singular values of a general matrix.
- What is the connection between singular values and eigenvalues of a matrix?
  - ⋄ singular value = $|$eigenvalue$|$, if Hermitian matrices.
  - ⋄ How about general matrices?
- Can we create matrices with prescribed singular values and eigenvalues?
  - ⋄ Desirable for test matrices.

Weyl-Horn Theorem

- Given vectors $\lambda \in C^n$ and $\alpha \in \mathbb{R}^n$,
  - ◇ Assume

$$\begin{aligned} |\lambda_1| &\geq \ldots \geq |\lambda_n|, \\ \alpha_1 &\geq \ldots \geq \alpha_n. \end{aligned}$$

  - ◇ Then a matrix with eigenvalues $\lambda_1, \ldots, \lambda_n$ and singular values $\alpha_1, \ldots, \alpha_n$ exists if and only if

$$\begin{aligned} \prod_{j=1}^{k} |\lambda_j| &\leq \prod_{j=1}^{k} \alpha_j, \quad k = 1, \ldots, n-1, \\ \prod_{j=1}^{n} |\lambda_j| &= \prod_{j=1}^{n} \alpha_j. \end{aligned}$$

    - ▷ If $|\lambda_n| > 0$, then $\log \alpha$ majorizes $\log |\lambda|$.
- How to solve the inverse singular eigenvalue problem numerically?

A Recursive Algorithm

- The Building Block — 2×2 Case
- The Original Proof by Induction
- An Innocent Mistake
- A Recursive Clause in Programming

The 2×2 Case

- The Weyl-Horn Condition:

$$\begin{cases} |\lambda_1| \leq \alpha_1, \\ |\lambda_1||\lambda_2| = \alpha_1\alpha_2. \end{cases}$$
$$\Downarrow$$
$$\begin{cases} \alpha_2 \leq |\lambda_2| \leq |\lambda_1| \leq \alpha_1 \\ |\lambda_1|^2 + |\lambda_2|^2 \leq \alpha_1^2 + \alpha_2^2. \end{cases}$$

- The building block — A triangular matrix

$$A = \begin{bmatrix} \lambda_1 & \mu \\ 0 & \lambda_2 \end{bmatrix}$$

has singular value $\{\alpha_1, \alpha_2\}$ if and only if

$$\mu = \sqrt{\alpha_1^2 + \alpha_2^2 - |\lambda_1|^2 - |\lambda_2|^2}.$$

  ◇ A is complex-valued when eigenvalues are complex.

  ◇ A stable way of computing μ:

$$\mu = \begin{cases} 0, & \text{if } |(\alpha_1-\alpha_2)^2-(|\lambda_1|-|\lambda_2|)^2| \leq \epsilon \\ \sqrt{|(\alpha_1-\alpha_2)^2-(|\lambda_1|-|\lambda_2|)^2|}, & \text{otherwise.} \end{cases}$$

Ideas in Horn's Proof

- Reduce the original inverse problem to two problems of *smaller sizes.*
- Problems of smaller sizes are guaranteed to be solvable by the *induction hypothesis.*
- The subproblems are *affixed* together by working on a suitable 2×2 *corner.*
- The 2×2 problem has an explicit solution.

Key to the Algorithmic Success

- The eigenvalues and singular values of each of the two subproblems can be derived *explicitly.*
- Each of the two subproblems can further be down-sized.
- The original problem is *divided* into subproblems of size 2×2 or 1×1.
- The smaller problems can be *conquered* to build up the original size.
- In an environment that allows a subprogram to invoke itself recursively, only one-step of the divide-and-conquer procedure will be enough.
- Very similar to the radix-2 FFT $\Longrightarrow$ fast algorithm.

Outline of Proof

- Suppose $\alpha_i > 0$ for all $i = 1, \ldots, n$. So $\lambda_i \neq 0$ for all i.
  - ◇ The case of zero singular values can be handled in a similar way.
- Define
$$\begin{cases} \sigma_1 &:= \alpha_1, \\ \sigma_i &:= \sigma_{i-1}\frac{\alpha_i}{|\lambda_i|}, \quad \text{for } i = 2, \ldots, n-1. \end{cases}$$
  - ◇ Assume $\sigma := \min_{1 \leq i \leq n-1} \sigma_i$ occurs at the index j.
- Define
$$\rho := \frac{|\lambda_1 \lambda_n|}{\sigma}.$$
- The following three sets of inequalities are true. The numbers satisfy the Weyl-Horn conditions.
$$\begin{cases} |\lambda_1| &\geq |\lambda_n|, \\ \sigma &\geq \rho. \end{cases}$$
$$\begin{cases} \sigma &\geq |\lambda_2| \geq \ldots \geq |\lambda_j|, \\ \alpha_1 &\geq \alpha_2 \geq \ldots \geq \alpha_j. \end{cases}$$
$$\begin{cases} |\lambda_{j+1}| \geq \ldots \geq |\lambda_{n-1}| &\geq \rho, \\ \alpha_{j+1} \geq \ldots \geq \alpha_{n-1} &\geq \alpha_n. \end{cases}$$

- By induction hypothesis,
  - ◇ There exist unitary matrices U_1, $V_1 \in C^{j\times j}$ and *triangular* matrices A_1 such that

$$U_1 \begin{bmatrix} \alpha_1 & 0 & \dots & 0 \\ 0 & \alpha_2 & & 0 \\ \vdots & \ddots & & \\ 0 & 0 & \dots & \alpha_j \end{bmatrix} V_1^* = A_1 = \begin{bmatrix} \sigma & \times & \times & \dots & \times \\ 0 & \lambda_2 & & & \times \\ & & & & \\ \vdots & & & \ddots & \\ 0 & 0 & & & \lambda_j \end{bmatrix}.$$

  - ◇ There exist unitary matrices U_2, $V_2 \in C^{(n-j)\times(n-j)}$, and *triangular* matrix A_2 such that

$$U_2 \begin{bmatrix} \alpha_{j+1} & 0 & \dots 0 \\ 0 & \alpha_{j+2} & 0 \\ \vdots & & \ddots \\ 0 & 0 & \dots \alpha_n \end{bmatrix} V_2^* = A_2 = \begin{bmatrix} \lambda_{j+1} & \times & \dots & \times & \times \\ 0 & \lambda_{j+2} & & & \times \\ \vdots & & \ddots & & \vdots \\ & & & \lambda_{n-1} & \times \\ 0 & 0 & \dots & 0 & \rho \end{bmatrix}.$$

- Horn's claim: The block matrix

$$\begin{bmatrix} A_1 & \bigcirc \\ \bigcirc & A_2 \end{bmatrix}$$

can be *permuted* to the triangular matrix

$$\begin{bmatrix} \lambda_2 & \times & \dots & \times & \times & & & & & \\ 0 & & & & \times & & & & & \\ \vdots & & \ddots & & \vdots & & & \bigcirc & & \\ & & & \lambda_j & \times & & & & & \\ 0 & & \dots & 0 & \sigma & 0 & & & & \\ 0 & 0 & \dots & 0 & 0 & \rho & \times & \times & \dots & \times \\ & & & & & & \lambda_{j+1} & & & \times \\ & \bigcirc & & & & & & & & \\ & & & & & \vdots & & & \ddots & \\ & & \dots & & & 0 & 0 & & & \lambda_{n-1} \end{bmatrix}$$

- The 2×2 corner can now be glued together by

$$U_0 \begin{bmatrix} \sigma & 0 \\ 0 & \rho \end{bmatrix} V_0^* = A_0 = \begin{bmatrix} \lambda_1 & \mu \\ 0 & \lambda_n \end{bmatrix}.$$

- How to do the permutation, or is it a mistake?
  - ◇ It takes more than permutation to rearrange the diagonals of a triangular matrix.

A MATLAB Program

```
function [A]=svd_eig(alpha,lambda);
n = length(alpha);
if n == 1                                  % The 1 by 1 case
   A = [lambda(1)];
elseif n == 2                              % The 2 by 2 case
   [U,V,A] = two_by_two(alpha,lambda);
else                                       % Check zero singular values
   tol = n*alpha(1)*eps;
   k = sum(alpha > tol); m = sum(abs(lambda) > tol);
   if k == n                               % Nonzero singular values
      j = 1; s = alpha(1); temp = s;
      for i = 2:n-1
         temp = temp*alpha(i)/abs(lambda(i));
         if temp < s, j = i; s = temp; end
      end
      rho = abs(lambda(1)*lambda(n))/s;
      [U0,V0,A0] = two_by_two([s;rho],[lambda(1);lambda(n)]);
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
      [A1] = svd_eig(alpha(1:j),[s;lambda(2:j)]);          % RECURSIVE %
      [A2] = svd_eig(alpha(j+1:n),[lambda(j+1:n-1);rho]); %  CALLING  %
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
      A = [A1,zeros(j,n-j);zeros(n-j,j),A2];
      Temp = A;
         A(1,:)=U0(1,1)*Temp(1,:)+U0(1,2)*Temp(n,:);
         A(n,:)=U0(2,1)*Temp(1,:)+U0(2,2)*Temp(n,:);
      Temp = A;
         A(:,1)=V0(1,1)*Temp(:,1)+V0(1,2)*Temp(:,n);
         A(:,n)=V0(2,1)*Temp(:,1)+V0(2,2)*Temp(:,n);
   else                                    % Zero singular values
      beta = prod(abs(lambda(1:m)))/prod(alpha(1:m-1));
      [U3,V3,A3] = svd_eig([alpha(1:m-1);beta],lambda(1:m));
      A = zeros(n); A(1:m,1:m) = V3'*A3*V3;
      for i = m+1:k, A(i,i+1) = alpha(i); end
      A(m,m+1) = sqrt(abs(alpha(m)^2-beta^2));
   end
end
```


Matrix Structure

- A Modified Proof
- A Symbolic Example

Correct the "Mistake"

- Horn's requirement:
  - ◇ Both intermediate matrices A_1 and A_2 are upper triangular matrices.
  - ◇ Diagonal entries are arranged in a certain order.
    - ▷ Valid from the Schur decomposition theorem.
    - ▷ More than permutation, not easy for computation.
    - ▷ To rearrange diagonal entries via unitary similarity transformations while maintaining the upper triangular structure is expensive.
- Our contribution:
  - ◇ The triangular structure is entirely unnecessary.
  - ◇ The matrix A produced from our algorithm is generally not triangular.
  - ◇ Do not need to rearrange the diagonal entries
  - ◇ Modify the first and the last rows and columns of the block diagonal matrix $\begin{bmatrix} A_1 & \bigcirc \\ \bigcirc & A_2 \end{bmatrix}$, *as if nothing happened*, is enough.

- Algorithm:
  - ◇ Denote $U_0 = [u_{0,st}]$ and $V_0 = [v_{0,st}]$.
  - ◇ Then

$$\begin{bmatrix} u_{0,11} & 0 & u_{0,12} \\ 0 & I_{n-1} & 0 \\ u_{0,21} & 0 & u_{0,22} \end{bmatrix} \begin{bmatrix} U_1 & 0 \\ 0 & U_2 \end{bmatrix} \begin{bmatrix} \alpha_1 & 0 & \dots & 0 \\ 0 & \alpha_2 & & 0 \\ \vdots & & \ddots & \\ 0 & & & \alpha_n \end{bmatrix} \begin{bmatrix} V_1^* & 0 \\ 0 & V_2^* \end{bmatrix} \begin{bmatrix} v_{0,11} & 0 & v_{0,12} \\ 0 & I_{n-1} & 0 \\ v_{0,21} & 0 & v_{0,22} \end{bmatrix}^*$$

    is the desired matrix.
- A has the structure

$$A = \begin{bmatrix} \lambda_1 & \otimes & \dots & \otimes & \otimes & * & * & & & \mu \\ \otimes & \lambda_2 & & & \times & 0 & 0 & & & * \\ \vdots & & \ddots & & \vdots & & & \bigcirc & & \\ & & & \lambda_{j-1} & \times & & & & & \\ \otimes & \times & \dots & \times & \lambda_j & & & & & * \\ * & 0 & \dots & 0 & 0 & \lambda_{j+1} & \times & \times & \dots & \otimes \\ * & & & & 0 & \times & \lambda_{j+2} & & & \otimes \\ & & \bigcirc & & & & & & & \\ & & & & & \vdots & & & \ddots & \\ 0 & * & \dots & * & * & \otimes & \otimes & & & \lambda_n \end{bmatrix}.$$

  - ◇ $\times$ = unchanged, original entries from A_1 or A_2.
  - ◇ $\otimes$ = entries of A_1 or A_2 that are modified by scalar multiplications.
  - ◇ $*$ = possible new entries that were originally zero.

A Variation of Horn's Proof

- Does the algorithm really works?
  - ◇ Clearly, A has singular values $\{\alpha_1, \ldots, \alpha_n\}$.
  - ◇ Need to show that A has eigenvalues $\{\lambda_1, \ldots, \lambda_n\}$.
- What has been changed?

(P1) Diagonal entries of A_1 and A_2 are in fixed orders, $\sigma, \lambda_2, \ldots, \lambda_j$ and $\lambda_{j+1}, \ldots, \lambda_{n-1}, \rho$, respectively.

(P2) Each A_i is similar through permutations, which need not to be known, to a lower triangular matrix whose diagonal entries constitute the same set as the diagonal entries of A_i. (Thus, each A_i has precisely its own diagonal entries as its eigenvalues.)

(P3) The first row and the last row have the same zero pattern except that the lower-left corner is always zero.

(P4) The first column and the last column have the same zero pattern except that the lower-left corner is always zero.

- Use graph theory to show that the affixed matrix A has exactly the same properties.

A Symbolic Example

- Dividing process:

$$\boxed{\left\{\begin{array}{cccccc}\lambda_1 & \lambda_2 & \lambda_3 & \lambda_4 & \lambda_5 & \lambda_6\\ \alpha_1 & \alpha_2 & \alpha_3 & \alpha_4 & \alpha_5 & \alpha_6\end{array}\right.}$$

$$j_1 = 5 \quad \Downarrow \quad \left\{\begin{array}{cc}\lambda_1 & \lambda_6\\ \sigma_1 & \rho_1\end{array}\right.$$

$$\boxed{\left\{\begin{array}{ccccc}\sigma_1 & \lambda_2 & \lambda_3 & \lambda_4 & \lambda_5\\ \alpha_1 & \alpha_2 & \alpha_3 & \alpha_4 & \alpha_5\end{array}\right.} \; \boxed{\left\{\begin{array}{c}\rho_1\\ \alpha_6\end{array}\right.}$$

$$j_2 = 2 \quad \Downarrow \quad \left\{\begin{array}{cc}\sigma_1 & \lambda_5\\ \sigma_2 & \rho_2\end{array}\right.$$

$$\boxed{\left\{\begin{array}{cc}\sigma_2 & \lambda_2\\ \alpha_1 & \alpha_2\end{array}\right.} \; \boxed{\left\{\begin{array}{ccc}\lambda_3 & \lambda_4 & \rho_2\\ \alpha_3 & \alpha_4 & \alpha_5\end{array}\right.} \; \boxed{}$$

$$j_3 = 1 \quad \Downarrow \quad \left\{\begin{array}{cc}\lambda_3 & \rho_2\\ \sigma_3 & \rho_3\end{array}\right.$$

$$\boxed{} \; \boxed{\left\{\begin{array}{c}\sigma_3\\ \alpha_3\end{array}\right.} \; \boxed{\left\{\begin{array}{cc}\lambda_4 & \rho_3\\ \alpha_4 & \alpha_5\end{array}\right.} \; \boxed{}$$

- Conquering process:

$$\boxed{\begin{bmatrix} \lambda_1 & \otimes & 0 & 0 & \otimes & * \\ 0 & \lambda_2 & 0 & 0 & 0 & 0 \\ \otimes & 0 & \lambda_3 & 0 & \times & * \\ \otimes & 0 & \times & \lambda_4 & \times & * \\ 0 & \times & 0 & 0 & \lambda_5 & 0 \\ 0 & * & 0 & 0 & * & \lambda_6 \end{bmatrix}}$$

$$j_1 = 5 \quad \Uparrow \quad \begin{bmatrix} \sigma_1 & \times & 0 & 0 & \times & 0 \\ 0 & \lambda_2 & 0 & 0 & 0 & 0 \\ \times & 0 & \lambda_3 & 0 & \times & 0 \\ \times & 0 & \times & \lambda_4 & \times & 0 \\ 0 & \times & 0 & 0 & \lambda_5 & 0 \\ 0 & 0 & 0 & 0 & 0 & \rho_1 \end{bmatrix}$$

$$\boxed{\begin{bmatrix} \sigma_1 & \otimes & 0 & 0 & * \\ 0 & \lambda_2 & 0 & 0 & 0 \\ * & 0 & \lambda_3 & 0 & \otimes \\ * & 0 & \times & \lambda_4 & \otimes \\ 0 & * & 0 & 0 & \lambda_5 \end{bmatrix}} \quad \boxed{\begin{bmatrix} \rho_1 \end{bmatrix}}$$

$$j_2 = 2 \quad \Uparrow \quad \begin{bmatrix} \sigma_2 & \times & 0 & 0 & 0 \\ 0 & \lambda_2 & 0 & 0 & 0 \\ 0 & 0 & \lambda_3 & 0 & \times \\ 0 & 0 & \times & \lambda_4 & \times \\ 0 & 0 & 0 & 0 & \rho_2 \end{bmatrix}$$

$$\boxed{\begin{bmatrix} \sigma_2 & * \\ 0 & \lambda_2 \end{bmatrix}} \quad \boxed{\begin{bmatrix} \lambda_3 & 0 & * \\ * & \lambda_4 & \otimes \\ 0 & 0 & \rho_2 \end{bmatrix}} \quad \boxed{}$$

$$j_3 = 1 \quad \Uparrow \quad \begin{bmatrix} \sigma_3 & 0 & 0 \\ 0 & \lambda_4 & \times \\ 0 & 0 & \rho_3 \end{bmatrix}$$

$$\boxed{} \quad \boxed{\begin{bmatrix} \sigma_3 \end{bmatrix}} \quad \boxed{\begin{bmatrix} \lambda_4 & * \\ 0 & \rho_3 \end{bmatrix}} \quad \boxed{}$$

Numerical Experiment

- The divide-and-conquer feature brings on fast computation.
- The overall cost is estimated at the order of $O(n^2)$.
- A numerical simulation:

Rosser Test

- Rosser matrix R:

$$R = \begin{bmatrix} 611 & 196 & -192 & 407 & -8 & -52 & -49 & 29 \\ 196 & 899 & 113 & -192 & -71 & -43 & -8 & -44 \\ -192 & 113 & 899 & 196 & 61 & 49 & 8 & 52 \\ 407 & -192 & 196 & 611 & 8 & 44 & 59 & -23 \\ -8 & -71 & 61 & 8 & 411 & -599 & 208 & 208 \\ -52 & -43 & 49 & 44 & -599 & 411 & 208 & 208 \\ -49 & -8 & 8 & 59 & 208 & 208 & 99 & -911 \\ 29 & -44 & 52 & -23 & 208 & 208 & -911 & 99 \end{bmatrix}.$$

  ◇ Has one double eigenvalue, three nearly equal eigenvalues, one zero eigenvalue, two dominant eigenvalues of opposite sign and one small nonzero eigenvalue.

  ◇ The *computed* eigenvalues and singular values of R are

$$\lambda = \begin{bmatrix} -1.020049018429997e{+}03 \\ 1.020049018429997e{+}03 \\ 1.020000000000000e{+}03 \\ 1.019901951359278e{+}03 \\ 1.000000000000001e{+}03 \\ 9.999999999999998e{+}02 \\ 9.804864072152601e{-}02 \\ 4.851119506099622e{-}13 \end{bmatrix}, \alpha = \begin{bmatrix} 1.020049018429997e{+}03 \\ 1.020049018429996e{+}03 \\ 1.020000000000000e{+}03 \\ 1.019901951359279e{+}03 \\ 1.000000000000000e{+}03 \\ 9.999999999999998e{+}02 \\ 9.804864072162672e{-}02 \\ 1.054603342667098e{-}14 \end{bmatrix}.$$

- Using the above λ and α,

  ◇ A nonsymmetric matrix is produced:

$$\begin{bmatrix} 1.0200e{+}03 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1.0200e{+}03 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1.0200e{+}03 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1.0199e{+}03 & 0 & 0 & 1.4668e{-}09 & 0 \\ 0 & 0 & 0 & 0 & 1.0000e{+}03 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1.0000e{+}03 & 0 & 0 \\ 0 & 0 & 0 & -1.5257e{-}05 & 0 & 0 & 9.8049e{-}02 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1.4045e{-}07 & 0 \end{bmatrix}.$$

  ◇ The re-computed eigenvalues and singular values of A are

$$\hat{\lambda} = \begin{bmatrix} -1.020049018429997e{+}03 \\ 1.020049018429997e{+}03 \\ 1.020000000000000e{+}03 \\ 1.019901951359278e{+}03 \\ 1.000000000000001e{+}03 \\ 9.999999999999998e{+}02 \\ 9.80486407215721e{-}02 \\ 0 \end{bmatrix}, \hat{\alpha} = \begin{bmatrix} 1.020049018429997e{+}03 \\ 1.020049018429997e{+}03 \\ 1.020000000000000e{+}03 \\ 1.019901951359279e{+}03 \\ 1.000000000000001e{+}03 \\ 9.999999999999998e{+}02 \\ 9.804864072162672e{-}02 \\ 0 \end{bmatrix}.$$

  ◇ The re-computed eigenvalues and singular values agree with those of R up to the machine accuracy.

Wilkinson Test

- Wilkinson's matrices:
  - ◇ All are symmetric and tridiagonal.
  - ◇ Have nearly, but not exactly, equal eigenvalue pairs.
- Using these data:
  - ◇ Discrepancy in eigenvalues and singular values between our constructed matrices and Wilkinson's matrices.
  - ◇ Matrices constructed are nearly but not symmetric.

Conclusion

- Weyl-Horn Theorem completely characterizes the relationship between eigenvalues and singular values of a general matrix.
- The original proof has been modified.
- With the aid of programming languages that allow a subprogram to invoke itself recursively, an induction proof can be implemented as a recursive algorithm.
- The resulting algorithm is fast. The cost of construction is approximately $O(n^2)$.
- The matrix being constructed usually is not symmetric and is complex-valued, if complex eigenvalues are present.
- Numerical experiment on some very challenging problems suggests that our method is quite robust.

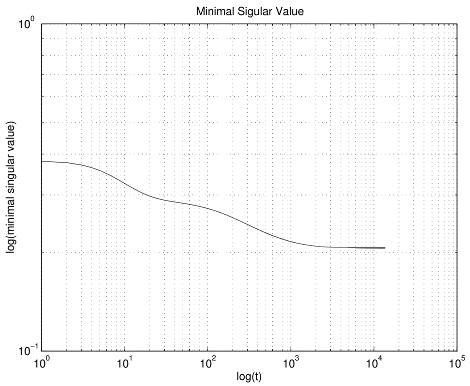


Figure 11: History of the smallest singular value for Example 3.

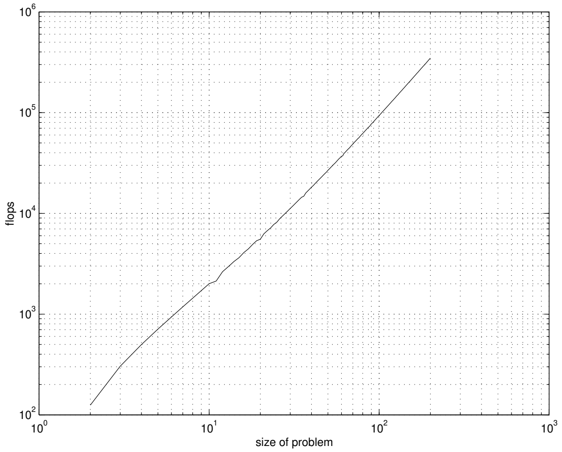


Figure 12: log-log plot of computational flops versus problem sizes

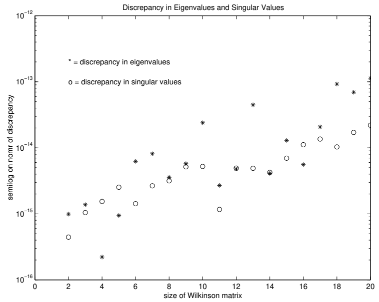


Figure 13: L_2 norm of discrepancy in eigenvalues and singular values.

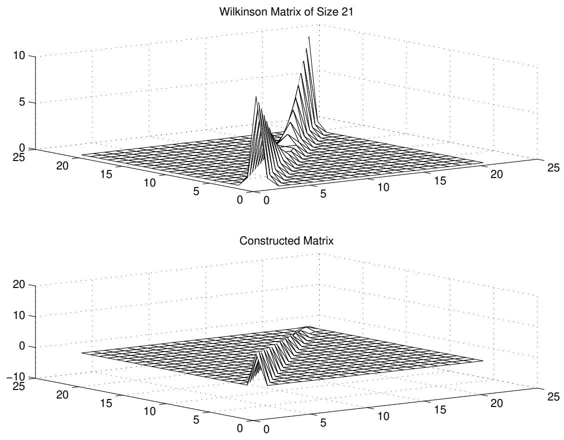


Figure 14: 3-D mesh representation of 21×21 matrices

Chapter 5

Least Squares Inverse Eigenvalue Problems

Overview

- The information of spectral constraint and the structrual constraint may not be obtained precisely in practice.
- It may occur in practice that one of the two constraints should be enforced more critically than the other.
  - ◇ Without the physical realizability, the physical system simply cannot be built. So structrual constraint is emphasized.
- It may occur that one constraint could be more relaxed than the other.
  - ◇ For complex system there is no accurate way to measure the spectrum or to obtain the entire information. Physical uncertainty can be tolerated up to a certain degree.
- When the two constraints cannot be settled simultaneously, the IEP could be formulated in a least squares setting.

Formulation

- All IEP's discussed so far have a natural generalization to least squares formulation.
- Depends upon which constraint is to be enforced, there are two ways to formulate the least squares IEP.

Least Squares Approximating the Spectrum

- Given:
  - ◇ Symmetric matrices $A(d) \in \mathbb{R}^{n\times n}$,
  - ◇ Real numbers $\lambda_1^*, \cdots, \lambda_m^*$,
  - ◇ $m \le n$,
- Solve:

$$\min_{d\in\mathbb{R}^l,\sigma} F(d,\sigma) = \sum_{i=1}^{m}(\lambda_{\sigma_i}(d) - \lambda_i^*)^2,$$

$$= \|\Lambda_\sigma(d) - \Lambda_m^*\|_F^2.$$

  - ◇ $\sigma :=$ a permutation;
  - ◇ $\Lambda_m^* := \mathrm{diag}(\lambda_1^*, ..., \lambda_m^*)$.

Least Squares Approximating the Structure

- Let
  - $\Lambda_m^* := \mathrm{diag}(\lambda_1^*, ..., \lambda_m^*)$.
  - $D_{n-m} := \{\text{diag matrices}\} \subseteq \mathbb{R}^{(n-m)\times(n-m)}$.
  - $\mathcal{O}(n) := \{\text{orthogonal matrices}\} \subseteq \mathbb{R}^{n\times n}$
- Define:

$$\Gamma := \left\{ Q \begin{bmatrix} \Lambda_m^* & 0 \\ 0 & \Lambda_{n-m} \end{bmatrix} Q^T \mid Q \in \mathcal{O}(n), \Lambda_{n-m} \in D_{n-m} \right\}.$$

- Given:
  - Symmetric matrices $A(d) \in \mathbb{R}^{n\times n}$,
  - Real numbers $\lambda_1^*, \cdots, \lambda_m^*$,
  - $m \leq n$,
- Solve:

$$\mathrm{dist}(\mathcal{A}(d), \Gamma) = \min_{d\in\mathbb{R}^l, B\in\Gamma} \|A(d) - B\|_F^2.$$

Main Theorem

- At a global minimizer, LSIEP1 and LSIEP2 are equivalent.
  - Both problems have the same objective values.

$$\min_{d,\sigma} \|\Lambda_\sigma(d) - \Lambda_m^*\|_F^2 = \min_{d,B} \|A(d) - B\|_F^2.$$

  - If d_1, σ solve **LSIEP1** and d_2, B solve **LSIEP2**, then
    - ▷ $d_1 = d_2$,
    - ▷ $B = Q(d_1) \begin{bmatrix} \Lambda_m^* & 0 \\ 0 & \Lambda_{\overline{\sigma}}(d_1) \end{bmatrix} Q(d_1)^T$.
      - · $Q(d_1)^T A(d_1) Q(d_1) = \begin{bmatrix} \Lambda_\sigma(d_1) & 0 \\ 0 & \Lambda_{\overline{\sigma}}(d_1) \end{bmatrix}$.
      - · $\mathrm{diag}[\Lambda_\sigma(d_1), \Lambda_{\overline{\sigma}}(d_1)]$ has same ordering as $\mathrm{diag}[\Lambda_m^*, \Lambda_{\overline{\sigma}}(d_1$
      - · $\overline{\sigma} := \{1, ..., n\} - \sigma$.
  - If so

$$\min_{d,B} \|A(d) - B\|_F^2 = \sum_{i=0}^{m} |\lambda_{\sigma_i} - \lambda_i^*|^2.$$

One Particular Case

- Consider the special case where

$$A(d) := A_0 + \sum_{i=1}^{l} d_i A_i \in \mathcal{A}(d) \text{ (affine subspace)}$$

- Lift & Project:
  1. Find
  $$Z^{(k)} := \arg\min_{B\in\Gamma} \|A(d^{(k)}) - B\|_F \quad \textbf{(Lift)}$$
  by the Wielandt-Hoffman Theorem!
  2. Find
  $$d^{(k+1)} := \arg\min_{d\in\mathbb{R}^l} \|Z^{(k)} - \mathcal{A}(d)\|_F \quad \textbf{(Project)}$$
  by solving a linear system.
- The topology of Γ is not clear. But *Step 1* can be accomplished by considering a "substructure".

$$\mathcal{M}_k := \left\{ Q \begin{bmatrix} \Lambda_m^* & 0 \\ 0 & \Lambda_{\overline{\sigma}}(d^{(k)}) \end{bmatrix} Q^T \mid Q \in \mathcal{O}(n) \right\}$$

which is known.

Geometric Sketch

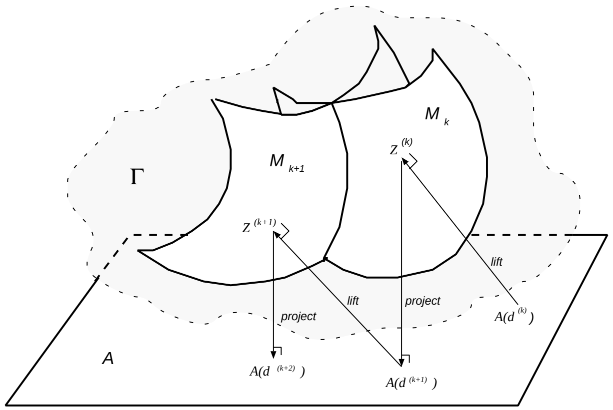


Figure 1: Geometry of life and projection.

- This a descent method!

$$\|Z^{(k+1)} - A(d^{(k+1)})\|_F \le \|Z^{(k)} - A(d^{(k+1)})\|_F$$
$$\le \|Z^{(k)} - A(d^{(k)})\|_F$$

Algorithm

- Given $d^{(0)}$.
- For k = 0,1,2,...
  1. Compute $Q(d^{(k)})$ and $\Lambda(d^{(k)})$.
  2. Find $\sigma = \{\sigma_1, ..., \sigma_m\}$. Form $\Lambda_{\overline{\sigma}}$
  3. (**lift**) Form
  $$Z^{(k)} = Q(d^{(k)})diag(\Lambda^*, \Lambda_{\overline{\sigma}}(d^{(k)}))Q(d^{(k)})^T.$$
  4. (**Project**) Compute $d^{(k+1)}$ from
  $$\sum_{i=1}^{l} < A_i, A_j > d_i^{(k+1)} =< Z^{(k)} - A_0, A_j > .$$
  5. stop if $\|d^{(k+1)} - d^{(k)}\| < \varepsilon$

Chapter 6

Partially Described Inverse Eigenvalue Problems

- Overview
- Generic Form
- PDIEP for Toeplitz Matrices

Overview

- The physical system is too complicated or the size is too large,
  - ◇ No reasonable analytical tools are available to evaluate the entire spectral information.
  - ◇ Through vibration tests where the excitation and the response of the structure at selected points are measured experimentally, there are identification techniques to extract a portion of eigenpair information from the measurements.
- It is unwise to use experimental values of high natural frequencies to reconstruct a model because a discrete model with n degrees of freedom can provide accurate values for only about $\frac{n}{3}$ natural frequencies.
- Eigenpair information sometimes provides additional intrinsic relationships. A few eigenpairs can determine much of the desirable reconstruction.

Generic Form

- Given
  - ◇ Vectors $\{\mathbf{v}^{(1)}, \ldots, \mathbf{v}^{(k)}\} \subset \mathbb{F}^n$,
  - ◇ Values $\{\lambda_1, \ldots \lambda_k\} \subset \mathbb{F}$,
  - ◇ A set $\mathcal{N}$ of structured matrices,

  Find $X \in \mathcal{N}$ such that

$$X\mathbf{v}^{(i)} = \lambda_i \mathbf{v}^{(i)}, \quad , i = 1, \ldots, k.$$

- Given
  - ◇ Two sets of real vectors $\{x_1, \ldots, x_p\}$ and $\{y_1, \ldots y_p\}$, $p \leq n$,
  - ◇ An arbitrary set of complex numbers $\mathcal{L} = \{\lambda_1, \ldots, \lambda_n\}$,

  Find a real matrix A such that

$$\begin{aligned} Ax_i &= y_i, \\ \sigma(A) &= \mathcal{L} \end{aligned}$$

- Open Question: How many pairs of information are needed to determine such a structured matrix?

PDIEP for Toeplitz Matrices

- Eigenvectors of a Toeplitz matrix have a special structure [8, 55, 113]:
  - ◇ Eigenvectors of any symmetric and centro-symmetric matrix must be either symmetric or skew-symmetric.
- The dimension of Toeplitz matrices with a single prescribed eigenvector in $\mathbb{R}^n$ should be at least $[\frac{n+1}{2}]$ [85].
- The dimension of Toeplitz matrices with two prescribed eigenvectors is independent of n [75].
- Define

$$\begin{aligned} S(\mathbf{v}) &:= \{\mathbf{c} \in \mathbb{R}^n | T(\mathbf{c})\mathbf{v} = \lambda\mathbf{v} \text{ for some } \lambda \in \mathbb{R}\}, \\ \pi(\mathbf{u}, \mathbf{v}) &:= \dim(S(\mathbf{u}) \bigcap S(\mathbf{v})) \end{aligned}$$

- Let η denote the dimension of the affine subspace of symmetric Toeplitz matrices with two prescribed eigenpairs. Then for almost all eigenvectors $\mathbf{u}$ and $\mathbf{v}$, and for any eigenvalues λ_1 and λ_2, the pair $\pi(\mathbf{u}, \mathbf{v})/\eta$ is summarized in the following table.

n = odd (even)	symmetric	skew-symmetric
symmetric	2/0 (3/1)	2/0 (2/0)
skew-symmetric	2/0 (2/0)	4/0 (3/1)

  - ◇ The symmetric Toeplitz matrix is uniquely determined, if
    - ▷ n is odd and if at least one of the given eigenvectors is symmetric, or
    - ▷ n is even and one eigenvector is symmetric and the other is skew-symmetric.

Chapter 7

Spectrally Constrained Approximation

- Overview
- Reformulation
- Least Squares Approximation
- Toeplitz Inverse Eigenvalue Problem
- Eigenvalue Computation
- Simultaneous Reduction
- Nearest Normal Matrix Approximation

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 approximating general matrices subject to singular value constraints.
- Notation:

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

$$\begin{aligned}
\Sigma &:= \text{ A given general matrix in } R^{m\times n}\\
W(\Sigma) &:= \{Q_1\Sigma Q_2 | Q_1 \in \mathcal{O}(m), Q_2 \in \mathcal{O}(n)\}\\
\mathcal{U} &:= \text{ A single matrix or a subspace in } \mathbb{R}^{m\times n}
\end{aligned}$$

Spectrally Constrained Problem

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

- Special cases:
  - ◇ Problem A: Given a symmetric matrix, find its least squares approximation with prescribed spectrum.
  - ◇ Problem B: Construct a symmetric Toeplitz matrix that has a prescribed set of eigenvalues.
  - ◇ Problem C: Find the spectrum of a given a symmetric matrix.

Singular-Value Constrained Problem

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

- Special cases:
  - ◇ Problem D: Given a general real $m \times n$ matrix, find its least square approximation that has a prescribed set of singular values.
  - ◇ Problem E: Construct a general real $m \times n$ matrix, find its singular values.

Reformulation

- Idea:
  1. $X \in M(\Lambda)$ satisfies the spectral constraint.
  2. $P(X) \in V$ has the desirable structure in V.
  3. Minimize the undesirable part $\|X - P(X)\|$.
- Working with the parameter Q is easier:

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

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

Feasible Set $O(n)$ & Gradient of F

- The set $O(n)$ is a regular surface.
- The tangent space of $O(n)$ at any orthogonal matrix Q is given by

$$T_Q O(n) = QK(n)$$

  where

$$K(n) = \{\text{All skew-symmetric matrices}\}.$$

- The normal space of $O(n)$ at any orthogonal matrix Q is given by

$$N_Q O(n) = QS(n).$$

- 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 $R^{n\times n}$:

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

- A unique orthogonal splitting of $X \in R^{n\times n}$:

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

- The projection of $\nabla F(Q)$ into the tangent space:

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

An 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 $M(\Lambda)$:

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

- The entire concept can be obtained by utilizing the Riemannian geometry on the Lie group $O(n)$.

The 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:

$$\begin{aligned} G'(Z)H \quad & = H[P(Z^T\Lambda Z), Z^T\Lambda Z] \\ & +Z[P(Z^T\Lambda Z), Z^T\Lambda H + H^T\Lambda Z] \\ & +Z[P'(Z^T\Lambda Z)(Z^T\Lambda H + H^T\Lambda Z), Z^T\Lambda Z]. \end{aligned}$$

- The projected Hessian at a critical point $X = Q^T\Lambda Q$ for the tangent vector QK with $K \in K(n)$:

$$\begin{aligned} & \langle G'(Q)QK, QK\rangle = \\ & \langle [P(X), K] - P'(X)[X, K], [X, K]\rangle. \end{aligned}$$

Least Squares Approximation

- Let the given matrix be $\hat{A}$ and $\Lambda := \mathrm{diag}\{\lambda_1, \ldots, \lambda_n\}$. The projection is $P(X) = \hat{A}$.
- The projected gradient is given by:

$$g(Q) = Q[\hat{A}, Q^T\Lambda Q].$$

- The descent flow is given by the IVP:

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

Sorting Property

- Assume the given eigenvalues are $\lambda_1 > \ldots > \lambda_n$.
- Assume the eigenvalues of $\hat{A}$ are $\mu_1 > \ldots > \mu_n$.
- Assume Q is a critical point on $O(n)$ and define

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

- The first order condition $[\hat{A}, X] = 0$ implies E must be a diagonal matrix. Hence, the diagonals of E must be a permutation of $\mu_1, \ldots, \mu_n$.
- The second order derivative is reduced to

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

Wielandt-Hoffman Theorem

- We have shown that if a matrix Q is optimal, then the columns $q_1, \ldots, q_n$ of Q^T must be the normalized eigenvectors of $\hat{A}$ corresponding respectively to $\mu_1, \ldots, \mu_n$. The solution to Problem A is unique and is given by

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

- Let A and $A + E$ be symmetric matrices with eigenvalues $\mu_1 > \ldots \mu_n$ and $\lambda_1 > \ldots > \lambda_n$, respectively. Then

$$\sum_{i=1}^{n}(\lambda_i - \mu_i)^2 \leq ||E||^2.$$

Toeplitz Inverse Eigenvalue Problem

- Let $\mathcal{T}$ be the subspace of all symmetric Toeplitz matrices and $\Lambda := \mathrm{diag}\{\lambda_1, \ldots, \lambda_n\}$.
- The subspace $\mathcal{T}$ has a natural orthogonal basis, say $E_1, \ldots, E_n$. So the projection of any matrix X is given by

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

- The projected gradient is given by:

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

- The descent flow is given by the IVP:

$$\begin{aligned} \frac{dX}{dt} &= [[P(X), X], X] \\ X(0) &= \text{any thing on } M(\Lambda) \text{ but diagonal matrices.} \end{aligned}$$

- Open Question: With an arbitrary structured affined subspace $\mathcal{V}$ (See the IEP with Prescribed Entries), characterize the critical points of the descent flow.

Toeplitz Annihilator

- To stay on the surface $\mathcal{M}(\Lambda)$, a differential equation must take the form

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

where $k : \mathcal{S}(n) \longrightarrow \mathcal{S}(n)^{\perp}$.

- Require k to be a linear Toeplitz annihilator:
  - ◇ $k(X) = 0$ if and only if $X \in \mathcal{T}$.
- What is the idea?
  - ◇ Suppose all elements in Λ are distinct.
  - ◇ $[X, k(X)] = 0$ if and only if $k(X)$ is a polynomial of X.
  - ◇ $k(X) \in \mathcal{S}(n) \cap \mathcal{S}(n)^{\perp} = \{0\}$.
  - ◇ $||X(t)|| = ||\Lambda||$ for all $t \in R$.
  - ◇ A bounded flow on a compact set must have a nonempty ω-limit set.

- Can such a k be defined?
  - ◇ The simpliest choice:

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

- Open Question: Starting with the unique centro-symmetric Jacobi matrix as the initial value, must the annihilator flow converge? [119]

Eigenvalue Computation

- Let V be the subspace of all diagonal matrices and $\Lambda = X_0$ be the matrix whose eigenvalues are to be found.
- The objective of Problem C is the same as that of the Jacobi method, i.e., to minimize the off-diagonal elements.
- The descent flow is given by the IVP:

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

- The necessary condition for X to be critical is

$$[\mathrm{diag}(X), X] = 0.$$

Simultaneous Reduction

- Simultaneous reduction of real matrices by either orthogonal similarity or orthogonal equivalence transformation is hard [64].
  - ◇ Little is known in both theory and practice on how reduction for more than two matrices.
  - ◇ The project gradient method based on the Jacobi idea can be formulated.
- Simultaneous reduction flow:

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

- Nearest normal matrix problem [64]

$$\begin{aligned} \frac{dW}{dt} &= \left[W, \frac{1}{2}[W, diag(W^*)] - [W, diag(W^*)]^*\right] \\ W(0) &= A. \end{aligned}$$

Chapter 8

Structured Low Rank Approximation

- Overview
- Low Rank Toeplitz Approximation
- Low Rank Circulant Approximation
- Low Rank Covariance Approximation
- Eculidean Distance Matrix Approximation
- Approximate GCD

Overview

- Given
  - ◇ A target matrix $A \in R^{n\times n}$,
  - ◇ An integer k, $1 \leq k < \text{rank}(A)$,
  - ◇ A class of matrices Ω with linear structure,
  - ◇ a fixed matrix norm $\|\cdot\|$;

  Find
  - ◇ A matrix $\hat{B} \in \Omega$ of rank k, and
  - ◇
  $$\|A - \hat{B}\| = \min_{B\in\Omega, \text{rank}(B)=k} \|A - B\|. \tag{1}$$
- Example of linear structure:
  - ◇ Toeplitz or block Toeplitz matrices.
  - ◇ Hankel or banded matrices.
- Applications:
  - ◇ Signal and image processing with Toeplitz structure.
  - ◇ Model reduction problem in speech encoding and filter design with Hankel structure.
  - ◇ Regularization of ill-posed inverse problems.

Difficulties

- No easy way to characterize, either algebraically or analytically, a given class of structured lower rank matrices.
- Lack of explicit description of the feasible set $\Longrightarrow$ Difficult to apply classical optimization techniques.
- Little discussion on whether lower rank matrices with specified structure actually exist.

An Example of Existence

- Physics sometimes sheds additional light.
- The Toeplitz matrix

$$H := \begin{bmatrix} h_n & h_{n+1} & \dots & h_{2n-1} \\ \vdots & & & \vdots \\ h_2 & h_3 & \dots & h_{n+1} \\ h_1 & h_2 & \dots & h_n \end{bmatrix}$$

  with

$$h_j := \sum_{i=1}^{k} \beta_i z_i^j, \quad j = 1, 2, \dots, 2n-1,$$

  where $\{\beta_i\}$ and $\{z_i\}$ are two sequences of arbitrary nonzero numbers satisfying $z_i \neq z_j$ whenever $i \neq j$ and $k \leq n$, is a Toeplitz matrix of rank k.
- The general Toeplitz structure preserving rank reduction problem as described in (1) remains open.
  - ◇ Existence of lower rank matrices of specified structure does not guarantee *closest* such matrices.
  - ◇ No $x > 0$ for which $1/x$ is minimum.

- For other types of structures, the existence question usually is a hard algebraic problem.

Another Hidden Catch

- The set of all $n \times n$ matrices with rank $\leq k$ is a *closed* set.
- The approximation problem

$$\min_{B \in \Omega, \mathrm{rank}(B) \leq k} \|A - B\|$$

  is *always* solvable, so long as the feasible set is non-empty.
  - ◇ The rank condition is to be less than or equal to k, but not necessarily exactly equal to k.
- It is possible that a given target matrix A does not have a nearest rank k structured matrix approximation, but does have a nearest rank $k-1$ or lower structured matrix approximation.

Low Rank Toeplitz Approximation

- Algebraic Structure of Low Rank Toeplitz Matrices.
- Constructing Low Rank Toeplitz Matrices.
  - ◇ Lift and Project Method
  - ◇ Parameterization by SVD
- Implicit Optimization
  - ◇ Engineerers' Misconception
  - ◇ Simplex Search Method
- Explicit Optimization
  - ◇ **constr** in MATLAB
  - ◇ **LANCELOT** on NEOS

A General Remark

- Introduce two procedures to tackle the structure preserving rank reduction problem numerically.
- The procedures can be applied to problems of any norm, any linear structure, and any matrix norm.
- Use the symmetric Toeplitz structure with Frobenius matrix norm to illustrate the ideas.

Algebraic Structure

- Identify a *symmetric* Toeplitz matrix by its first row,

$$T = T([t_1, \ldots, t_n]) = \begin{bmatrix} t_1 & t_2 & \ldots & & t_n \\ t_2 & t_1 & \ddots & & t_{n-1} \\ \vdots & \ddots & \ddots & & \\ t_{n-1} & & & & t_2 \\ t_n & t_{n-1} & \ldots & t_2 & t_1 \end{bmatrix}.$$

  ◇ $\mathcal{T}$ = The affine subspace of all $n \times n$ symmetric Toeplitz matrices.

- Spectral decomposition of symmetric rank k matrices:

$$M = \sum_{i=1}^{k} \alpha_i y^{(i)} {y^{(i)}}^T. \tag{2}$$

- Write $T = T([t_1, \ldots, t_n])$ in terms of (2) $\Longrightarrow$

$$\sum_{i=1}^{k} \alpha_i y_j^{(i)} y_{j+s}^{(i)} = t_{s+1},\ s = 0, 1, \ldots, n-2,\ 1 \leq j \leq n-s \tag{3}$$

  ◇ Lower rank matrices form an *algebraic variety*, i.e, solutions of polynomial systems.

Some Examples

- The case $k = 1$ is trivial.

  ◇ Rank-one Toeplitz matrices form two simple one-parameter families,

$$\begin{aligned} T &= \alpha_1 T([1, \ldots, 1]), \quad \text{or} \\ T &= \alpha_1 T([1, -1, 1, \ldots, (-1)^{n-1}]) \end{aligned}$$

  with arbitrary $\alpha_1 \neq 0$.

- For 4×4 symmetric Toeplitz matrices of rank 2, there are 10 unknowns in 6 equations.

$$\left\{ \begin{array}{lcl} \alpha_1 & := & \frac{\alpha_2\left({y_1^{(2)}}^2 - {y_2^{(2)}}^2\right)}{-{y_1^{(1)}}^2 + {y_2^{(1)}}^2}, \\ y_3^{(1)} & := & \frac{y_2^{(1)} y_1^{(2)} y_1^{(1)} + 2\, y_2^{(2)} {y_2^{(1)}}^2 - y_2^{(2)} {y_1^{(1)}}^2}{y_2^{(1)} y_1^{(2)} + y_1^{(1)} y_2^{(2)}}, \\ y_4^{(1)} & := & -\frac{{y_2^{(1)}}^3 {y_1^{(2)}}^2 - 4\, {y_2^{(1)}}^3 {y_2^{(2)}}^2 - 4\, y_1^{(1)} y_1^{(2)} y_2^{(2)} {y_2^{(1)}}^2 - 2\, y_2^{(1)} {y_1^{(1)}}^2 {y_1^{(2)}}^2 + 3\, y_2^{(1)} {y_2^{(2)}}^2 {y_1^{(1)}}^2 + 2\, y_1^{(2)} y_2^{(2)} {y_1^{(1)}}^3}{{y_2^{(1)}}^2 {y_1^{(2)}}^2 + 2\, y_2^{(1)} y_1^{(2)} y_1^{(1)} y_2^{(2)} + {y_1^{(1)}}^2 {y_2^{(2)}}^2}, \\ y_3^{(2)} & := & -\frac{y_2^{(1)} {y_1^{(2)}}^2 - 2\, y_2^{(1)} {y_2^{(2)}}^2 - y_1^{(2)} y_2^{(2)} y_1^{(1)}}{y_2^{(1)} y_1^{(2)} + y_1^{(1)} y_2^{(2)}}, \\ y_4^{(2)} & := & -\frac{3\, {y_2^{(1)}}^2 {y_1^{(2)}}^2 y_2^{(2)} - 4\, {y_2^{(1)}}^2 {y_2^{(2)}}^3 + 2\, y_2^{(1)} y_1^{(1)} {y_1^{(2)}}^3 - 4\, y_2^{(1)} y_1^{(1)} {y_2^{(2)}}^2 y_1^{(2)} - 2\, y_2^{(2)} {y_1^{(1)}}^2 {y_1^{(2)}}^2 + {y_1^{(1)}}^2 {y_2^{(2)}}^3}{{y_2^{(1)}}^2 {y_1^{(2)}}^2 + 2\, y_2^{(1)} y_1^{(2)} y_1^{(1)} y_2^{(2)} + {y_1^{(1)}}^2 {y_2^{(2)}}^2}. \end{array} \right.$$

  ◇ Explicit description of algebraic equations for higher dimensional lower rank symmetric Toeplitz matrices becomes unbearably complicated.

Let's See It!

- Rank deficient $T([t_1, t_2, t_3])$
  - ◇ $\det(T) = (t_1 - t_3)(t_1^2 + t_1 t_3 - 2t_2^2) = 0$.
  - ◇ A union of two algebraic varieties.

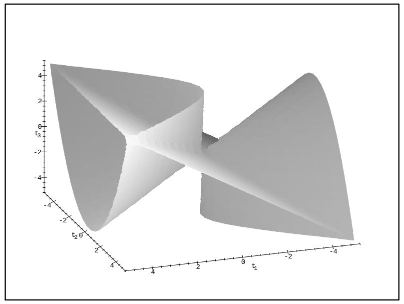


Figure 1: Lower rank, symmetric, Toeplitz matrices of dimension 3 identified in R^3.

- The number of *local* solutions to the structured lower rank approximation problem is not unique.

Constructing Lower Rank Toeplitz Matrices

- Idea:
  - ◇ Rank k matrices in $R^{n\times n}$ form a *surface* $\mathcal{R}(k)$.
  - ◇ Rank k Toeplitz matrices $= \mathcal{R}(k) \bigcap \mathcal{T}$.
- Two approaches:
  - ◇ Parameterization by SVD:
    - ▷ Identify $M \in \mathcal{R}(k)$ by the triplet (U, Σ, V) of its singular value decomposition $M = U\Sigma V^T$.
      - · U and V are orthogonal matrices, and
      - · $\Sigma = \mathrm{diag}\{s_1, \ldots, s_k, 0, \ldots, 0\}$ with $s_1 \geq \ldots \geq s_k > 0$.
    - ▷ Enforce the structure.
  - ◇ Alternate projections between $\mathcal{R}(k)$ and $\mathcal{T}$ to find intersections. (Cheney & Goldstein'59, Catzow'88)

Lift and Project Algorithm

- Given $A^{(0)} = A$, repeat projections until convergence:
  - ◇ **LIFT**. Compute $B^{(\nu)} \in \mathcal{R}(k)$ nearest to $A^{(\nu)}$:
    - ▷ From $A^{(\nu)} \in \mathcal{T}$, first compute its SVD

$$A^{(\nu)} = U^{(\nu)}\Sigma^{(\nu)}V^{(\nu)^T}.$$

    - ▷ Replace $\Sigma^{(\nu)}$ by $\mathrm{diag}\{s_1^{(\nu)}, \ldots, s_k^{(\nu)}, 0, \ldots, 0\}$ and define

$$B^{(\nu)} := U^{(\nu)}\Sigma^{(\nu)}V^{(\nu)^T}.$$

  - ◇ **PROJECT**. Compute $A^{(\nu+1)} \in \mathcal{T}$ nearest to $B^{(\nu)}$:
    - ▷ From $B^{(\nu)}$, choose $A^{(\nu+1)}$ to be the matrix formed by replacing the diagonals of $B^{(\nu)}$ by the averages of their entries.
- The general approach remains applicable to any other linear structure, and symmetry can be enforced.
  - ◇ The only thing that needs to be modified is the projection in the projection (second) step.

Geometric Sketch

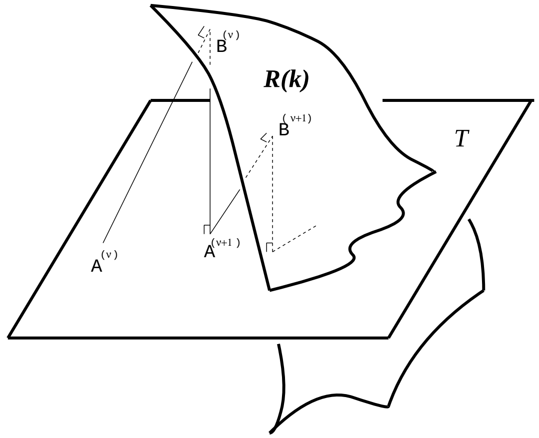


Figure 2: Algorithm 1 with intersection of lower rank matrices and Toeplitz matrices

Black-box Function

- Descent property:

  $$\|A^{(\nu+1)} - B^{(\nu+1)}\|_F \leq \|A^{(\nu+1)} - B^{(\nu)}\|_F \leq \|A^{(\nu)} - B^{(\nu)}\|_F.$$

  ◇ Descent with respect to the Frobenius norm which is not necessarily the norm used in the structure preserving rank reduction problem.

- If all $A^{(\nu)}$ are distinct then the iteration converges to a Toeplitz matrix of rank k.

  ◇ In principle, the iteration could be trapped in an impasse where $A^{(\nu)}$ and $B^{(\nu)}$ would not improve any more, but not experienced in practice.

- The lift and project iteration provides a means to define a *black-box function*

  $$P : \mathcal{T} \longrightarrow \mathcal{T} \bigcap \mathcal{R}(k).$$

  ◇ The $P(T)$ is *presumably* piecewise continuous since all projections are continuous.

The graph of $P(T)$

- Consider $P : R^2 \longrightarrow R^2$:

  ◇ Use the xy-plane to represent the domain of P for 2×2 symmetric Toeplitz matrices $T(t_1, t_2)$.

  ◇ Use the z-axis to represent the image $p_{11}(T)$ and $p_{12}(T)$), respectively.

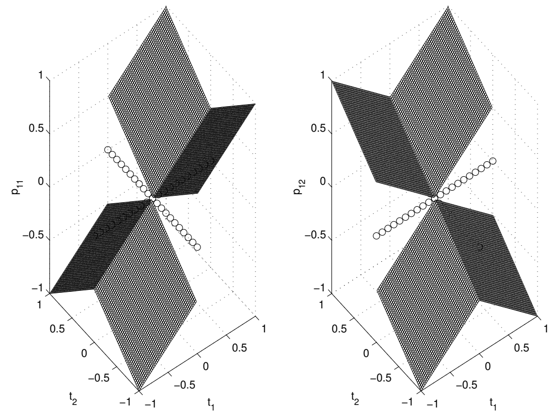


Figure 3: Graph of $P(T)$ for 2-dimensional symmetric Toeplitz T.

- Toeplitz matrices of the form $T(t_1, 0)$ or $T(0, t_2)$, corresponding to points on axes, converge to the zero matrix.

Implicit Optimization

- Implicit formulation:

$$\min_{T=\text{toeplitz}(t_1,\dots,t_n)} \|T_0 - P(T)\|. \tag{4}$$

  - ◇ T_0 is the given target matrix.
  - ◇ $P(T)$, regarded as a black box function evaluation, provides a handle to manipulate the objective function $f(T) := \|T_0 - P(T)\|$.
  - ◇ The norm used in (4) can be any matrix norm.
- Engineers' misconception:
  - ◇ $P(T)$ is *not* necessarily the closest rank k Toeplitz matrix to T.
  - ◇ In practice, $P(T_0)$ has been used "as a cleansing process whereby any corrupting noise, measurement distortion or theoretical mismatch present in the given data set (namely, T_0) is removed."
  - ◇ More needs to be done in order to find the *closest* lower rank Toeplitz approximation to the given T_0 as $P(T_0)$ is merely known to be in the feasible set.

Numerical Experiment

- An ad hoc optimization technique:
  - ◇ The simplex search method by Nelder and Mead requires only function evaluations.
  - ◇ Routine **fmins** in MATLAB, employing the simplex search method, is ready for use in our application.
- An example:
  - ◇ Suppose $T_0 = T(1, 2, 3, 4, 5, 6)$.
  - ◇ Start with $T^{(0)} = T_0$, and set worst case precision to 10^{-6}.
  - ◇ Able to calculate *all* lower rank matrices while maintaining the symmetric Toeplitz structure. Always so?
  - ◇ Nearly machine-zero of smallest calculated singular value(s) $\Longrightarrow T_k^*$ is computationally of rank k.
  - ◇ T_k^* is only a local solution.
  - ◇ $\|T_k^* - T_0\| < \|P(T_0) - T_0\|$ which, though represents only a slight improvement, clearly indicates that $P(T_0)$ alone does not give rise to an optimal solution.

rank k	5	4	3	2	1
# of iterations	110	81	46	36	17
# of SVD calls	1881	4782	2585	2294	558
optimal solution	$\begin{bmatrix}1.1046\\1.8880\\3.1045\\3.9106\\5.0635\\5.9697\end{bmatrix}$	$\begin{bmatrix}1.2408\\1.8030\\3.0352\\4.1132\\4.8553\\6.0759\end{bmatrix}$	$\begin{bmatrix}1.4128\\1.7980\\2.8171\\4.1089\\5.2156\\5.7450\end{bmatrix}$	$\begin{bmatrix}1.9591\\2.1059\\2.5683\\3.4157\\4.7749\\6.8497\end{bmatrix}$	$\begin{bmatrix}2.9444\\2.9444\\2.9444\\2.9444\\2.9444\\2.9444\end{bmatrix}$
$\|T_0 - T_k^*\|$	0.5868	0.9851	1.4440	3.2890	8.5959
singular values	$\begin{bmatrix}17.9851\\7.4557\\2.2866\\0.9989\\0.6164\\3.4638e{-15}\end{bmatrix}$	$\begin{bmatrix}17.9980\\7.4321\\2.2836\\0.8376\\2.2454e{-14}\\2.0130e{-14}\end{bmatrix}$	$\begin{bmatrix}18.0125\\7.4135\\2.1222\\1.9865e{-14}\\9.0753e{-15}\\6.5255e{-15}\end{bmatrix}$	$\begin{bmatrix}18.2486\\6.4939\\2.0884e{-14}\\7.5607e{-15}\\3.8479e{-15}\\2.5896e{-15}\end{bmatrix}$	$\begin{bmatrix}17.6667\\2.0828e{-14}\\9.8954e{-15}\\6.0286e{-15}\\2.6494e{-15}\\2.1171e{-15}\end{bmatrix}$

Table 1: Test results for a case of $n = 6$ symmetric Toeplitz structure

Explicit Optimization

- Difficult to compute the gradient of $P(T)$.
- Other ways to parameterize structured lower rank matrices:
  - ◇ Use eigenvalues and eigenvectors for symmetric matrices;
  - ◇ Use singular values and singular vectors for general matrices.
  - ◇ Robust, but might have *overdetermined* the problem.

An Illustration

- Define

$$M(\alpha_1,\ldots,\alpha_k,y^{(1)},\ldots,y^{(k)}) := \sum_{i=1}^{k}\alpha_i y^{(i)}{y^{(i)}}^T.$$

- Reformulate the symmetric Toeplitz structure preserving rank reduction problem *explicitly* as

$$\begin{array}{ll} \min & \|T_0 - M(\alpha_1,\ldots,\alpha_k,y^{(1)},\ldots,y^{(k)})\| \quad (5)\\ \text{subject to} & m_{j,j+s-1} = m_{1,s}, \quad (6)\\ & s = 1,\ldots n-1,\\ & j = 2,\ldots,n-s+1, \end{array}$$

  if $M = [m_{ij}]$.
  - ◇ Objective function in (5) is described in terms of the non-zero eigenvalues $\alpha_1,\ldots,\alpha_k$ and the corresponding eigenvectors $y^{(1)},\ldots,y^{(k)}$ of M.
  - ◇ Constraints in (6) are used to ensure that M is symmetric and Toeplitz.
- For other types of structures, we only need modify the constraint statement accordingly.
- The norm used in (5) can be arbitrary but is fixed.

Redundant Constraints

- Symmetric centro-symmetric matrices have special spectral properties:
  - ◇ $\lceil n/2\rceil$ of the eigenvectors are symmetric; and
  - ◇ $\lfloor n/2\rfloor$ are skew-symmetric.
    - ▷ $v = [v_i] \in R^n$ is symmetric (or skew-symmetric) if $v_i = v_{n-i}$ (or $v_i = -v_{n-i}$).
- Symmetric Toeplitz matrices are symmetric and centro-symmetric.
- The formulation in (5) does not take this spectral structure into account in the eigenvectors $y^{(i)}$.
  - ◇ More variables than needed have been introduced.
  - ◇ May have overlooked any internal relationship among the $\frac{n(n-1)}{2}$ equality constraints.
  - ◇ May have caused, inadvertently, additional computation complexity.

Using Existing Optimization Codes

- Using **constr** in MATLAB
  - ◇ Routine **constr** in MATLAB:
    - ▷ Uses a sequential quadratic programming method.
    - ▷ Solve the Kuhn-Tucker equations by a quasi-Newton updating procedure.
    - ▷ Can estimate derivative information by finite difference approximations.
    - ▷ Readily available in Optimization Toolbox.
  - ◇ Our experiments:
    - ▷ Use the same data as in the implicit formulation.
    - ▷ Case $k = 5$ is computationally the same as before.
    - ▷ Have trouble in cases $k = 4$ or $k = 3$,
      - · Iterations will not improve approximations at all.
      - · MATLAB reports that the optimization is terminated successfully.

- Using **LANCELOT** on NEOS
  - ◇ Reasons of failure of MATLAB are not clear.
    - ▷ Constraints might no longer be linearly independent.
    - ▷ Termination criteria in **constr** might not be adequate.
    - ▷ Difficult geometry means hard-to-satisfy constraints.
  - ◇ Using more sophisticated optimization packages, such as **LANCELOT**.
    - ▷ A standard Fortran 77 package for solving large-scale nonlinearly constrained optimization problems.
    - ▷ Break down the functions into sums of *element functions* to introduce sparse Hessian matrix.
    - ▷ Huge code. See

      http://www.rl.ac.uk/departments/ccd/numerical/lancelot/sif/sifhtml.html.
    - ▷ Available on the NEOS Server through a socket-based interface.
    - ▷ Uses the **ADIFOR** automatic differentiation tool.

◇ **LANCELOT** works.

- ▷ Find optimal solutions of problem (5) for all values of k.
- ▷ Results from **LANCELOT** agree, up to the required accuracy 10^{-6}, with those from **fmins**.
- ▷ Rank affects the computational cost nonlinearly.

rank k	5	4	3	2	1
# of variables	35	28	21	14	7
# of f/c calls	108	56	47	43	19
total time	12.99	4.850	3.120	1.280	.4300

Table 3: Cost overhead in using **LANCELOT** for $n = 6$.

Conclusions

- Structure preserving rank reduction problems arise in many important applications, particularly in the broad areas of signal and image processing.
- Constructing the nearest approximation of a given matrix by one with any rank and any linear structure is difficult in general.
- We have proposed two ways to formulate the problems as standard optimization computations.
- It is now possible to tackle the problems numerically via utilizing standard optimization packages.
- The ideas were illustrated by considering Toeplitz structure with Frobenius norm.
- Our approach can be readily generalized to consider rank reduction problems for any given linear structure and of any given matrix norm.

Low Rank Circulant Approximation

- Basic Properties
- (Inverse) Eigenvalue Problem
- Conjugate Evenness
- Low Rank Approximation
- Tree Structure
- Numerical Experiment

Basic Properties

- A circulant matrix $C = Circul(c)$

$$C = \begin{bmatrix} c_0 & c_1 & & \dots & c_{n-1} \\ c_{n-1} & c_0 & c_1 & \dots & c_{n-2} \\ c_{n-2} & c_{n-1} & c_0 & \dots & c_{n-3} \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ c_1 & c_2 & & c_{n-1} & c_0 \end{bmatrix}$$

  is uniquely determined by the first row c.

  ◇ Define

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

  Then

$$Circul(c) = \sum_{k=0}^{n-1} c_k \Pi^k = P_c(\Pi)$$

  with characteristic polynomial

$$P_c(x) = \sum_{k=0}^{n-1} c_k x^k.$$

Elementary Spectral Properties

- Define
$$\Omega := \mathrm{diag}(1, \omega, \omega^2, \ldots, \omega^{n-1}), \quad \omega := \exp(\frac{2\pi i}{n}).$$
- Define the Fourier matrix F where
$$F^* := \frac{1}{\sqrt{n}} \begin{bmatrix} 1 & 1 & 1 & \ldots & 1 \\ 1 & \omega & \omega^2 & \ldots & \omega^{n-1} \\ 1 & \omega^2 & \omega^4 & \ldots & \omega^{2n-2} \\ \vdots & & & & \vdots \\ 1 & \omega^{n-1} & \omega^{n-2} & \ldots & \omega \end{bmatrix}.$$
  - ◇ F is unitary.

- The forward shift matrix Π is unitarily diagonalizable.
$$\Pi = F^* \Omega F.$$
- The circulant matrix $Circul(c)$ with any given row vector c has a spectral decomposition
$$Circul(c) = F^* P_c(\Omega) F.$$
- Spectral properties:
  - ◇ Closely related to the discrete Fourier transform.
  - ◇ Explicit solution for eigenvalue and inverse eigenvalue problems.
  - ◇ FFT calculation.

(Inverse) Eigenvalue Problem

- Forward problem:
  - ◇ Eigenvalues of $Circul(c)$:
  $$\lambda = [P_c(1), \dots P_c(\omega^{n-1})].$$
  - ◇ Can be computed from
  $$\lambda^T = \sqrt{n} F^* c^T.$$
- Inverse problem:
  - ◇ Given any vector $\lambda := [\lambda_0, \dots, \lambda_{n-1}] \in C^n$, define
  $$c^T = \frac{1}{\sqrt{n}} F \lambda^T.$$
  - ◇ $Circul(c)$ has eigenvalues in vector λ.
- Both matrix-vector products involved done in $O(n \log_2 n)$ flops.
- If all the eigenvalues are distinct, there are precisely $n!$ distinct circulant matrices with the prescribed spectrum.

Conjugate Evenness

- $c^T = \frac{1}{\sqrt{n}} F \lambda^T$ is real if and only if $\lambda^T = \sqrt{n} F^* c^T$ is conjugate-even.
  - ◇ If $n = 2m$,
  $$\lambda = [\lambda_0, \lambda_1, \dots, \lambda_{m-1}, \lambda_m, \overline{\lambda_{m-1}}, \dots, \overline{\lambda_1}].$$
    - ▷ $\lambda_0, \lambda_m \in \mathbb{R}$. (Absolutely real, others real or complex.)
  - ◇ If $n = 2m + 1$,
  $$\lambda := [\lambda_0, \lambda_1, \dots, \lambda_m, \overline{\lambda_m}, \dots, \overline{\lambda_1}].$$
    - ▷ $\lambda_0 \in \mathbb{R}$. (Absolutely real.)
- Singular value decomposition of $Circul(c)$:
  $$Circul(c) = (F^* P_c(\Omega) |P_c(\Omega)|^{-1}) |P_c(\Omega)| F$$
  - ◇ Singular values are $|P_c(\omega^k)|, k = 0, 1, \cdots n - 1$.
  - ◇ At most $\lceil \frac{n+1}{2} \rceil$ distinct singular values.

Low Rank Approximation

- Given $A \in R^{n \times n}$, its nearest circulant matrix approximation $Circul(c)$ is given by the projection (T. Chan)

$$c_k := \frac{1}{n}\langle A, \Pi^k \rangle, \quad k = 0, \dots, n-1,$$

  - ◇ $Circul(c)$ is generally of **full rank** even if A has lower rank.
- How to reduce the rank of $Circul(c)$?
  - ◇ The truncated singular value decomposition (TSVD) gives rise to the nearest low rank approximation in Frobenius norm.
  - ◇ The TSVD of $Circul(c)$ is automatically circulant.
  - ◇ But: the TSVD can lead to a **complex** circulant approximation.

Trivial $O(n \log n)$ TSVD Algorithm

- Given a real matrix A and a fixed rank $\ell \leq n$,
  1. Use the projection to find the nearest real circulant matrix approximation $Circul(c)$ of A.
  2. Use the FFT to calculate the spectrum λ of the matrix $Circul(c)$.
  3. Arrange all elements of $|\lambda|$ in descending order, including those with equal modulus.
  4. Let $\hat{\lambda}$ be the vector consisting of elements of λ, but those corresponding to the last $n-\ell$ singular values in the descending order are set to zero.
  5. Apply the inverse FFT to $\hat{\lambda}$ to determine a nearest circulant matrix $Circul(\hat{c})$ of rank ℓ to A.
- The resulting matrix $Circul(\hat{c})$ is complex-valued in general.
  - ◇ Need to preserve the conjugate-even structure.
  - ◇ Need to modify the TSVD strategy.

Data Matching Problem

- The low rank "real" circulant approximation problem is equivalent to a data matching problem:

  (DMP) *Given a conjugate-even vector $\lambda \in C^n$, find its nearest conjugate-even approximation $\hat{\lambda} \in C^n$ subject to the constraint that $\hat{\lambda}$ has exactly $n - \ell$ zeros.*

- How to solve the DMP?
  - ◇ Write $\hat{\lambda} = [\hat{\lambda}_1, 0] \in C^n$ with $\hat{\lambda}_1 \in C^\ell$ being arbitrary.
  - ◇ Consider the problem of minimizing

    $$F(P, \hat{\lambda}) = \|P\hat{\lambda}^T - \lambda^T\|^2$$

    with a permutation matrix P.
    - ▷ P is used to search for the match.
  - ◇ Write $P = [P_1, P_2]$ with $P_1 \in R^{n\times\ell}$.

  - ◇ A least squares problem:

    $$F(P, \hat{\lambda}) = \|P_1\hat{\lambda}_1^T - \lambda^T\|^2$$

  - ◇ The optimal solution is

    $$\hat{\lambda}_1 = \lambda P_1.$$

    - ▷ The entries of $\hat{\lambda}_1$ must be a portion of λ.
  - ◇ The objective function becomes

    $$F(P, \hat{\lambda}) = \|(P_1P_1^T - I)\lambda\|^2.$$

    - ▷ $P_1P_1^T - I$ is just a projection.
    - ▷ The optimal permutation P should be such that $P_1P_1^T$ projects λ to its first ℓ components with largest modulus.
- Without the conjugate-even constraint, the answer to the data matching problem corresponds precisely to the usual TSVD selection criterion.
- With the conjugate-even constraint, the above criterion remains effective subject to the conjugate-even structure inside λ.

An Example using a Tree Structure

- Consider the case $n = 6$.
- Suppose λ_1, λ_2 are complex and distinct.
- Six possible conjugate-even structures.
- Tree graph:
  - ◇ Each node in the tree represents an element of λ.
  - ◇ Arrange the nodes from top to bottom in descending order of their moduli.
  - ◇ In case of a tie,
    - ▷ Complex conjugate nodes stay at the same level.
    - ▷ Real node is below the complex nodes.
- If $\lambda_1, \overline{\lambda_1}, \lambda_0, \lambda_2, \overline{\lambda_2}, \lambda_3$, then the tree is given by:

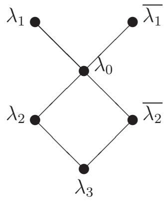


Figure 4: Tree graph of $\lambda_1, \overline{\lambda_1}, \lambda_0, \lambda_2, \overline{\lambda_2}, \lambda_3$ with $|\lambda_1| \geq |\lambda_0| > |\lambda_2| \geq |\lambda_3|$.

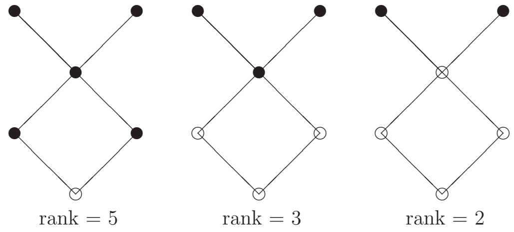


Figure 5: Tree graphs of $\hat{\lambda}$ with rank 5, 3, and 2.

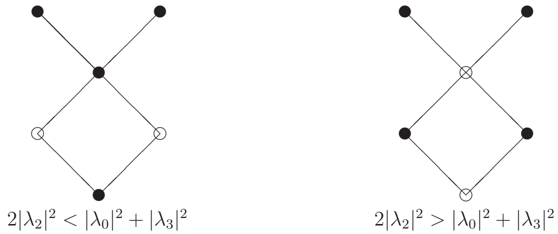


Figure 6: Tree graphs of $\hat{\lambda}$ with rank 4.

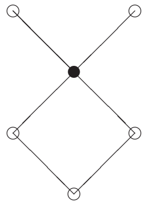


Figure 7: Tree graph of $\hat{\lambda}$ with rank 1.

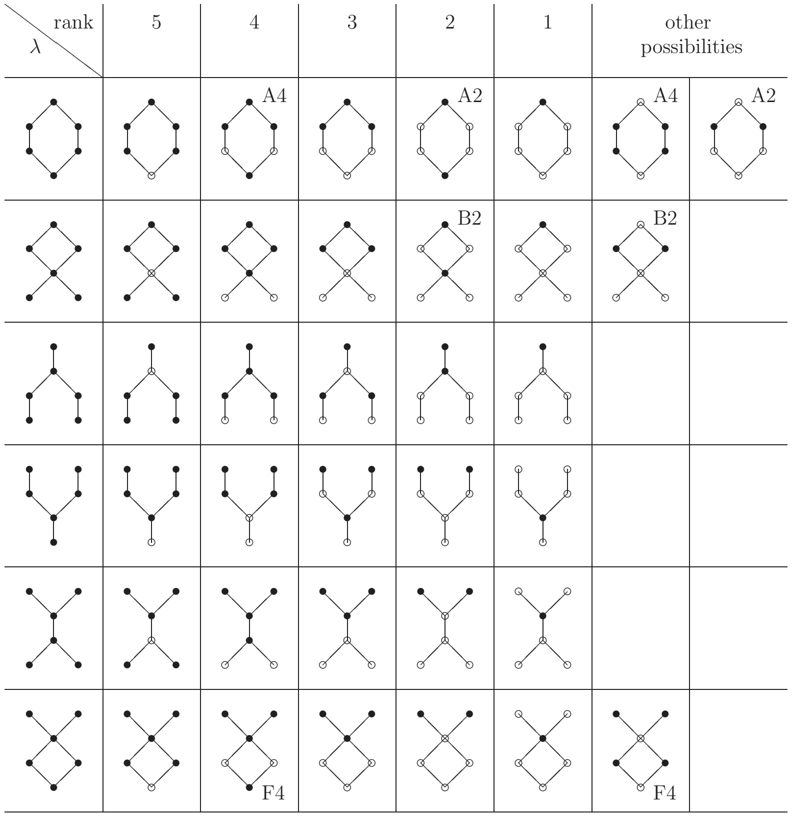


Figure 8: Possible solutions to the DMP when $n = 6$.

Numerical Experiment

- The low rank approximation algorithm needs to be smart enough to explore the conjugate-even structure, to truncate, and to reassemble the conjugate-even structure.
- Numerical complexity is $O(n \log n)$ flops.

Example 1: Symmetric Illustration

Consider the 8×8 symmetric $Circul(c)$:

$$c = \left[0.5404, 0.2794, 0.1801, \text{-}0.0253, \text{-}0.2178, \text{-}0.0253, 0.1801, 0.2794\right].$$

- Eigenvalues (in descending order):

$$\left[1.1909, 1.1892, 1.1892, 0.3273, 0.3273, \mathbf{0.1746}, \text{-}0.0376, \text{-}0.0376\right]$$

- For rank 7 approximation, the usual TSVD would set -0.0376 to zero, resulting in a complex matrix.
- Use the conjugate-even eigenvalues

$$\hat{\lambda} = \left[1.1909, 1.1892, 0.3273, \text{-}0.0376, \mathbf{0}\ \text{-}0.0376, 0.3273, 1.1892\right],$$

  to obtain the best real-valued, rank 7, approximation $Circul(\hat{c})$ via the FFT:

$$\hat{c} = \left[0.5186, 0.3657, 0.0670, \text{-}0.0680, \text{-}0.0572, \text{-}0.0680, 0.0670, 0.3657\right].$$

- To obtain the best real-value, rank 4, circulant approximation, use eigenvalues $\hat{\lambda}$

$$\hat{\lambda} = \left[1.1909, 1.1892, 0, 0, 0.3273, 0, 0, 1.1892\right].$$

Example 2: Complex Illustration

Consider the 9×9 $Circul(c)$ with

$$c = \left[1.6864, 1.7775, 1.9324, 2.9399, 1.9871, 1.7367, 4.0563, 1.2848, 2.5989\right].$$

- Eigenvalues: structure given by

$$\begin{aligned}&\left[\mathbf{20.0000},\right.\\ &\text{-}2.8130 + 1.9106i, \text{-}2.8130 - 1.9106i, 3.0239 - 1.0554i, 3.0239 + 1.0554i,\\ &\left.\text{-}1.3997 + 0.7715i, \text{-}1.3997 - 0.7715i, \text{-}1.2223 - 0.2185i, \text{-}1.2223 + 0.2185i\right].\end{aligned}$$

- To obtain a real-valued circulant approximation of rank 8, we have no choice but to select the set the *largest* eigenvalue (singular value) of $Circul(c)$ to zero.
  - ◇ Setting the largest singular value to zero to obtain the nearest real low rank approximation is quite counter-intuitive to the usual sense of TSVD.
  - ◇ Apply algorithm to reduce the rank further, to 7.

Example 3: Perturbed Case

- Let $C_\kappa \in R^{n\times n}$ be a given circulant matrix of rank κ. Random noise added to C_κ will destroy the circulant structure as well as the rank condition.
- Let $E \in R^{n\times n}$ denote a random but fixed circulant matrix with unit Frobenius norm, and let

$$W_j = C_\kappa + 10^{-j}E, \quad j = 1, \ldots, 12.$$

- W_j will almost certainly be of full rank. Note that $\|W_j - C_\kappa\| = 10^{-j}$. It will be interesting to see if W_j has any closer circulant matrix approximation of rank κ other than C_κ, especially when j is large.
- Test case with $n = 100$, $\kappa = 73$, and a predetermined matrix C_{73}.
- Using our algorithm to find the best circulant approximation Z_j to W_j, we find that it is always the case that

$$\|W_j - Z_j\| < \|W_j - C_\kappa\|$$

  for all j, i.e., our real circulant approximation is closest.

Conclusion

- For any given real data matrix, its nearest real circulant approximation can simply be determined from the average of its diagonals.
- The nearest low rank (possibly complex) approximation to the circulant matrix can be determined effectively from the TSVD and the FFT.
- To construct a real circulant matrix with specified spectrum, the eigenvalues must appear in conjugate-even form. So, the truncation criteria for a nearest low rank, real, circulant matrix approximation must be modified.
- We have proposed a fast algorithm with $O(n \log n)$ complexity to accomplish all of these objectives.

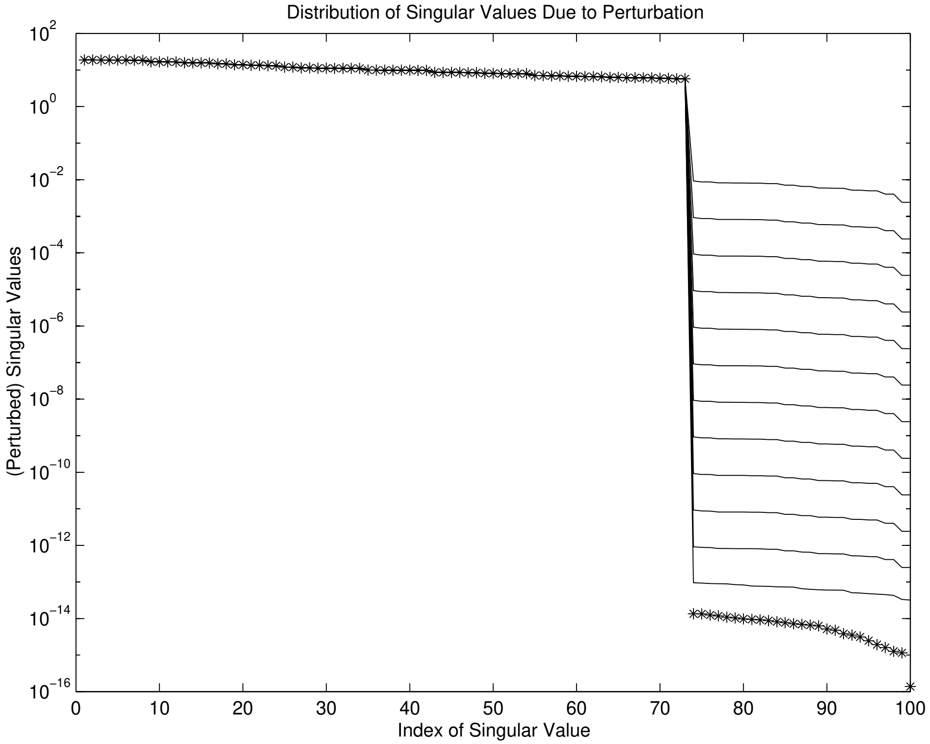


Figure 9: Distribution of Singular Values.

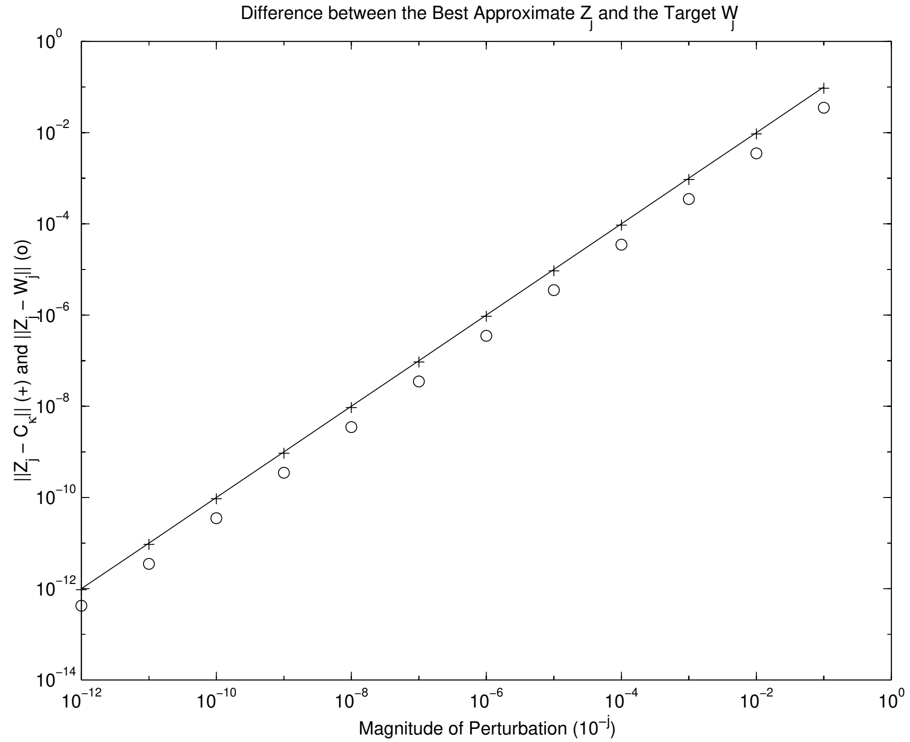


Figure 10: Errors in Approximation.

Lor Rank Covarance Approximation

Euclidian Distance Matrix Approximation

Approximate GCD

f-COUNT	FUNCTION	MAX{g}	STEP	Procedures
29	0.958964	8.65974e-15	1	
77	0.958964	2.66454e-14	1.91e-06	
131	0.958964	2.70894e-14	2.98e-08	Hessian modified twice
185	0.958964	2.70894e-14	2.98e-08	
239	0.958964	2.73115e-14	2.98e-08	
289	0.958964	2.77556e-14	4.77e-07	
337	0.958964	2.77556e-14	1.91e-06	
393	0.958964	2.77556e-14	7.45e-09	Hessian modified twice
445	0.958964	5.28466e-14	1.19e-07	
501	0.958964	5.68434e-14	7.45e-09	
557	0.958964	5.70655e-14	7.45e-09	Hessian not updated
613	0.958964	5.66214e-14	7.45e-09	
667	0.958964	5.55112e-14	2.98e-08	Hessian modified twice
713	0.958964	3.17302e-13	7.63e-06	
761	0.958964	2.61569e-13	1.91e-06	
812	0.958964	2.60014e-13	-2.38e-07	Hessian modified twice
856	0.958964	2.57794e-13	3.05e-05	Hessian modified twice
900	0.958964	2.56462e-13	3.05e-05	Hessian modified twice
948	0.958964	2.57128e-13	1.91e-06	
994	0.958964	2.56684e-13	7.63e-06	
1038	0.958964	3.42837e-13	3.05e-05	
1083	0.958964	3.41727e-13	-1.53e-05	Hessian modified twice
1124	0.958964	3.92575e-13	0.000244	Hessian modified twice
1161	0.958964	5.04485e-13	0.00391	Hessian modified twice
1200	0.958964	5.12923e-13	0.000977	Hessian modified twice
1233	0.958964	5.61551e-13	0.0625	Hessian modified twice
1272	0.958964	5.86642e-13	0.000977	Hessian modified twice
1308	0.958964	4.84279e-13	0.00781	Hessian modified twice
1309	0.958964	4.84723e-13	1	Hessian modified twice

Optimization Converged Successfully

Table 2: A typical output of intermediate results from **constr**.

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