

**Group Theory, Linear Transformations, and Flows:  
(Some) Dynamical Systems on Manifolds**

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# Motivation

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

– V. I. Arnold

Geometric Methods in the Theory of Ordinary Differential Equations, 1988

- What is the simplest form referred to here?
- What kind of continuous change can be employed?

# Realization Process

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- Realization process, in a sense, means any deducible procedure that we use to rationalize and solve problems.
  - ◊ The simplest form refers to the agility to think and draw conclusions.
- In mathematics, a realization process often appears in the form of an iterative procedure or a differential equation.
  - ◊ The steps taken for the realization, i.e., the changes, could be discrete or continuous.

# Continuous Realization

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

# Build the Bridge

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

# Characteristics of a Bridge

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



# Two Examples

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- Eigenvalue Computation
- Constrained Least Squares Approximation

# The Eigenvalue Problem

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- The mathematical problem:
  - ◊ A symmetric matrix  $A_0$  is given.
  - ◊ Solve the equationfor a nonzero vector  $x$  and a scalar  $\lambda$ .
- An iterative method :
  - ◊ The  $QR$  decomposition:

$$A_0x = \lambda x$$

$$A = QR$$

where  $Q$  is orthogonal and  $R$  is upper triangular.

- ◊ The  $QR$  algorithm (Francis'61):

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

- ◊ The sequence  $\{A_k\}$  converges to a diagonal matrix.
- ◊ Every matrix  $A_k$  has the same eigenvalues of  $A_0$ , i.e., ( $A_{k+1} = Q_k^T A_k Q_k$ ).

- A continuous method:
  - ◊ Lie algebra decomposition:
 
$$X = X^o + X^+ + X^-$$
 where  $X^o$  is the diagonal,  $X^+$  the strictly upper triangular, and  $X^-$  the strictly lower triangular part of  $X$ .
  - ◊ Define  $\Pi_0(X) := X^- - X^{-\top}$ .
  - ◊ The Toda lattice (Symes'82, Deift et al'83):
 
$$\begin{aligned} \frac{dX}{dt} &= [X, \Pi_0(X)] \\ X(0) &= X_0. \end{aligned}$$
- Sampled at integer times,  $\{X(k)\}$  gives the same sequence as does the  $QR$  algorithm applied to the matrix  $A_0 = \exp(X_0)$ .
  - Evolution starts from  $X_0$  and converges to the limit point of Toda flow, which is a diagonal matrix, maintains the spectrum.
    - ◊ The construction of the Toda lattice is based on the physics.
      - ▷ This is a Hamiltonian system.
      - ▷ A certain physical quantities are kept at constant, i.e., this is a *completely integrable* system.
    - ◊ The convergence is guaranteed by “nature”?

# Least Squares Matrix Approximation

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

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

- ◊ Equality Constrained Optimization:
  - ▷ Augmented Lagrangian methods.
  - ▷ Sequential quadratic programming methods.
- ◊ None of these techniques is easy.
  - ▷ The constraint carries lots of redundancies.

- A continuous approach:
  - ◊ The projection of the gradient of  $F$  can easily be calculated.
  - ◊ Projected gradient flow (Brockiet'88, Chu&Driessel'90):
 
$$\begin{aligned} \frac{dX}{dt} &= [X, [X, N]] \\ X(0) &= \Lambda. \end{aligned}$$
    - ▷  $X := Q^T \Lambda Q$ .
    - ▷ Flow  $X(t)$  moves in a descent direction to reduce  $\|X - N\|^2$ .
  - ◊ The optimal solution  $X$  can be fully characterized by the spectral decomposition of  $N$  and is unique.
- Evolution starts from an initial value and converges to the limit point, which solves the least squares problem.
  - ◊ The flow is built on the basis of systematically reducing the difference between the current position and the target position.
  - ◊ This is a descent flow.

# Equivalence

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- (Bloch'90) Suppose  $X$  is tridiagonal. Take

$$N = \text{diag}\{n, \dots, 2, 1\},$$

then

$$[X, N] = \Pi_0(X).$$

- A gradient flow hence becomes a Hamiltonian flow.

# Basic Form

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- Lax dynamics:

$$\begin{aligned} \frac{dX(t)}{dt} &:= [X(t), k_1(X(t))] \\ X(0) &:= X_0. \end{aligned}$$

- Parameter dynamics:

$$\begin{aligned} \frac{dg_1(t)}{dt} &:= g_1(t)k_1(X(t)) \\ g_1(0) &:= I. \end{aligned}$$

and

$$\begin{aligned} \frac{dg_2(t)}{dt} &:= k_2(X(t))g_2(t) \\ g_2(0) &:= I. \end{aligned}$$

$$\diamond k_1(X) + k_2(X) = X.$$

# Similarity Property

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

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

- Check

$$\begin{aligned} \frac{dZ}{dt} &= \frac{dg_1}{dt} X g_1^{-1} + g_1 \frac{dX}{dt} g_1^{-1} + g_1 X \frac{dg_1^{-1}}{dt} \\ &= (g_1 k_1(X)) X g_1^{-1} \\ &\quad + g_1 (X k_1(X) - k_1(X) X) g_1^{-1} \\ &\quad + g_1 X (-k_1(X) g_1^{-1}) \\ &= 0. \end{aligned}$$

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



# Decomposition Property

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

- Trivially  $\exp(X_0t)$  satisfies the IVP
- Define  $Z(t) = g_1(t)g_2(t)$ .
- Then  $Z(0) = I$  and

$$\frac{dZ}{dt} = X_0Z, Z(0) = I.$$

$$\begin{aligned} \frac{dZ}{dt} &= \frac{dg_1}{dt}g_2 + g_1\frac{dg_2}{dt} \\ &= (g_1k_1(X))g_2 + g_1(k_2(X)g_2) \\ &= g_1Xg_2 \\ &= X_0Z \quad (\text{by Similarity Property}). \end{aligned}$$

- By the uniqueness theorem in the theory of ordinary differential equations,  $Z(t) = \exp(X_0t)$ .

# Reversal Property

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

- By Decomposition Property,

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

# Abstraction

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- *QR*-type Decomposition:
  - ◊ Lie algebra decomposition of  $gl(n) \iff$  Lie group decomposition of  $Gl(n)$  in the neighborhood of  $I$ .
  - ◊ Arbitrary subspace decomposition  $gl(n) \iff$  Factorization of a *one-parameter semigroup* in the neighborhood of  $I$  as the product of two nonsingular matrices , i.e.,
 
$$\exp(X_0 t) = g_1(t)g_2(t).$$
  - ◊ The product  $g_1(t)g_2(t)$  will be called the *abstract  $g_1g_2$  decomposition* of  $\exp(X_0 t)$ .
- *QR*-type Algorithm:
  - ◊ By setting  $t = 1$ , we have
 
$$\begin{aligned} \exp(X(0)) &= g_1(1)g_2(1) \\ \exp(X(1)) &= g_2(1)g_1(1). \end{aligned}$$
  - ◊ The dynamical system for  $X(t)$  is autonomous  $\implies$  The above phenomenon will occur at every feasible integer time.
  - ◊ Corresponding to the abstract  $g_1g_2$  decomposition, the above iterative process for all feasible integers will be called the *abstract  $g_1g_2$  algorithm*.

# Matrix Groups

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- A subset of nonsingular matrices (over any field) which are closed under matrix multiplication and inversion is called a *matrix group*.
  - ◊ Matrix groups are central in many parts of mathematics and applications.
- A smooth manifold which is also a group where the multiplication and the inversion are smooth maps is called a *Lie group*.
  - ◊ The most remarkable feature of a Lie group is that the structure is the same in the neighborhood of each of its elements.
- (Howe'83) Every (non-discrete) matrix group is in fact a Lie group.
  - ◊ Algebra and geometry are intertwined in the study of matrix groups.
- Lots of realization processes used in numerical linear algebra are the results of group actions.

Group	Subgroup	Notation	Characteristics
General linear		$GL(n)$	$\{A \in \mathbb{R}^{n \times n} \mid \det(A) \neq 0\}$
	Special linear	$SL(n)$	$\{A \in GL(n) \mid \det(A) = 1\}$
Upper triangular		$\mathcal{U}(n)$	$\{A \in GL(n) \mid A \text{ is upper triangular}\}$
	Unipotent	$\mathcal{U}nip(n)$	$\{A \in \mathcal{U}(n) \mid a_{ii} = 1 \text{ for all } i\}$
Orthogonal		$\mathcal{O}(n)$	$\{Q \in GL(n) \mid Q^T Q = I\}$
Generalized orthogonal		$\mathcal{O}_S(n)$	$\{Q \in GL(n) \mid Q^T S Q = S\}; \quad S \text{ is a fixed matrix}$
	Symplectic	$Sp(2n)$	$\mathcal{O}_J(2n); \quad J := \begin{bmatrix} 0 & I \\ -I & 0 \end{bmatrix}$
	Lorentz	$\mathcal{L}or(n, k)$	$\mathcal{O}_L(n+k); \quad L := \text{diag}\{\underbrace{1, \dots, 1}_n, \underbrace{-1, \dots, -1}_k\}$
Affine		$\mathcal{A}ff(n)$	$\left\{ \begin{bmatrix} A & \mathbf{t} \\ \mathbf{0} & 1 \end{bmatrix} \mid A \in GL(n), \mathbf{t} \in \mathbb{R}^n \right\}$
	Translation	$\mathcal{T}rans(n)$	$\left\{ \begin{bmatrix} I & \mathbf{t} \\ \mathbf{0} & 1 \end{bmatrix} \mid \mathbf{t} \in \mathbb{R}^n \right\}$
	Isometry	$\mathcal{I}som(n)$	$\left\{ \begin{bmatrix} Q & \mathbf{t} \\ \mathbf{0} & 1 \end{bmatrix} \mid Q \in \mathcal{O}(n), \mathbf{t} \in \mathbb{R}^n \right\}$
Center of $G$		$Z(G)$	$\{z \in G \mid zg = gz, \text{ for every } g \in G\}, \quad G \text{ is a given group}$
Product of $G_1$ and $G_2$		$G_1 \times G_2$	$\{(g_1, g_2) \mid g_1 \in G_1, g_2 \in G_2\}; \quad (g_1, g_2) * (h_1, h_2) := (g_1 h_1, g_2 h_2); \quad G_1 \text{ and } G_2 \text{ are given groups}$
Quotient		$G/N$	$\{Ng \mid g \in G\}; \quad N \text{ is a fixed normal subgroup of } G$
	Hessenberg	$\mathcal{H}ess(n)$	$\mathcal{U}nip(n)/\mathcal{Z}_n$

# Group Actions

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- A function  $\mu : G \times \mathbb{V} \longrightarrow \mathbb{V}$  is said to be a *group action* of  $G$  on a set  $\mathbb{V}$  if and only if
  - ◊  $\mu(gh, \mathbf{x}) = \mu(g, \mu(h, \mathbf{x}))$  for all  $g, h \in G$  and  $\mathbf{x} \in \mathbb{V}$ .
  - ◊  $\mu(e, \mathbf{x}) = \mathbf{x}$ , if  $e$  is the identity element in  $G$ .
- Given  $\mathbf{x} \in \mathbb{V}$ , two important notions associated with a group action  $\mu$ :
  - ◊ The *stabilizer* of  $\mathbf{x}$  is
$$Stab_G(\mathbf{x}) := \{g \in G \mid \mu(g, \mathbf{x}) = \mathbf{x}\}.$$
  - ◊ The *orbit* of  $\mathbf{x}$  is
$$Orb_G(\mathbf{x}) := \{\mu(g, \mathbf{x}) \mid g \in G\}.$$

Set $V$	Group $G$	Action $\mu(g, A)$	Application
$\mathbb{R}^{n \times n}$	Any subgroup	$g^{-1}Ag$	conjugation
$\mathbb{R}^{n \times n}$	$\mathcal{O}(n)$	$g^{\top}Ag$	orthogonal similarity
$\underbrace{\mathbb{R}^{n \times n} \times \dots \times \mathbb{R}^{n \times n}}_k$	Any subgroup	$(g^{-1}A_1g, \dots, g^{-1}A_kg)$	simultaneous reduction
$S(n) \times SPD(n)$	Any subgroup	$(g^{\top}Ag, g^{\top}Bg)$	symm. positive definite pencil reduction
$\mathbb{R}^{n \times n} \times \mathbb{R}^{n \times n}$	$\mathcal{O}(n) \times \mathcal{O}(n)$	$(g_1^{\top}Ag_2, g_1^{\top}Bg_2)$	$QZ$ decomposition
$\mathbb{R}^{m \times n}$	$\mathcal{O}(m) \times \mathcal{O}(n)$	$g_1^{\top}Ag_2$	singular value decomp.
$\mathbb{R}^{m \times n} \times \mathbb{R}^{p \times n}$	$\mathcal{O}(m) \times \mathcal{O}(p) \times \mathcal{G}(n)$	$(g_1^{\top}Ag_3, g_2^{\top}Bg_3)$	generalized singular value decomp.

## Some Exotic Group Actions (yet to be studied!)

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- In numerical analysis, it is customary to use actions of the orthogonal group to perform the change of coordinates for the sake of cost efficiency and numerical stability.
  - ◊ What could be said if actions of the isometry group are used?
    - ▷ Being isometric, stability is guaranteed.
    - ▷ The inverse of an isometry matrix is easy.
 
$$\begin{bmatrix} Q & \mathbf{t} \\ \mathbf{0} & 1 \end{bmatrix}^{-1} = \begin{bmatrix} Q^\top & -Q^\top \mathbf{t} \\ \mathbf{0} & 1 \end{bmatrix}.$$
    - ▷ The isometry group is larger than the orthogonal group.

- What could be said if actions of the orthogonal group plus shift are used?

$$\mu((Q, s), A) := Q^\top A Q + sI, \quad Q \in \mathcal{O}(n), s \in \mathbb{R}_+.$$

- What could be said if action of the orthogonal group with scaling are used?

$$\mu((Q, s), A) := sQ^\top A Q, \quad Q \in \mathcal{O}(n), s \in \mathbb{R}_+,$$

or

$$\mu((Q, \mathbf{s}, \mathbf{t}), A) := \text{diag}\{\mathbf{s}\} Q^\top A Q \text{diag}\{\mathbf{t}\}, \quad Q \in \mathcal{O}, \mathbf{s}, \mathbf{t} \in \mathbb{R}_+^n.$$



# Tangent Space and Project Gradient

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- Given a group  $G$  and its action  $\mu$  on a set  $\mathbb{V}$ , the associated orbit  $Orb_G(\mathbf{x})$  characterizes the rule by which  $\mathbf{x}$  is to be changed in  $\mathbb{V}$ .
  - ◊ Depending on the group  $G$ , an orbit is often too “wild” to be readily traced for finding the “simplest form” of  $\mathbf{x}$ .
  - ◊ Depending on the applications, a path/bridge/highway/differential equation needs to be built on the orbit to connect  $\mathbf{x}$  to its simplest form.
- A differential equation on the orbit  $Orb_G(\mathbf{x})$  is equivalent to a differential equation on the group  $G$ .
  - ◊ Lax dynamics on  $X(t)$ .
  - ◊ Parameter dynamics on  $g_1(t)$  or  $g_2(t)$ .
- To stay in either the orbit or the group, the vector field of the dynamical system must be distributed in the tangent space of the corresponding manifold.
- Most of the tangent spaces for the matrix groups can be calculated explicitly.
- If some kind of objective function has been used to control the connecting bridge, its gradient should be projected to the tangent space.

# Tangent Space in General

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- Given a matrix group  $G \leq \mathcal{GL}(n)$ , the *tangent space* to  $G$  at  $A \in G$  can be defined as
 
$$\mathcal{T}_A G := \{\gamma'(0) \mid \gamma \text{ is a differentiable curve in } G \text{ with } \gamma(0) = A\}.$$
- The tangent space  $\mathfrak{g} = \mathcal{T}_I G$  at the identity  $I$  is critical.
  - ◊  $\mathfrak{g}$  is a Lie subalgebra in  $\mathbb{R}^{n \times n}$ , i.e.,
 
$$\text{If } \alpha'(0), \beta'(0) \in \mathfrak{g}, \text{ then } [\alpha'(0), \beta'(0)] \in \mathfrak{g}$$
  - ◊ The tangent space of a matrix group has the same structure everywhere, i.e.,
 
$$\mathcal{T}_A G = A\mathfrak{g}.$$
  - ◊  $\mathcal{T}_I G$  can be characterized as the *logarithm* of  $G$ , i.e.,
 
$$\mathfrak{g} = \{M \in \mathbb{R}^{n \times n} \mid \exp(tM) \in G, \text{ for all } t \in \mathbb{R}\}.$$

Group $G$	Algebra $\mathfrak{g}$	Characteristics
$GL(n)$	$gl(n)$	$\mathbb{R}^{n \times n}$
$SL(n)$	$sl(n)$	$\{M \in gl(n) \mid \text{trace}(M) = 0\}$
$Aff(n)$	$aff(n)$	$\left\{ \begin{bmatrix} M & \mathbf{t} \\ \mathbf{0} & 0 \end{bmatrix} \mid M \in gl(n), \mathbf{t} \in \mathbb{R}^n \right\}$
$O(n)$	$o(n)$	$\{K \in gl(n) \mid K \text{ is skew-symmetric}\}$
$Isom(n)$	$isom(n)$	$\left\{ \begin{bmatrix} K & \mathbf{t} \\ \mathbf{0} & 0 \end{bmatrix} \mid K \in o(n), \mathbf{t} \in \mathbb{R}^n \right\}$
$G_1 \times G_2$	$\mathcal{T}_{(e_1, e_2)} G_1 \times G_2$	$\mathfrak{g}_1 \times \mathfrak{g}_2$

# An Illustration of Projection

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- The tangent space of  $\mathcal{O}(n)$  at any orthogonal matrix  $Q$  is

$$\mathcal{T}_Q\mathcal{O}(n) = Q\mathbb{K}(n)$$

where

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

- The normal space of  $\mathcal{O}(n)$  at any orthogonal matrix  $Q$  is

$$\mathcal{N}_Q\mathcal{O}(n) = Q\mathbb{S}(n).$$

- The space  $\mathbb{R}^{n \times n}$  is split as

$$\mathbb{R}^{n \times n} = Q\mathbb{S}(n) \oplus Q\mathbb{K}(n).$$

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

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

- The projection of  $X$  onto the tangent space  $\mathcal{T}_Q\mathcal{O}(n)$  is given by

$$\text{Proj}_{\mathcal{T}_Q\mathcal{O}(n)} X = Q \left\{ \frac{1}{2}(Q^T X - X^T Q) \right\}.$$

# Canonical Forms

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- A canonical form refers to a “specific structure” by which a certain conclusion can be drawn or a certain goal can be achieved.
- The superlative adjective “simplest” is a relative term which should be interpreted broadly.
  - ◊ A matrix with a specified pattern of zeros, such as a diagonal, tridiagonal, or triangular matrix.
  - ◊ A matrix with a specified construct, such as Toeplitz, Hamiltonian, stochastic, or other linear varieties.
  - ◊ A matrix with a specified algebraic constraint, such as low rank or nonnegativity.

Canonical form	Also know as	Action
Bidiagonal $J$	Quasi-Jordan Decomp., $A \in \mathbb{R}^{n \times n}$	$P^{-1}AP = J,$ $P \in \mathcal{G}l(n)$
Diagonal $\Sigma$	Sing. Value Decomp., $A \in \mathbb{R}^{m \times n}$	$U^T AV = \Sigma,$ $(U, V) \in \mathcal{O}(m) \times \mathcal{O}(n)$
Diagonal pair $(\Sigma_1, \Sigma_2)$	Gen. Sing. Value Decomp., $(A, B) \in \mathbb{R}^{m \times n} \times \mathbb{R}^{p \times n}$	$(U^T AX, V^T BX) = (\Sigma_1, \Sigma_2),$ $(U, V, X) \in \mathcal{O}(m) \times \mathcal{O}(p) \times \mathcal{G}l(n)$
Upper quasi-triangular $H$	Real Schur Decomp., $A \in \mathbb{R}^{n \times n}$	$Q^T AQ = H,$ $Q \in \mathcal{O}(n)$
Upper quasi-triangular $H$ Upper triangular $U$	Gen. Real Schur Decomp., $A, B \in \mathbf{R}^{n \times n}$	$(Q^T AZ, Q^T BZ) = (H, U),$ $Q, Z \in \mathcal{O}(n)$
Symmetric Toeplitz $T$	Toeplitz Inv. Eigenv. Prob., $\{\lambda_1, \dots, \lambda_n\} \subset \mathbb{R}$ is given	$Q^T \text{diag}\{\lambda_1, \dots, \lambda_n\}Q = T,$ $Q \in \mathcal{O}(n)$
Nonnegative $N \geq 0$	Nonneg. inv. Eigenv. Prob., $\{\lambda_1, \dots, \lambda_n\} \subset \mathbb{C}$ is given	$P^{-1} \text{diag}\{\lambda_1, \dots, \lambda_n\}P = N,$ $P \in \mathcal{G}l(n)$
Linear variety $X$ with fixed entries at fixed locations	Matrix Completion Prob., $\{\lambda_1, \dots, \lambda_n\} \subset \mathbb{C}$ is given $X_{i,j,\nu} = a_\nu, \nu = 1, \dots, \ell$	$P^{-1}\{\lambda_1, \dots, \lambda_n\}P = X,$ $P \in \mathcal{G}l(n)$
Nonlinear variety with fixed singular values and eigenvalues	Test Matrix Construction, $\Lambda = \text{diag}\{\lambda_1, \dots, \lambda_n\}$ and $\Sigma = \text{diag}\{\sigma_1, \dots, \sigma_n\}$ are given	$P^{-1}\Lambda P = U^T \Sigma V$ $P \in \mathcal{G}l(n), U, V \in \mathcal{O}(n)$
Maximal fidelity	Structured Low Rank Approx. $A \in \mathbb{R}^{m \times n}$	$(\text{diag}(USS^T U^T))^{-1/2} USV^T,$ $(U, S, V) \in \mathcal{O}(m) \times \mathbb{R}_x^k \times \mathcal{O}(n)$

# Objective Functions

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- The orbit of a selected group action only defines the rule by which a transformation is to take place.
- Properly formulated objective functions helps to control the construction of a bridge between the current point and the desired canonical form on a given orbit.
  - ◊ The bridge often assumes the form of a differential equation on the manifold.
  - ◊ The vector field of the differential equation must distributed over the tangent space of the manifold.
  - ◊ Corresponding to each differential equation on the orbit of a group action is a differential equation on the group, and vice versa.
- **How to choose appropriate objective functions?**

## Some Flows on $Orb_{\mathcal{O}(n)}(X)$ under Conjugation

- Toda lattice arises from a special mass-spring system (Symes'82, Deift et al'83),

$$\frac{dX}{dt} = [X, \Pi_0(X)], \quad \Pi_0(X) = X^{-1} - X^{-T},$$

$X(0)$  = tridiagonal and symmetric.

- ◇ No specific objective function is used.
  - ▷ Physics law governs the definition of the vector field.
- ◇ Generalization to general matrices is totally by brutal force and blindness (*and by the then young and desperate researchers*) (Chu'84, Watkins'84).
 
$$\frac{dX}{dt} = [X, \Pi_0(G(X))], \quad G(z) \text{ is analytic over spectrum of } X(0).$$
  - ▷ But nicely explains the pseudo-convergence and convergence behavior of the classical QR algorithm for general and normal matrices, respectively.
  - ▷ Sorting of eigenvalues at the limit point is observed, but not quite clearly understood.



- Double bracket flow (Brockett'88),
 
$$\frac{dX}{dt} = [X, [X, N]], \quad N = \text{fixed and symmetric.}$$
  - ◊ This is the projected gradient flow of the objective function
 
$$\text{Minimize } F(Q) := \frac{1}{2} \|Q^T \Lambda Q - N\|^2,$$
 Subject to  $Q^T Q = I$ .
    - ▷ Sorting is necessary in the first order optimality condition (Wielandt&Hoffman'53).
- Take a special  $N = \text{diag}\{n, n - 1, \dots, 2, 1\}$ ,
  - ◊  $X$  is tridiagonal and symmetric  $\implies$  Double bracket flow  $\equiv$  Toda lattice (Bloch'90).
    - ▷ **Bingo!** The classical Toda lattice does have an objective function in mind.
  - ◊  $X$  is a general symmetric matrix  $\implies$  Double bracket = A specially scaled Toda lattice.
- Scaled Toda lattice (Chu'95),
 
$$\frac{dX}{dt} = [X, K \circ X], \quad K = \text{fixed and skew-symmetric.}$$
  - ◊ Flexible in componentwise scaling.
  - ◊ Enjoy very general convergence behavior.
  - ◊ But still no explicit objective function in sight.

## Some Flows on $Orb_{\mathcal{O}(m) \times \mathcal{O}(n)}(X)$ under Equivalence

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- Any flow on the orbit  $Orb_{\mathcal{O}(m) \times \mathcal{O}(n)}(X)$  under equivalence must be of the form

$$\frac{dX}{dt} = X(t)h(t) - k(t)X(t), \quad h(t) \in \mathbb{K}(n), \quad k(t) \in \mathbb{K}(m).$$

- $QZ$  flow (Chu '86),

$$\begin{aligned} \frac{dX_1}{dt} &= X_1 \Pi_0 (X_2^{-1} X_1) - \Pi_0 (X_1 X_2^{-1}) X_1, \\ \frac{dX_2}{dt} &= X_2 \Pi_0 (X_2^{-1} X_1) - \Pi_0 (X_1 X_2^{-1}) X_2, \end{aligned}$$

- $SVD$  flow (Chu '86),

$$\begin{aligned} \frac{dY}{dt} &= Y \Pi_0 (Y(t)^\top Y(t)) - \Pi_0 (Y(t) Y(t)^\top) Y, \\ Y(0) &= \text{bidiagonal}. \end{aligned}$$

- ◊ The "objective" in the design of this flow was to maintain the bidiagonal structure of  $Y(t)$  for all  $t$ .
- ◊ The flow gives rise to the Toda flows for  $Y^\top Y$  and  $Y Y^\top$ .

# Projected Gradient Flows

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- Given
  - ◊ A continuous matrix group  $G \subset \mathcal{GL}(n)$ .
  - ◊ A fixed  $X \in \mathbb{V}$  where  $\mathbb{V} \subset \mathbb{R}^{n \times n}$  be a subset of matrices.
  - ◊ A differentiable map  $f : \mathbb{V} \rightarrow \mathbb{R}^{n \times n}$  with a certain “inherent” properties, e.g., symmetry, isospectrum, low rank, or other algebraic constraints.
  - ◊ A group action  $\mu : G \times \mathbb{V} \rightarrow \mathbb{V}$ .
  - ◊ A projection map  $P$  from  $\mathbb{R}^{n \times n}$  onto a singleton, a linear subspace, or an affine subspace  $\mathbb{P} \subset \mathbb{R}^{n \times n}$  where matrices in  $\mathbb{R}$  carry a certain desired structure, e.g., the canonical form.

- Consider the functional  $F : G \rightarrow \mathbb{R}$

$$F(g) := \frac{1}{2} \|f(\mu(g, X)) - P(\mu(g, X))\|_F^2.$$

- ◊ Want to minimize  $F$  over  $G$ .
- Flow approach:
  - ◊ Compute  $\nabla F(g)$ .
  - ◊ Project  $\nabla F(g)$  onto  $\mathcal{T}_g G$ .
  - ◊ Follow the projected gradient until convergence.

## Some Old Examples

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- Brockett's double bracket flow (Brockett'88).
- Least squares approximation with spectral constraints (Chu&Driessel'90).

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

- Simultaneous reduction problem (Chu'91),

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

$$X_i(0) = A_i$$

- Nearest normal matrix problem (Chu'91),

$$\frac{dW}{dt} = \left[ W, \frac{1}{2} \{ [W, \text{diag}(W^*)] - [W, \text{diag}(W^*)]^* \} \right]$$

$$W(0) = A.$$

- Matrix with prescribed diagonal entries and spectrum (Schur-Horn Theorem) (Chu'95),

$$\dot{X} = [X, [\text{diag}(X) - \text{diag}(a), X]]$$

- Inverse generalized eigenvalue problem for symmetric-definite pencil (Chu&Guo'98).

$$\dot{X} = -((XW)^T + XW),$$

$$\dot{Y} = -((YW)^T + YW),$$

$$W := X(X - P_1(X)) + Y(Y - P_2(Y)).$$

- Various structured inverse eigenvalue problems (Chu&Golub'02).
- Remember the list of applications that Nicoletta gave on Monday!?!??

# New Thoughts

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- The idea of group actions, least squares, and the corresponding gradient flows can be generalized to other structures such as
  - ◊ Stiefel manifold  $\mathcal{O}(p, q) := \{Q \in \mathbb{R}^{p \times q} \mid Q^T Q = I_q\}$ .
  - ◊ The manifold of oblique matrices  $\mathcal{OB}(n) := \{Q \in \mathbb{R}^{n \times n} \mid \text{diag}(Q^T Q) = I_n\}$ .
  - ◊ Cone of nonnegative matrices.
  - ◊ Semigroups.
  - ◊ Low rank approximation.
- Using the product topology to describe separate groups and actions might broaden the applications.
- Any advantages of using the isometry group over the orthogonal group?

# Stochastic Inverse Eigenvalue Problem

- Construct a stochastic matrix with prescribed spectrum
  - ◊ A hard problem (Karpelevic'51, Minc'88).

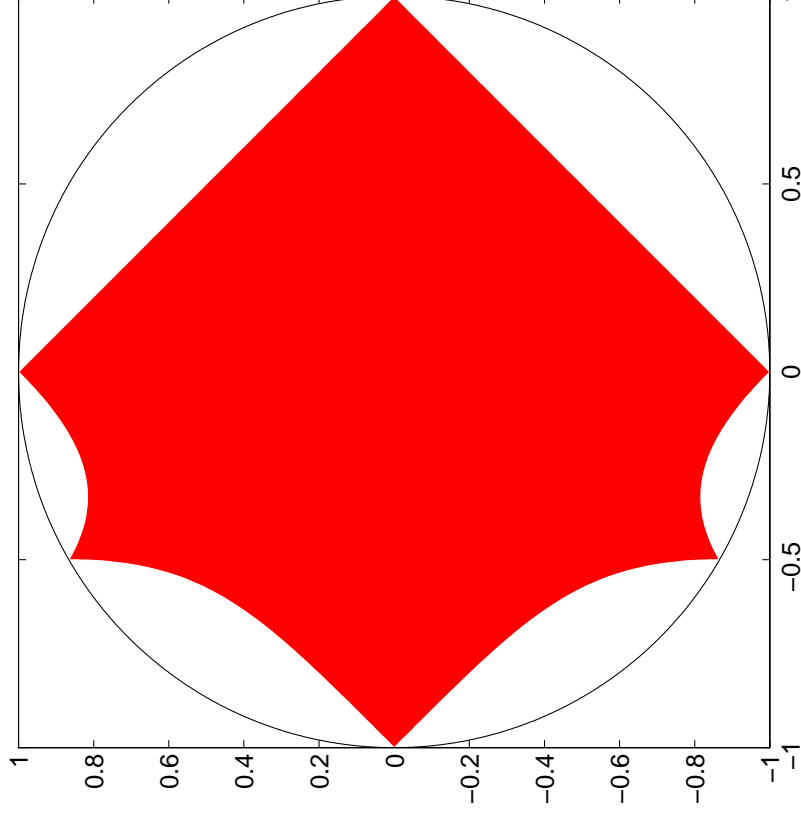


Figure 1:  $\Theta_4$  by the Karpelevič theorem.

- ◊ Would be done if the nonnegative inverse eigenvalue problem is solved – a long standing open question.

- Least squares formulation:

$$\text{Minimize } F(g, R) := \frac{1}{2} \|gJg^{-1} - R \circ R\|^2$$

Subject to  $g \in Gl(n), R \in gl(n)$ .

◇  $J$  = Real matrix carrying spectral information.

◇  $\circ$  = Hadamard product.

- Steepest descent flow:

$$\begin{aligned} \frac{dg}{dt} &= [(gJg^{-1})^T, \alpha(g, R)]g^{-T} \\ \frac{dR}{dt} &= 2\alpha(g, R) \circ R. \end{aligned}$$

◇  $\alpha(g, R) := gJg^{-1} - R \circ R$ .



- ASVD flow for  $g$  (Bunse-Gerstner et al'91, Wright'92):

$$\begin{aligned} g(t) &= X(t)S(t)Y(t)^T \\ \dot{g} &= \dot{X}SY^T + X\dot{S}Y^T + XSY^T \\ X^T \dot{g} Y &= \underbrace{X^T \dot{X}}_Z S + \dot{S} + S \underbrace{\dot{Y}^T Y}_W \end{aligned}$$

Define  $Q := X^T \dot{g} Y$ . Then

$$\begin{aligned} \frac{dS}{dt} &= \text{diag}(Q), \\ \frac{dX}{dt} &= XZ, \\ \frac{dY}{dt} &= YW. \end{aligned}$$

- ◊  $Z, W$  are skew-symmetric matrices obtainable from  $Q$  and  $S$ .

# Nonnegative Matrix Factorization

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- For various applications, given a nonnegative matrix  $A \in \mathbb{R}^{m \times n}$ , want to

$$\min_{0 \leq V \in \mathbb{R}^{m \times k}, 0 \leq H \in \mathbb{R}^{k \times n}} \frac{1}{2} \|A - VH\|_F^2.$$

- ◊ Relatively new techniques for dimension reduction applications.

- ▷ Image processing — no negative pixel values.
- ▷ Data mining — no negative frequencies.
- ◊ No firm theoretical foundation available yet (Tropp'03).

- Relatively easy by flow approach!

$$\min_{E \in \mathbb{R}^{m \times k}, F \in \mathbb{R}^{k \times n}} \frac{1}{2} \|A - (E \circ E)(F \circ F)\|_F^2.$$

- Gradient flow:

$$\begin{aligned} \frac{dV}{dt} &= V \circ (A - VH)H^T, \\ \frac{dH}{dt} &= H \circ (V^T(A - VH)). \end{aligned}$$

- ◊ Once any entry of either  $V$  or  $H$  hits 0, it stays zero. This is a natural barrier!
- ◊ The first order optimality condition is clear.

## Image Articulation Library

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- Assume images are composite objects in many articulations and poses.
- Factorization would enable the identification and classification of intrinsic “parts” that make up the object being imaged by multiple observations.
- Each column  $\mathbf{a}_j$  of a nonnegative matrix  $A$  now represents  $m$  pixel values of one image.
- The columns  $\mathbf{v}_k$  of  $V$  are  $k$  basis elements in  $\mathbb{R}^m$ .
- The columns of  $H$ , belonging to  $\mathbb{R}^k$ , can be thought of as coefficient sequences representing the  $n$  images in the basis elements.

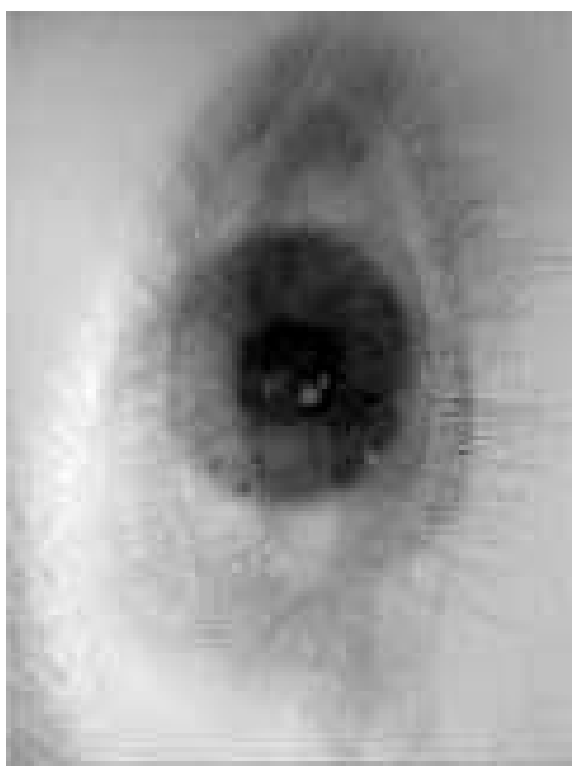
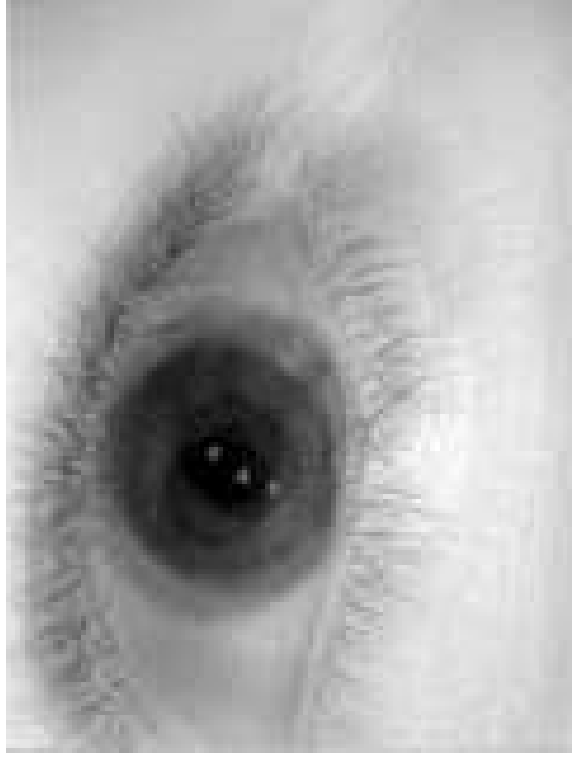
$A \in \mathbb{R}^{19200 \times 10}$  Representing 10 Gray-scale  $120 \times 160$  Irises

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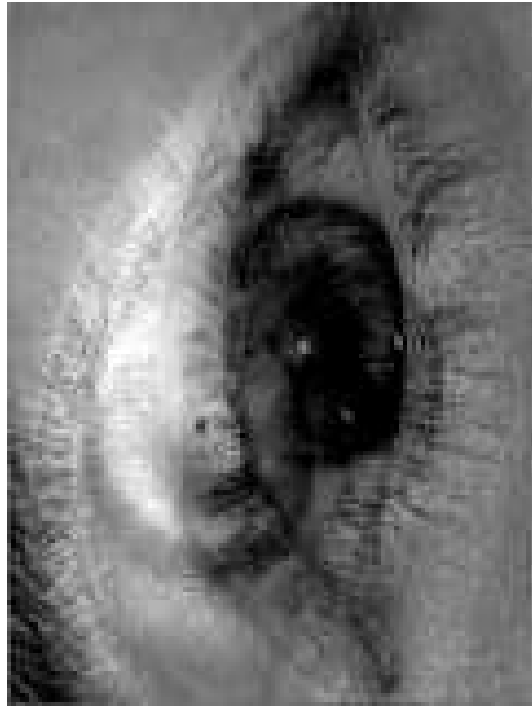
## Basis Irises with $k = 2$

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(Wrong?) Basis Irises with  $k = 4$

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# Conclusion

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- Many operations used to transform matrices can be considered as matrix group actions.
- The view unifies different transformations under the same framework of tracing orbits associated with corresponding group actions.
  - ◊ More sophisticated actions can be composed that might offer the design of new numerical algorithms.
  - ◊ As a special case of Lie groups, (tangent space) structure of a matrix group is the same at every of its element. Computation is easy and cheap.
- It is yet to be determined how a dynamical system should be defined over a group so as to locate the simplest form.
  - ◊ The notion of “simplicity” varies according to the applications.
  - ◊ Various objective functions should be used to control the dynamical systems.
  - ◊ Usually offers a global method for solving the underlying problem.
- Continuous realization methods often enable to tackle existence problems that are seemingly impossible to be solved by conventional discrete methods.
- Group actions together with properly formulated objective functions can offer a channel to tackle various classical or new and challenging problems.

- Some basic ideas and examples have been outlined in this talk.
- ◊ More sophisticated actions can be composed that might offer the design of new numerical algorithms.
- ◊ The list of application continues to grow.
- New computational techniques for structured dynamical systems on matrix group will further extend and benefit the scope of this interesting topic.
- ◊ Need ODE techniques specially tailored for gradient flows.
- ◊ Need ODE techniques suitable for very large-scale dynamical systems.
- ◊ **Help! Help! Help!**