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

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Motivation

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

- 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

- 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

- 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

- 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

- Eigenvalue Computation
- Constrained Least Squares Approximation

The Eigenvalue Problem

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

$$A_0 x = \lambda x$$

    for a nonzero vector x and a scalar λ.
- An iterative method :
  - ◇ The QR decomposition:

$$A = QR$$

    where Q is orthogonal and R is upper triangular.
  - ◇ The QR algorithm (Francis'61):

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

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

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

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

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

- A continuous approach:
  - ◇ The projection of the gradient of F can easily be calculated.
  - ◇ Projected gradient flow (Brocket'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

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

  $$N = \mathrm{diag}\{n, \ldots, 2, 1\},$$

  then

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

- A gradient flow hence becomes a Hamiltonian flow.

Basic Form

- 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

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

  - ◇ $k_1(X) + k_2(X) = X$.

Similarity Property

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

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

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

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

Decomposition Property

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

- Trivially $exp(X_0t)$ satisfies the IVP

$$\frac{dY}{dt} = X_0Y, Y(0) = I.$$

- Define $Z(t) = g_1(t)g_2(t)$.
- Then $Z(0) = I$ and

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

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

Reversal Property

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

- By Decomposition Property,

$$\begin{aligned} g_2(t)g_1(t) &= g_1(t)^{-1}exp(X_0t)g_1(t) \\ &= exp(g_1(t)^{-1}X_0g_1(t)t) \\ &= exp(X(t)t). \end{aligned}$$

Abstraction

- QR-type Decomposition:
  - ◇ Lie algebra decomposition of $gl(n) \Longleftrightarrow$ Lie group decomposition of $Gl(n)$ in the neighborhood of I.
  - ◇ Arbitrary subspace decomposition $gl(n) \Longleftrightarrow$ 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 $g_1 g_2$ 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 $\Longrightarrow$ The above phenomenon will occur at every feasible integer time.
  - ◇ Corresponding to the abstract $g_1 g_2$ decomposition, the above iterative process for all feasible integers will be called the *abstract $g_1 g_2$ algorithm*.

Matrix Groups

- 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		$\mathcal{G}l(n)$	$\{A \in \mathbb{R}^{n\times n} \vert \det(A) \neq 0\}$
	Special linear	$\mathcal{S}l(n)$	$\{A \in \mathcal{G}l(n) \vert \det(A) = 1\}$
Upper triangular		$\mathcal{U}(n)$	$\{A \in \mathcal{G}l(n) \vert A \text{ is upper triangular}\}$
	Unipotent	$\mathcal{U}nip(n)$	$\{A \in \mathcal{U}(n) \vert a_{ii} = 1 \text{ for all } i\}$
Orthogonal		$\mathcal{O}(n)$	$\{Q \in \mathcal{G}l(n) \vert Q^\top Q = I\}$
Generalized orthogonal		$\mathcal{O}_S(n)$	$\{Q \in \mathcal{G}l(n) \vert Q^\top SQ = S\}$; S is a fixed matrix
	Symplectic	$\mathcal{S}p(2n)$	$\mathcal{O}_J(2n)$; $J := \begin{bmatrix} 0 & I \\ -I & 0 \end{bmatrix}$
	Lorentz	$\mathcal{L}or(n,k)$	$\mathcal{O}_L(n+k)$; $L := \mathrm{diag}\{\underbrace{1,\ldots,1}_{n}, \underbrace{-1,\ldots -1}_{k}\}$
Affine		$\mathcal{A}ff(n)$	$\left\{\begin{bmatrix} A & \mathbf{t} \\ \mathbf{0} & 1 \end{bmatrix} \vert A \in \mathcal{G}l(n), \mathbf{t} \in \mathbb{R}^n\right\}$
	Translation	$\mathcal{T}rans(n)$	$\left\{\begin{bmatrix} I & \mathbf{t} \\ \mathbf{0} & 1 \end{bmatrix} \vert \mathbf{t} \in \mathbb{R}^n\right\}$
	Isometry	$\mathcal{I}som(n)$	$\left\{\begin{bmatrix} Q & \mathbf{t} \\ \mathbf{0} & 1 \end{bmatrix} \vert Q \in \mathcal{O}(n), \mathbf{t} \in \mathbb{R}^n\right\}$
Center of G		$Z(G)$	$\{z \in G \vert zg = gz, \text{ for every } g \in G\}$, G is a given group
Product of G_1 and G_2		$G_1 \times G_2$	$\{(g_1,g_2) \vert g_1 \in G_1, g_2 \in G_2\}$; $(g_1,g_2) * (h_1,h_2) := (g_1h_1, g_2h_2)$; G_1 and G_2 are given groups
Quotient		G/N	$\{Ng \vert g \in G\}$; N is a fixed normal subgroup of G
	Hessenberg	$\mathcal{H}ess(n)$	$\mathcal{U}nip(n)/\mathcal{Z}_n$

Group Actions

- 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 μ:
  - ◇ The *stabilizer* of $\mathbf{x}$ is
  $$Stab_G(\mathbf{x}) := \{g \in G | \mu(g, \mathbf{x}) = \mathbf{x}\}.$$
  - ◇ The *orbit* of $\mathbf{x}$ is
  $$Orb_G(\mathbf{x}) := \{\mu(g, \mathbf{x}) | g \in G\}.$$

Set $\mathbb{V}$	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
$\underbrace{\mathbb{R}^{n\times n} \times \ldots \times \mathbb{R}^{n\times n}}_{k}$	Any subgroup	$(g^{-1}A_1g, \ldots, g^{-1}A_kg)$	simultaneous reduction
$\mathbb{S}(n) \times \mathbb{S}_{PD}(n)$	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.
$\mathbb{R}^{m\times n} \times \mathbb{R}^{p\times n}$	$\mathcal{O}(m) \times \mathcal{O}(p) \times \mathcal{G}l(n)$	$(g_1^\top Ag_3, g_2^\top Bg_3)$	generalized singular value decomp.

Some Exotic Group Actions (yet to be studied!)

- 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?

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

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

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

or

$$\mu((Q,\mathbf{s},\mathbf{t}),A) := \mathrm{diag}\{\mathbf{s}\}Q^\top AQ\mathrm{diag}\{\mathbf{t}\}, \quad Q \in \mathcal{O}, \mathbf{s}, \mathbf{t} \in \mathbb{R}^n_\times.$$

Tangent Space and Project Gradient

- Given a group G and its action μ 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

- Given a matrix group $G \leq \mathcal{G}l(n)$, the *tangent space* to G at $A \in G$ can be defined as

$$\mathcal{T}_A G := \{\gamma'(0) | \gamma \text{ is a differentiable curve in } G \text{ with } \gamma(0) = A\}.$$

- 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.,

$$\mathfrak{g} = \{M \in \mathbb{R}^{n \times n} | \exp(tM) \in G, \text{ for all } t \in \mathbb{R}\}.$$

Group G	Algebra $\mathfrak{g}$	Characteristics
$\mathcal{G}l(n)$	$gl(n)$	$\mathbb{R}^{n\times n}$
$\mathcal{S}l(n)$	$sl(n)$	$\{M \in gl(n) \vert \mathrm{trace}(M) = 0\}$
$\mathcal{A}ff(n)$	$aff(n)$	$\{\begin{bmatrix} M & \mathbf{t} \\ \mathbf{0} & 0 \end{bmatrix} \mid M \in gl(n), \mathbf{t} \in \mathbb{R}^n\}$
$\mathcal{O}(n)$	$o(n)$	$\{K \in gl(n) \vert \mathrm{K\ is\ skew\text{-}symmetric}\}$
$\mathcal{I}som(n)$	$isom(n)$	$\{\begin{bmatrix} K & \mathbf{t} \\ \mathbf{0} & 0 \end{bmatrix} \mid K \in o(n), \mathbf{t} \in \mathbb{R}^n\}$
$G_1 \times G_2$	$\mathcal{T}_{(e_1,e_2)}G_1 \times G_2$	$\mathfrak{g}_1 \times \mathfrak{g}_2$

An Illustration of Projection

- 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 $X \in \mathbb{R}^{n\times n}$:
$$X = Q(Q^TX) = Q\left\{\frac{1}{2}(Q^TX - X^TQ)\right\} + Q\left\{\frac{1}{2}(Q^TX + X^TQ)\right\}.$$
- The projection of X onto the tangent space $\mathcal{T}_Q\mathcal{O}(n)$ is given by
$$\text{Proj}_{\mathcal{T}_Q\mathcal{O}(n)}X = Q\left\{\frac{1}{2}(Q^TX - X^TQ)\right\}.$$

Canoncial Forms

- 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 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 Σ	Sing. Value Decomp., $A \in \mathbb{R}^{m\times n}$	$U^\top AV = \Sigma$, $(U, V) \in \mathcal{O}(m) \times \mathcal{O}(n)$
Diagonal pair (Σ_1, Σ_2)	Gen. Sing. Value Decomp., $(A, B) \in \mathbb{R}^{m\times n} \times \mathbb{R}^{p\times n}$	$(U^\top AX, V^\top BX) = (\Sigma_1, \Sigma_2)$, $(U, V, X) \in \mathcal{O}(m) \times \mathcal{O}(p) \times \mathcal{G}l(n)$
Upper quasi-triangular H	Real Schur Decomp., $A \in \mathbb{R}^{n\times n}$	$Q^\top AQ = H$, $Q \in \mathcal{O}(n)$
Upper quasi-triangular H Upper triangular U	Gen. Real Schur Decomp., $A, B \in \mathbf{R}^{n\times n}$	$(Q^\top AZ, Q^\top BZ) = (H, U)$, $Q, Z \in \mathcal{O}(n)$
Symmetric Toeplitz T	Toeplitz Inv. Eigenv. Prob., $\{\lambda_1, \ldots, \lambda_n\} \subset \mathbb{R}$ is given	$Q^\top \mathrm{diag}\{\lambda_1, \ldots, \lambda_n\}Q = T$, $Q \in \mathcal{O}(n)$
Nonnegative $N \geq 0$	Nonneg. inv. Eigenv. Prob., $\{\lambda_1, \ldots, \lambda_n\} \subset \mathbb{C}$ is given	$P^{-1}\mathrm{diag}\{\lambda_1, \ldots, \lambda_n\}P = N$, $P \in \mathcal{G}l(n)$
Linear variety X with fixed entries at fixed locations	Matrix Completion Prob., $\{\lambda_1, \ldots, \lambda_n\} \subset \mathbb{C}$ is given $X_{i_\nu, j_\nu} = a_\nu, \nu = 1, \ldots, \ell$	$P^{-1}\{\lambda_1, \ldots, \lambda_n\}P = X$, $P \in \mathcal{G}l(n)$
Nonlinear variety with fixed singular values and eigenvalues	Test Matrix Construction, $\Lambda = \mathrm{diag}\{\lambda_1, \ldots, \lambda_n\}$ and $\Sigma = \mathrm{diag}\{\sigma_1, \ldots \sigma_n\}$ are given	$P^{-1}\Lambda P = U^\top \Sigma V$ $P \in \mathcal{G}l(n), \quad U, V \in \mathcal{O}(n)$
Maximal fidelity	Structured Low Rank Approx. $A \in \mathbb{R}^{m\times n}$	$\left(\mathrm{diag}\left(USS^\top U^\top\right)\right)^{-1/2} USV^\top$, $(U, S, V) \in \mathcal{O}(m) \times \mathbb{R}^k_\times \times \mathcal{O}(n)$

Objective Functions

- 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 el al'83),

$$\begin{aligned} \frac{dX}{dt} &= [X, \Pi_0(X)], \quad \Pi_0(X) = X^- - X^{-\top}, \\ X(0) &= \text{tridiagonal and symmetric.} \end{aligned}$$

  - ◇ 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),

$$\frac{dX}{dt} = [X, [X, N]], \qquad N = \text{fixed and symmetric.}$$

  - ◇ This is the projected gradient flow of the objective function

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

    - ▷ Sorting is necessary in the first order optimality condition (Wielandt&Hoffman'53).

- Take a special $N = \mathrm{diag}\{n, n-1, \ldots, 2, 1\}$,
  - ◇ X is tridiagonal and symmetric $\Longrightarrow$ 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 $\Longrightarrow$ Double bracket = A specially scaled Toda lattice.

- Scaled Toda lattice (Chu'95),

$$\frac{dX}{dt} = [X, K \circ X], \qquad K = \text{fixed and skew-symmetric.}$$

  - ◇ 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

- 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),

$$\begin{aligned} \frac{dX_1}{dt} &= X_1\Pi_0(X_2^{-1}X_1) - \Pi_0(X_1X_2^{-1})X_1, \\ \frac{dX_2}{dt} &= X_2\Pi_0(X_2^{-1}X_1) - \Pi_0(X_1X_2^{-1})X_2, . \end{aligned}$$

- SVD flow (Chu'86),

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

  - ⋄ 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 $YY^\top$.

Projected Gradient Flows

- Given
  - ◇ A continuous matrix group $G \subset \mathcal{G}l(n)$.
  - ◇ A fixed $X \in \mathbb{V}$ where $\mathbb{V} \subset \mathbb{R}^{n\times n}$ be a subset of matrices.
  - ◇ A differentiable map $f : \mathbb{V} \longrightarrow \mathbb{R}^{n\times n}$ with a certain "inherent" properties, e.g., symmetry, isospectrum, low rank, or other algebraic constraints.
  - ◇ A group action $\mu : G \times \mathbb{V} \longrightarrow \mathbb{V}$.
  - ◇ 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 $F : G \longrightarrow \mathbb{R}$

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

  - ◇ 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

- 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),

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

- Nearest normal matrix problem (Chu'91),

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

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

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

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

$$\begin{aligned} \dot{X} &= -\left((XW)^T + XW\right), \\ \dot{Y} &= -\left((YW)^T + YW\right), \\ W &:= X(X - P_1(X)) + Y(Y - P_2(Y)). \end{aligned}$$

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

New Thoughts

- The idea of group actions, least squares, and the corresponding gradient flows can be generalized to other structures such as
  - ◇ Stiefel manifold $\mathcal{O}(p,q) := \{Q \in \mathbb{R}^{p\times q} | Q^T Q = I_q\}$.
  - ◇ The manifold of oblique matrices $\mathcal{OB}(n) := \{Q \in \mathbb{R}^{n\times n} | \mathrm{diag}(Q^\top Q) = I_n\}$.
  - ◇ 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).

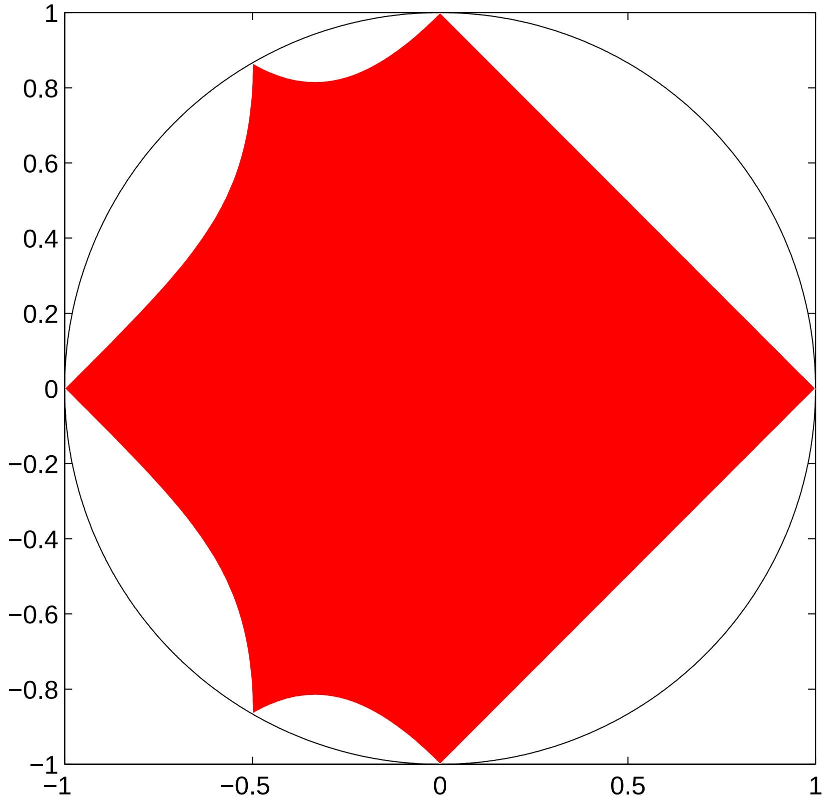


Figure 1: Θ_4 by the Karpelevič theorem.

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

- Least squares formulation:

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

  - ◇ 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):

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

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

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

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

Nonnegative Matrix Factorization

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

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

  - ◇ 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:

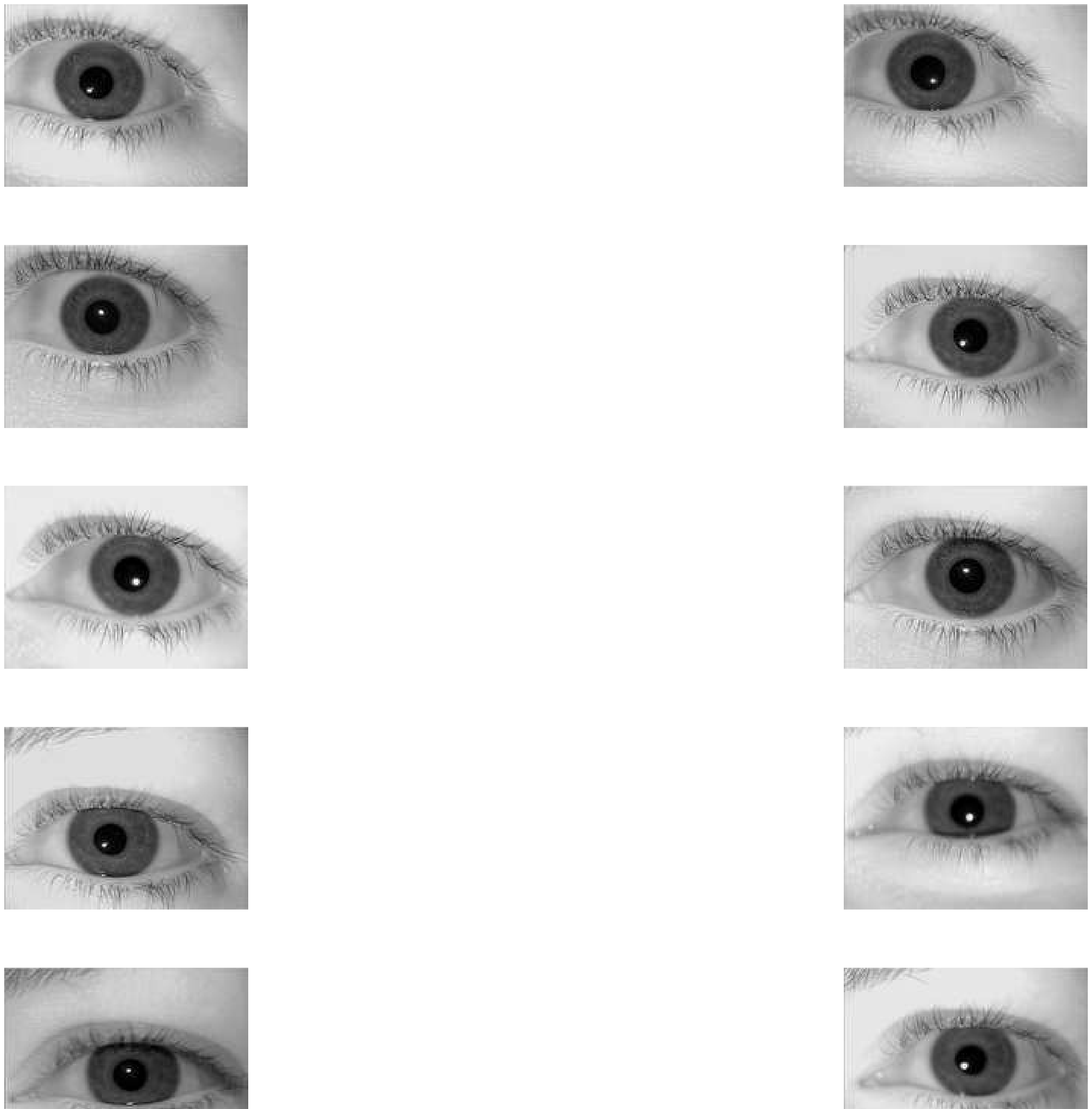
$$\begin{aligned} \frac{dV}{dt} &= V \circ (A - VH)H^\top), \\ \frac{dH}{dt} &= H \circ (V^\top (A - VH)). \end{aligned}$$

  - ◇ 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.

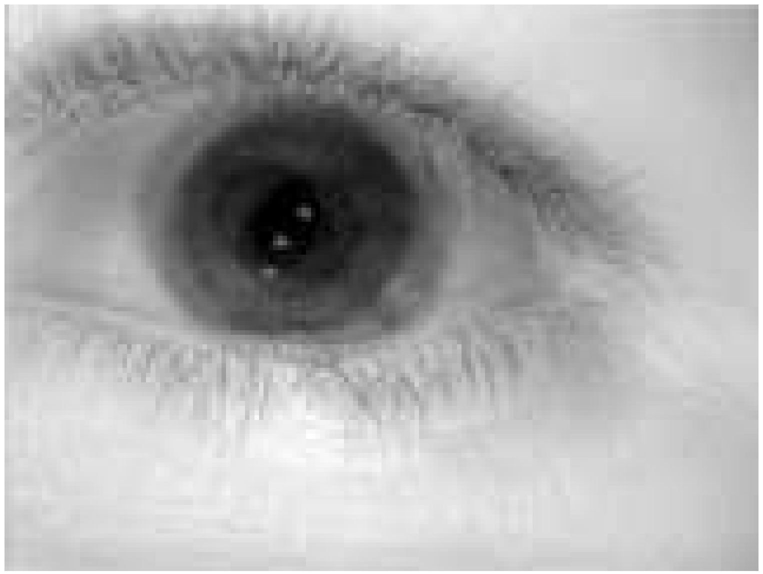
Image Articulation Library

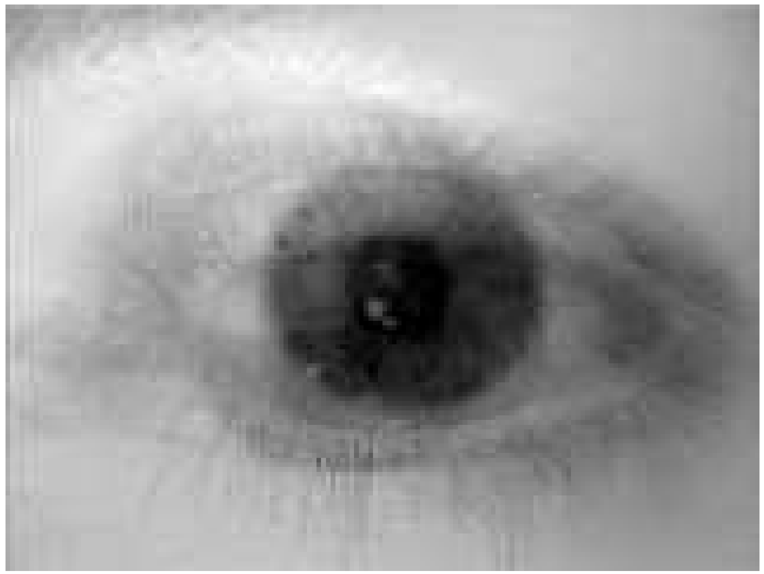
- Assume images are composite objects in many articulations and poses.
- Factorization would enable the identification and classification of intrinsic "parts" that make up the object being imaged by multiple observations.
- Each column $\mathbf{a}_j$ of a nonnegative matrix A now represents m pixel values 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 120×160 Irises

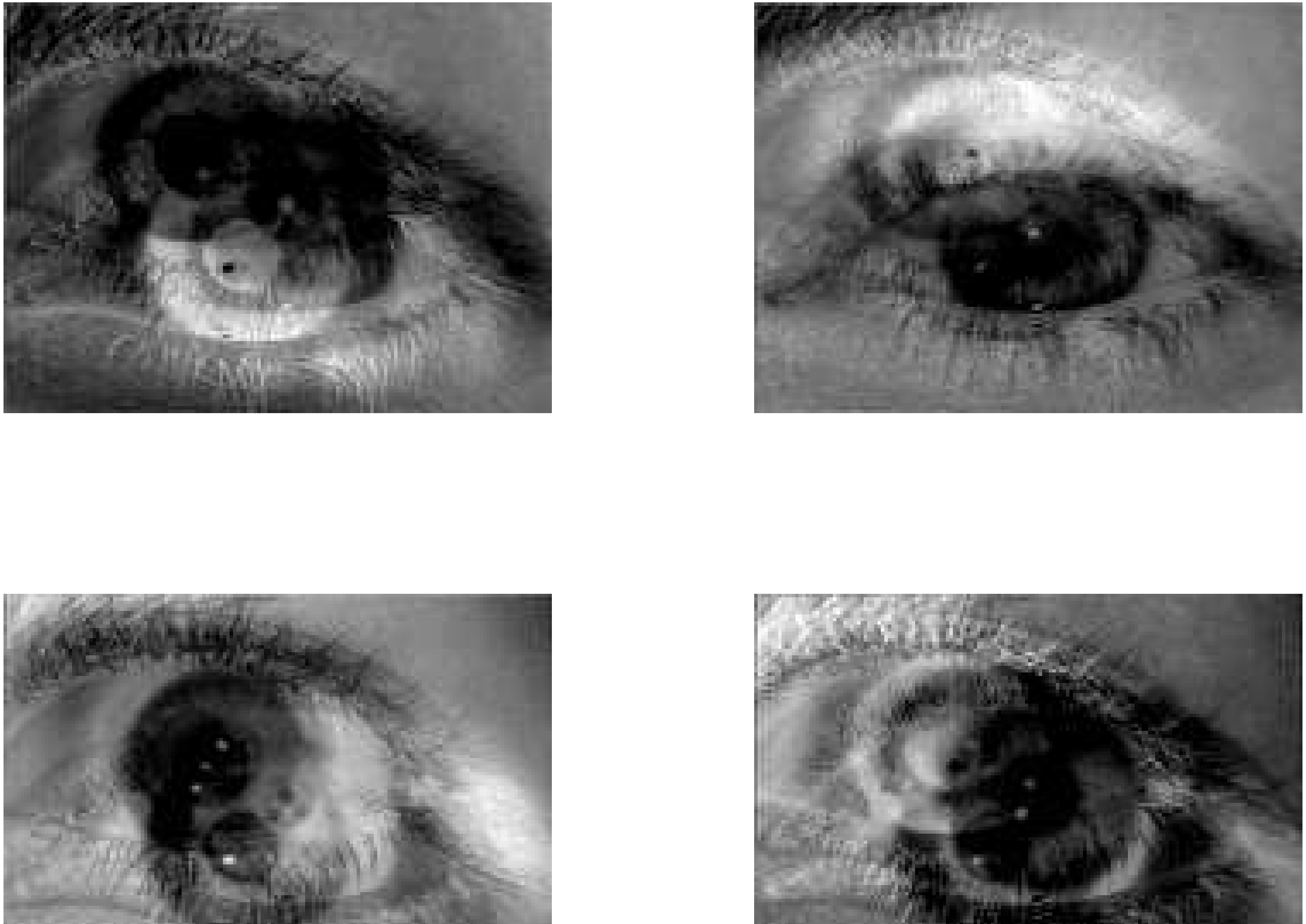


Basis Irises with $k = 2$





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



Conclusion

- 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!