A PATH TO PROCESS GENERAL MATRIX FIELDS

joint work with Bernhard Burgeth

Dagstuhl Seminar 18442 | November 1, 2018 | Andreas Kleefeld | Jülich Supercomputing Centre, Germany

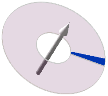
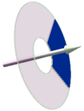
TABLE OF CONTENTS

Part I: Introduction & motivation

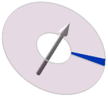
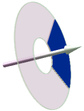
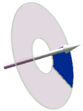
INTRODUCTION & MOTIVATION

Processing fields of rotation matrices

- Interpolation of rotation matrices?

$\frac{1}{2} \cdot$  $+ \; \frac{1}{2} \cdot$  $= \; ?$

- Interpolation specific for rotation matrices (M. Moakher, SIAM, 2002).

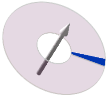
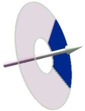
$\frac{1}{2} \odot$  $\oplus \; \frac{1}{2} \odot$  $=$ 

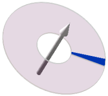
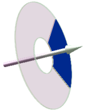
- What about further operations?
- What about other classes of matrices?

INTRODUCTION & MOTIVATION

Beyond symmetric matrices (B. Burgeth & A. K., Springer, 2017)

- Unifying concept for $\mathrm{psup}/\mathrm{pinf}$ of rotations R_1, R_2 in $\mathbb{R}^d$?

$\mathrm{psup}\Big($  ,  $\Big) = $?

$\mathrm{pinf}\Big($  ,  $\Big) = $?

- What about other classes of non-symmetric matrices?
- Generalize $\mathrm{Sym}(n)$.
- Idea: Complexification, Hermitian matrices, $\mathrm{Her}(n)$.

Part II: Calculus for Hermitian matrices

CALCULUS FOR HERMITIAN MATRICES

Basic properties

- $\mathrm{Her}(n) = \{\mathbf{H} \in \mathbb{C}^{n\times n} \,|\, \mathbf{H} = \mathbf{H}^*\}$ is $\mathbb{R}$-vector space.
  - * stands for transposition with complex conjugation.
- $\mathbf{H} = \mathrm{Re}(\mathbf{H}) + \mathrm{Im}(\mathbf{H})\mathrm{i}\,,$
  - Symmetric real part $\mathrm{Re}(\mathbf{H})\,.$
  - Skew-symmetric imaginary part $\mathrm{Im}(\mathbf{H})\,.$
- $\mathbf{H}$ unitarily diagonalizable: $\mathbf{H} = \mathbf{U}\mathbf{D}\mathbf{U}^*\,,$
  - $\mathbf{U}$ unitary: $\mathbf{U}^*\mathbf{U} = \mathbf{U}\mathbf{U}^* = \mathbf{I}\,.$
  - $\mathbf{D} = \mathrm{diag}(d_1, \ldots, d_n)$ diagonal matrix with real-valued $d_1 \geq \ldots \geq d_n\,.$
- Loewner order: $\mathbf{H}_1 \geq \mathbf{H}_2 \iff \mathbf{H}_1 - \mathbf{H}_2$ positive semidefinite.

CALCULUS FOR HERMITIAN MATRICES

Dictionary for Hermitian matrices

Setting	Scalar-valued	Matrix-valued
Function	$f : \begin{cases} \mathbb{R} \longrightarrow \mathbb{R} \\ x \mapsto f(x) \end{cases}$	$F : \begin{cases} \mathrm{Her}(n) \longrightarrow \mathrm{Her}(n) \\ \mathbf{H} \mapsto \mathbf{U}\,\mathrm{diag}(f(d_1), \dots, f(d_n))\,\mathbf{U}^* \end{cases}$
Partial derivatives	$\partial_\omega h$, $\omega \in \{t, x_1, \dots, x_d\}$	$\overline{\partial}_\omega \mathbf{H} := (\partial_\omega h_{ij})_{ij}$, $\omega \in \{t, x_1, \dots, x_d\}$
Gradient	$\nabla h(x) := (\partial_{x_1} h(x), \dots, \partial_{x_d} h(x))^\top$, $\nabla h(x) \in \mathbb{R}^d$	$\overline{\nabla}\mathbf{H}(x) := (\overline{\partial}_{x_1} \mathbf{H}(x), \dots, \overline{\partial}_{x_d} \mathbf{H}(x))^\top$, $\overline{\nabla}\mathbf{H}(x) \in (\mathrm{Her}(n))^d$

CALCULUS FOR HERMITIAN MATRICES

Dictionary for Hermitian matrices

Setting	Scalar-valued	Matrix-valued
Length	$\|w\|_p := \sqrt[p]{\|w_1\|^p + \cdots + \|w_d\|^p}$, $\|w\|_p \in [0, +\infty[$	$\|\|\|\mathbf{W}\|\|\|_p := \sqrt[p]{\|\mathbf{W}_1\|^p + \cdots + \|\mathbf{W}_d\|^p}$, $\|\|\|\mathbf{W}\|\|\|_p \in \mathrm{Her}^+(n)$
Supremum	$\sup(a, b)$	$\mathrm{psup}(\mathbf{A}, \mathbf{B}) = \frac{1}{2}(\mathbf{A} + \mathbf{B} + \|\mathbf{A} - \mathbf{B}\|)$
Infimum	$\inf(a, b)$	$\mathrm{pinf}(\mathbf{A}, \mathbf{B}) = \frac{1}{2}(\mathbf{A} + \mathbf{B} - \|\mathbf{A} - \mathbf{B}\|)$

Image processing tools for symmetric matrices carry over to Hermitian matrices.

CALCULUS FOR HERMITIAN MATRICES

Embedding $\mathrm{M}_{\mathbb{R}}(n)$ into $\mathrm{Her}(n)$

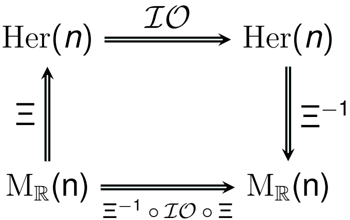
- Linear mapping $\Xi : \mathrm{M}_{\mathbb{R}}(\mathrm{n}) \longrightarrow \mathrm{Her}(n)$

$$\Xi : \mathbf{M} \longmapsto \frac{1}{2}(\mathbf{M} + \mathbf{M}^{\top}) + \frac{\mathrm{i}}{2}(\mathbf{M} - \mathbf{M}^{\top})$$

- Inverse mapping $\Xi^{-1} : \mathrm{Her}(n) \longrightarrow \mathrm{M}_{\mathbb{R}}(\mathrm{n})$

$$\Xi^{-1} : \mathbf{H} \longmapsto \frac{1}{2}(\mathbf{H} + \mathbf{H}^{\top}) - \frac{\mathrm{i}}{2}(\mathbf{H} - \mathbf{H}^{\top})$$

- Processing strategy:



- Operations on Hermitian matrices via operator $\mathcal{IO}$.
- $\mathcal{IO}$ represents averaging, psup, pinf, time-step in numerical scheme, etc.

Part III: Processing orthogonal matrices

PROCESSING ORTHOGONAL MATRICES

Processing orthogonal matrices, $\mathbf{Q} \in \mathrm{O}(n)$

- $\mathrm{O}(n) \subset \mathrm{M}_{\mathbb{R}}(\mathrm{n})$
- There is a problem.
  - **Before** processing: $\mathbf{Q} \in \mathrm{O}(n)$.
  - **After** processing: $(\Xi^{-1} \circ \mathcal{IO} \circ \Xi)(\mathbf{Q}) \notin \mathrm{O}(n)$.
- There is a remedy.
  - Projection from $\mathrm{M}_{\mathbb{R}}(\mathrm{n})$ back to $\mathrm{O}(n)$ via best Frobenius norm approximation $\tilde{\mathbf{Q}} \in \mathrm{O}(n)$

$$\|(\Xi^{-1} \circ \mathcal{O} \circ \Xi)(\mathbf{Q}) - \tilde{\mathbf{Q}}\|_{\mathrm{F}}^2 \longrightarrow \min .$$

- This **nearest matrix problem** allows for explicit solution:
  - Orthogonal factor in polar decomposition of $\mathbf{M}$.
  - $\tilde{\mathbf{Q}} = \mathcal{P}_{\mathrm{O}(n)}(\mathbf{M}) = \mathbf{M} \left(\mathbf{M}^\top \mathbf{M}\right)^{-1/2}$.

PROCESSING ORTHOGONAL MATRICES

Projection into $\mathrm{O}(n)$

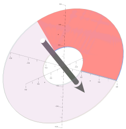
- Augmented processing strategy

$$
\begin{array}{ccccc}
 & \mathrm{Her}(n) & \xrightarrow{\;\mathcal{I}\mathcal{O}\;} & \mathrm{Her}(n) & \\
 & \Xi \Big\Uparrow & & \Big\Downarrow \Xi^{-1} & \\
\mathrm{O}(n) \subset & \mathrm{M}_{\mathbb{R}}(\mathrm{n}) & \xrightarrow[\Xi^{-1} \circ \mathcal{I}\mathcal{O} \circ \Xi]{} & \mathrm{M}_{\mathbb{R}}(\mathrm{n}) & \xrightarrow[\mathcal{P}_{\mathrm{O}(n)}]{} \mathrm{O}(n)
\end{array}
$$

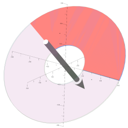
- General strategy allows for processing of
  - any square real matrix $\in \mathrm{M}_{\mathbb{R}}(\mathrm{n})$.
  - any matrices from an “interesting” subset $\mathrm{S} \subset \mathrm{M}_{\mathbb{R}}(\mathrm{n})$.
- But $\mathcal{P}_{\mathrm{S}}$ needs to be calculated.

PROCESSING ORTHOGONAL MATRICES

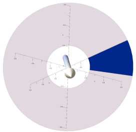
Experiments in $\mathrm{SO}(3)$



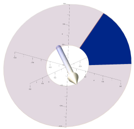
$\mathbf{R}_1$



$\mathrm{psup}(\mathbf{R}_1, \mathbf{R}_2)$



$\mathrm{pinf}(\mathbf{R}_1, \mathbf{R}_2)$



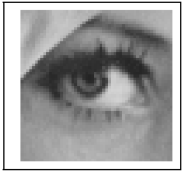
$\mathbf{R}_2$

Pseudo-supremum and pseudo-infimum of two rotations.

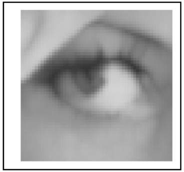
PROCESSING ORTHOGONAL MATRICES

Experiments in $\mathrm{SO}(2)$ and $\mathrm{SO}(3)$, B. Burgeth & A. K., LNCS 10225, 2017

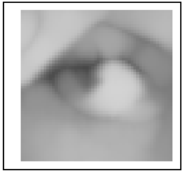
- Scalar ($\rightarrow$ angle ϕ) image as rotations in $\mathrm{SO}(2)$.



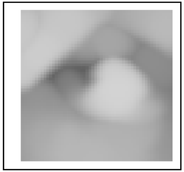
Original



Dilation, $T = 2$



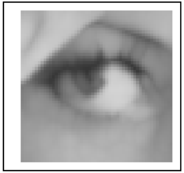
Dilation, $T = 4$



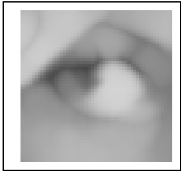
Dilation, $T = 6$

- Scalar ($\rightarrow$ angle ϕ) image as rotations in $\mathrm{SO}(3)$, **single axis**.

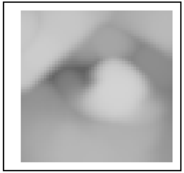
Original



Dilation, $T = 2$



Dilation, $T = 4$

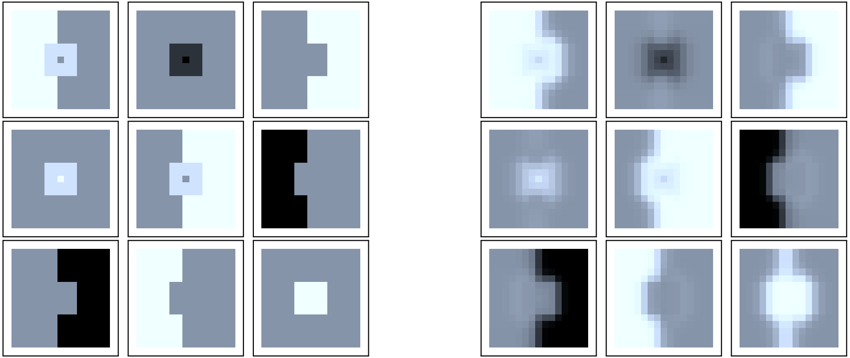


Dilation, $T = 6$

PROCESSING ORTHOGONAL MATRICES

Experiment in $\mathrm{SO}(3)$

- Tiled view: original 15×15-field of $\mathrm{SO}(3)$-matrices, its dilation with $T = 1$.

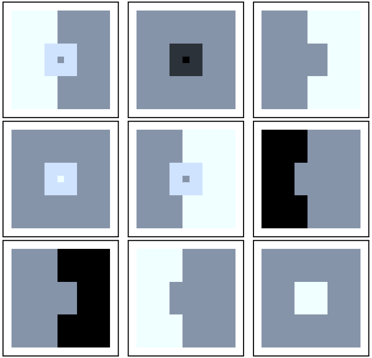


Original $\mathrm{SO}(3)$ field   Dilated $\mathrm{SO}(3)$ field, $T = 1$

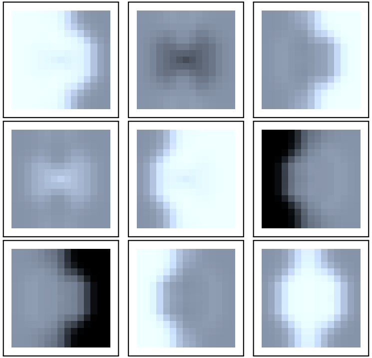
PROCESSING ORTHOGONAL MATRICES

Experiment in $\mathrm{SO}(3)$

- Tiled view: original 15×15-field of $\mathrm{SO}(3)$-matrices, its dilation with $T = 2$.



Original $\mathrm{SO}(3)$ field



Dilated $\mathrm{SO}(3)$ field, $T = 2$

Part IV: Processing Moebius transformations

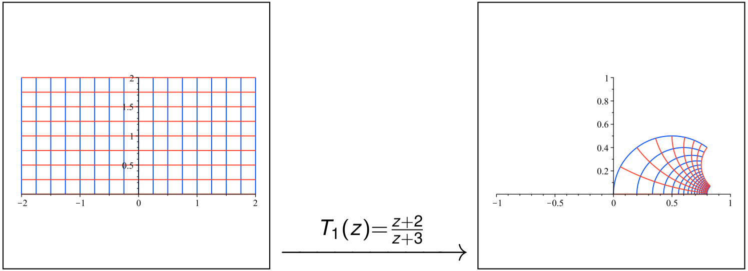
PROCESSING MOEBIUS TRANSFORMATIONS

Setup and illustrative example

- Moebius transformations are given by

$$T(z) = \frac{az+b}{cz+d}\,, \qquad ad - bc \neq 0\,.$$

- Play an important role in hyperbolic geometry.
- They represent motions in the Poincaré half-space model.



PROCESSING MOEBIUS TRANSFORMATIONS

Setup and illustrative example

- Algebraic description via matrices of the form

$$\mathbf{T} = \begin{pmatrix} a & b \\ c & d \end{pmatrix} .$$

  with $a, b, c, d \in \mathbb{R}$ and $ad - bc \neq 0$.
- Matrices are elements of $\mathrm{M}_{\mathbb{R}}(2)$ with determinant $\neq 0$.
- Hence, $\mathbf{T} \in \mathrm{Gl}_2(\mathbb{R})$.
- Pointcaré half model

$$\mathbb{H} = \{z = x + \mathrm{i}y \in \mathbb{C} \,:\, x \in \mathbb{R} \,,\ y > 0\}$$

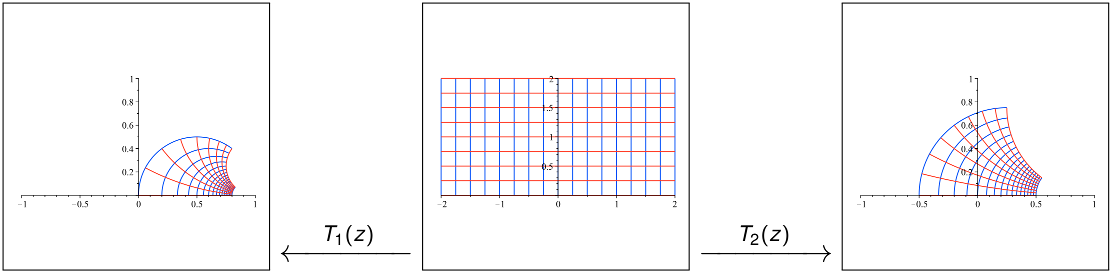
  is invariant under Moebius transformations.

PROCESSING MOEBIUS TRANSFORMATIONS

Example

$$T_1(z) = \frac{z+2}{z+3}, \quad \mathbf{T}_1 = \begin{pmatrix} 1 & 2 \\ 1 & 3 \end{pmatrix}$$

$$T_2(z) = \frac{z+1}{z+4}, \quad \mathbf{T}_2 = \begin{pmatrix} 1 & 1 \\ 1 & 4 \end{pmatrix}$$



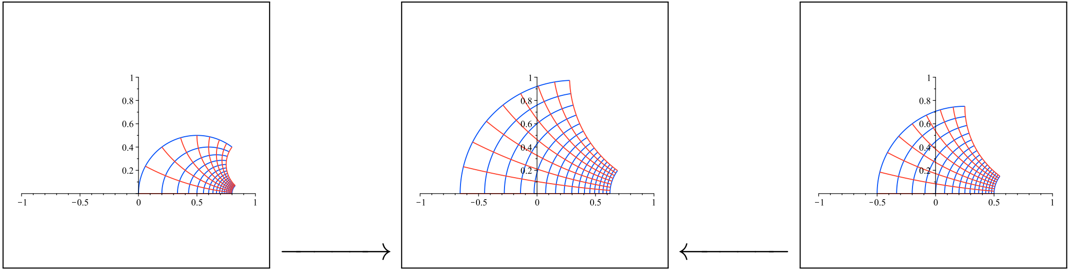
What is the pseudo supremum and infimum of two Moebius transformations?

PROCESSING MOEBIUS TRANSFORMATIONS

Example pseudo supremum

$$\mathbf{T}_1 = \begin{pmatrix} 1 & 2 \\ 1 & 3 \end{pmatrix}, \qquad \mathbf{T}_2 = \begin{pmatrix} 1 & 1 \\ 1 & 4 \end{pmatrix},$$

$$\mathbf{T}_{\mathrm{psup}} = \mathrm{psup}\left(\mathbf{T}_1, \mathbf{T}_2\right) \approx \begin{pmatrix} 1.2887 & 1.2113 \\ 1.0000 & 4.0774 \end{pmatrix}$$



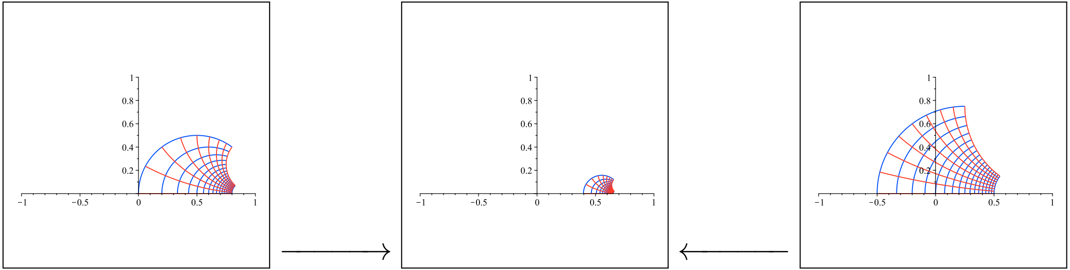
$\mathbf{T}_1$ $\qquad$ $\mathbf{T}_{\mathrm{psub}}$ $\qquad$ $\mathbf{T}_2$

PROCESSING MOEBIUS TRANSFORMATIONS

Example pseudo infimum

$$\mathbf{T}_1 = \begin{pmatrix} 1 & 2 \\ 1 & 3 \end{pmatrix}, \qquad \mathbf{T}_2 = \begin{pmatrix} 1 & 1 \\ 1 & 4 \end{pmatrix},$$

$$\mathbf{T}_{\mathrm{pinf}} = \mathrm{pinf}\,(\mathbf{T}_1, \mathbf{T}_2) \approx \begin{pmatrix} 0.7113 & 1.7887 \\ 1.0000 & 2.9226 \end{pmatrix}$$



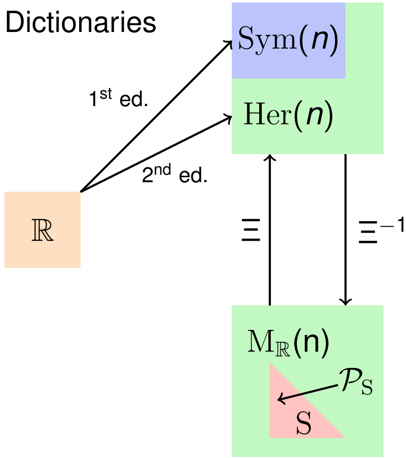
$\mathbf{T}_1$ $\qquad$ $\mathbf{T}_{\mathrm{pinf}}$ $\qquad$ $\mathbf{T}_2$

Part V: Summary & outlook

SUMMARY & OUTLOOK

Summary

- Transition from scalar calculus to calculus for symmetric matrices.
- Proposed an extension to Hermitian matrices.
- 1-to-1 link to general square matrices.
- Specialization to "interesting" matrix subsets possible, for example $\mathrm{S} = \mathrm{O}(n)$.



SUMMARY & OUTLOOK

Outlook

- Extending the "dictionary".
- Considering other interesting classes of matrices.
- Solving (numerically) nearest matrix problems.
- Looking for interesting fields of applications:
  - Material science (crack formation), problem size: $10^3 \times 10^3 \times 10^3$-grid, 10 matrix entries, 10^3-iterations.
  - Processing of correlation matrices within "big data".
  - High resolution 10^7, multispectral $(10^2)^2$ images, 10^3-iterations.
- Visualization is a problem.
- Increasing the efficiency of computations.
- HPC for real applications are necessary.

REFERENCES

Partial list

- B. Burgeth & A. Kleefeld, *Towards Processing Fields of General Real-Valued Square Matrices*, Modeling, Analysis, and Visualization of Anisotropy, Springer, 115–144 (2017).
- B. Burgeth & A. Kleefeld, *A Unified Approach to PDE-Driven Morphology for Fields of Orthogonal and Generalized Doubly-Stochastic Matrices*, Springer LNCS 10225, 284–295 (2017).
- A. Kleefeld, A. Meyer-Baese, & B. Burgeth, *Elementary Morphology for SO(2)- and SO(3)-Orientation Fields*, Springer LNCS 9082, 458–469 (2015).