



A PATH TO PROCESS GENERAL MATRIX FIELDS

joint work with Bernhard Burgeth

Workshop Data Science | January 30, 2019 | Andreas Kleefeld | Jülich Supercomputing Centre, Germany

INTRODUCTION

Mathematics Division

Head: Prof. Dr. Johannes Grotendorst



Methods, Algorithms & Tools Lab



Daniel Abele



Dr. Andreas Kleefeld



Christof Päßler



Lukas Pieronek

INTRODUCTION & MOTIVATION

Data processing (difficulty: **easy**)

- E.g. **gray-valued** image processing.
- Tools: mathematical morphology (discrete or continuous).
- PDE-based processing (e.g. Perona-Malik diffusion, coherence-enhancing anisotropic diffusion).
- Prerequisites: linear combinations, discretizations of derivatives, roots/powers, max/min.



INTRODUCTION & MOTIVATION

Data processing (difficulty: **medium**)

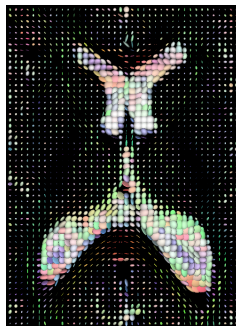
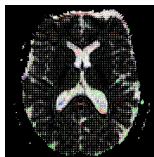
- What about color images/multispectral images (**vector-valued** data)?
- No standard ordering available.
- Channel-wise approach, lexicographic ordering, etc.
- Problem: false-colors phenomenon (interchannel relationships are ignored).



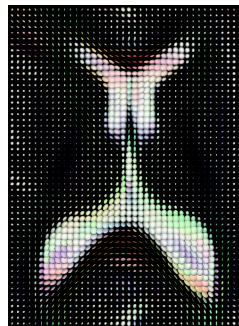
INTRODUCTION & MOTIVATION

Data processing (difficulty: **hard**)

- What about **matrix-valued** data, e.g. positive semi-definite matrices (DT-MRI)?
- Linear combinations, roots/powers, discretization of derivatives ready for use.
- Max/min is available (Loewner ordering).
- **Catch:** only partial ordering.



Real DT-MRI data



MCED

- In other applications: matrices of a matrix field are **not** symmetric!
- E.g. material science: stress/strain tensors can lose symmetry; diagonalization: rotation fields.

INTRODUCTION & MOTIVATION

Data processing (difficulty: **bring it on**)

- Interpolation of rotation matrices?

$$\frac{1}{2} \cdot \text{[Diagram 1]} + \frac{1}{2} \cdot \text{[Diagram 2]} = ?$$

The diagram shows two ellipses representing rotation matrices. The first ellipse is light purple with a white circle in the center, a black arrow pointing up-right, and a blue arrow pointing down-right. The second ellipse is light purple with a white circle in the center, a black arrow pointing up-left, and a blue arrow pointing down-left. The result is a question mark.

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

$$\frac{1}{2} \odot \text{[Diagram 1]} \oplus \frac{1}{2} \odot \text{[Diagram 2]} = \text{[Diagram 3]}$$

The diagram shows two ellipses representing rotation matrices. The first ellipse is light purple with a white circle in the center, a black arrow pointing up-right, and a blue arrow pointing down-right. The second ellipse is light purple with a white circle in the center, a black arrow pointing up-left, and a blue arrow pointing down-left. The result is a single ellipse representing the interpolated rotation matrix, which is light purple with a white circle in the center, a black arrow pointing up-right, and a blue arrow pointing down-left.

- What about further operations?
- What about other classes of non-symmetric matrices?
- **Idea:** complexification, Hermitian matrices, $\text{Her}(n)$.

CALCULUS FOR HERMITIAN MATRICES

Basic properties

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

CALCULUS FOR HERMITIAN MATRICES

Dictionary for Hermitian matrices

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

CALCULUS FOR HERMITIAN MATRICES

Dictionary for Hermitian matrices

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

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

CALCULUS FOR HERMITIAN MATRICES

Embedding $M_{\mathbb{R}}(n)$ into $\text{Her}(n)$

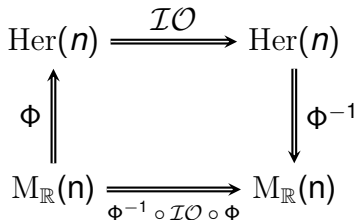
- Linear mapping $\Phi : M_{\mathbb{R}}(n) \longrightarrow \text{Her}(n)$

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

- Inverse mapping $\Phi^{-1} : \text{Her}(n) \longrightarrow M_{\mathbb{R}}(n)$

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

- Processing strategy:



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

PROCESSING ORTHOGONAL MATRICES

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

- $O(n) \subset M_{\mathbb{R}}(n)$
- There is a problem.
 - **Before** processing: $\mathbf{Q} \in O(n)$.
 - **After** processing: $(\Phi^{-1} \circ \mathcal{IO} \circ \Phi)(\mathbf{Q}) \notin O(n)$.
- There is a remedy.
 - Projection from $M_{\mathbb{R}}(n)$ back to $O(n)$ via best Frobenius norm approximation $\tilde{\mathbf{Q}} \in O(n)$
$$\|(\Phi^{-1} \circ \mathcal{O} \circ \Phi)(\mathbf{Q}) - \tilde{\mathbf{Q}}\|_F^2 \longrightarrow \min .$$
- This **nearest matrix problem** allows for explicit solution:
 - Orthogonal factor in polar decomposition of $\mathbf{M}$.
 - $\tilde{\mathbf{Q}} = \mathcal{P}_{O(n)}(\mathbf{M}) = \mathbf{M} (\mathbf{M}^T \mathbf{M})^{-1/2}$.

PROCESSING ORTHOGONAL MATRICES

Projection into $O(n)$

- Augmented processing strategy

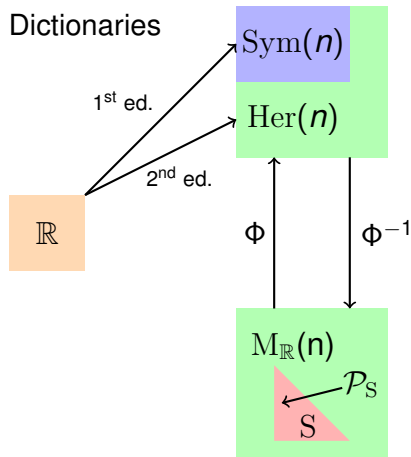
$$\begin{array}{ccccc} \text{Her}(n) & \xrightarrow{\mathcal{IO}} & \text{Her}(n) & & \\ \uparrow \Phi & & \downarrow \Phi^{-1} & & \\ O(n) \subset M_{\mathbb{R}}(n) & \xrightarrow[\Phi^{-1} \circ \mathcal{IO} \circ \Phi]{} & M_{\mathbb{R}}(n) & \xrightarrow[\mathcal{P}_{O(n)}]{} & O(n) \end{array}$$

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

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 $S = O(n)$.



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.
 - 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 is 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 & B. BURGETH, *Processing Multispectral Images via Mathematical Morphology*, Mathematics and Visualization, Springer, 129–148 (2015).
-  A. KLEEFELD, A. MEYER-BAESE, & B. BURGETH, *Elementary Morphology for $SO(2)$ - and $SO(3)$ -Orientation Fields*, Springer LNCS 9082, 458–469 (2015).