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

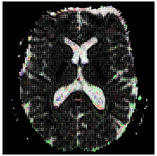
Data processing (difficulty: medium)

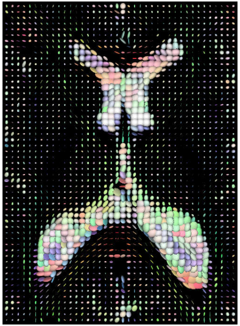
- What about color images/multispectral images (**vector-valued** data)?
- No standard ordering available.
- Channel-wise approach, lexicographic ordering, etc.
- Problem: false-colors phenomenon (interchannel relationships are ignored).

INTRODUCTION & MOTIVATION

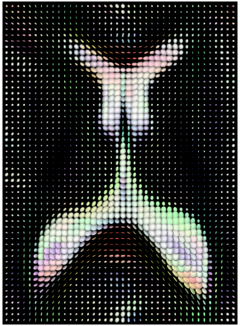
Data processing (difficulty: hard)

- 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



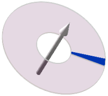
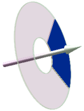
MCED

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

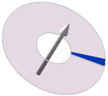
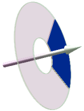
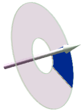
INTRODUCTION & MOTIVATION

Data processing (difficulty: bring it on)

- 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 non-symmetric matrices?
- Idea: complexification, Hermitian matrices, $\mathrm{Her}(n)$.

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 ordering: $\mathbf{H}_1 \geq \mathbf{H}_2 \Longleftrightarrow \mathbf{H}_1 - \mathbf{H}_2$ positive semi-definite.

CALCULUS FOR HERMITIAN MATRICES

Dictionary for Hermitian matrices

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

CALCULUS FOR HERMITIAN MATRICES

Dictionary for Hermitian matrices

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

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

CALCULUS FOR HERMITIAN MATRICES

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

- Linear mapping $\quad \Phi \;:\; \mathrm{M}_{\mathbb{R}}(\mathsf{n}) \longrightarrow \mathrm{Her}(n)$

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

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

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

- Processing strategy:

$$\begin{array}{ccc} \mathrm{Her}(n) & \xRightarrow{\;\mathcal{IO}\;} & \mathrm{Her}(n) \\ \Phi \Big\Uparrow & & \Big\Downarrow \Phi^{-1} \\ \mathrm{M}_{\mathbb{R}}(\mathsf{n}) & \xRightarrow[\;\Phi^{-1} \circ \mathcal{IO} \circ \Phi\;]{} & \mathrm{M}_{\mathbb{R}}(\mathsf{n}) \end{array}$$

- 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, $\mathbf{Q} \in \mathrm{O}(n)$

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

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

- 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

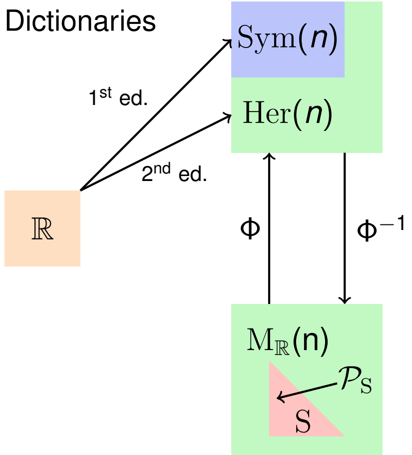
$$\begin{array}{ccccc} \mathrm{Her}(n) & \xrightarrow{\mathcal{IO}} & \mathrm{Her}(n) & & \\ \Phi \Big\Uparrow & & \Big\Downarrow \Phi^{-1} & & \\ \mathrm{O}(n) \subset \mathrm{M}_{\mathbb{R}}(n) & \xrightarrow[\Phi^{-1} \circ \mathcal{IO} \circ \Phi]{} & \mathrm{M}_{\mathbb{R}}(n) & \xrightarrow[\mathcal{P}_{\mathrm{O}(n)}]{}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

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



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.
  - 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).