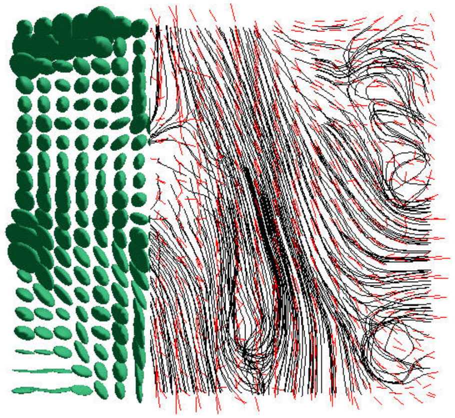
Constrained Flows of Matrix-Valued Functions and Applications to Image Processing



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Context: PDE-based image regularization and enhancement

Idea: Use a nonlinear PDE to eliminate noise and artifacts from an image $\mathbf{I}_0 : \Omega \to \mathbb{R}$ while preserving large global features (such as object contours).

- Solution obtained by deforming $\mathbf{I}_0$ through a regularizing flow. One introduces a family $t \mapsto \mathbf{I}(t)$ of images, solution of an evolution equation:

$$\partial_t \mathbf{I} = \mathbf{V}(\mathbf{I}),\ \ \mathbf{I}(0) = \mathbf{I}_0,$$

  where $\mathbf{V}$ usually includes an anisotropic diffusion operator.

- One often defines this equation as a gradient flow $\partial_t \mathbf{I} = -\nabla \mathcal{E}(\mathbf{I})$ corresponding to the minimization of a cost functional $\mathcal{E}$, such as

$$\mathcal{E}(\mathbf{I}) = \int_\Omega \frac{\alpha}{2} \|\mathbf{I}(\mathbf{x}) - \mathbf{I}_0(\mathbf{x})\|^2 \ + \phi(\|\nabla_\mathbf{x} \mathbf{I}(\mathbf{x})\|)\, d\mathbf{x}.$$

Objective: Regularizing PDEs for constrained matrix-valued datasets

The extension of this approach to multi-valued datasets:

$\longrightarrow$ Color images, direction fields, camera orientations, DT-MRI volumes, ...

is generally nontrivial, since additional constraints are involved:

$\longrightarrow$ Unit-norm, orthogonality, positive definiteness, ...

In these cases, one needs to build a PDE acting on some nonlinear subset $\mathcal{M}$ of a linear space of matrix-valued mappings $\mathcal{F}(\Omega, \mathbb{R}^{n \times p})$.

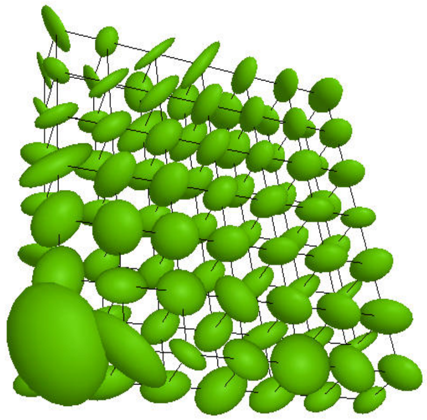
- How to design evolution equations on this nonlinear functional space $\mathcal{M}$?
- How to build a suitable, constraint-preserving, numerical approximation of the corresponding flows ?

Example of application: DT-MRI regularization - 1

- DT-MRI, What is it ?: Diffusion Tensor Imaging is an MRI acquisition technique that measures the motion of water molecules along the fibers in the white matter of the brain.

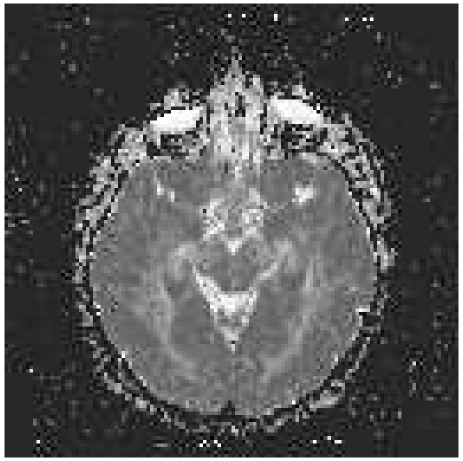
- Model: After estimation, each voxel of a DT-MRI volume is modeled as a symmetric positive definite matrix $\mathbf{X} \in \mathrm{P}(3)$ (a diffusion tensor).

- A diffusion tensor field $\mathbf{X} : \Omega \subset \mathbb{R}^3 \to \mathrm{P}(3)$ is generally represented using ellipsoids:



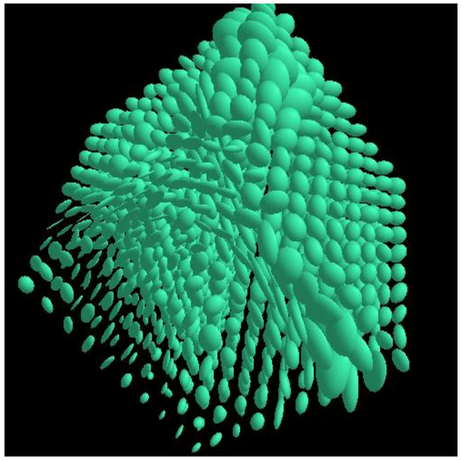
Example of application: DT-MRI regularization - 2

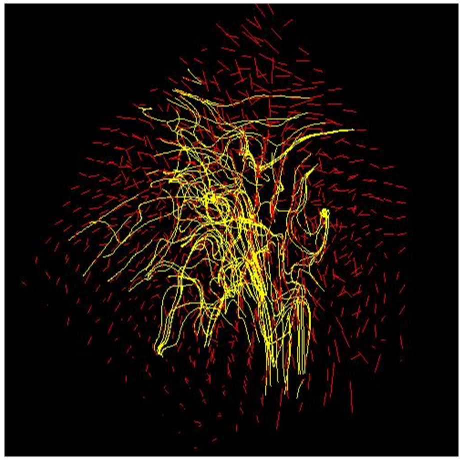
- One can reconstruct fiber maps from a DT-MRI field by tracking at each voxel the direction given by the eigenvector of largest eigenvalue:



Slice of the trace of a DT-MRI volume

$128 \times 128 \times 56$





Diffusion Tensors (left) and tracked fibers

(right) of a 16^3 subvolume.

- Why regularizing a DT-MRI field ?

$\longrightarrow$ Denoising and computation of more coherent physiological attributes.

$\longrightarrow$ Easier retrieval of global fiber bundle structures (toward a model of cerebral connectivity).

Related works

- PDEs acting on constrained multi-valued datasets (orientation diffusion, harmonic maps):

  - *P. Perona, 98.*
  - *B. Tang, G. Sapiro, V. Caselles, 00.*
  - *T. Chan, J. Shen, 00.*
  - *D. Tschumperlé, R. Deriche, 01.*
  - *L. Vese, S. Osher, 01.*
  - *R. Kimmel, N. Sochen, 02.*

- Regularization of DT-MRI fields:

  - *C. Westin et al., 99.*
  - *O. Coulon, D. Alexander, S. Arridge, 01.*
  - *B. Vemuri et al., 01.*

Constrained flows: A geometric viewpoint

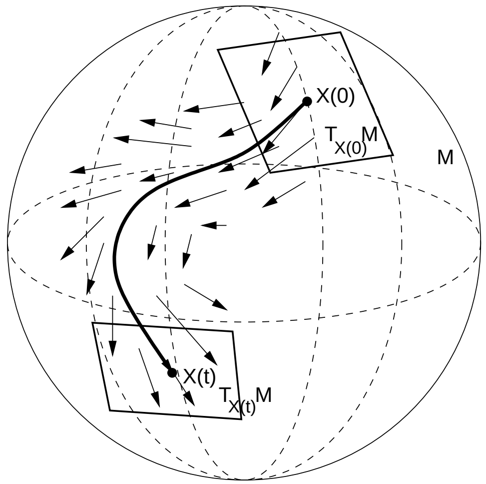
- Consider a matrix-valued function $\mathbf{X}$ in a suitable linear set of functions $\mathcal{F}(\Omega, \mathbb{R}^{n\times p})$.

- Formally, taking into account additional constraints reduces our configuration space to a given "submanifold" $\mathcal{M}$ of $\mathcal{F}(\Omega, \mathbb{R}^{n\times p})$.

- By analogy with finite dimensional problems, a constrained flow on $\mathcal{M}$ is induced from a vector field $\mathbf{V}$ that belongs to the tangent space of $\mathcal{M}$ at any given point.

$$\partial_t \mathbf{X} = \mathbf{V}(\mathbf{X}),\ \mathbf{X}(0) \in \mathcal{M},\quad \mathbf{V}(\mathbf{X}) \in T_{\mathbf{X}}\mathcal{M}$$

$$\Rightarrow\ \mathbf{X}(t) \in \mathcal{M}$$



Constrained flows: Orthogonality, spectral constraints - 1

Many constraints on matrices (orthogonality, rank and other spectral constraints) can be expressed in terms of Lie groups and homogeneous spaces.

We applied some of these ideas to define and study three constrained sets of matrix-valued mappings:

- **1 - Fields of orthonormal vector sets (Stiefel)**

$$\mathcal{M} = \mathcal{F}(\Omega, \mathrm{St}(n,p))$$

where $\mathrm{St}(n,p) = \{\mathbf{X} \in \mathbb{R}^{n\times p} \;/\; \mathbf{X}^T\mathbf{X} = \mathbf{I}_p\}$ is the Stiefel manifold.

Note that $\mathrm{St}(n,n) = \mathrm{O}(n)$ and $\mathrm{St}(n,1) = \mathrm{S}^{n-1}$.

Constrained flows: Orthogonality, spectral constraints - 2

- **2 - Fields of symmetric matrices with prescribed eigenvalues (isospectral)**

$$\mathcal{M} = \{\mathbf{U}^T \mathbf{X}_0 \mathbf{U} \ / \ \mathbf{U} \in \mathcal{F}(\Omega, \mathrm{O}(n))\}$$

where $\mathbf{X}_0$ is a field of real symmetric matrices with prescribed eigenvalues.

- **3 - Fields of symmetric matrices with prescribed rank/signature**

$$\mathcal{M} = \mathcal{F}(\Omega, \mathrm{S}(r, n))$$

where $\mathrm{S}(r, n) = \{\mathbf{X} \in \mathbb{R}^{n \times n} \ / \ \mathbf{X}^T = \mathbf{X}, \ \mathrm{Rank}(X) = r\}$.

Constrained flows: Generic forms

- **Orthogonal (Stiefel)**

$$\boxed{\partial_t \mathbf{X} = \mathbf{X}\mathbf{A}(\mathbf{X}) + \mathbf{X}_\perp \mathbf{B}(\mathbf{X})}$$

with $\mathbf{A}(\mathbf{X}) \in \mathcal{F}(\Omega, \mathfrak{so}(p))$, $\mathbf{B}(\mathbf{X}) \in \mathcal{F}(\Omega, \mathbb{R}^{(n-p)\times p})$ and $\mathbf{X}\mathbf{X}^T + \mathbf{X}_\perp \mathbf{X}_\perp^T = \mathbf{I}_n$.

- **Isospectral**

$$\boxed{\partial_t \mathbf{X} = [\mathbf{X}, \mathbf{A}(\mathbf{X})]}$$

with $\mathbf{A}(\mathbf{X}) \in \mathcal{F}(\Omega, \mathfrak{so}(n))$, $[\mathbf{A}, \mathbf{B}] = \mathbf{A}\mathbf{B} - \mathbf{B}\mathbf{A}$.

- **Symmetric rank/signature preserving**

$$\boxed{\partial_t \mathbf{X} = \mathbf{A}(\mathbf{X})\mathbf{X} + \mathbf{X}(\mathbf{A}(\mathbf{X}))^T}$$

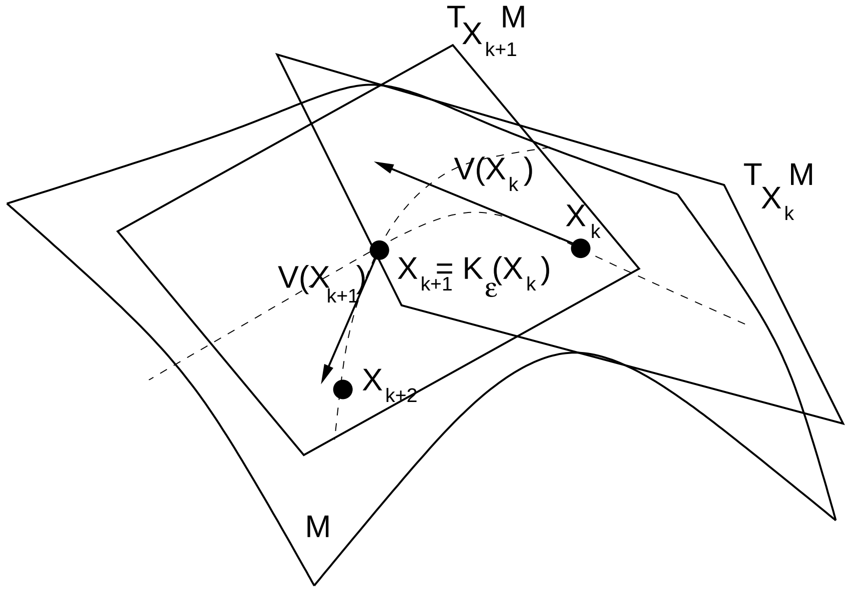
with $\mathbf{A}(\mathbf{X}) \in \mathcal{F}(\Omega, \mathbb{R}^{n\times n})$.

Objective: Build a discrete approximation of a continuous flow on a manifold $\mathcal{M}$.

$$\partial_t \mathbf{X} = \mathbf{V}(\mathbf{X}) \quad \longleftrightarrow \quad \mathbf{X}_{k+1} = \mathrm{K}_\varepsilon(\mathbf{X}_k)$$

Problem: How to design a step-forward operator K_ε which is consistent with the continuous flow ?

$$\begin{cases} \mathrm{K}_\varepsilon(\mathbf{X}) \in \mathcal{M} \\ \mathrm{K}_0(\mathbf{X}) = \mathbf{X} \\ \partial_\varepsilon \mathrm{K}_\varepsilon(\mathbf{X})|_{\varepsilon=0} = \mathbf{V}(\mathbf{X}) \end{cases}$$



Note: the usual Euler step $\mathrm{K}_\varepsilon(\mathbf{X}) = \mathbf{X} + \varepsilon \mathbf{V}(\mathbf{X})$ only works when $\mathcal{M}$ is a linear space.

Geometric numerical integrators - $\mathcal{M} = \mathcal{F}(\Omega, \mathrm{St}(n,p))$

On $\mathrm{St}(n,p)$, the equation of a **geodesic** of tangent $\mathbf{H}$ at point $\mathbf{X}$ is given by

$$\mathrm{Geo}_{\mathbf{X}}(\varepsilon\mathbf{H}) = \mathbf{X}\mathbf{M}(\varepsilon) + \mathbf{Q}\mathbf{N}(\varepsilon), \text{ with } \begin{pmatrix} \mathbf{M}(\varepsilon) \\ \mathbf{N}(\varepsilon) \end{pmatrix} = e^{\varepsilon\begin{pmatrix} \mathbf{X}^T\mathbf{H} & -\mathbf{R}^T \\ \mathbf{R} & \mathbf{0} \end{pmatrix}} \begin{pmatrix} \mathbf{I}_p \\ \mathbf{0} \end{pmatrix}$$

where $\mathbf{Q}$ and $\mathbf{R}$ are obtained by QR-decomposition of $(\mathbf{I}_n - \mathbf{X}\mathbf{X}^T)\mathbf{H}$.

We use this geodesic to define a suitable **step-forward operator** on $\mathcal{M}$:

$$\boxed{\text{Given } \mathbf{V} \in T_{\mathbf{X}}\mathcal{F}(\Omega, \mathrm{St}(n,p)),\ \forall \mathbf{x} \in \Omega, \quad \mathrm{K}_\varepsilon(\mathbf{X})(\mathbf{x}) = \mathrm{Geo}_{\mathbf{X}(\mathbf{x})}(\varepsilon\mathbf{V}(\mathbf{X})(\mathbf{x}))}$$

Note:

- Case $\mathrm{St}(n,1) = \mathrm{S}^{n-1} \quad \longrightarrow \quad \mathrm{Geo}_{\mathbf{X}}(\varepsilon\mathbf{H}) = \mathbf{X}\cos(\varepsilon\|\mathbf{H}\|) + \frac{\mathbf{H}}{\|\mathbf{H}\|}\sin(\varepsilon\|\mathbf{H}\|)$.
- Case $\mathrm{St}(n,n) = \mathrm{O}(n) \quad \longrightarrow \quad \mathrm{Geo}_{\mathbf{X}}(\varepsilon\mathbf{H}) = \mathbf{X}e^{\varepsilon\mathbf{X}^T\mathbf{H}}$.

Geometric numerical integrators - Other cases

- **Isospectral**

$$\partial_t \mathbf{X} = [\mathbf{X}, \mathbf{A}(\mathbf{X})]$$

$$\longleftrightarrow \quad \forall \mathbf{x} \in \Omega,\ \mathrm{K}_\varepsilon(\mathbf{X}_k)(\mathbf{x}) = e^{-\varepsilon \mathbf{A}(\mathbf{X}_k)(\mathbf{x})} \mathbf{X}_k(\mathbf{x}) e^{\varepsilon \mathbf{A}(\mathbf{X}_k)(\mathbf{x})}$$

- **Symmetric rank/signature preserving**

$$\partial_t \mathbf{X} = \mathbf{A}(\mathbf{X})\mathbf{X} + \mathbf{X}(\mathbf{A}(\mathbf{X}))^T$$

$$\longleftrightarrow \quad \forall \mathbf{x} \in \Omega,\ \mathrm{K}_\varepsilon(\mathbf{X}_k)(\mathbf{x}) = e^{\varepsilon \mathbf{A}(\mathbf{X}_k)(\mathbf{x})} \mathbf{X}_k(\mathbf{x}) e^{\varepsilon (\mathbf{A}(\mathbf{X}_k)(\mathbf{x}))^T}$$

Building minimizing flows

Idea: We want to minimize a cost functional $\mathcal{E} : \mathcal{M} \to \mathbb{R}$ using a suitable gradient flow:

$$\partial_t \mathbf{X} = -\nabla \mathcal{E}(\mathbf{X})$$

Gradient definition:

$$\begin{cases} \nabla \mathcal{E}(\mathbf{X}) \in T_{\mathbf{X}}\mathcal{M} \\ d\mathcal{E}(\mathbf{X}) \cdot \mathbf{H} = g_{\mathbf{X}}(\nabla \mathcal{E}(\mathbf{X}), \mathbf{H}), \ \forall \ \mathbf{H} \in T_{\mathbf{X}}\mathcal{M} \end{cases}$$

where $g_{\mathbf{X}}(\mathbf{V}_1, \mathbf{V}_2)$ is a suitable metric on $\mathcal{M}$.

Example of metric on $\mathcal{F}(\Omega, \mathrm{St}(n,p))$:

$$g_{\mathbf{X}}(\mathbf{V}_1, \mathbf{V}_2) = \int_{\Omega} \mathrm{Trace}((\mathbf{V}_1)^T(\mathbf{I}_n - \frac{1}{2}\mathbf{X}\mathbf{X}^T)\mathbf{V}_2) \ d\mathbf{x}$$

Natural gradients

$$d\mathcal{E}(\mathbf{X})\cdot\mathbf{H} = \int_\Omega \mathrm{Trace}((\mathbf{G}(\mathbf{X})(\mathbf{x}))^T\mathbf{H}(\mathbf{x}))\; d\mathbf{x}$$

- **Unconstrained**

$$\nabla\mathcal{E}(\mathbf{X}) = \mathbf{G}(\mathbf{X})$$

- **Orthogonal (Stiefel)**

$$\nabla\mathcal{E}(\mathbf{X}) = \mathbf{G}(\mathbf{X}) - \mathbf{X}\mathbf{G}(\mathbf{X})^T\mathbf{X}$$

- **Isospectral**

$$\nabla\mathcal{E}(\mathbf{X}) = \left[\mathbf{X}, \left[\mathbf{X}, \left(\mathbf{G}(\mathbf{X}) + \mathbf{G}(\mathbf{X})^T\right)\right]\right]$$

- **Symmetric rank/signature preserving**

$$\nabla\mathcal{E}(\mathbf{X}) = \left(\left(\mathbf{G}(\mathbf{X}) + \mathbf{G}(\mathbf{X})^T\right)\mathbf{X}^2 + \mathbf{X}^2\left(\mathbf{G}(\mathbf{X}) + \mathbf{G}(\mathbf{X})^T\right)\right)$$

Application: A cost functional for matrix-valued image regularization

- We consider a generic regularization functional on $\mathcal{F}(\Omega, \mathbb{R}^{n\times p})$

$$\mathcal{E}(\mathbf{X}) = \int_\Omega \frac{\alpha}{2}\|\mathbf{X}(\mathbf{x}) - \mathbf{X}_0(\mathbf{x})\|^2 + \phi(\|\nabla_\mathbf{x}\mathbf{X}(\mathbf{x})\|)\ d\mathbf{x}$$

  The computation of its first variation yields the unconstrained gradient $\mathbf{G}(\mathbf{X})$:

$$\mathbf{G}_{i,j}(\mathbf{X}) = \alpha(\mathbf{X}_{i,j} - \mathbf{X}_{0_{i,j}}) - \operatorname{div}\left(\frac{\phi^{'}(\|\nabla_\mathbf{x}\mathbf{X}\|)}{\|\nabla_\mathbf{x}\mathbf{X}\|}\nabla_\mathbf{x}\mathbf{X}_{i,j}\right)$$

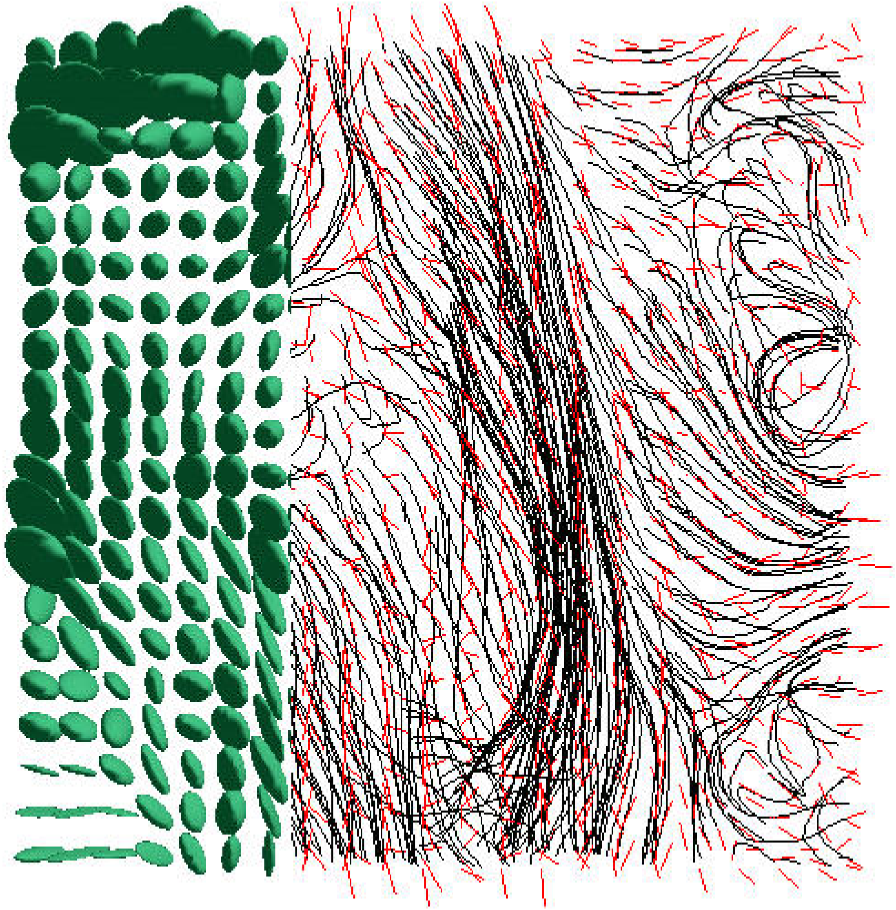
- Given a specific constraint, compute the natural gradient $\nabla\mathcal{E}(\mathbf{X})$ from $\mathbf{G}(\mathbf{X})$ and implement the constrained flow

$$\partial_t\mathbf{X} = -\nabla\mathcal{E}(\mathbf{X})$$

  starting from $\mathbf{X}_0$.

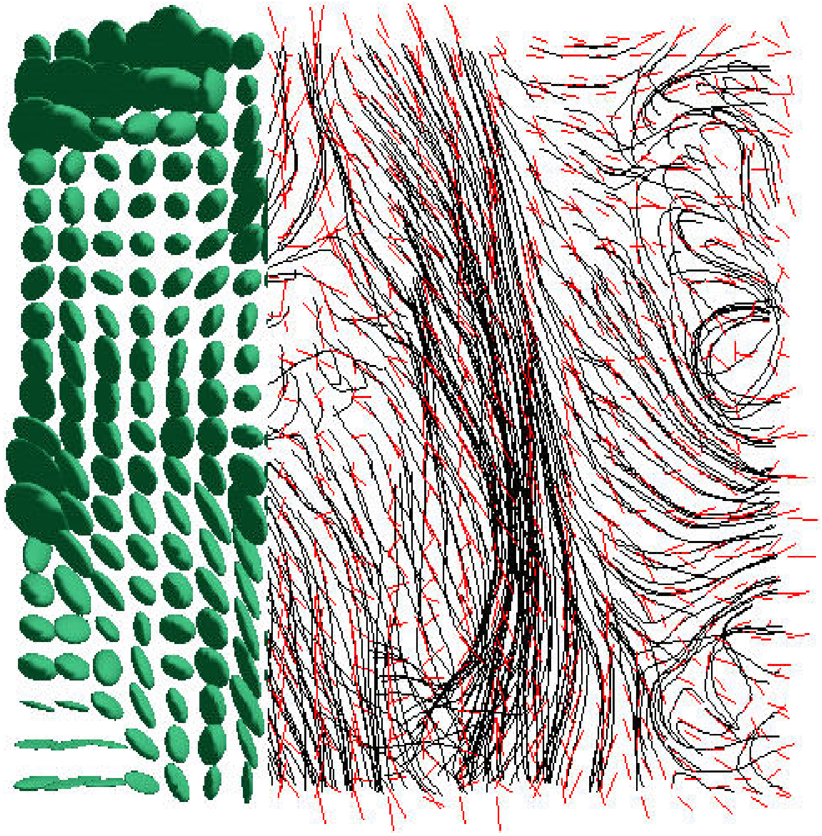
Application to DT-MRI data

Slice of a DT-MRI of the brain (mean diffusivity)

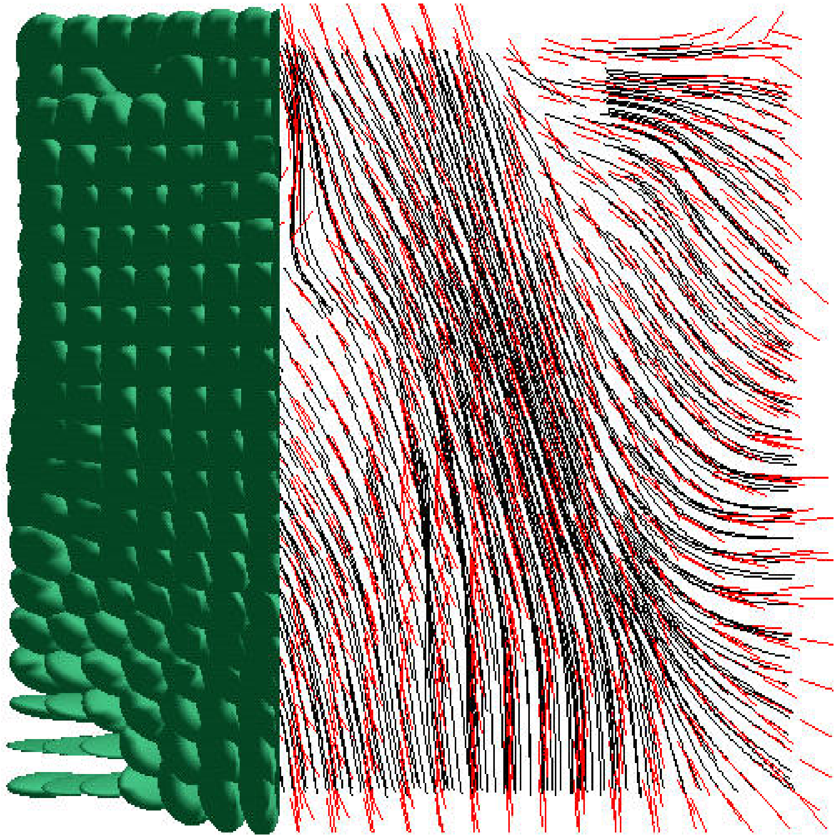


Local tensors/streamlines corresponding to the white square area

Application to DT-MRI data - Symmetric rank/signature preserving flow



Original

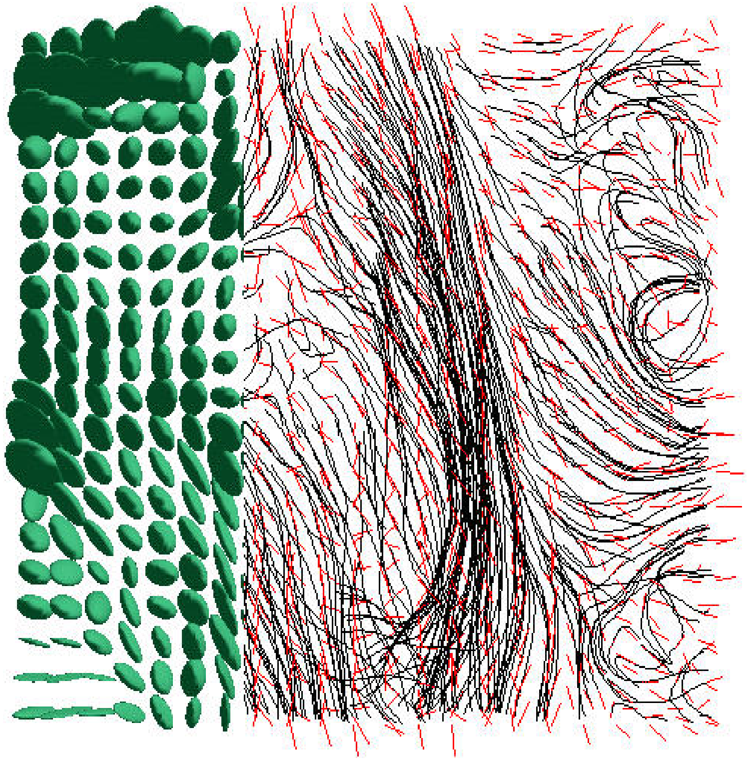


Symmetric rank/preserving flow

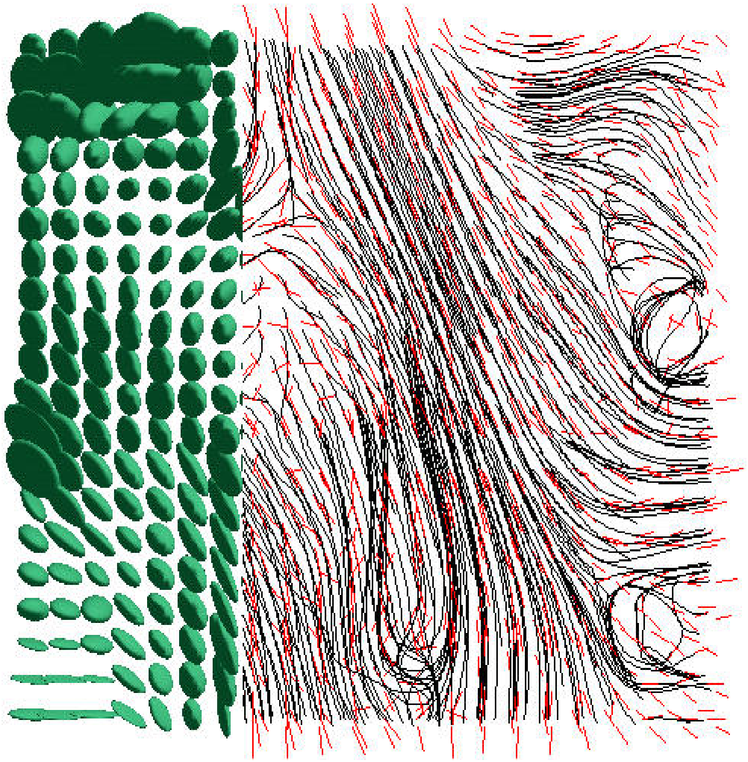
$$\partial_t \mathbf{X} = -\left(\left(\mathbf{G}(\mathbf{X}) + \mathbf{G}(\mathbf{X})^T\right)\mathbf{X}^2 + \mathbf{X}^2\left(\mathbf{G}(\mathbf{X}) + \mathbf{G}(\mathbf{X})^T\right)\right)$$

We observe an eigenvalue swelling effect ($\rightarrow$ loss of the orientation feature).

Application to DT-MRI data - Decomposition and orthogonal flow



Original



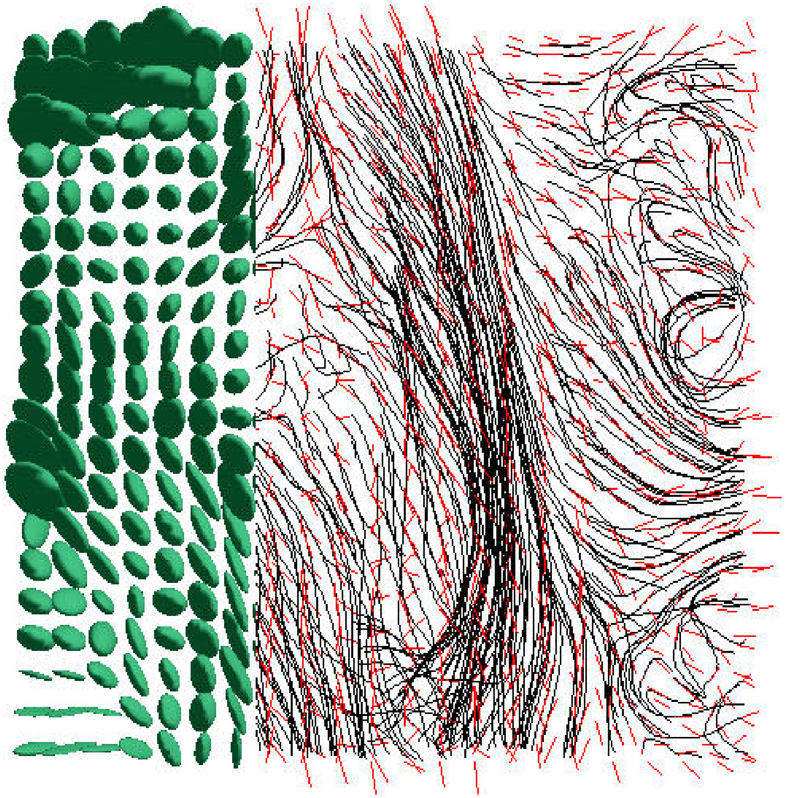
Orthogonal flow, with local alignment

We compute a spectral decomposition of each diffusion tensor $\mathbf{X}(\mathbf{x}) = \mathbf{U}(\mathbf{x})^T \Lambda(\mathbf{x}) \mathbf{U}(\mathbf{x})$ and regularize the orientation field $\mathbf{U} \in \mathcal{F}(\Omega, \mathrm{O}(n))$ separately by minimizing $\mathcal{E}(\mathbf{U})$ with the orthogonal flow:

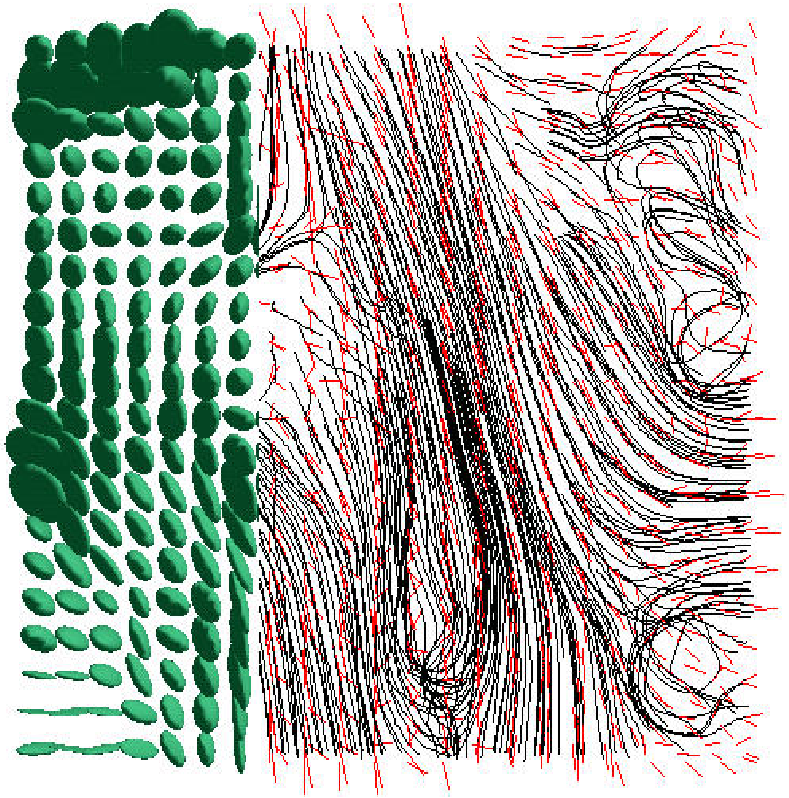
$$\partial_t \mathbf{U} = \mathbf{U}\mathbf{G}(\mathbf{U})^T \mathbf{U} - \mathbf{G}(\mathbf{U})$$

Good results but require an additional alignment step.

Application to DT-MRI data - Isospectral flow



Original



Isospectral flow

$$\partial_t \mathbf{X} = \left[\mathbf{X}, \left[\mathbf{X}, -\left(\mathbf{G}(\mathbf{X}) + \mathbf{G}(X)^T\right)\right]\right]$$

Preservation of the eigenvalues (diffusivities). No need for an explicit tensor decomposition ($\rightarrow$ faster).

Conclusion and perspectives - 1

We presented:

- A geometric characterization of evolution equations on three constrained sets of matrix-valued mappings.
- A simple method to transform unconstrained gradient flows into their constrained counterparts.
- Structure-preserving numerical integrators that respect the geometry of the constrained sets.
- An application to the regularization of DT-MRI volumes in medical imaging.

Conclusion and perspectives - 2

Future developments:

- Study of the well-posedness of the continuous flows and the convergence of the numerical algorithms.
  $\rightarrow$ *Product formulas for flows and semiflows on Hilbert manifolds [Chorin et al., 78].*

- Incorporate directly the geometry of the constrained sets of mappings in the design of the cost functionals.
  $\rightarrow$ *Theory of harmonic maps into Lie groups and homogeneous spaces [Dai et al., 97].*