Fast and Scalable Optimal Transport for Brain Tractograms

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Robust and Regularized Optimal Transport

- Let χ be a feature space, $\alpha = \sum_{i=1}^{N} \alpha_i \delta_{x_i}$, $\beta = \sum_{j=1}^{M} \beta_j \delta_{y_j}$ two weighted point clouds on χ. The robust and regularized optimal transport problem reads:

$$OT_{\varepsilon,\rho}(\alpha,\beta) = \boxed{\boxed{\text{Transport cost}} + \varepsilon\,.\,\text{Regularization}} + \rho\,.\,\text{Relaxation}$$

$$= \min_{\pi \in \mathbb{R}^{N\times M}_{\geq 0}} \langle \pi, C\rangle + \varepsilon \mathrm{KL}(\pi, \alpha \otimes \beta) + \rho \mathrm{KL}(\pi \mathbf{1}, \alpha) + \rho \mathrm{KL}(\pi^T \mathbf{1}, \beta)$$

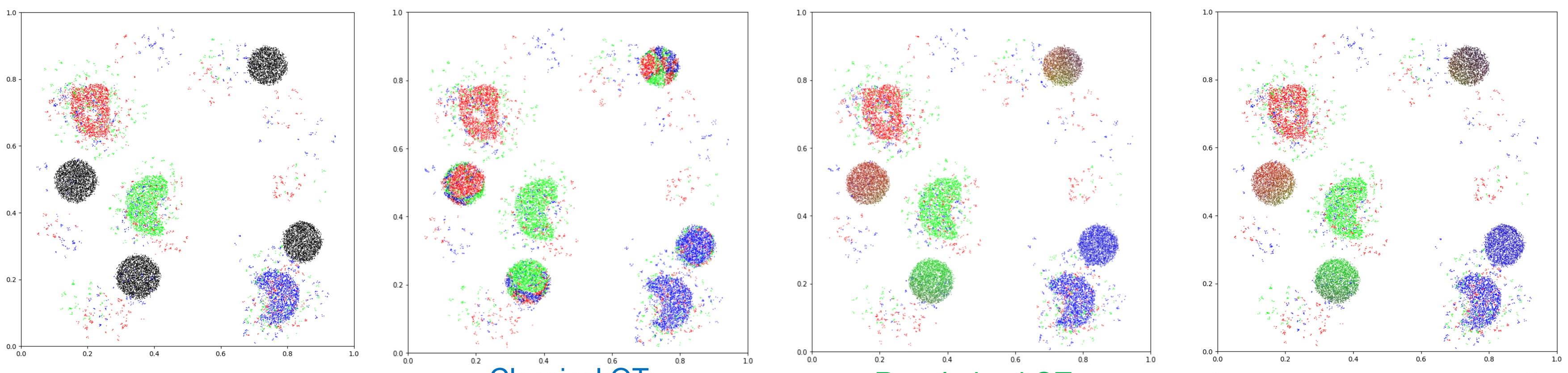
- 3 hyperparameters : ε, ρ and the cost C matrix (usually $C(x,y) = \frac{1}{2}|x-y|^2$)

OT for Label Transfer

If the target distribution β is labelled with L classes, the transport plan $(\pi_{i,j})$ can be used as a soft-assignement to transfert the labels on α:

$$Lab_i = 1/\alpha_i \sum_{j=1}^{M} \pi_{i,j} l_j$$

one-hot vector of labels in $\mathbb{R}^L$



Toy data-set of 2D points. Atlas has three coloured labels. Target is in black.

Classical OT: optimal assignment between the point clouds, generalizes sorting [3]

Regularized OT: "Blurs" the transport problem and improve robustness [2]

Regularized, unbalanced OT: Introduces a maximum "reach" to discard outliers. [1,4]

Wasserstein Barycenter

By minimizing $\frac{1}{K}\sum_{k=1}^{M} OT_{\varepsilon,\rho}(\alpha,\beta_k)$ with respect to the position x_i of α, where α is the atlas, we estimate the Wasserstein barycenter of the β_k. Here α and β_k are images and so $\beta_k = \sum_{j=1}^{M} \beta_{j,k} \delta_{y_{j,k}}$ where $\beta_{j,k}$ are intensities and $\delta_{y_{j,k}}$ the voxel positions.

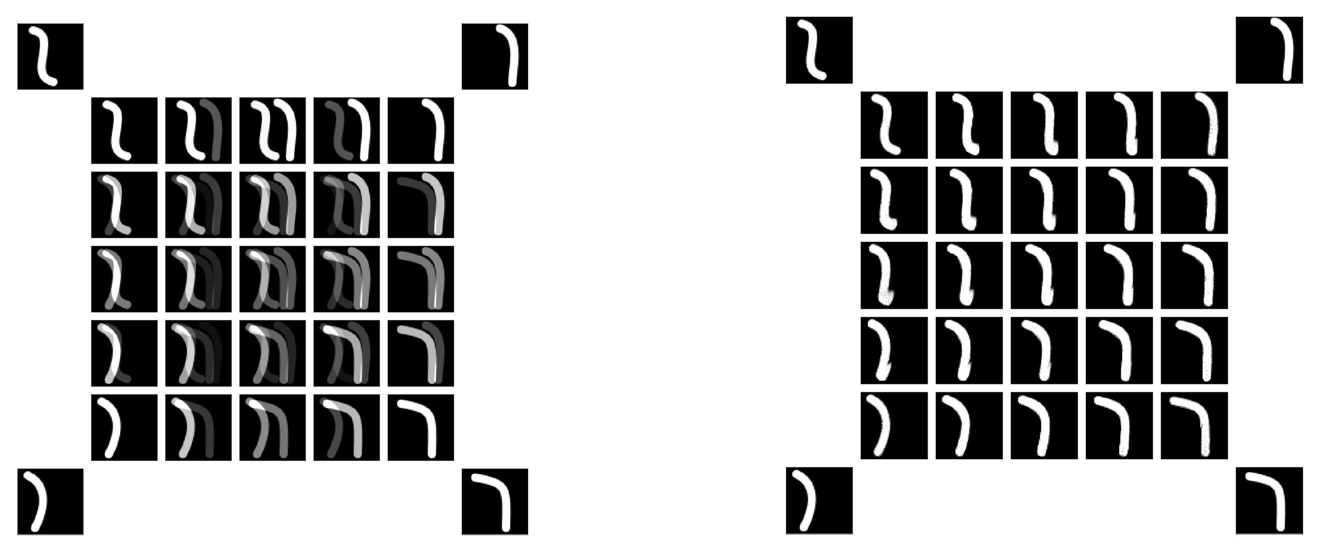
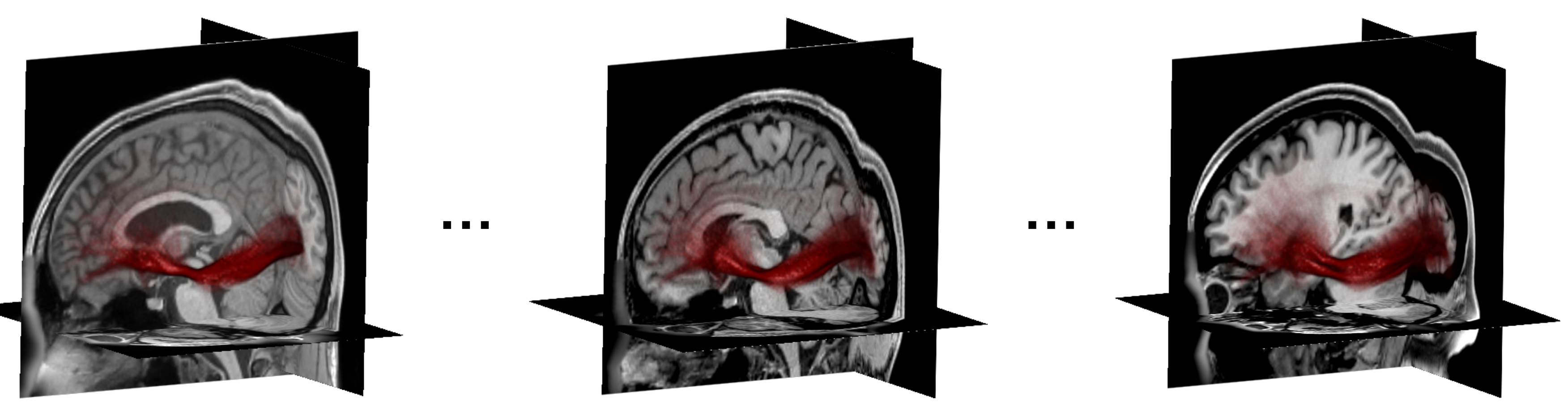


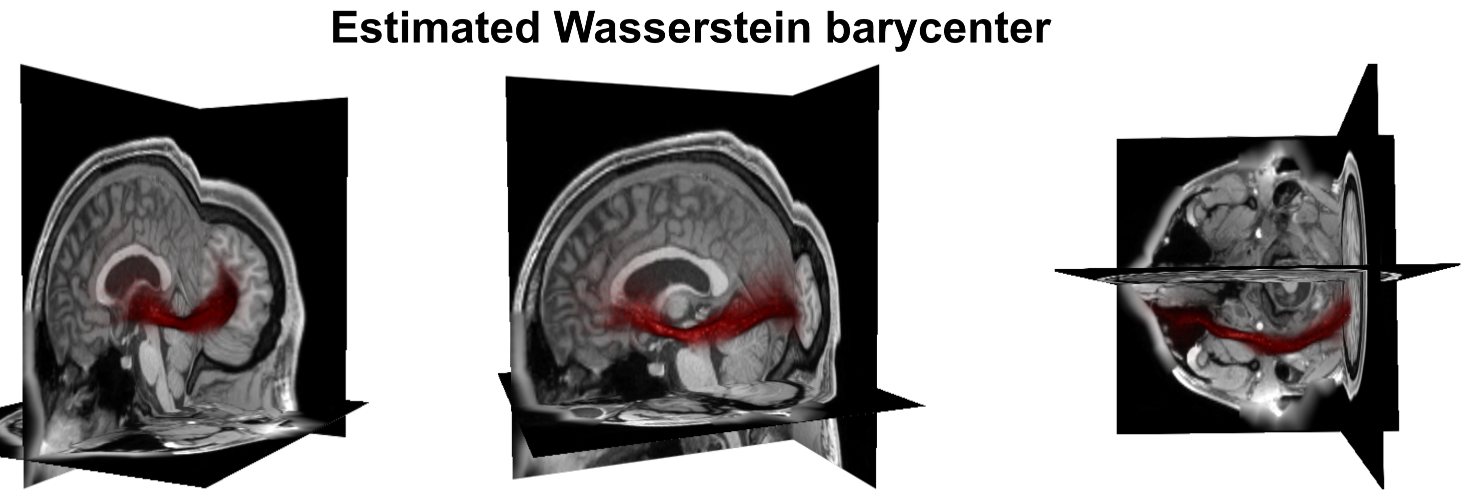
Fig: Linear (left) vs Wasserstein (right) interpolations between 4 images (corners). The OT interpolation is a *cheap* way *of* computing a *geometric* barycenter.

Application on Track Density Maps

Barycenter of 5 track density maps of the left IFOF computed with MrTrix. Left IFOF were manually segmented. Track density maps are 3D probability distributions $\Longrightarrow$ OT is a natural tool to study these data.



Estimated Wasserstein barycenter



Our Contribution

- **Multiscale algorithm** for solving the regularized OT problem
→ x10-1,000 speed-up compared with the baseline Sinkhorn algorithm [2].

- GPU implementation with a **linear footprint memory (KeOps library)**
→ We scale up to millions of points.

- User-friendly PyTorch interface available
→ `pip install geomloss` and www.kernel-operations.io/geomloss.

- Applications to **barycenter estimations** on track density maps, and **segmentation transfer** on brain tractograms.

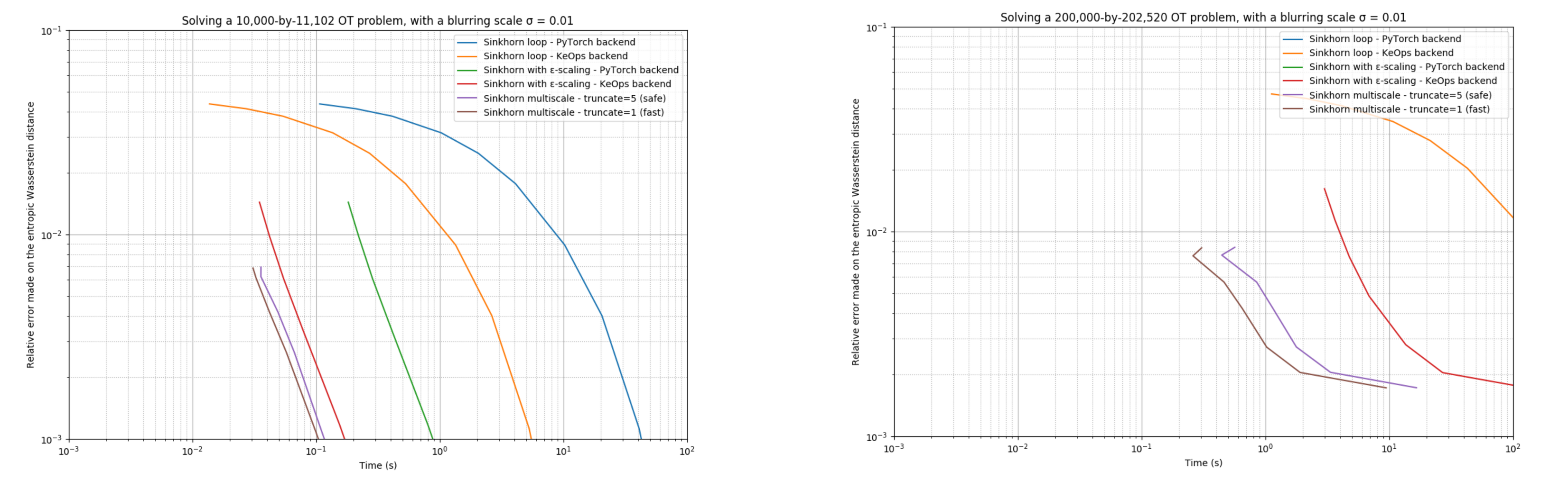


Fig: Relative error on the entropic OT with respect to computational time, for different backends (PyTorch or Keops) and different strategies.

Label Transfer on Brain Tractograms

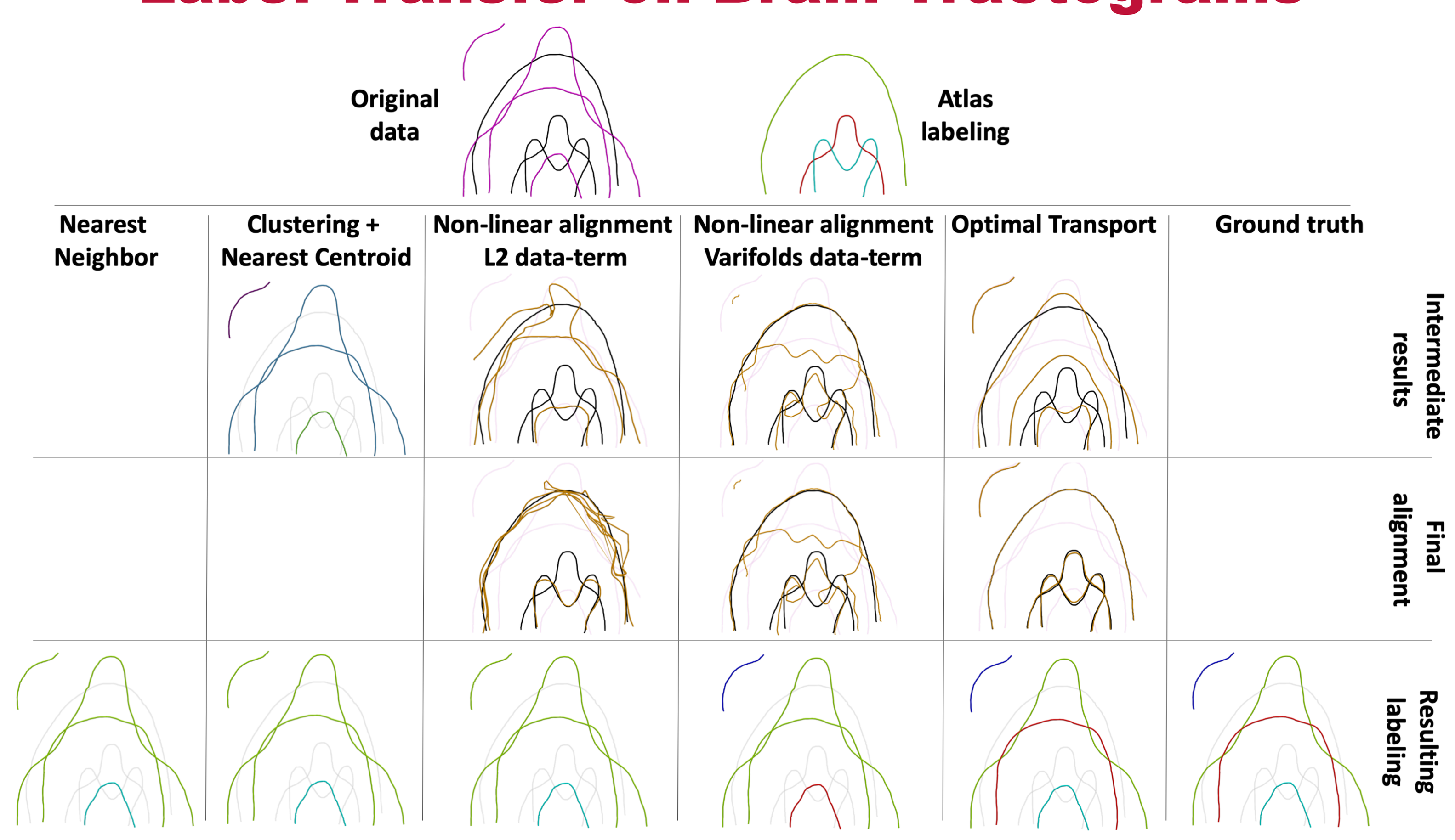
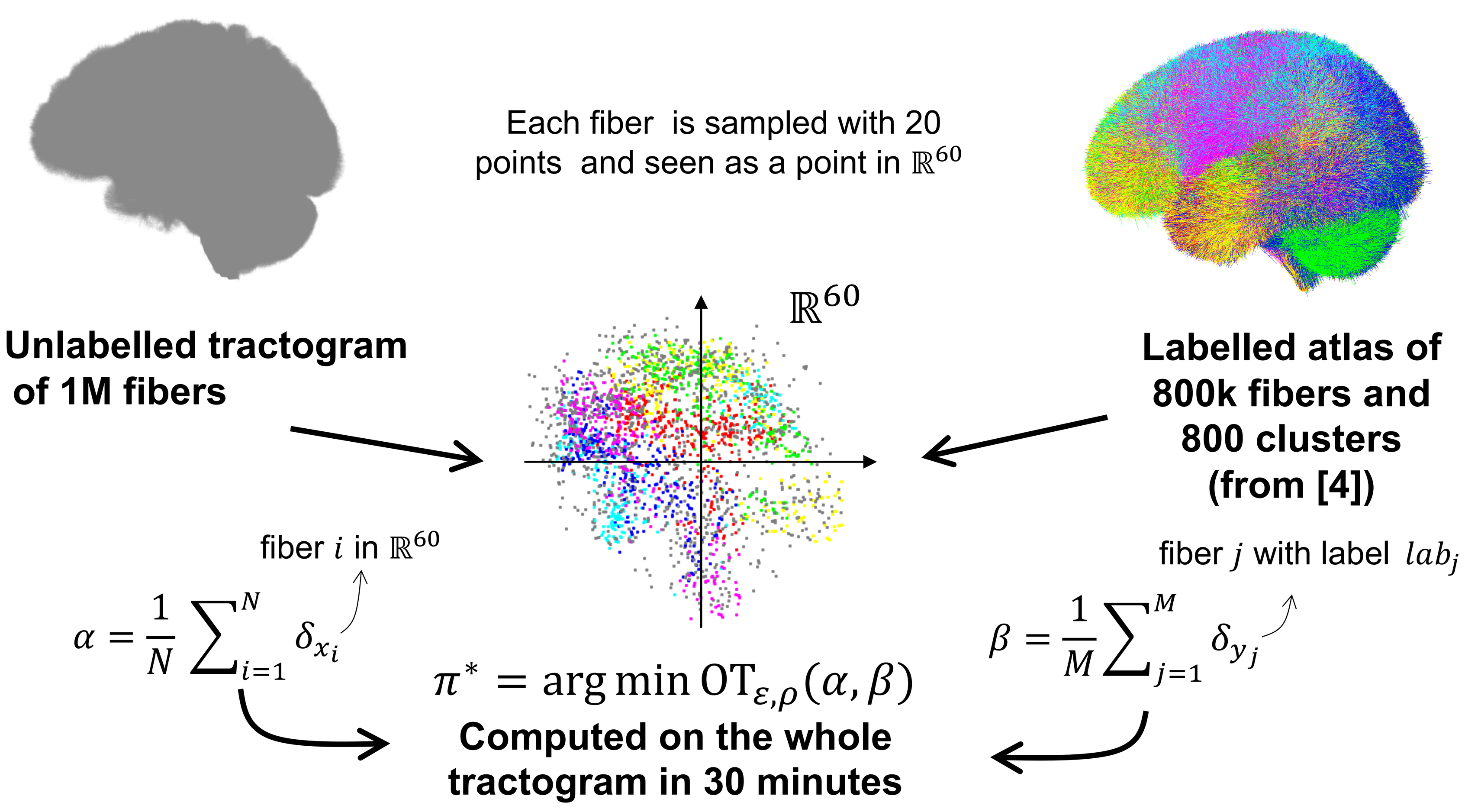


Fig: Label transfer between an atlas (black) and a subject (magenta) using different strategies. In the last row fibers detected as outliers are shown in dark blue.



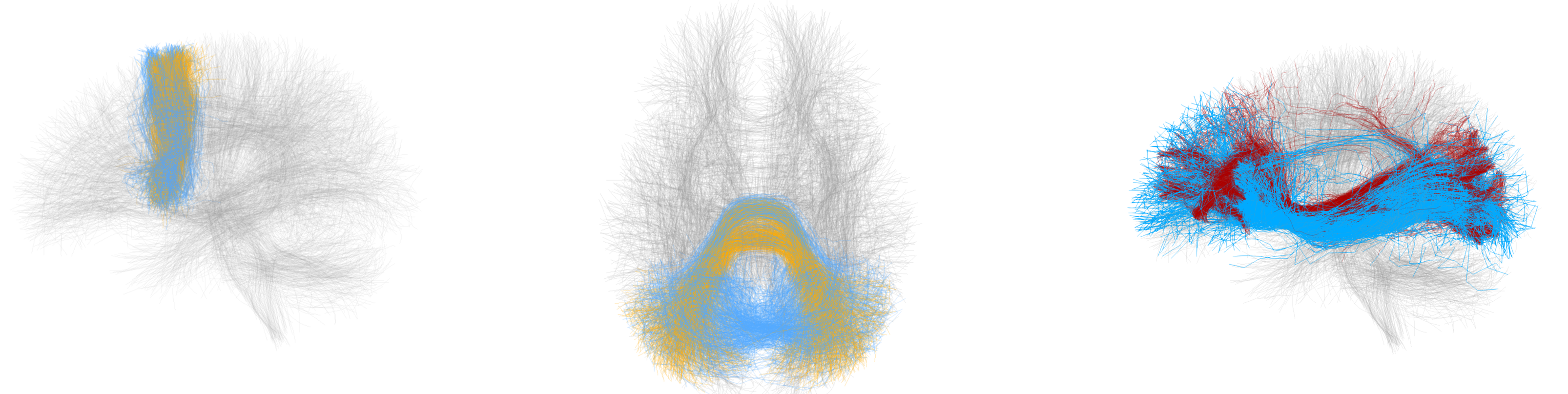


Fig: Some clusters of the atlas (in orange) with their respective segmentations (in light blue) of one random subject. On the right: comparison of a manual segmentation (in red) vs the segmentation obained with our method (light blue).

[1] Chizat, L. et. al. « An interpolating distance between optimal transport and Fisher-Rao metrics. Foundations of Computational Mathematics 2018. **[2]** Cuturi, M « Sinkhorn distances : Lightspeed computation of optimal transport ». NIPS 2013. **[3]** Kantorovich, L. « On the transfer of masses », 1942. **[4]** Peyré, G. and Cuturi, M. « Computational optimal transport. » Foundatios and Trends in Machine Learning 2019. **[5]** Zhang, F. et. al. « An anatomically currated fiber clustering white matter atlas for consistent white matter tract parcellation across lifespan. NeuroImage 2018. **Data are from the HCP project : https://db.humanconnectome.org.**

Contacts