Metric learning for diffeomorphic image registration.

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Outline

Example of problems of interest

Given two shapes, find a diffeomorphism of $\mathbb{R}^3$ *that maps one shape onto the other*

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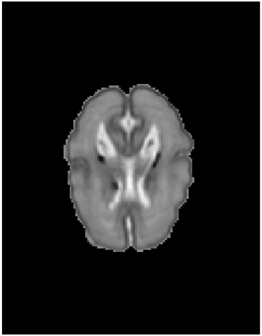
Different data types and different way of representing them.



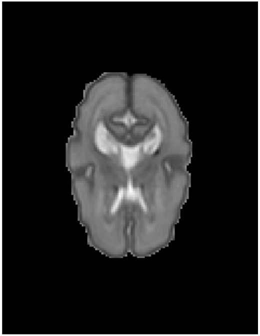


Figure – Two slices of 3D brain images of the same subject at different ages

Example of problems of interest

Given two shapes, find a diffeomorphism of $\mathbb{R}^3$ that maps one shape onto the other

Deformation by a diffeomorphism

Figure – Diffeomorphic deformation of the image

Variety of shapes

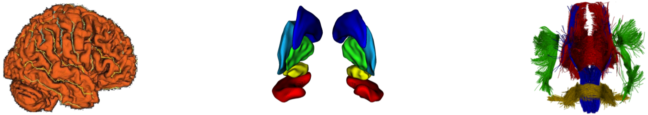


Figure – Different anatomical structures extracted from MRI data

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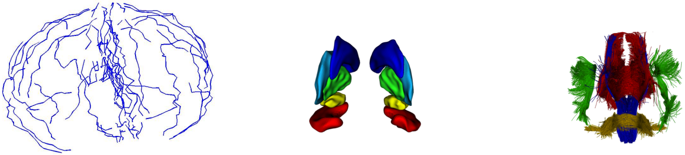

Figure – Different anatomical structures extracted from MRI data

A Riemannian approach to diffeomorphic registration

Several diffeomorphic registration methods are available:

- Free-form deformations B-spline-based diffeomorphisms by D. Rueckert
- Log-demons (X.Pennec et al.)
- Large Deformations by Diffeomorphisms (M. Miller,A. Trouvé, L. Younes)
- ANTS

Only the two last ones provide a Riemannian framework.

A Riemannian approach to diffeomorphic registration

- $v_t \in V$ a time dependent vector field on $\mathbb{R}^n$.
- $\varphi_t \in \mathit{Diff}$, the flow defined by

$$\partial_t \varphi_t = v_t(\varphi_t)\,. \tag{1}$$

Action of the group of diffeomorphism G_0 (flow at time 1):

$$\Pi : G_0 \times \mathcal{C} \to \mathcal{C}\,,$$
$$\Pi(\varphi, X) \doteq \varphi.X$$

Right-invariant metric on G_0: $d(\varphi_{0,1}, \mathrm{Id})^2 = \frac{1}{2}\int_0^1 |v_t|_V^2 dt$.
$\longrightarrow$ Strong metric needed on V
(Mumford and Michor: *Vanishing Geodesic Distance on...*)

Matching problems in a diffeomorphic framework

1. U a domain in $\mathbb{R}^n$
2. V a Hilbert space of C^1 vector fields such that:

$$\|v\|_{1,\infty} \leqslant C|v|_V .$$

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V is a Reproducing kernel Hilbert Space (RKHS): (pointwise evaluation continuous)
$\Longrightarrow$ Existence of a matrix function k_V (kernel) defined on $U \times U$ such that:

$$\langle v(x), a \rangle = \langle k_V(.,x)a, v \rangle_V .$$

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Right invariant distance on G_0

$$d(\mathrm{Id}, \varphi)^2 = \inf_{v \in L^2([0,1],V)} \int_0^1 |v_t|_V^2 dt \,,$$

$\longrightarrow$ geodesics on G_0.

Variational formulation

Find the best deformation, minimize

$$\mathcal{J}(\varphi) = \inf_{\varphi \in G_V} \underbrace{d(\varphi.A, B)^2}_{\text{similarity measure}} \tag{2}$$

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Tychonov regularization:

$$\mathcal{J}(\varphi) = \underbrace{R(\varphi)}_{\text{Regularization}} + \underbrace{\frac{1}{2\sigma^2} d(\varphi.A, B)^2}_{\text{similarity measure}} . \quad (3)$$

Riemannian metric on G_V:

$$R(\varphi) = \frac{1}{2} \int_0^1 |v_t|_V^2 \, dt \quad (4)$$

is a **right-invariant metric** on G_V.

Optimization problem

Minimizing

$$\mathcal{J}(v) = \frac{1}{2}\int_0^1 |v_t|_V^2 dt + \frac{1}{2\sigma^2} d(\varphi_{0,1}.A, B)^2 \,.$$

In the case of landmarks:

$$\mathcal{J}(\varphi) = \frac{1}{2}\int_0^1 |v_t|_V^2 dt + \frac{1}{2\sigma^2} \sum_{i=1}^{k} \|\varphi(x_i) - y_i\|^2 \,,$$

In the case of images:

$$d(\varphi_{0,1}.I_0, I_{target})^2 = \int_U |I_0 \circ \varphi_{1,0} - I_{target}|^2 dx \,.$$

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$$\mathcal{J}(v) = \frac{1}{2}\int_0^1 |v_t|_V^2\, dt + \frac{1}{2\sigma^2} d(\varphi_{0,1}.A, B)^2\,.$$

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Main issues for practical applications:

- choice of the metric (prior),
- choice of the similarity measure.

Why does the Riemannian framework matter?

Generalizations of statistical tools in Euclidean space:

- Distance often given by a Riemannian metric.
- Straight lines $\rightarrow$ geodesic defined by

$$\text{Variational definition: } \arg\min_{c(t)} \int_0^1 \|\dot{c}\|^2_{c(t)}\, dt = 0\,,$$

$$\text{Equivalent (local) definition: } \nabla_{\dot{c}}\dot{c} = \ddot{c} + \Gamma(c)(\dot{c},\dot{c}) = 0\,.$$

- Average $\rightarrow$ Fréchet/Karcher mean.

$$\text{Variational definition: } \quad \arg\min\{x \rightarrow E[d^2(x,y)]d\mu(y)\}$$

$$\text{Critical point definition: } \quad E[\nabla_x d^2(x,y)]d\mu(y)] = 0\,.$$

- PCA $\rightarrow$ Tangent PCA or PGA.
- Geodesic regression, cubic regression...(variational or algebraic)

Karcher mean on 3D images

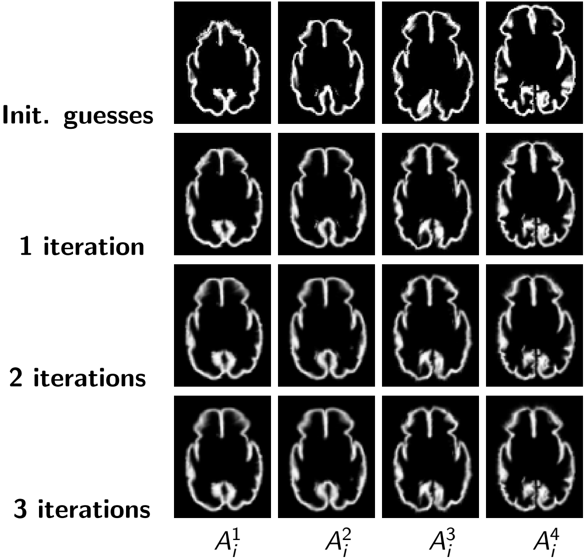

Figure – Average image estimates A_i^m, $m \in \{1, \cdots, 4\}$ after i =0, 1, 2 and 3 iterations.

Interpolation, Extrapolation

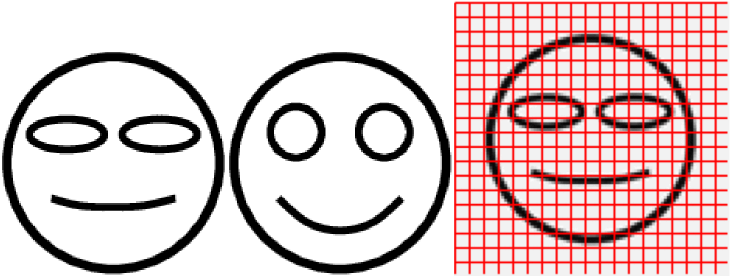

Figure – Geodesic regression (MICCAI 2011)

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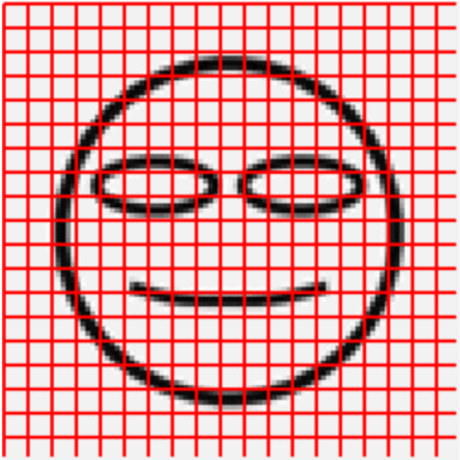

Figure – Extrapolation of happiness

What metric to choose?

Choosing the right-invariant metric

Right-invariant metric: Eulerian fluid dynamic viewpoint on regularization.
Space V of vector fields is defined equivalently by

- its kernel K such as Gaussian kernel,
- its differential operator, for instance $(\mathrm{Id} - \sigma \Delta)^n$ for Sobolev spaces.

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The norm on V is simply

$$\|v\|_V^2 = \int_\Omega \langle v(x), (Lv)(x) \rangle \, dx = \int_\Omega (L^{1/2} v)^2(x) \, dx \,.$$

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Scale parameter important!

$$k_\sigma(x,y) = e^{-\frac{\|x-y\|^2}{\sigma^2}} \text{ kernel/operator } (\mathrm{Id} - \sigma\Delta)^n \tag{5}$$

- σ small: good matching but non regular deformations and more local minima.
- σ large: poor matching but regular deformations and more global minima.

Sum of kernels and multiscale

Choice of mixture of Gaussian kernels: (Risser, Vialard et al. 2011)

$$K(x,y) = \sum_{i=1}^{n} \alpha_i e^{-\frac{\|x-y\|^2}{\sigma_i^2}} \tag{6}$$

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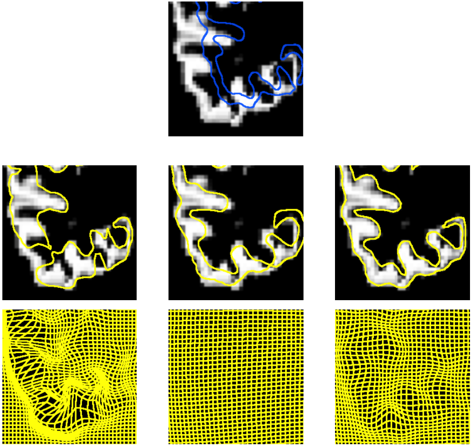

Figure – Left to right: Small scale, large scale and multi scale.

Decomposition over different scales

Try to disentangle contributions at each scale: (Bruveris, Risser, Vialard, 2012, Siam MMS) using semi-direct product of groups. Consider $G_{\sigma_1}, G_{\sigma_2}$ two diffeomorphism groups at different scales associated with V_{σ_1} and V_{σ_2}.

Semi-direct product of groups $G_{\sigma_1} \ltimes G_{\sigma_2}$.

Non-linear extension of the infimal convolution of norms:

$$\|v\|^2 = \min_{(v_1,v_2)\in V_1\times V_2} \left\{ \|v_1\|^2_{V_1} + \|v_2\|^2_{V_2} \,\middle|\, v = v_1 + v_2 \right\} . \quad (7)$$

Non-linear extension $\longrightarrow$ semi-direct product of groups.

From Eulerian to Lagrangian viewpoints

Spatial correlation of the deformation: need for local deformability on the tissues.
Toward a more Lagrangian point of view.

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Toward a more Lagrangian point of view.

How to introduce spatially varying metric?

Using kernels: χ_i being a partition of unity of the domain.

$$K = \sum_{i=1}^{n} \chi_i K_i \chi_i \,, . \tag{8}$$

This kernel is associated to the following variational interpretation:

$$\|v\|^2 = \min_{(v_1,\ldots,v_n) \in V_1 \times \ldots \times V_n} \left\{ \sum_{i=1}^{n} \|v_i\|_{V_i}^2 \;\middle|\; \sum_{i=1}^{n} \chi_i v_i = v \right\} . \tag{9}$$

$\longrightarrow$ possibility to introduce soft-symmetries...

Left-invariant metrics

Miccai 2013, Marsden's Fields volume, Schmah, Risser, Vialard
Change of point of view: choose body-coordinates and convective velocity:

$$\mathcal{J}(\varphi) = \frac{1}{2}\int_0^1 \|v(t)\|_V^2\, dt + E(\varphi(1)\cdot I, J), \tag{10}$$

under the convective velocity constraint:

$$\partial_t \varphi(t) = d\varphi(t)\cdot v(t)\,, \tag{11}$$

where $d\varphi(t)$ is the tangent map of $\varphi(t)$.

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- More natural interpretation of spatially varying metrics.
- Left action + left invariant metric $\implies$ no induced Riemannian metric.

Difference with LDDMM

The path look different:

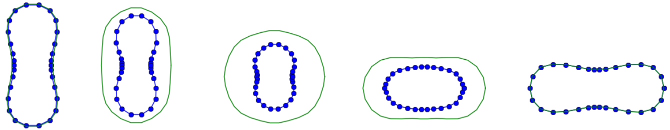
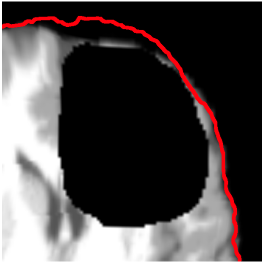
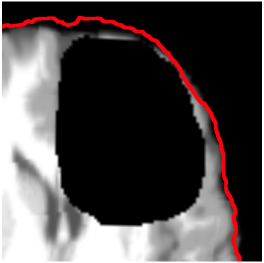


Figure – The green curves Right-LDM geodesic path, The blue curves Left-LDM geodesic path.



LDDMM



LIDM

What's next

Left-invariance is more Lagrangian but the metric is fixed as in the Eulerian situation!

- On a template, learning the metric.

Motivation:

- Better matching results: i.e better regularization or matching.
- Better matching quality for organs with (segmented) tumors.

Metric learning

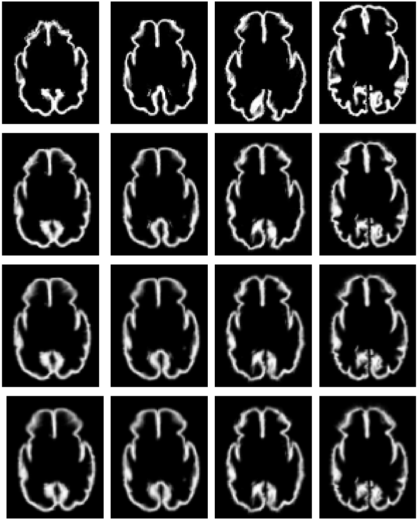


Figure – Given a collection of shape and a template, learn the metric.

Metric learning: High-dimensional inverse problem

(Miccai 2014: Vialard, Risser)

- $(I_n)_{n=1,\dots,N}$ be a population of N images.
- T be a template (Karcher mean for instance).

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Registering the template T onto the image I_n consists in minimizing:

$$\mathcal{J}_{I_n,K}(v) = \frac{1}{2}\int_0^1 \|v(t)\|_V^2 \, dt + d(T \circ \varphi(1)^{-1}, I_n)\,, \tag{12}$$

where

$$\partial_t \varphi(t) = v(t) \circ \varphi(t)\,.$$

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Equivalent to minimize

$$\mathcal{J}_{I_n,K}(v) = \frac{1}{2}\int_0^1 \langle P(t)\nabla I(t), K\star(P(t)\nabla I(t)\rangle \, dt + d(T \circ \varphi(1)^{-1}, I_n) \,, \qquad (13)$$

Optimize over K? Ill posed!

- Incorporate the smoothness constraint by defining

$$\mathcal{K} = \{\hat{K} M \hat{K} \mid M \text{ SDP operator on } L^2(\mathbb{R}^d, \mathbb{R}^d)\}\,, \tag{14}$$

M symmetric positive definite matrix.

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M symmetric positive definite matrix.

- Regularization on M. Prior for M close to Id. Minimize

$$\mathcal{F}(M) = \frac{\beta}{2} d^2_{S^{++}}(M, Id) + \frac{1}{N} \sum_{n=1}^{N} \min_{v} \mathcal{J}_{I_n}(v, M)\,, \tag{15}$$

where d^2 can be chosen as

- Affine invariant metric (Pennec et al.) $g_1 = \mathrm{Tr}(M^{-1}(\delta M) M^{-1}(\delta M))$.
- (Modified) Wasserstein metric.

Problem

Problem: matrix M is huge: $(dn)^2$ where $d = 2, 3$ dimension and n number of voxels.
Computing the logarithm is costly.

Wasserstein metric

Pros: Easy to compute
Cons: Non complete metric.

Trick

The map $N \mapsto NN^T$ is a Riemannian submersion from $M_n(\mathbb{R})$ equipped with the Frobenius norm to the space of SDP matrices equipped with the Wasserstein metric

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Encode the symmetric matrix as NN^T and perform the optimization on N. The regularization reads $\frac{1}{2}\|N - Id\|^2$
The gradient is

$$\nabla_{L^2}\mathcal{F}(N) = \beta(N - Id) - \tag{16}$$

$$\frac{1}{2N}\sum_{n=1}^{N}\int_0^1 (\hat{K} \star P_n(t)) \otimes (N\hat{K} \star P_n(t)) + (N\hat{K} \star P_n(t)) \otimes (\hat{K} \star P_n(t))dt\,, \tag{17}$$

Reducing the problem dimension

Idea

Learn at large scales and not at fine scale.

Introduce:

$$\mathcal{K} = \{\hat{K} M \Pi \hat{K} + \hat{K}(Id - \Pi)\hat{K} \,|\, M \text{ SDP operator on } L^2(\mathbb{R}^d, \mathbb{R}^d)\} \,. \tag{18}$$

with Π an orthogonal projection on a finite dimensional parametrization of vector fields: use of splines.

Experiments

- 40 subjects of the LONI Probabilistic Brain Atlas (LPBA40).
- All 3D images were affinely aligned to subject 5 using ANTS.

Table – Reference results

	No Reg	SyN	K_{fine}	K_{ref}
TO	0.665	0.750	0.732	0.712
$DetJ_{Max}$	1	3.17	4.65	1.66
$DetJ_{Min}$	1	0.047	0.46	0.67
$DetJ_{Std}$	0	0.17	0.11	0.063

Table – Average results.

	DiagM	GridM1	GridM2	K_{20}	K_{30}
TO	0.711	0.710	**0.704**	0.710	**0.704**
$DetJ_{Max}$	1.66	1.61	**1.41**	1.62	**1.50**
$DetJ_{Min}$	0.68	0.70	0.67	0.73	0.66
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For a given quality of overlap, better smoothness of the deformations.

Main issues

- The metric is fixed in Eulerian coordinates.
- The metric is template based.

Make the method adaptive to any pairs of images on a simpler model.

SVF model: A simple model

Based on *Metric learning for image registration*, CVPR 2019, Niethammer, Kwitt, Vialard.
Let $v(x)$ be a vector field. Find a v minimizer of

$$\frac{1}{2}\|v\|_V^2 + \mathrm{Sim}(I \circ \varphi_1^{-1}, J) \tag{19}$$

$$\partial_t \varphi_t = v(\varphi_t)\,. \tag{20}$$

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Equivalent momentum formulation: Find $m \in L^2(\Omega, \mathbb{R}^d) \subset V^*$ such that

$$\frac{1}{2}\langle m, K \star m \rangle + \mathrm{Sim}(I \circ \varphi_1^{-1}, J) \tag{21}$$

s.t.

$$\partial_t \varphi^{-1}(t,x) + D\varphi^{-1}(t,x)(K \star m(t,x)) = 0\,. \tag{22}$$

Numerical discretization: Central differences in space and 20 timesteps in time of RK4.

Parametrization of the metric

Fix a collection of scales $\sigma_0 < \ldots < \sigma_{N-1}$ and set $G_i(x) = e^{-|x|^2/\sigma_i^2}$.

$$v_0(x) \overset{\text{def.}}{=} (K(w) \star m_0)(x)$$
$$\overset{\text{def.}}{=} \sum_{i=0}^{N-1} \sqrt{w_i(x)} \int_y G_i(|x-y|)\sqrt{w_i(y)} m_0(y)\, \mathrm{d}y \,, \quad (23)$$

Problem: w_i should be sufficiently smooth to guarantee diffeomorphisms.
Introduce *pre-weights* $\omega_i(x)$ and fix K_σ, with σ small:

$$K_\sigma \star \omega_i = w_i$$

and

$$\sum_i w_i(x) = 1\,.$$

Learning the metric is still ill-posed:

$$\widehat{\mathrm{OMT}}(w) = \left|\log \frac{\sigma_{N-1}}{\sigma_0}\right|^{-r} \sum_{i=0}^{N-1} w_i \, \left|\log \frac{\sigma_{N-1}}{\sigma_i}\right|^{r} \quad (24)$$

Is 0 for $(w_i) = (0, \ldots, 0, 1)$.

Objective function

Optimize momentum + metric.

$$\mathrm{Obj}_{0,1}(m,\omega) = \underset{m_0}{\mathrm{argmin}}\ \lambda\langle m_0, v_0\rangle\ + \mathrm{Sim}[I_0 \circ \Phi^{-1}(1), I_1] +$$

$$\lambda_{\mathrm{OMT}} \int \widehat{\mathrm{OMT}}(w(x))\,\mathrm{dx} +$$

$$\lambda_{\mathrm{TV}} \sqrt{\sum_{l=0}^{N-1} \left(\int \gamma(\|\nabla I_0(x)\|)\|\nabla \omega_l(x)\|_2\,\mathrm{dx} \right)^2}\,, \quad (25)$$

where $\gamma(x) \in \mathbb{R}^+$ is an edge indicator function

$$\gamma(\|\nabla I\|) = (1 + \alpha\|\nabla I\|)^{-1},\ \alpha > 0\,.$$

Then, minimize

$$\sum_{i,j} \mathrm{Obj}_{0,1}(m_{i,j}, \omega^i)\,, \quad (26)$$

where $\omega^i = f_\theta(I_i)$.

Parametrize and learn the pre-weights ω_i

The pre-weights are parametrized by a 2-layers net:

$$(\omega_i)_{i=1,\dots,N} = \mathrm{ShallowNet}(I)\,.$$

Input: current image, Output: pre-weights.

ShallowNet $= \texttt{conv}(d, n_1) \to \texttt{BatchNorm} \to \texttt{lReLU} \to \texttt{conv}(n_1, N) \to \texttt{BatchNorm} \to \texttt{weighted-linear-softmax}$

$$\sigma_w(z)_j = \frac{\mathrm{clamp}_{0,1}(w_j + z_j - \overline{z})}{\sum_{i=0}^{N-1} \mathrm{clamp}_{0,1}(w_i + z_i - \overline{z})}\,, \qquad (27)$$

The weights w_j are reasonably initialized: $w_i = \sigma_i^2 / (\sum_{j=0}^{N-1} \sigma_j^2)$

Optimization

Shared parameters: ShallowNetwork parameters,
Individual parameters: Momentum for each pair.

1. (1) initialize with reasonable weights and optimize over momentums,
2. (2) Jointly optimize on the shared and individual parameters: use SGD with (Nesterov) momentum, different batch size in 2d/3d, 50 epochs in 2d, less in 3D.

Experiments on synthetic data

1) Generate concentric circular regions with random radii and associate different multi-Gaussian weights to these regions. We associate a fixed multi-Gaussian weight to the background.
2) Randomly create vector momenta at the borders of the concentric circles.
3) Add noise (for texture) and compute forward model, to obtain source image, similar for target image.

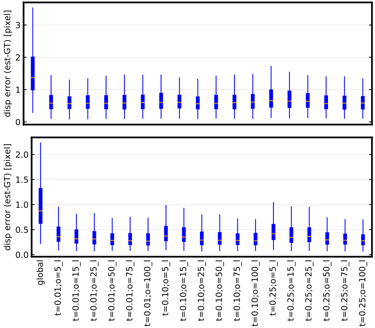


Figure – *Displacement error* (in pixel) with respect to the ground truth

Experiments on synthetic data

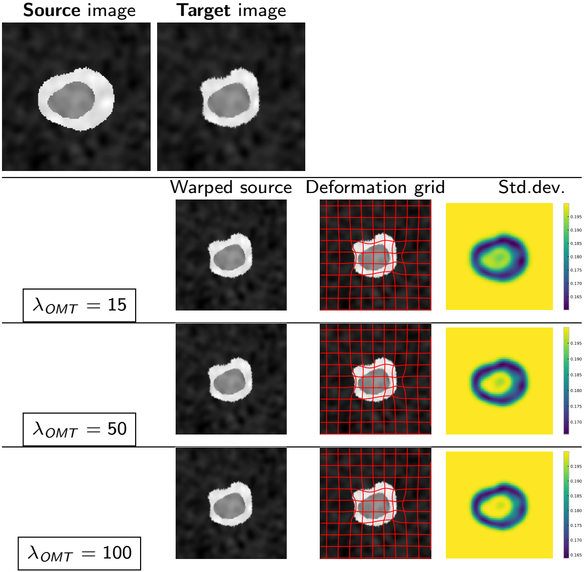
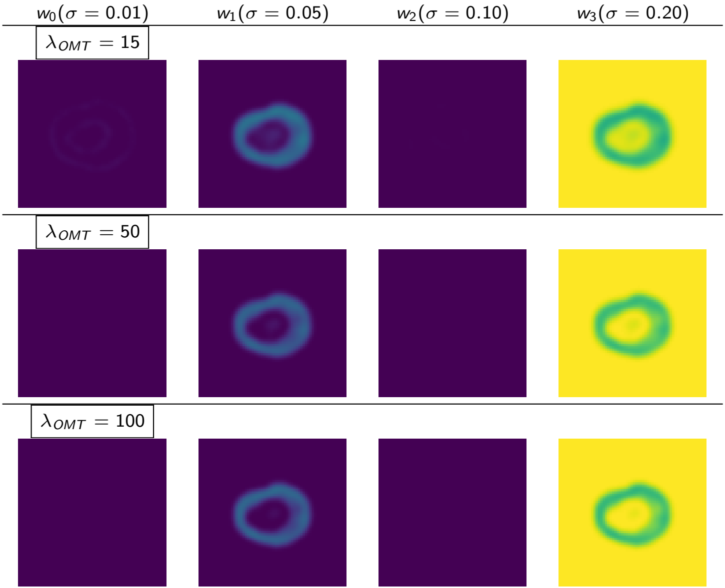


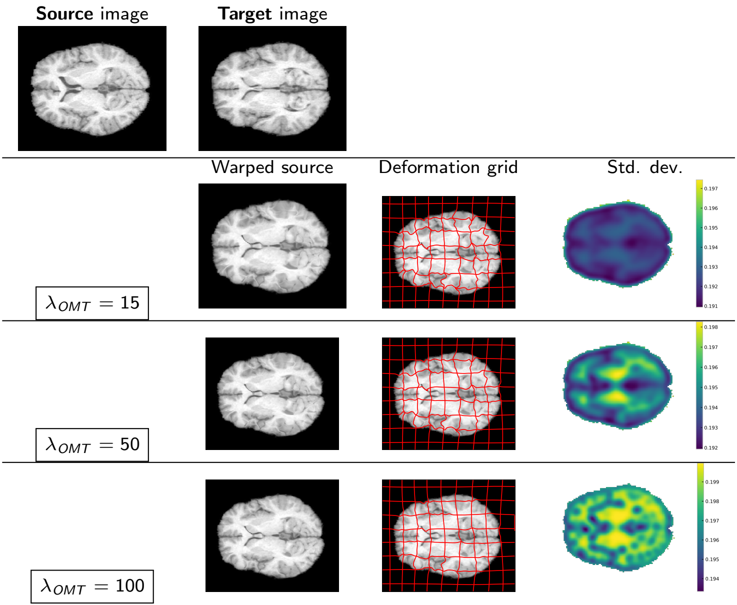
Figure – $\lambda_{TV} = 0.1$. Overall variance is similar but the true weights are not recovered: weights on the outer ring $[0.05, 0.55, 0.3, 0.1]$

Experiments



Figure

On 2D real data: LPBA40



Performance on 3D data: CUMC12

Training on different dataset:

- Trained on different dataset, test on CUMC12
- Training 132 image pairs on CUMC12, 90 image pairs on MGH10, 150 image pairs on IBSR18.

Method	mean	std	1%	5%	50%	95%	99%	p	MW-stat	sig?
FLIRT	0.394	0.031	0.334	0.345	0.396	0.442	0.463	<1e−10	17394.0	✓
AIR	0.423	0.030	0.362	0.377	0.421	0.483	0.492	<1e−10	17091.0	✓
ANIMAL	0.426	0.037	0.328	0.367	0.425	0.483	0.498	<1e−10	16925.0	✓
ART	0.503	0.031	0.446	0.452	0.506	0.556	0.563	<1e−4	11177.0	✓
Demons	0.462	**0.029**	0.407	0.421	0.461	0.510	0.531	<1e−10	15518.0	✓
FNIRT	0.463	0.036	0.381	0.410	0.463	0.519	0.537	<1e−10	15149.0	✓
Fluid	0.462	0.031	0.401	0.410	0.462	0.516	0.532	<1e−10	15503.0	✓
SICLE	0.419	0.044	0.300	0.330	0.424	0.475	0.504	<1e−10	17022.0	✓
SyN	0.514	0.033	0.454	0.460	0.515	0.565	0.578	0.072	9677.0	✗
SPM5N8	0.365	0.045	0.257	0.293	0.370	0.426	0.455	<1e−10	17418.0	✓
SPM5N	0.420	0.031	0.361	0.376	0.418	0.471	0.494	<1e−10	17160.0	✓
SPM5U	0.438	0.029	0.373	0.394	0.437	0.489	0.502	<1e−10	16773.0	✓
SPM5D	0.512	0.056	0.262	0.445	0.523	0.570	0.579	0.315	9043.0	✗
m/c global	0.480	0.031	0.421	0.430	0.482	0.530	0.543	<1e−10	13864.0	✓
m/c local	0.517	0.034	0.454	0.461	0.521	0.568	0.578	0.263	9163.0	✗
c/c global	0.480	0.031	0.421	0.430	0.482	0.530	0.543	<1e−10	13864.0	✓
c/c local	**0.520**	0.034	**0.455**	**0.463**	**0.524**	**0.572**	**0.581**	-	-	-
i/c global	0.480	0.031	0.421	0.430	0.482	0.530	0.543	<1e−10	13863.0	✓
i/c local	0.518	0.035	0.454	0.460	0.522	0.571	0.581	0.338	8972.0	✗

Table – Statistics for mean target overlap ratios for CUMC12 for different methods.

Conclusion

Summary

- Adaptive metric learning in SVF.
- Avoid end to end training for preserving diffeomorphic properties.
- Diffeomorphic guarantees at test time (no guarantee for DL methods: VoxelMorph).

Perspectives

- Combine it with momentum prediction (QuickSilver like).
- Use it in LDDMM.
- Incorporate richer deformations descriptors.

Paper to appear: *Metric learning for image registration*, CVPR 2019, Niethammer, Kwitt, Vialard.