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Application of optimal transport to data assimilation

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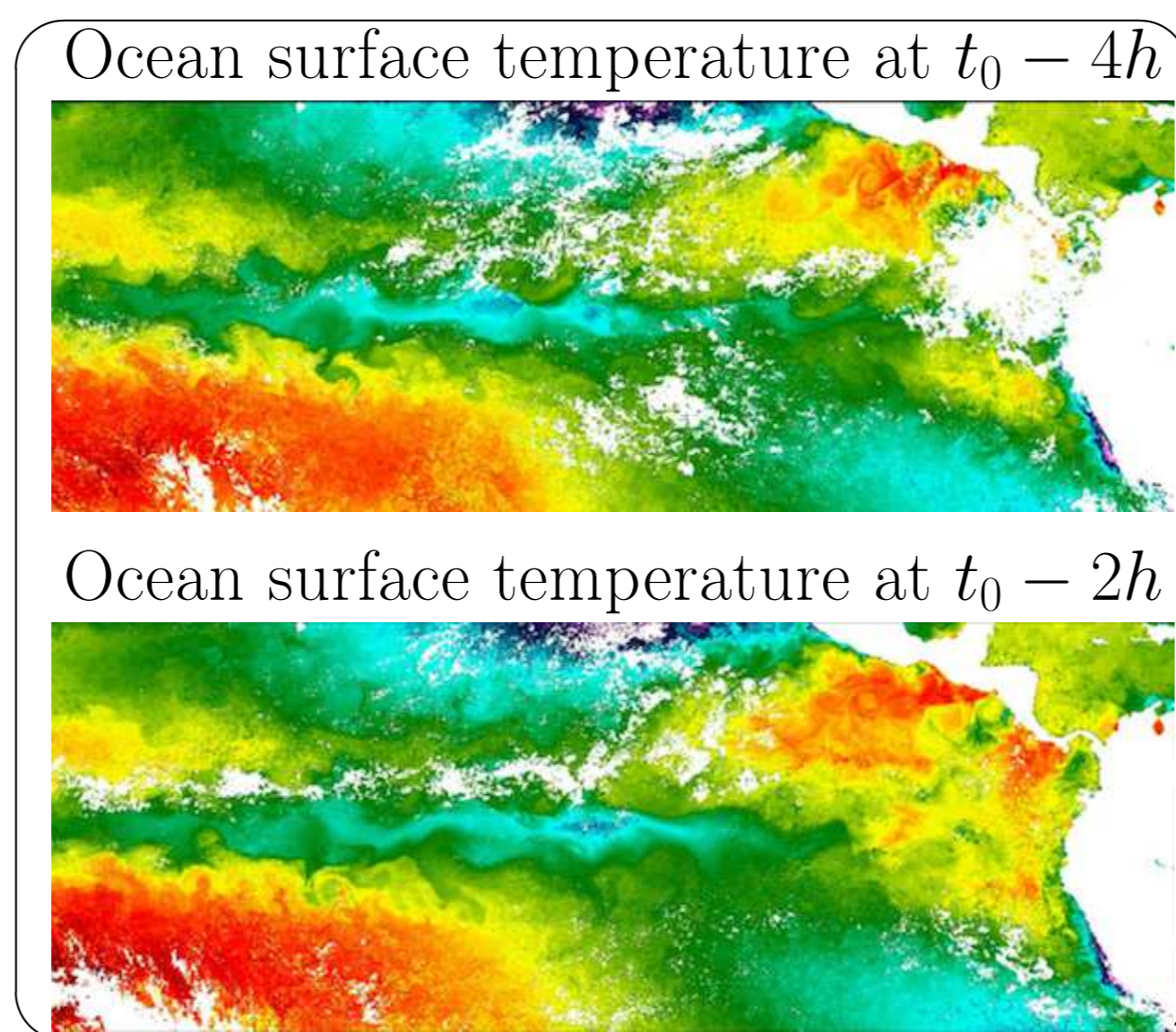
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EXAMPLE OF OCEANOGRAPHIC DATA ASSIMILATION

Given a state \mathbf{x} whose evolution is simulated through a model \mathcal{M} , **data assimilation** is an inverse problem aiming at reconstructing an initial condition \mathbf{x}_0 of \mathbf{x} given only several partial observations $(\mathbf{y}_i^o)_i$ of \mathbf{x} . For example, the state $\mathbf{x}(t, x, y, z)$ of the ocean gathers :



- Temperature $T(t, x, y, z)$
- Velocities $\mathbf{u}(t, x, y, z)$
- Salinity $S(t, x, y, z)$
- Water height $h(t, x, y)$

The question is then: What is the complete state of the ocean at $t = 0$, $\mathbf{x}_0(x, y, z)$?

In variational data assimilation this is done by minimizing a cost function \mathcal{J} defined as

$$\mathcal{J}(\mathbf{x}_0) = \frac{1}{2} \sum_i d(\mathcal{H}_i(\mathbf{x}_0), \mathbf{y}_i^o)^2 + \frac{\gamma}{2} d(\mathbf{x}_0, \mathbf{x}_0^b)^2, \quad (1)$$

$$\approx d(\mathbf{x}_0, \mathbf{x}_0^b)^2$$

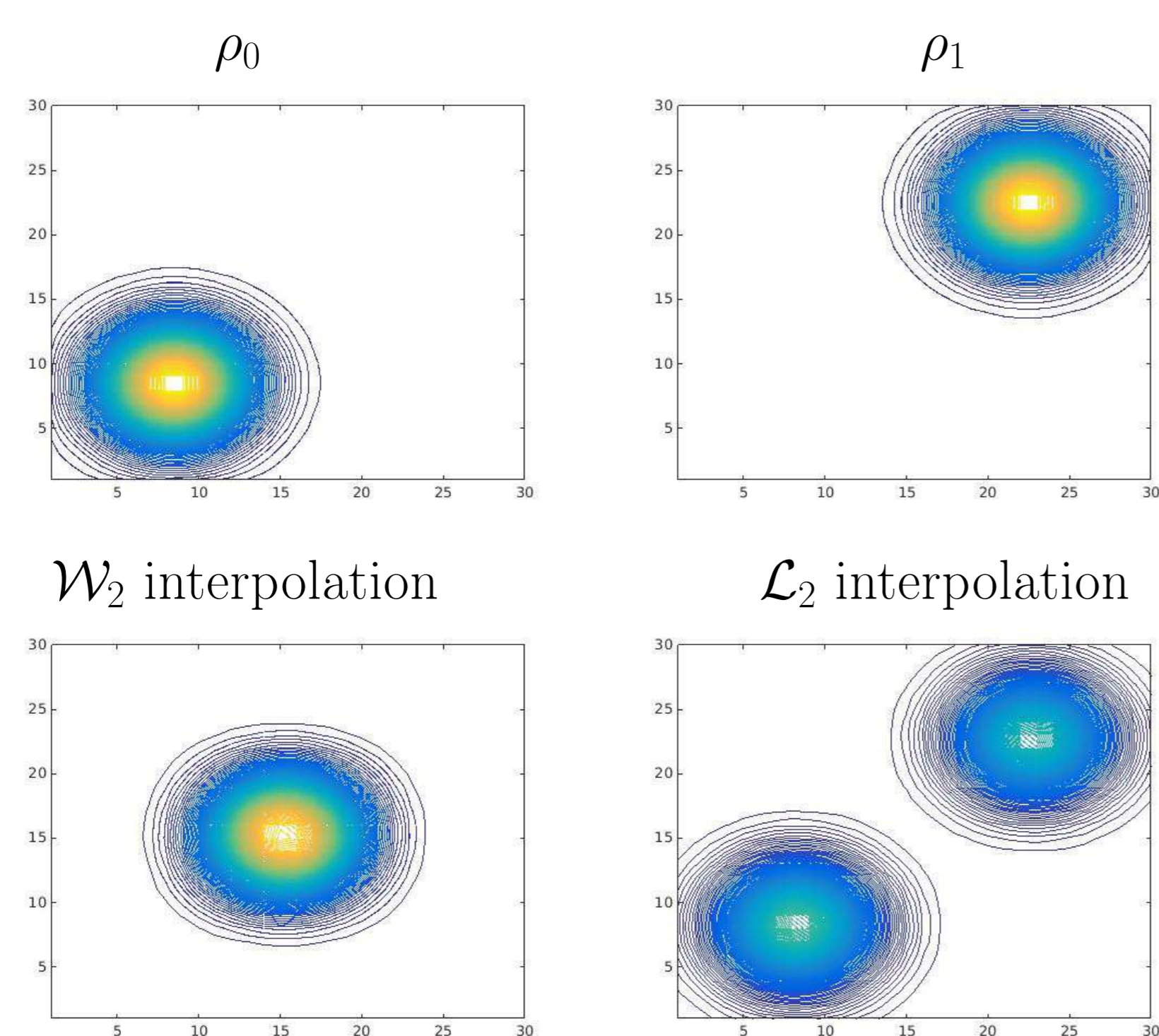
It is common for the distance d to be a weighted \mathcal{L}_2 distance. Yet, with this \mathcal{L}_2 distance, variational data assimilation cannot well cope with displacement errors. By choosing distances d that take into account the data more in its entirety, we hope get a more realistic variational data assimilation. That is why we are interested in the Wasserstein distance $d = \mathcal{W}_2$.

ADVANTAGES OF OPTIMAL TRANSPORTATION IN CASE OF DISPLACEMENT ERROR

Knowing two densities $\rho_0(x)$ and $\rho_1(x)$, the **Wasserstein distance** $\mathcal{W}_2(\rho_0, \rho_1)$ is defined as

$$\mathcal{W}_2^2(\rho_0, \rho_1) := \inf_{\substack{(\rho(t, x), v(t, x)) \\ \partial_t \rho + \text{div}(\rho v) = 0 \\ \rho(0, x) = \rho_0(x), \rho(1, x) = \rho_1(x)}} \int \int_{[0,1] \times \Omega} \rho(t, x) |v(t, x)|^2 dt dx.$$

Example of interpolation using Wasserstein and \mathcal{L}_2 distances. (Interpolation in the sense of minimizing $d(\rho, \rho_0)^2 + d(\rho, \rho_1)^2$).



For Wasserstein distance to be defined, one needs $\rho_0 \geq 0$, $\rho_1 \geq 0$ and $\int_{\Omega} \rho_0 = \int_{\Omega} \rho_1$.

GRADIENT DESCENT WITH THE WASSERSTEIN DISTANCE

Assuming \mathbf{x}_0 , $\mathcal{H}_i(\mathbf{x}_0)$ and \mathbf{y}_i^o are probability measures, the cost function \mathcal{J}_W is

$$\mathcal{J}_W(\mathbf{x}_0) = \frac{1}{2} \sum_i \mathcal{W}_2^2(\mathcal{H}_i(\mathbf{x}_0), \mathbf{y}_i^o)$$

The gradient descent algorithm for minimizing \mathcal{J}_W consists in using the following iterative algorithm

$$\mathbf{x}_0^{n+1} = \mathbf{x}_0^n - \alpha \text{grad} \mathcal{J}_W(\mathbf{x}_0^n)$$

so that $\mathcal{J}_W(\mathbf{x}_0^{n+1}) < \mathcal{J}_W(\mathbf{x}_0^n)$. To get the gradient, the **differential** must be computed and also an **inner product**. Indeed, $\text{grad} \mathcal{J}(\mathbf{x}_0)$ is such that for all η , $(\eta, \text{grad} \mathcal{J}(\mathbf{x}_0)) = D\mathcal{J}[\mathbf{x}_0].\eta$.

The differential:

Let's differentiate \mathcal{J}_W by computing $\mathcal{J}_W(\mathbf{x}_0 + \epsilon \eta)$:

- $\mathcal{H}_i(\mathbf{x}_0 + \epsilon \eta) = \mathcal{H}_i(\mathbf{x}_0) + \epsilon L[t_i, \mathbf{x}_0].\eta$ with L the tangent model.
- $\frac{1}{2} \mathcal{W}_2^2(\mathbf{y} + \epsilon \mu, \mathbf{y}') = \epsilon \langle \mu, \psi \rangle_2$ with ψ the **Kantorovich potential** of optimal transportation between \mathbf{y} and \mathbf{y}' .

Then,

$$D\mathcal{J}_W[\mathbf{x}_0].\eta = \sum_i \left\langle L[t_i, \mathbf{x}_0].\eta, \psi_i \right\rangle_2$$

with ψ_i the Kantorovich potential of the optimal transportation between $\mathcal{H}_i(\mathbf{x}_0)$ and \mathbf{y}_i^o .

The inner product:

For convergence reason, instead of using the \mathcal{L}_2 inner product, we use the \mathcal{W}_2 inner product defined in \mathbf{x}_0 by

$$(\eta, \eta') = \int_{\Omega} \mathbf{x}_0 \nabla \Phi \cdot \nabla \Phi',$$

with Φ, Φ' s.t. $\eta = -\text{div}(\mathbf{x}_0 \nabla \Phi)$, $\eta' = -\text{div}(\mathbf{x}_0 \nabla \Phi')$

Finally, the gradient of \mathcal{J}_W w.r.t. \mathcal{W}_2 inner product is, (L^* is the **adjoint model**),

$$\text{grad} \mathcal{J}_W(\mathbf{x}_0) = -\text{div} \left(\mathbf{x}_0 \nabla \left(\sum_i L^*[t_i, \mathbf{x}_0].\psi_i \right) \right).$$

ASSIMILATION OF NON-PROBABILITY MEASURE VARIABLES

In the case where $\mathcal{H}_i(\mathbf{x}_0)$ and \mathbf{y}_0 are probability measures, but *not* \mathbf{x}_0 , it is not possible to write the background term \mathcal{J}^b with \mathcal{W}_2 . For example, for the Shallow-water system

$$\begin{cases} \partial_t h + \text{div}(hu) = 0 \\ \partial_t u + (u \cdot \nabla)u + g \nabla h = \mu \Delta u \end{cases} \quad (2)$$

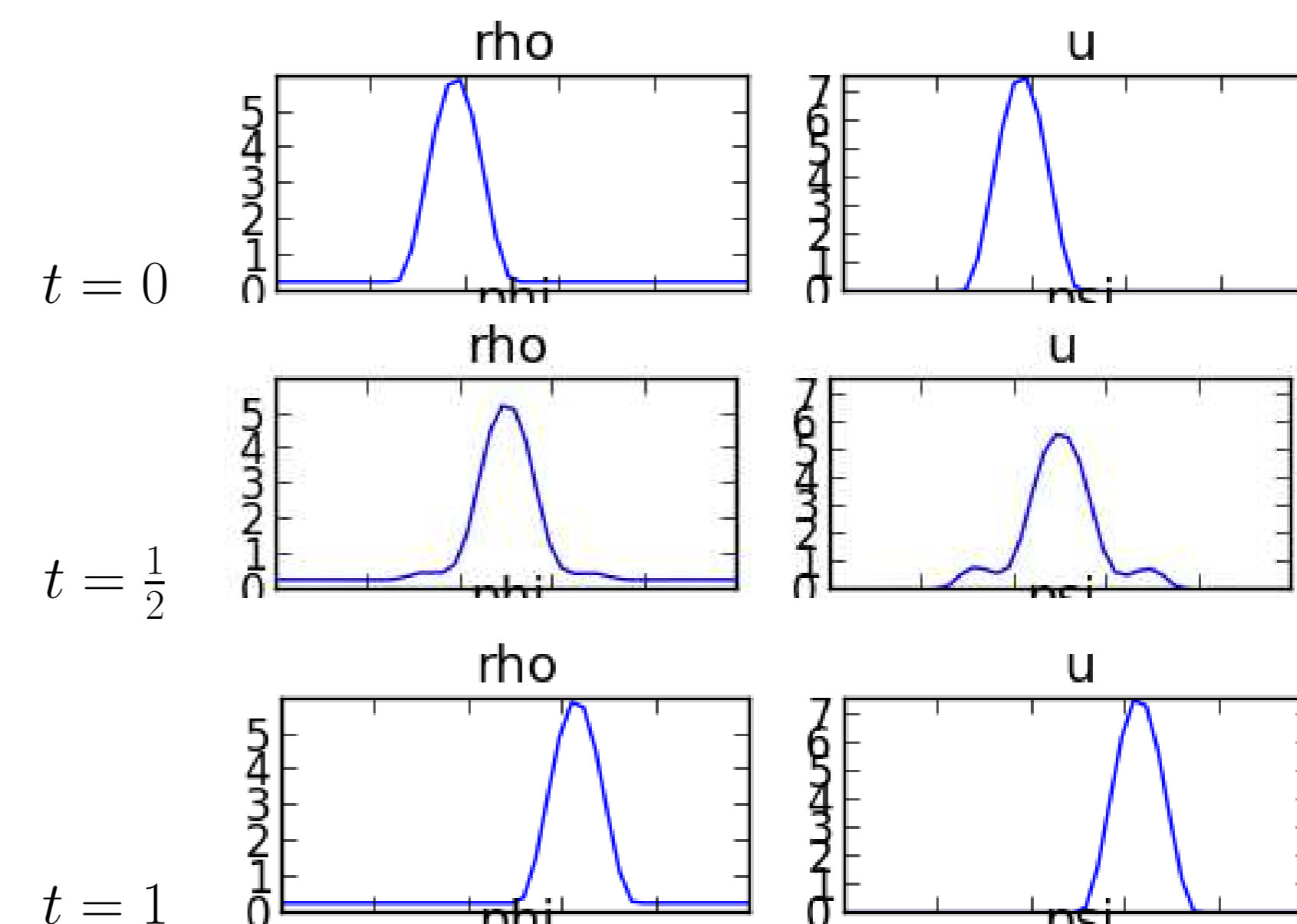
where (h_0, u_0) are to be assimilated using observations of h only. The cost function writes

$$\mathcal{J}(h_0, u_0) = \frac{1}{2} \sum_i \mathcal{W}_2^2(\mathcal{H}_i(h_0, u_0), h_i^o) + \gamma \mathcal{J}^b(h_0, u_0).$$

As it is impossible to write $\mathcal{W}_2^2(u_0, u_0^b)$, we rather use the following background term

$$\mathcal{J}^b(h_0, u_0) = \inf_{\substack{\partial_t \rho + \text{div}(\rho v) = 0 \\ \partial_t u + \text{div}(\rho w) = 0 \\ \rho(0, x) = h_0, \rho(1, x) = h_0^b \\ u(0, x) = u_0, u(1, x) = u_0^b}} \int \int_{[0,1] \times \Omega} (|v|^2 + |w|^2) \rho dt dx, \quad (3)$$

Using this, the interpolation of two shifted (h_0, u_0) and (h_1, u_1) is in-between:



The inner product to be chosen for computing the gradient will be

$$\left(\begin{pmatrix} \eta \\ v \end{pmatrix}, \begin{pmatrix} \eta' \\ v' \end{pmatrix} \right) = \int_{\Omega} h_0 \nabla \Phi \cdot \nabla \Phi' + \int_{\Omega} h_0 \nabla \Psi \cdot \nabla \Psi'$$

with Φ, Φ', Ψ, Ψ' such that

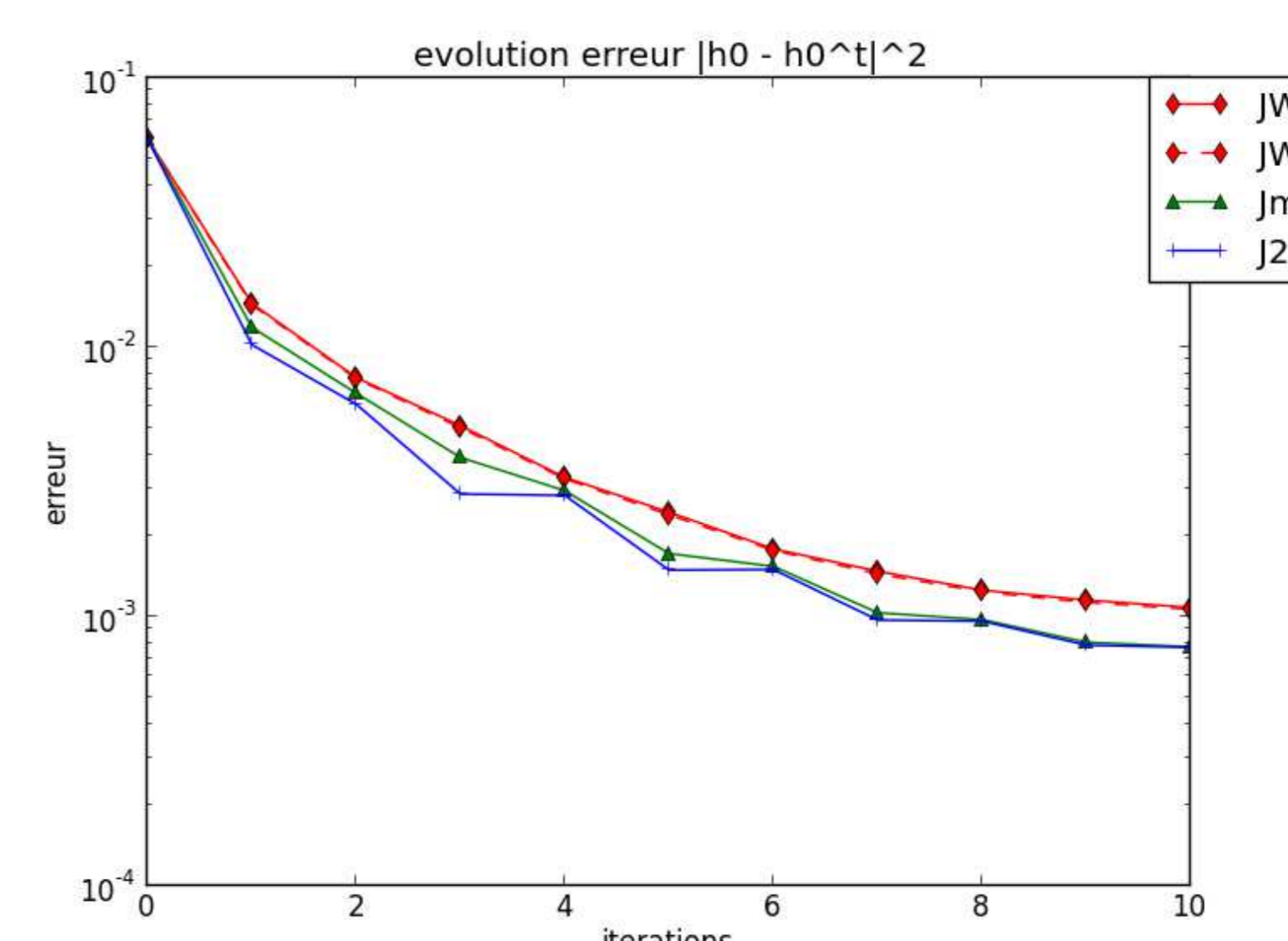
$$\begin{aligned} \eta &= -\text{div}(h_0 \nabla \Phi), & \eta' &= -\text{div}(h_0 \nabla \Phi') \\ v &= -\text{div}(h_0 \nabla \Psi), & v' &= -\text{div}(h_0 \nabla \Psi'). \end{aligned}$$

DIFFICULTIES OF USING THE WASSERSTEIN DISTANCE

- The Wasserstein distance is only defined for probability measures.
- When $\rho_0, \rho_1 \approx 1$, the \mathcal{W}_2 interpolation looks like \mathcal{L}_2 interpolation...
- When $\mathcal{J}(h_0^n) \rightarrow \min_{h_0} \mathcal{J}(h_0)$, one only has $h_0^n \rightarrow \arg \min_{h_0} \mathcal{J}(h_0)$.
- The computing time is larger for \mathcal{W}_2 than for \mathcal{L}_2 [Peyré, Papadakis, Oudet, 2013].

RESULTS AND PROPECTS

With some tests on the assimilation of (2), we compare the error $\|h_0 - h_0^b\|_2^2$ by using $d = \mathcal{L}_2$ and $d = \mathcal{W}_2$ in the cost function. The behaviors seem correct.



The background term (3) is still to be implemented.