Application of optimal transport to data assimilation

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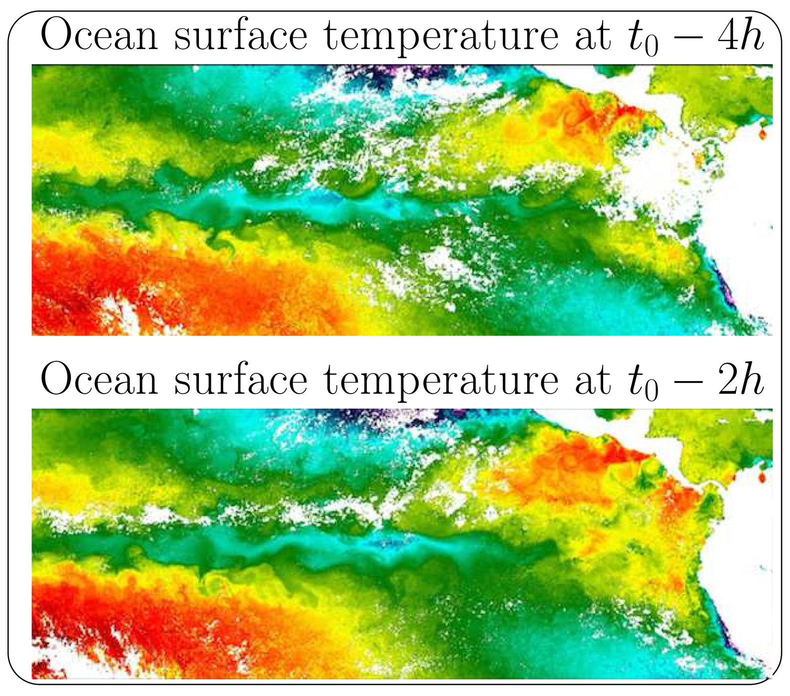
Example of oceanographic data assimilation

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

$$\mathcal{J}(\mathbf{x}_0)=\underbrace{\frac{1}{2}\sum_i d\Big(\mathcal{H}_i(\mathbf{x}_0),\mathbf{y}_i^o\Big)^2}_{\approx d\left(\mathbf{x}_0,\mathbf{x}_0^t\right)^2}+\frac{\gamma}{2}d\Big(\mathbf{x}_0,\mathbf{x}_0^b\Big)^2, \qquad (1)$$

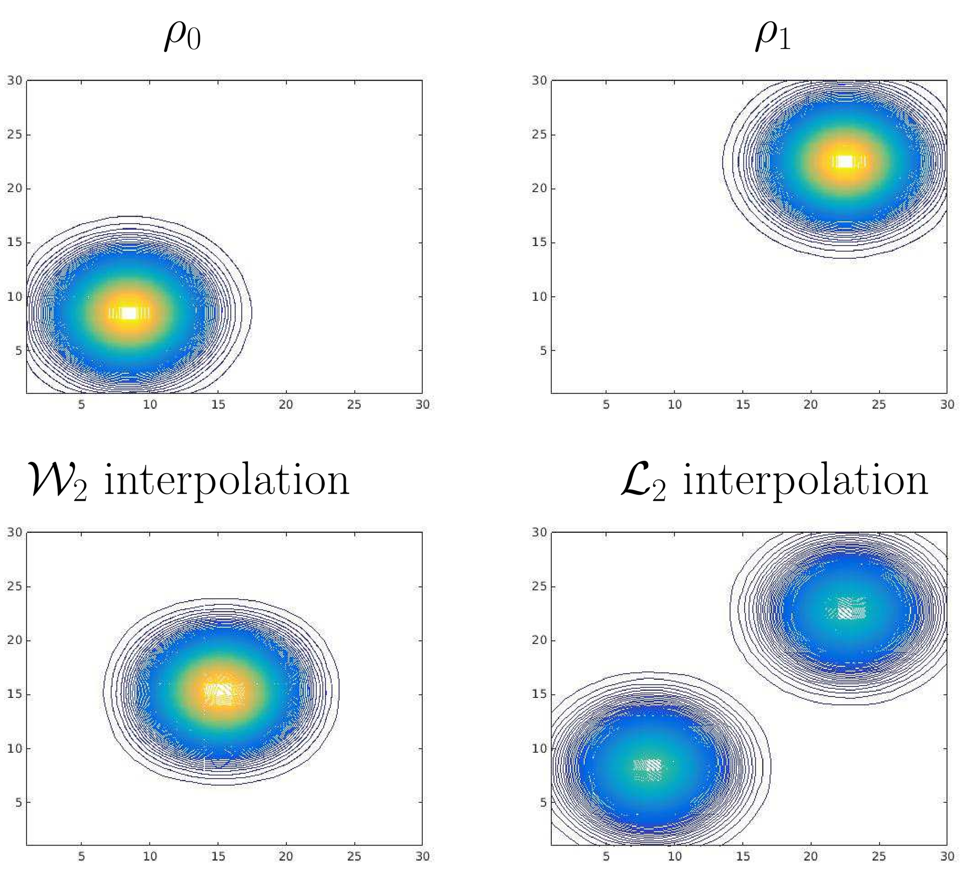
It is common for the distance d to be a weighted $\mathcal{L}_2$ distance. Yet, with this $\mathcal{L}_2$ distance, variational data assimilation cannot well cope with displacement errors. By choosing distances d that take into account the datas more in its entirety, we hope get a more realistic variational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

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

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

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

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

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

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, $\mathrm{grad}\mathcal{J}(\mathbf{x}_0)$ is such that for all η, $(\eta,\mathrm{grad}\mathcal{J}(\mathbf{x}_0))=D\mathcal{J}[\mathbf{x}_0].\eta$.

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,

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

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

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

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

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

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

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

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

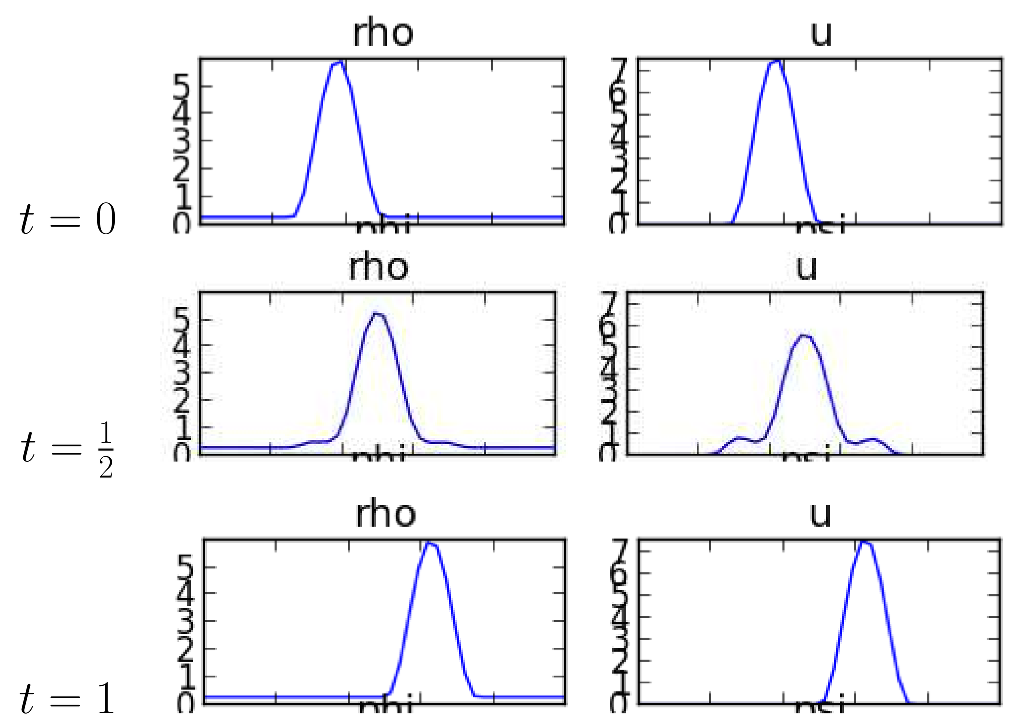
where (h_0,u_0) are to be assimilated using observations of h only. The cost function writes

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

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

$$J^b(h_0,u_0)=\inf_{\substack{\partial_t\rho+\mathrm{div}(\rho v)=0\\ \partial_t u+\mathrm{div}(\rho w)=0\\ \rho(0,x)=h_0,\,\rho(1,x)=h_0^b\\ u(0,x)=u_0,\,u(1,x)=u_0^b}}\iint_{[0,1]\times\Omega}(|v|^2+|w|^2)\,\rho\,\mathrm{d}t\mathrm{d}x,\qquad (3)$$

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

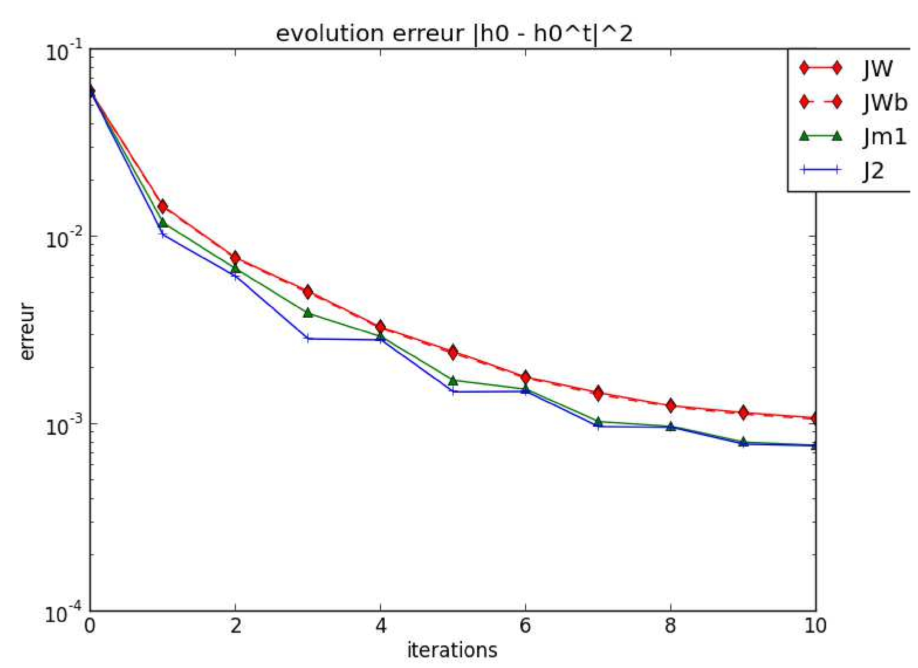
$$\begin{aligned}\eta&=-\mathrm{div}(h_0\nabla\Phi), & \eta'&=-\mathrm{div}(h_0\nabla\Phi')\\ v&=-\mathrm{div}(h_0\nabla\Psi), & v'&=-\mathrm{div}(h_0\nabla\Psi').\end{aligned}$$

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 $\mathcal{J}(h_0^n)\to\min_{h_0}\mathcal{J}(h_0)$, one only has $h_0^n\rightharpoonup\arg\min_{h_0}\mathcal{J}(h_0)$.
- 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 $\|h_0-h_0^t\|_2^2$ 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.

This work has been supported by the region Rhône-Alpes.