Application of optimal transport to data assimilation

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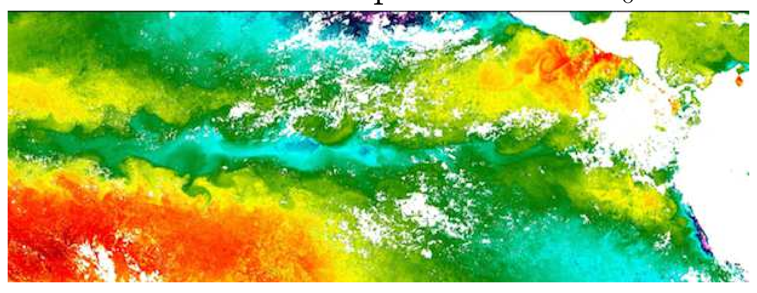
Example of oceanographic data assimilation

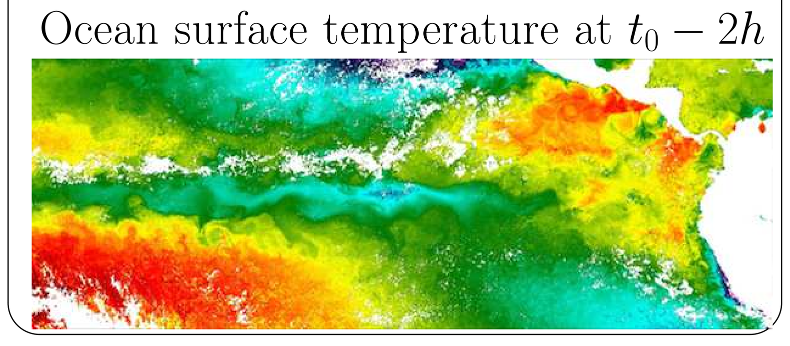
Given a state $\mathbf{x}$ whose evolution is simulated through a model $\mathcal{M}$, **data assimilation** is an inverse problem aiming at reconstructing an initial condition $\mathbf{x}_0$ of $\mathbf{x}$ given only several partial observations $(\mathbf{y}_i^o)_i$ of $\mathbf{x}$. For example, the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

Ocean surface temperature at $t_0 - 4h$



Ocean surface temperature at $t_0 - 2h$



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

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

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 $d = \mathcal{W}_2$.

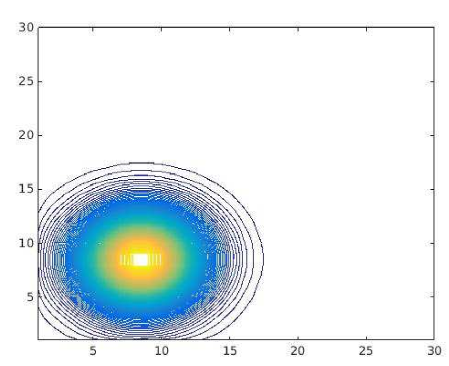
Advantages of optimal transportation in case of displacement error

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

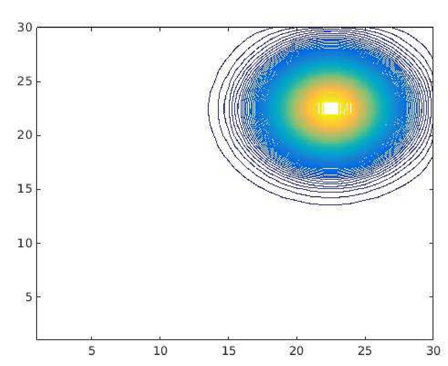
$$\mathcal{W}_2^2(\rho_0,\rho_1) := \inf_{\substack{(\rho(t,x),v(t,x)) \\ \partial_t\rho + \mathrm{div}(\rho v) = 0 \\ \rho(0,x)=\rho_0(x),\, \rho(1,x)=\rho_1(x)}} \iint_{[0,1]\times\Omega} \rho(t,x)|v(t,x)|^2 \,\mathrm{d}t\mathrm{d}x.$$

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

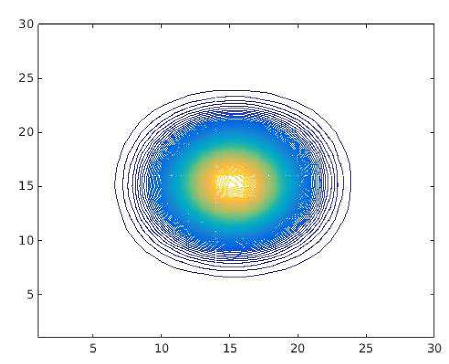
ρ_0



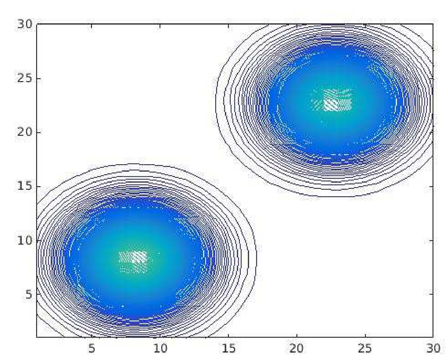
ρ_1



$\mathcal{W}_2$ interpolation



$\mathcal{L}_2$ interpolation



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

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

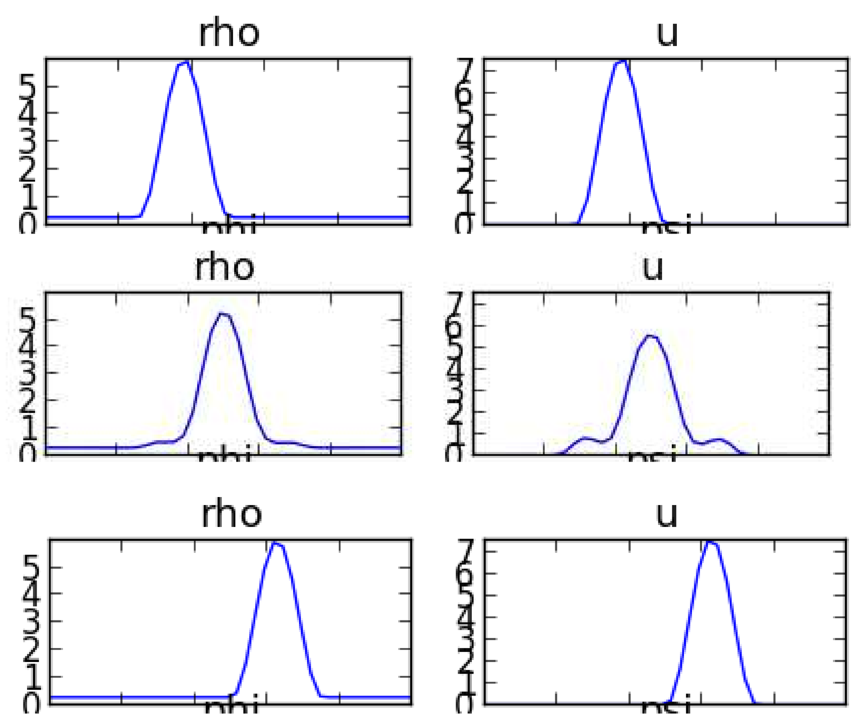
where (h_0,u_0) are to be assimilated using observations of h only. The cost function writes

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

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

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

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

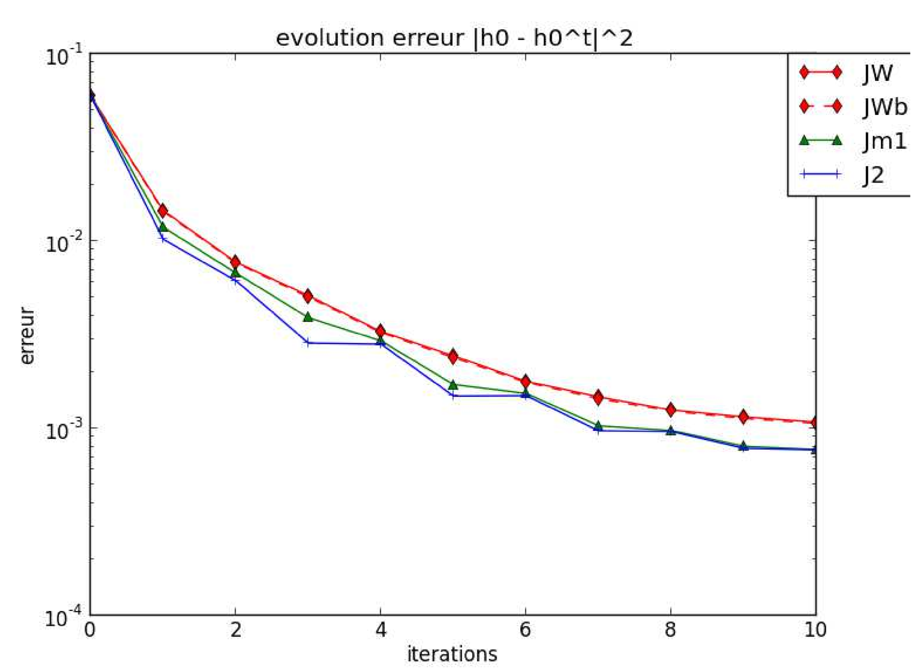
$$\begin{aligned} \eta &= -\mathrm{div}(h_0\nabla\Phi), & \eta' &= -\mathrm{div}(h_0\nabla\Phi') \\ v &= -\mathrm{div}(h_0\nabla\Psi), & v' &= -\mathrm{div}(h_0\nabla\Psi'). \end{aligned}$$

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.

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