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RESEARCH ARTICLE

Deep prior in variational assimilation to estimate ocean circulation without explicit regularization

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Abstract

Many applications in geosciences require solving inverse problems to estimate the state of a physical system. Data assimilation provides a strong framework to do so when the system is partially observed and its underlying dynamics is known to some extent. In the variational flavor, it can be seen as an optimal control problem where initial conditions are the control parameters. Such problems being often ill-posed, regularization may be needed using explicit prior knowledge to enforce satisfying solution. In this work we propose to use a deep prior, a neural architecture that generates potential solution and acts as implicit regularization. The architecture is trained in an fully-unsupervised manner using the variational data assimilation cost so that gradients are backpropagated through the dynamical model and then through the neural network. To demonstrate its use, we set a twin experiment using a shallow-water toy model, where we test various variational assimilation algorithms on a ocean-like circulation estimation.

1. Introduction

Physics-driven numerical weather prediction requires to estimate initial conditions before making a forecast. To do so, one should exploit all the knowledge at disposal which can be observations, a dynamical model or errors statistics. It formalizes as an inverse problem and data assimilation offers a large panel of methods to solve it [2]. A subset of these methods are variational so that the system state is estimated via the minimization of a cost function as in the 4D-Var algorithm [10]. Many similarities with machine learning have been highlighted [1] as both can be used to perform Bayesian inversion by gradient descent.

Even though variational data assimilation has a long standing experience in model-constrained optimization, deep learning techniques have revolutionized ill-posed inverse problems solving [14]. And methods combining neural architectures and differentiable physical models already exists [6, 17, 12]. Most of the time, a large database is leveraged to learn a regularization adapted to the task.

Fitting observations respecting the dynamical model can be seen as a form of regularization but an additional regularizer may be required to promote acceptable solution [9]. Recently a very original idea called deep prior [18] has been developed. A neural architecture is used to generate the solution of an inverse problem and acts like an implicit regularization. Astonishingly the whole architecture is trained in an unsupervised manner on one example and provides results comparable to supervised methods.

In this work, we propose a hybrid methodology bridging deep prior and variational data assimilation and we test it in a twin experiment. The algorithm is evaluated on an ocean-like motion estimation task requiring regularization, then compared to adapted data assimilation algorithms [3, 4]. All algorithms are implemented using tools from the deep learning community. The code is available in Github¹.

2. Methodology

2.1. Data assimilation Framework

A dynamical system is considered where a state \mathbf{X} evolves over time following perfectly-known dynamics \mathbb{M} , see Eq. (1). Partial and noisy observations \mathbf{Y} are available through an observation operator \mathbb{H} , Eq. (2). A background \mathbf{X}_b gives prior information about the initial system state, Eq. (3).

$$\text{Evolution:} \quad \mathbf{X}_{t+1} = \mathbb{M}_t(\mathbf{X}_t) \quad (1)$$

$$\text{Observation:} \quad \mathbf{Y}_t = \mathbb{H}_t(\mathbf{X}_t) + \varepsilon_{R_t} \quad (2)$$

$$\text{Background:} \quad \mathbf{X}_0 = \mathbf{X}_B + \varepsilon_B \quad (3)$$

Additive noise ε_B and ε_R represent uncertainties about the observations and the background, respectively. These noises are quantified by their assumed known covariance matrices \mathbf{B} and \mathbf{R} , respectively. The dynamics is here considered perfect, but the framework could easily be extended to an imperfect dynamics. For any given matrix \mathbf{A} , we note $\|x - y\|_{\mathbf{A}}^2 = \langle (x - y) | \mathbf{A}^{-1} (x - y) \rangle$ the associated Mahalanobis distance.

¹https://github.com/ArFilоче/Deepprior4DVar_CI22

2.2. Variational assimilation

The objective of data assimilation is to provide an estimation of the system state \mathbf{X} by optimally combining available data \mathbf{X}_B , \mathbf{Y} and the dynamical model \mathbb{M} . In the variational formalism [10], this is done via the minimization of a cost function which is the sum of background errors and observational errors, $\mathcal{J}_{4DVar} = \frac{1}{2} \|\varepsilon_b\|_{\mathbf{B}}^2 + \frac{1}{2} \sum_{t=0}^T \|\varepsilon_{R_t}\|_{\mathbf{R}_t}^2$. The optimization problem is model-constrained as described in Eq. (4). What motivates this cost function is that minimizing it leads to the maximum *a posteriori* estimation of the state under independent Gaussian errors, linear observation operator and linear model hypothesis. The corresponding optimization algorithm is named 4D-Var.

$$\begin{aligned} \arg \min_{\mathbf{X}_0} \quad & \mathcal{J}_{4DVar}(\mathbf{X}_0) = \frac{1}{2} \|\mathbf{X}_0 - \mathbf{X}_b\|_{\mathbf{B}}^2 + \frac{1}{2} \sum_{t=0}^T \|\mathbf{Y}_t - \mathbb{H}_t(\mathbf{X}_t)\|_{\mathbf{R}_t}^2 \\ \text{s.t.} \quad & \mathbf{X}_{t+1} = \mathbb{M}_t(\mathbf{X}_t) \end{aligned} \quad (4)$$

The link between variational assimilation and Tikhonov regularization is well described in [9]. For example, choosing a particular matrix \mathbf{B} will promote a particular set of solutions. Therefore, making alike choices can be seen as a handcrafted regularization to take advantage of expert prior knowledge.

2.3. Deep prior 4D-Var

The idea behind deep prior is that using a well-suited neural architecture to generate a solution of the variational problem can act as a handcrafted regularization. This means that the control parameters are shifted from the system state space to the neural network parameters space. From a practical standpoint, a latent variable z is fixed and a generator network g_θ outputs the solution from it such that $g_\theta(z) = \mathbf{X}_0$.

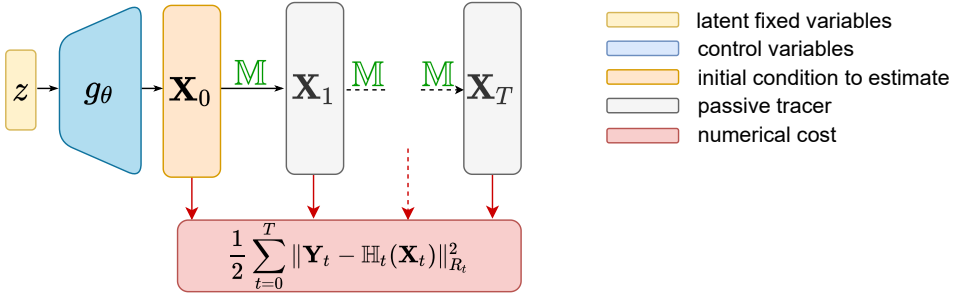


Figure 1. Schematic view of the forward integration in Deep Prior 4D-Var.

2.3.1. Cost function

The generator is then trained with the variational assimilation cost $\mathcal{J}(\theta)$. To emphasize the regularizing effect of the deep prior method, we choose to fix $\mathbf{B} = \mathbf{0}$ so that no background information is used. It means that $\mathcal{J}(\theta) = \frac{1}{2} \sum_{t=0}^T \|\varepsilon_{R_t}\|_{\mathbf{R}_t}^2$ and by denoting multiple integration between two times $\mathbb{M}_{t_1 \rightarrow t_2}$, the cost can be developed as in Eq. (5).

$$\mathcal{J}(\theta) = \frac{1}{2} \sum_{t=0}^T \|\mathbf{Y}_t - \mathbb{H}_t(\mathbb{M}_{0 \rightarrow t}(g_\theta(z)))\|_{\mathbf{R}_t}^2 \quad (5)$$

It is important to note that this approach is unsupervised, the architecture being trained from scratch on one assimilation window with no pre-training. All the prior information should be contained in the architecture choice.

2.3.2. Gradient

The gradients of this cost function can be determined analytically. First, the chain rule gives Eq. (6). Then using the adjoint state method we can develop $\nabla_{\mathbf{X}_0} \mathcal{J}(\mathbf{X}_0)$ as in Eq. (7), a detailed proof can be found in [2]. In the differentiable programming paradigm, such analytical expression is not needed to obtain gradients, adjoint modeling is implicitly performed as gradients are backpropagated automatically.

$$\nabla_{\theta} \mathcal{J}(\theta) = \nabla_{\mathbf{X}_0} \mathcal{J}(\mathbf{X}_0) \nabla_{\theta} \mathbf{X}_0 = \nabla_{\mathbf{X}_0} \mathcal{J}(\mathbf{X}_0) \nabla_{\theta} g_{\theta}(z) \quad (6)$$

$$\nabla_{\mathbf{X}_0} \mathcal{J}(\mathbf{X}_0) = \sum_{t=0}^T \left[\frac{\partial (\mathbb{H}_t \mathbb{M}_{0 \rightarrow t})}{\partial \mathbf{X}_0} \right]^{\top} \mathbf{R}_t^{-1} \varepsilon_{R_t} \quad (7)$$

2.3.3. Algorithm

The algorithm seeks to numerically optimize the cost function and simply consists of alternating forward and backward integration to update control parameters by gradient descent (see Algorithm 1). A schematic view of the forward integration can be found in Figure 1.

Algorithm 1 – Deep prior 4D-Var

Initialize fixed latent variables z

Initialize control variables θ

while stop criterion **do**

forward: integrate $\mathbb{M}_{0 \rightarrow T}(g_{\theta}(z))$ and compute \mathcal{J}

backward: automatic differentiation returns $\nabla_{\theta} \mathcal{J}$

update: $\theta = \text{optimizer}(\theta, \mathcal{J}, \nabla_{\theta} \mathcal{J})$

end while

return θ, \mathbf{X}_0

3. Case study

3.1. Twin experiment

The proposed methodology is tested within a twin experiment where data are generated from a numerical dynamical model. Observations are then created by sub-sampling and adding noise. The aim of this experiment is to highlight the implicit regularizing effect of the deep generative network. To do so, we compare various algorithms on the observation assimilation task. The considered algorithms are 4D-Var with no regularization, 4D-Var with Tikhonov regularization, and deep prior 4D-Var. All the algorithms are implemented with tools based on automatic differentiation such that no adjoint modeling is required, as described in [7]. In all the assimilation experiments, the dynamical model is perfectly known.

3.2. Dynamical system

3.2.1. State

State variables of the considered system are η , the height deviation of the horizontal pressure surface from its mean height, and \mathbf{w} , the associated velocity field. \mathbf{w} can be decomposed in u and v , the zonal

and meridional velocity, respectively. At each time t , the system state is then $\mathbf{X}_t = (\eta_t \mathbf{w}_t^\top)^\top$. The considered temporal window has a fixed size.

3.2.2. Shallow water model

The dynamical model used here corresponds to a discretization of the shallow water equations system in Eq. (8) with first order upwind numerical schemes. These schemes are implemented using a natively differentiable software. H represents the mean height of the horizontal pressure surface and g the acceleration due to gravity. After reaching an equilibrium starting from Gaussian random initial conditions, system trajectories are simulated as shown in Figure 2.

$$\begin{cases} \frac{\partial \eta}{\partial t} + \frac{\partial(\eta + H)u}{\partial x} + \frac{\partial(\eta + H)v}{\partial y} = 0 \\ \frac{\partial u}{\partial t} + g \frac{\partial \eta}{\partial x} = 0 \\ \frac{\partial v}{\partial t} + g \frac{\partial \eta}{\partial y} = 0 \end{cases} \quad (8)$$

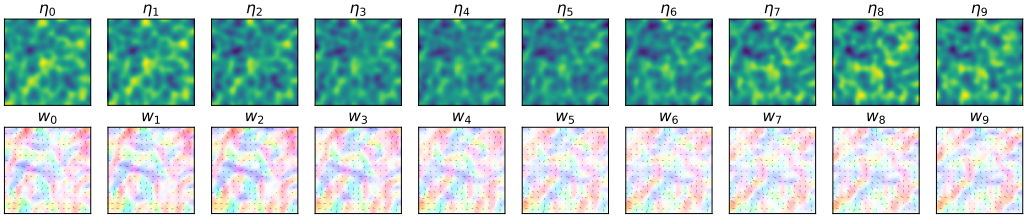


Figure 2. Example of simulated trajectory with the shallow water numerical model.

3.2.3. Observations

At regular observational dates, η is fully observed up to an additive white noise, see Figure 3. The velocity field \mathbf{w} is never observed. This means that at observational date t , the observation operator \mathbb{H}_t is then a linear projector so that $\eta_t = \mathbb{H}_t \mathbf{X}_t$.

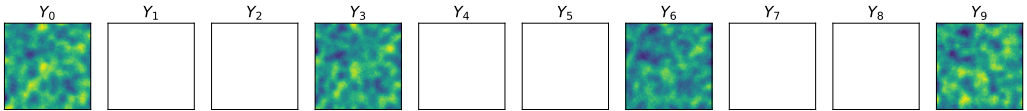


Figure 3. Example of simulated system observations.

3.3. Regularization

The role of the assimilation task is then to estimate the velocity field from successive observations of η . Such motion estimation inverse problem can be ill-posed and may need regularization. The dynamical model being considered perfect, all the velocity fields within the window are determined by the initial field \mathbf{w}_0 .

3.3.1. No regularization

The 4D-Var version without regularization only optimizes the fit-to-data term in the cost function. This means that no prior knowledge on the solution can be used, the background covariance matrix \mathbf{B} vanishes.

3.3.2. Tikhonov regularization

On the other hand, the ‘‘Tikhonov’’ 4D-Var algorithm optimizes the fit-to-data term and also a penalty term. The estimated motion field is forced to be smooth by constraining $\|\nabla \mathbf{w}_0\|_2^2$ and $\|\nabla \cdot \mathbf{w}_0\|_2^2$ to be small. As proved in [11], these terms can be directly included in the background error using a particular matrix \mathbf{B} such that $\alpha \|\nabla \mathbf{w}_0\|_2^2 + \beta \|\nabla \cdot \mathbf{w}_0\|_2^2 = \|\mathbf{X}_0 - \mathbf{X}_b\|_{B_{\alpha,\beta}}^2$ where α and β are parameters to be tuned. Such regularization is a classical optical flow penalty [8] and can be used for ocean motion estimation [3].

3.3.3. Deep prior

As depicted in the method, the only assumption made is about the architecture of the network g_θ generating the solution \mathbf{w}_0 . Obviously, the chosen architecture is critical for performances. In this experiment, we use a neural architecture similar to the generative convolutional network presented in [16], but replacing deconvolution operations to avoid checkerboard artifacts as described in [13]. The exact architecture is provided in Appendix A.1.

4. Results

The first results to look at is the plot of the velocity fields estimated by the algorithms, see Figure 4. The 2D-field of arrows represents the direction and the intensity of the velocity, the colormap provides the same information but helps visualization. Without regularization, the 4D-Var estimation is sharp and seems to suffer from numerical optimization artifacts. On the contrary the deep prior estimate looks less precise but far smoother. The regularized provides the most accurate and smooth estimation. Others examples can be found in Appendix A.2.

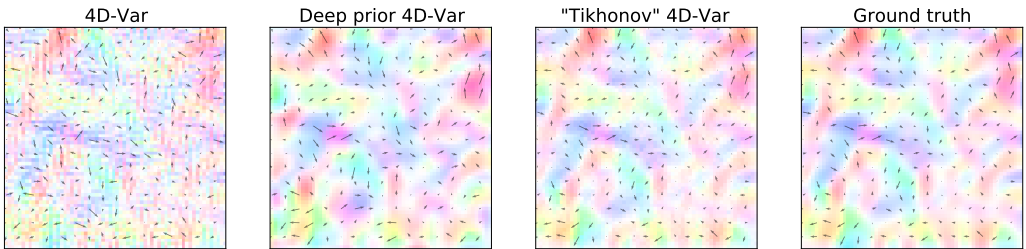


Figure 4. Example of estimated motion fields \mathbf{w}_0 with various algorithms.

Several metrics are calculated to quantify the quality of the estimations. The endpoint error and the angular error are classical optical flow scores, they calculate the Euclidean distance and the average angular deviation between the estimation and the ground truth, respectively. At first glance, there is no statistical difference between deep prior 4D-Var and 4D-Var without regularization.

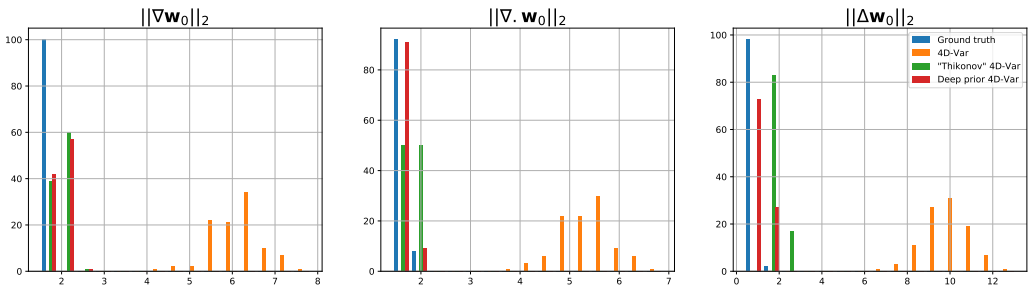
However, if we dig into smoothness statistics of the estimated fields, $\|\nabla \cdot \mathbf{w}_0\|_2$, $\|\nabla \mathbf{w}_0\|_2$ and $\|\Delta \mathbf{w}_0\|_2$, it seems that deep prior is able to capture complex statistics of the true motion field. Similar behavior has been noticed in [19]. Looking closer in the histograms, Figure 5, we see that deep prior and ‘‘Tikhonov’’ 4D-Var estimations have smoothness statistics very close to that of the original motion field. Whether it has been explicitly constrained or by deep network design, smooth solutions are

Table 1. Metrics quantifying the quality of estimated motion field \mathbf{w}_0 over the assimilated database

Metric ¹	Assimilation Score		Smoothness statistics		
	Endpoint error ($\times 10^2$)	Angular error	$\ \nabla \mathbf{w}_0\ _2$	$\ \nabla \cdot \mathbf{w}_0\ _2$	$\ \Delta \mathbf{w}_0\ _2$
4D-Var	4.2 ± 0.4	28.4 ± 9.8	6.1 ± 0.6	5.3 ± 0.5	9.9 ± 1.0
Deep Prior 4D-Var	4.6 ± 2.0	26.7 ± 5.0	1.9 ± 0.1	1.6 ± 0.9	1.0 ± 0.3
“Tikhonov” 4D-Var	1.6 ± 0.6	9.9 ± 9.8	2.0 ± 0.1	1.8 ± 0.1	1.9 ± 0.1
Ground truth	0	0	1.7 ± 0.9	1.6 ± 0.1	0.7 ± 0.3

¹All the metrics are averaged on images

unforced by regularization.

**Figure 5.** Histograms of smoothness statistics from estimated motion field \mathbf{w}_0 with various algorithms.

It has to be noted that the “Tikhonov” 4D-Var is the only algorithm here that has been treated with hyper-parameters tuning which can explain the large differences in scores. It can be argued that the neural architecture, which is known as a good baseline to generate images, has been tuned through many image processing experiments. However, grid-searching hyper-parameters particularly suited for this experiment should enhance performances.

5. Conclusion

We proposed an original method bridging ideas from the image processing and the geosciences communities to solve a variational inverse problem. More precisely we used a neural network as implicit regularization to generate the solution of an initial value problem. To demonstrate its efficiency, we set up a twin experiment comparing different algorithms in a data assimilation task derived from shallow water model. The results show that this kind of regularization can provide an interesting alternative when prior knowledge is not available. However in our case, we observed that expert-driven handcrafted regularization provides better performances. Finally, this work opens the way for further developments on the architecture design, but also in a more realistic context where the numerical dynamics is imperfect.

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A. Appendix. Experiment details

A.1. Neural network architecture

Layer (type)	Output Shape	Param #
ConvTranspose2d-1	[-1, 512, 4, 4]	819,200
BatchNorm2d-2	[-1, 512, 4, 4]	1,024
ReLU-3	[-1, 512, 4, 4]	0
Upsample-4	[-1, 512, 8, 8]	0
ReflectionPad2d-5	[-1, 512, 10, 10]	0
Conv2d-6	[-1, 256, 8, 8]	1,179,904
BatchNorm2d-7	[-1, 256, 8, 8]	512
ReLU-8	[-1, 256, 8, 8]	0
Upsample-9	[-1, 256, 16, 16]	0
ReflectionPad2d-10	[-1, 256, 18, 18]	0
Conv2d-11	[-1, 128, 16, 16]	295,040
BatchNorm2d-12	[-1, 128, 16, 16]	256
ReLU-13	[-1, 128, 16, 16]	0
Upsample-14	[-1, 128, 32, 32]	0
ReflectionPad2d-15	[-1, 128, 34, 34]	0
Conv2d-16	[-1, 64, 32, 32]	73,792
BatchNorm2d-17	[-1, 64, 32, 32]	128
ReLU-18	[-1, 64, 32, 32]	0
Upsample-19	[-1, 64, 64, 64]	0
ReflectionPad2d-20	[-1, 64, 66, 66]	0
Conv2d-21	[-1, 3, 64, 64]	1,731
Tanh-22	[-1, 3, 64, 64]	0
=====		
Total params: 2,371,587		
Trainable params: 2,371,587		
Non-trainable params: 0		
=====		
Input size (MB): 0.00		
Forward/backward pass size (MB): 11.03		
Params size (MB): 9.05		
Estimated Total Size (MB): 20.08		
=====		

A.2. Supplementary examples

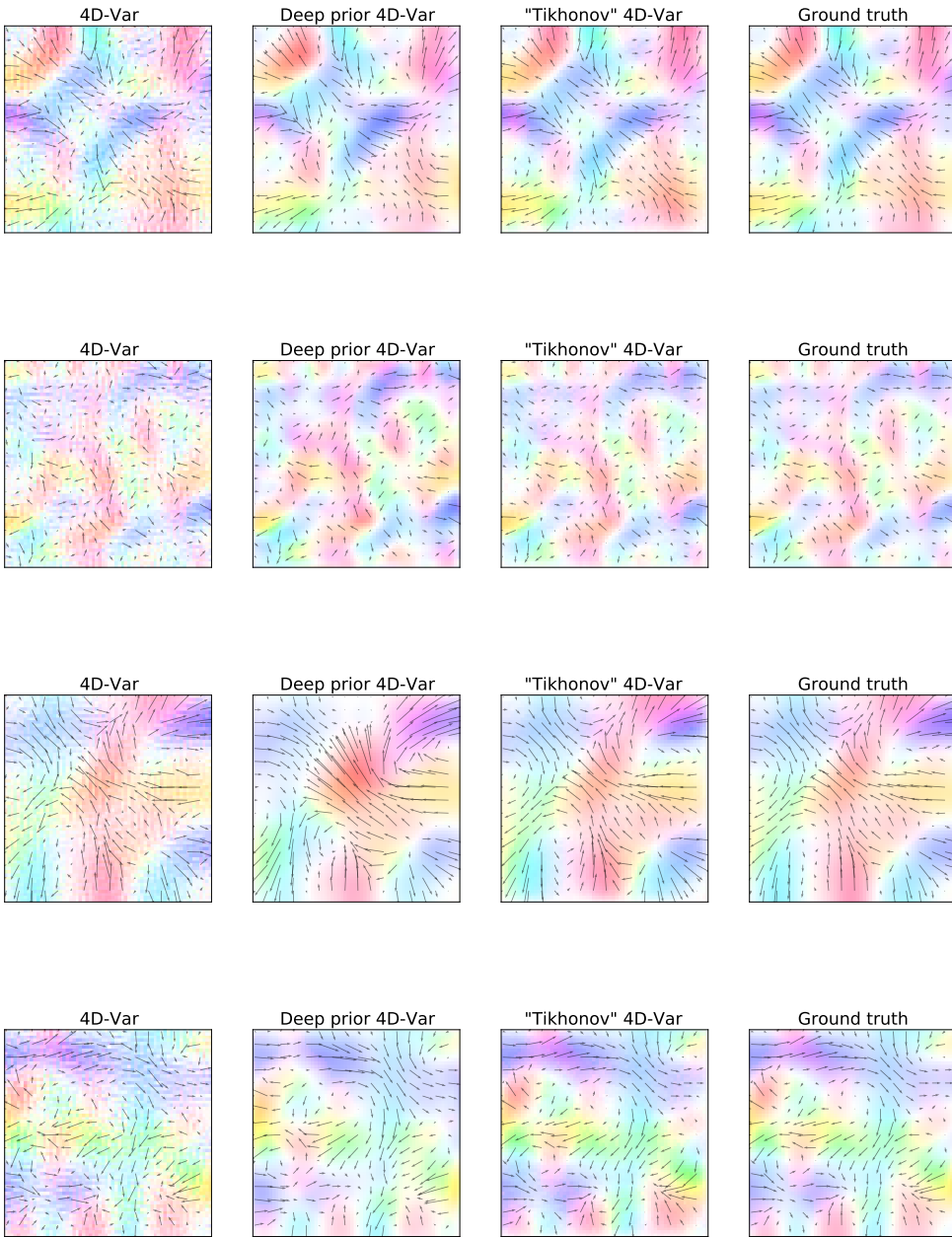


Figure 6. *Examples of estimated motion fields \mathbf{w}_0 with various algorithms, each line corresponds to a different assimilation window.*