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Deterministic Predictability of the Most Probable State and Reformulation of Variational Data Assimilation

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Introduction

- EnKF and variational methods are approximate data assimilation methods for nonlinear systems or non-Gaussian PDFs.
- Theoretical comparison of the two methods for nonlinear systems will provide insight into further advances of data assimilation.
- The present study addresses the above issue by investigating deterministic predictability and by reformulating the variational method.

Contents

Evolution of the most probable state

- The initial condition of deterministic prediction is usually set to the most probable state (the mode of PDF) estimated from data assimilation.

- In the present study, if the most probable state evolves according to the equations of the system, it is said that deterministic prediction is possible.

- The evolution of PDF of the state variables $p(\mathbf{x},t)$ is described by the Liouville equation:

$$\frac{\partial p}{\partial t}+\mathrm{Tr}\left[\frac{\partial}{\partial \mathbf{x}}\left(p\mathbf{F}\right)\right]=0,$$

for a deterministic system: $$\frac{d\mathbf{x}}{dt}=\mathbf{F}(\mathbf{x},t).$$

Evolution of the most probable state – cont'd

- Prediction equation of the mode of PDF $\mathbf{x}_M(t)$:

$$\frac{d\mathbf{x}_M}{dt} = \mathbf{F}(\mathbf{x}_M, t) - \mathbf{P}_M \underline{\frac{\partial}{\partial \mathbf{x}} \mathrm{Tr}\left[\frac{\partial \mathbf{F}}{\partial \mathbf{x}}\right]}\Bigg|_{\mathbf{x}_M},$$

where the error covariance matrix $\mathbf{P}_M(t)$ is defined by Gaussian fitting to the PDF at the mode:

$$\mathbf{P}_M := -\left(\frac{1}{p}\frac{\partial^2 p}{\partial \mathbf{x}\partial \mathbf{x}}\right)\Bigg|_{\mathbf{x}_M}^{-1}.$$

- Prediction equation of $\mathbf{P}_M(t)$:

$$\frac{d\mathbf{P}_M}{dt} = \frac{\partial \mathbf{F}}{\partial \mathbf{x}}\bigg|_{\mathbf{x}_M} \mathbf{P}_M + \mathbf{P}_M \frac{\partial \mathbf{F}}{\partial \mathbf{x}}\bigg|_{\mathbf{x}_M}^{\mathrm{T}} - \mathbf{P}_M \left(\underline{\frac{\partial^2}{\partial \mathbf{x}\partial \mathbf{x}} \mathrm{Tr}\left[\frac{\partial \mathbf{F}}{\partial \mathbf{x}}\right]}\right)\Bigg|_{\mathbf{x}_M} \mathbf{P}_M$$
$$- \mathbf{P}_M \left(\frac{1}{p}\frac{\partial^3 p}{\partial \mathbf{x}\partial \mathbf{x}\partial \mathbf{x}}\right)\Bigg|_{\mathbf{x}_M} \mathbf{P}_M \underline{\frac{\partial}{\partial \mathbf{x}} \mathrm{Tr}\left[\frac{\partial \mathbf{F}}{\partial \mathbf{x}}\right]}\Bigg|_{\mathbf{x}_M} \mathbf{P}_M .$$

Evolution of the most probable state – cont'd

- If the trace condition

$$\frac{\partial}{\partial \mathbf{x}} \mathrm{Tr}\left[\frac{\partial \mathbf{F}}{\partial \mathbf{x}}\right] \equiv \mathbf{0}$$

holds, the first equation is reduced to

$$\frac{d\mathbf{x}_M}{dt} = \mathbf{F}(\mathbf{x}_M, t),$$

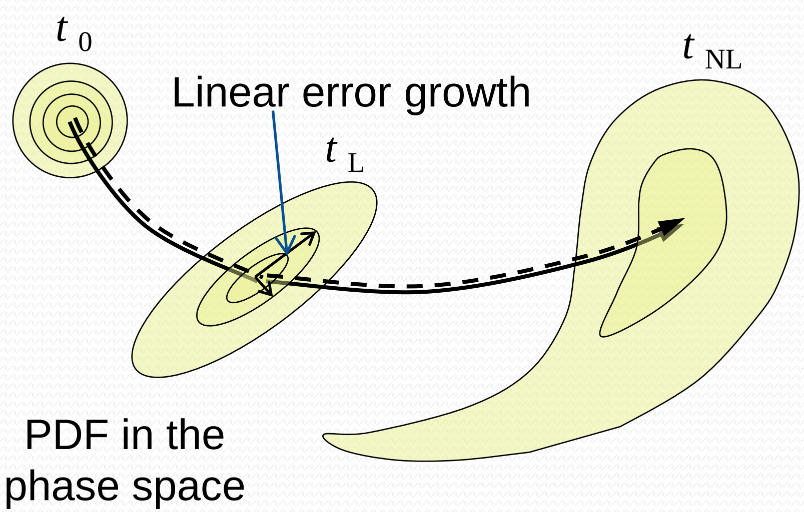
and deterministic prediction is possible.

- Prediction equation of the error covariance matrix $\mathbf{P}_M$ is given by:

$$\frac{d\mathbf{P}_M}{dt} = \left.\frac{\partial \mathbf{F}}{\partial \mathbf{x}}\right|_{\mathbf{x}_M} \mathbf{P}_M + \mathbf{P}_M \left.\frac{\partial \mathbf{F}}{\partial \mathbf{x}}\right|_{\mathbf{x}_M}^{\mathrm{T}}.$$

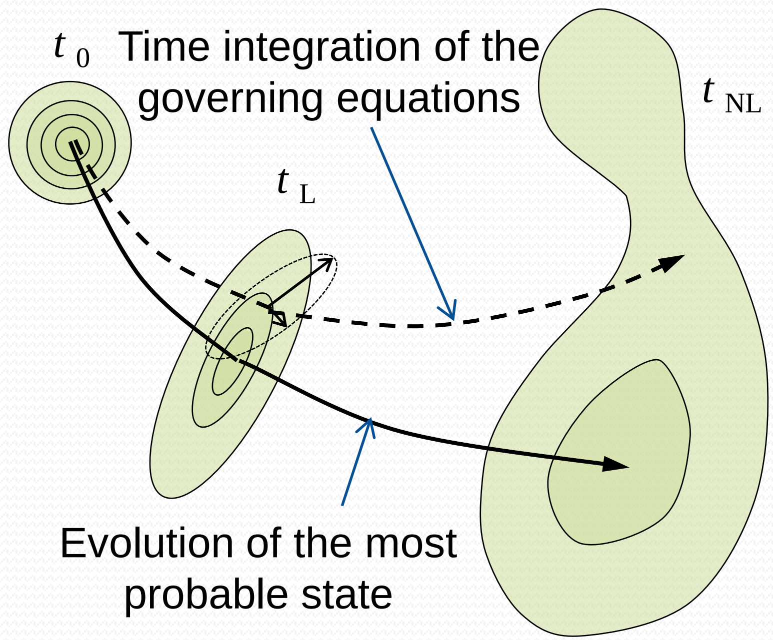
Evolution of the most probable state – cont'd

Nonlinear system satisfying the trace condition



Canonical Hamiltonian systems, Lorenz-63 and -96 models, etc.

Nonlinear system not satisfying the trace condition



Cumulus convection, chemical reactions, etc.

Hamiltonian fluid dynamics

- Equation of motion with Hamiltonian $H(\mathbf{x},t)$:

$$\frac{d\mathbf{x}}{dt} = \mathbf{F} = \{\mathbf{x}, H\}, \qquad \{f,g\} := \left(\frac{\partial f}{\partial \mathbf{x}}\right)^{\mathrm{T}} \mathbf{J} \frac{\partial g}{\partial \mathbf{x}},$$

  where $\{f,g\}$ is the Poisson bracket.

- Canonical Hamiltonian systems satisfy the trace condition due to the Liouville theorem:

$$\mathbf{J} = \begin{pmatrix} \mathbf{0} & \mathbf{I} \\ -\mathbf{I} & \mathbf{0} \end{pmatrix} \quad \Rightarrow \quad \mathrm{Tr}\left[\frac{\partial \mathbf{F}}{\partial \mathbf{x}}\right] \equiv 0 \quad \Rightarrow \quad \frac{\partial}{\partial \mathbf{x}} \mathrm{Tr}\left[\frac{\partial \mathbf{F}}{\partial \mathbf{x}}\right] \equiv \mathbf{0}.$$

- Fluid dynamics with Lagrangian variables is transformed into a canonical Hamiltonian system.

- Fluid dynamics with Eulerian variables is generally not a canonical Hamiltonian system.

Trace condition

- Since the trace is invariant under invertible linear transformations, the trace condition is also invariant.

If $\quad \hat{\mathbf{x}} = \mathbf{L}\mathbf{x}, \qquad \mathbf{L}$: nonsingular matrix,

then $\quad \dfrac{\partial}{\partial \mathbf{x}} \mathrm{Tr}\left[\dfrac{\partial \mathbf{F}}{\partial \mathbf{x}}\right] \equiv \mathbf{0} \quad \Leftrightarrow \quad \dfrac{\partial}{\partial \hat{\mathbf{x}}} \mathrm{Tr}\left[\dfrac{\partial \hat{\mathbf{F}}}{\partial \hat{\mathbf{x}}}\right] \equiv \mathbf{0}.$

- If fluids are unbounded, it is found from a Fourier expansion that the trace condition generally holds for Eulerian fluid dynamics.

Quasi-geostrophic equation

- Governing equations with bottom topography h_B :

$$\frac{\partial q}{\partial t} = -J[\psi, f + q], \qquad \frac{\partial \theta_B}{\partial t} = -J[\psi_B, \theta_B + fSh_B], \qquad \frac{\partial \theta_T}{\partial t} = -J[\psi_T, \theta_T],$$

$$q = L[\psi] := \nabla^2 \psi + \frac{\partial}{\partial \zeta}\left[\frac{\rho_s(\zeta)^2}{S(\zeta)} \frac{\partial \psi}{\partial \zeta} \right], \qquad \zeta(z) := \int_0^z \rho_s(z')dz'.$$

- Boundary conditions for a multiply-connected domain:

$$\psi = \psi_i(\zeta) \quad \text{on LB}_i, \qquad \left.\frac{\partial \psi}{\partial \zeta}\right|_{\zeta_B} = \frac{\theta_B}{\rho_s(\zeta_B)}, \qquad \left.\frac{\partial \psi}{\partial \zeta}\right|_{\zeta_T} = \frac{\theta_T}{\rho_s(\zeta_T)}.$$

- It is found from an expansion in the following complete orthogonal system $\{\varphi_k(\mathbf{r})\}$ that the trace condition holds.

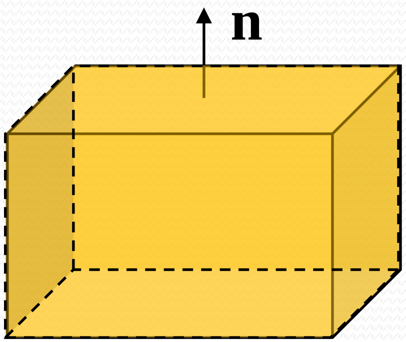
$$L[\varphi_k] = -\lambda_k \varphi_k(\mathbf{r}), \qquad \varphi_k = 0 \quad \text{on LB}_i, \qquad \left.\frac{\partial \varphi_k}{\partial \zeta}\right|_{\zeta_B} = \left.\frac{\partial \varphi_k}{\partial \zeta}\right|_{\zeta_T} = 0.$$

Boussinesq approximation

- Governing equations:

$$\frac{\partial \mathbf{v}}{\partial t} = -(\mathbf{v}\cdot\nabla)\mathbf{v} - f\,\mathbf{k}\times\mathbf{v} - \frac{1}{\rho_0}\nabla p - \frac{\rho}{\rho_0} g\mathbf{k},$$

$$\frac{\partial \rho}{\partial t} = -\mathbf{v}\cdot\nabla\rho, \qquad \nabla\cdot\mathbf{v} = 0.$$



- Boundary condition:

$$\mathbf{v}\cdot\mathbf{n} = 0 \quad \text{at the boundary.}$$

- It is found from a Fourier expansion that the trace condition holds for a cuboid domain.
- For complex domains, calculation in grid space may be necessary.

Shallow-water equations

- Governing equations with bottom topography h_B :

$$\frac{\partial \mathbf{u}}{\partial t} = -(\mathbf{u}\cdot\nabla)\mathbf{u} - f\mathbf{k}\times\mathbf{u} - g\nabla\eta, \qquad \frac{\partial \eta}{\partial t} = -\nabla\cdot\left(H+\eta-h_B\right)\mathbf{u}.$$

- Boundary condition for a rectangular domain:

$$\mathbf{u}\cdot\mathbf{n} = 0 \quad \text{at the lateral boundary.}$$

- It is found from a Fourier expansion that the trace condition does not hold. The trace depends only on divergence at the boundary.

$$\mathrm{Tr}\left[\frac{\partial \hat{\mathbf{F}}}{\partial \hat{\mathbf{x}}}\right] = \frac{N}{4}\sum_{m=1}^{M}\hat{D}_{2m0} + \frac{M}{4}\sum_{n=1}^{N}\hat{D}_{02n} - \frac{1}{8}\sum_{m=1}^{M}\sum_{n=1}^{N}\hat{D}_{2m2l}.$$

- If error correlation between vorticity and divergence is negligible, the evolution of the mode of vorticity is not directly affected by the trace term.

Summary of deterministic predictability in fluid dynamics

- The trace condition holds for the quasi-geostrophic equation and the Boussinesq approximation.

- Deterministic prediction of geostrophic motion and oceanic circulation is possible, if nonlinearity in forcing and dissipation is weak.

- The trace condition does not hold for the shallow-water equations with lateral boundaries.

- Deterministic prediction of divergent motion with a free surface is difficult near lateral boundaries.

Reformulation of variational data assimilation

Assumption: The trace condition holds.

- Since the analysis $\mathbf{x}_{k-1}^a$ is the mode of posterior PDF, the background state (prediction) $\mathbf{x}_k^f$ at the next analysis time is the mode of prior PDF.
- If $\mathbf{x}_k^f$ is close to the true state, the first two terms of the expansion of the logarithm of prior PDF $p(\mathbf{x}_k)$ around $\mathbf{x}_k^f$ give a good approximation.

$$\log p(\mathbf{x}_k) = \log p(\mathbf{x}_k^f) - \frac{1}{2}\left(\mathbf{x}_k - \mathbf{x}_k^f\right)^{\mathrm{T}}\left(\mathbf{P}_k^f\right)^{-1}\left(\mathbf{x}_k - \mathbf{x}_k^f\right) + O(\left|\mathbf{x}_k - \mathbf{x}_k^f\right|^3),$$

where the background error covariance $\mathbf{P}_k^f$ is defined by Gaussian fitting to the prior PDF at $\mathbf{x}_k^f$.

Reformulation of variational data assimilation – cont'd

- Cost function:

$$J(\mathbf{x}_k) = \frac{1}{2}\left(\mathbf{x}_k - \mathbf{x}_k^f\right)^{\mathrm{T}}\left(\mathbf{P}_k^f\right)^{-1}\left(\mathbf{x}_k - \mathbf{x}_k^f\right) - \log p(\mathbf{y}_k^o \mid \mathbf{x}_k) + O(\left|\mathbf{x}_k - \mathbf{x}_k^f\right|^3),$$

  The third term may be identified as a penalty term.

- Analysis error covariance $\mathbf{P}_k^a$ is defined by Gaussian fitting to the posterior PDF at $\mathbf{x}_k^a$:

$$\mathbf{P}_k^a := \left[\frac{\partial^2 J}{\partial \mathbf{x} \partial \mathbf{x}}\right]_{\mathbf{x}_k^a}^{-1}.$$

- The evolution of the error covariance $\mathbf{P}_M$ defined by Gaussian fitting to PDF at the mode is given by:

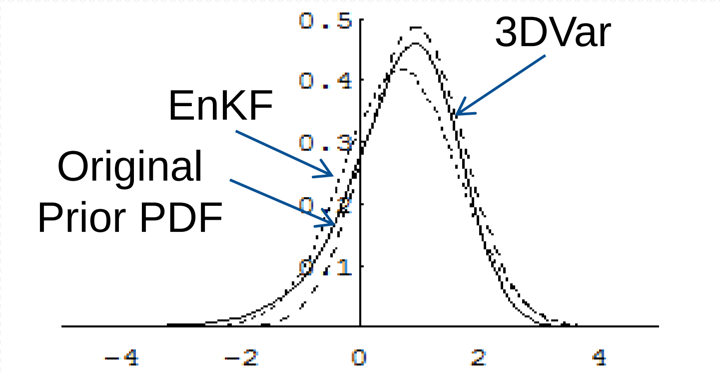
$$\frac{d\mathbf{P}_M}{dt} = \left.\frac{\partial \mathbf{F}}{\partial \mathbf{x}}\right|_{\mathbf{x}_M} \mathbf{P}_M + \mathbf{P}_M \left.\frac{\partial \mathbf{F}}{\partial \mathbf{x}}\right|_{\mathbf{x}_M}^{\mathrm{T}}.$$

No approximation except the expansion of prior PDF.

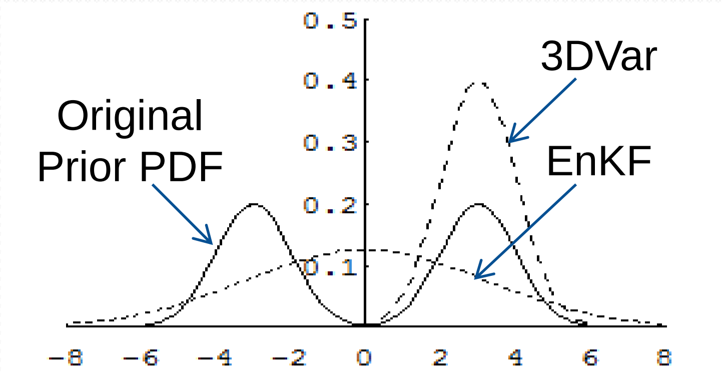
Comparison of EnKF and variational methods

For nonlinear systems that satisfy the trace condition:

- EnKF vs. 3DVar with flow-dependent $\mathbf{P}_k^f$



Weak non-Gaussianity



Strong non-Gaussianity

- EnKF vs. 4DVar with flow-dependent $\mathbf{P}_k^f$

  - EnKF needs more Gaussian fitting.

  - 4DVar needs no more Gaussian fitting with less weight to the prior PDF.

Comparison of EnKF and variational methods – cont'd

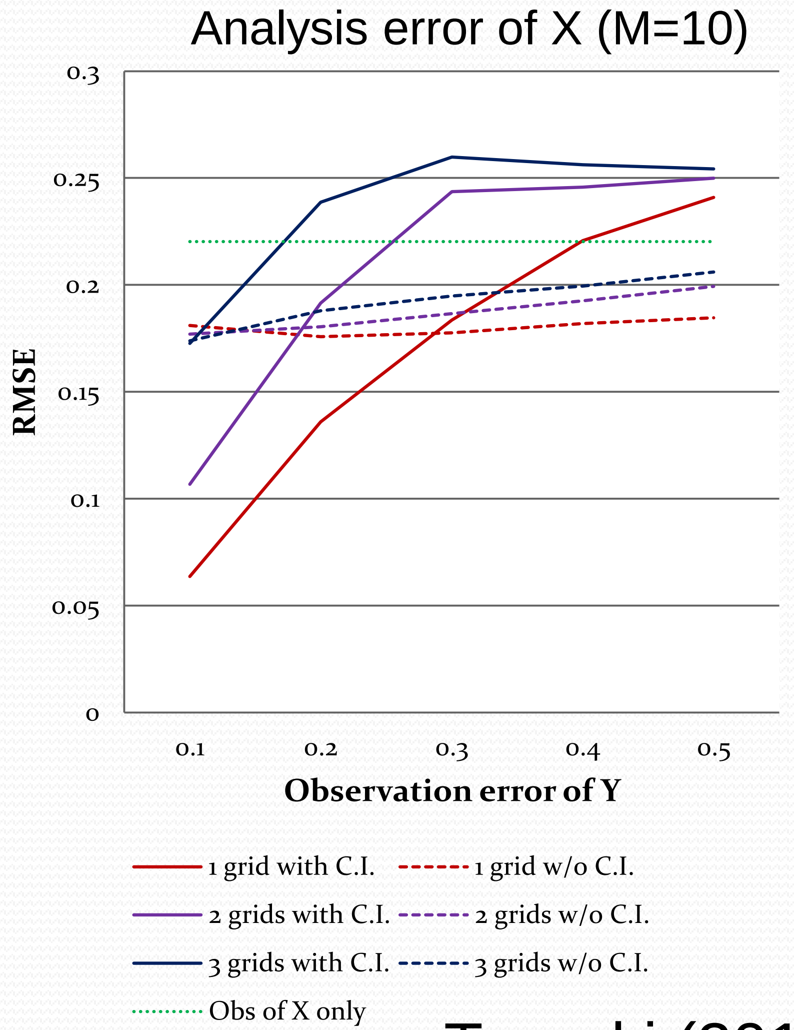
Ultimate data assimilation methods:

- Particle filter with enough ensemble members to neglect sampling error, for the mean,
- 4DVar with an enough length assimilation window to neglect the prior PDF, for the mode.

- 4DVar with flow-dependent background error is suitable for deterministic prediction of a nonlinear system that satisfies the trace condition.
- EnKF is suitable for ensemble prediction of a nonlinear system not satisfying the trace condition. Further advances are needed for non-Gaussianity.

Multi-scale data assimilation experiment with LETKF

- Lorenz-96 two-scale model: 36 large-scale variables X, 360 small-scale variables Y.
- The problem observed when precision or density of small-scale obs. data is not enough is not due to sampling error, but due to Gaussian assumption.



Tsuyuki (2012)

Conclusions

- Deterministic prediction is possible for fluid motion governed by the quasi-geostrophic equation or, possibly, by the Boussinesq approximation.
- Deterministic prediction of divergent motion with a free surface is difficult near lateral boundaries.
- If a nonlinear system satisfies the trace condition, variational data assimilation is formulated with less approximations.
- 4DVar with flow-dependent background error is suitable for deterministic prediction of a nonlinear system that satisfies the trace condition.

Thank you.

Hamiltonian fluid dynamics – cont'd

- The Liouville theorem also holds for a noncanonical Hamiltonian system with the Lie-Poisson bracket:

$$J_{ij} = \sum_{k=1}^{n} c_{ij}^{k} x_k \quad (c_{ij}^{k}\text{: structure constants}), \text{ if } \sum_{i=1}^{n} c_{ij}^{i} = 0.$$

- A couple of fluid equations with Eulerian variables are written with the Lie-Poisson bracket satisfying the above condition. An example is the 2-dimensional nondivergent vorticity equation:

$$\frac{\partial \zeta}{\partial t} = \{\zeta, H\}, \quad H = \frac{1}{2}\int_D |\nabla \psi|^2 d^2\mathbf{r}, \quad \{f, g\} := \int_D \zeta J\left[\frac{\delta f}{\delta \zeta}, \frac{\delta g}{\delta \zeta}\right] d^2\mathbf{r}.$$

- The Lie-Poisson bracket is not a necessary condition for the Liouville theorem to hold. Hence, Hamiltonian fluid dynamics is not of much help for the present purpose.

We are lucky the weather at large scales is predictable by deterministic NWP.