Thanks to Kevin Judd

Vorticity : iteration 10



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The Geometry of Data Assimilation 2: Gradient Decent (GD) and the Indistinguishable States Importance Sampler (ISIS)

Leonard A Smith

LSE CATS/Grantham

Pembroke College, Oxford

Not possible without:

H Du, A. Jarman, K Judd, A Lopez,

D. Stainforth, N. Stern & Emma Suckling







Smith (2002) Chaos and Predictability in Encyc Atmos Sci



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ISIS provides a coherent scheme for forming ensembles, given a perfect model.

This graph shows the evolution of an accountable PDF under a perfect model.

It is accountable in the sense that it suffers only from being a <u>finite</u> sample.

In "Bayesian" terms, the prior is the invariant measure of the system; we often have unconstructive proofs that establish that this measure is geometrically interesting (and thus extremely expensive to sample).

Indistinguishable states (ISIS) approach provides a more computationally tractable means of generating a sample.

But what is the point of DA when the model is imperfect?

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20.0

0.0



Your choice of DA algorithm will depend on your aims, as well as quality of your model and the accuracy of your obs.

One my aim to form an ensemble directly (this is preferred) or to find a reference trajectory and then form an ensemble using that trajectory and the observations. I also aim to learn about model error from the forecast system (not have to specify it *a priori*!)

Gradient Decient (GD) is a method for finding a reference trajectory or p-orbit.

ISIS seeks an ensemble from the indistinguishable states of the ref trajectory.

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Outside the perfect model scenario, there is no "optimal".

(But there are better and worse)



(Winning group gets copies of my book)





Inside the perfect model scenario, I know what I am looking for:

The model and the system are effectively identical. There is a state ("Truth") that is defines the future of the system.

In chaotic systems "Truth" is not identifiable given noisy observations.

The most likely state, given with observations (and the noise model) will fall in the set H(x), the indistinguishable states of x, which are in turn a subset of the unstable manifold of x.

K Judd & LA Smith (2001) <u>Indistinguishable states I: the perfect model</u> <u>scenario</u> *Physica D* 151: 125-141

Even if you do not believe in the mathematical niceties of Indistinguishable States, if you are aiming to make decisions PDFs from ensembles, you must be targeting something similar! (No?)



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ISIS ensembles fall near the attractor, like this:

Consider a series of spheres of radius ε ("ε -balls") centred on "Truth."

Count how many times each method "wins" by putting more probability mass within ε of the "Truth" (as a function







-0.5

-0.6

-0.8

-0.9

But the point today is that all the grey dots, the target for PDF forecasting, go away when the model is imperfect!

Given an imperfect model, we can test against additional observations in "now cast" mode, but the aim of a relevant (PDF) ensemble has vanished. (and would be a function of lead-time if resurrected!)

(See Du's thesis for much discussion and examples)

We'll return to using imperfect models soon.

Figure 3.6: Compare the EnKF and ISIS results via ϵ -ball, the blue line denotes the proportion of EnKF method wins and the red line denotes the proportion of ISIS method wins a) Ikeda experiment, Noise level 0.05 (Details of the experiment are listed in Appendix B Table B.3); b) Lorenz96 experiment, Noise level 0.5 (Details of the experiment are listed in Appendix B Table B.4)

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How to find a reference trajectory?



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Finding reference trajectory via GD

$${}^{0}\boldsymbol{u} = \{S_{-n}, ..., S_{0}\}$$

Given a sequence of n observations of m dimension system, we define a sequence space a $m \times n$ dimensional space, which contains any series of n model states.

Define the mismatch error cost function:

 $C_{GD}(\mathbf{u}) = \sum_{t=-n+1}^{0} |F(\mathbf{u}_t) - \mathbf{u}_{t+1}|^2$ Applying a Gradient Descent algorithm, starting at the observations

and evolving so as to minimise the cost function.





Finding reference trajectory

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Thanks to Kevin Judd

Vorticity : iteration 10





GD is NOT 4DVAR



- difficulties of locating the global minima with long assimilation window
- Iosing information of model dynamics and observations without long window



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T21L3 QG model (in PMS); suggesting a 20-ish day window.

Distance of original and best and trajectories from truth





Kevin's Blue Movie



Real "time" not algorithmic GD time!



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Draw ensemble members according to likelihood



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Given a shadowing reference trajectory (if we have one), we then look for its set of Indistinguishable States

Ikeda System

$$\tilde{x}_{i+1} = 1 + \mu(\tilde{x}_i \cos \theta - \tilde{y}_i \sin \theta)$$

$$\tilde{y}_{i+1} = \mu(\tilde{x}_i \sin \theta - \tilde{y}_i \cos \theta)$$

$$\theta = a - b/(1 + \tilde{x}_i^2 + \tilde{y}_i^2)$$

$a = 0.4, b = 0.6, \mu = 0.83$



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Two model states (say, x and y) are *indistinguishable states* (IS) if likely observations of the historical trajectory of x might well have come from y.

A model trajectory *i-shadows* the observations if that trajectory might well have generated the observations, given the noise model.

The distinction between shadows and IS is that *shadowing* relates a model trajectory to a set of observations, while being IS is a relation between two model trajectories *given* a noise model.





Ikeda : Some sets of indistinguishable states (Model is perfect)





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So within PMS we can use H(x) as an importance sampler, and form ISIS ensembles: one DA method sketched!

And in all simple systems tested so far, ISIS puts more ensemble members (and probabilty mass) near truth, than (shree's) EnKF or a pure Bayesian approach (each given equal cpu)



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CATS CENTRE FOR THE ANALYSIS OF TIME SERIES A (good) Imperfect Model for the Ikeda System



A good but imperfect model may be constructed using a finite truncation of the trigonometric expansions.

Aside: Which parameter values *should* be used in that case?

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And what about the set of indistinguishable states? In short: H(x) is empty.

As t goes to minus infinity, three are no trajectories consistent with the given observations (including the trajectory that ends at $x_0 =$ the "true x").

But what is the aim of DA in this case?

Before going there, lets look at the case of missing observations...

Passive tracers in the flow of two point vortices for example...



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Missing k components $\mathbf{s} = s_1, ..., s_{m-k}, s_{m-k+1}^{\star}, ..., s_m^{\star}$ Initialize GD using $\mathbf{u}^0 = s_1, ..., s_{m-k}, s_{m-k+1}, ..., s_m$ After l iterations $\mathbf{u}^l = z_1, ..., z_{m-k}, z_{m-k+1}, ..., z_m$ Initialize GD using $\mathbf{u}^0 = s_1, ..., s_{m-k}, z_{m-k+1}, ..., z_m$





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A good but imperfect model may be constructed using a finite truncation of the trigonometric expansions.

Aside: Which parameter values *should* be used in that case?

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Ignored subspace model : Maximum likelihood states (Model assumed perfect)





Ignored subspace model : Maximum likelihood states (Model assumed perfect)





Traditional aims of state estimation:

 $P(\mathbf{x}(\mathbf{t}_0) | \mathbf{s}_i, \mathbf{F}_a(\mathbf{x}), \mathbf{a}, n)$

Traditional aim of forecasting (in statistics)

 $P(x(t > t_0) | s_i, F_a(x), a, n)$

In cases where $F_a(x)$ is imperfect (*i.e.* in practice), these two procedures may have different target different distributions for $P(x(t_0))$.

Evaluation of $P(x(t_0))$ via data denial is not expected to yield the same ranking as forecast evaluation of $P(x(t>t_0))$.



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- In the IPMS, model state and system state are living in the different state space.
- Let x_t be a projection of system trajectory into model state space R^d .
- The chaotic model has dynamics $y_{t+1} = f(y_t), y_t \in \mathbb{R}^d$.
- Let f(.) be the best model we have.
- Observations: $s_t = x_t + \epsilon_t$ where ϵ is *IID*.
- Define the model error, $\omega_t^* = x_t f(x_{t-1}), \omega_t^* \in \mathbb{R}^d$

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- No model trajectories are able to be consistent with the infinite observations.
- There are pseudo-orbits, with non-zero mismatch error, that are consistent with the observations. We define pseudo-orbit $z_t, t = 0, -1, -2, ...$ $z_{i+1} = f(z_i) + \omega_i, \omega_i \text{ is not IID}$
- Confounding of observational noise and model error prevents one identifying either of them.
- Data assimilation can explore the model dynamics by employing pseudo-orbits.





Ikeda system:

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$$x_{n+1} = \gamma + u(x_n \cos \theta - y_n \sin \theta)$$

$$y_{n+1} = u(x_n \sin \theta + y_n \cos \theta),$$

where $\theta = \beta - \alpha/(1 + x_n^2 + y_n^2)$

Imperfect model is obtained by using the truncated polynomial, i.e.

$$\cos\theta = \cos(\omega + \pi) \mapsto -\omega + \omega^3/6 - \omega^5/120$$



 $\sin\theta = \sin(\omega + \pi) \mapsto -1 + \omega^2/2 - \omega^4/24$

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Toy model-system pairs

Lorenz96 system:

$$\begin{aligned} \frac{dx_i}{dt} &= -x_{i-2}x_{i-1} + x_{i-1}x_{i+1} - x_i + F - \frac{h_x c}{b}\sum_{j=1}^n y_{i,j} \\ \frac{dy_{j,i}}{dt} &= cby_{j+1,i}(y_{j-1,i} - y_{j+2,i}) - cy_{j,i} + -\frac{h_y c}{b}x_i \end{aligned}$$

Imperfect model:

$$\frac{dx_i}{dt} = -x_{i-2}x_{i-1} + x_{i-1}x_{i+1} - x_i + F$$

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ATS CENTRE FOR THE ANALYSIS OF TIME SERIES Insight of Gradient Descent

Given a sequence of n observations of m dimension system, we define a sequence space a $m \times n$ dimensional space, which contains any series of n model states.

Define the mismatch error cost function:

$$C_{GD}(\mathbf{u}) = \sum_{t=-n+1}^{0} |f(\mathbf{u}_t) - \mathbf{u}_{t+1}|^2$$

Applying a Gradient Descent algorithm, starting at the observations and evolving so as to minimise the cost function.

Define the implied noise to be $\delta_i = \mathbf{s}_i - \mathbf{u}_i$

and the imperfection error to be $\omega_i = \mathbf{u}_i - \mathbf{u}_{i-1}$





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Knowing the model is imperfect, we interpret the mismatch and the implied noise differently. And we no long run GD all the way to a trajectory. Ut when to stop?







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for both higher dimension Lorenz96 system-model pair experiment (left) and low dimension Ikeda system-model pair experiment (right). the Environment

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GD with stopping criteria

- GD minimization with "intermediate" runs produces more consistent pseudo-orbits
- Certain criteria need to be defined in advance to decide when to stop or how to tune the number of iterations.
- □ The stopping criteria are suggested **out-of-sample** by computing consistency between implied noise and the noise model
- or by minimizing other relevant utility function



Imperfection error vs model error



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WC4DVAR cost function:

$$C_{wc \, 4d \, var} = \frac{1}{2} (x_0 - x_0^b)^T B_0^{-1} (x_0 - x_0^b) + \frac{1}{2} \sum_{t=0}^N (x_t - s_t)^T \Gamma^{-1} (x_t - s_t)$$
$$+ \frac{1}{2} \sum_{t=1}^N (x_t - F(x_{t-1}))^T Q^{-1} (x_t - F(x_{t-1}))$$

We have good reason to believe that model error is not IID (and empirical evidence for ECMWF, see Orrell et al 2001)

D Orrell, LA Smith, T Palmer & J Barkmeijer (2001) <u>Model Error in Weather</u> <u>Forecasting</u>, *Nonlinear Processes in Geophysics 8: 357-371*



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Options for Forming ensemble outside PMS

Apply the GD method on perturbed observations.

Apply the GD method on the results of other data assimilation methods.






Evaluate ensemble via Ignorance

The Ignorance Score is defined by:

where Y is the verification.

$$S(p(y), Y) = -log(p(Y))$$

Systems	Ignorance		Lower		Upper	
	EnKF	GD	EnKF	GD	EnKF	GD
Ikeda	-2.67	-3.62	-2.77	-3.70	-2.52	-3.55
Lorenz96	-3.52	-4.13	-3.60	-4.18	-3.39	-4.08

Ikeda system-model pair and Lorenz96 system-model pair, the noise model is N(0, 0.5) and N(0, 0.05) respectively. Lower and Upper are the 90 percent bootstrap resampling bounds of Ignorance score



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CATS CENTRE FOR THE ANALYSIS Deployed: m=2, m=18, T20/T21, NOGAPS

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Thanks to Kevin Judd

Vorticity : iteration 10



"teleconnections of the day(s)"

Mismatch Directions Reveal Model Error



Figure 10: Direction error for T47L24 and T79L30 models. Contour lines show mean error and shading shows standard deviation. Details as in figure9

Grantham Research Institute on Climate Change and the Environment K Judd, CA Reynolds, LA Smith & TE Rosmond (2008) <u>The Geometry of Model Error</u>. Journal of Atmospheric Sciences 65 (6), 1749-1772

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This is not a stochastic fix:

After a flight, the series of control perturbations required to keep a bydesign-unstable aircraft in the air look are a random time series and arguably are Stochastic.

But you cannot fly very far by specifying the perturbations randomly!

Think of WC4dVar/ISIS/GD perturbations as what is required to keep the model flying near the observations: we can learn from them, but no "stochastic model" could usefully provide them. With the Eurofighter Typhoon, in subsonic flight the pressure point lies in front of the centre of gravity, therefore making the aircraft aerodynamically unstable, and is why Eurofighter Typhoon has such a complex Flight Control System – computers react quicker than a pilot.



When Eurofighter Typhoon

crosses into supersonic flight, the pressure point moves behind the centre of gravity, giving a stable aircraft.

The advantages of an intentionally unstable design over that of a stable arrangement include greater agility – particularly at subsonic speeds - reduced drag, and an overall increase in lift (also enhancing STOL performance).

Which is NOT to say stochastic models are not a good idea: Physically it makes more sense to include a realization of a process rather than it mean! But a better model class will not resolve the issue of model inadequacy!

It will not yield decision-relevant PDFs!



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The Geometry of Model Error

Projection Error



This of this as the control perturbation required to keep the model near the observations, NOT as a stochastic forcing!

NOGAPS T79L30 October – NAVDAS Analysis

Note that this information on (state dependent) model error comes out of the algorithm!

We can also watch how a state evolves during gradient decent:

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Direction Error

The aim of DA is ensemble formation.

If the model evolves on a natural manifold, there are huge resource and dynamical advantages to initialization on that manifold. (Balance was just a co-dimension 10⁶ first step.)

Inside PMS, ISIS will be pretty hard to beat if the model is chaotic.

Outside PMS all bets are off.

Model inadequacy suggests ISIS or WC 4DVAR if the model still has a natural manifold.

ISIS has the advantage that it tells you about state dependency of model error where 4DVAR requires a statistical description of model error *as in input*!

Geometrical insight may save some statistical gnashing of teeth.

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Starting the ensemble off the manifold is likely a waste of cpu time

The Geometry of Model Error





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Assuming PMS when the model is imperfect introduces state-dependent systematic errors:

Ignored subspace model : Maximum likelihood states (Model assumed perfect)



State estimation using pseudo-orbits out-performs those that assume PMS... GD beats EnKF and (WC)4DVAR, perhaps PF's.... But what is the point? What is the goal?

Ignored subspace model : Q-density of indistinguishable states (Model is imperfect)



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Papers

R Hagedorn and LA Smith (2009) <u>Communicating the value of probabilistic forecasts with weather roulette</u>. *Meteorological Applications*16 (2): 143-155. <u>Abstract</u>

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Internal (in)consistency... Model Inadequacy



A weather modification team with different goals and differing beliefs.



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