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EVOLVING TOPICS IN DATA ASSIMILATION

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In the early 1980's Eugenia Kalnay was my postdoc advisor at the Goddard Modeling and Simulation Facility (GMSF), a precursor to the current Goddard Modeling and Assimilation Office (GMAO). One of the great things about being a postdoc at Goddard was the great range of scientists, collaborators, and visitors. There were many new interesting ideas—including new interesting ideas for data assimilation (DA). For context, for the younger audience members, optimum interpolation (OI) was the cutting edge DA method at this point.

Thanks to Eugenia, I was introduced to a wide range of topics in predictability, ensembles, and data assimilation. Many of these topics became personal research interests and have evolved and morphed into new areas of research of wider interest, with potential or actual impacts on operations. My postdoc research experiences—in what were then new research areas—included trying to answer the questions listed on this slide.

- How can we use ensembles to improve forecasts, skill vs. spread, etc.?
- How can we use the data assimilation cycle to identify and correct model bias?
- How should observing system simulation experiments (OSSEs) be designed?
- Can we solve variational data assimilation with nonlinear obs operators by using conjugate gradient minimization?
- What can we do when a feature (a storm) is in the wrong place in the background?
- What can we do when only half of a feature is observed by a satellite?
- Would it be possible/better to use radiances in data assimilation instead of retrievals?
- Can we determine time continuous solutions to the governing equations that best fit some observation? (Can we solve the 4d-VAR problem?)

I will describe some advances in some of these areas and make some predictions of the future evolution of data assimilation. In principle, modern approaches answer these questions. In practice, approximations and short cuts are required and keeping these topics in mind can help to understand results from modern systems, and point the way to improving them. Please, remember, this is my personal view. In DA, we have to focus in on the problem at hand, but DA systems are complex and are impacted by many different design choices. I will show some details as examples, but basically, I want to take a top level view of DA.

Usually we try to find a balance between our prior knowledge and current observations by minimizing a cost function, usually called J. This approach is optimal (maximum likelihood or least squares sense) if some assumptions are true about the observation and model errors—that they are unbiased or have a known bias that can be removed, that the covariances are known, that the errors are Gaussian. Of course, these assumptions and the real world don't match.

We can view the advance of DA as making better and better approximations and transformations so that these assumptions are better satisfied. Characterization of the errors is important. We want not just the standard deviations and correlations of the observations themselves. We must also account for

- Representativeness error; and
- Forward model error, which includes what might be called
- Geophysical "bias" (which is usually caused by ignoring something that is present in real life).

Correlated errors will occur even in radiances due to geophysical biases and other forward model errors.

Transformation of the observations and control variable are important, in order to have errors that are Gaussian, and if possible uncorrelated. Intuition helps to obtain parsimonious error characterizations. Transformations help to limit correlations or to make them easier (more parsimonious) to represent. With enough transforms and assumptions the background error covariance matrix becomes the identity matrix, and J_b is simply a dot product of the transformed analysis increments with themselves.

What will the future bring? We will squeeze more out of the data we have. Coupled data assimilation will efficiently use data with signals from two (or more) components of the earth system. This will include cloudy radiances, microwave observations impacted by the surface and even observations at the land sea boundary. We will extract more information from hyperspectral instruments. Current subsets of channels used in DA, from AIRS for example, tend to not include interesting signals from the boundary layer and from water vapor.

And even further in the future: Will quantum computing solve the DA problem once and for all? I'm going out on a limb here, but then, I won't be around if I'm wrong. While quantum computing can deal with nonlinearity, it still requires defining some metric of optimality.

Now I'll get back to reviewing some of the work that started when I was a postdoc.

Lagged averaged forecasting (*Hoffman and Kalnay* 1983) is my most cited paper. But on Eugenia's list, it's not even in the top 10. This is not DA paper, but there is an important lesson for DA. During the linear growth of errors, the ensemble mean stays on the attractor, but in the nonlinear regime the ensemble mean trajectory is very likely not a solution of the governing equations. And add to this that the attractor is the model attractor, the real atmosphere is doing something different, perhaps very different.

I used the same toy model, developed for my thesis and used in the lagged average forecasting study, to solve the 4d-Var problem (*Hoffman* 1986). Since I did not know what an adjoint was, this was either brave or foolish. I won't go into the details but highlight one finding—a finding that is obvious after you know the answer. And that is that the 4d-Var initial conditions will have both growing and decaying perturbations relative to the truth at the beginning of the 4d-Var interval. At the end of the interval, all that's left are growing modes and the forecast errors amplify at a very fast rate. In other words: a superior analysis may not produce a superior forecast.

At the time of my postdoc minimizing a function of several hundred variables was novel. I realized that coding J and coding the gradient of J would lead to problems and instead it was important to code J and then determine the gradient of the code for J. So I ended up coding the equivalent of an adjoint by applying the chain rule to my code for J in developing the variational analysis method (VAM). Originally the VAM was developed as an ambiguity removal technique for scatterometer winds (*Hoffman* 1984). In this case J_b and J_o were nonlinear. The VAM has continued to be used to produce the cross-calibrated multi-platform (CCMP) surface wind products from microwave wind speeds and scatterometer wind vectors (*Atlas et al.* 2011). (CCMP was one of the data products highlighted on the NASA hyperwall in the exhibits hall.)

As a postdoc, my VAM test case was 12 Z 10 Sep 1978 at the height of the QE2 storm, a N. Atlantic storm that damaged the ocean liner QE2. At that time we had scatterometer data for only a 3 month period from the Seasat-A satellite scatterometer (SASS). There were two important lessons for me:

- A single ship report can have a huge influence. (The *Asia Hawk* wind report was probably from 35 degrees not from 350!)
- Observing half a strong storm with a weak background in the wrong place creates huge challenges for DA.

In scatterometer data analysis we explored two possible forms for the observation function (*Hoffman et al.* 2003). The first uses the radar backscatter values, the second uses the retrieved, but ambiguous, wind vectors. These are quite different but have minima in the same place and give similar results.

More generally, should one use radiances or retrievals in DA. In our simulation study of 3d-retrievals (*Hoffman and Nehrkorn* 1989), we examined an intermediate approach. 3d-retrievals like radiances assimilation uses information on the smoothness of the temperature field in the horizontal as prior knowledge, information not available in the usual 1d retrieval setting. In this study we examined how to handle the effect of cloud, which has both large scale structure and substantial variations on small scales equal to the size of the observations. It's worth noting at this point, that a modern 1d retrieval is in fact a 1d DA methods that minimize J in the 1d setting.

More recently, I returned to this question on the side of retrievals (*Hoffman* 2011). Within DA if we have to linearize the observation operator, then we could adopt the averaging kernel representation. This provides several advantages, including the possibility of implementing interactive retrievals within an EnKF DA.

The fact that the scatterometer observed only half the QE2 storm lead to the formulation of the Feature Calibration and Alignment (FCA, *Hoffman et al.* 1995) technique. Our insights into the weather allow us to subjectively identify features, say an intense storm. When a storm in the wrong place, a static background error covariance will be in error. 4dVar and EnKF should improve this situation, but FCA or other techniques, like running-in-place, can help. Recently the feature alignment part of FCA was implemented in the WRFDA system, as a preprocessor called dWRF (*Nehrkorn et al.* 2015).

Some things that should be kept in mind for the future: First, I think we will embrace strong signals even if they are nonlinear—clouds, precip, etc.—and even if the signals are from two or more earth system components. One promising approach for coupled DA is through coupled obs operators. That is use each component model as needed to evaluate $H(x_1, x_2,\ldots.)$ and then use the resulting observation innovations in *all* of the component model EnKFs.

In addition, it is important to have

- Highly accurate data;
- Knowledge of the structure of the observation and model errors.

The question of "ensemble vs. variational DA" might be replaced today with the question "Can we afford to implement and maintain a 4d-Var system?" And it is important to keep in mind the large sensitivity of DA systems to QC and data selection.

A few closing thoughts: First, representing and estimating model error should viewed as a stop gap measure. Obviously, it is best to improve our models. Yes, you can tune model parameters, adding stochasticity, or inflate an ensemble. But these fixes can be expected to be non-physical in some way. In terms of the model attractor these fixes correct only one projection, or we might say, one shadow, of the model attractor. While doing that, they may make a mess of things when viewed from other vantage points. Finally, what do we mean by optimal. We might say an optimal forecast minimizes lives lost and maximizes damage averted. In the future, will we actually use such metrics to define optimal in DA?

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