

ATMOSPHERIC SCIENCES Ave Arellano

STATE AUGMENTATION

Joint Estimation of State and Emissions ASP AQ Colloquium, Boulder, CO August 4, 2016



How do you find a black box? Ask a Bayesian

Mathematical probability tools are used in diverse areas, such as crashed plane recovery, insurance and spam filtering



In June 2009, en route from Rio de Janeiro to Paris, Air France flight AF447 crashed into the Atlantic. **Bayesian analysis** played a crucial role in the location of the flight recorders and the recovery of the deceased passengers and crew. So what is Bayesian analysis?



Approximate flight path of AF 447. The solid red line shows the actual route. The dashed line indicates the planned route beginning with the position of the last transmission heard. All times are UTC.

wikipedia

Bayes' rule found AF 447 May 11, 2012

Tags: AF 447, Air France flight 447, Bayes, Metron, Theory That Would Not Die

Few realize the key role played by a long-discredited 18th century mathematical theory in finding and recovering the wreckage of AF 447.

After a fruitless two-year search for Air France Flight 447, Bayes' rule pointed to its most probable location—where it was found after only one week of undersea searching.

The 2009 crash of AF 447 was one of the most mysterious accidents in aviation history. The Airbus took off from Rio de Janeiro on May 31, 2009, bound overnight for Paris. Early in the morning it met an intense high-altitude electrical storm over the South Atlantic and disappeared without a trace with 228 aboard.

Bureau d'Enquêtes et d'Analyses (BEA), the French equivalent of the U.S. Federal Aviation Agency, coordinated the longest, most difficult, most high-tech, and most expensive undersea search ever launched.

To understand why the jet crashed, the BEA needed to find the black boxes housing the cockpit and flight data recordings. But the aviation industry's standard black box is the size of a shoebox, and they were lost somewhere in an undersea area similar in size and mountainous topography to Switzerland.

After almost two years of fruitless searching, the French agency turned to an American consulting firm to make an exhaustive Bayesian review of the entire search effort. Bayes' rule, discovered by English and French mathematicians in the 1700s, has recently swept through the computer world.

> see related article by s. mcgrayne @ <u>http://</u> www.mcgrayne.com/blog.htm?post=854513

It says that by updating our initial beliefs with objective new information, we can get a new and improved belief. So analysts for Metron Inc. in Reston, Virginia, started their search for AF 447 by incorporating everything that was known before the accident about airplane flight dynamics, area winds and currents, and other aircraft accidents involving loss of control. Metron assigned 70% probability to the credibility of these data. The positions and recovery times of bodies found drifting on the ocean surface were also incorporated into the prior probability but were assigned only a 30% probability because of the turbulent equatorial waters. All this information was organized into consistent scenarios and their uncertainties quantified and weighted.

To update this pre-search information, all available data from the air, surface, and underwater searches were assembled. Finally, Bayes' rule was used to update the prior pre-search information with the search data.

Introducing the possibility that the pinging alarm signals attached to the black boxes had malfunctioned during the crash pointed to a high-priority area that sonar had not yet explored.

After a one-week undersea search, the wreckage of AF 447 was found on April 3, 2011 under almost 2.5 miles of ocean.

see related article by s. mcgrayne @ <u>http://</u> www.mcgrayne.com/blog.htm?post=854513



Bayesed and Confused

It was all about our initial beliefs (and how you trust them), updating our beliefs with 'objective' (but incomplete/imperfect) information







Bayesed and Confused

the use of our initial belief (and its uncertainty) to make inference in light of limited information



Bayesian Update

 $\triangleright p(x)$ from propagation step for one-dimensional example: state x is a scalar



Bayesian Update

▷ observation likelihood p(y|x) for y = 0.8



Bayesian Update updated p(x|y) $\underline{p(\mathbf{x}_k|\mathbf{y}_k^o, Y_{k-1}^o)} = \frac{p(\mathbf{y}_k^o|\mathbf{x}_k, Y_{k-1}^o)p(\mathbf{x}_k|Y_{k-1}^o)}{p(\mathbf{y}_k^o|Y_{k-1}^o)}$ \triangleright 5 4 3 (x)d 2 1 0 0.2 0.4 0.6 0.8 1.2 1.4 1.6 1.8 2 0 1

Χ

Importance of Covariances

The effect of the update step on an unobserved variable.



Source: Chris Snyder/NCAR (in Blayo et al., 2015) - Oxford Univ. Press

1.5

1.5

1

X₁

2

1

2

Kalman Filter (Review)

Forecast Step

$$\mathbf{x}_{k+1}^f = \mathbf{M}_k \mathbf{x}_k^f$$

 \mathbf{X}_{k}^{J} is nxl state vector at time k

 \mathbf{M}_k is nxn state transition matrix (propagator, dynamical model)

 \mathbf{x}_{k+1}^{f} is nxl state vector at time k+l

Forecast Step

$$\mathbf{x}_{k+1}^f = \mathbf{M}_k \mathbf{x}_k^f$$

Without observations to assimilate, the evolution of the state can be written as:

$$\mathbf{x}_{1}^{f} = \mathbf{M}_{0}\mathbf{x}_{0}^{f}$$
$$\mathbf{x}_{2}^{f} = \mathbf{M}_{1}\mathbf{x}_{1}^{f} = \mathbf{M}_{1}\mathbf{M}_{0}\mathbf{x}_{0}^{f}$$
$$\mathbf{x}_{3}^{f} = \mathbf{M}_{2}\mathbf{x}_{2}^{f} = \mathbf{M}_{3}\mathbf{M}_{1}\mathbf{M}_{0}\mathbf{x}_{0}^{f}$$
$$\mathbf{x}_{k}^{f} = \mathbf{M}_{k-1}\mathbf{x}_{k-1}^{f} = \mathbf{M}_{k-1}\mathbf{M}_{k-2}\cdots\mathbf{M}_{0}\mathbf{x}_{0}^{f}$$

Forecast Step

$$\mathbf{x}_{k+1}^f = \mathbf{M}_k \mathbf{x}_k^f$$

$$\mathbf{P}_{k+1}^{f} = \mathbf{M}_{k} \mathbf{P}_{k}^{f} \mathbf{M}_{k} + \mathbf{Q}_{k} = \mathbf{P}_{k}^{p} + \mathbf{Q}_{k}$$

- \mathbf{P}_{k}^{f} is nxn error covariance matrix of the state at time k \mathbf{P}_{k+1}^{f} is nxn error covariance matrix of the state at time k+1
- \mathbf{P}_{k}^{p} is called the predictability term
- \mathbf{Q}_k is an nxn random error covariance (model error)

The evolution of the error covariance is the main difference between an OI (3D-Var) and KF

Forecast Step

$$\mathbf{x}_{k+1}^{f} = \mathbf{M}_{k} \mathbf{x}_{k}^{f}$$
$$\mathbf{P}_{k+1}^{f} = \mathbf{M}_{k} \mathbf{P}_{k}^{f} \mathbf{M}_{k} + \mathbf{Q}_{k} = \mathbf{P}_{k}^{p} + \mathbf{Q}_{k}$$

But this is challenging (in fact infeasible) for large dimensions ($n \sim 10^6$).

This is where approximations come into play.

Analysis Step

$$\mathbf{x}_{k+1}^{a} = \mathbf{x}_{k+1}^{f} + \mathbf{K}_{k+1} (\mathbf{y}_{k+1}^{o} - \mathbf{H}_{k+1} \mathbf{x}_{k+1}^{f})$$
$$\mathbf{K}_{k+1} = \mathbf{P}_{k+1}^{f} \mathbf{H}_{k+1}^{T} (\mathbf{H}_{k+1} \mathbf{P}_{k+1}^{f} \mathbf{H}_{k+1}^{T} + \mathbf{R}_{k+1})^{-1}$$

 \mathbf{y}_{k+1}^{o} is an mxl observation vector at time k+l \mathbf{H}_{k+1} is an mxn observation operator at time k+l \mathbf{R}_{k+1} is an mxm observation error covariance at time k+l

 \mathbf{x}_{k+1}^{a} is an n×1 analysis state vector at time k+1

Analysis Step

$$\mathbf{x}_{k+1}^{a} = \mathbf{x}_{k+1}^{f} + \mathbf{K}_{k+1} (\mathbf{y}_{k+1}^{o} - \mathbf{H}_{k+1} \mathbf{x}_{k+1}^{f})$$
$$\mathbf{K}_{k+1} = \mathbf{P}_{k+1}^{f} \mathbf{H}_{k+1}^{T} (\mathbf{H}_{k+1} \mathbf{P}_{k+1}^{f} \mathbf{H}_{k+1}^{T} + \mathbf{R}_{k+1})^{-1}$$

 \mathbf{y}_{k+1}^{o} is an mxl observation vector at time k+l

Since the observation error is typically assumed as diagonal (independent), one can also assimilate sequentially for each observation, rather than assimilating the whole observation vector (saves space and minimize numerical errors).

Analysis Step

$$\mathbf{x}_{k+1}^{a} = \mathbf{x}_{k+1}^{f} + \mathbf{K}_{k+1} (\mathbf{y}_{k+1}^{o} - \mathbf{H}_{k+1} \mathbf{x}_{k+1}^{f})$$
$$\mathbf{K}_{k+1} = \mathbf{P}_{k+1}^{f} \mathbf{H}_{k+1}^{T} (\mathbf{H}_{k+1} \mathbf{P}_{k+1}^{f} \mathbf{H}_{k+1}^{T} + \mathbf{R}_{k+1})^{-1}$$

 \mathbf{H}_{k+1} is an nxm observation operator at time k+1

This operator can be linear or non-linear. In many cases, this matrix is sparse. But errors in formulating this can also exist (not exactly representing reality).

Analysis Step

$$\begin{aligned} \mathbf{x}_{k+1}^{a} &= \mathbf{x}_{k+1}^{f} + \mathbf{K}_{k+1} \left(\mathbf{y}_{k+1}^{o} - \mathbf{H}_{k+1} \mathbf{x}_{k+1}^{f} \right) \\ \mathbf{K}_{k+1} &= \mathbf{P}_{k+1}^{f} \mathbf{H}_{k+1}^{T} \left(\mathbf{H}_{k+1} \mathbf{P}_{k+1}^{f} \mathbf{H}_{k+1}^{T} + \mathbf{R}_{k+1} \right)^{-1} \end{aligned}$$
The Kalman gain matrix can be approximated as well (sub-optimal) based on our approximations of the forecast error covariance.

hink toy example:

$$T_{a,0} = T_{b,0} + \frac{\rho_{0,1}\sigma_b^2}{\left(\sigma_{o,1}^2 + \sigma_{b,1}^2\right)} \left(T_{o,1} - T_{b,1}\right)$$

$$W = \left(\rho_{0,1}\frac{\sigma_{b,0}}{\sigma_{b,1}}\right) \left(\frac{\sigma_{b,1}^2}{\sigma_{o,1}^2 + \sigma_{b,1}^2}\right) = \left(\frac{\sigma_{0,1}^2}{\sigma_{b,1}^2}\right) \left(\frac{\sigma_{b,1}^2}{\sigma_{o,1}^2 + \sigma_{b,1}^2}\right), \quad \frac{\sigma_{b,0}}{\sigma_{b,1}} = 1$$

Analysis Step

$$\mathbf{x}_{k+1}^{a} = \mathbf{x}_{k+1}^{f} + \mathbf{K}_{k+1} (\mathbf{y}_{k+1}^{o} - \mathbf{H}_{k+1} \mathbf{x}_{k+1}^{f})$$
$$\mathbf{K}_{k+1} = \mathbf{P}_{k+1}^{f} \mathbf{H}_{k+1}^{T} (\mathbf{H}_{k+1} \mathbf{P}_{k+1}^{f} \mathbf{H}_{k+1}^{T} + \mathbf{R}_{k+1})^{-1}$$
$$\mathbf{P}_{k+1}^{a} = \mathbf{P}_{k+1}^{f} - \mathbf{K}_{k+1} \mathbf{H}_{k+1} \mathbf{P}_{k+1}^{f}$$

Has many forms:

$$\mathbf{P}_{k+1}^{a} = (\mathbf{I} - \mathbf{K}_{k+1}\mathbf{H}_{k+1})\mathbf{P}_{k+1}^{f}$$

$$\mathbf{P}_{k+1}^{a} = \mathbf{P}_{k+1}^{f} - \mathbf{P}_{k+1}^{f}\mathbf{H}_{k+1}^{T}(\mathbf{H}_{k+1}\mathbf{P}_{k+1}^{f}\mathbf{H}_{k+1}^{T} + \mathbf{R}_{k+1})^{-1}\mathbf{H}_{k+1}\mathbf{P}_{k+1}^{f}$$

$$\mathbf{P}_{k+1}^{a} = \left[\left(\mathbf{P}_{k+1}^{f}\right)^{-1} + \mathbf{H}_{k+1}^{T}(\mathbf{R}_{k+1})^{-1}\mathbf{H}_{k+1}\right]^{-1}$$

 $\mathbf{P}_{k+1}^{a} = (\mathbf{I} - \mathbf{K}_{k+1}\mathbf{H}_{k+1})\mathbf{P}_{k+1}^{f}(\mathbf{I} - \mathbf{K}_{k+1}\mathbf{H}_{k+1})^{T} + \mathbf{K}_{k+1}\mathbf{R}_{k+1}\mathbf{K}_{k+1}^{T}$

Extensions of the Kalman filter can be used to estimate unknown system parameters.

These parameters can be either related to the dynamics and/or observation operator. It is also possible to estimate parameters related to the statistics of the errors involved in the problem.

Forward Model

$$\frac{dC_i}{dt} = \frac{s_i}{n_a}$$

$$\boldsymbol{x}^{t}(t_{k+1}) = \boldsymbol{M}_{k}[\boldsymbol{x}^{t}(t_{k})] + \eta_{k}, \qquad \eta_{k} \sim N(0, q^{2})$$

$$\frac{\partial \rho_{i}}{\partial t} = \left[\frac{\partial \rho_{i}}{\partial t}\right]_{adv} + \left[\frac{\partial \rho_{i}}{\partial t}\right]_{mix} + \left[\frac{\partial \rho_{i}}{\partial t}\right]_{conv} + \left[\frac{\partial \rho_{i}}{\partial t}\right]_{scav} + \left[\frac{\partial \rho_{i}}{\partial t}\right]_{chem} + \left[\frac{\partial \rho_{i}}{\partial t}\right]_{em} + \left[\frac{\partial \rho_{i}}{\partial t}\right]_{dep}$$

Eq. 4.10 of Brasseur and Jacob, 2016

Hierarchical Models

p(state, parameters|data) ∝ p(data|state, parameter) x p(state|parameter) p(parameter)

for Gaussian statistics, this is equivalent to Generalized Inverse formulation

Wikle and Berliner (2007), Evensen (2009)

Let's look back at our discrete system:

$$\mathbf{x}_{k+1}^t = \mathbf{M}_k(\boldsymbol{\theta})\mathbf{x}_k^t + \mathbf{e}_k^t$$

and the following observational process:

$$\mathbf{y}_{k+1}^{o} = \mathbf{H}_{k+1}\mathbf{x}_{k+1}^{t} + \mathbf{v}_{k+1}^{o}$$

where the sequence of the noises are Gaussian and mutually uncorrelated, i.e.

$$\mathbf{e}_k^t \sim N(0, \mathbf{Q}_k), \mathbf{v}_k^o \sim N(0, \mathbf{R}_k)$$

dynamical process:
$$\mathbf{x}_{k+1}^t = \mathbf{M}_k(\boldsymbol{\theta})\mathbf{x}_k^t + \mathbf{e}_k^t$$

observational process: $\mathbf{y}_{k+1}^o = \mathbf{H}_{k+1}\mathbf{x}_{k+1}^t + \mathbf{v}_{k+1}^o$

The system does not however represent the most general form for problems of parameter estimation, since we are assuming that the equations are linear in the state variable.

Another simplification in this system is that the observation function is taken as known, with no parameters to be determined to describe it.

Even with all these simplifications, the system is sufficient to exemplify the main idea of the approach of parameter estimation.

dynamical process:
$$\mathbf{x}_{k+1}^t = \mathbf{M}_k(\boldsymbol{\theta})\mathbf{x}_k^t + \mathbf{e}_k^t$$

observational process: $\mathbf{y}_{k+1}^o = \mathbf{H}_{k+1}\mathbf{x}_{k+1}^t + \mathbf{v}_{k+1}^o$

The variable θ represents an p-vector of constant, but unknown, coefficients that we intend to estimate.

If we imagine that the parameters θ are functions of time, the fact that they are in reality constant can be expressed as:

$$\boldsymbol{\theta} = \boldsymbol{\theta}_{k+1}^t = \boldsymbol{\theta}_k^t$$

dynamical process:
$$\mathbf{x}_{k+1}^t = \mathbf{M}_k(\boldsymbol{\theta})\mathbf{x}_k^t + \mathbf{e}_k^t$$

observational process: $\mathbf{y}_{k+1}^o = \mathbf{H}_{k+1}\mathbf{x}_{k+1}^t + \mathbf{v}_{k+1}^o$

This produces an extra equation that we can append to the system above, to augment the state vector, that is:

$$\mathbf{u}_{k+1}^t \equiv \begin{pmatrix} \mathbf{x}_{k+1}^t \\ \boldsymbol{\theta}_{k+1}^t \end{pmatrix}$$

where n+p vector \mathbf{u}^t is now re-defined state variable. Unfortunately, this procedure does not lead to anything in terms of estimating $\boldsymbol{\theta}$.

dynamical process:
$$\mathbf{x}_{k+1}^t = \mathbf{M}_k(\boldsymbol{\theta})\mathbf{x}_k^t + \mathbf{e}_k^t$$

observational process: $\mathbf{y}_{k+1}^o = \mathbf{H}_{k+1}\mathbf{x}_{k+1}^t + \mathbf{v}_{k+1}^o$

To be able to actually estimate θ through say the Kalman filter, it is necessary to treat the vector of deterministic, constant and unknown parameters as if it were a random vector. Thus we write the equation for the parameters to be estimated as:

$$\boldsymbol{\theta}_{k+1}^t = \boldsymbol{\theta}_k^t + \boldsymbol{\alpha}_k$$

where α_k is a p-random vector with assumed known statistics $\alpha_k \sim N(0, \mathbf{S}_k)$ taken to be uncorrelated from the errors of the system.

dynamical process:
$$\mathbf{x}_{k+1}^t = \mathbf{M}_k(\boldsymbol{\theta})\mathbf{x}_k^t + \mathbf{e}_k^t$$

observational process: $\mathbf{y}_{k+1}^o = \mathbf{H}_{k+1}\mathbf{x}_{k+1}^t + \mathbf{v}_{k+1}^o$

The above equations can be re-written in the form:

$$\mathbf{u}_{k+1}^{t} = \boldsymbol{f}(\mathbf{u}_{k}^{t}) + \begin{pmatrix} \mathbf{e}_{k}^{t} \\ \boldsymbol{\alpha}_{k} \end{pmatrix}$$
$$\mathbf{y}_{k+1}^{o} = (\mathbf{H}_{k+1} \quad \mathbf{0}) \begin{pmatrix} \mathbf{x}_{k+1}^{t} \\ \boldsymbol{\theta}_{k+1}^{t} \end{pmatrix} + \mathbf{v}_{k+1}^{o}$$

The above equations can be re-written in the form:

$$\mathbf{u}_{k+1}^{t} = \boldsymbol{f}(\mathbf{u}_{k}^{t}) + \begin{pmatrix} \mathbf{e}_{k}^{t} \\ \boldsymbol{\alpha}_{k} \end{pmatrix}$$
$$\mathbf{y}_{k+1}^{o} = (\mathbf{H}_{k+1} \quad \mathbf{0}) \begin{pmatrix} \mathbf{x}_{k+1}^{t} \\ \boldsymbol{\theta}_{k+1}^{t} \end{pmatrix} + \mathbf{v}_{k+1}^{o}$$
$$(\mathbf{u}_{k}^{t}) \equiv \begin{pmatrix} \mathbf{M}_{k}(\boldsymbol{\theta}_{k}^{t}) & \mathbf{0} \\ \mathbf{0} & \mathbf{I} \end{pmatrix} \mathbf{u}_{k}^{t} = \begin{pmatrix} \mathbf{M}_{k}(\boldsymbol{\theta}_{k}^{t})\mathbf{u}_{k}^{t} \\ \boldsymbol{\theta}_{k}^{t} \end{pmatrix}$$

Let us assume that initially, at k=0, the estimates \mathbf{x}_0^t , $\boldsymbol{\theta}_0^t$

$$\mathbf{u}_0^a \equiv \begin{pmatrix} \mathbf{x}_0^a \\ \boldsymbol{\theta}_0^a \end{pmatrix} = \begin{pmatrix} E\{\mathbf{x}_0^t\} \\ \boldsymbol{\theta}_0 \end{pmatrix}$$

with error covariance

$$\mathbf{P}_0^a = \begin{pmatrix} cov\{\mathbf{x}_0^t, \mathbf{x}_0^t\} & \mathbf{0} \\ \mathbf{0} & \mathbf{\Theta}_0 \end{pmatrix}$$

Following the extended Kalman filter equations, we need to calculate the Jacobian of the modified dynamics.

$$\boldsymbol{F}'(\mathbf{u}_k^a) \equiv \frac{\partial \boldsymbol{f}(\mathbf{u}_k^t)}{\partial (\mathbf{u}_k^t)^T} \bigg|_{\mathbf{u}_k^t = \mathbf{u}_k^a} \qquad \boldsymbol{f}(\mathbf{u}_k^t) = \begin{pmatrix} \mathbf{M}_k(\boldsymbol{\theta}_k^t)\mathbf{u}_k^t \\ \boldsymbol{\theta}_k^t \end{pmatrix}$$

$$F'(\mathbf{u}_{k}^{a}) = \begin{pmatrix} \frac{\partial \mathbf{M}(\boldsymbol{\theta}_{k}^{t})\mathbf{x}_{k}^{t}}{\partial(\mathbf{x}_{k}^{t})^{T}} \Big|_{\mathbf{u}_{k}^{t}=\mathbf{u}_{k}^{a}} & \frac{\partial \mathbf{M}(\boldsymbol{\theta}_{k}^{t})\mathbf{x}_{k}^{t}}{\partial(\boldsymbol{\theta}_{k}^{t})^{T}} \Big|_{\mathbf{u}_{k}^{t}=\mathbf{u}_{k}^{a}} \\ \frac{\partial \boldsymbol{\theta}_{k}^{t}}{\partial(\mathbf{x}_{k}^{t})^{T}} \Big|_{\mathbf{u}_{k}^{t}=\mathbf{u}_{k}^{a}} & \frac{\partial \boldsymbol{\theta}_{k}^{t}}{\partial(\boldsymbol{\theta}_{k}^{t})^{T}} \Big|_{\mathbf{u}_{k}^{t}=\mathbf{u}_{k}^{a}} \\ F'(\mathbf{u}_{k}^{a}) = \begin{pmatrix} \mathbf{M}(\boldsymbol{\theta}_{k}^{a}) & \frac{\partial \mathbf{M}(\boldsymbol{\theta}_{k}^{t})}{\partial(\boldsymbol{\theta}_{k}^{t})^{T}} \Big|_{\boldsymbol{\theta}_{k}^{t}=\boldsymbol{\theta}_{k}^{a}} \end{pmatrix} \\ \mathbf{0} & \mathbf{I} \end{pmatrix}$$

Then the forecast step of the Kalman filter becomes

$$\begin{pmatrix} \mathbf{x}_{k+1}^f \\ \boldsymbol{\theta}_{k+1}^f \end{pmatrix} = \begin{pmatrix} \mathbf{M}(\boldsymbol{\theta}_k^a) \mathbf{x}_k^a \\ \boldsymbol{\theta}_k^a \end{pmatrix}$$

$$\mathbf{P}_{k+1}^{f} = \begin{pmatrix} \mathbf{M}(\boldsymbol{\theta}_{k}^{a}) & \frac{\partial \mathbf{M}(\boldsymbol{\theta}_{k}^{t})}{\partial(\boldsymbol{\theta}_{k}^{t})^{T}} \Big|_{\boldsymbol{\theta}_{k}^{t} = \boldsymbol{\theta}_{k}^{a}} \mathbf{x}_{k}^{a} \end{pmatrix} \mathbf{P}_{k}^{a} \begin{pmatrix} \mathbf{M}(\boldsymbol{\theta}_{k}^{a}) & \frac{\partial \mathbf{M}(\boldsymbol{\theta}_{k}^{t})}{\partial(\boldsymbol{\theta}_{k}^{t})^{T}} \Big|_{\boldsymbol{\theta}_{k}^{t} = \boldsymbol{\theta}_{k}^{a}} \mathbf{x}_{k}^{a} \end{pmatrix}^{T} + \begin{pmatrix} \mathbf{Q}_{k} & \mathbf{0} \\ \mathbf{0} & \mathbf{I} \end{pmatrix}$$

$$\mathbf{P}_{k+1}^{f} = \begin{pmatrix} \mathbf{P}_{xx_{k+1}}^{f} & \mathbf{P}_{x\theta_{k+1}}^{f} \\ \left(\mathbf{P}_{x\theta_{k+1}}^{f} \right)^{T} & \mathbf{P}_{\theta\theta_{k+1}}^{f} \end{pmatrix}$$

and the analysis step becomes

$$\mathbf{K}_{k+1} = \mathbf{P}_{k+1}^{f} (\mathbf{H}_{k+1} \quad \mathbf{0})^{T} \left((\mathbf{H}_{k+1} \quad \mathbf{0}) \mathbf{P}_{k+1}^{f} (\mathbf{H}_{k+1} \quad \mathbf{0})^{T} + \mathbf{R}_{k+1} \right)^{-1}$$
$$\stackrel{\text{def}}{=} \begin{pmatrix} \mathbf{K}_{\mathbf{x}_{k+1}} \\ \mathbf{K}_{\mathbf{\theta}_{k+1}} \end{pmatrix}$$

$$P_{k+1}^{a} = [I - K_{k+1}(H_{k+1} \ 0)]P_{k+1}^{f}$$

$$\begin{pmatrix} x_{k+1}^{a} \\ \theta_{k+1}^{a} \end{pmatrix} = \begin{pmatrix} x_{k+1}^{f} \\ \theta_{k+1}^{f} \end{pmatrix} + K_{k+1}(y_{k+1}^{o} - H_{k+1}x_{k+1}^{f})$$

$$K_{x_{k+1}} = P_{xx_{k+1}}^{f}H_{k+1}^{T}(H_{k+1}P_{xx_{k+1}}^{f}H_{k+1}^{T} + R_{k+1})^{-1}$$

$$K_{\theta_{k+1}} = P_{x\theta_{k+1}}^{f}H_{k+1}^{T}(H_{k+1}P_{xx_{k+1}}^{f}H_{k+1}^{T} + R_{k+1})^{-1}$$

Forecast Step

$$\begin{pmatrix} \mathbf{x}_{k+1}^{f} \\ \boldsymbol{\theta}_{k+1}^{f} \end{pmatrix} = \begin{pmatrix} \mathbf{M}(\boldsymbol{\theta}_{k}^{a})\mathbf{x}_{k}^{a} \\ \boldsymbol{\theta}_{k}^{a} \end{pmatrix}$$

$$\mathbf{P}_{k+1}^{f} = \begin{pmatrix} \mathbf{M}(\boldsymbol{\theta}_{k}^{a}) & \frac{\partial \mathbf{M}(\boldsymbol{\theta}_{k}^{t})}{\partial(\boldsymbol{\theta}_{k}^{t})^{T}} \Big|_{\boldsymbol{\theta}_{k}^{t} = \boldsymbol{\theta}_{k}^{a}} \mathbf{x}_{k}^{a} \end{pmatrix} \mathbf{P}_{k}^{a} \begin{pmatrix} \mathbf{M}(\boldsymbol{\theta}_{k}^{a}) & \frac{\partial \mathbf{M}(\boldsymbol{\theta}_{k}^{t})}{\partial(\boldsymbol{\theta}_{k}^{t})^{T}} \Big|_{\boldsymbol{\theta}_{k}^{t} = \boldsymbol{\theta}_{k}^{a}} \mathbf{x}_{k}^{a} \end{pmatrix}^{T} + \begin{pmatrix} \mathbf{Q}_{k} & \mathbf{0} \\ \mathbf{0} & \mathbf{I} \end{pmatrix}$$

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Analysis Step

$$\mathbf{K}_{k+1} = \mathbf{P}_{k+1}^{f} (\mathbf{H}_{k+1} \ \mathbf{0})^{T} \left((\mathbf{H}_{k+1} \ \mathbf{0}) \mathbf{P}_{k+1}^{f} (\mathbf{H}_{k+1} \ \mathbf{0})^{T} + \mathbf{R}_{k+1} \right)^{-1}$$
$$\mathbf{P}_{k+1}^{a} = \left[\mathbf{I} - \mathbf{K}_{k+1} (\mathbf{H}_{k+1} \ \mathbf{0}) \right] \mathbf{P}_{k+1}^{f}$$
$$\binom{\mathbf{x}_{k+1}^{a}}{\boldsymbol{\theta}_{k+1}^{a}} = \binom{\mathbf{x}_{k+1}^{f}}{\boldsymbol{\theta}_{k+1}^{f}} + \mathbf{K}_{k+1} (\mathbf{y}_{k+1}^{o} - \mathbf{H}_{k+1} \mathbf{x}_{k+1}^{f})$$

Let's look at an example. (kalman_filter_augmented2b.m)

Consider a slightly modified system of our previous tutorial:

$$\frac{\partial [a]}{\partial t} + \mu \frac{\partial [a]}{\partial x} = D \frac{\partial^2 [a]}{\partial x^2} + E[a]$$

The numerical solution of of which is:

$$a_{j}^{i+1} = (Df + Cr)a_{j-1}^{i} + (1 - 2Df - Cr)a_{j}^{i} + (Df)a_{j+1}^{i} + (E\Delta t)a_{j}^{i}$$

What if we do not know the wind speed μ and production rate E? Here, we also want to estimate these as our parameters together with estimating our state [a]?



Let's run kalman_filter_augmented2b.m

Chem DA Applications

ESTIMATING SOURCES OF CARBON MONOXIDE: Some Top-down Approaches

TOP-DOWN APPROACHES USING CAM-CHEM/DART OR WRF-CHEM/DART

 BAYESIAN SYNTHESIS INVERSION (INVERSE MODELING OR IM)
 JOINT STATE-SOURCE ESTIMATION (DATA ASSIMILATION OR DA)
 TWO-STEP APPROACH (DA + IM)

<u>CARBON MONOXIDE IN THE ATMOPSHERE</u>

Source: incomplete combustion Sink: oxidation by OH (lifetime of 2 months)

	Range of estimates (Tg CO yr $^{-1}$)
Sources	1800-2700
Fossil fuel combustion / industry	300-550
Biomass burning	300-700
Vegetation	60-160
Oceans	20-200
Oxidation of methane	400-1000
Oxidation of other hydrocarbons	200-600
Sinks	2100-3000
Tropospheric oxidation by OH	1400-2600
Stratosphere	~ 100
Soil uptake	250-640





THE BASIC IDEA IS TO DECOMPOSE THE STATE AS CONTRIBUTIONS OF CO SOURCES TO THE CO STATE.

n sources

 $X_{t+\Delta t}^{i} = M(X_{t}^{i}, \mu_{t}^{i}, \{met\}_{t}, \theta) \text{ such that } X_{t+\Delta t} = \sum X_{t+\Delta t}^{i}$

IN THE CASE OF A MODEL GRID POINT:

$$x_{t+\Delta t} = [k^1, k^2, \cdots, k^{nsourrces}]_{t+\Delta t} \begin{bmatrix} \mu^1 \\ \mu^2 \\ \vdots \\ \mu^{nsources} \end{bmatrix}$$

<u>Note:</u> CO tracers do not affect OH (They are treated as passive tracers)

NOW, IF WE HAVE A SET OF OBSERVATIONS, AND WE ASSUME THE OBSERVATIONS ARE RELATED TO THE SOURCES BY:

 $Y = H(K\mu) + e, \quad where \quad e \sim N(0, S_e)$ AND $\mu \sim N(\mu_a, S_a)$

THEN, WE CAN FIND AN ESTIMATE OF THE SOURCES BY: $p(\mu|Y) = \alpha \ p(Y|\mu)p(\mu)$

THE MEAN, COVARIANCE, & AVERAGING KERNEL OF WHICH ARE:

 $\hat{\mu} = \mu_{a} + S_{a}(HK)^{T} [(HK)S_{a}(HK)^{T} + S_{e}]^{-1} [Y - (HK)\mu_{a}]$ $\hat{S} = [(HK)^{T}S_{e}^{-1}(HK) + S_{a}^{-1}]^{-1}$ $\hat{A} = I - \hat{S}S_{a}^{-1}$

IN THE PAST, WE SOLVE FOR REGIONAL/SECTORAL SCALING FACTORS (ASSUMING THE SPATIOTEMPORAL DISTRIBUTION OF THE PRIOR SOURCES ARE WELL-KNOWN). E.G.,





MAIN LIMITATIONS:

1. ESTIMATES SENSITIVE TO ERROR ASSUMPTIONS AND OBS CHOICE



HEALD ET AL (2004)

MAIN LIMITATIONS:

1. ESTIMATES SENSITIVE TO ERROR ASSUMPTIONS AND OBS CHOICE



ARELLANO ET AL (2004)

MAIN LIMITATIONS: 1.ESTIMATES SENSITIVE TO ERROR ASSUMPTIONS AND OBS CHOICE



HOOGHIEMESTRA ET AL (2012)

MAIN LIMITATIONS: 2.ESTIMATES SENSITIVE TO INVERSE METHODOLOGY AND CONFIGURATION



KOPACZ ET AL (2007)

MAIN LIMITATIONS:

3. ESTIMATES SENSITIVE TO MODEL TREATMENT OF TRANSPORT (CONVECTION, BOUNDARY LAYER)

differences in response functions differences in inverse results





ARELLANO AND HESS (2006)

MAIN LIMITATIONS:

3.A POSTERIORI CO STATES STILL EXHIBIT LARGE BIASES



KOPACZ ET AL (2010)

MAIN LIMITATIONS: 3.A posteriori CO states still exhibit Large biases





[%]

(2004)

30

< -30

-15

0

HEALD ET AL

15



JOINT STATE-SOURCE ESTIMATION

DART EAKF



 $x_{\alpha}^{l} = x_{1}^{l} + \nabla x_{ANDERSON}^{I}$ (2001, 2003), ANDERSON ET AL., (2009)

JOINT STATE-SOURCE ESTIMATION

STATE-AUGMENTATION:

FOLLOWING E.G., EVENSEN (2009) FOR PARAMETER AND STATE ESTIMATION, WE CAN AUGMENT OUR STATE VECTOR WITH THE 2D-3D SOURCES OF CO. WE CAN USE THE SAME EAKF FORMULATION IN DART.



MAIN ISSUE:

WE DONT HAVE A MODEL TO SIMULATE THE EVOLUTION OF SOURCES (THEY ARE PRESCRIBED). SPURIOUS CORRELATIONS CAN EXIST RESULTING TO 'NOISY' ESTIMATES



<u>CAMCHEM/DART MOPITT CO REANALYSIS</u> Evaluation of Emission Sensitivities



ENSEMBLE-BASED EMISSION SENSITIVITIES



GAUBERT ET AL IN PREP

MEAN CORRELATION BETWEEN SPECIES IN THE FORECAST ERROR CORRELATION MATRIX ESTIMATED FROM CHASER/LETKF (MIYAZAKI ET AL., ACP, 2012)

Surface





JOINT STATE-SOURCE ESTIMATION

RECENT ENKF Application

Inversion of CO emissions over Beijing and its surrounding areas with ensemble Kalman filter

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JOINT STATE-SOURCE ESTIMATION

Prior

Posterior



Sensitivity experiments to investigate the sensitivity of the inverse emission estimates to the sensitivity factors.

Experiments	Sensitivity factors	Tests
SE01	Length of assimilation window	From 1 day to 12 days
SE02	Perturbing model error	Removed
SE03	Using nighttime observation	Removed
SE04	Boundary conditions	Doubled
SE05	Adjusting CO concentrations	Removed
SE06	Localization scale	27 km; 63 km

JOINT STATE-SOURCE ESTIMATION SNIPPET OF THEIR CONCLUSIONS

Several issues have been highlighted in this study and should be addressed in further analysis. Firstly, regarding the ill-posed inverse problem, the inverse estimation with the relatively sparse observations in the current study is sensitive to several factors such as localization scale, boundary conditions, and length of assimilation window. Further investigation or application of the inverse estimation scheme should pay particular attention to the optimization of these factors. For example, assimilating more observations over the region with few assimilation stations should be helpful to reduce the sensitivity of the inverse estimation to localization scale and improve the inverse emission inventory obtained in the current study. Secondly, the inverse estimation approach with sequential assimilation enables combining the information of model and observation data in a consistent and synchronous way. However, the rapid fluctuation of the hourly estimates suggests that a smoother for the sequential estimations is necessary to filter the influence from the random model errors and produce stable estimation. Last but not the least, the error in the meteorological simulations constitutes a major concern for the CO simulation over some periods. Reducing the bias or accurately simulating the meteorological uncertainty might improve the inversion estimation

- \triangleright suppose p(x) and $p(y^{o}|x)$ are exponential pdfs
- ▷ analysis variance depends on y^o : $var(x|y^o) = 0.15^2$ for $y^o = 1.3$



Source: Chris Snyder/NCAR (in Blayo et al., 2015) - Oxford Univ. Press

- \triangleright suppose p(x) and $p(y^{o}|x)$ are exponential pdfs
- ▷ analysis variance depends on y^o : $var(x|y^o) = 0.23^2$ for $y^o = 1.7$



 \triangleright $p(x_1, x_2)$ for 2D state (x_1, x_2) ; thin lines indicate marginal pdfs



- \triangleright observation $y^o = x_1 + \epsilon = 1.1$
- $\triangleright p(y^o|x_1, x_2)$ does not depend on x_2



- $\triangleright p(x_1, x_2|y^o)$
- \triangleright marginal variances increase, marginal for x_2 becomes bimodal



Source: Chris Snyder/NCAR (in Blayo et al., 2015) - Oxford Univ. Press

Toward a chemical reanalysis in a coupled chemistry-climate model: An evaluation of MOPITT CO assimilation and its impact on tropospheric composition

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Abstract We examine in detail a 1 year global reanalysis of carbon monoxide (CO) that is based on joint assimilation of conventional meteorological observations and Measurement of Pollution in The Troposphere (MOPITT) multispectral CO retrievals in the Community Earth System Model (CESM). Our focus is to assess the impact to the chemical system when CO distribution is constrained in a coupled full chemistry-climate model like CESM. To do this, we first evaluate the joint reanalysis (MOPITT Reanalysis) against four sets of independent observations and compare its performance against a reanalysis with no MOPITT assimilation (Control Run). We then investigate the CO burden and chemical response with the aid of tagged sectoral CO tracers. We estimate the total tropospheric CO burden in 2002 (from ensemble mean and spread) to be $371 \pm 12\%$ Tg for MOPITT Reanalysis and $291 \pm 9\%$ Tg for Control Run. Our multispecies analysis of this difference suggests that (a) direct emissions of CO and hydrocarbons are too low in the inventory used in this study and (b) chemical oxidation, transport, and deposition processes are not accurately and consistently represented in the model. Increases in-CO led to net reduction of OH and subsequent longer lifetime of CH₄ (Control Run: 8.7 years versus MOPITT Reanalysis: 9.3 years). Yet at the same time, this increase led to 5–10% enhancement of Northern Hemisphere O_3 and overall photochemical activity via HO_x recycling. Such nonlinear effects further complicate the attribution to uncertainties in direct emissions alone. This has implications to chemistry-climate modeling and inversion studies of longer-lived species.

 $\frac{Final Thoughts}{\partial C_i} + \mathbf{v} \cdot \nabla C_i = \frac{s_i}{S_i}$ Better characterization of model emors (covariances) is key! Need to be careful about 'mis-attribution'. Posterior diagnostics have to be investigated incl. comparison with independent datasets. $dC_i \ s_i$ Non-linearity and Non-Gautsianity continue to be an issue. Ensemble-based approaches show promise (localization is critical).

Need to reconcile with bottom-up estimates.

$$\boldsymbol{x}^{t}(t_{k+1}) = \boldsymbol{M}_{k}[\boldsymbol{x}^{t}(t_{k})] + \eta_{k}, \qquad \eta_{k} \sim N(0, q^{2})$$
$$\frac{\partial \rho_{i}}{\partial t} = \left[\frac{\partial \rho_{i}}{\partial t}\right]_{adv} + \left[\frac{\partial \rho_{i}}{\partial t}\right]_{mix} + \left[\frac{\partial \rho_{i}}{\partial t}\right]_{conv} + \left[\frac{\partial \rho_{i}}{\partial t}\right]_{scav} + \left[\frac{\partial \rho_{i}}{\partial t}\right]_{chem} + \left[\frac{\partial \rho_{i}}{\partial t}\right]_{em} + \left[\frac{\partial \rho_{i}}{\partial t}\right]_{dep}$$

Eq. 4.10 of Brasseur and Jacob, 2016

References

