# **Emission Estimation**

## NCAR/ASP 2016 Summer Colloquium on Air Quality

Dylan Jones Department of Physics University of Toronto Top-down emission estimation requires the solution of a delicate, and potentially noise sensitive, 'inverse problem'



[Courtesy of Ian McDade]

#### But there is hope!



Bayes' theorem:  $p(\mathbf{y}|\mathbf{x})p(\mathbf{x}) = p(\mathbf{x},\mathbf{y}) = p(\mathbf{x}|\mathbf{y})p(\mathbf{y})$ 

$$p(\mathbf{x}|\mathbf{y}) = \frac{p(\mathbf{y}|\mathbf{x})p(\mathbf{x})}{p(\mathbf{y})}$$



## **The Bayesian Approach**

$$p(\mathbf{x}|\mathbf{y}) = \frac{p(\mathbf{y}|\mathbf{x})p(\mathbf{x})}{p(\mathbf{y})}$$

How do we get **x**?

For the MAP estimator, we want to find the state that maximized the conditional pdf

Consider the linear model:  $y = Hx + \varepsilon$ 

Assuming Gaussian error statistics,

$$-2\ln p(\mathbf{y}|\mathbf{x}) = (\mathbf{y} - \mathbf{H}\mathbf{x})^T \mathbf{R}^{-1} (\mathbf{y} - \mathbf{H}\mathbf{x}) + c_1$$
  
$$-2\ln p(\mathbf{x}) = (\mathbf{x} - \mathbf{x}^b)^T \mathbf{B}^{-1} (\mathbf{x} - \mathbf{x}^b) + c_2$$
  
$$-2\ln p(\mathbf{x}|\mathbf{y}) = (\mathbf{y} - \mathbf{H}\mathbf{x})^T \mathbf{R}^{-1} (\mathbf{y} - \mathbf{H}\mathbf{x}) + (\mathbf{x} - \mathbf{x}^b)^T \mathbf{B}^{-1} (\mathbf{x} - \mathbf{x}^b) + c_3$$

where  $\mathbf{R} = E[\varepsilon \varepsilon^T]$  and  $\mathbf{B} = E[(\mathbf{x} - \mathbf{x}^b)(\mathbf{x} - \mathbf{x}^b)^T]$ 

## **The Bayesian Approach**

For the MAP estimate we require

$$\frac{\partial}{\partial \mathbf{x}} \ln p(\mathbf{x} | \mathbf{y}) = 0$$

$$-2\ln p(\mathbf{x}|\mathbf{y}) = (\mathbf{y} - \mathbf{H}\mathbf{x})^T \mathbf{R}^{-1}(\mathbf{y} - \mathbf{H}\mathbf{x}) + (\mathbf{x} - \mathbf{x}^b)^T \mathbf{B}^{-1}(\mathbf{x} - \mathbf{x}^b) + c_3$$

Thus 
$$-\mathbf{H}^T \mathbf{R}^{-1}(\mathbf{y} - \mathbf{H}\mathbf{x}) + \mathbf{B}^{-1}(\mathbf{x} - \mathbf{x}^b) = 0$$

which yields the MAP solution:

$$\mathbf{x}^{a} = \mathbf{x}^{b} + (\mathbf{H}^{T}\mathbf{R}^{-1}\mathbf{H} + \mathbf{B}^{-1})^{-1}\mathbf{H}^{T}\mathbf{R}^{-1}(\mathbf{y} - \mathbf{H}\mathbf{x}^{b})$$
$$\mathbf{P}^{a} = (\mathbf{H}^{T}\mathbf{R}^{-1}\mathbf{H} + \mathbf{B}^{-1})^{-1}$$

# **The Bayesian Approach**



The small ellipsoid is the contour of the posterior pdf. It represents the region consistent with the prior information and the measurement [Rogers, 2000].

Averaging kernel:  $\mathbf{A} = \mathbf{I} - \mathbf{P}^a \mathbf{B}^{-1}$ 

## **Resolution of the Inversion**

 $\mathbf{x}^{a} = \mathbf{x}^{b} + (\mathbf{H}^{T}\mathbf{R}^{-1}\mathbf{H} + \mathbf{B}^{-1})^{-1}\mathbf{H}^{T}\mathbf{R}^{-1}(\mathbf{y} - \mathbf{H}\mathbf{x}^{b}) = \mathbf{x}^{b} + \mathbf{K}(\mathbf{y} - \mathbf{H}\mathbf{x}^{b})$ But  $\mathbf{y} = \mathbf{H}\mathbf{x} + \boldsymbol{\varepsilon}$ 

$$\mathbf{x}^{a} = \mathbf{x}^{b} + \mathbf{K}\mathbf{H}(\mathbf{x} - \mathbf{x}^{b}) + \mathbf{K}\varepsilon$$
$$= \mathbf{x}^{b} + \mathbf{A}(\mathbf{x} - \mathbf{x}^{b}) + \mathbf{K}\varepsilon$$

Averaging kernel matrix:

$$\mathbf{A} = \mathbf{K}\mathbf{H}$$
  
=  $(\mathbf{H}^T \mathbf{R}^{-1}\mathbf{H} + \mathbf{B}^{-1})^{-1}\mathbf{H}^T \mathbf{R}^{-1}\mathbf{H}$   
=  $(\mathbf{I} - \mathbf{P}^a \mathbf{B}^{-1})$ 

Degrees of freedom for signal (DOFs) = trace(A)

### **Resolution of the Inversion**



 $\mathbf{A} = \mathbf{I} - \mathbf{P}^a \mathbf{B}^{-1}$ 

Palmer et al. 2003, Inverting for emissions of carbon monoxide from Asia using aircraft observations over the western Pacific, JGR, 2003



## **Filtering Properties**

$$\mathbf{x}^{a} = \mathbf{x}^{b} + \mathbf{B}\mathbf{H}^{T}(\mathbf{H}\mathbf{B}\mathbf{H}^{T} + \mathbf{R})^{-1}(\mathbf{y} - \mathbf{H}\mathbf{x}^{b})$$

Let  $\mathbf{d} = \mathbf{y} - \mathbf{H}\mathbf{x}^b$ 

If we assume that H = I, we can write the analysis increment as

$$\mathbf{z} = \mathbf{x}^a - \mathbf{x}^b = \mathbf{B}(\mathbf{B} + \mathbf{R})^{-1}\mathbf{d} = (\mathbf{I} + \mathbf{R}\mathbf{B}^{-1})^{-1}\mathbf{d}$$

Additional simplifications 
$$\mathbf{R} = (\boldsymbol{\sigma}^r)^2 \mathbf{I}$$
 and  $\mathbf{B} = (\boldsymbol{\sigma}^b)^2 \mathbf{C}$ 

where  ${\bf C}$  is a correlation matrix with eigenvectors and eigenvalues  ${\bf e}$  and  $\lambda$ 

So we have 
$$\mathbf{Be} = (\sigma^b)^2 \lambda \mathbf{e}$$
 and  $\mathbf{Re} = (\sigma^r)^2 \mathbf{Ie} = (\sigma^r)^2 \mathbf{e}$ 

Thus  $(\mathbf{I} + \mathbf{RB}^{-1})^{-1} \mathbf{e} = \left(\frac{1}{1 + \frac{(\sigma^r)^2}{(\sigma^b)^2 \lambda}}\right) \mathbf{e} = \left(\frac{1}{1 + \frac{\alpha}{\lambda}}\right) \mathbf{e}$ 

where  $\alpha = \frac{(\sigma^r)^2}{(\sigma^b)^2}$ 

#### **Filtering Properties**

Increment:  $z = x^{a} - x^{b} = B(B + R)^{-1} d = (I + RB^{-1})^{-1} d$ 

Expand the innovation in terms of the eigenvectors of C

$$\mathbf{d} = \sum_{i=1}^{N} c_i \mathbf{e}_i$$

So the increment becomes

$$\mathbf{z} = (\mathbf{I} + \mathbf{R}\mathbf{B}^{-1})^{-1}\mathbf{d} = \sum_{i=1}^{N} c_i \left(\frac{1}{1 + \frac{\alpha}{\lambda_i}}\right) \mathbf{e}_i$$

- Modes with the largest  $\lambda_i$  are damped the least.
- The ratio of the observation error to the prior error ( $\alpha$ ) also determines the damping.

# How well do we constrain the state given the a priori and measurement uncertainties?

Our linear forward model is:  $y = Hx + \varepsilon$ 

$$\mathbf{y} - \mathbf{y}^b = \mathbf{H}(\mathbf{x} - \mathbf{x}^b) + \varepsilon$$
  
Let  $\tilde{\mathbf{x}} = \mathbf{B}^{-1/2}(\mathbf{x} - \mathbf{x}^b)$   $\tilde{\mathbf{y}} = \mathbf{R}^{-1/2}(\mathbf{y} - \mathbf{y}^b)$ 

Our model  
becomes:  

$$\mathbf{\tilde{y}} = \mathbf{H}\mathbf{B}^{1/2}\mathbf{\tilde{y}} + \mathbf{E}$$

$$\mathbf{\tilde{y}} = \mathbf{R}^{-1/2}\mathbf{H}\mathbf{B}^{1/2}\mathbf{\tilde{x}} + \mathbf{R}^{-1/2}\mathbf{E}$$

$$= \mathbf{\tilde{H}}\mathbf{\tilde{x}} + \mathbf{\tilde{\varepsilon}} \quad \text{where} \quad \mathbf{\tilde{H}} = \mathbf{R}^{-1/2}\mathbf{H}\mathbf{B}^{1/2} \quad \mathbf{\tilde{\varepsilon}} = \mathbf{R}^{-1/2}\mathbf{\varepsilon}$$

$$\mathbf{B}_{\mathbf{\tilde{x}}} = E[\mathbf{B}^{-1/2}(\mathbf{x} - \mathbf{x}^{b})(\mathbf{x} - \mathbf{x}^{b})^{T}\mathbf{B}^{-1/2}] = \mathbf{B}^{-1/2}E[(\mathbf{x} - \mathbf{x}^{b})(\mathbf{x} - \mathbf{x}^{b})^{T}]\mathbf{B}^{-1/2} = \mathbf{I}$$

$$\mathbf{R}_{\mathbf{\tilde{\varepsilon}}} = E[\mathbf{\tilde{\varepsilon}}\mathbf{\tilde{\varepsilon}}^{T}] = E[\mathbf{R}^{-1/2}\mathbf{\varepsilon}\mathbf{\varepsilon}^{T}\mathbf{R}^{-1/2}] = \mathbf{I}$$

$$\mathbf{R}_{\mathbf{\tilde{y}}} = E[\mathbf{\tilde{y}}\mathbf{\tilde{y}}^{T}] = E[(\mathbf{\tilde{H}}\mathbf{\tilde{x}} + \mathbf{\tilde{\varepsilon}})(\mathbf{\tilde{H}}\mathbf{\tilde{x}} + \mathbf{\tilde{\varepsilon}})^{T}]$$

$$= \mathbf{\tilde{H}}E[\mathbf{\tilde{x}}\mathbf{\tilde{x}}^{T}]\mathbf{\tilde{H}}^{T} + E[\mathbf{\tilde{\varepsilon}}\mathbf{\tilde{\varepsilon}}^{T}]$$

$$= \mathbf{\tilde{H}}\mathbf{\tilde{H}}^{T} + \mathbf{I}$$
See Chapter 2 of Rodgers

12

# How well do we constrain the state given the a priori and measurement uncertainties?

The transformed observation covariance  $\mathbf{R}_{\tilde{\mathbf{y}}} = \tilde{\mathbf{H}}\tilde{\mathbf{H}}^T + \mathbf{I}$ 

 $\tilde{\mathbf{H}}\tilde{\mathbf{H}}^{T}$  is the contribution from the variability of the state

I contribution from the measurement noise

What are the modes of variability of the state that are above the noise?



# **CO Inversion Example**

Heald, C. L., et al. (2004), Comparative inverse analysis of satellite (MOPITT) and aircraft (TRACE-P) observations to estimate Asian sources of carbon monoxide, JGR, 109.

#### Aircraft observations



**Observations averaged 26 Feb - 9 Apr 2001** 



# **CO Inversion Example**

- Emissions from India project strongly onto the vector with singular value 58.4 with MOPITT data, with aircraft data the corresponding singular value is <1
- Southeast Asia and the Philippines project onto the vector with 26.1 with MOPITT data, with aircraft data the corresponding singular value is 2.1
- With MOPITT data, 10/11 modes are clearly above the noise
- With the aircraft data, only 4/11 modes are above the noise

[Heald et al. 2004]

# What is the appropriate resolution at which to conduct the inversion?

The inversion analysis should be conducted at a spatial and temporal resolution that is consistent with the variability of the state, subject to the information in the measurements

Conduct the inversion at the highest resolution possible; use the singular vectors of the transformed Jacobian to determine the scales on which you can reliably constrain the state

#### **Impact of Model Biases: Sensitivity to Transport and Chemistry**



# **Inconsistencies in Top-down CO Source Estimates**

	This	This Study		Kopacz et al	Fortems-Cheinev et al	Hooghiemstra et al
Region	Stations	MOPITT	[2009]	[2010]	[2011]	[2011]
Nam	$108 \pm 21$	$132 \pm 22$	146	71	199	166
Europe	$94 \pm 15$	$97\pm24$	111	95	137	92
Asia	$439\pm56$	$468 \pm 48$	531	660	506	597
Sam	$117 \pm 37$	$117 \pm 24$	141	183	184	156
Africa	$243\pm 62$	$272\pm38$	304	343	283	338
Oceania	$110 \pm 26$	$21 \pm 19$	185	-	117	-
Subtotal	$1118\pm88$	$1110\pm71$	1417	1350	1441	1390
NMVOC-CO	$704\pm78$	$733\pm60$	1344	1290	1176	410
CH <sub>4</sub> -CO	865	865				887
Total	2687	2708	2762	2642	2602	2646

**Table 2.** Comparison of Our Derived Total Emissions (Sum of Anthropogenic and Biomass Burning Emissions) Using Either NOAA Stations or MOPITT Observations With Recent Values From Literature<sup>a</sup>

<sup>a</sup>All studies shown here performed an inversion for the year 2004 (or parts of that year). The global estimate of CO from oxidation of NMVOCs and methane and the total CO production for 2004 are also given. For studies that only reported an oxidation source of CO (from methane and NMVOCs), we report that number.

Hooghiemstra et al. (JGR, 2012)

- The global mean source is well constrained
- Regional source estimates differ due to different:
  - inversion approaches
  - datasets
  - atmospheric models



#### Impact of OH on CO Source Estimates

Tropospheric column (10<sup>12</sup> cm<sup>-2</sup>) in July 2004

Mean NH midlatitude (20N-40N) OH (10<sup>6</sup> cm<sup>-3</sup>)

Tracer	V5 OH	V8 ОН
US 48 States	25	49
Alaska and Canada	41	55
Mexico	3	4
SE Asia/India	35	39
Eastern Asia	66	92
Europe	47	68
South America	52	54
Southern Africa	60	63
Northern Africa	31	40

Jiang et al. (ACP, 2015)

CO estimates (Tg CO) based on inversion of MOPITT V5J data in the GEOS-Chem 4D-Var system for June-August 2004.

#### **GEOS-Chem 4D-Var Inversion of MOPITT, OMI, and TES Data (Nov 2009)**



#### **GEOS-Chem 4D-Var Inversion of MOPITT, OMI, and TES Data (Nov 2009)**



#### **GEOS-Chem 4D-Var Inversion of MOPITT, OMI, and TES Data (Nov 2009)**



Excessive correction in NOx emissions to help optimize O3 initial conditions <sup>22</sup>

#### **Strong Constraint 4D-Var**



In strong Constraint 4D-Var the model is assumed to be perfect:

$$\mathbf{x}_{i+1} = \boldsymbol{M}_i(\mathbf{x}_i)$$

$$J(\mathbf{x}_0) = \frac{1}{2} \sum_{i=0}^{N} \left[ \mathbf{y}_i - H_i(M_i(\mathbf{x}_0)) \right]^T \mathbf{R}_i^{-1} \left[ \mathbf{y}_i - H_i(M_i(\mathbf{x}_0)) \right]$$
$$+ \frac{1}{2} (\mathbf{x}_0 - \mathbf{x}^b)^T \mathbf{B}^{-1} (\mathbf{x}_0 - \mathbf{x}^b)$$

Here we optimize only the initial state.

#### QUARTERLY JOURNAL

#### OF THE

#### ROYAL METEOROLOGICAL SOCIETY

Vol. 132 OCTOBER 2006 Part B N
--------------------------------

Q. J. R. Meteorol. Soc. (2006), 132, pp. 2483–2504

doi: 10.1256/qj.05.224

#### Accounting for an imperfect model in 4D-Var

#### By YANNICK TRÉMOLET\*

European Centre for Medium-Range Weather Forecasts, Reading, UK

(Received 14 November 2005; revised 24 May 2006)

#### SUMMARY

In most operational implementations of four-dimensional variational data assimilation (4D-Var), it is assumed that the model used in the data assimilation process is perfect or, at least, that errors in the model can be neglected when compared to other errors in the system. In this paper, we study how model error could be accounted for in 4D-Var.

We present three approaches for the formulation of weak-constraint 4D-Var: estimating explicitly a modelerror forcing term, estimating a representation of model bias or, estimating a four-dimensional model state as the control variable. The consequences of these approaches with respect to the implementation and the properties of 4D-Var are discussed.

We show that 4D-Var with an additional model-error representation as part of the control variable is essentially an initial-value problem and that its characteristics are very similar to that of strong constraint 4D-Var. Taking the four-dimensional state as the control variable, however, leads to very different properties. In that case, weak-constraint 4D-Var can be interpreted as a coupling between successive strong-constraint assimilation cycles. A possible extension towards long-window 4D-Var and possibilities for evolutions of the data assimilation system are presented.

### **Accounting for Model Errors in 4D-Var**

Account for the imperfect model:  $\mathbf{x}_i = M_i(\mathbf{x}_{i-1}) + \eta_i$ 

#### Weak Constraint 4D-Var

$$J(\mathbf{x}) = \frac{1}{2} \sum_{i=0}^{n} [\mathbf{y}_{i} - H_{i}(\mathbf{x}_{i})]^{T} \mathbf{R}_{i}^{-1} [\mathbf{y}_{i} - H_{i}(\mathbf{x}_{i})]$$
$$+ \frac{1}{2} \sum_{i=1}^{n} [\mathbf{x}_{i} - M_{i}(\mathbf{x}_{i-1})]^{T} \mathbf{Q}_{i}^{-1} [\mathbf{x}_{i} - M_{i}(\mathbf{x}_{i-1})]$$
$$+ \frac{1}{2} (\mathbf{x}_{0} - \mathbf{x}^{b})^{T} \mathbf{B}^{-1} (\mathbf{x}_{0} - \mathbf{x}^{b})$$

The control variable is the full 4-D state vector.

### Weak Constraint 4D-Var: Estimating Model Bias

 $\mathbf{x}_i = M_i(\mathbf{x}_0) + \boldsymbol{\beta}$ 

$$J(\mathbf{x}_0, \boldsymbol{\beta}) = \frac{1}{2} \sum_{i=0}^n [\mathbf{y}_i - H_i(M_i(\mathbf{x}_0) + \boldsymbol{\beta})]^T \mathbf{R}_i^{-1} [\mathbf{y}_i - H_i(M_i(\mathbf{x}_0) + \boldsymbol{\beta})]$$
$$+ \frac{1}{2} \boldsymbol{\beta}^T \mathbf{Q}^{-1} \boldsymbol{\beta} + \frac{1}{2} (\mathbf{x}_0 - \mathbf{x}^b)^T \mathbf{B}^{-1} (\mathbf{x}_0 - \mathbf{x}^b)$$

The control variable is the initial state and the model bias.



### Weak Constraint 4D-Var: Estimating Model Errors

M (-- ) + e

$$\mathbf{x}_{i} = M_{i}(\mathbf{x}_{i}) + \eta_{i}$$

$$J(\mathbf{x}_{0}, \eta) = \frac{1}{2} \sum_{i=0}^{n} [\mathbf{y}_{i} - H_{i}(\mathbf{x}_{i})]^{T} \mathbf{R}_{i}^{-1} [\mathbf{y}_{i} - H_{i}(\mathbf{x}_{i})]$$

$$+ \frac{1}{2} \sum_{i=1}^{n} \eta_{i}^{T} \mathbf{Q}_{i}^{-1} \eta_{i} + \frac{1}{2} (\mathbf{x}_{0} - \mathbf{x}^{b})^{T} \mathbf{B}^{-1} (\mathbf{x}_{0} - \mathbf{x}^{b})$$

The control variable is the initial state and the model error forcing.



# Weak Constraint 4D-Var Inversion of CO Emissions

#### Initial Implementation in GEOS-Chem

- Assimilated MOPITT V5J data for March 2006 in the GEOS-Chem weak constraint 4D-Var system
- The constraint vector consists of the initial CO distribution, the model-error forcing, and the CO sources.
- The model forcing terms are estimated only in the tropics and subtropics, 30°S-30°N
- The forcing is kept constant over a time window of 5 days and is applied only in the free troposphere
- We assume  $\mathbf{Q} = \boldsymbol{\sigma}_{Q} \mathbf{I}$
- Assume that **B** is diagonal, whereas **R** accounts for vertical correlations in the MOPITT retrievals

## Weak Constraint 4D-Var Inversion of CO Emissions





## Weak Constraint 4D-Var Inversion of CO Emissions



Strong constraint inversion has a large residual bias in the lower troposphere, which is reduced somewhat in the weak constraint inversions.



# Estimated Mean Model-Error Forcing for Nov 2009

- The forcing terms are weaker with a stronger penalty
- Negative forcing in the southern tropics and positive forcing in the northern tropics
- Negative forcing in the tropics is along the ITCZ

[Martin Keller, U. Toronto]

# **Estimating Model Errors With Weak Constraint 4D-Var**

#### **Benefits**

- Can be used to mitigate impact of model errors on estimated emissions
- Can be used to study structure and physical origin of model errors from the estimated forcing terms

#### **Challenges**

- Results are sensitive to the setup of the weak constraint system
- The spatial and temporal sampling of the observations limit the ability of the inversion system to estimate the forcing terms
- The ability of the inversion system to accurately capture model transport errors depends on the vertical resolution of the data
- It is difficult to disentangle model biases, emission errors, and observation biases