Inverse estimation of surface exchanges of greenhouse gases

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This document discusses the determination of sources of a trace gas given measurements of its concentration. It aims to lay out the basic principles of inverse methods, illustrate these with some examples using CO_2 and finally sketch the current status. Throughout I am heavily indebted to four key references: *Enting* (2002) provides the most complete treatment of inverse problems applied to atmospheric tracers. *Rodgers* (2000) and *Tarantola* (2004) provide more general treatment of inverse problems. These books can be regarded as alternative choices depending on the preference and mathematical background of the student. Finally, *Evans and Stark* (2002) provides a highly abstract treatment of the area. Its most useful contribution is the unification of the language of applied mathematics and statistics. Previously both fields have pursued parallel developments in inverse problems and caused considerable confusion. *Enting* (2002) and *Rodgers* (2000) both provide exercises and some "hands-on" exercises are also provided by *Rayner et al.* (2000).

The Problem

Our aim is to deduce a description of the sources of an atmospheric tracer given

1. Possible prior estimates of the sources
2. A set of measurements of tracer concentration
3. Knowledge of atmospheric transport.

Modern practice is to express this problem in probabilistic terms. This is necessary since our knowledge of any of the above items is incomplete. We describe the measurements and prior estimates by multivariate probability density functions $P(\mathbf{d})$ and $\mathbf{s}$ respectively. If we have a complete (though probably incorrect) description of atmospheric transport then we can generate a realization of the data consistent with any chosen source field. That is we have a mapping $\mathbf{M}$ between the PDFs of sources and data. Our task is to generate a PDF for the sources given the PDFs and measurement mapping. We write this as $P(\mathbf{s}|\mathbf{d})$.[1] This is accomplished using Bayes' Theorem which states

$$P(\mathbf{s}|\mathbf{d}) = \frac{P(\mathbf{d}|\mathbf{s})P(\mathbf{s})}{P(\mathbf{d})} \tag{1}$$

Note that the denominator on the rhs is a constant since we assume a given measurement. It is usually absorbed in normalizing the PDF.

Eq. 1 shows that the posterior PDF of sources (given a particular measurement) is the combination of the prior PDF of sources (with no measurement) and the PDF of the data given a particular value for the source $\mathbf{s}_0$. As Rodgers points out, this makes the calculation rather easy. For example, if $P(\mathbf{d}|\mathbf{s}_0)$ is invariant up to translation, i.e has a fixed shape then we can simply apply $\mathbf{M}$ to $\mathbf{s}_0$, calculate $P(\mathbf{d}|\mathbf{s}_0)$ based on this calculated value and we

[1] We have already made the simplification that the measurement is deterministic, strictly speaking we should include a PDF for this as well

have all we need to calculate $P(\mathbf{s}|\mathbf{d})$. Note that $P(\mathbf{d}|\mathbf{s}_0)$ can be thought of as a description of the measurement error. We often broaden this to include errors in the forward model.

Although Eq. 1 gives us a complete description of the PDF, it does not give us any particular quantities of interest such as the most likely value, the expected value or the variance. For these we must operate on the posterior PDF, e.b. maximize it to find the most likely value or calculate various moments to produce means, variances etc. For this we need to know both the structure of the PDFs and be able to operate with $\mathbf{M}$.

Linear, Gaussian Problem

By far the most common and tractable form of the inverse problem occurs if all the PDFs are Gaussian and $\mathbf{M}$ is linear. Gaussian have the form

$$P(x) \propto e^{-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2} \tag{2}$$

They have most likely value and mean both equal to μ and variance by σ^2. We assume $P(\mathbf{s})$ is Gaussian with mean $\mathbf{s}_0$ (a prior estimate for sources) and standard deviation σ_s while $P(\mathbf{d})$ is normal with mean $\mathbf{d}_m$ (measured value) and standard deviation σ_d. Substituting yields

$$P(\mathbf{s}|\mathbf{d}) \propto e^{-\frac{1}{2}\left[\left(\frac{\mathbf{Ms}-\mathbf{d}_m}{\sigma_d}\right)^2+\left(\frac{\mathbf{s}-\mathbf{s}_0}{\sigma_s}\right)^2\right]} \tag{3}$$

We can find the most likely value of this PDF by minimizing the expression in square brackets. This constitutes the solution of a least squares problem and is the usual starting point for atmospheric inversions (*Enting et al.*, 1995; *Rayner et al.*, 1999; *Rödenbeck et al.*, 2003; *Baker et al.*, 2005, e.g.) who explicitly solve the minimization problem. Minimization by hand of expressions like this had previously been used by *Keeling et al.* (1989) and *Tans et al.* (1990) who derived the first important spatial information on carbon fluxes from atmospheric measurements.

Beyond this, the minimization of the bracketed term in Eq. 3 for a given $\mathbf{M}$, $\mathbf{s}_0$ and $\mathbf{d}_m$ is a standard optimization problem (consult e.g. *Gill et al.*, 1981, for methods of solution). The nature of atmospheric transport may allow us to develop a simple solution. The continuity equation for a passive tracer can be written

$$\frac{\partial c}{\partial t} = s - \vec{U} \cdot \nabla c \tag{4}$$

where c is the concentration field s the sources and $\vec{U}$ the velocity. c is linear in s and so we can express c as a linear Green's function as

$$c(\vec{x},t) = \int T(\vec{\xi},t_0,\vec{x},t)c(\vec{\xi},t_0)d\vec{\xi} + \int_{t_0}^{t} T(\vec{\xi},\tau,\vec{x},t)s(\vec{\xi},\tau)d\vec{\xi},d\tau \tag{5}$$

which states that the concentration is the sum of transport acting on the initial condition plus the integral of transport acting on the total source field before the current time.[2]

More importantly both these integrations can be performed piecewise with the transport representing the response to a δ-function in either sources or initial concentration. Also, the diffusive nature of atmospheric transport means that if $t \gg t_0$ the first integral can be replaced by a constant depending only on the global integral of $c(\vec{x},t_0)$. The required time-scale is long compared to atmospheric mixing in the domain of the problem. In practice, since we currently use only tropospheric observations, this means two years.

Discretizing c and s yields the result:

$$\vec{C} = C_0 + \mathbf{J}\vec{S} \tag{6}$$

[2]In practice, many transport models use nonlinear advection schemes to improve accuracy. *Law et al.* (2003) demonstrated the implications of this for inversions.

For convenience we usually absorb the initial concentration into the source vector; *Enting et al.* (1995) call this a pseudosource.

We can now minimize the bracketed term in Eq. 3 to solve directly for $\vec{S}$. At the same time we introduce the slight generalization of possible uncertainty covariances among (but not between) sources and data. We write these covariances as $\mathbf{C}(\vec{S})$ and $\mathbf{C}(\vec{D})$ respectively. There are several ways of writing the resulting solution (e.g. *Rodgers*, 2000, chapter 4). I find the most informative to be

$$\vec{S} = \vec{S}_0 + \mathbf{C}(\vec{S})\mathbf{J}\mathbf{C}(\vec{D})^{-1}\left(\vec{D} - \mathbf{J}\vec{S}_0\right) \tag{7}$$

where $\mathbf{C}(\vec{S})$ is given by:

$$\mathbf{C}(\vec{S})^{-1} = \mathbf{C}(\vec{S}_0)^{-1} + \mathbf{J}^T\mathbf{C}(\vec{D})^{-1}\mathbf{J} \tag{8}$$

Eq. 7 shows that the update to the initial estimate $\vec{S}_0$ depends on the mismatch between simulated and observed concentrations $\vec{D} - \mathbf{J}\vec{S}_0$, the weight given to the data $\mathbf{C}(\vec{D})^{-1}$, the sensitivity of concentrations to sources $\mathbf{J}$ and finally freedom of movement of the sources $\mathbf{C}(\vec{S})$. If we regard the inverse uncertainty covariance as a measure of the information content (often we use its logarithm) we see from Eq.8 that the information content of sources is given by its initial value plus the information content of the data projected back into the source space. Hence either very uncertain data or a weak relationship between sources and data will yield a final uncertainty covariance close to the initial value. Note also that $\mathbf{C}(\vec{S})$ does not depend on either $\vec{D}$ or $\vec{S}$. This independence is an outcome of the linear and Gaussian assumptions. It means we can assess the information content added by new measurements before these measurements are made. This realization underlies the network design work of *Rayner et al.* (1996); *Gloor et al.* (2000); *Law et al.* (2004). There is an alternative form for Eq. 7 as

$$\vec{S} = \vec{S}_0 + \mathbf{C}(\vec{S}_0)\mathbf{J}^T\left(\mathbf{J}\mathbf{C}(\vec{S}_0)\mathbf{J}^T + \mathbf{C}(\vec{D})\right)^{-1}\left(\vec{D} - \mathbf{J}\vec{S}_0\right) \tag{9}$$

Note that this form is both computationally more efficient and analogous to the update step in the Kalman Filter (see, e.g. *Gelb*, 1974, for details).

Although the matrices involved in the solution of Eq. 9 and Eq. 8 can be large, the real cost in these offline methods is the construction of $\mathbf{J}$. The traditional solution is to generate the Green's functions directly by inserting a unit pulse of tracer into an atmospheric transport model, running the model forward and sampling the output at observing locations. This was the approach used by most authors until recently (*Enting et al.*, 1995; *Rayner et al.*, 1999; *Bousquet et al.*, 2000; *Baker et al.*, 2005, e.g.). this requires one tracer run for every dimension in source space, potentially every gridpoint at every timestep. The first simplification is to assume that all CO_2 sources are at the surface. This is roughly correct but see the recent work of *Folberth et al.* (2005) for important corrections. More drastic is a large reduction in source resolution by assuming fixed patterns of surface exchange over large regions of the globe and solving for scaling magnitudes for these patterns. The carbon cycle is active and variable at almost every spatial scale so these patterns are unlikely to be correct. *Kaminski et al.* (2001) showed errors in their structure could seriously bias the solution even at large scale. This finding, along with the computational inefficiency inherent in the direct calculation of Green's functions with more unknowns than observations, has stimulated the development of adjoint methods. Here a tracer representing an observation is run backwards through the transport model to calculate the sensitivity of that observation to fluxes at all places and previous times. The use of adjoint methods in this field was pioneered by *Kaminski et al.* (1999a,b) and have since been applied in several studies (*Rödenbeck et al.*, 2003; *Peylin et al.*, 2005, e.g.). These studies, however, still used the explicit solutions of Eq. 9 and Eq. 8.

Construction and manipulation of the Green's function is only possible where the number of observations or source components is limited. The first of these has been a longstanding problem since CO_2 observations have traditionally been made by gathering flask samples at about one hundred sites at roughly biweekly intervals (*Conway et al.*, 1994, see e.g.). The sparsity of observations has meant that the posterior uncertainties (from

Eq. 8) are often too large to make useful inferences. This is especially true for the tropical continents where a combination of logistical difficulties and rapid vertical mixing in the atmosphere makes the task of the insitu network especially difficult.

Fortunately the situation is changing rapidly. The flask measurement network is being augmented by devices that measure concentration continuously. *Law et al.* (2002, 2003) used the solution of Eq. 8 to demonstrate the extra information content in these measurements. The information content comes partly from the better constraint on mean concentrations implied by more measurements. More important is the interaction of changing atmospheric flow with continuous sampling. Different parts of the source field are sampled as the flow changes. If we assume we can predict the sources from these regions when they are *not* being sampled (e.g. by assuming sources change only slowly) we get an improved prediction. *Peylin et al.* (2005) have demonstrated the application of such measurements. Early results suggest their widespread use will severely challenge existing transport models.

Finally, a series of papers have suggested the utility of remotely-sensed concentration for constraining inversion. Starting with the idealized study of *Rayner and O'Brien* (2001) followed by more detailed studies (*Rayner et al.*, 2002; *Houweling et al.*, 2004, e.g.), these studies suggest that the constraint on surface sources can be improved, perhaps greatly improved, using remotely-sensed concentration measurements with challenging but achievable precision. Both these later studies caution that the control of measurement biases must be very good to realize these goals. Concepts for measurement techniques have been presented by several authors e.g. *Aoki et al.* (1993); *Clerbaux et al.* (1998); *Engelen et al.* (2001); *O'Brien and Rayner* (2002); *Chedin et al.* (2003); *Dufour and Breon* (2003). There are missions under development for dedicated CO_2 measurement (*Crisp et al.*, 2003; *hamazaki et al.*, 2004). Finally various authors have already retrieved CO_2 concentration from instruments not originally intended for that purpose (*Chédin et al.*, 2002; *Chedin et al.*, 2003; *Crevoisier et al.*, 2004; *Engelen et al.*, 2004; *Chahine et al.*, 2005; *Engelen and McNally*, 2005, e.g.).

This tremendous expansion in data availability has prompted several groups to implement new algorithms whose cost depends on the assimilation window more than the number of data or observations. *Peters et al.* (2005) has adapted the Ensemble Kalman Filter technique (*Evensen*, 2003) to the flux inversion problem. In such an inversion problem, with no underlying dynamical model, the Kalman Filter is really a sequential assimilation technique (see *Enting*, 2002, for a comparison of Green's function and Kalman Filter approaches). The Ensemble Kalman Filter avoids the explicit computation of the immense covariance matrices associated with such problems at the expense of an approximation of this matrix. By contrast, *Chevallier et al.* (2005) has applied a variational technique in which the bracketed term in Eq. 3 is minimized using knowledge of its gradient. That gradient, in turn, is calculated via an adjoint model. This variational method also calculates an approximate covariance matrix. There is a significant methodological debate within the inversion community about the best method to use. The key advantages of the Ensemble Kaalman Filter are its implicit parallelism and the simplicity of implementation since it does not require the construction of an adjoint model. The key advantages of the variational method are its ability to consider the impact of all the data at once and its ability to include serial correlations in data. These are probably important in the highly time-resolved datasets coming on stream.

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