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Bayesian Estimation of Prior Variance in Source Term Determination

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The problem of determination of source term of an atmospheric release is studied. We assume that the observations y are obtained as linear combination of the source term, x, and source-receptor sensitivities, which can be written in matrix notation as $y = Mx$ with source receptor sensitivity matrix M.

Direct estimation of the source term vector x is not possible since the system is often ill-conditioned. The solution is thus found by minimization of a cost function with regularization terms. A typical cost function is:

$$C(x) = (y - Mx)^T R^{-1} (y - Mx) + \alpha x^T D^T D x, \tag{1}$$

where the first term minimizes the error of the measurements with covariance matrix R, and the second term is the regularization with weight α. Various types of regularization arise for different choices of matrix D. For example, Tikhonov regularization arises for D in the form of identity matrix, and smoothing regularization for D in the form of a tri-diagonal matrix (Laplacian operator). Typically, the form of matrix D is assumed to be known, and the weight α is optimized manually by a trial and error procedure.

In this contribution, we use the probabilistic formulation of the problem, where term $(\alpha D^T D)^{-1}$ is interpreted as a covariance matrix of the prior distribution of x. Following the Bayesian approach, we relax the assumption of known α and D and assume that these are unknown and estimated from the data. The general problem is not analytically tractable and approximate estimation techniques has to be used. We present Variational Bayesian solution of two special cases of the prior covariance matrix.

First, the structure of D is assumed to be known and only the weight α is estimated. Application of the Variational Bayes method to this case yields an iterative estimation algorithm. In the first step, the usual optimization problem is solved for an estimate of α. In the next step, the value of α is re-estimated and the procedure returns to the first step. Positivity of the solution is guaranteed by using truncated Gaussian priors.

In the second case, we assume that $\alpha = 1$ and the matrix $D^T D$ is diagonal with all diagonal elements unknown. The resulting estimation procedure is only minor modification of that for the first case. This choice is known in the machine-learning community as the automatic relevance determination prior. In effect, this prior favors sparse solutions of the inverse problem.

Performance of both methods is evaluated on a chosen tracer experiment.

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