Bayesian error covariance estimates in variational retrieval algorithms.

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The well known basic problem of variational methods:

$$J(\mathbf{x}) = \frac{1}{2}(\mathbf{x} - \mathbf{x}^b)^T \mathbf{B}_{\mathbf{x}}^{-1}(\mathbf{x} - \mathbf{x}^b) + \frac{1}{2}(\mathbf{y}^o - \mathbf{H}(\mathbf{x}))^T \mathbf{O}_{\mathbf{y}}^{-1}(\mathbf{y}^o - \mathbf{H}(\mathbf{x}))$$

The problem is: What are **O** and **B** actually? - And what about biases?

Desroziers relations puts some restriction on errors

Notation in refractivity space:

$\mathbf{o} = \mathbf{y}_o, \mathbf{b} = H(\mathbf{x}_b), \mathbf{O} = \mathbf{O}_\mathbf{y}$ and $\mathbf{B} = \mathbf{H}\mathbf{B}_\mathbf{x}\mathbf{H}^T$

Desroziers et al. (2005): $\langle(\mathbf{o}-\mathbf{b})(\mathbf{o}-\mathbf{b})^T\rangle = \mathbf{B} + \mathbf{O}$, and 3 more (redundant) equations.

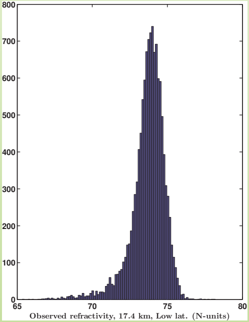
- Only constrains the sum of the error covariances. One must assume that either background noise or observation noise are known, to fix **O** and **B**.
- Implies, of cource, that IF one has either the **O** or **B** matrix, both matrices can be found.

The error covariances are hidden in the data

The model

$$
\begin{aligned}
\mathbf{o} &= \mathbf{t} + \omega + \varepsilon_o,\ \varepsilon_o \sim N(\varepsilon_o|0, \mathbf{O}) \\
\mathbf{b} &= \mathbf{t} + \beta + \varepsilon_b,\ \varepsilon_b \sim N(\varepsilon_b|0, \mathbf{B})
\end{aligned}
$$

Where $\mathbf{t} \sim N(\mathbf{t}|0, \mathbf{T})$, and $\omega, \beta, \varepsilon_o$ and ε_b are vectors.



Example of refractivity histogram

We shall not assume anything

The likelihood, of observations **o** and **b**, given the true values:

$$L(\mathbf{o},\mathbf{b}|\mathbf{t},\omega,\beta,\mathbf{O},\mathbf{B}) = \frac{1}{(2\pi|\mathbf{O}|^{\frac{1}{2}}|\mathbf{B}|^{\frac{1}{2}})^N}\times$$
$$\exp\{-\tfrac{1}{2}\sum_{n=1}^{N}[(\mathbf{b}_n-\mathbf{t}_n)^T\mathbf{B}^{-1}(\mathbf{b}_n-\mathbf{t}_n)+(\mathbf{o}_n-\mathbf{t}_n)^T\mathbf{O}^{-1}(\mathbf{o}_n-\mathbf{t}_n)]\}$$

Posterior:

$$P(\mathbf{O},\mathbf{B}|\mathbf{o},\mathbf{b},\mathbf{t},\omega,\beta)\propto$$
$$L(\mathbf{o},\mathbf{b}|\mathbf{t},\omega,\beta,\mathbf{O},\mathbf{B})p(\omega)p(\beta)p(\mathbf{t}|\mathbf{T})p(\mathbf{T})p(\mathbf{O})p(\mathbf{B}),$$

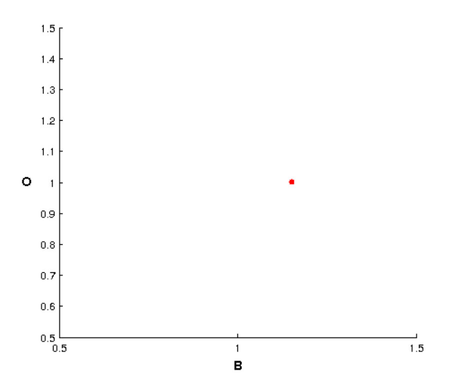
where

$$p(\mathbf{t}|\mathbf{T}) = \frac{1}{(2\pi|\mathbf{T}|)^{\frac{N}{2}}}\exp\{-\tfrac{1}{2}\sum_{n=1}^{N}(\mathbf{t}_n)^T\mathbf{T}^{-1}(\mathbf{t}_n)\}$$

and $p(\mathbf{O}), p(\mathbf{B}), p(\mathbf{T}), p(\omega)$ and $p(\beta)$ are chosen to be flat priors.

Example of sampling, $O_{30,30}$ and $B_{30,30}$

Rather than performing the integrals $P(\mathbf{O}) = \int d\mathbf{t} d\mathbf{B} d\omega d\beta$ $P(\mathbf{O}, \mathbf{B}|\mathbf{o}, \mathbf{b}, \mathbf{t}, \omega, \beta)$, we find the marginal distribution of the parameters with a Markov Chain Monte Carlo algorithm, that samples $\mathbf{t}, \omega, \beta, \mathbf{O}$ and $\mathbf{B}$.



The EUMETSAT Network of Satellite Application Facilities

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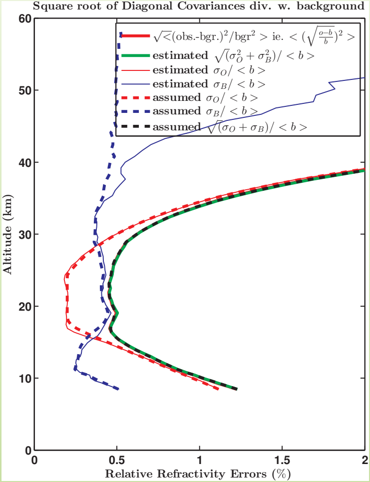
Rather than providing a mathematical prove:

You give me two data series

$$
\begin{aligned}
o &= t + \omega + \varepsilon_o,\ \varepsilon_o \sim N(\varepsilon_o|0, \sigma_o^2) \\
b &= t + \beta + \varepsilon_b,\ \varepsilon_b \sim N(\varepsilon_b|0, \sigma_b^2)
\end{aligned}
$$

Where $t \sim N(t|0, \sigma_t^2)$ Then I give you σ_o^2, σ_b^2 and $\omega - \beta$

Covariance diagonals (surrogate data with bias)

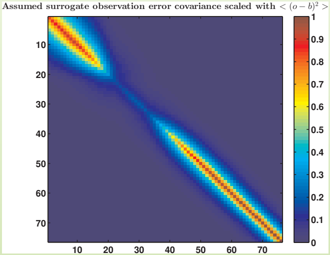


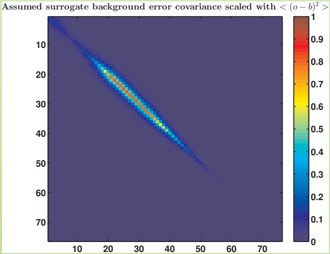
Two artificial data sets "observation" and "background" with known error characteristics are produced from 2000 true refractivity profiles (Metop A and B, latitude < 30 deg.):

$o = t + \varepsilon_o$ and $b = t + \varepsilon_b$, where ε_o and ε_b are noise terms. A Bayesian estimate of the two error covariance matrices is obtained by a MCMC method

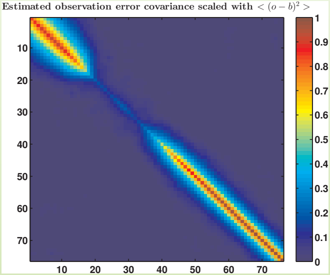
Finding **O** and **B** matrices

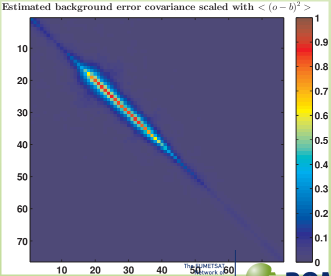
Surrogate



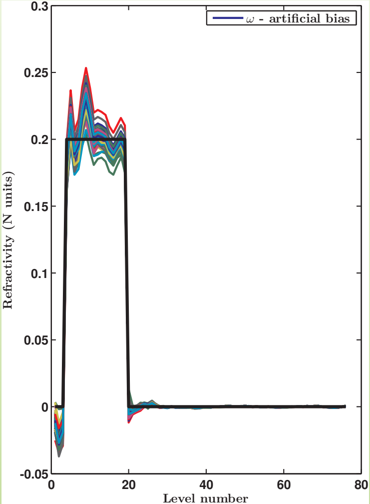


Estimated with MCMC



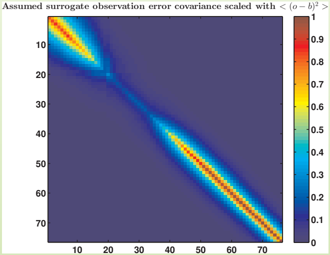


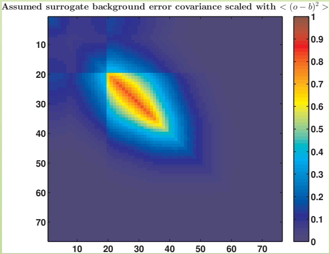
Finding bias



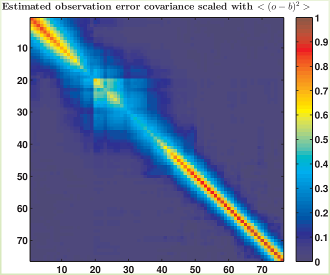
Finding **O** and **B** matrices from biased data

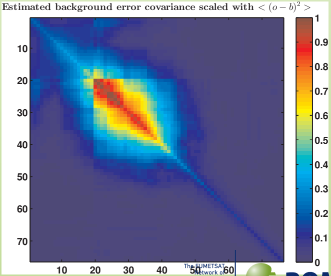
Surrogate



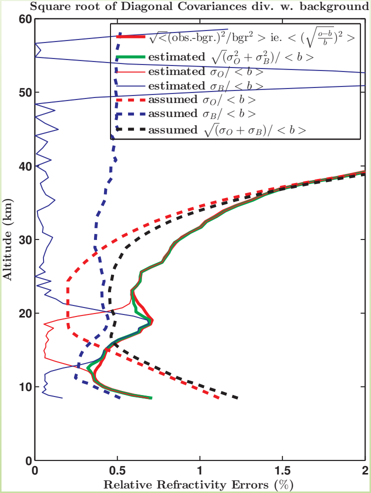


Estimated with MCMC





Finding real covariances



Conclusions

- Observation error covariances can be obtained from two data series measuring the same property.
- Alternative method for error estimates.
- Alternative method for validation.
- Problems with (inter) correlations and too large correlations.
- It is certainly not “plug and play”.