Environment Canada
Air Quality Research Division

Convergence of the Desroziers scheme: New results

Richard Ménard

Air Quality Research Division – Environment Canada
Richard.Menard@ec.gc.ca

Abstract

The convergence of the Deroziers' scheme to estimate observation and background error variances based on *OmF*, *OmA* and *AmF* is studied from a theoretical point of view. The general properties of the fixed point of the scheme are discussed and illustrated with a scalar and 1D domain with **H**=**I**. Analysis of the problem shows that the scheme converges but not to the truth unless addition information is provided. In 1D, if the true observation and background error correlation are known then the Desroziers' scheme converges to the truth error variances. An augmented scheme is proposed to estimate correlation length-scales in addition to the error variances. The scheme is nonlinear, but if the initial guess is not too far away from the true error statistics, the estimated variances and correlation lengths converges to the truth. In particular the scheme can estimate the observation error correlation length-scale.

Desroziers' scheme

Starting with the innovation covariance

$$\left\langle (O-F)(O-F)^T \right\rangle = \mathbf{HBH}^T + \mathbf{R}$$

and a first estimate on observation and background error covariances

$$\overline{\mathbf{R}}_{k+1} = \overline{\mathbf{R}}_k (\mathbf{H}\overline{\mathbf{B}}_k\mathbf{H}^T + \overline{\mathbf{R}}_k)^{-1}(\mathbf{HBH}+\mathbf{R}) = \left\langle (O-A)(O-F)^T \right\rangle_{k+1}$$

$$\mathbf{H}\overline{\mathbf{B}}_{k+1}\mathbf{H}^T = \mathbf{H}\overline{\mathbf{B}}_k\mathbf{H}^T (\mathbf{H}\overline{\mathbf{B}}_k\mathbf{H}^T + \overline{\mathbf{R}}_k)^{-1}(\mathbf{HBH}+\mathbf{R}) = \left\langle (A-F)(O-F)^T \right\rangle_{k+1}$$

The overbar denotes the estimates, and k the iteration index

General properties of the Desroziers' scheme

(1) If $\overline{\mathbf{R}}^*$ and $\overline{\mathbf{B}}^*$ are fixed points, then

$$\mathbf{H}\overline{\mathbf{B}}^*\mathbf{H}^T + \overline{\mathbf{R}}^* = (\mathbf{HBH}+\mathbf{R})$$

(2) When the iterate k is such that

$$\mathbf{H}\overline{\mathbf{B}}_k\mathbf{H}^T + \overline{\mathbf{R}}_k = (\mathbf{HBH}+\mathbf{R})$$

no more updates on the individual components $\overline{\mathbf{R}}_k$ and $\overline{\mathbf{B}}_k$ can occur.

1D Periodic domain

Assume an homogeneous **B** in a 1D periodic domain with observations at each grid points, **H = I**. Diagonalizing the system using a Fourier unitary transform matrix, gives the following spectral equ.s

$$\overline{R}_{k+1}(n) = \frac{\overline{R}_k(n)}{\overline{B}_k(n)+\overline{R}_k(n)}\left[B(n)+R(n)\right]$$

$$\overline{B}_{k+1}(n) = \frac{\overline{B}_k(n)}{\overline{B}_k(n)+\overline{R}_k(n)}\left[B(n)+R(n)\right]$$

Illustration - scalar case

Iteration on observation error

$$\left\langle (O-A)(O-F)^T \right\rangle = \overline{\mathbf{R}}(\mathbf{H}\overline{\mathbf{B}}\mathbf{H}^T + \overline{\mathbf{R}})^{-1}(\mathbf{HBH}+\mathbf{R})$$

where $\left\langle (O-F)(O-F)^T \right\rangle = \mathbf{HBH}^T + \mathbf{R}$ is obtained from innovations and overbar denotes *prescribed* error covariances

i)- Correctly prescribed forecast error variance

$$\overline{\mathbf{B}} = \mathbf{B} = \sigma_f^2 \qquad \overline{\mathbf{R}} = \alpha\mathbf{R} = \alpha\sigma_o^2 \qquad \text{optimal value } \alpha = 1$$

$$\left\langle (O-A)(O-F) \right\rangle = \frac{\alpha\sigma_o^2}{\alpha\sigma_o^2+\sigma_f^2}(\sigma_o^2+\sigma_f^2) = \alpha\sigma_o^2\left(\frac{\gamma+1}{\alpha\gamma+1}\right)$$

where $\gamma = \dfrac{\sigma_o^2}{\sigma_f^2}$

Let $\left\langle (O-A)(O-F) \right\rangle = \alpha_{n+1}\sigma_o^2$ be the next iterate

so the iteration on α_n takes the form

$$\alpha_{n+1} = \alpha_n\left(\frac{\gamma+1}{\alpha_n\gamma+1}\right) = G(\alpha_n)$$

Define a *mapping* G

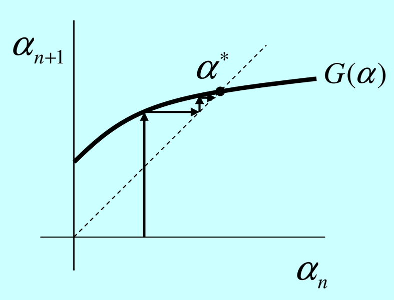
$$G(\alpha) = \alpha\left(\frac{\gamma+1}{\alpha\gamma+1}\right)$$

The fixed-point is

$$\alpha^* = G(\alpha^*)$$

condition for convergence

$$\left|G'(\alpha^*)\right| < 1$$



and so for this case we get $\alpha^* = 1$

$$G'(\alpha^*) = \frac{1}{\gamma+1} = \frac{\sigma_f^2}{\sigma_o^2+\sigma_f^2} = K \le 1$$

the scheme is always convergent and converges to the true value $\alpha = 1$

ii)- Incorrectly prescribed forecast error variance

$$\overline{\mathbf{B}} = \beta\mathbf{B} = \beta\sigma_f^2 \qquad \overline{\mathbf{R}} = \alpha\mathbf{R} = \alpha\sigma_o^2$$

the mapping is now different

$$\alpha_{n+1} = \alpha_n\left(\frac{\gamma+1}{\alpha_n\gamma+\beta}\right) = G(\alpha_n)$$

The fixed-point is

$$\alpha^* = 1 + \frac{1-\beta}{\gamma} = 1 + \frac{\left(\sigma_f^2 - \overline{\sigma}_f^2\right)}{\sigma_o^2}$$

that is *not the true observation error* value.

- If forecast error variance is underestimated, obs error is overestimated
- If forecast error variance is overestimated, obs error is underestimated

$$G'(\alpha^*) = \frac{\beta}{\gamma+1} = \frac{\beta\sigma_f^2}{\sigma_o^2+\sigma_f^2}$$

Will not converge if: $\beta\sigma_f^2 = \overline{\sigma}_f^2 > \sigma_o^2 + \sigma_f^2$

In practice the estimated forecast error variance will never be larger than the innovation error variance, so for all practical cases the scheme converges.

B - Iteration of both, observation and background error variances

Consider the case of tuning together α and β in each iteration

$$\alpha_{n+1} = \alpha_n\left(\frac{\gamma+1}{\alpha_n\gamma+\beta_n}\right) = G(\alpha_n,\beta_n)$$

$$\beta_{n+1} = \beta_n\left(\frac{\gamma+1}{\alpha_n\gamma+\beta_n}\right) = F(\alpha_n,\beta_n)$$

then the ratio

$$\mu_{n+1} = \frac{\alpha_{n+1}}{\beta_{n+1}} = \frac{\alpha_n}{\beta_n} = \mu_n = \cdots = \mu_0$$

is constant.

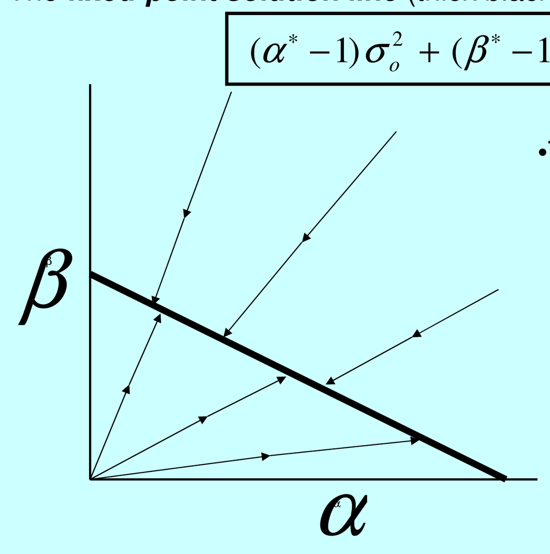
The mapping $(\alpha_n,\beta_n) \leftrightarrow (\alpha_{n+1},\beta_{n+1})$ is in fact ill-defined, since the Jacobian

$$\frac{\partial(G,F)}{\partial(\alpha_n,\beta_n)} = \frac{\gamma+1}{(\alpha_n\gamma+\beta_n)}\begin{pmatrix}\beta_n & -\alpha_n \\ -\beta_n\gamma & \alpha_n\gamma\end{pmatrix}$$

is rank deficient ! and its determinant is 0. So the scheme is ***strongly convergent***

The ***fixed-point solution line*** (thick black line) is a very strong attractor

$$\boxed{(\alpha^*-1)\sigma_o^2 + (\beta^*-1)\sigma_f^2 = 0}$$



- The convergence occur in a single iteration, and in the scalar case or 1D case with no constraint on correlations, any point on the solution line is a fixed point. ***Additional information on the error correlations is thus needed to have a scheme that can converge to the truth***

1D with spatial correlation models

Let $r(n), b(n)$ be the spectral components of the obs and background error correlation, then

$$\sum r(n) = 1, \quad \sum b(n) = 1$$

Also assume that $r(n), b(n), \overline{r}(n), \overline{b}(n)$ are all derived from a correlation model (eg. SOAR) with either given or estimated correlation-scale.
The iteration equation then becomes

$$\alpha_{i+1} = \alpha_i \sum \overline{r}_i(n;L_R)\,\chi_i^2(n)$$

$$\beta_{i+1} = \beta_i \sum \overline{b}_i(n;L_B)\,\chi_i^2(n)$$

where the spectral

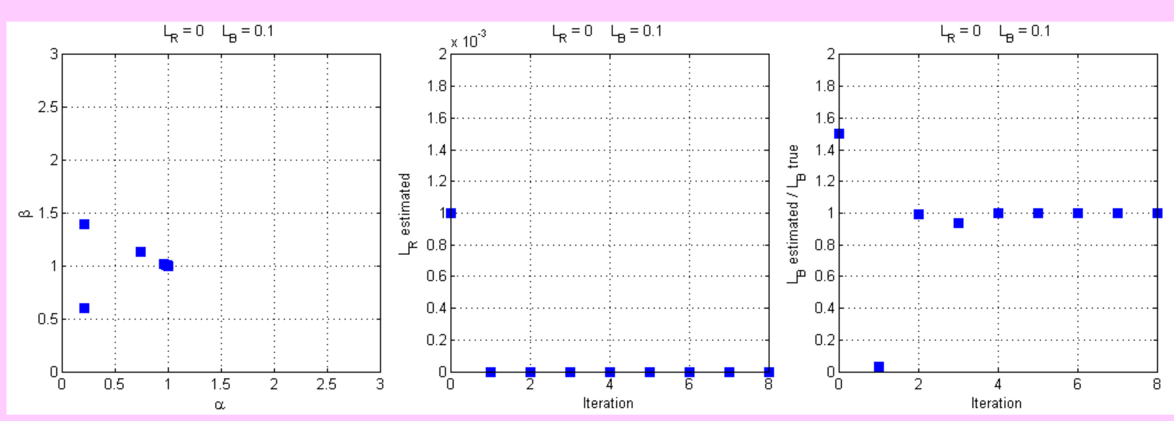
$$\chi_i^2(n) \equiv \chi_i^2(n;\,\alpha_i,\beta_i,\,L_R,L_B,\,L_{\overline{R}},L_{\overline{B}}) = \frac{b(n;L_B)+\gamma r(n;L_R)}{\beta_i\overline{b}(n;L_{\overline{B}})+\alpha_i\gamma\overline{r}(n;L_{\overline{R}})}$$

and we add to this an estimation of the length-scales based on a maximum likelihood estimation

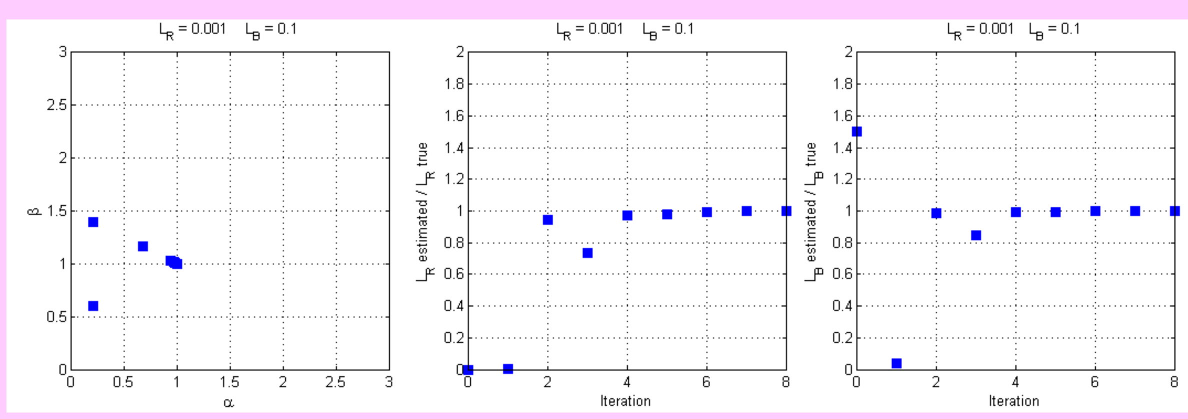
$$\left[L_{\overline{R}},L_{\overline{B}}\right] \underset{\min}{\Leftarrow} \mathcal{L}(\chi_i^2,\alpha_i,\beta_i)$$

where $\mathcal{L}$ is the log-likelihood function

Experiment 1 – The true obs error is spatially uncorrelated, but we assume initially that obs error are correlated



Experiment 2 – The true obs error is spatially correlated, but we assume initially that obs errors are spatially uncorrelated



Summary and Conclusions

- The convergence of the Desroziers' et al (2005) scheme has been investigated from a theoretical point of view

- Iteration on either observation error variance or background error variance generally converges, but will not converge to the truth unless other information is provided

- By estimating the observation and background error correlation length scale (here done using a maximum likelihood method) as part of the Desroziers' algorithm, convergence to the truth is obtained. In particular the scheme can estimate correctly if the observation error is spatially uncorrelated and otherwise estimate the obs error correlation length scale, and this simultaneously with a correct estimation of the background error correlation length and observation and background error variances.

- The scheme is however, nonlinear and the regime of validity is currently not known. However, if the correlation models are known then the variance estimates always converge to the truth