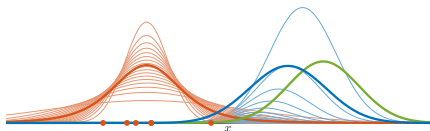
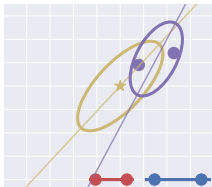


EnKF – FAQ

(Ensemble Kalman filter – Frequently asked questions)



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Marc Bocquet, Alberto Carrassi



EnKF workshop, Voss, June 4, 2019

Adaptive covariance inflation in the ensemble Kalman filter by Gaussian scale mixtures

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Also answered these questions about the EnKF:

- Why do we use $(N-1)$ in $\frac{1}{N-1} \sum_n (x_n - \bar{x})^2$?

- About **nonlinearity**:

- Why does it create **sampling error**?

- Why does it cause **divergence**?

This paper studies multiplicative inflation: the complementary scaling of the state covariance in the ensemble Kalman filter (EnKF). Firstly, error sources in the EnKF are catalogued and discussed in relation to inflation; nonlinearity is given particular attention as a source of sampling error. In response, the “finite-size” refinement known as the EnKF- N is re-derived via a Gaussian scale mixture, again demonstrating how it yields adaptive inflation. Existing methods for adaptive inflation estimation are reviewed, and several insights are gained from a comparative analysis.

One such adaptive inflation method is used to complement the EnKF- N to make a hybrid that is suitable for contexts where model error is present and imperfectly parametrized. Benchmark results are obtained from experiments with the two-scale inflation model and its hybrid. The proposed hybrid EnKF- N method of adaptive inflation is found to yield systematic accuracy improvements in comparison to the existing methods, albeit to a moderate degree.

adaptive filtering, ensemble inference, covariance inflation, data assimilation, scale mixture

Revising the stochastic iterative ensemble smoother

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Abstract

Ensemble randomized maximum likelihood (EnRML) is an iterative (stochastic) ensemble smoother, used for large and nonlinear inverse problems, such as history matching and data assimilation. Its current formulation is overly complicated and has issues with computational costs, noise, and covariance localization, even causing some practitioners to omit crucial prior information. This paper resolves these difficulties and streamlines the algorithm, without changing its output. These simplifications are achieved through the careful treatment of the linearizations and subspaces. For example, it is shown (a) how ensemble linearizations relate to average sensitivity, and (b) that the ensemble does not lose rank during updates. The paper also draws significantly on the theory of the (deterministic) iterative ensemble Kalman smoother (IEnKS). Comparative benchmarks are obtained with the Lorenz-96 model with these two smoothers and the ensemble smoother using multiple data assimilation (ES-MDA).

Also answered these questions about the EnKF:

- Why do we prefer the Kalman **gain** "form"?
- About **ensemble linearizations**:
 - **What** are they?
 - Why is this **rarely discussed**?
 - How does it relate to **analytic derivatives**?

Ensemble linearizations

Traditional EnKF presentation

Recall the KF gain:

$$\mathbf{K} = \mathbf{C}_x \mathbf{H}^\top (\mathbf{H} \mathbf{C}_x \mathbf{H}^\top + \mathbf{R})^{-1}. \quad (1)$$

1st idea: substitute $\mathbf{C}_x \leftarrow \bar{\mathbf{C}}_x = \frac{1}{N-1} \mathbf{X} \mathbf{X}^\top$

$$\implies \bar{\mathbf{K}} = \bar{\mathbf{C}}_x \mathbf{H}^\top (\mathbf{H} \bar{\mathbf{C}}_x \mathbf{H}^\top + \mathbf{R})^{-1} \quad (2)$$

$$= \mathbf{X} \mathbf{Y}^\top (\mathbf{Y} \mathbf{Y} + (N-1) \mathbf{R})^{-1} \quad (3)$$

$$\text{with } \mathbf{Y} = \mathbf{H} \mathbf{X} \quad (4)$$

$$= \mathcal{H}(\mathbf{X}) \quad (5)$$

$$= \mathcal{H}(\mathbf{E}) - \text{mean}. \quad (6)$$

2nd idea: use eqn. (6) also in nonlinear case (when $\nabla \mathbf{H}$).

What is the ensemble's linearization?

Recall $\bar{\mathbf{C}}_x = \frac{1}{N-1} \mathbf{X}\mathbf{X}^\top$ and suppose \mathcal{H} is nonlinear.

Question: Is there a matrix $\bar{\mathbf{H}}$ such that
$$\begin{cases} \frac{1}{N-1} \mathbf{X}\mathbf{Y}^\top = \bar{\mathbf{C}}_x \bar{\mathbf{H}}^\top \\ \frac{1}{N-1} \mathbf{Y}\mathbf{Y}^\top = \bar{\mathbf{H}} \bar{\mathbf{C}}_x \bar{\mathbf{H}}^\top \end{cases} \quad ?$$

Answer: Yes (mostly): $\bar{\mathbf{H}} = \mathbf{Y}\mathbf{X}^+$.

Follow up questions:

- How come this is rarely discussed?
- Why $\mathbf{Y}\mathbf{X}^+$?
- Does it relate to the analytic derivative (\mathcal{H}') ?

Does $\bar{\mathbf{H}} = \mathbf{Y}\mathbf{X}^+$ relate to \mathcal{H}' ?

$$\begin{aligned} \text{Theorem: } \lim_{N \rightarrow \infty} \bar{\mathbf{H}} &= \mathbb{E}[\mathcal{H}'(\mathbf{x})] \\ &= \lim_{N \rightarrow \infty} \mathbf{Y}\mathbf{X}^+ &= \mathbf{C}_{yx}\mathbf{C}_x^{-1} \\ &= \lim_{N \rightarrow \infty} \mathbf{Y}\mathbf{X}^T(\mathbf{X}\mathbf{X}^T)^{-1} &(\text{by Stein/IBP}) \\ &= \lim_{N \rightarrow \infty} \bar{\mathbf{C}}_{yx}\bar{\mathbf{C}}_x^{-1} \\ &= \mathbf{C}_{yx}\mathbf{C}_x^{-1} \quad (\text{a.s., by Slutsky, sub. to reg.}) \end{aligned}$$

I.e. $\bar{\mathbf{H}}$ may (indeed) be called the “average” derivative.

Assumptions:

- Ensemble (behind $\bar{\mathbf{H}}$) and \mathbf{x} share the **same distribution**.
- This is **Gaussian**.

How come $\bar{\mathbf{H}} = \mathbf{Y}\mathbf{X}^+$ is rarely discussed?

Substitute $\mathbf{H} \leftarrow \bar{\mathbf{H}}$ in $\bar{\mathbf{K}}$:

$$\bar{\mathbf{K}} = \bar{\mathbf{C}}_x \bar{\mathbf{H}}^T (\bar{\mathbf{H}} \bar{\mathbf{C}}_x \bar{\mathbf{H}}^T + \mathbf{R})^{-1} \quad (7)$$

$$= \mathbf{X}\mathbf{Y}^T (\mathbf{Y} \mathbf{\Pi}_{\mathbf{X}^T} \mathbf{Y}^T + (N-1)\mathbf{R})^{-1}, \quad (8)$$

where $\mathbf{\Pi}_{\mathbf{X}^T} = \mathbf{X}^+ \mathbf{X}$, which is scary... But $\mathbf{\Pi}_{\mathbf{X}^T}$

- is just a projection;
- vanishes if \mathcal{H} is linear, or $(N-1) \leq M$;
- is present for any/all linearization of \mathcal{H} ;

Why $\bar{\mathbf{H}} = \mathbf{Y}\mathbf{X}^+$?

$\bar{\mathbf{H}}$ is:

- Linear least-squares (LLS) estimate of \mathcal{H} given \mathbf{Y} and \mathbf{X} .
- BLUE ?
- MVUE ?

$\bar{\mathbf{H}}$ is LLS because $\bar{\mathbf{K}}$ is LLS, and the chain rule applies.

Why the “gain form”?

Not equivalent when $(N-1) < M$:

$$\bar{\mathbf{P}} = [\mathbf{I} - \bar{\mathbf{K}}\mathbf{H}]\bar{\mathbf{B}} \quad (9)$$

$$\bar{\mathbf{P}} = (\bar{\mathbf{B}}^+ + \mathbf{H}^T \mathbf{R}^{-1} \mathbf{H})^{-1} \quad (10)$$

Why is the Kalman gain form (9) better?

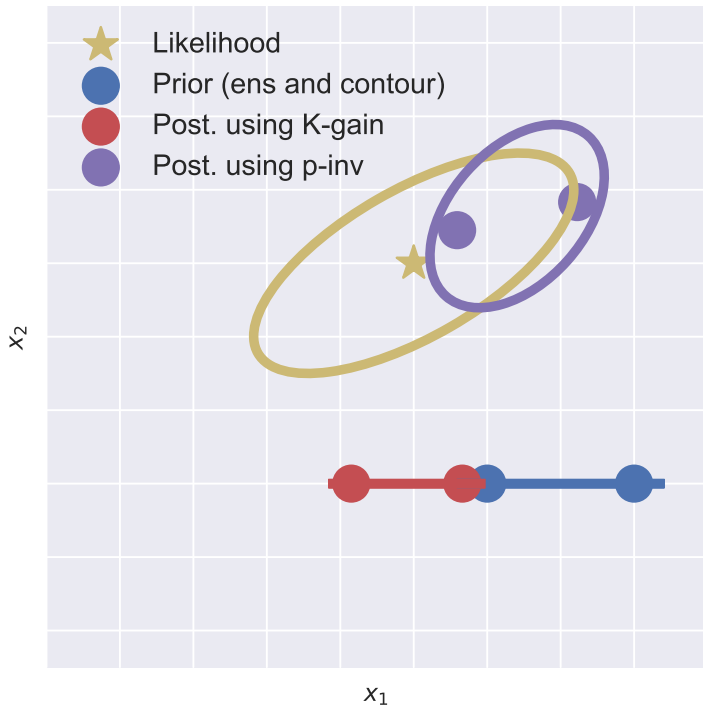
Note that eqn. (10) follows from

$$\text{prior} \propto \exp[-\frac{1}{2}(\mathbf{x} - \bar{\mathbf{x}})^T \bar{\mathbf{B}}^+ (\mathbf{x} - \bar{\mathbf{x}})], \quad (11)$$

which is “flat” in the directions outside of $\text{col}(\bar{\mathbf{B}})$.

\implies eqn. (10) yields “opposite” of the correct update.

Note: further complications in case $\bar{\mathbf{P}}$ not defined in eqn. (10).

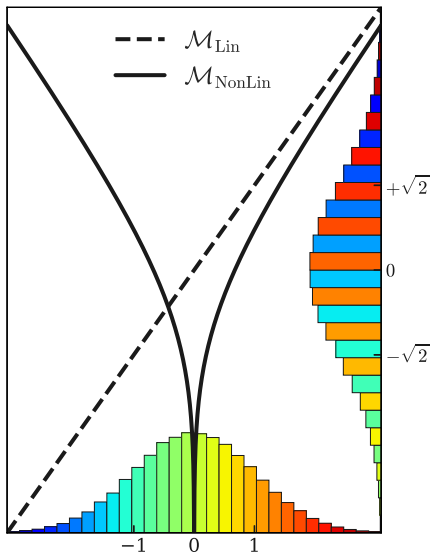


Nonlinearity,
sampling error, and divergence.

Aim: study **sampling error**,
due to **nonlinearity**,
without worrying about
non-Gaussianity.

$$\mathcal{M}_{\text{Lin}}(x) = \sqrt{2}x,$$

$$\mathcal{M}_{\text{NonLin}}(x) = \sqrt{2}F_{\mathcal{N}}^{-1}(F_{\chi}(x^2))$$



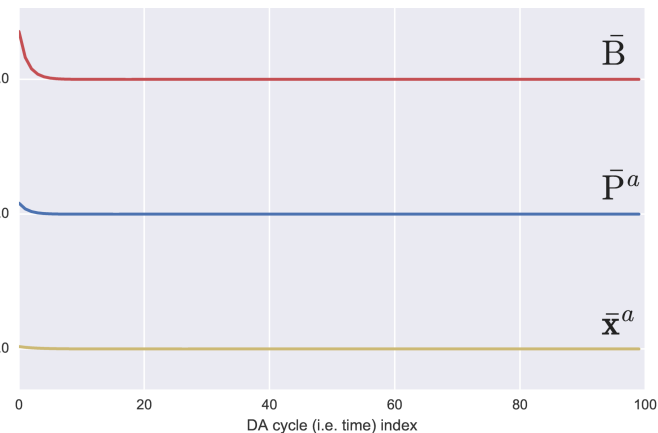
Motivational problem

$$\text{prior} = \mathcal{N}(x|0, \underline{2}),$$

$$\text{likelihood} = \mathcal{N}(0|x, 2),$$

$$\Rightarrow \text{posterior} = \mathcal{N}(x| \underline{0}, \underline{1}).$$

$$\text{dyn. model} = \mathcal{M}_{\text{Lin}}(x) = \sqrt{2}x \text{ dyn. model} = \cancel{\mathcal{M}_{\text{Lin}}(x)} = \cancel{\sqrt{2}x} \text{ dyn. model}$$



Sampling error from nonlinearity – why?

Consider the error
in the m -th sample moment
of the forecast (f) ensemble,
propagated by a degree- d model.
It can be shown that

$$\text{Error}_m^f = \sum_{i=1}^{md} C_{m,i} \text{Error}_i^a, \quad (12)$$

i.e. the moments get coupled, which defeats moment-matching.

Riccati recursion

Assume constant, linear dynamics (\mathbf{M}), $\mathbf{Q} = 0$, $\mathbf{H} = \mathbf{I}$, and a deterministic EnKF.

The **ensemble covariance** obeys:

■ Forecast:
$$\bar{\mathbf{B}}_k = \mathbf{M}^2 \bar{\mathbf{P}}_{k-1}. \quad (13)$$

■ Analysis:
$$\bar{\mathbf{P}}_k = (\mathbf{I} - \bar{\mathbf{K}}_k) \bar{\mathbf{B}}_k \quad (14)$$

$$\iff \bar{\mathbf{P}}_k^{-1} = \bar{\mathbf{B}}_k^{-1} + \mathbf{R}^{-1}. \quad (15)$$

\implies The “Riccati recursion”:

$$\bar{\mathbf{P}}_k^{-1} = (\mathbf{M}^2 \bar{\mathbf{P}}_{k-1})^{-1} + \mathbf{R}^{-1}. \quad (16)$$

Attenuation

Stationary Riccati:

$$\bar{\mathbf{P}}_{\infty}^{-1} = (\mathbf{M}^2 \bar{\mathbf{P}}_{\infty})^{-1} + \mathbf{R}^{-1} \quad (17)$$

$$\iff \bar{\mathbf{P}}_{\infty} = \bar{\mathbf{K}}_{\infty} \mathbf{R}, \quad \bar{\mathbf{K}}_{\infty} = \begin{cases} \mathbf{I} - \mathbf{M}^{-2} & \text{if } \mathbf{M} \geq 1, \\ 0 & \text{otherwise.} \end{cases} \quad (18)$$

Initial conditions (ICs) don't appear

\implies ICs are "forgotten".

\implies Sampling error is attenuated.

Why $(N - 1)$?

Suppose we **re-define** the EnKF algorithm to use a different normalization factor, i.e.

$$\tilde{\mathbf{P}}_k \tilde{\mathbf{P}}_0 = \frac{\alpha}{N-1} \mathbf{X}_k \mathbf{X}_k^T \frac{\alpha}{N-1} \mathbf{X}_0 \mathbf{X}_0^T = \alpha \bar{\mathbf{P}}_k \alpha \bar{\mathbf{P}}_0. \quad (19)$$

But,

$$\text{the ensemble forecast yields } \tilde{\mathbf{B}}_k = \mathbf{M}^2 \tilde{\mathbf{P}}_{k-1}, \quad (20)$$

$$\text{the analysis using } \tilde{\mathbf{B}}_k \text{ yields } \tilde{\mathbf{P}}_k^{-1} = \tilde{\mathbf{B}}_k^{-1} + \mathbf{R}^{-1}. \quad (21)$$

$$\implies \text{The Riccati recursion: } \tilde{\mathbf{P}}_k^{-1} = (\mathbf{M}^2 \tilde{\mathbf{P}}_{k-1})^{-1} + \mathbf{R}^{-1} \quad (22)$$

Note: α does not appear.

\implies its impact is attenuated, just like ICs.

$$\implies \tilde{\mathbf{P}}_k \xrightarrow[k \rightarrow \infty]{} \bar{\mathbf{P}}_k.$$

$$\implies \tilde{\mathbf{x}}_k \xrightarrow[k \rightarrow \infty]{} \bar{\mathbf{x}}_k.$$

Filter divergence

Recall Riccati:

$$\bar{\mathbf{P}}_k = \underbrace{(\mathbf{I} - \bar{\mathbf{K}}_k)}_{\xrightarrow[k \rightarrow \infty]{} \mathbf{M}^{-2}} \mathbf{M}^2 \bar{\mathbf{P}}_{k-1}. \quad (23)$$

Now consider $\delta \bar{\mathbf{P}}_k$. Its recursion is:

$$\delta \bar{\mathbf{P}}_k \approx (\mathbf{I} - \bar{\mathbf{K}}_k)^2 [\mathbf{M}^2 + \mathcal{M}\mathcal{M}'''] \delta \bar{\mathbf{P}}_{k-1}, \quad (24)$$

Yielding $\delta \bar{\mathbf{P}}_k \xrightarrow[k \rightarrow \infty]{} 0$ in the linear case ($\mathcal{M}''' = 0$),
as we found previously.

By contrast, no such guarantee exists when $\mathcal{M}''' \neq 0$
 \implies filter divergence.

Also, \mathcal{M}''' may grow worse with k
 \implies vicious circle.

Revising
EnRML

EnRML issues

Gauss-Newton version:

(Reynolds et al., 2006; Gu and Oliver, 2007; Chen and Oliver, 2012):

- Requires “model sensitivity” matrix.
- ... which requires pseudo-inverse of the “anomalies”.

⇒ Levenberg-Marquardt version (Chen and Oliver, 2013):

- Modification *inside* Hessian, simplifying *likelihood increment*.
- Further complicates *prior increment*, which is sometimes dropped!

⇒ New version Raanes, Evensen, Stordal, 2019:

- No explicit computation of the model sensitivity matrix
- Computing its product with the prior covariance is efficient.
- Does not require any pseudo-inversions.

Algorithm simplification

Chen and Oliver (2013):

$d^o \leftarrow d_{\text{obs}} + \epsilon;$ * perturb observations, $\epsilon \sim N[0, C_D];$
 $\Delta m_{\text{pr}} \leftarrow C_{\text{sc}}^{-1/2} (m_{\text{pr}} - \overline{m_{\text{pr}}}) / \sqrt{N_e - 1};$
 $U_{m_0}^{p_{m_0}} W_{m_0}^{p_{m_0}} (V_{m_0}^{p_{m_0}})^T \leftarrow \Delta m_{\text{pr}};$ * truncated SVD;
 $A_m \leftarrow U_{m_0}^{p_{m_0}} (W_{m_0}^{p_{m_0}})^{-1};$
 $m_0 \leftarrow m_{\text{pr}}; \quad d_0 \leftarrow g(m_0);$
 $S_0 \leftarrow (d_0 - d^o)^T C_D^{-1} (d_0 - d^o);$
while $\ell < \ell_{\text{max}}$ **do**
 $\Delta m \leftarrow C_{\text{sc}}^{-1/2} (m_{\ell-1} - \overline{m_{\ell-1}}) / \sqrt{N_e - 1};$
 $\Delta d \leftarrow C_D^{-1/2} (d_{\ell-1} - \overline{d_{\ell-1}}) / \sqrt{N_e - 1};$
 $U_d^{p_d} W_d^{p_d} (V_d^{p_d})^T \leftarrow \Delta d;$ * truncated SVD;
 $X_1 \leftarrow (U_d^{p_d})^T C_D^{-1/2} (d_{\ell-1} - d^o);$
 $X_2 \leftarrow (-I_{p_d} + (W_d^{p_d})^2)^{-1} X_1;$
 $X_3 \leftarrow V_d^{p_d} W_d^{p_d} X_2;$
 $\delta m_1 \leftarrow -C_{\text{sc}}^{1/2} \Delta m X_3;$
 $X_4 \leftarrow A_m^T C_{\text{sc}}^{-1/2} (m - m_{\text{pr}});$
 $X_5 \leftarrow A_m X_4;$
 $X_6 \leftarrow \Delta m^T X_5;$
 $X_7 \leftarrow V_d^{p_d} (I_{p_d} + (W_d^{p_d})^2)^{-1} (V_d^{p_d})^T X_6;$
 $\delta m_2 \leftarrow -C_{\text{sc}}^{1/2} \Delta m X_7;$
 $m_{\ell} \leftarrow m_{\ell-1} + \delta m_1 + \delta m_2; \quad d_{\ell} \leftarrow g(m_{\ell});$

Raanes, Evensen, Stordal (2019):

Require: prior ens. \mathbf{E} , obs. perturb's \mathbf{D}

$$\bar{\mathbf{x}} = \mathbf{E} \mathbf{1} / N$$

$$\mathbf{X} = \mathbf{E} - \bar{\mathbf{x}} \mathbf{1}^T$$

$$\mathbf{W} = \mathbf{I}_N$$

repeat:

Run model (on each col.) to get $\mathcal{M}(\mathbf{E})$

$$\mathbf{Y} = \mathcal{M}(\mathbf{E}) (\mathbf{W} \mathbf{I}_1^T)^+$$

$$\nabla J_{\mathbf{W}}^{\text{klhd}} = \mathbf{Y}^T \mathbf{C}_D^{-1} [\mathbf{y} \mathbf{1}^T + \mathbf{D} - \mathcal{M}(\mathbf{E})]$$

$$\nabla J_{\mathbf{W}}^{\text{prior}} = (N-1) [\mathbf{I}_N - \mathbf{W}]$$

$$\bar{\mathbf{C}}_{\mathbf{w}} = (\mathbf{Y}^T \mathbf{C}_D^{-1} \mathbf{Y} + (N-1) \mathbf{I}_N)^{-1}$$

$$\mathbf{W} = \mathbf{W} + \bar{\mathbf{C}}_{\mathbf{w}} [\nabla J_{\mathbf{W}}^{\text{prior}} + \nabla J_{\mathbf{W}}^{\text{klhd}}]$$

$$\mathbf{E} = \bar{\mathbf{x}} \mathbf{1}^T + \mathbf{X} \mathbf{W}$$

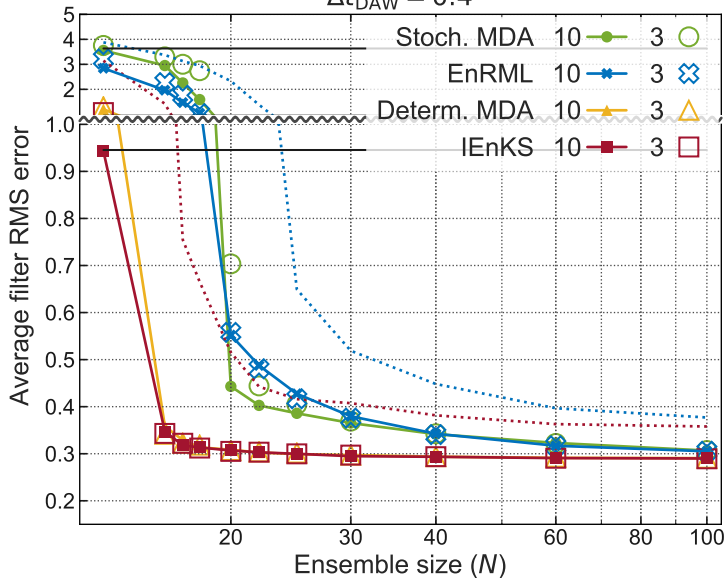
Available from github.com/nansencenter/DAPPER

```
if MDA: # View update as annealing (progressive assimilation).
    Cow1 = Cow1 @ T # apply previous update
    dw = dy @ Y.T @ Cow1
    if 'PertObs' in upd_a:          #== "ES-MDA". By Emerick/Reynolds.
        D = mean0(randn(Y.shape)) * sqrt(nIter)
        T -= (Y + D) @ Y.T @ Cow1
    elif 'Sqrt' in upd_a:          #== "ETKF-ish". By Raanes.
        T = Cowp(0.5) * sqrt(za) @ T
    elif 'Order1' in upd_a:       #== "DEnKF-ish". By Emerick.
        T -= 0.5 * Y @ Y.T @ Cow1
    # Tinv = eye(N) [as initialized] coz MDA does not de-condition.

else: # View update as Gauss-Newton optimzt. of log-posterior.
    grad = Y0@dy - w*za          # Cost function gradient
    dw = grad@Cow1              # Gauss-Newton step
    if 'Sqrt' in upd_a:          #== "ETKF-ish". By Bocquet/Sakov.
        T = Cowp(0.5) * sqrt(N1) # Sqrt-transforms
        Tinv = Cowp(-.5) / sqrt(N1) # Saves time [vs tinv(T)] when Nx<N
    elif 'PertObs' in upd_a:     #== "EnRML". By Oliver/Chen/Raanes/Evensen/Stordal.
        D = mean0(randn(Y.shape)) if iteration==0 else D
        gradT = -(Y+D)@Y0.T + N1*(eye(N) - T)
        T = T + gradT@Cow1
        # Tinv= tinv(T, threshold=N1) # unstable
        Tinv = inv(T+1)           # the +1 is for stability.
    elif 'Order1' in upd_a:     #== "DEnKF-ish". By Raanes.
        # Included for completeness; does not make much sense.
        gradT = -0.5*Y@Y0.T + N1*(eye(N) - T)
        T = T + gradT@Cow1
        Tinv = tinv(T, threshold=N1)
```

$$\Delta t_{\text{obs}} = 0.2$$

$$\Delta t_{\text{DAW}} = 0.4$$



Summary

- In the **linear** case, ICs are forgotten by Riccati.
 - \implies Sampling error **attenuates**.
 - \implies The covariance **normalization factor** is inconsequential.
- By contrast, **nonlinearity**
 - undoes the attenuation, causing filter **divergence**.
 - creates **sampling error** by cascading higher-order error down through the moments.
- Gain **form** $>$ Precision-matrix **form**.
- The **ensemble linearizations**
 - are **LLS regression** estimates.
 - converge to the **average, analytic sensitivity**.

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Appendix

Sampling error from nonlinearity – why?

- Consider the m -th “true” and “sample” moments:

$$\mu_m = \mathbb{E}[x^m], \quad (25)$$

$$\hat{\mu}_m = N^{-1} \sum_{n=1}^N x_n^m. \quad (26)$$

- Define: $\text{Error}_m = \hat{\mu}_m - \mu_m$.
- Define: $\mu_m^f = \mathbb{E}[(\mathcal{M}(x))^m]$.
- Assume degree- d Taylor-exp. of \mathcal{M} is accurate. Then

$$\mu_m^f = \sum_{i=1}^{md} C_{m,i} \mu_i. \quad (27)$$

- Hence, Due to coupling of moments,

$$\text{Error}_m^f = \sum_{i=1}^{md} C_{m,i} \text{Error}_i^a \text{Error}_i, \quad (28)$$

which defeats moment-matching.