A data-driven method for improving the correlation estimation in serial ensemble Kalman filter

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Outline

1. Correlation statistics in EnKF

2. Learning algorithm for improving the correlation estimation

3. Serial EnKF with transformed correlations

4. Numerical experiments on the Lorenz-96 model

5. Conclusion
Correlation statistics in EnKF
EnKF in linear and Gaussian settings

- In the linear and Gaussian, and under certain assumptions (controllability, observability, uncorrelated noises), the Kalman posterior error covariance matrix $P^a$ will converge to the fixed point $\hat{C}$ of

$$
\hat{C} = (I - KH)(F\hat{C}F^T + Q),
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where $K = \hat{C}H^T(H\hat{C}H^T + R)^{-1}$ is the Kalman gain, $F$ is the deterministic linear forecast model with noise covariance matrix $Q$, $H$ is the linear observation operator, and $R$ is the observation error covariance matrix.
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- The scheme approximates both prior and posterior covariances by the ensemble covariance matrix, e.g.,

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P^a \approx \frac{1}{K-1}XX^T,
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where $X$ is the matrix $\mathbb{R}^{N \times K}$ of analysis ensemble perturbations from the ensemble mean (the $k^{th}$ column of $X$ is $X^{a,k} = x^{a,k} - \bar{x}^{a,k}$).
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- In the linear and Gaussian setting, the EnKF solution is optimal with finite ensemble if

$$x^{a,k}_t - \overline{x}^a_t \sim \mathcal{N}(0, \hat{C})$$

in the limit as $t \to \infty$. 
Motivation

- **Nonlinear and non-Gaussian case**: estimating the correlation \( \rho = D^{-1/2}CD^{-1/2} \), \( D = \text{diag}(C) \), is much more difficult because \( \rho \) is time-dependent and does not equilibrate to an invariant \( \rho_{\text{eq}} \). Furthermore, the EnKF sample correlation, \( r^K \), is such that

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\hat{r}(t) \equiv \lim_{K \to \infty} r^K(t) \neq \rho(t), \quad \forall t.
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- Since estimating the true correlation \( \rho \) is very difficult, then instead, we try to estimate \( \hat{r} \).

How can we transform \( r^K \) into \( \hat{r} \)?

- The idea:
  1. Find a linear map \( L \) that transforms the undersampled correlation matrix \( r^K \) into a sample of improved correlation matrix:
     \[
     L^T r^K \approx \hat{r}, \quad L \in \mathbb{R}^{N \times N \times M}.
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  2. Implement the map \( L \) into the serial LLS EnKF of Anderson (2003).
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EnKF $L=500$

- Implement the map $\mathcal{L}$ into the serial LLS EnKF of Anderson (2003).
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Learning algorithm for improving the correlation estimation
A minimization problem

- For nonlinear filtering problems, where \( h(x) : \mathbb{R}^N \rightarrow \mathbb{R}^M \), we consider the sample cross correlation:

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r^K_{xy} = D_X^{-1/2} \left( \frac{1}{K-1} XY^\top \right) D_Y^{-1/2} \in \mathbb{R}^{N \times M}.
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[The \( K^{th} \) column of \( Y \) is \( Y_k = h(x^{a,k}) - \bar{y}^a \), where \( \bar{y}^a = \sum_{k=1}^K h(x^{a,k}) / K \)]
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\textit{Onward:} suppress the subscript \( xy \) (write \( r_{xy}^K \) as \( r^K \); \( \hat{r} = \lim_{K \to \infty} r^K \)).
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- We seek to find a linear map $\mathcal{L}$ such that for every pair $(i,j)$, $\mathcal{L}(\cdot, i, j)$ takes the sample correlations $r^K(\cdot, y_j)$ to the limiting correlation $\hat{r}(x_i, y_j)$.
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Inspired by Anderson (2012), we formulate:

\[
\min_{\mathcal{L}(\cdot,i,j)} \int_{[-1,1] \times [-1,1]} (r^K(\cdot,y_j)^\top \mathcal{L}(\cdot,i,j) - \hat{r}(x_i,y_j))^2 p(r^K | \hat{r}) p(\hat{r}) dr^K d\hat{r}.
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- In practice, can use any reliable correlation statistics $r^L$ to approximate the limiting correlation $\hat{r}$, so that $r^L \sim p(\hat{r})$. (e.g. EnKF with large ensemble $L$).
Learning the map $\mathcal{L}$

1. **Train offline**: Generate an OSSE assimilation analysis ensemble $\{x_{t}^{a,k}\}^{T,L}_{t,k=1}$ with $L \gg 1$ and $T$ assimilation cycles.
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or $\text{LSP} : \min_{\parallel u \parallel_1} \parallel Au - b \parallel_1^2$ when $u = (A^T A)^{-1} A^T b$.
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4. Monte Carlo approximation to the minimization problem:

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- Offline training, little computational overhead, almost no tuning ($K$, $T$, $L$).
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- Offline training, little computational overhead, almost no tuning $(K, T, L)$.
- $\mathcal{L}$ is a scalar: the map found can be viewed as a type of data-driven localization function ($\mathcal{L}_{d}$).
Serial EnKF with transformed correlations
Adapted serial LLS EnKF (Anderson, 2013)

LLS EnKF assimilates observations \( j = 1, \ldots, M \) one at a time:

\[
\begin{align*}
1 & \text{ for } j = 1 \text{ to } M \text{ do } \quad /* \text{ Loop over observations */} \\
2 & \quad y_j^a = y_j^b + (P_{y_j y_j} + R_{jj})^{-1} P_{y_j y_j} (y_j^o - y_j^b) ; \\
3 & \quad y_j^{a,k} = y_j^a + \sqrt{\frac{R_{jj}}{R_{jj} + P_{y_j y_j}}} (y_j^{b,k} - y_j^b) ; \\
4 & \quad \Delta y_j^k = y_j^{a,k} - y_j^{b,k} ; \quad /* \text{ compute the obs update */} \\
5 & \quad x_j^{a,k} = x_j^{b,k} + \frac{P_{x y_j}}{P_{y_j y_j}} \Delta y_j^k ; \quad /* \text{ regresses the update onto } x */
\end{align*}
\]

The straightforward modification is to replace in line 5:

\[
P_{x y_j}^b = D_X^{1/2} r(\cdot, y_j) D_Y^{1/2} \quad \leftarrow \quad D_X^{1/2} \mathcal{L}(\cdot, \cdot, j)^\top r(\cdot, y_j) D_Y^{1/2} ,
\]

where \( D_X \), \( D_Y \) and \( r \) are estimated from the EnKF with ensemble size \( K \).
Numerical experiments on the Lorenz-96 model
**Linear direct observations**

Maps $\mathcal{L}$ and $\mathcal{L}_d$ found by regressing onto ETKF L500

$N = 40$ state variables, 10 (top) and 40 (bottom) observations
observation time steps 1 (left) and 10 (right)

(a) 5 ensemble members. 
(b) 40 ensemble members.

Localized structure of the mappings; $\mathcal{L}_d$ (dashed black) is an envelope for the mappings $\mathcal{L}$. 
Linear direct observations
Filtering results with adapted LLS EnKF + covariance inflation

(c) $\mathcal{L}$.  
(d) $\mathcal{L}_d$.

Time mean RMSE normalized by the RMSE of the ETKF using 500 ensemble members shown for the serial EnKF using $\mathcal{L}$ and $\mathcal{L}_d$, plotted against inflation factor and $K$. 
Linear direct observations
Filtering results – Best tuned inflation values

10 observations, observation time step $n = 1$, comparison of 3 localization methods

Time mean of RMSE (left) and spread (right) as a function of ensemble size

$GC$ is more performant for $K > 10$ but is extensively tuned!
Linear direct observations
Regression using different products

20 observations, observation time step $n = 1$, all use best tuned inflation values

Two choices of regression products: (1) ETKF with 500 ensemble members and (2) serial EnKF with GC localization with optimal half-width.
Linear indirect observations
Maps $\mathcal{L}$ and $\mathcal{L}_d$ found by regressing onto ETKF L500

20 observations, 5 ensemble members
Linear indirect observations
Filtering results with localization and best tuned inflation values

20 observations, observation time step $n = 5$

Time mean of RMSE (left) and spread (right)
Summary

- A data-driven method for improving the correlation estimation in serial ensemble Kalman filter is introduced.
- The method finds a linear map that transforms, at each assimilation cycle, the poorly estimated sample correlation into a sample of improved correlation.
- This map is obtained from an offline training procedure with almost no tuning as the solution of a linear regression problem that uses appropriate sample correlation statistics obtained from historical data assimilation product.
- In numerical tests with the Lorenz-96 model for ranges of cases of linear and nonlinear observation models, the proposed scheme improves the filter estimates, especially when ensemble size is small relative to the dimension of the state space.