A generalised and fully Bayesian framework for ensemble updating

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Abstract
We propose a generalised framework for the updating of a prior ensemble to a posterior ensemble, an essential yet challenging part in ensemble-based filtering methods. The proposed framework is based on a generalised and fully Bayesian view on the traditional ensemble Kalman filter (EnKF). In the EnKF, the updating of the ensemble is based on Gaussian assumptions, whereas in our general setup the updating may be based on another parametric family. In addition, we propose to formulate an optimality criterion and to find the optimal update with respect to this criterion. The framework is fully Bayesian in the sense that the parameters of the assumed forecast model are treated as random variables. As a consequence, a parameter vector is simulated, for each ensemble member, prior to the updating. In contrast to existing fully Bayesian approaches, where the parameters are simulated conditionally on all the forecast samples, the parameters are in our framework simulated conditionally on both the data and all the forecast samples, except the forecast sample which is to be updated. The proposed framework is studied in detail for two parametric families. The first is for continuous variables, for which we use the family of linear-Gaussian models and the optimality criterion is to minimise the expected Mahalanobis distance between corresponding prior and posterior ensemble members. For this situation, we find that the optimal filter is a particular square root filter. The second parametric family we study is the finite state-space hidden Markov model, where the optimality criterion is to maximise the expected number of elements in corresponding prior and posterior state vectors that are equal. For both cases, we present simulation examples and compare the results with existing ensemble-based filtering methods. The results of the proposed approach indicate a promising performance. In particular, the filter based on the linear-Gaussian model gives a more realistic representation of the uncertainty than the traditional EnKF, and the effect of not conditioning on the forecast sample which is to be updated when simulating the parameters is remarkable.

Keywords: Bayesian updating; ensemble Kalman filter; linear-Gaussian model; Markov chains; square root filter; update step

1 Introduction
The ensemble Kalman filter (EnKF) [Burgers et al. 1998; Evensen 2003] is a recursive Monte Carlo algorithm which provides an approximate solution to the filtering problem in statistics. The EnKF has been successfully applied to problems in several scientific fields, including reservoir modelling, oceanography and weather forecasting. Although the filter relies on a linear-Gaussian assumption about the underlying state-space model, it has shown to work well even in non-linear, non-Gaussian situations, and it also scales well to problems with very high-dimensional state vectors. The literature on the EnKF is extensive, and several modifications of the original algorithm of [Evensen 1994] have been proposed and studied.
Much of the literature is quite geophysical-oriented with limited focus on the statistical foundations of the methodology. In recent years, however, the EnKF has gained increasing attention also from statisticians, see for instance Katzfuss et al. (2016). In the current report, we take a Bayesian perspective on the EnKF and use it to formulate a new and general class of ensemble filtering methods which also includes filtering of categorical variables.

The EnKF alternates between a forecast step and an update step. The main challenge, and the focus of this report, is the update step. The goal of the update step is to condition an ensemble of (approximate) realisations from a prior, or so-called forecast, distribution on new observations so that a new ensemble of (approximate) realisations from the corresponding posterior, or so-called filtering, distribution is obtained. What causes trouble is that the forecast and filtering distributions are generally intractable. To cope with this issue, the EnKF introduces Gaussian approximations and updates the forecast samples in the form of a linear shift closely related to the linear update of the mean in the traditional Kalman filter (Kalman, 1960). Since the resulting filtering ensemble is obtained from a linear shift of a possibly non-Gaussian forecast ensemble, non-Gaussian properties may have been captured.

An important feature about the linear update of the EnKF is that it implicitly involves the construction of a Gaussian approximation to the forecast distribution. In practice, only a covariance matrix is estimated. Combined with the assumption that the likelihood model is linear-Gaussian, the Gaussian approximation to the forecast distribution yields a Gaussian approximation to the filtering distribution according to Bayes’ rule. Under the assumption that the forecast ensemble contains independent samples from the Gaussian approximation to the forecast model, the linear shift corresponds to conditional simulation from a Gaussian distribution with mean and covariance so that each updated sample marginally is distributed according to the Gaussian approximation to the filtering distribution. Loe and Tjelmeland (2021) present a generalisation of these underlying features of the EnKF and formulate a general class of ensemble updating procedures. The overall idea behind the framework they propose is that more generally another parametric model than the Gaussian can be pursued for the approximation to the forecast distribution. Likewise, another parametric model than the linear-Gaussian can be pursued for the likelihood model. From Bayes’ rule, a corresponding approximation to the filtering distribution follows. To update the prior samples, the authors propose to simulate samples from a distribution conditional on the forecast ensemble such that, given that the forecast samples are distributed according to the constructed approximation to the forecast distribution, the updated samples are distributed according to the corresponding approximation to the filtering distribution, which corresponds to the property of the EnKF linear update.

The traditional EnKF algorithm is known to have a tendency to underestimate the variances in the forecast and filtering distributions, and the filter may in some cases even diverge. Various modifications have been proposed to correct for these issues, e.g. localisation (Houtekammer and Mitchell, 2001; Hamill and Whitaker, 2001; Ott et al., 2004) and inflation (Anderson and Anderson, 1999). One possible reason for the unstable behaviour of the EnKF is that uncertainty about the covariance matrix which is estimated from the forecast samples is not taken into account. That is, prior to the ensemble update, the covariance matrix of the Gaussian forecast approximation is estimated from the forecast ensemble, and thereafter the linear update proceeds as if this estimated covariance matrix were correct, which obviously is not really the case even in a true linear-Gaussian situation. Myrseth and Omre (2010) address this issue and propose a Bayesian hierarchical EnKF (HEnKF) algorithm where the mean and the covariance of the Gaussian forecast approximation are treated as random variables with prior distributions selected from the Gaussian conjugate family. Prior to the linear updating of the ensemble, the covariance matrix is then simulated rather than estimated. Myrseth and Omre (2010) present simulation examples where their proposed HEnKF algorithm provides more reliable results than the traditional EnKF and reduces the undesirable effect of underestimating the variance. An improved version of the HEnKF algorithm is presented by Tsyrulnikov and Rakitko (2017). Other strategies for incorporating parameter uncertainty in the EnKF are proposed by Stroud et al. (2018) and Katzfuss et al. (2020). All studies indicate that it is advantageous to take parameter uncertainty into account.
In the present report, we propose a fully Bayesian version of the framework proposed in Loe and Tjelmeland (2021). The framework is fully Bayesian in the sense that the model parameters of the assumed forecast distribution are treated as random variables. While the framework of Loe and Tjelmeland (2021) can be seen as a generalisation of the traditional EnKF, the framework proposed in the present report can be seen as a generalisation of the HEnKF of Myrseth and Omre (2010), with one important modification.

In Myrseth and Omre (2010), a covariance matrix is simulated for each ensemble member by simulating from the distribution of the covariance matrix given all the forecast samples. In a more general context, if we denote the parameters of the forecast model by $\theta$ and the forecast samples by $x^{(1)}, \ldots, x^{(M)}$, where $M$ is the ensemble size, this would translate to simulating, for each ensemble member, a parameter vector $\theta^{(i)}$ from the distribution of $\theta$ given $x^{(1)}, \ldots, x^{(M)}$. In the present report, however, we propose to adopt a Bayesian model for the update from which it follows that also the incoming observation, say $y$, must be included in the conditioning, whilst the forecast sample $x^{(i)}$ to be updated must be excluded. In other words, prior to the updating of $x^{(i)}$, we propose in this report to simulate a parameter $\theta^{(i)}$ conditionally on $y$ and $x^{(1)}, \ldots, x^{(i-1)}, x^{(i+1)}, \ldots, x^{(M)}$. Similarly to Loe and Tjelmeland (2021), we investigate two particular applications of the proposed framework: firstly, the case where the chosen forecast and likelihood approximations constitute a linear-Gaussian model, which corresponds to the model assumptions of the EnKF, and secondly, the case where the chosen forecast and likelihood approximations constitute a hidden Markov model (HMM) with categorical states. In contrast to Loe and Tjelmeland (2021), where the core focus is on the situation with the finite state-space HMM, this report also gives considerable focus to the linear-Gaussian model and the EnKF. In particular, we formulate a class of EnKF algorithms, in a fully Bayesian setting, of which the traditional EnKF and the square root EnKF (Tippett et al., 2003) represent special cases.

The remains of the report take the following outline. First, Section 2 provides some background material on state-space models and the EnKF. Next, our general ensemble updating framework is presented in Section 3. In Sections 4 and 5 we consider two applications of the proposed framework, namely the linear-Gaussian model and the finite state-space HMM, respectively. In Sections 6 and 7 we present simulation examples for the same two cases. Finally, we finish off in Section 8 with a few closing remarks.

2 Preliminaries

In this section, we describe state-space models and the related filtering problem in more detail. We also review the ensemble Kalman filter (EnKF).

2.1 State-space models

A general state-space model consists of a latent process, $\{x^t\}_{t=1}^T$, $x^t = (x^t_1, \ldots, x^t_n) \in \Omega_x$, and a corresponding observed process, $\{y^t\}_{t=1}^T$, $y^t = (y^t_1, \ldots, y^t_m) \in \Omega_y$, with one observation $y^t$ for each $x^t$. The latent $x^t$-process, usually called the state process, constitutes a first order Markov chain with initial distribution $p(x^1)$ and transition probabilities $p_{x^t|x^{t-1}}(x^t|x^{t-1})$, $t \geq 2$, so that the joint distribution of $x^{1:T} = (x^1, \ldots, x^T)$ can be written as

$$p_{x^{1:T}}(x^{1:T}) = p_{x^1}(x^1) \prod_{t=2}^T p_{x^t|x^{t-1}}(x^t|x^{t-1}).$$

The observations $\{y^t\}_{t=1}^T$ are assumed conditionally independent given $\{x^t\}_{t=1}^T$, with $y^t$ depending on $\{x^t\}_{t=1}^T$ only through $x^t$. Hence the joint likelihood for the observations $y^{1:T} = (y^1, \ldots, y^T)$ can be written as

$$p_{y^{1:T}|x^{1:T}}(y^{1:T}|x^{1:T}) = \prod_{t=1}^T p_{y^t|x^t}(y^t|x^t).$$
called filtering distribution, report, is the filtering problem. The objective of the filtering problem is, for each
term state-space model may refer to either a categorical or a continuous situation.

A graphical illustration of the general state-space model is shown in Figure 1. When the variables of
the series of filtering distributions can be computed recursively according to a two-step procedure as follows:

$$p_{x^t | y^{1:t-1}}(x^t | y^{1:t-1}) = \int_{\Omega_x} p_{x^t | x^{t-1}}(x^t | x^{t-1}) p_{x^{t-1} | y^{1:t-1}}(x^{t-1} | y^{1:t-1})dx^{t-1},$$  \hspace{1cm} (2.1)

$$p_{x^t | y^t}(x^t | y^t) = \int_{\Omega_x} p_{x^t | y^t-1}(x^t | y^t-1) p_{y^t | x^t}(y^t | x^t) \int_{\Omega_x} p_{x^t | y^t-1}(x^t | y^t-1) p_{y^t | x^t}(y^t | x^t)dx^t.$$  \hspace{1cm} (2.2)

The first step is called the prediction step and computes the forecast distribution $p_{x^t | y^{1:t-1}}(x^t | y^{1:t-1})$.
The second step is called the update step and uses Bayes’ rule to condition the forecast distribution
on the incoming observation $y^t$ to compute the filtering distribution $p_{x^t | y^t}(x^t | y^t)$. The update step
can be viewed as a standard Bayesian inference problem where $p_{x^t | y^{1:t-1}}(x^t | y^{1:t-1})$ represents the prior,
$p_{y^t | x^t}(y^t | x^t)$ the likelihood, and $p_{x^t | y^t}(x^t | y^t)$ the posterior. For this reason, the terms prior and forecast,
and the terms posterior and filtering, are used interchangeably in this report.

A graphical illustration of a general state-space model.

Figure 1: Graphical illustration of a general state-space model.

Although conceptually simple, the filtering recursions in Eqs. (2.1) and (2.2) are generally intractable
because we are unable to evaluate the integrals. Approximate solutions therefore become necessary. The
most common approach is the class of simulation-based methods, or ensemble methods, where a set of
samples, typically called an ensemble, is used to empirically represent the series of prediction and filtering
distributions. Starting from an initial ensemble of independent realisations from the initial model $p_{x^1}(x^1)$,
the idea is to advance the ensemble forward in time according to the state-space model dynamics. Similarly
to the recursions in Eqs. (2.1) and (2.2), ensemble methods alternate between a forecast step and an
update step. Assuming at time $t$ that an ensemble $\{x^{t-1,1}, \ldots, x^{t-1,M}\}$ of $M$ independent realisations
from the previous filtering distribution $p_{x^t | y^{1:t-1}}(x^t | y^{1:t-1})$ is available, the forecast step is carried out
by simulating $x^{t,1}, x^{t-1,1} \sim p_{x^t | x^{t-1}}(x^t | x^{t-1})$ independently for each $i$. This yields a forecast ensemble,
$\{x^{t,1}, \ldots, x^{t,M}\}$, with independent realisations from the forecast distribution $p_{x^t | y^{1:t-1}}(x^t | y^{1:t-1})$.

Typically in practical applications, we are able to simulate from $p_{x^t | x^{t-1}}(x^t | x^{t-1})$, but often to a high
computational cost, which restricts the ensemble size $M$ to be small. After the forecast step, the forecast
ensemble needs to be updated taking the new observation $y^t$ into account, in order to obtain a new filtering
ensemble, $\{x^{t,1}, \ldots, x^{t,M}\}$, with independent realisations from the filtering distribution $p_{x^t | y^t}(x^t | y^t)$
at time $t$. However, in contrast to the prediction step, there is no straightforward way to proceed with
this updating. Therefore, ensemble filtering methods require approximations in the update step. In the
present report, we propose one such approximate updating method.

There exist two main classes of ensemble filtering methods: particle filters (Doucet et al., 2001) and
ensemble Kalman filters (EnKFs). Hybrid versions of these filters have also been proposed (e.g., Frei and
[Künsch 2012, 2013]. In this report, we focus on the EnKF, and a brief review of the EnKF follows in the next section.

2.2 The ensemble Kalman filter

The EnKF is an ensemble filtering method which relies on Gaussian approximations in the update step. The filter was first introduced in Evensen (1994) and several modifications of the algorithm have been presented in the literature since then. The variety of EnKF methods can be classified into two main categories, stochastic filters and deterministic filters, differing in whether the updating of the ensemble is carried out in a stochastic or deterministic manner. Deterministic filters are also known as square root filters, and this is the term we use in this report.

To understand the EnKF, consider first a linear-Gaussian model where \( x \sim N(x; \mu, Q) \) and \( y \mid x \sim N(y; Hx, R) \), \( \mu \in \mathbb{R}^n \), \( Q \in \mathbb{R}^{n \times n} \), \( H \in \mathbb{R}^{m \times n} \), and \( R \in \mathbb{R}^{m \times m} \). The posterior model corresponding to this linear-Gaussian model is a Gaussian, \( N(x^*; Q^*) \), with mean \( \mu^* \in \mathbb{R}^n \) and covariance matrix \( Q^* \in \mathbb{R}^{n \times n} \) analytically available from the Kalman filter equations as

\[
\mu^* = \mu + K(y - H\mu)
\]

(2.3) and

\[
Q^* = (I_n - KH)Q
\]

(2.4) respectively, where \( I_n \in \mathbb{R}^{n \times n} \) is the n x n identity matrix and

\[
K = QH^\top \left( HQH^\top + R \right)^{-1}
\]

(2.5) is the so-called Kalman gain matrix, where we have introduced the notation \( A^\top \) to denote the transpose of a matrix \( A \). Now, suppose \( x \sim N(x; \mu, Q) \) and \( \epsilon \sim N(\epsilon; 0, R) \) are independent random samples, and consider the linear transformation

\[
\tilde{x} = x + K(y - Hx + \epsilon).
\]

(2.6) It is then a straightforward matter to show that \( \tilde{x} \mid y \) is distributed according to the Gaussian distribution \( N(x^*; Q^*) \) with mean \( \mu^* \) and covariance \( Q^* \) given by Eqs. (2.3) and (2.4), respectively (e.g., Burgers et al., 1998). This result is used in the EnKF.

At a given time step \( t \), the EnKF starts by making a linear-Gaussian assumption about the true (unknown) underlying model. Specifically, the forecast samples \( x^{t,(1)}, \ldots, x^{t,(M)} \) are assumed to be distributed according to a Gaussian distribution \( N(x^t; \mu^t, Q^t) \) where the parameters \( \mu^t \) and \( Q^t \) are set equal to the sample mean and the sample covariance of the forecast ensemble, and the likelihood model is assumed to be a Gaussian distribution with mean \( H^tx^t \) and covariance \( R^t \). Under the assumption that the assumed linear-Gaussian model is correct we have \( x^{t,(i)} \sim N(x^t; \mu^t, Q^t) \) for each \( i \), and the goal is to update \( x^{t,(i)} \) so that \( \tilde{x}^{t,(i)} \sim N(x^t; \mu^{t*}, Q^{t*}) \), where \( \mu^{t*} \) and \( Q^{t*} \) are given by Eqs. (2.3) and (2.4), respectively, with a superscript \( t \) included in the notations, i.e.

\[
\mu^{t*} = \mu^t + K^t(y^t - H^t\mu^t)
\]

(2.7) and

\[
Q^{t*} = (I_n - K^tH^t)Q^t
\]

(2.8) respectively, where \( K^t \) is given by Eq. (2.5), with a superscript \( t \) included, \( K^t = Q^t(H^t)^\top (H^tQ^t(H^t)^\top + R^t)^{-1} \). The stochastic EnKF and the square root EnKF obtain this result in different ways. The stochastic EnKF proceeds by simulating \( \epsilon^{t,(i)} \sim N(\epsilon^t; 0, R^t) \) for \( i = 1, \ldots, M \), and then exploits Eq. (2.6), which now takes
the form
\[ x^{\ell,(i)} = x^{\ell,(i)} + K^t(y^t - H^t x^{\ell,(i)} + \epsilon^t). \] (2.9)

The square root EnKF takes a different approach and instead performs a non-random linear transformation of \( x^{\ell,(i)} \),
\[ \tilde{x}^{\ell,(i)} = B^t(x^{\ell,(i)} - \mu^t) + \mu^t + K^t(y^t - H^t \mu^t), \] (2.10)
where \( B^t \in \mathbb{R}^{n \times n} \) is a solution to the quadratic matrix equation
\[ B^t Q^t (B^t)^\top = (I_n - K^t H^t) Q^t. \] (2.11)

If the underlying state-space model really is linear-Gaussian, the EnKF is consistent in the sense that the distribution of each updated sample converges to the true (Gaussian) filtering distribution as \( M \to \infty \). In all other cases, the update is biased. However, since the posterior ensemble is obtained from a linear shift of a possibly non-Gaussian prior ensemble, non-Gaussian properties of the true prior and posterior models can, to some extent, be captured.

3 A general and fully Bayesian ensemble updating framework

In this section, we formulate a general class of ensemble updating procedures. As described in previous sections, the goal is to update a given ensemble of prior realisations, \( \{x^{\ell,(1)}, \ldots, x^{\ell,(M)}\} \), to a corresponding ensemble of posterior realisations, \( \{\tilde{x}^{\ell,(1)}, \ldots, \tilde{x}^{\ell,(M)}\} \), taking the new observation \( y^t \) into account. To cope with this task, we propose to separately update each of the \( x^{\ell,(i)} \) samples in the prior ensemble to a corresponding \( \tilde{x}^{\ell,(i)} \) sample in the posterior ensemble, and to base the updating of \( \tilde{x}^{\ell,(i)} \) on an assumed Bayesian model. As mentioned previously in the report, the proposed framework can be viewed as a generalisation of the hierarchical EnKF algorithm of Myrseth and Omre (2010) with the modification that the parameters are simulated in a different manner. The key steps of the proposed updating framework are summarised in Algorithm 1.

Algorithm 1: General ensemble updating procedure

1. Select the assumed distributions \( f_0(\theta^t) \), \( f_{x^t|\theta^t}(x^t|\theta^t) \) and \( f_{y^t|x^t}(y^t|x^t) \) introduced in Section 3.1.
2. for \( i = 1, \ldots, M \) do
   a) Simulate \( \theta^{\ell,(i)}|x^{\ell,(i)}\), \( y^t \sim f_{\theta^t|x^{\ell,(i)},y^t}(\theta^t|x^{\ell,(i)},y^t) \) as described in Section 3.3.
   b) Construct the model \( q(\tilde{x}^{\ell,(i)}|x^{\ell,(i)},\theta^{\ell,(i)},y^t) \) specified in Sections 3.2 and 3.3.
   c) Simulate \( \tilde{x}^{\ell,(i)}|x^{\ell,(i)},\theta^{\ell,(i)},y^t \sim q(\tilde{x}^{\ell,(i)}|x^{\ell,(i)},\theta^{\ell,(i)},y^t) \)
end

3.1 Assumed Bayesian model

For the updating of the forecast sample \( x^{\ell,(i)} \) we adopt an assumed Bayesian model. A graphical illustration of this assumed Bayesian model is shown in Figure 2. The model includes an unknown parameter vector \( \theta^t \in \Omega_s \), and the forecast samples \( x^{\ell,(1)}, \ldots, x^{\ell,(M)} \) and the latent state vector \( x^t \) are assumed to be conditionally independent and identically distributed given \( \theta^t \). Moreover, the observation \( y^t \) is assumed to be conditionally independent of \( x^{\ell,(1)}, \ldots, x^{\ell,(M)} \) and \( \theta^t \) given \( x^t \), and the updated sample \( \tilde{x}^{\ell,(i)} \) is restricted to be conditionally independent of \( x^t \) and
\[ x^{\ell,(-i)} = \{x^{\ell,(1)}, \ldots, x^{\ell,(i-1)}, x^{\ell,(i+1)}, \ldots, x^{\ell,(M)}\} \].
given $x^{t,(i)}$, $\theta^i$ and $y^i$.  

To distinguish the assumed Bayesian model from the true and unknown underlying model, we use in the following the notation $f(\cdot)$ to denote distributions associated with the assumed Bayesian model, while, as in previous sections, $p(\cdot)$ is reserved for the truth. Under the assumed Bayesian model, the joint distribution of $\theta^i$, $x^i$, $x^{t,(1)}, \ldots, x^{t,(M)}$ and $y^i$ then reads 

$$f_{\theta^i,x^i,x^{t,(1)},\ldots,x^{t,(M)},y^i}(\theta^i, x^i, x^{t,(1)}, \ldots, x^{t,(M)}, y^i) = f_{\theta^i}(\theta^i) f_{x^i|\theta^i}(x^i|\theta^i) f_{x^{t,(i)}|x^i}(x^{t,(i)}|x^i) \prod_{t=1}^M f_{x^{t,(i)}|\theta^i}(x^{t,(i)}|\theta^i),$$

where $f_{\theta^i}(\theta^i)$ is an assumed prior model for $\theta^i$, $f_{x^i|\theta^i}(x^i|\theta^i)$ is an assumed prior model for $x^i|\theta^i$ and $f_{y^i|x^i}(y^i|x^i)$ is an assumed likelihood model. The prior $f_{x^{t,(i)}|\theta^i}(x^{t,(i)}|\theta^i)$ can be interpreted as an approximation to the intractable forecast model $p_{x^{t,(i)}|x^{t,-1}}(x^{t,(i)}|x^{t,-1})$. The model $f_{\theta^i}(\theta^i)$ for $\theta^i$ should be chosen as a conjugate prior for $f_{x^i|\theta^i}(x^i|\theta^i)$, while the models $f_{x^{t,(i)}|\theta^i}(x^{t,(i)}|\theta^i)$ and $f_{y^i|x^i}(y^i|x^i)$ must be chosen so that the corresponding posterior model 

$$f_{x^i|\theta^i, y^i}(x^i|\theta^i, y^i) \propto f_{x^i|\theta^i}(x^i|\theta^i) f_{y^i|x^i}(y^i|x^i)$$

is tractable.

### 3.2 Class of updating distributions

Under the assumption that the assumed Bayesian model introduced above is correct, a naïve updating procedure is to sample $\tilde{x}^{t,(i)}$ from $f_{\tilde{x}^{t,(i)}|x^{t,(1)},\ldots,x^{t,(M)},y^i}(\tilde{x}^{t,(i)}|x^{t,(1)},\ldots,x^{t,(M)},y^i)$. However, this procedure may be very sensitive to the assumptions of the assumed Bayesian model. To get an updating procedure which is more robust against the assumptions of the assumed model, a better approach is to generate $\tilde{x}^{t,(i)}$ as a modified version of $x^{t,(i)}$ and require 

$$f_{\tilde{x}^{t,(i)}|x^{t,\cdot}, y^i}(x^{t,\cdot}|x^{t,\cdot}, y^i) = f_{x^{t,\cdot}|x^{t,\cdot}, y^i}(x^{t,\cdot}|x^{t,\cdot}, y^i).$$

This way, we use the randomness in $x^{t,(i)}$ to generate randomness in $\tilde{x}^{t,(i)}$. The forecast sample $x^{t,(i)}$ is therefore not included in the conditioning in Eq. (3.1). To generate $\tilde{x}^{t,(i)}$ as a modified version of $x^{t,(i)}$ under this restriction, we introduce a distribution $q(\tilde{x}^{t,(i)}|x^{t,(i)}, \theta^i, y^i)$ which fulfills Eq. (3.1), and simulate $\tilde{x}^{t,(i)}|x^{t,(i)}, \theta^i, y^i \sim q(\tilde{x}^{t,(i)}|x^{t,(i)}, \theta^i, y^i)$. To construct such a $q(\tilde{x}^{t,(i)}|x^{t,(i)}, \theta^i, y^i)$, we first note that the constraint in Eq. (3.1) can be rewritten as 

$$\int_{\Theta_\theta} f_{\theta^i, x^{t,(i)}, y^i}(\theta^i, x^{t,\cdot}|x^{t,\cdot}, y^i) d\theta^i = \int_{\Theta_\theta} f_{\theta^i, x^{t,(i)}, y^i}(\theta^i, x^{t,\cdot}|x^{t,\cdot}, y^i) d\theta^i.$$
Using that both \( x^t \) and \( \tilde{x}^{t, (i)} \) are conditionally independent of \( x^{t, -i} \) given \( \theta^t \) and \( y^t \), this can be rewritten as
\[
\int_{\Omega_0} f_{\theta^t|x^{t, -i}, y^t}(\theta^t|x^{t, -i}, y^t) f_{x^{t, (i)}|y^t, \theta^t}(x^t|y^t, \theta^t) d\theta^t = \int_{\Omega_0} f_{\theta^t|x^{t, -i}, y^t}(\theta^t|x^{t, -i}, y^t) f_{x^{t, (i)}|y^t, \theta^t}(x^t|y^t, \theta^t) d\theta^t.
\]
(3.2)

A sufficient condition for this restriction to hold is
\[
f_{x^{t, (i)}|\theta^t, y^t}(x^t|\theta^t, y^t) = f_{x^{t, (i)}|\theta^t, y^t}(x^t|\theta^t, y^t)
\]
for all \( x^t, \theta^t \), and \( y^t \). Thereby, if for a given \( \theta^t \) we can manage to construct a \( q(\tilde{x}^{t, (i)}|x^{t, (i)}, \theta^t, y^t) \) consistent with Eq. (3.3), we can update \( x^{t, (i)} \) by first simulating \( \tilde{x}^{t, (i)} \sim f_{\theta^t|x^{t, -i}, y^t}(\theta^t|x^{t, -i}, y^t) \) and thereafter simulate \( \tilde{x}^{t, (i)}|x^{t, (i)}, \tilde{x}^{t, (i)} \sim q(\tilde{x}^{t, (i)}|x^{t, (i)}, \theta^t, y^t) \). How to simulate \( \tilde{x}^{t, (i)}|x^{t, -i}, y^t \) is discussed in Section 3.4. To construct a \( q(\tilde{x}^{t, (i)}|x^{t, (i)}, \theta^t, y^t) \) consistent with Eq. (3.3) we note that for \( f_{x^{t, (i)}|\theta^t, y^t}(x^t|\theta^t, y^t) \) in Eq. (3.3) we have
\[
f_{x^{t, (i)}|\theta^t, y^t}(\tilde{x}^{t, (i)}|\theta^t, y^t) = \int_{\Omega_0} f_{x^{t, (i)}|\theta^t, y^t}(x^t|\theta^t, y^t) q(\tilde{x}^{t, (i)}|x^t, \theta^t, y^t) dx^t.
\]
Thereby, from Eq. (3.3), it follows that \( q(\tilde{x}^{t, (i)}|x^{t, (i)}, \theta^t, y^t) \) must fulfil
\[
f_{x^{t, (i)}|\theta^t, y^t}(\tilde{x}^{t, (i)}|\theta^t, y^t) = \int_{\Omega_0} f_{x^{t, (i)}|\theta^t, y^t}(x^t|\theta^t, y^t) q(\tilde{x}^{t, (i)}|x^t, \theta^t, y^t) dx^t
\]
for all \( \tilde{x}^{t, (i)}, \theta^t \) and \( y^t \).

The criterion in Eq. (3.4) defines a class of updating distributions in the sense that there may be infinitely many solutions \( q(\tilde{x}^{t, (i)}|x^{t, (i)}, \theta^t, y^t) \) which fulfill Eq. (3.4). It should be noted that if the assumed model is correct it does not matter which \( q(\tilde{x}^{t, (i)}|x^{t, (i)}, \theta^t, y^t) \) within this class we choose; the distribution of \( \tilde{x}^{t, (i)}|x^{t, -i}, y^t \) then equals \( f_{x^{t, (i)}|\theta^t, y^t}(x^t|x^{t, -i}, y^t) \) regardless. Generally, however, the assumed model is wrong, and the choice of \( q(\tilde{x}^{t, (i)}|x^{t, -i}, \theta^t, y^t) \) can have a substantial effect on the actual distribution of \( \tilde{x}^{t, (i)}|x^{t, -i}, y^t \). The simplest solution is to set \( q(\tilde{x}^{t, (i)}|x^{t, -i}, \theta^t, y^t) \) equal to \( f_{x^{t, (i)}|\theta^t, y^t}(x^t|\theta^t, y^t) \) which entails that we simulate \( \tilde{x}^{t, (i)} \) independently of \( x^{t, (i)} \). However, this naive approach is very sensitive to the assumptions of the assumed model and is not a good way to proceed as we lose a lot of valuable information from \( x^{t, (i)} \) about the true (unknown) model that we may not have been able to capture with the assumed model. As discussed above, we want to generate \( \tilde{x}^{t, (i)} \) as a modified version of \( x^{t, (i)} \). That way, we retain more information from \( x^{t, (i)} \) about the true model. An optimal solution \( q(\tilde{x}^{t, (i)}|x^{t, (i)}, \theta^t, y^t) \) within the class of distributions can be found if an optimality criterion is specified, which we discuss in the next section.

### 3.3 Optimality criterion

Generally, an optimal solution, denoted \( q^*(\tilde{x}^{t, (i)}|x^{t, (i)}, \theta^t, y^t) \), within the class of distributions defined in the previous section can for example be defined as the solution which minimises the expected value of some function \( g(x^{t, (i)}, \tilde{x}^{t, (i)}) \),
\[
q^*(\tilde{x}^{t, (i)}|x^{t, (i)}, \theta^t, y^t) = \arg\min_{q(i)} \mathbb{E} \left[ g(x^{t, (i)}, \tilde{x}^{t, (i)}) \right],
\]
where the expectation is taken over the distribution \( f_{x^{t, (i)}|\theta^t, y^t}(x^t|\theta^t, y^t) \), i.e. the joint distribution of \( x^{t, (i)} \) and \( \tilde{x}^{t, (i)} \) given \( \theta^t, y^t \). In the present report, we propose to choose the function \( g(x^{t, (i)}, \tilde{x}^{t, (i)}) \) as the Mahalanobis distance between \( x^{t, (i)} \) and \( \tilde{x}^{t, (i)} \),
\[
g(x^{t, (i)}, \tilde{x}^{t, (i)}) = \left( x^{t, (i)} - \tilde{x}^{t, (i)} \right)^\top \Sigma^{-1} \left( x^{t, (i)} - \tilde{x}^{t, (i)} \right),
\]
(3.5)
where \( \Sigma \in \mathbb{R}^{n \times n} \) is some positive definite matrix. If \( \Sigma \) equals the identity matrix, \( g(x^{t,(i)}, \tilde{x}^{t,(i)}) \) reduces to the squared Euclidean distance between \( x^{t,(i)} \) and \( \tilde{x}^{t,(i)} \),

\[
g(x^{t,(i)}, \tilde{x}^{t,(i)}) = \sum_{j=1}^{n} (x^{t,(i)}_j - \tilde{x}^{t,(i)}_j)^2.
\]

(3.6)

Basically, the optimality criterion then states that we want to make minimal changes to each prior sample \( x^{t,(i)} \). To us, this seems like a reasonable criterion since we want to capture as much information from \( x^{t,(i)} \) as possible. Of course, one must value the information that comes with the observation \( y' \), but there is no reason to make more changes to \( x^{t,(i)} \) than necessary.

If \( x' \) is a vector of categorical variables, \( x'_j \in \{0, 1, \ldots, K-1\} \), an alternative is to select \( g(x^{t,(i)}, \tilde{x}^{t,(i)}) \) as the number of corresponding elements of \( x^{t,(i)} \) and \( \tilde{x}^{t,(i)} \) that are different,

\[
g(x^{t,(i)}, \tilde{x}^{t,(i)}) = \sum_{j=1}^{n} 1(x^{t,(i)}_j \neq \tilde{x}^{t,(i)}_j),
\]

(3.7)

where \( 1(\cdot) \) denotes the usual indicator function. If each component \( x'_j \) is binary, the functions in Eqs. (3.6) and (3.7) are equal.

### 3.4 Parameter simulation

In this section, we describe how to simulate \( \theta^{t,(i)} | x^{t,(i)}, y' \sim f_{\theta|x,y}(\theta | x^{t,(i)}, y') \) when \( f_{\theta|x}(\theta) \) is chosen as a conjugate prior for \( f_{\theta|x,y}(\theta | x^{t,(i)}, y') \).

Specifically, we can then introduce \( x' \) as an auxiliary variable and simulate \( (x', \theta') \) from the joint distribution

\[
f_{x', \theta|x^{t,(i)}, y'}(x', \theta' | x^{t,(i)}, y') \propto f_{\theta|x,y}(\theta | x^{t,(i)}, y') f_{x'| \theta, x^{t,(i)}}(x' | \theta) f_{y'| x, x^{t,(i)}}(y' | x^{t,(i)}) \prod_{j \neq i} f_{\theta|x,y}(x^{t,(j)} | \theta)
\]

by constructing a Gibbs sampler which alternates between drawing \( x' \) from the full conditional distribution \( f_{x'| \theta, x^{t,(i)}}(x' | \theta') \) and \( \theta' \) from the full conditional distribution \( f_{\theta|x,y}(\theta' | x^{t}, x^{t,(i)}, y') \).

Using that \( x^{t} \) and \( x^{t,(i)} \) are conditionally independent given \( \theta' \) (see Figure 2), it follows that the full conditional distribution \( f_{x'| \theta, x^{t,(i)}}(x' | \theta, x^{t,(i)}, y') \) is given as

\[
f_{x'| x^{t,(i)}, y'}(x' | \theta', x^{t,(i)}, y') = f_{x'| \theta, x^{t,(i)}}(x' | \theta', y')
\]

Simulating from \( f_{x'| \theta, x^{t,(i)}}(x' | \theta', y') \) should be achievable, since \( f_{x'| \theta, x^{t,(i)}}(x' | \theta', y') \) and \( y'_i \) are chosen so that \( f_{x'| \theta, x^{t,(i)}}(x' | \theta', y') \) is tractable. Using that \( \theta' \) and \( y' \) are conditionally independent given \( x' \), the other full conditional distribution, \( f_{\theta|x, x^{t,(i)}, y'}(\theta | x', x^{t,(i)}, y') \), is given as

\[
f_{\theta|x, x^{t,(i)}, y'}(\theta | x', x^{t,(i)}, y') = f_{\theta|x, x^{t,(i)}, y'}(\theta | x', x^{t,(i)}, y')
\]

Since \( f_{\theta|x,y}(\theta | x^{t,(i)}, y') \) is chosen as a conjugate prior for \( f_{x'| \theta, x^{t,(i)}}(x' | \theta', y') \), and since \( x^{t}, x^{t,(1)}, \ldots, x^{t,(M)} \) are independent and identically distributed given \( \theta' \), it follows that \( f_{\theta|x, x^{t,(i)}, y'}(\theta | x', x^{t,(i)}, y') \) is tractable and belongs to the same family of distributions as \( f_{\theta|x,y}(\theta | x', x^{t,(i)}, y') \).

### 4 Application 1: Linear-Gaussian assumed model

In this section, we consider how the updating procedure described in Section 3 can be applied when the elements of the state vector \( x' \) are continuous variables. Specifically, we then propose to let the distributions \( f_{x'| \theta}(x' | \theta) \) and \( f_{y'| x}(y' | x) \) of the assumed Bayesian model constitute a linear-Gaussian model. As we shall see, the resulting optimal updating procedure then corresponds to a fully Bayesian version of a square root EnKF.
4.1 Specification of the assumed model

Suppose \( x^t = (x_1^t, \ldots, x_n^t) \in \mathbb{R}^n \) and \( y^t = (y_1^t, \ldots, y_m^t) \in \mathbb{R}^m \). Let \( \theta^t = (\mu^t, Q^t) \) where \( \mu^t \in \mathbb{R}^n \), \( Q^t \in \mathbb{R}^{n \times n} \), and \( Q^t \) is positive definite. Select \( f_{x^t|y^t}(x^t|\theta^t) \) as a Gaussian distribution with mean vector \( \mu^t \) and covariance matrix \( Q^t \),

\[
f_{x^t|y^t}(x^t|\theta^t) = N(x^t; \mu^t, Q^t),
\]

and choose \( f_{y^t|x^t}(y^t|x^t) \) as a Gaussian distribution with mean \( H^t x^t \), \( H^t \in \mathbb{R}^{m \times n} \) and covariance matrix \( R^t \in \mathbb{R}^{m \times m} \),

\[
f_{y^t|x^t}(y^t|x^t) = N(y^t; H^t x^t, R^t).
\]

Given \( \theta^t \), this model corresponds to the linear-Gaussian model introduced in Section 2.2. The corresponding posterior model \( f_{x^t|\theta^t, y^t}(x^t|\theta^t, y^t) \) is then a Gaussian distribution with mean vector \( \mu^* \) and covariance matrix \( Q^* \) given by Eqs. (2.7) and (2.8), respectively. Following Section 3, we adopt a conjugate prior for \( \theta^t \), where the posterior sample \( \tilde{\theta}^t \) is distributed according to a Gaussian distribution with mean \( \mu^* \) and covariance matrix \( S^* \),

\[
f_{\theta^t}(\tilde{\theta}^t) = \mathcal{N}(\tilde{\theta}^t; \mu^*, S^*),
\]

and a Gaussian distribution for \( \mu^t|Q^t \),

\[
f_{\mu^t|Q^t}(\mu^t) = \mathcal{N}(\mu^t; \mu_0, \kappa^{-1} Q^t),
\]

where \( \nu, \kappa \in \mathbb{R} \), \( \mu_0 \in \mathbb{R}^n \) and \( V \in \mathbb{R}^{n \times n} \) are known hyperparameters.

4.2 Derivation of the class of updating distributions

The restriction in Eq. (3.3) now entails that the updating distribution \( q(\tilde{x}^{t,(i)}|x^{t,(i)}, \theta^t, y^t) \) must be chosen so that the integral on the right hand side of Eq. (3.4) returns a Gaussian distribution with mean vector equal to \( \mu^* \) in Eq. \( \ref{eq:2.7} \) and covariance matrix equal to \( Q^* \) in Eq. \( \ref{eq:2.8} \). To obtain this, we start by selecting \( q(\tilde{x}^{t,(i)}|x^{t,(i)}, \theta^t, y^t) \) as a Gaussian distribution with mean vector \( B^t x^{t,(i)} + C^t y^t + d^t \) and covariance matrix \( S^t \),

\[
q(\tilde{x}^{t,(i)}|x^{t,(i)}, \theta^t, y^t) = \mathcal{N}(\tilde{x}^{t,(i)}; B^t x^{t,(i)} + C^t y^t + d^t, S^t),
\]

where \( B^t \in \mathbb{R}^{n \times n} \), \( C^t \in \mathbb{R}^{n \times m} \), \( d^t \in \mathbb{R}^n \) and \( S^t \in \mathbb{R}^{n \times n} \) are quantities that we need to decide so that Eq. (3.4) is fulfilled. The \( B^t \), \( C^t \), \( d^t \) and \( S^t \) can all be functions of \( \theta^t \) and \( y^t \). From Eq. \( \ref{eq:3.3} \), it follows that the posterior sample \( \tilde{x}^{t,(i)} \) can be obtained as a linear shift of \( x^{t,(i)} \) plus a zero-mean Gaussian noise term \( \tilde{\epsilon}^{t,(i)} \sim \mathcal{N}(0; S^t) \),

\[
\tilde{x}^{t,(i)} = B^t x^{t,(i)} + C^t y^t + d^t + \tilde{\epsilon}^{t,(i)}.
\]

Using that \( x^{t,(i)} \) in a similar fashion can be obtained as \( x^{t,(i)} = \mu^t + \omega^{t,(i)} \), where \( \omega^{t,(i)} \sim \mathcal{N}(\omega^t; 0, Q^t) \), we can rewrite Eq. (4.1) as

\[
x^{t,(i)} = B^t \mu^t + C^t y^t + d^t + B^t \omega^{t,(i)} + \tilde{\epsilon}^{t,(i)}.
\]

Given \( (\theta^t, y^t) \), the stochastic components on the right hand side of this equation are \( \omega^{t,(i)} \) and \( \tilde{\epsilon}^{t,(i)} \) which are independent and Gaussian. Thereby, since \( \tilde{x}^{t,(i)} \) is a linear combination of \( \omega^{t,(i)} \) and \( \tilde{\epsilon}^{t,(i)} \), we find that \( \tilde{x}^{t,(i)} \) given \( (\theta^t, y^t) \) is distributed according to a Gaussian distribution \( \mathcal{N}(\tilde{x}^{t,(i)}; \mu^t, \tilde{Q}^i) \) with mean vector \( \tilde{\mu}^i \) and covariance matrix \( \tilde{Q}^i \) respectively given as

\[
\tilde{\mu}^i = B^t \mu^t + C^t y^t + d^t
\]

and

\[
\tilde{Q}^i = B^t Q^t (B^t)^\top + S^t.
\]

The requirement in Eq. \( \ref{eq:3.3} \) now states that the mean vector \( \tilde{\mu}^i \) in Eq. (4.5) must be equal to \( \mu^* \) in
Eq. (2.7) and the covariance matrix $\tilde{Q}^t$ in Eq. (4.6) must be equal to $Q^{*t}$ in Eq. (2.8). That is, we must have
\begin{equation}
B^t\mu^t + C^ty^t + d^t = \mu^t + K^t(y^t - H^t\mu^t)
\end{equation}
(4.7)
and
\begin{equation}
B^tQ^t(B^t)^\top + S^t = (I_n - K^tH^t)Q^t.
\end{equation}
(4.8)
Solving Eq. (4.7) with respect to $C^ty^t + d^t$ and inserting the result into Eq. (4.4), we obtain
\begin{equation}
\tilde{x}^{t,(i)} = B^t(x^{t,(i)} - \mu^t) + \mu^t + K^t(y^t - H^t\mu^t) + \hat{\epsilon}^{t,(i)}. \tag{4.9}
\end{equation}
Thereby, we see that in order to update $x^{t,(i)}$ we must specify appropriate $B^t$ and $S^t$. To choose a procedure, one may either first choose $S^t$ and thereafter compute $B^t$ consistent with Eq. (4.8), or one may first choose $B^t$ and then compute $S^t$ consistent with Eq. (4.8). Below, we list some solutions that are particularly interesting.

**Example 1.** By choosing all elements of $B^t$ equal to zero, we obtain $\tilde{x}^{t,(i)}$ independent of $x^{t,(i)}$,
\begin{equation}
\tilde{x}^{t,(i)} = \mu^t + K^t(y^t - H^t\mu^t) + \hat{\epsilon}^{t,(i)}.
\end{equation}
We then have $S^t = (I_n - K^tH^t)Q^t$, and $q(\tilde{x}^{t,(i)}|x^{t,(i)}, \theta^t, y^t)$ is simply equal to the assumed posterior model $f_{x^{t,(i)}}(x^{t,(i)}|\theta^t, y^t)$, i.e. the Gaussian distribution with mean and covariance given by Eqs. (2.7) and (2.8), respectively.

**Example 2.** By choosing all elements of $S^t$ equal to zero, the update of $x^{t,(i)}$ becomes deterministic and equivalent to a square root EnKF. Specifically, Eq. (4.9) becomes equal to Eq. (2.10), and Eq. (4.8) becomes equal to Eq. (2.11). The distribution $q(\tilde{x}^{t,(i)}|x^{t,(i)}, \theta^t, y^t)$ is then a degenerate Gaussian distribution, or a delta function.

**Example 3.** By choosing
\begin{equation}
B^t = I_n - K^tH^t
\end{equation}
(4.10)
and
\begin{equation}
S^t = (I_n - K^tH^t)Q^t(I_n - K^tH^t)^\top
\end{equation}
(4.11)
the update in Eq. (4.9) becomes equivalent to the stochastic EnKF update in Eq. (2.9). This result is proved in Appendix A.

### 4.3 The optimal solution

The optimality criterion we consider for this situation is to minimise the expected value of the Mahalanobis distance $g(x^{t,(i)}, \tilde{x}^{t,(i)})$ in Eq. (3.3) for a general positive definite matrix $\Sigma$. The minimisation is to be solved with respect to $B^t$ and $S^t$ under the restriction in Eq. (4.8) and, since $S^t$ is a covariance matrix, the additional restriction that $S^t$ is positive semidefinite.

To compute the optimal solution with respect to these criteria, we start out using that $\Sigma^{-1} = A^\top A$, $A \in \mathbb{R}^{n\times n}$. Hence, the function to be minimised, with respect to $B^t$ and $S^t$, is
\begin{equation}
E[g(x^{t,(i)}, \tilde{x}^{t,(i)})] = E\left[\left(A(\tilde{x}^{t,(i)} - x^{t,(i)})\right)^\top A(\tilde{x}^{t,(i)} - x^{t,(i)})\right],
\end{equation}
(4.12)
where the expectation is taken over the joint distribution $f_{x^{t}(\theta^t)}(x^{t,(i)}|x^{t}, \theta^t, y^t)$. Using Eq. (4.9), we can write $A(\tilde{x}^{t,(i)} - x^{t,(i)})$ as
\begin{equation}
A(\tilde{x}^{t,(i)} - x^{t,(i)}) = A\left((B^t - I_n)(x^{t,(i)} - \mu^t) + K^t(y^t - H^t\mu^t) + \hat{\epsilon}^{t,(i)}\right).
\end{equation}
(4.13)
Since $\theta^t$ and $y^t$ are treated as constants, the only stochastic components on the right hand side of Eq. (4.13) are $x^t$ and $\hat{\epsilon}^{t,(i)}$ which are independent and Gaussian. Thereby, $A(\tilde{x}^{t,(i)} - x^{t,(i)})$ is Gaussian since
it is a linear combination of independent Gaussian variables. Moreover, from Eq. (4.13) we see that
\[ E[A(x^{t,i}) - x^{t,i}] = AK'(y^t - H^t\mu^t) \]
and
\[ \text{Cov}[A(x^{t,i}) - x^{t,i}] = A(B^t - I_n)Q'(B^t - I_n)^\top A^\top + AS'A^\top. \]
Using that for any stochastic vector \( w \) we have \( E[w^\top w] = \text{tr}(\text{Cov}(w)) + E[w^\top E[w]) \), we can write Eq. (4.12) as
\[ E \left[ (A(x^{t,i}) - x^{t,i})^\top (A(x^{t,i}) - x^{t,i}) \right] = \text{tr}(A(B^t - I_n)Q'(B^t - I_n)^\top A^\top) + \text{tr}(AS'A^\top) + \left( AK'(y^t - H^t\mu^t) \right)^\top \left( AK'(y^t - H^t\mu^t) \right). \] (4.14)
We see that the last term in this equation is constant as a function of \( B^t \) and \( S^t \). Thereby, to minimise Eq. (4.12) with respect to \( B^t \) and \( S^t \) we only need to minimise the sum of the two traces in Eq. (4.14). According to the restriction in Eq. (4.8) we must have
\[ S^t = (I_n - K'H^t)Q' - B^tQ'(B^t)^\top. \] (4.15)
Using Eq. (4.15), we can write the sum of the two traces in Eq. (4.14) as a function of \( B^t \) only,
\[ \text{tr} \left\{ A(B^t - I_n)Q'(B^t - I_n)^\top A^\top \right\} + \text{tr} \left\{ AS'A^\top \right\} = \text{tr} \left\{ -2AB^tQ'A^\top + 2AQ'A^\top - AK'H^tQ'A^\top \right\}. \]
Here, only the first term is a function of \( B^t \). Hence, minimising Eq. (4.12) with respect to \( B^t \) is equivalent to maximising
\[ c(B^t) = \text{tr}\left\{ AB^tQ'A^\top \right\} \] (4.16)
with respect to \( B^t \) under the restriction that the matrix \( S^t \) in Eq. (4.15) is positive semidefinite.

To solve the optimisation problem stated above, we first rephrase it to a standardised form. To do so, we start with singular value decompositions of the two covariance matrices \( Q' \) and \( (I_n - K'H^t)Q' \),
\[ Q' = VDV^\top, \]
\[ (I_n - K'H^t)Q' = UAU^\top, \]
where \( U, V \in \mathbb{R}^{n \times n} \) are orthogonal matrices, i.e. \( UU^\top = VV^\top = I \) and \( VV^\top = V^\top V = I_n \), and \( D, \Lambda \in \mathbb{R}^{n \times n} \) are diagonal matrices. Inserting Eqs. (4.17) and (4.18) into Eq. (4.15) and defining
\[ \tilde{S}^t = \Lambda^{-\frac{1}{2}}U^\top S^tU\Lambda^{-\frac{1}{2}} \]
and
\[ \tilde{B}^t = \left( \Lambda^{-\frac{1}{2}}U^\top B^t V D^\frac{1}{2} \right)^\top \]
we get that Eq. (4.15) is equivalent to
\[ \tilde{S}^t = I_n - (\tilde{B}^t)^\top \tilde{B}^t \] (4.19)
and the objective function \( c(B^t) \) in Eq. (4.16) can be rephrased in terms of \( \tilde{B}^t \) as
\[ \tilde{c}(\tilde{B}^t) = \text{tr}\left\{ A\Lambda^\frac{1}{2}(\tilde{B}^t)^\top D^\frac{1}{2}V^\top A^\top \right\} \]
\[ = \text{tr}\left\{ B\Lambda^\frac{1}{2}U^\top A^\top AQ^\top V D^\frac{1}{2} \right\} \]
\[ = \text{tr}\left\{ \tilde{B}^t \tilde{Z}^t \right\}, \] (4.20)
where

\[ Z^t = \Lambda^{\frac{1}{2}} U^\top A Q^t V D^{-\frac{1}{2}}. \quad (4.21) \]

Recognising that the matrix \( \hat{S}^t \) is positive semidefinite if and only if \( S^t \) is positive semidefinite, the rephrased optimisation problem is thereby to maximise \( \tilde{c}(\hat{B}^t) \) in Eq. 4.20 with respect to \( \hat{B}^t \) under the constraint that \( \hat{S}^t \) in Eq. 4.19 is positive semidefinite. To solve this standardised optimisation problem we can apply the following theorem for which a proof is given in Appendix B.

**Theorem 1.** For a square matrix \( Z \in \mathbb{R}^{n \times n} \) of full rank and with singular value decomposition \( Z = P G F^\top \) the maximum value for \( \text{tr}(\hat{B} Z) \), \( \hat{B} \in \mathbb{R}^{n \times n} \) under the restriction that \( \hat{S} = I_n - \hat{B}^\top \hat{B} \) is positive semidefinite occurs only for

\[ \hat{B} = FP^\top. \]

To apply Theorem 1 we first need to argue why the matrix \( Z^t \) in Eq. 4.21 has full rank. Since \( Q^t \) and \( (I_n - K^t H^t)Q^t \) are positive definite matrices, \( D \) and \( \Lambda \) are invertible. Thereby also \( D^{\frac{1}{2}} \) and \( \Lambda^{\frac{1}{2}} \) are invertible. \( V \) and \( U \) are both orthogonal and thereby invertible. Finally, as we have required \( \Sigma \) to be positive definite, \( \Sigma \) is invertible, and when \( \Sigma \) is invertible, \( A \) is also invertible. Thereby, \( Z^t \) is given as a product of invertible matrices and is therefore itself invertible and has full rank.

According to Theorem 1 the solution to our optimisation problem in standardised form is \( \hat{B}^t = FP^\top \). We thereby get that

\[ \hat{S}^t = I_n - (FP^\top)^\top FP^\top = I_n - PP^\top FP^\top = 0, \]

i.e. all elements in \( \hat{S}^t \), and hence all elements in \( S^t \), are zero. The solution to our optimisation problem thereby corresponds to a square root EnKF. The corresponding optimal value for \( B^t \) is

\[ B^t = U\Lambda^{\frac{1}{2}} p F^\top D^{-\frac{1}{2}} V^\top. \]

### 4.4 Parameter simulation

According to step 2a) in Algorithm 1 we need to simulate \( \theta^t|x^t,\cdot,\cdot;\cdot \sim f_{\theta^t|x^t,\cdot,\cdot;\cdot}(\theta^t|x^t,\cdot,\cdot;\cdot) \) prior to constructing \( q(\hat{x}^t,\cdot|\cdot) \sim \tilde{Q} \). For this, we can construct a Gibbs sampler as explained in Section 3.4. For the linear-Gaussian model we now consider, we have \( \theta^t = (\mu^t, Q^t) \). To construct the Gibbs sampler we need to derive the full conditional distributions \( f_{\theta^t|x^t,\cdot,\cdot;\cdot}(\theta^t|x^t,\cdot,\cdot;\cdot) \) and \( f_{\theta^t|x^t,\cdot,\cdot;\cdot}(\theta^t|x^t,\cdot,\cdot;\cdot) \). From previous sections, we know that \( f_{\theta^t|x^t,\cdot,\cdot;\cdot}(\theta^t|x^t,\cdot,\cdot;\cdot) \) is a Gaussian distribution, \( N(\theta^t|x^t,\cdot,\cdot;\cdot ; \mu^t, Q^t) \), with parameters \( \mu^t \) and \( Q^t \) given by Eqs. (2.7) and (2.8), respectively. To simulate from \( f_{\theta^t|x^t,\cdot,\cdot;\cdot}(\theta^t|x^t,\cdot,\cdot;\cdot) \), we first factorise it as

\[ f_{\theta^t|x^t,\cdot,\cdot;\cdot}(\theta^t|x^t,\cdot,\cdot;\cdot) = f_{Q^t|x^t,\cdot,\cdot;\cdot}(Q^t|x^t,\cdot,\cdot;\cdot) f_{\theta^t|x^t,\cdot,\cdot;\cdot}(\theta^t|x^t,\cdot,\cdot;\cdot) = f_{Q^t|x^t,\cdot,\cdot;\cdot}(Q^t|x^t,\cdot,\cdot;\cdot) f_{\theta^t|x^t,\cdot,\cdot;\cdot}(\theta^t|x^t,\cdot,\cdot;\cdot). \]

Since conjugate priors are chosen for \( \mu^t \) and \( Q^t \), it can be shown that \( f_{Q^t|x^t,\cdot,\cdot;\cdot}(Q^t|x^t,\cdot,\cdot;\cdot) \) is an inverse Wishart distribution,

\[ f_{Q^t|x^t,\cdot,\cdot;\cdot}(Q^t|x^t,\cdot,\cdot;\cdot) = W^{-1}(Q^t; \bar{V}, \tilde{\nu}), \]

where

\[ \tilde{\nu} = \nu + M \]

and

\[ \bar{V} = V + C^t, \tilde{\nu} + \frac{\kappa M}{\kappa + M} \left( \hat{x}^t, \cdot, \cdot - \mu_0 \right) \left( \hat{x}^t, \cdot, \cdot - \mu_0 \right)^\top, \]

where

\[ \hat{x}^t, \cdot, \cdot = \frac{1}{M} \left( x^t + \sum_{j \neq t} x^t, j \right). \]
and
\[ C^t_{i,i} = \left( x^t - x^t_i \right) \left( x^t - x^t_i \right)^\top + \sum_{j \neq i} \left( x^t_j - x^t_i \right) \left( x^t_j - x^t_i \right)^\top, \]
and \( f_{\mu^t|Q^t,x^t_i,x^t_{-i}} (\nu^t|Q^t, x^t, x^t_{-i}) \) is a Gaussian distribution,
\[ f_{\mu^t|Q^t,x^t_i,x^t_{-i}} (\nu^t|Q^t, x^t, x^t_{-i}) = \mathcal{N} (\mu^t; \tilde{\mu}_0, \kappa^{-1} Q^t), \]
where
\[ \tilde{\mu}_0 = \frac{\kappa \mu_0 + M \bar{x}^t_i}{\kappa + M}, \]
and
\[ \kappa = \kappa + M. \]

5 Application 2: First-order Markov chain assumed model

In this section, we describe how the general updating procedure described in Section 3 can be applied when the elements of the state vector \( x' \) are categorical variables, \( x'_j \in \{0, 1, \ldots, K - 1\} \), and \( x^t \) is restricted to have a one-dimensional spatial arrangement. We then propose to let \( f_{\theta^t|x^t} (x^t|x^t_i) \) and \( f_{\theta^t|x^t} (y^t|x^t) \) constitute a hidden Markov model (HMM). The following material can be seen as a generalised and fully Bayesian version of the updating method for binary state vectors proposed in Loe and Tjelmeland (2021).

5.1 Specification of the assumed model

Suppose \( x^t = (x^t_1, \ldots, x^t_n) \) is a vector of \( n \) categorical variables, \( x^t_j \in \{0, 1, \ldots, K - 1\} \), and suppose \( x^t \) has a one-dimensional spatial arrangement (i.e., the vector is spatially arranged along a line). A natural choice of model for \( f_{\theta^t|x^t} (x^t|x^t_i) \) is then a first-order Markov chain,
\[ f_{\theta^t|x^t} (x^t|x^t_i) = f(x^t_i|x^t_i) \prod_{j=2}^n f(x^t_j|x^t_{j-1}, \theta^t). \tag{5.1} \]
Moreover, suppose \( y^t = (y^t_1, \ldots, y^t_n) \) is a vector of \( n \) variables, \( y^t_j \in \mathbb{R} \), so that we have one observation \( y^t_j \) for each component \( x^t_j \) of \( x^t \), and assume that the \( y^t_j \)'s are conditionally independent given \( x^t \),
\[ f_{\theta^t|x^t} (y^t|x^t) = \prod_{j=1}^n f_{y^t_j|x^t_j} (y^t_j|x^t_j). \]
Given \( \theta^t \), the pair \( f_{\theta^t|x^t} (x^t|x^t_i) \) and \( f_{\theta^t|x^t} (y^t|x^t) \) constitute a HMM. The corresponding posterior model \( f_{\theta^t|x^t,y^t} (x^t|x^t_i, y^t) \) is then also a first-order Markov chain whose initial and transition probabilities can be computed with the the forward-backward algorithm for HMMs (e.g., Künsch 2000).

The parameter \( \theta^t \) may in this context represent the initial and transition probabilities of the assumed first-order Markov chain \( f_{\theta^t|x^t} (x^t|x^t_i) \). In the following, we let
\[ \theta^t = \left( \{ \theta^t_1(i) \}_{i=0}^{K-1}, \{ \theta^t_{1,k}(i) \}_{i,k=0}^{K-1}, \ldots, \{ \theta^t_{n,k}(i) \}_{i,k=0}^{K-1} \right), \]
where \( \theta^t_1(i), \theta^t_{j,k}(i) \in (0, 1) \), \( \sum_{i=0}^{K-1} \theta^t_{j,k}(i) = 1 \), and
\[ f(x^t_i = i|\theta^t) = \theta^t_1(i) \]
and
\[ f(x^t_j = i|x^t_{j-1} = k, \theta^t) = \theta^t_{j,k}(i). \]
for \(i, k = 0, \ldots, K - 1\) and \(j = 2, \ldots, n\). For convenience, we also define

\[
\theta_i^t = (\theta_i^t(0), \theta_i^t(1), \ldots, \theta_i^t(K - 1))
\]

and

\[
\theta_{j,k}^t = (\theta_{j,k}^t(0), \theta_{j,k}^t(1), \ldots, \theta_{j,k}^t(K - 1)).
\]

As discussed in Section 3.4, the prior \(\theta\) should be chosen as conjugate for \(f_{\omega}(x^i|\theta)\). To obtain this, we first assume that all the vectors \(\theta_1^t, \theta_2^t, \ldots, \theta_{K-1}^t, \theta_0^t, \ldots, \theta_{K-1}^t, \theta_1^t, \ldots, \theta_{K-1}^t\) are a priori independent, so that

\[
f_{\omega}(\theta^t) = f_{\omega}(\theta_1^t) \prod_{j,k} f_{\omega}(\theta_{j,k}^t),
\]

and then choose \(f_{\omega}(\theta_1^t)\) as a Dirichlet distribution with parameters \(\alpha_1^t(0), \ldots, \alpha_1^t(K - 1)\),

\[
f_{\omega}(\theta_i^t) \propto \prod_{i=0}^{K-1} \theta_i^t(i),
\]

and choose each \(f_{\omega}(\theta_{j,k}^t)\) as a Dirichlet distribution with parameters \(\alpha_{j,k}^t(0), \ldots, \alpha_{j,k}^t(K - 1)\),

\[
f_{\omega}(\theta_{j,k}^t) \propto \prod_{i=0}^{K-1} \theta_{j,k}^t(i)^{\alpha_{j,k}^t(i)}.
\]

The hyperparameters \(\alpha_1^t(i)\) and \(\alpha_{j,k}^t(i)\), \(i, k = 0, \ldots, K - 1, j = 2, \ldots, n\), are all assumed to be known.

### 5.2 Class of updating distributions

Because of the discrete context of the current situation, the criterion in Eq. (5.1) can be written as a sum,

\[
f_{x^1|y^t, \omega^t}(\tilde{x}^{1, t(i)}, y^t) = \sum_{x^{1, t(i)} \in \mathcal{D}_x} f_{x^1|y^t}(x^{1, t(i)}|\theta^t)q(\tilde{x}^{1, t(i)}|x^{1, t(i)}, \theta^t, y^t).
\]  \hspace{1cm} (5.2)

Brute force, the updating distribution \(q(\tilde{x}^{1, t(i)}|x^{1, t(i)}, \theta^t, y^t)\) now represents a transition matrix, and there are \(K^n(K^n-1)\) transition probabilities that need to be specified. Even when \(n\) is only moderately large this becomes too computationally demanding. To simplify the situation, we therefore enforce a certain dependency structure for \(q(\tilde{x}^{1, t(i)}|x^{1, t(i)}, \theta^t, y^t)\) as illustrated in Figure 3. We can then factorise \(q(\tilde{x}^{1, t(i)}|x^{1, t(i)}, \theta^t, y^t)\) as

\[
q(\tilde{x}^{1, t(i)}|x^{1, t(i)}, \theta^t, y^t) = q(z_1^{1, t(i)}|z_2^{1, t(i)}, \theta^t, y^t) \prod_{j=2}^n q(z_j^{1, t(i)}|z_{j-1}^{1, t(i)}, z_j^{1, t(i)}, \theta^t, y^t).
\]  \hspace{1cm} (5.3)

The number of quantities required to specify \(q(\tilde{x}^{1, t(i)}|x^{1, t(i)}, \theta^t, y^t)\) thereby reduces to \(K(K + (n - 1)K^2(K - 1)\), or more specifically \(K(K - 1)\) quantities for \(q(z_1^{1, t(i)}|z_2^{1, t(i)}, \theta^t, y^t)\) and \(K^2(K - 1)\) quantities for each factor \(q(z_j^{1, t(i)}|z_{j-1}^{1, t(i)}, z_j^{1, t(i)}, \theta^t, y^t)\), \(j = 2, \ldots, n\). As this is a linear, rather than an exponential, function of \(n\), \(n\) can be large without causing trouble.

According to the requirement in Eq. (5.2), \(q(\tilde{x}^{1, t(i)}|x^{1, t(i)}, \theta^t, y^t)\) must be constructed such that marginalising out \(x^{1, t(i)}\) from the joint distribution \(f_{x^1|y^t}(x^{1, t(i)}|\theta^t)q(\tilde{x}^{1, t(i)}|x^{1, t(i)}, \theta^t, y^t)\) returns the posterior Markov chain model \(f_{x^1|y^t}(\tilde{x}^{1, t(i)}|\theta^t, y^t)\). However, the problem of constructing such a \(q(\tilde{x}^{1, t(i)}|x^{1, t(i)}, \theta^t, y^t)\) itself, is generally too intricate to solve. Therefore, we need to settle with an approximate approach. As in Loe and Tjelmeland (2021), we propose to replace the requirement of retaining the whole Markov chain model \(f_{x^1|y^t}(x^{1, t(i)}|\theta^t, y^t)\) with the requirement that only the bivariate
probabilities \( f_{x^j_t, x^j_{t+1} | \theta^t, y^t}(x^j_t, x^j_{t+1} | \theta^t, y^t) \) are retained, i.e.

\[
f_{\tilde{x}^j_t, \tilde{x}^j_{t+1} | \theta^t, y^t}(x^j_t, x^j_{t+1} | \theta^t, y^t) = f_{x^j_t, x^j_{t+1} | \theta^t, y^t}(x^j_t, x^j_{t+1} | \theta^t, y^t), \quad j = 1, \ldots, n - 1.
\] (5.4)

This means that, under the assumption that the assumed model is correct, the distribution of the updated sample \( \tilde{x}^j_t \) given \( \theta^t, y^t \) is not equal to the first-order Markov chain \( f_{x^j_t, x^j_{t+1} | \theta^t, y^t} \), but that each pair \( (\tilde{x}^j_t, \tilde{x}^j_{t+1}) \), \( j = 1, \ldots, n - 1 \), is marginally distributed according to the bivariate distribution \( f_{x^j_t, x^j_{t+1}}(x^j_t, x^j_{t+1}|\theta^t, y^t) \) of the Markov chain.

5.3 The optimal solution

The optimality criterion we consider for this situation is to minimise the expected number of components of \( x^j_t \) that are different from their corresponding components in \( \tilde{x}^j_t \); that is, we want to minimise the expected value of the function \( g(x^j_t, \tilde{x}^j_t) \) in Eq. (3.7). Minimising \( E \left[ g(x^j_t, \tilde{x}^j_t) \right] \) is equivalent to maximising

\[
E \left[ \sum_{j=1}^{n} 1(x^j_t = \tilde{x}^j_t) \right]
\] (5.5)

where the expectation is taken over \( f_{x^j_t | \theta^t, y^t}(x^j_t) \) and \( q(x^j_t) \). We are thereby faced with a constrained optimisation problem where we want to maximise, with respect to \( q(x^j_t) \), the function in Eq. (5.5) under the condition in Eq. (5.4) and under the condition that \( q(\tilde{x}^j_t | x^j_t, \theta^t, y^t) \) can be factorised as in Eq. (5.5).

Loe and Tjelmeland (2021) propose a dynamic programming algorithm for solving the optimisation problem stated above when \( x^j_t \) is binary, \( x^j_t \in \{0, 1\} \). The proposed algorithm is based on that the maximum value of Eq. (5.5) can be computed recursively since

\[
\max \frac{q_k}{n} \sum_{j=k}^{n} 1(x^j_k = \tilde{x}^j_k) = \max \frac{q_k}{n} \left[ 1(x^j_k = \tilde{x}^j_k) + \sum_{j=k+1}^{n} 1(x^j_k = \tilde{x}^j_k) \right]
\]

\[
= \max \frac{q_k}{n} \left[ 1(x^j_k = \tilde{x}^j_k) + \max \frac{q_k}{n} \sum_{j=k+1}^{n} 1(x^j_k = \tilde{x}^j_k) \right]
\] (5.6)

where \( q_k = q(\tilde{x}^j_k | x^j_{k-1}, x^j_k, \theta^t, y^t) \), \( q_1 = q(\tilde{x}^j_t) \), and \( q_{kn} = (q_k, \ldots, q_n) \). The algorithm starts with a 'backward' recursion where, for \( k = n, n - 1, \ldots, 1 \), Eq. (5.6) and the optimal value of \( q_k \) are computed as functions of \( q_{k-1} = (q_1, \ldots, q_{k-1}) \). At the final step of the backward recursion the whole expectation in Eq. (5.5) is thereby computed, along with the optimal value for \( q_1 \). The algorithm then proceeds with a 'forward' recursion where, for \( k = 2, \ldots, n \), we recursively compute the optimal values for \( q_2, \ldots, q_n \). Using linear programming, we are currently in the process of developing an alternative algorithm for solving the optimisation problem when the number of possible values of \( x^j_t \) is larger than two.
5.4 Parameter simulation

To construct the Gibbs sampler described in Section 3.4 for simulating \( \theta^{(t)} \mid x^{t-1}, y^t \) we need to be able to simulate from the distributions \( f_{\theta \mid y^t, y^t(x^t \mid \theta^t, y^t)} \) and \( f_{\theta \mid x^t, x^{t-1}}(\theta^t \mid x^t, x^{t-1}) \). From Section 5.1 we know that \( f_{\theta \mid y^t, y^t(x^t \mid \theta^t, y^t)} \) now is a first-order Markov chain with transition probabilities that are easy to compute with the forward-backward algorithm for HMMs. When it comes to \( f_{\theta \mid x^t, x^{t-1}}(\theta^t \mid x^t, x^{t-1}) \), it can easily be shown that \( \theta_i^t \mid x^t, x^{t-1} \) is Dirichlet distributed with parameters

\[
\tilde{\alpha}_i^t(r) = \alpha_i^t(r) + 1(x_{1}^t = r) + \sum_{m \neq i} 1 \left( x_{1}^t(m) = r \right),
\]

for \( r = 0, \ldots, K - 1 \). Similarly, it can be shown that each \( \theta_j^t \mid x^t, x^{t-1} \) is Dirichlet distributed with parameters

\[
\tilde{\alpha}_j^t(r) = \alpha_j^t(r) + 1(x_{j-1}^t = k, x_j^t = r) + \sum_{m \neq j} 1 \left( x_{j-1}^t(m) = k, x_j^t(m) = r \right)
\]

for \( r = 0, \ldots, K - 1 \). Moreover, all the parameters are independent a posteriori,

\[
f_{\theta \mid y^t, y^t(x^t \mid \theta^t, y^t)}(\theta^t \mid x^t, x^{t-1}) = f_{\theta \mid x^t, x^{t-1}}(\theta^t \mid x^t, x^{t-1}) \prod_{j,k} f_{\theta_j^t \mid x^{t-1}}(\theta_j^t \mid x^{t-1}).
\]

6 Simulation experiment with a linear-Gaussian assumed model

In this section, we present a simulation experiment for the situation described in Section 4. We adopt an experimental setup previously used in Myrseth and Omre (2010). In the following, we first describe how we generate a reference time series and simulate corresponding observations. Thereafter, we specify the precise assumed model we are using, and finally we present and discuss simulation results.

6.1 Experimental setup

To generate a reference time series \( \{x^t\}_{t=1}^T \) that we consider as the true unobserved state process we adopt the same setup as in Myrseth and Omre (2010). At each time \( t \), we assume that the state vector \( x^t = (x_1^t, \ldots, x_n^t) \) consists of \( n = 100 \) continuous variables so that \( \Omega_x = \mathbb{R}^{100} \). The latent process is defined from time 1 to time \( T = 11 \). The values of the initial state vector, \( x^1 \), is generated from a Gaussian distribution with zero mean, where the variance of each component is 20 and where the correlation between elements \( r \) and \( s \) in \( x^1 \) is

\[
c(r, s) = \exp \left\{ - \frac{3|r - s|}{20} \right\}.
\]

Myrseth and Omre (2010) define two deterministic ways to generate \( x^t, t = 2, \ldots, T \) from \( x^1 \), one linear forward function and one non-linear. We adopt the same linear forward function as used there, but not the same non-linear function. The non-linear forward function used in Myrseth and Omre (2010) induces a light-tailed bi-modal marginal distribution for each component in the state vector at time \( t = T \). We construct instead a forward function which produces a heavy-tailed one-mode marginal distribution for time \( t > 1 \).

For \( t = 2, \ldots, T \), the linear forward function we use is defined by

\[
x^t = \xi^{t-1} x^{t-1},
\]

where \( \xi^{t-1} \) is an \( n \times n \) matrix defined so that for \( j = 5t - 4, \ldots, 5t + 5 \), element \( j \) in \( x^t \) is set equal to the average of elements \( \max\{1, j - 4\} \) to \( j + 5 \) in \( x^{t-1} \), whereas the remaining elements in \( x^t \) equal the corresponding elements in \( x^{t-1} \). The effect of this forward function is that the first part of the vector \( x^t \) is a smoothed version of the first part of \( x^1 \), whereas the rest of \( x^t \) equals the corresponding part of \( x^1 \).

When the time \( t \) increases, the part that has been smoothed also increases.
Figure 4: The reference state vector (red crosses) at time \( t = T \) for the (a) linear and (b) non-linear forward model cases, and the simulated observations (green circles) at the same time. Note that a few of the observations are outside the range of the vertical axis.

For the non-linear forward function, we simply transform the Gaussian distributed elements in the state vector at time \( t = 1 \) to be from a (scaled) \( t \)-distribution at any later time \( t > 1 \). More specifically, element \( j \) in \( x^2 \) is defined from the corresponding element in \( x^1 \) by

\[
x^2_j = \sqrt{20F^{-1}_T} \left( \Phi \left( \frac{x^1_j}{\sqrt{20}} \right), 100 \right),
\]

where \( F_T(\cdot, \nu) \) and \( \Phi(\cdot) \) are the cumulative distribution functions for a \( t \)-distribution with \( \nu \) degrees of freedom and a standard normal distribution, respectively. Thus, the marginal distribution of each element in \( x^2 \) is a \( t \)-distribution with \( 100 \) degrees of freedom. For later times \( t > 2 \), each element \( j \) in \( x^t \) is defined from the corresponding element in \( x^{t-1} \) by

\[
x^t_j = \sqrt{20F^{-1}_T} \left( F_T \left( \frac{x^{t-1}_j}{\sqrt{20}}, \nu_{t-1} \right), \nu_t \right),
\]

where \( \nu_t = 100/(2t - 3) \). Thus, the marginal distribution for each element gets heavier and heavier tails when the time \( t \) increases.

Having generated a reference time series \( \{x^t\}_{t=1}^T \) as described above, observations are simulated for each time \( t = 1, \ldots, T \). For each time \( t = 1, \ldots, T \) an observation vector \( y^t \) is simulated according to

\[
y^t | x^t \sim N \left( y^t; x^t, 20I_n \right).
\]

The reference state vectors for the linear and the non-linear models at time \( t = T \) and the corresponding simulated observations at that time step are shown in Figure 4.

### 6.2 Details of the assumed model

The assumed model is as specified in Section 4.1. The hyperprior in Eqs. (4.1) and (4.2) for \( \theta^t = (\mu^t, Q^t) \) is specified by four hyperparameters: \( \mu_0, \kappa, \nu \) and \( V \). We choose values for these hyperparameters to get a vague, but proper prior for \( \theta^t \), and use the same values for all time steps. We set all the elements of \( \mu_0 \in \mathbb{R}^n \) equal to zero, and set \( \kappa = 10, \nu = n + 1.1 \) and \( V = (\nu - n - 1)I_n \). Note that this in particular gives \( E[Q^t] = I_n \) a priori. For the likelihood \( f_{y^t | x^t}(y^t | x^t) \) we use the same distribution as the one we used to simulate the data, i.e. \( f_{y^t | x^t}(y^t | x^t) \) is specified by Eq. (6.5).

### 6.3 Simulation results

When evaluating the performance of the proposed approach, the results are compared with several other variants of EnKF. When updating one of the ensemble members, there are two important steps. The first step is how to generate or estimate \( \mu^t \) and \( Q^t \) based on the prediction ensemble. The second step is how to
use these $\mu^t$ and $Q^t$ values to update the ensemble member in question. We consider tree variants of the first step. The first is what we propose in this report, to sample $\mu^t$ and $Q^t$ from a posterior distribution given the new observation $y^t$ and all ensemble members, except the member which is to be updated. For the function $g(x^t, \tilde{x}^t)$ we here use the Euclidean distance, i.e. $\Sigma = I_n$. The second is what [Myrseth and Omre (2010)] are advocating, to sample $\mu^t$ and $Q^t$ from a posterior distribution given all the ensemble members, including also the member that is going to be updated, but not given the new observation $y^t$. The third is the standard procedure in EnKF, to estimate $\mu^t$ and $Q^t$ based on all the ensemble members.

For how to update an ensemble member when values of $\mu^t$ and $Q^t$ are given, we consider two variants. The first is the square-root filter we found to be optimal in Section 4.3 and the second is the standard stochastic EnKF update procedure specified in Eq. (2.9). By combining each of the three variants of how to generate $\mu^t$ and $Q^t$ with each of the two variants of how to update the ensemble members, one can define six updating procedures. We present results for all the six combinations.

Using the linear forward model described in Section 6.1, the prediction ensembles at time $T = 11$ in one run of each of the six procedures considered, with $M = 19$ ensemble members, are shown in Figure 5. The ensemble members, drawn with solid lines in the figure, should thus be considered as (approximate) samples from the distribution $p_{x_{11}|y_{1:10}}(x_{11}|y_{1:10})$. For comparison, the latent true state vector at time $T = 11$ is also shown, with red crosses. The upper, middle and lower lines show results when using our
proposed procedure for generating $\mu_t$ and $Q_t$, when using the procedure in [Myrseth and Omre (2010)] for the same, and when using empirical estimates, respectively. The left and right columns show results when using our optimal square-root filter to update the ensemble members, and when using the standard stochastic EnKF update, respectively.

The most striking difference between the six cases is the spread of the ensemble members. In the four lower figures the spread is very small, and as a result the latent true value is in most places outside the spread of the ensemble members. For the standard stochastic EnKF procedure, shown in the lower right figure, this should come as no surprise as it is well known that this procedure tends to underestimate the uncertainty. What is more surprising is that the increase of the spread is so small when instead using the procedure proposed in [Myrseth and Omre (2010)], shown in the middle right figure. The difference in the spread of the ensemble members in each of the figures in the middle row and the corresponding figure in the upper row is also striking, when remembering the very small difference in the procedures used to generate the figures. The only difference between the procedures is what to condition on when generating values for $\mu_t$ and $Q_t$. In the procedures used to generate the figures in the middle row one is conditioning on all the ensemble members, but not the new data. In the procedure for the upper row one is conditioning on the new data and all the ensemble members except the ensemble member that is to be updated. Other simulation runs not included in this report show that most of the difference in the results comes from not conditioning on the ensemble member that is to be updated. The effect of including the new data in the conditioning set is clearly visible, but still small compared to the effect of not conditioning on the ensemble member that is to be updated.

In the four lower plots in Figure 5 the latent true state vector is in most positions outside the spread of the ensemble members. As such, these ensemble members do not give a realistic representation of our information about $x_{11}$. In the two upper plots in the same figure, the latent true state is in most positions inside the spread of the ensemble members. These ensembles may therefore give a better representation of the uncertainty. However, the spread in the ensemble members is larger in the upper left plot than in the upper right plot. So an interesting question is therefore which of the two that gives the best representation of our information about $x_{11}$. It is of course not necessarily the procedure that gives the largest spread that gives the best representation of uncertainty. To provide one answer to this question, one can first observe that in a perfect model, the variables $x_t^{1(1)}, \ldots, x_t^{1(M)}, x_t$ are exchangeable. One way to measure to what degree the spread of the ensemble members gives a realistic representation of the uncertainty is therefore to study the distribution of

$$Z = \frac{M}{n} \sum_{i=1}^{M} 1(x_t^{1(i)} \leq x_t^1),$$

where the index $j$ is sampled uniformly on the integers from 1 to $n$. In the perfect model $Z$ has a uniform distribution on the integers zero to $M$. Repeating the simulation procedures leading to the plots in Figure 5 one thousand times, randomising also over the latent state vector, the plots in Figure 6 show the estimated distributions for $Z$ for each of the six filtering procedures. The four lower plots in this figure just confirm what we saw in Figure 5, the latent state value is very often more extreme than all the ensemble members. The distributions in the two upper plots are neither perfectly uniform, but we see that the distribution in the upper left plot is slightly closer to being uniform than the upper right one. We thereby conclude that of the six procedures tried here, it is our proposed procedure that best represents our knowledge about $x_{11}$.

Above, we presented simulation experiments for the six ensemble updating procedures we have defined, for a linear forward model and with $M = 19$ ensemble members. We have also done similar simulation experiments for both smaller and larger ensemble sizes $M$, and for the non-linear forward function discussed in Section 6.1. There are two main lessons to learn from these experiments. The first is that the differences between the six methods gradually reduce when the number of ensemble members increases, and for $M$ large enough they all behave essentially the same. It should, however, be remembered that in typical applications of the EnKF, the dimension of the state vector, $n$, is much larger than the number of ensemble members,
Figure 6: Gaussian linear example: Estimated distribution for $Z$ when using $M = 19$ ensemble members. The upper, middle and lower rows are when using our proposed procedure for generating $\mu^t$ and $Q^t$, when using the procedure of [Myrseth and Omre (2010)] for the same, and when using empirical estimates, respectively. The left and right columns are when updating with our optimal square-root filter and when using the standard stochastic EnKF procedure, respectively.
Figure 7: Gaussian linear example: Estimated distribution for $Z$ when using $M = 199$ ensemble members. The upper, middle and lower rows are when using our proposed procedure for generating $\mu$ and $Q$, when using the procedure of Myrseth and Omre (2010) for the same, and when using empirical estimates, respectively. The left and right columns are when updating with our optimal square-root filter and when using the standard stochastic EnKF procedure, respectively.

$M$. As one example, the plots in Figure 7 are the same type of plots as in Figure 6, but for runs with $M = 199$ ensemble members.

The second lesson we learn from the simulation experiments, is that the results when using our non-linear forward function is quite similar to what we have for the linear forward function. As one example, Figures 8 and 9 show similar plots as in Figures 5 and 6, but for the non-linear forward function defined by Eqs. (6.3) and (6.4). Again we see that the upper left plot in Figure 9 is the one closest to being uniform. Also when using the non-linear forward function the differences between the six methods gradually vanish when the number of ensemble members, $M$, increases. Of course, that the results for our non-linear forward function are similar to the results for the linear function, does not imply that this is generally true for all non-linear forward functions. We have for example not studied how the various procedures perform with a forward function inducing skewed distributions for the state vector.

7 Simulation experiment with a first-order Markov chain assumed model

In this section, we demonstrate the proposed updating procedure in a simulation example where the state vector consists of binary variables and $f_{x_{t+1}|x_{t}}(x_{t+1}|\theta_{t})$ and $f_{y_{t}|x_{t}}(y_{t}|x_{t})$ constitute a hidden Markov model as described in Section 6. The experimental setup of the simulation example is the same as in the simulation example presented in Loe and Tjelmeland (2021). Below, we first describe the experimental setup of the
Figure 8: Gaussian non-linear example: Prediction ensemble at time $T = 11$ when using $M = 19$ ensemble members. The upper, middle and lower rows are when using our proposed procedure for generating $\mu_t$ and $Q_t$, when using the procedure of Myrseth and Omre (2010) for the same, and when using empirical estimates, respectively. The left and right columns are when updating with our optimal square-root filter and when using the standard stochastic EnKF procedure, respectively. The ensemble members are shown with solid lines and the latent true state is shown with red crosses.
Figure 9: Gaussian non-linear example: Estimated distribution for $Z$ when using $M = 19$ ensemble members. The upper, middle and lower rows are when using our proposed procedure for generating $\mu^t$ and $Q^t$, when using the procedure of Myrseth and Omre (2010) for the same, and when using empirical estimates, respectively. The left and right columns are when updating with our optimal square-root filter and when using the standard stochastic EnKF procedure, respectively.
Figure 10: First-order Markov chain simulation example: (a) the latent state process, (b) the observations, (c) estimates of marginal filtering probabilities obtained with the proposed Bayesian updating approach, and (d) estimates of marginal filtering probabilities obtained with the non-Bayesian updating approach. In all figures, the colour black represents the value zero and the colour white represent the value one.

Simulation example in Section 7.1 and thereafter we present and discuss the simulation results in Section 7.2.

7.1 Experimental setup

The simulation example involves a state process \{x^t\}_{t=1}^T \text{ with } T=100 \text{ time steps, and the state vector } \mathbf{x}_t \text{ at each time step is a vector of } n=400 \text{ binary variables, } x^t_j \in \{0,1\}. \text{ The initial distribution } p_{x^1}(x^1) \text{ and the forward model } p_{x^t|x^{t-1}}(x^t|x^{t-1}) \text{ of the unobserved } x^t\text{-process} \text{ are the same as in the simulation example of } \text{Loe} \text{ and } \text{Tjelmeland} \text{ (2021). For simplicity, we do not discuss the technical details of this model here, but one should note that the generated state vector } x^t \text{ at any time } t \text{ is not a first-order Markov chain.}

The process is inspired by how water comes through to an oil-producing well in a petroleum reservoir. In this context, we let the \( t \) in \( x^t_j \) represent time and \( j \) the location in the well, and the values zero and one represent oil and water, respectively. Hence, the event \( x^t_j = 0 \) indicates the presence of oil in location \( j \) at time \( t \), while the event \( x^t_j = 1 \) indicates the presence of water.

An image of a state process \( \{x^t\}_{t=1}^T \) generated using the true model specified above is shown in Figure 10(a), where the colours black and white represent the values zero (oil) and one (water), respectively. Based on this reference state process, a corresponding observation process \( \{y^t\}_{t=1}^T \) is generated by simulating, independently for each time step \( t = 1, \ldots, T \) and for each node \( j = 1, \ldots, n \), an observation \( y^t_j \) from a Gaussian distribution with mean \( x^t_j \) and variance \( \sigma^2 = 2^2 \). Figure 10(b) shows a grey-scale image of the generated observation process. Pretending that only the observations are available, the goal is to assess the filtering distribution \( p_{x^t|y^{1:t}}(x^t|y^{1:t}) \) for each time step \( t = 1, \ldots, T \).

As described in Section 5, the assumed model \( f_{x^t|\theta^t}(x^t|\theta^t) \) is a first-order Markov chain, and the parameter \( \theta^t \) represents its initial and transition probabilities. Moreover, \( \theta^t \) is a vector of the Dirichlet distributed random variables

\[
\theta^t_1 = (\theta^t_1(0), \theta^t_1(1)),
\]

\[
\theta^t_j = (\theta^t_j(0), \theta^t_j(1)),
\]

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and

\[ \theta_j^{-1} = (\theta_j^0(0), \theta_j^1(1)), \]

for \( j = 2, \ldots, n \). The corresponding hyperparameters \( \alpha^j_0(0), \alpha^j_1(1), \alpha^j_0(0), \alpha^j_1(0), \alpha^j_1(1) \) are all set equal to 2 at every time step. For each of the two methods, we thereby obtain five samples, and we perform five independent runs of each method and estimate the marginal filtering probabilities in each

From a visual inspection, the output from the two approaches look very similar. To investigate this further, we consider the maximum values of the five samples. Equivalent output from other time steps \( t = 1 \) to 100 at the (arbitrarily chosen) time step \( j \) parameter value \( \theta_j \) is treated as random in the Bayesian approach. More specifically, the Bayesian approach simulates a

Methodologically, the main difference between the Bayesian and the non-Bayesian approach is that \( \theta^* \) is treated as random in the Bayesian approach. More specifically, the Bayesian approach simulates a parameter value \( \theta^{(i)} \) for each ensemble member \( x^{(i)} \), while the non-Bayesian approach instead computes an estimate, \( \hat{\theta} \), and this same estimate \( \hat{\theta} \) is used to update all the forecast samples. Therefore, since the Bayesian approach incorporates randomness in \( \theta^* \), one would expect the spread, or the variability, in the samples from the Bayesian approach to be greater than the variability in the samples from the non-Bayesian approach, which is also what Myrseth and Omre (2010) observed in their work and what we observed in the simulation example with the linear-Gaussian model presented in the previous section. However, it appears that this is not the case for the binary simulation experiment studied here. For continuous variables, variability is easy to measure and visualise, but for categorical variables, other techniques are necessary.

To evaluate the performance of the proposed approach, we compare our results with corresponding results obtained using the method of Loe and Tjelmeland (2021). For simplicity, we refer in the following to the method proposed in the present report as the Bayesian approach, and the method proposed in Loe and Tjelmeland (2021) as the non-Bayesian approach.

Figures 10(c) and (d) show grey-scale images of estimated values \( \hat{p}(x_j = 1|y^{1:t}) \) of the marginal filtering probabilities \( p_{x_j|y_t}(x_j = 1|y^{1:t}), j = 1, \ldots, n, t = 1, \ldots, T \) obtained with the Bayesian and the non-Bayesian approach, respectively, where the estimate \( \hat{p}(x_j = 1|y^{1:t}) \) is the empirical mean of the \( \bar{x}_j^{(i)} \) samples,

\[ \hat{p}(x_j = 1|y^{1:t}) = \frac{1}{M} \sum_{i=1}^{M} \bar{x}_j^{(i)}. \] (7.1)

From a visual inspection, the output from the two approaches look very similar. To investigate this further, we perform five independent runs of each method and estimate the marginal filtering probabilities in each run. For each of the two methods, we thereby obtain five samples, \( \hat{p}^{(i)}(x_j = 1|y^{1:t}), r = 1, \ldots, 5 \), of \( \hat{p}(x_j = 1|y^{1:t}) \) in Eq. (7.1). Figure 11 shows plots of the empirical means of these five samples for locations \( j = 1 \) to 100 at the (arbitrarily chosen) time step \( t = 50 \), along with the corresponding minimum and maximum values of the five samples. Equivalent output from other time steps \( t \) and for other locations \( j \) follow the same trend and are therefore, for simplicity, not included. As seen in Figure 11 the results from the two methods look very much the same. This may suggest that the Bayesian approach offers no considerable advantage over the non-Bayesian approach, at least not when it comes to estimating marginal filtering probabilities.

To study the variability of the results in the categorical context of this example, we consider the coefficient of unalikeability (CU) of Kader and Perry (2007). Given a set of independent random samples taking values in a categorical sample space, the CU provides a measure for how unalike the samples are. In the present simulation example, we are interested in computing the CU of the filtering ensemble \( \{\hat{x}^{(1)}, \ldots, \hat{x}^{(M)}\} \) at each of the time steps \( t = 1, \ldots, T \). Hereafter, we denote the CU of \( \{\hat{x}^{(1)}, \ldots, \hat{x}^{(M)}\} \) by \( u^t \). Since \( \hat{x}^{(i)} \) is a vector of \( n = 400 \) binary variables, there are \( 2^{400} \) possible configurations for \( \hat{x}^{(i)} \). Each configuration can be interpreted as a (unique) category. Hence, each realisation \( \hat{x}^{(i)} \) of the posterior ensemble corresponds to one of the \( 2^{400} \) possible categories. However, we only have \( M = 20 \) ensemble members, which is not enough to give an informative value for \( u^t \) when the number of categories is so high. Therefore, we consider first
Figure 11: First-order Markov chain simulation example: The left plot shows the empirical means (solid red line) of five estimated values \( \hat{p}(x_t^j = 1 | y^{1:t}) \) for the marginal filtering probability \( p_{x_t^j | y^{1:t}}(x_t^j = 1 | y^{1:t}) \) obtained from five independent runs of the Bayesian approach, along with the corresponding minimum and maximum values (dotted black lines) of the five estimates. The right plot shows corresponding output from the non-Bayesian approach.

each four-tuple \( x^t_{j,j+3} = (x^t_j, x^t_{j+1}, x^t_{j+2}, x^t_{j+3}) \), \( j = 1, \ldots, n - 3 \), of \( x^t \) separately. The number of possible configurations for each such four-tuple is \( 2^4 = 16 \), and from the posterior samples \( \tilde{x}^{t,(i)}_{j,j+3} \) we can compute a coefficient of unalikeability \( u^t_j \). After having computed \( u^t_j \) for each four-tuple \( x^t_{j,j+3} \) of \( x^t \), we compute the mean, \( \bar{u}^t \), of all of them. This \( \bar{u}^t \) then serves as an approximation for the actual CU, \( u^t \), of \( \{\tilde{x}^{t,(1)}, \ldots, \tilde{x}^{t,(M)}\} \). Figure 12 shows a plot of the values of \( \bar{u}^t \), \( t = 1, \ldots, T \), obtained with the Bayesian approach (red line) and the non-Bayesian approach (blue line). As one can see, the values of \( \bar{u}^t \) from the Bayesian approach very much coincide with the values from the non-Bayesian approach, which indicates a similar variability in the samples.

After various additional tests, both with different data \( \{y^t\}_{t=1}^T \), different values for the observation noise \( \sigma \) and different values for the ensemble size \( M \), it seems that the variability in the results from the two approaches, and the results from the two approaches in general, are very much alike. One possible reason for this, is the optimality criterion for \( q(\tilde{x}^{t,(i)} | x^{t,(i)}, \hat{\theta}^t, y^t) \), i.e. the criterion of maximising the expected number of unchanged components of \( x^{t,(i)} \). Basically, the optimality criterion states that we want to make minimal changes to the forecast samples, and this results in that the distributions \( q(\tilde{x}^{t,(i)} | x^{t,(i)}, \hat{\theta}^t, y^t) \), \( i = 1, \ldots, M \), from the Bayesian approach and the distribution \( q(\tilde{x}^{t,(i)} | x^{t,(i)}, \theta^{t,(i)}, y^t) \) from the non-Bayesian approach are all drawn towards each other. Consequently, the generated posterior samples from the two approaches will be similar to each other. Another possible reason for the lack of differing variability is the binary nature of the problem. More specifically, since both approaches capture the mean of \( x^t_j \) quite well, they must also capture the variance, as there is a one-to-one relationship between the mean and variance for a binary random variable.

8 Closing remarks

In this report, a general framework for updating a prior ensemble to a posterior ensemble is presented. Being able to update a prior ensemble to a posterior ensemble is a crucial step in ensemble-based solutions to the filtering, or data assimilation, problem. The proposed method is based on an assumed Bayesian model and a proposed optimality criterion.

Two special applications of the general framework are investigated, one where the elements of the state
vector are continuous variables and one where the elements are binary variables. In the continuous case, an assumed Gaussian distribution is adopted for the state vector and a linear-Gaussian model for the observation. This results in a class of updating methods where a fully Bayesian version of the EnKF is a special case, and we prove that a particular version of the square root EnKF is optimal with respect to the optimality criterion of making minimal changes to each ensemble member. In the binary application, the state and observation vectors are instead assumed to follow a finite state-space HMM. The corresponding updating procedure is then essentially the same as the one for binary vectors proposed in [Loe and Tjelmeland, 2021], except now the transition probabilities of the assumed Markov chain model are treated as random.

When studying the results of the presented simulation examples, the most striking aspect is that the proposed approach is substantially better in representing the uncertainty in the situation with the linear-Gaussian model. When comparing results from the proposed approach with results obtained using the procedure of [Myrseth and Omre, 2010], we really see the importance of not using the same information twice. That we do not get the same dramatic effect in the example for the assumed HMM may be because in that model the same parameters control both the mean and the variance. As the non-Bayesian ensemble filtering method seems to capture the mean quite well, it must then also give a good representation of the variance.

Computational efficiency is not a main focus in the present report. The dynamic programming procedure developed for the assumed HMM requires computing time proportional to the number of elements in the state vector and is thereby computationally efficient. The updating procedure of the assumed linear-Gaussian model requires inversion of \( n \times n \) matrices, where \( n \) is the dimension of the state vector, so this procedure is only computationally feasible for sufficiently small values of \( n \). In typical applications of the EnKF, the state vector is very large and computational efficiency is therefore essential. In the EnKF, the prior covariance matrix is estimated by the empirical covariance matrix of the prior ensemble. The rank of the (estimated) covariance matrix is thereby limited by the number of ensemble members, which is typically much smaller than the dimension of the state vector. The low rank of the covariance matrix makes it possible to rephrase the EnKF updating equation so that efficient computation is possible. In the proposed approach for the assumed linear-Gaussian model, the generated covariance matrices are by construction of full rank. It should, however, be possible to get computational efficiency by restricting the inverse covariance matrices, i.e. precision matrices, to be sparse. To achieve this, a prior tailored to produce sparse precision matrices must be constructed and the class of updating distributions must be restricted to ensure that all necessary computations for the updating can be performed on sparse matrices. The details of this is a direction of future research.

In the present report, we have studied in detail two applications of the proposed framework. In the
future, it is of interest to explore also other assumed models and other optimality criteria. It would in particular be interesting to consider a situation where the state vector represents a two-dimensional lattice of categorical variables. A possible assumed prior model is then a Markov mesh model [Abend et al., 1965]. It would also be interesting to apply the proposed framework in a mixed discrete and continuous situation, i.e. a model where the state vector consists of both discrete and continuous variables.

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Loe, M. K. and Tjelmeland, H. (2021). Ensemble updating of binary state vectors by maximising the expected number of unchanged components. *Scandinavian Journal of Statistics*, To Appear. DOI: 10.1111/sjos.12483.
A Proof of the result in Example 3

Here we prove the result stated in Example 3 that is, we prove that when $B^t$ and $S^t$ are as specified in Eqs. (4.10) and (4.11), respectively, the linear update in Eq. (4.9) corresponds to the stochastic EnKF update in Eq. (2.9).

We start by inserting the expression for $B^t$ in Eq. (4.10) into Eq. (4.9). This gives

$$x^{t,(i)} = x^{t,(i)} + K^t(y^t - H^tx^{t,(i)}) + \epsilon^{t,(i)}.$$  \hfill (A.1)

Comparing Eq. (A.1) with the stochastic EnKF update in Eq. (2.9), we see that it remains to show that the distribution of $\hat{x}^{t,(i)}$ in Eq. (A.1) is identical to the distribution of $K^t \epsilon^{t,(i)}$ in Eq. (2.9). As both $\epsilon^{t,(i)}$ and $x^{t,(i)}$ are Gaussian with zero mean, the distributions of $\hat{x}^{t,(i)}$ and $K^t \epsilon^{t,(i)}$ are equal if

$$\text{Cov}[\hat{x}^{t,(i)}] = \text{Cov}[K^t \epsilon^{t,(i)}].$$

Since we have $\text{Cov}[\hat{x}^{t,(i)}] = S^t$, with $S^t$ given by Eq. (4.11), and $\text{Cov}[K^t \epsilon^{t,(i)}] = K^t R^t (K^t)^\top$, this means that we need to show that

$$(I_n - K^t H^t) Q^t (K^t (H^t)^\top) = K^t R^t (K^t)^\top,$$

or rather

$$(I_n - K^t H^t) Q^t (H^t)^\top = K^t R^t.$$ \hfill (A.2)

In order to prove Eq. (A.2) we first prove that

$$((Q^t)^{-1} + (H^t)^\top (R^t)^{-1} H^t)^{-1} (Q^t)^{-1} = I_n - K^t H^t$$ \hfill (A.3)

and

$$((Q^t)^{-1} + (H^t)^\top (R^t)^{-1} H^t)^{-1} (H^t)^\top (R^t)^{-1} = K^t.$$ \hfill (A.4)

To prove Eqs. (A.3) and (A.4) we make use of the following two formulations of the Woodbury matrix identity,

$$((Q^t)^{-1} + (H^t)^\top (R^t)^{-1} H^t)^{-1} = Q^t + Q^t (H^t)^\top (R^t + H^t Q^t (H^t)^\top)^{-1} H^t Q^t,$$ \hfill (A.5)

$$(R^t + H^t Q^t (H^t)^\top)^{-1} = (R^t)^{-1} - (R^t)^{-1} H^t ((Q^t)^{-1} + (H^t)^\top (R^t)^{-1} H^t)^{-1} (H^t)^\top (R^t)^{-1}.$$ \hfill (A.6)

To prove Eq. (A.3) we start by inserting Eq. (A.5) on the left hand side in Eq. (A.3) and use that the
Kalman gain is given as \( K^t = Q^t (H^t)^\top (H^t Q^t H^t)^\top + R^t \)^\top, \]
\[
\left( (Q^t)^{-1} + (H^t)^\top (R^t)^{-1} H^t \right)^{-1} K^t = \left( Q^t + Q^t (H^t)^\top \left( R^t + H^t Q^t (H^t)^\top \right)^{-1} H^t Q^t \right) (Q^t)^{-1} = I_n - K^t H^t.
\]

Hence we see that Eqs. (A.8) and (A.9) are equal, and the proof is complete.

The Cauchy-Schwarz inequality, \(|\langle M, N \rangle|^2 \leq \langle M, M \rangle \langle N, N \rangle\), then gives
\[
\langle M N^\top \rangle^2 \leq \langle M M^\top \rangle \langle N N^\top \rangle
\]
with equality if and only if there exists a constant \( c \in \mathbb{R} \) such that \( M = cN \).
Using the singular value decomposition of $Z$, i.e. $Z = P G F^\top$, we can write
\[
\text{tr}(\tilde{B}Z) = \text{tr}(\tilde{B}P G F^\top) = \text{tr}(\tilde{B}PG^\frac{1}{2} (FG^\frac{1}{2})^\top).
\] (B.1)

The Cauchy-Schwarz inequality for $\text{tr} \left( BPG^\frac{1}{2} (FG^\frac{1}{2})^\top \right)$ with $M = BPG^\frac{1}{2}$ and $N = FG^\frac{1}{2}$ then gives
\[
\text{tr} \left( \tilde{B}Z \right)^2 \leq \text{tr} \left( BPG^\frac{1}{2} (BPG^\frac{1}{2})^\top \right) \text{tr} \left( FG^\frac{1}{2} (FG^\frac{1}{2})^\top \right)
\] (B.2)
with equality if and only if there exists a number $c \in \mathbb{R}$ such that
\[
BPG^\frac{1}{2} = cFG^\frac{1}{2} \iff \tilde{B} = cFP^\top.
\]

Using basic trace properties and that $\tilde{B}^\top \tilde{B} = I_n - \tilde{S}$ and $F^\top F = P^\top P = I_n$, the right hand side in (B.2) can be rewritten as
\[
\text{tr} \left( BPG^\frac{1}{2} (BPG^\frac{1}{2})^\top \right) \text{tr} \left( FG^\frac{1}{2} (FG^\frac{1}{2})^\top \right) = \text{tr} \left( PGP^\top \tilde{B}^\top \right) \text{tr} \left( G F^\top \right)
= \text{tr} \left( PGP^\top (I - \tilde{S}) \right) \text{tr} (G)
= \left( \text{tr} \left( PGP^\top \right) - \text{tr} \left( PGP^\top \tilde{S} \right) \right) \text{tr} (G)
= \left( \text{tr} (G) - \text{tr} (PGP^\top \tilde{S}) \right) \text{tr} (G).
\]

When $\tilde{S} = 0$, we see that the Cauchy-Schwarz inequality yields
\[
\text{tr}(\tilde{B}Z)^2 \leq \text{tr}(G)^2
\]
with equality if and only if there exists $c \in \mathbb{R}$ such that $\tilde{B} = cFP^\top$. The condition that $\tilde{S} = I_n - \tilde{B}^\top \tilde{B} = 0$ gives restrictions on the allowed values for $c$. Specifically,
\[
I_n - \tilde{B}^\top \tilde{B} = I_n - (cFP^\top)^\top (cFP^\top) = I_n - c^2 PP^\top F F^\top
= (1 - c^2)I_n = 0 \iff c = \pm 1.
\]
Hence, when $\tilde{S} = 0$, the maximum value of $\text{tr}(\tilde{B}Z)^2$ is $\text{tr}(G)^2$ and this occurs only for $\tilde{B} = \pm FP^\top$. The maximum value of $\text{tr}(\tilde{B}Z)$ is thereby $\text{tr}(G)$ which occurs when $c = 1$, i.e. for $\tilde{B} = FP^\top$.

When $\tilde{S} \neq 0$, we need to study the sign of $\text{tr} \left( PGP^\top \tilde{S} \right)$. Since $G$ is a diagonal matrix we get
\[
\text{tr} \left( PGP^\top \tilde{S} \right) = \text{tr} \left( GP^\top \tilde{S} P \right) = \sum_{i=1}^{n} G_{ii} (P^\top SP)_{ii}.
\]
We have assumed $Z$ to have full rank, so all singular values of $Z$ are strictly positive, i.e. $G_{ii} > 0$ for each $i$. Let $\tilde{S}$ have singular value decomposition $\tilde{S} = WJW^\top$. We then get
\[
(P^\top SP)_{ii} = \left( P^\top WJW^\top P \right)_{ii} = \left( (W^\top P)^\top JW^\top P \right)_{ii}
= \sum_{k=1}^{n} J_{kk} \left( W^\top P \right)^2_{ki}.
\]
Since we have assumed $\tilde{S} \neq 0$ at least one of the singular values of $\tilde{S}$ must be strictly positive, i.e. we have at least one $J_{kk} > 0$. Without loss of generality we assume in the following that $J_{11} > 0$. Since both $P$ and $W$ are orthogonal matrices $W^\top P$ is also orthogonal. Thereby there exists at least one index $i$ such
that \((W^TP)_{ii} > 0\). For this value of \(i\) we then have

\[(P^T\tilde{S}P)_{ii} \geq J_{ii}(W^TP)^2_{ii} > 0.\]

Thereby, since \(P^T\tilde{S}P\) is positive semidefinite,

\[\text{tr}\left(PP^T\tilde{S}\right) \geq G_{ii}(P^T\tilde{S}P)_{ii} > 0.\]

Thus,

\[|\text{tr}(\tilde{B}Z)| \leq \sqrt{\left(\text{tr}(G) - \text{tr}(PP^T\tilde{S})\right)\text{tr}(G)} < \text{tr}(G).\]

We thereby see that the maximum value of \(\text{tr}(\tilde{B}Z)\) when \(\tilde{S} \neq 0\) is smaller than its maximum value when \(\tilde{S} = 0\). The maximum value of \(\text{tr}(\tilde{B}Z)\) must therefore occur when \(\tilde{S} = 0\) and \(\tilde{B} = PP^T\), and the proof is complete.