Ensemble filter techniques for intermittent data assimilation - a survey

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September 3, 2012

Abstract

This survey paper is written with the intention of giving a mathematical introduction to filtering techniques for intermittent data assimilation, and to survey some recent advances in the field. The paper is divided into three parts. The first part introduces Bayesian statistics and its application to statistical inference and estimation. Basic aspects of Markov processes, as they typically arise from scientific models in the form of stochastic differential and/or difference equations, are covered in the second part. The third and final part describes the filtering approach to estimation of model states by assimilation of observational data into scientific models. While most of the material is of survey type, very recent advances in the field of nonlinear data assimilation covered in this paper include a discussion of Bayesian inference in the context of optimal transportation and coupling of random variables, as well as a discussion of recent advances in ensemble transform filters. References and sources for further reading material will be listed at the end of each section.
1 Introduction to Bayesian statistics

In this section, we summarize the Bayesian approach to statistical inference and estimation, in which probability is interpreted as a measure of uncertainty (of the system state, for example). Contrary to closely related inverse problem formulations, all variables involved are considered to be uncertain, and are described as random variables. Furthermore uncertainty is only discussed in the context of available information, requiring the computation of conditional probabilities; Bayes’ formula is used for statistical inference. We start with a short introduction to random variables.

1.1 Preliminaries

We start with a sample space $\Omega$ which characterizes all possible outcomes of an experiment. An event is a subset of $\Omega$ and we assume that the set $\mathcal{F}$ of all events forms a $\sigma$-algebra (i.e., $\mathcal{F}$ is non-empty, and closed over complementation and countable unions). For example, suppose that $\Omega = \mathbb{R}$. Then events can be defined by taking all possible countable unions and complements of intervals $(a, b] \subset \mathbb{R}$; these are known as the Borel sets.

Definition (Probability measure). A probability measure is a function $P: \mathcal{F} \rightarrow [0, 1]$ with the following properties:

(i) Total probability equals one: $P(\Omega) = 1$.

(ii) Probability is additive for independent events: If $A_1, A_2, \ldots, A_n, \ldots$ is a finite or countable collection of events $A_i \in \mathcal{F}$ and $A_i \cap A_j = \emptyset$ for $i \neq j$, then

$$P(\bigcup_i A_i) = \sum_i P(A_i)$$

The triple $(\Omega, \mathcal{F}, P)$ is called a probability space.

Definition (Random variable). A function $X : \Omega \rightarrow \mathbb{R}$ is called a (univariate) random variable if

$$\{ \omega \in \Omega : X(\omega) \leq x \} \in \mathcal{F}$$

for all $x \in \mathbb{R}$. The (cumulative) probability distribution function of $X$ is given by

$$F_X(x) = P(\{ \omega \in \Omega : X(\omega) \leq x \}).$$

The cumulative probability distribution function implies a probability measure on $\mathbb{R}$ which we denote by $\mu_X$.

Often, when working with a random variable $X$, the underlying probability space $(\Omega, \mathcal{F}, P)$ is not emphasised; one typically only specifies the target space $\mathcal{X} = \mathbb{R}$ and the probability distribution or measure $\mu_X$ on $\mathcal{X}$. We then say that $\mu_X$ is the law of $X$ and write $X \sim \mu_X$. A probability measure $\mu_X$ introduces an integral over $\mathcal{X}$ and

$$\mathbb{E}_X[f] = \int_{\mathcal{X}} f(x) \mu_X(dx)$$

is called the expectation value of a function $f : \mathbb{R} \rightarrow \mathbb{R}$ (if $f$ is called a measurable function where the integral exists). We also use the notation $\text{law}(X) = \mu_X$ to indicate that $\mu_X$ is the probability measure for a random variable $X$. Two important choices for $f$ are $f(x) = x$, which leads to the mean $\bar{x} = \mathbb{E}_X[x]$ of $X$, and $f(x) = (x - \bar{x})^2$, which leads to the variance $\sigma^2 = \mathbb{E}_X[(x - \bar{x})^2]$ of $X$.

Univariate random variables naturally extend to the multivariate case, i.e. $\mathcal{X} = \mathbb{R}^N$, $N > 1$. A probability measure $\mu_X$ on $\mathcal{X}$ is called absolutely continuous (with respect to the standard Lebesgue integral $dx$ on $\mathbb{R}^N$) if there exists a probability density function (PDF) $\pi_X : \mathcal{X} \rightarrow \mathbb{R}$ with $\pi_X(x) \geq 0$, and

$$\mathbb{E}_X[f] = \int_{\mathcal{X}} f(x) \mu_X(dx) = \int_{\mathbb{R}^N} f(x) \pi_X(x) dx,$$
for all measurable functions $f$. The shorthand $\mu_X(dx) = \pi_X dx$ is often adopted. The implication is that one can, for all practical purposes, work within the classical Riemann integral framework and does not need to resort to Lebesgue integration. Again we can define the mean $\bar{x} \in \mathbb{R}^N$ of a multivariate random variable and its covariance matrix

$$
P = \mathbb{E}_X[(x - \bar{x})(x - \bar{x})^T] \in \mathbb{R}^{N \times N}.
$$

Here $a^T$ denotes the transpose of a vector $a$. We now discuss a few standard distributions.

**Example** (Gaussian distribution). We use the notation $X \sim N(m, \sigma^2)$ to denote a univariate Gaussian random variable with mean $\bar{x}$ and variance $\sigma^2$, with PDF given by

$$
\pi_X(x) = \frac{1}{\sqrt{2\pi\sigma}} e^{-\frac{1}{2\sigma^2}(x-\bar{x})^2},
$$

$x \in \mathbb{R}$. In the multivariate case, we use the notation $X \sim N(\bar{x}, \Sigma)$ to denote a Gaussian random variable with PDF given by

$$
\pi_X(x) = \frac{1}{(2\pi)^{N/2}|\Sigma|^{1/2}} \exp\left(-\frac{1}{2}(x - \bar{x})^T \Sigma^{-1}(x - \bar{x})\right),
$$

$x \in \mathbb{R}^N$.

**Example** (Laplace distribution and Gaussian mixtures). The univariate Laplace distribution has PDF

$$
\pi_X(x) = \frac{\lambda}{2} e^{-\lambda|x|},
$$

$x \in \mathbb{R}$. This may be rewritten as

$$
\pi_X(x) = \int_{0}^{\infty} \frac{1}{\sqrt{2\pi\sigma}} e^{-x^2/(2\sigma^2)} \frac{\lambda^2}{2} e^{-\lambda^2\sigma^2/2} d\sigma,
$$

which is a weighted Gaussian PDF with mean zero and variance $\sigma^2$, integrated over $\sigma$. Replacing the integral by a Riemann sum over a sequence of quadrature points $\{\sigma_j\}_{j=1}^J$, we obtain

$$
\pi_X(x) \approx \sum_{j=1}^{J} \alpha_j \frac{1}{\sqrt{2\pi\sigma_j}} e^{-x^2/(2\sigma_j^2)}, \quad \alpha_j \propto \frac{\lambda^2}{2} e^{-\lambda^2\sigma_j^2/2} (\sigma_j - \sigma_{j-1})
$$

and the constant of proportionality is chosen such that the weights $\alpha_j$ sum to one. This is an example of a **Gaussian mixture** distribution, namely a weighted sum of Gaussians. In this case, the Gaussians are all centred on $x = 0$; the most general form of a Gaussian mixture is

$$
\pi_X(x) = \sum_{j=1}^{J} \alpha_j \frac{1}{\sqrt{2\pi\sigma_j}} e^{-(x-x_j)^2/(2\sigma_j^2)},
$$

with weights $\alpha_j > 0$ subject to $\sum_{j=1}^{J} \alpha_j = 1$, and locations $-\infty < x_j < \infty$. Univariate Gaussian mixtures generalize to mixtures of multi-variate Gaussians in the obvious manner.

**Example** (Point distribution). As a final example, we consider the point measure $\mu_{x_0}$ defined by

$$
\int_X f(x) \mu_{x_0}(dx) = f(x_0).
$$

Using the Dirac delta notation $\delta(\cdot)$ this can be formally written as $\mu_{x_0}(dx) = \delta(x - x_0) dx$. The associated random variable $X$ has the certain outcome $X(\omega) = x_0$ for almost all $\omega \in \Omega$. One can call such a random variable deterministic, and write $X = x_0$ for short. Note that the point measure is not absolutely continuous with respect to the Lebesgue measure, i.e., there is no corresponding probability density function.
We now briefly discuss pairs of random variables $X_1$ and $X_2$ over the same target space $\mathcal{X}$. Formally, we can treat them as a single random variable $Z = (X_1, X_2)$ over $\mathcal{Z} = \mathcal{X} \times \mathcal{X}$ with a joint distribution $\mu_{X_1, X_2}(x_1, x_2) = \mu_Z(z)$.

**Definition** (Marginals, independence, conditional probability distributions). Let $X_1$ and $X_2$ denote two random variables on $\mathcal{X}$ with joint PDF $\pi_{X_1, X_2}(x_1, x_2)$. The two PDFs
\[
\pi_{X_1}(x_1) = \int_{\mathcal{X}} \pi_{X_1, X_2}(x_1, x_2)dx_2
\]
and
\[
\pi_{X_2}(x_2) = \int_{\mathcal{X}} \pi_{X_1, X_2}(x_1, x_2)dx_1,
\]
respectively, are called the marginal PDFs, i.e. $X_1 \sim \pi_{X_1}$ and $X_2 \sim \pi_{X_2}$. The two random variables are called independent if
\[
\pi_{X_1, X_2}(x_1, x_2) = \pi_{X_1}(x_1) \pi_{X_2}(x_2).
\]
We also introduce the conditional PDFs
\[
\pi_{X_1|X_2}(x_1|x_2) = \frac{\pi_{X_1, X_2}(x_1, x_2)}{\pi_{X_2}(x_2)}
\]
and
\[
\pi_{X_2|X_1}(x_2|x_1) = \frac{\pi_{X_1, X_2}(x_1, x_2)}{\pi_{X_1}(x_1)}.
\]

**Example** (Gaussian joint distributions). A Gaussian joint distribution $\pi_{XY}(x, y)$, $x, y \in \mathbb{R}$, with mean $(\bar{x}, \bar{y})$ and covariance matrix
\[
\Sigma = \begin{bmatrix}
\sigma^2_{xx} & \sigma^2_{xy} \\
\sigma^2_{yx} & \sigma^2_{yy}
\end{bmatrix}
\]
leads to a Gaussian conditional distribution
\[
\pi_X(x|y) = \frac{1}{\sqrt{2\pi\sigma^2_c}} e^{-(x-x_c)^2/(2\sigma^2_c)},
\]
with conditional mean
\[
\bar{x}_c = \bar{x} + \sigma^2_{xy}\sigma^2_{yy}^{-1}(y - \bar{y})
\]
and conditional variance
\[
\sigma^2_c = \sigma^2_{xx} - \sigma^2_{xy}\sigma^2_{yy}^{-1}\sigma^2_{yx}.
\]
For given $y$, we define $X|y$ as the random variable with conditional probability distribution $\pi_X(x|y)$, and write $X|y \sim \mathcal{N}(\bar{x}_c, \sigma^2_c)$.

### 1.2 Bayesian inference

We start this section by considering transformations of random variables. A typical scenario is the following one. Given a pair of independent random variables $\Xi$ with values in $\mathcal{Y} = \mathbb{R}^K$ and $X$ with values in $\mathcal{X} = \mathbb{R}^N$ together with a continuous map $h : \mathbb{R}^N \rightarrow \mathbb{R}^K$, we define a new random variable
\[
Y = h(X) + \Xi.
\]
The map $h$ is called the observation operator, which yields observed quantities given a particular value $x$ of the state variable $X$, and $\Xi$ represents measurement errors.

**Theorem** (PDF for transformed random variable). Assume that both $X$ and $\Xi$ are absolutely continuous, then $Y$ is absolutely continuous with PDF
\[
\pi_Y(y) = \int_{\mathcal{X}} \pi_\Xi(y-h(x))\pi_X(x)dx.
\]
If $X$ is a deterministic variable, i.e. $X = x_0$ for an appropriate $x_0 \in \mathbb{R}^N$, then the PDF simplifies to
\[
\pi_Y(y) = \pi_\Xi(y-h(x_0)).
\]
Proof. We start with \( X = x_0 \). Then \( Y - h(x_0) = \Xi \) which immediately implies the stated result. In the general case, consider the conditional probability

\[
\pi_Y(y|x_0) = \pi_{\Xi}(y - h(x_0)).
\]

Equation (3) then follows from the implied joint distribution

\[
\pi_{XY}(x,y) = \pi_Y(y|x)\pi_X(x)
\]

and subsequent marginalization, i.e.

\[
\pi_Y(y) = \int_{\mathcal{X}} \pi_{XY}(y,x)dx = \int_{\mathcal{X}} \pi_Y(y|x)\pi_X(x)dx.
\]

The problem of predicting the distribution \( \pi_Y \) of \( Y \) given a particular configuration of the state variable \( X = x_0 \) is called the forward problem. The problem of predicting the distribution of the state variable \( X \) given an observation \( Y = y_0 \) gives rise to an inference problem, which is defined more formally as follows.

**Definition (Bayesian inference).** Given a particular value \( y_0 \in \mathbb{R}^K \), we consider the associated conditional PDF \( \pi_X(x|y_0) \) for the random variable \( X \). From

\[
\pi_{XY}(x,y) = \pi_Y(y|x)\pi_X(x) = \pi_X(x|y)\pi_Y(y)
\]

we obtain Bayes’ formula

\[
\pi_X(x|y_0) = \frac{\pi_X(y_0|x)\pi_X(x)}{\pi_Y(y_0)}
\]  

(4)

The object of Bayesian inference is to obtain \( \pi_X(x|y_0) \).

Since \( \pi_Y(y_0) \neq 0 \) is a constant, Equation (4) can be written as

\[
\pi_X(x|y_0) \propto \pi_X(y_0|x)\pi_X(x) = \pi_{\Xi}(y_0 - h(x))\pi_X(x),
\]

where the constant of proportionality depends only on \( y_0 \). We denote \( \pi_X(x) \) the prior PDF of the random variable \( X \) and \( \pi_X(x|y_0) \) the posterior PDF. The function \( \pi(y_0|x) \) is called the likelihood function.

Having obtained a posterior PDF \( \pi_X(x|y_0) \), it is often necessary to provide an estimate of a “most likely” value of \( x \) conditioned on \( y_0 \). Bayesian estimators for \( x \) are defined as follows.

**Definition (Bayesian estimators).** Given a posterior PDF \( \pi_X(x|y_0) \) we define a Bayesian estimator \( \hat{x} \in \mathcal{X} \) by

\[
\hat{x} = \arg \min_{x' \in \mathcal{X}} \int \mathcal{L}(x',x)\pi_X(x|y_0)dx
\]

where \( \mathcal{L}(x',x) \) is an appropriate loss function. Popular choices include the maximum a posteriori (MAP) estimator with \( \hat{x} \) corresponding to the modal value of \( \pi_X(x|y_0) \). The MAP estimator formally corresponds to the loss function \( \mathcal{L}(x',x) = 1_{\{x' \neq x\}} \). The posterior median estimator corresponds to \( \mathcal{L}(x',x) = \|x' - x\| \) while the minimum mean square error estimator (or conditional mean estimator)

\[
\hat{x} = \int_{\mathcal{X}} x\pi_X(x|y_0)dx
\]

results from \( \mathcal{L}(x',x) = \|x' - x\|^2 \).

We now consider an important example for which the posterior can be computed analytically.
Example (Bayes’ formula for Gaussian distributions). Consider the case of a scalar observation, i.e. $K = 1$, with $\Xi \sim N(0, \sigma_{rr}^2)$. Then

$$
\pi_\Xi(h(x) - y) = \frac{1}{\sqrt{2\pi\sigma_{rr}}} e^{-\frac{1}{2\sigma_{rr}^2}(h(x) - y)^2}.
$$

We also assume that $X \sim N(\bar{x}, P)$ and that $h(x) = Hx$. Then the posterior distribution of $X$ given $y = y_0$ is also Gaussian with mean

$$
\bar{x}_c = \bar{x} - PH^T(HPH^T + \sigma_{rr}^2)^{-1}(H\bar{x} - y_0)
$$

and covariance matrix

$$
P_c = P - PH^T(HPH^T + \sigma_{rr}^2)^{-1}HP.
$$

These are the famous Kalman update formulas which follow from the fact that the product of two Gaussian distributions is also Gaussian, where the variance of $Y = HX + \Sigma$ is given by

$$
\sigma_{yy}^2 = HPH^T + \sigma_{rr}^2
$$

and the vector of covariances between $x \in \mathbb{R}^N$ and $y = Hx \in \mathbb{R}$ is given by $PH^T$. For Gaussian random variables, the MAP, posterior median, and minimum mean square error estimators coincide and are given by $\bar{x}_c$. The case of vector-valued observations will be discussed in Section 3.3. Finally note that $\bar{x}_c$ solves the minimization problem

$$
\bar{x}_c = \arg\min_{x \in \mathbb{R}^N} \left\{ \frac{1}{2} (x - \bar{x})^T P^{-1} (x - \bar{x}) + \frac{1}{2R} (Hx - y_0)^2 \right\},
$$

which can be viewed as a regularization of the ill-posed inverse problem

$$
y_0 = Hx, \quad x \in \mathbb{R}^N, \quad N > 1,
$$

in the sense of Tikhonov. A standard Tikhonov regularization would be based on $P^{-1} = \delta I$ with the regularization parameter $\delta > 0$ appropriately chosen. In the Bayesian approach to inverse problems the regularization term is instead determined by the Gaussian prior $\pi_X$.

We mention in passing that Bayes’ formula has to be replaced by the Radon-Nikodym derivative in the case where the prior distribution is not absolutely continuous with respect to the Lebesgue measure (or in case the space $\mathcal{X}$ does not admit a Lebesgue measure). Consider as an example the case of an empirical measure $\mu_X$ centered about the $M$ samples $x_i \in \mathcal{X}$, $i = 1, \ldots, M$, i.e. a weighted sum of point measures given by

$$
\mu_X(dx) = \frac{1}{M} \sum_{i=1}^M \mu_{x_i}(dx).
$$

Then the resulting posterior measure $\mu_X(\cdot | y_{obs})$ is absolutely continuous with respect to $\mu_X$, i.e. there exists a Radon-Nikodym derivative such that

$$
\int_{\mathcal{X}} f(x) \mu_X(dx | y_0) = \int_{\mathcal{X}} f(x) \frac{d\mu_X(x | y_0)}{d\mu_X(x)} \mu_X(dx)
$$

and the Radon-Nikodym derivative satisfies

$$
\frac{d\mu_X(x | y_0)}{d\mu_X(x)} \propto \pi_\Xi(h(x) - y_0).
$$

Furthermore, the explicit expression for the posterior measure is given by

$$
\mu_X(dx | y_0) = \sum_{i=1}^M w_i \mu_{x_i}(dx),
$$

with weights $w_i \geq 0$ defined by

$$
w_i \propto \pi_\Xi(h(x_i) - y_0),
$$

and the constant of proportionality is determined by the condition $\sum_{i=1}^M w_i = 1$. 

6
1.3 Coupling of random variables

We have seen that under Bayes’ formula a prior probability measure $\mu_X(\cdot)$ on $X$ is transformed into a posterior probability measure $\mu_X(\cdot|y_0)$ on $X$ conditioned on the observation $y_0 = Y(\omega)$. With each of the probability measures, we can associate random variables such that, e.g., $X_1 \sim \mu_X$ and $X_2 \sim \mu_X(\cdot|y_0)$. However, while Bayes’ formula leads to a transformation of measures, it does not imply a specific transformation on the level of the associated random variables; many different transformations of random variables lead to the same probability measure. In this section we will, therefore, introduce the concept of coupling two probability measures.

**Definition** (Coupling). Let $\mu_{X_1}$ and $\mu_{X_2}$ denote two probability measures on a space $X$. A coupling of $\mu_{X_1}$ and $\mu_{X_2}$ consists of a pair $Z = (X_1, X_2)$ of random variables such that $X_1 \sim \mu_{X_1}$, $X_2 \sim \mu_{X_2}$, and $Z \sim \mu_Z$. The joint measure $\mu_Z$ on the product space $Z = X \times X$, is called the *transference plan* for this coupling. The set of all transference plans is denoted by $\Pi(\mu_{X_1}, \mu_{X_2})$.

Here, we will discuss different forms of couplings assuming that both the source and target distributions are explicitly known, whilst applications to Bayes formula (4) will be discussed in Sections 1.4 and 3. In the context of Bayesian statistics, knowledge of the source (prior) distribution and the likelihood implies knowledge of the target (posterior) distribution.

Since prior distributions in Bayesian inference are generally assumed to be absolutely continuous, the discussion of couplings will be restricted to the less abstract case of $X = \mathbb{R}^N$ and $\mu_{X_1}(dx) = \pi_{X_1}(x)dx$, $\mu_{X_2}(dz) = \pi_{X_2}(z)dz$. In other words, we assume that the marginal measures are absolutely continuous. We will, in general, not assume that the coupling is absolutely continuous on $Z = X \times X = \mathbb{R}^{2N}$. Clearly, couplings always exist since one can use the trivial product coupling

$$\pi_Z(x_1, x_2) = \pi_{X_1}(x_1)\pi_{X_2}(x_2),$$

in which case the associated random variables $X_1$ and $X_2$ are independent. The more interesting case is that of a deterministic coupling.

**Definition** (Deterministic coupling). Assume that we have a random variable $X_1$ with law $\mu_{X_1}$ and a second probability measure $\mu_{X_2}$. A diffeomorphism $T : X \rightarrow X$ is called a *transport map* if the induced random variable $X_2 = T(X_1)$ satisfies

$$\int_X f(x_2)\mu_{X_2}(dx_2) = \int_X f(T(x_1))\mu_{X_1}(dx_1)$$

for all suitable functions $f : X \rightarrow \mathbb{R}$. The associated coupling

$$\mu_Z(dx_1, dx_2) = \delta(x_2 - T(x_1))\mu_{X_1}(dx_1)dx_2,$$

where $\delta(\cdot)$ is the standard Dirac distribution, is called a *deterministic coupling*. Note that $\mu_Z$ is not absolutely continuous even if both $\mu_{X_1}$ and $\mu_{X_2}$ are.

Using

$$\int_X f(x_2)\delta(x_2 - T(x_1))dx_2 = f(T(x_1)),$$

it indeed follows from the above definition of $\mu_Z$ that

$$\int_X f(x_2)\mu_{X_2}(dx_2) = \int_Z f(x_2)\mu_Z(dx_1, dx_2) = \int_X f(T(x_1))\mu_{X_1}(dx_1).$$

We discuss a simple example.

**Example** (One-dimensional transport map). Let $\pi_{X_1}(x) \geq 0$ and $\pi_{X_2}(x) > 0$ denote two PDFs on $X = \mathbb{R}$. We define the associated cumulative distribution functions by

$$F_{X_1}(x) = \int_{-\infty}^x \pi_{X_1}(x')dx', \quad F_{X_2}(x) = \int_{-\infty}^x \pi_{X_2}(x')dx'.$$
Since $F_{X_2}$ is monotonically increasing, it has a unique inverse $F_{X_2}^{-1}(p)$ for $p \in [0, 1]$. The inverse may be used to define a transport map that transforms $X_1$ into $X_2$ as follows,

$$X_2 = T(X_1) = F_{X_2}^{-1}(F_{X_1}(X_1)).$$

For example, consider the case where $X_1$ is a random variable with uniform distribution $U([0, 1])$ and $X_2$ is a random variable with standard normal distribution $N(0, 1)$. Then the transport map between $X_1$ and $X_2$ is simply the inverse of the cumulative distribution function

$$F_{X_2}(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{x} e^{-(x')^2/2} dx',$$

which provides a standard tool for converting uniformly distributed random numbers to normally distributed ones.

We now extend this transform method to random variables in $\mathbb{R}^N$ with $N = 2$.

**Example** (Knothe-Rosenblatt rearrangement). Let $\pi_{X_1}(x^1, x^2)$ and $\pi_{X_2}(x^1, x^2)$ denote two PDFs on $x = (x^1, x^2) \in \mathbb{R}^2$. A transport map between $\pi_{X_1}$ and $\pi_{X_2}$ can be constructed in the following manner. We first find the two one-dimensional marginals $\pi_{X_1}(x^1)$ and $\pi_{X_2}(x^1)$ of the two PDFs. In the previous example we have seen how to construct a transport map $X_1^3 = T_1(X_1^1)$ which couples these two one-dimensional marginal PDFs. Here $X_1^1$ denotes the first component of the random variables $X_i$, $i = 1, 2$. Next we write

$$\pi_{X_1}(x^1, x^2) = \pi_{X_1}(x^2 | x^1) \pi_{X_1}(x^1), \quad \pi_{X_2}(x^1, x^2) = \pi_{X_2}(x^2 | x^1) \pi_{X_2}(x^1)$$

and find a transport map $X_2^3 = T_2(X_1^1, X_2^1)$ by considering one-dimensional couplings between $\pi_{X_1}(x^2 | x^1)$ and $\pi_{X_2}(x^2 | T(x^1))$ with $x^1$ fixed. The associated joint distribution is given by

$$\pi_{Z}(x_1^1, x_1^2, x_2^1, x_2^2) = \delta(x_2^1 - T_1(x_1^1)) \delta(x_2^2 - T_2(x_1^1, x_1^2)) \pi_{X_1}(x_1^1, x_1^2).$$

This is called the *Knothe-Rosenblatt rearrangement*, also well-known to statisticians under the name of *conditional quantile transforms*. It can be extended to $\mathbb{R}^N$, $N \geq 3$ in the obvious way by introducing the conditional PDFs

$$\pi_{X_1}(x^3 | x^1, x^2), \quad \pi_{X_2}(x^3 | x^1, x^2),$$

and by constructing an appropriate map $X_3^3 = T_3(X_1^1, X_2^1, X_3^1)$ from those conditional PDFs for fixed pairs $(x_1^1, x_2^1)$ and $(x_2^1, x_3^1) = (T_1(x_1^1), T_2(x_1^1, x_2^1))$ etc. While the Knothe-Rosenblatt rearrangement can be used in quite general situations, it has the undesirable property that the map depends on the choice of ordering of the variables i.e., in two dimensions a different map is obtained if one instead first couples the $x^2$ components.

**Example** (Affine transport maps for Gaussian distributions). Consider two Gaussian distributions $N(\bar{x}_1, \Sigma_1)$ and $N(\bar{x}_2, \Sigma_2)$ in $\mathbb{R}^N$ with means $\bar{x}_1$ and $\bar{x}_2$ and covariance matrices $\Sigma_1$ and $\Sigma_2$, respectively. We first define the *square root* $\Sigma^{1/2}$ of a symmetric positive definite matrix $\Sigma$ as the unique symmetric positive definite matrix which satisfies $\Sigma^{1/2} \Sigma^{1/2} = \Sigma$. Then the affine transformation

$$x_2 = T(x_1) = \bar{x}_2 + \Sigma_2^{1/2} \Sigma_1^{-1/2}(x_1 - \bar{x}_1)$$

(5)

provides a deterministic coupling. Indeed, we find that

$$(x_2 - \bar{x}_2)^T \Sigma_2^{-1} (x_2 - \bar{x}_2) = (x_1 - \bar{x}_1)^T \Sigma_1^{-1} (x_1 - \bar{x}_1)$$

under the suggested coupling. The proposed coupling is, of course, not unique since

$$x_2 = T(x_1) = \bar{x}_2 + \Sigma_2^{1/2} Q \Sigma_1^{-1/2} (x_1 - \bar{x}_1),$$

where $Q$ is an orthogonal matrix, also provides a coupling. We will see in Section that a coupling between Gaussian random variables is also at the heart of the ensemble square root filter formulations of sequential data assimilation.
Deterministic couplings can be viewed as a special case of a Markov process \( \{X_n\}_{n \in \{1, 2\}} \) defined by

\[
\pi_{X_2}(x_2) = \int_{X_1} \pi(x_2|x_1)\pi_{X_1}(x_1)dx_1,
\]

where \( \pi(x_2|x_1) \) denotes an appropriate conditional PDF for the random variable \( X_2 \) given \( X_1 = x_1 \). Indeed, we simply have

\[
\pi(x_2|x_1) = \delta(x_2 - T(x_1))
\]

for deterministic couplings. We will come back to Markov processes in Section 2.

The trivial coupling \( \pi_Z(x_1, x_2) = \pi_{X_1}(x_1)\pi_{X_2}(x_2) \) leads to a zero correlation between the induced random variables \( X_1 \) and \( X_2 \) since their covariance is

\[
\text{cov}(X_1, X_2) = \mathbb{E}_Z[(x_1 - \bar{x}_1)(x_2 - \bar{x}_2)^T] = \mathbb{E}_Z[x_1x_2^T] - \bar{x}_1\bar{x}_2^T = 0,
\]

where \( \bar{x}_i = \mathbb{E}_{X_i}[x] \). A transport map leads instead to the covariance matrix

\[
\text{cov}(X_1, X_2) = \mathbb{E}_Z[x_1x_2^T] - \mathbb{E}_{X_1}[x_1](\mathbb{E}_{X_2}[x_2])^T = \mathbb{E}_{X_1}[x_1T(x_1)^T] - \bar{x}_1\bar{x}_2^T,
\]

which is non-zero in general. If several transport maps exist then one could choose the one that maximizes the covariance. Consider, for example, univariate random variables \( X_1 \) and \( X_2 \), then maximizing their covariance for given marginal PDFs has an important geometric interpretation: it is equivalent to minimizing the mean square distance between \( x_1 \) and \( T(x_1) = x_2 \) given by

\[
\mathbb{E}_Z[|x_2 - x_1|^2] = \mathbb{E}_{X_1}[|x_1|^2] + \mathbb{E}_{X_2}[|x_2|^2] - 2\mathbb{E}_Z[x_1x_2]
\]

\[
= \mathbb{E}_{X_1}[|x_1|^2] + \mathbb{E}_{X_2}[|x_2|^2] - 2\mathbb{E}_Z[(x_1 - \bar{x}_1)(x_2 - \bar{x}_2)] - 2\bar{x}_1\bar{x}_2
\]

\[
= \mathbb{E}_{X_1}[|x_1|^2] + \mathbb{E}_{X_2}[|x_2|^2] - 2\bar{x}_1\bar{x}_2 - 2\text{cov}(X_1, X_2).
\]

Hence finding a joint measure \( \mu \) that minimizes the expectation of \( (x_1 - x_2)^2 \) simultaneously maximizes the covariance between \( X_1 \) and \( X_2 \). This geometric interpretation leads to the celebrated Monge-Kantorovitch problem.

**Definition** (Monge-Kantorovitch problem). A transference plan \( \mu_Z^* \in \Pi(\mu_{X_1}, \mu_{X_2}) \) is called the solution to the Monge-Kantorovitch problem with cost function \( c(x_1, x_2) = \|x_1 - x_2\|^2 \) if

\[
\mu_Z^* = \arg\inf_{\mu_Z \in \Pi(\mu_{X_1}, \mu_{X_2})} \mathbb{E}_Z[\|x_1 - x_2\|^2]. \tag{6}
\]

The associated function

\[
W(\mu_{X_1}, \mu_{X_2}) = \mathbb{E}_Z[\|x_1 - x_2\|^2], \quad \text{law}(Z) = \mu_Z^*
\]

is called the \( L^2 \)-Wasserstein distance of \( \mu_{X_1} \) and \( \mu_{X_2} \).

**Theorem** (Optimal transference plan). If the measures \( \mu_{X_i} \), \( i = 1, 2 \), are absolutely continuous, then the optimal transference plan that solves the Monge-Kantorovitch problem corresponds to a deterministic coupling

\[
X_2 = T(X_1) = \nabla_x \psi(X_1),
\]

for some convex potential \( \psi : \mathbb{R}^N \to \mathbb{R} \).

**Proof.** We only demonstrate that the solution to the Monge-Kantorovitch problem is of the desired form when the infimum in (6) is restricted to deterministic couplings. See [19] for a complete proof and also for more general results in terms of subgradients and weaker conditions on the two marginal measures.

We denote the associated PDFs by \( \pi_{X_i} \), \( i = 1, 2 \). We also introduce the inverse transfer map \( X_1 = S(X_2) = T^{-1}(X_2) \) and consider the functional

\[
\mathcal{L}[S, \Psi] = \frac{1}{2} \int_{\mathbb{R}^N} \|S(x) - x\|^2\pi_{X_2}(x)dx + \int_{\mathbb{R}^N} [\Psi(S(x))\pi_{X_2}(x) - \Psi(x)\pi_{X_1}(x)]dx.
\]
in $S$ and a potential $\Psi : \mathbb{R}^N \to \mathbb{R}$. We note that
\[
\int_{\mathbb{R}^N} [\Psi(S(x)) \pi_{X_2}(x) - \Psi(x) \pi_{X_1}(x)] dx = \\
\int_{\mathbb{R}^N} \Psi(x) [\pi_{X_2}(T(x)) |DT(x)| - \pi_{X_1}(x)] dx
\]
by a simple change of variables. Here $|DT(x)|$ denotes the determinant of the Jacobian matrix of $T$ at $x$ and the potential $\Psi$ can be interpreted as a Lagrange multiplier enforcing the coupling of the two marginal PDFs under the desired transport map.

Taking variational derivatives with respect to $S$ and $\Psi$, we obtain two equations
\[
\frac{\delta \mathcal{L}}{\delta S} = \pi_{X_2}(x) \left((S(x) - x) + \nabla_x \Psi(S(x))\right) = 0
\]
and
\[
\frac{\delta \mathcal{L}}{\delta \Psi} = -\pi_{X_1}(x) + \pi_{X_2}(T(x)) |DT(x)| = 0
\]
characterizing critical points of the functional $\mathcal{L}$. The first equality implies
\[
x_2 = x_1 + \nabla_x \Psi(x_1) = \nabla_x \left(\frac{1}{2} \xi_x^T \xi_1 + \Psi(x_1)\right) =: \nabla_x \psi(x_1)
\]
and the second recovers our Ansatz that $T$ transforms $\pi_{X_1}$ into $\pi_{X_2}$ as a result of the Lagrange multiplier $\Psi$.

**Example** (Optimal transport maps for Gaussian distributions). Consider two Gaussian distributions $N(\bar{x}_1, \Sigma_1)$ and $N(\bar{x}_2, \Sigma_2)$ in $\mathbb{R}^N$ with means $\bar{x}_1$ and $\bar{x}_2$ and covariance matrices $\Sigma_1$ and $\Sigma_2$, respectively. We had previously discussed the deterministic coupling \([3]\). However, the induced affine transformation $x_2 = T(x_1)$ cannot not be generated from a potential $\psi$ since the matrix $\Sigma_2^{1/2} \Sigma_1^{-1/2}$ is not symmetric. Indeed the optimal coupling in the sense of Monge-Kantorovitch with cost function $c(x_1, x_2) = \|x_1 - x_2\|^2$ is provided by
\[
x_2 = T(x_1) := \bar{x}_2 + \Sigma_2^{1/2} \left[\Sigma_2^{1/2} \Sigma_1 \Sigma_2^{-1/2}\right]^{-1/2} \Sigma_2^{1/2} (x_1 - \bar{x}_1).
\]
See \([40]\) for a derivation. The following generalization will be used in Section \([3]\). Assume that a matrix $A \in \mathbb{R}^{N \times M}$ is given such that $\Sigma_2 = AA^T$. Clearly we can chose $A = \Sigma_2^{1/2}$ in which case $M = N$ and $A$ is symmetric. However we allow for $A$ to be non-symmetric and $M$ can be different from $N$. An important observation is that one can replace $\Sigma_2^{1/2}$ in \((3)\) by $A$ and $A^T$, respectively, i.e.
\[
T(x_1) = \bar{x}_2 + A \left[A^T \Sigma_1 A\right]^{-1/2} A^T (x_1 - \bar{x}_1).
\]

While optimal couplings are of broad theoretical and practical interest, their computational implementation can be very demanding. In Section \([3]\), we will discuss an embedding method originally due to Jürgen Moser \([37]\), which leads to a generally non-optimal but computationally more tractable formulation in the context of Bayesian statistics and data assimilation.

### 1.4 Monte Carlo methods

Monte Carlo methods, also called particle or ensemble methods depending on the context in which they are being used, can be used to approximate statistics, namely expectation values $E_X[f]$, for a random variable $X$. We begin by discussing the special case $f(x) = x$, namely, the mean.

**Definition** (Empirical mean). Given a sequence $X_i$, $i = 1, \ldots, M$, of independent random variables with identical measure $\mu_X$, the empirical mean is
\[
\bar{x}_M = \frac{1}{M} \sum_{i=1}^{M} X_i(\omega) = \frac{1}{M} \sum_{i=1}^{M} x_i
\]
with samples $x_i = X_i(\omega)$.
Of course, $\bar{x}_M$ itself is the realization of a random variable $X_M$ and we consider the mean squared error (MSE)

$$
\text{MSE}(\bar{x}) = \mathbb{E}_{X_M}[(\bar{x}_M - \bar{x})^2] = (\mathbb{E}_{X_M}[(\bar{x}_M - \bar{x})^2] + \mathbb{E}_{X_M}[(\bar{x}_M - \mathbb{E}_{X_M}[\bar{x}_M])^2])
$$

with respect to the exact mean value $\bar{x} = \mathbb{E}_{X}[x]$. We have broken down the MSE into two components: squared bias and variance. Such a decomposition is possible for any estimator and is known as the bias-variance decomposition. The particular estimator $X_M$ is called unbiased since $\mathbb{E}_{X_M}[X_M] = \bar{x}$ for any $M > 1$. Furthermore $X_M$ converges weakly to $\bar{x}$ under the central limit theorem provided $\mu_X$ has finite second-order moments, i.e.

$$
\lim_{M \to \infty} \mathbb{E}_{X_M}[(\bar{x}_M - \mathbb{E}_{X_M}[\bar{x}_M])^2] = 0.
$$

It remains to generate samples $x_i = X_1(\omega)$ from the required distribution. Methods to do this include the von Neumann rejection method and Markov chain Monte Carlo methods, which we will briefly discuss in Section 2. Often the prior distribution is assumed to be Gaussian, in which case explicit random number generators are available. We now turn to the situation where samples from the prior distribution are available, and are to be used to approximate the mean of the posterior distribution (or any other expectation value).

Importance sampling is a classical method to approximate expectation values of a random variable $X^t \sim \pi_{X^t}$ using samples from a random variable $X^p \sim \pi_{X^p}$, which requires that the target PDF $\pi_{X^t}$ is absolutely continuous with respect to proposal PDF $\pi_{X^p}$. This is the case for the prior and posterior PDFs from Bayes’ formula 1, i.e. we set the proposal distribution $\pi_{X^p}(x)$ equal to the prior distribution $\pi_X(x)$ and the posterior distribution $\pi_X(x|y_0) \propto \pi_Y(y_0|x)\pi_X(x)$ becomes the target distribution $\pi_{X^p}(x)$.

**Definition** (Importance sampling for Bayesian estimation). Let $x^\text{prior}_i, i = 1, \ldots, M$, denote samples from the prior PDF $\pi_X(x)$, then the importance sampler estimate of the mean of the posterior $\pi_X(x|y_0)$ is

$$
\bar{x}_M^\text{post} = \sum_{i=1}^M w_i x^\text{prior}_i
$$

with importance weights

$$
w_i = \frac{\pi_Y(y_0|x^\text{prior}_i)}{\sum_{i=1}^M \pi_Y(y_0|x^\text{prior}_i)}
$$

Importance sampling becomes statistically inefficient when the weights have largely varying magnitude, which becomes particularly significant for high-dimensional problems. To demonstrate this effect consider a uniform prior on the unit hypercube $V = [0, 1]^N$. Each of the $M$ samples $x_i$ from this prior formally represent a hypercube with volume $1/M$. However, the likelihood measures the distance of a sample $x_i$ to the observation $y_0$ in the Euclidean distance and the volume of a hypersphere decreases rapidly relative to that of an associated hypercube as $N$ increases. Within the framework of the bias-variance decomposition of a mean squared error such as 10, the curse of dimensionality manifests itself in large variances for finite $M$.

To counteract this curse of dimensionality, one may utilize the concept of coupling. In other words, assume that we have a transport map $x^\text{post} = T(x^\text{prior})$ which couples the prior and posterior distributions. Then, with transformed samples $x^\text{post}_i = T(x^\text{prior}_i), i = 1, \ldots, M$, we obtain the estimator

$$
\bar{x}_M^\text{post} = \sum_{i=1}^M \tilde{w}_i x^\text{post}_i
$$

with equal weights $\tilde{w}_i = 1/M$.

Sometimes one cannot couple the prior and posterior distribution directly, or the coupling is too expensive computationally. Then one can attempt to find a coupling between the prior PDF $\pi_X(x)$ and an approximation $\tilde{\pi}_X(x|y_0)$ to the posterior PDF $\pi_X(x|y_0) \propto \pi_Y(y_0|x)\pi_X(x)$. Given an associated transport map $X^\text{prop} = \tilde{T}(X^\text{prior})$, i.e.

$$
\tilde{\pi}_X(\tilde{T}(x)|y_0) = \pi_X(x)|D\tilde{T}(x)|^{-1},
$$
one then takes \( \tilde{\pi}_X(x|y_0) \) as the proposal density \( \pi_X(x) \) in an importance sampler with realizations \( x^\text{prop}_i \), \( i = 1, \ldots, M \), defined by
\[
x^\text{prop}_i = T(x^\text{prior}_i).
\]
An asymptotically unbiased estimator for the posterior mean is now provided by
\[
x^\text{post}_M = \sum_{i=1}^{M} \tilde{w}_i x^\text{prop}_i
\]
with weights
\[
\tilde{w}_i \propto \frac{\pi_Y(y_0|x^\text{prop}_i)\pi_X(x^\text{prop}_i)}{\hat{\pi}_X(x^\text{prop}_i|y_0)} = \pi_Y(y_0|x^\text{prop}_i)|D^T(x^\text{prior}_i)|\frac{\pi_X(x^\text{prop}_i)}{\hat{\pi}_X(x^\text{prior}_i)},
\]
i.e. \( \tilde{w}_i = \frac{\pi_Y(y_0|x^\text{prop}_i)\pi_X(x^\text{prop}_i)}{\hat{\pi}_X(x^\text{prop}_i|y_0)} \). For fixed \( \omega \), \( \pi_X(x) = \pi_X(x|y_0) = \pi_X(x) \) leads to standard importance sampling using prior samples, i.e. \( x^\text{prop}_i = x^\text{prior}_i \).

We will return to the subject of sampling from the posterior distribution in Sections 2.3 and 3.2.

References
An excellent introduction to many topics covered in this survey is [22]. Bayesian inference and a Bayesian perspective on inverse problems are discussed in [24], [38], [31]. The monographs [49, 50] provide an in depth introduction to optimal transportation and coupling of random variables. Monte Carlo methods are covered in [32]. We also point to [20] for a discussion of estimation and regression methods from a bias-variance perspective. A discussion of infinite-dimensional Bayesian inference problems can be found in [15].

2 Elementary stochastic processes

In this section, we collect basic results concerning stochastic processes which are of relevance for the data assimilation problem.

Definition (Stochastic process). Let \( T \) be a set of indices. A stochastic process is a family \( \{X_t\}_{t \in T} \) of random variables on a common space \( \mathcal{X} \), i.e. \( X_t(\omega) \) \( \in \mathcal{X} \).

In the context of dynamical systems, the variable \( t \) corresponds to time. We distinguish between continuous time \( t \in [0, t_{end}] \subset \mathbb{R} \) or discrete time \( t_n = n\Delta t, n \in \{0, 1, 2, \ldots\} = T \), with \( \Delta t > 0 \) a time-increment. In cases where subscript indices can be confusing we will also use the notations \( X(t) \) and \( X(t_n) \), respectively.

A stochastic process can be seen as a function of two arguments: \( t \) and \( \omega \). For fixed \( \omega \), \( X_t(\omega) \) becomes a function of \( t \in T \), which we call a realization or trajectory of the stochastic process. We will restrict to the case where \( X_t(\omega) \) is continuous in \( t \) (with probability 1) in the case of a continuous time. Alternatively, one can fix the time \( t \in T \) and consider the random variable \( X_t(\cdot) \) and its distribution. More generally, one can consider \( l \)-tuples \( (t_1, t_2, \ldots, t_l) \) and associated \( l \)-tuples of random variables \( (X_{t_1}(\cdot), X_{t_2}(\cdot), \ldots, X_{t_l}(\cdot)) \) and their joint distributions. This leads to concepts such as temporal correlation.

2.1 Discrete time Markov processes

First, we develop the concept of Markov processes for discrete time processes.

Definition (Discrete time Markov processes). The discrete time stochastic process \( \{X_n\}_{n \in T} \) with \( \mathcal{X} = \mathbb{R}^N \) and \( T = \{0, 1, 2, \ldots\} \) is called a (time-independent) Markov process if its joint PDFs can be written as
\[
\pi_n(x_0, x_1, \ldots, x_n) = \pi(x_n|x_{n-1})\pi(x_{n-1}|x_{n-2}) \cdots \pi(x_1|x_0)\pi_0(x_0)
\]
for all \( n \in \{0,1,2,\ldots\} = T \). The associated marginal distributions \( \pi_n = \pi_{X_n} \) satisfy the Chapman-Kolmogorov equation

\[
\pi_{n+1}(x') = \int_{\mathbb{R}^N} \pi(x'|x)\pi_n(x)dx
\]

and the process can be recursively repeated to yield a family of marginal distributions \( \{\pi_n\}_{n \in T} \) for given \( \pi_0 \). This family can also be characterized by the linear Frobenius-Perron operator

\[
\pi_{n+1} = P\pi_n,
\]

which is induced by (15).

The above definition is equivalent to the more traditional definition that a process is Markov if the conditional distributions satisfy

\[
\pi_n(x_n|x_0,x_1,\ldots,x_{n-1}) = \pi(x_n|x_{n-1}).
\]

Note that, contrary to Bayes’ formula (4), which directly yields marginal distributions, the Chapman-Kolmogorov equation (15) starts from a given coupling \( \pi_{X_{n+1}}(x_{n+1},x_n) = \pi(x_{n+1}|x_n)\pi_{X_n}(x_n) \) followed by marginalization to derive \( \pi_{X_{n+1}}(x_{n+1}) \). A Markov process is called time-dependent if the conditional PDF \( \pi(x'|x) \) depends on \( t_n \). While we have considered time-independent processes in this section, we will see in Section 3 that the idea of coupling applied to Bayes’ formula leads to time-dependent Markov processes.

### 2.2 Stochastic difference and differential equations

We start from the stochastic difference equation

\[
X_{n+1} = X_n + \Delta t f(X_n) + \sqrt{2\Delta t}Z_n, \quad t_{n+1} = t_n + \Delta t,
\]

where \( \Delta t > 0 \) is a small parameter (the step-size), \( f \) is a given (Lipschitz continuous) function, and \( Z_n \sim N(0,Q) \) are independent and identically distributed random variables with correlation matrix \( Q \).

The time evolution of the associated marginal densities \( \pi_{X_n} \) is governed by the Chapman-Kolmogorov equation with conditional PDF

\[
\pi(x'|x) = \frac{1}{(4\pi\Delta t)^{N/2}|Q|^{1/2}} \exp \left( -\frac{1}{4\Delta t}(x'-x - \Delta tf(x))^TQ^{-1}(x'-x - \Delta tf(x)) \right).
\]

**Proposition** (Stochastic differential and Fokker-Planck equation). Taking the limit \( \Delta t \to 0 \), one obtains the stochastic differential equation (SDE)

\[
dX_t = f(X_t)dt + \sqrt{2}Q^{1/2}dW_t
\]

for \( X_t \), where \( \{W_t\}_{t \geq 0} \) denotes standard \( N \)-dimensional Brownian motion, and the Fokker-Planck equation

\[
\frac{\partial \pi_X}{\partial t} = -\nabla_x \cdot (\pi_X f) + \nabla_x \cdot (Q \nabla_x \pi_X)
\]

for the marginal density \( \pi_X(x,t) \). Note that \( Q = 0 \) (no noise) leads to the Liouville, transport or continuity equation

\[
\frac{\partial \pi_X}{\partial t} = -\nabla_x \cdot (\pi_X f),
\]

which implies that we may interpret \( f \) as a given velocity field in the sense of fluid mechanics.
Proof. The difference equation (17) is called the Euler-Maruyama method for approximating the SDE (19). See [21, 26] for a discussion on the convergence of (17) to (19) at $\Delta t \to 0$.

The Fokker-Planck equation (20) is the linear combination of a drift and a diffusion term. To simplify the discussion we derive both terms separately from (17) by first considering $f = 0$, $Q \neq 0$ and then $Q = 0$, $f \neq 0$. To simplify the derivation of the diffusion term even further we also assume $x \in \mathbb{R}$ and $Q = 1$. In other words, we show that scalar Brownian motion

$$dX_t = \sqrt{2}dW_t$$

leads to the heat equation

$$\frac{\partial \pi}{\partial t} = \frac{\partial^2 \pi}{\partial x^2}.$$ 

We first note that the conditional PDF (18) reduces to

$$\pi(x'|x) = (4\pi\Delta t)^{-1/2} \exp\left(-\frac{(x' - x)^2}{4\Delta t}\right)$$

under $f(x) = 0$, $Q = 1$, $N = 1$, and the Chapman-Kolmogorov equation (15) becomes

$$\pi_{n+1}(x') = \int_{\mathbb{R}} \frac{1}{\sqrt{4\pi\Delta t}} e^{-y^2/(4\Delta t)} \pi_n(x' + y)dy$$

under the variable substitution $y = x - x'$. We now expand $\pi_n(x' + y)$ in $y$ about $y = 0$, i.e.

$$\pi_n(x' + y) = \pi_n(x') + y \frac{\partial \pi_n}{\partial x}(x') + \frac{y^2}{2} \frac{\partial^2 \pi_n}{\partial x^2}(x') + \cdots,$$

and substitute the expansion into (22).

$$\pi_{n+1}(x') = \int_{\mathbb{R}} \frac{1}{\sqrt{4\pi\Delta t}} e^{-y^2/(4\Delta t)} \pi_n(x')dy$$

$$+ \int_{\mathbb{R}} \frac{1}{\sqrt{4\pi\Delta t}} e^{-y^2/(4\Delta t)} y \frac{\partial \pi_n}{\partial x}(x')dy$$

$$+ \int_{\mathbb{R}} \frac{1}{\sqrt{4\pi\Delta t}} e^{-y^2/(4\Delta t)} \frac{y^2}{2} \frac{\partial^2 \pi_n}{\partial x^2}(x')dy + \cdots.$$ 

The integrals correspond to the zeroth, first and second-order moments of the Gaussian distribution with mean zero and variance $2\Delta t$. Hence

$$\pi_{n+1}(x') = \pi_n(x') + \Delta t \frac{\partial^2 \pi_n}{\partial x^2}(x') + \cdots$$

and it can also easily be shown that the neglected higher-order terms contribute with $O(\Delta t^2)$ terms. Therefore

$$\frac{\pi_{n+1}(x') - \pi_n(x_n)}{\Delta t} = \frac{\partial^2 \pi_n}{\partial x^2}(x') + O(\Delta t),$$

and the heat equation is obtained upon taking the limit $\Delta t \to 0$. The non-vanishing drift case, i.e. $f(x) \neq 0$, while being more technical, can be treated in the same manner.

One can also use (7) to derive Liouville’s equation (21) directly. We set

$$T(x) = x + \Delta tf(x)$$

and note that

$$|DT(x)| = 1 + \Delta t\nabla_x \cdot f + O(\Delta t^2).$$

Hence (7) implies

$$\pi_{X_1} = \pi_{X_2} + \Delta t\pi_{X_2} \nabla_x \cdot f + \Delta t(\nabla_x \pi_{X_2}) \cdot f + O(\Delta t^2)$$

and

$$\frac{\pi_{X_2} - \pi_{X_1}}{\Delta t} = -\nabla_x \cdot (\pi_{X_2}f) + O(\Delta t).$$

Taking the limit $\Delta t \to 0$, we obtain (21).
Following the work of Felix Otto (see, e.g., [41, 49]), we note that in the case of pure diffusion, i.e. \( f = 0 \), the Fokker-Planck equation can be rewritten as a gradient flow system. We first introduce some notation.

**Definition** (differential geometric structure on manifold of probability densities). We formally introduce the manifold of all PDFs on \( X = \mathbb{R}^N \)

\[
\mathcal{M} = \{ \pi : \mathbb{R}^N \to \mathbb{R} : \pi(x) \geq 0, \int_{\mathbb{R}^N} \pi(x)dx = 1 \}
\]

with tangent space

\[
T_{\pi} \mathcal{M} = \{ \phi : \mathbb{R}^N \to \mathbb{R} : \int_{\mathbb{R}^N} \phi(x)dx = 0 \}.
\]

The variational derivative of a functional \( F : \mathcal{M} \to \mathbb{R} \) is defined as

\[
\int_{\mathbb{R}^N} \frac{\delta F}{\delta \pi} \phi dx = \lim_{\epsilon \to 0} \frac{F(\pi + \epsilon \phi) - F(\pi)}{\epsilon}.
\]

where \( \phi \) is a function such that \( \int_{\mathbb{R}^N} \phi dx = 0 \), i.e. \( \phi \in T_{\pi} \mathcal{M} \).

Consider the potential

\[
V(\pi_X) = \int_{\mathbb{R}^N} \pi_X \ln \pi_X dx,
\]

which has functional derivative

\[
\frac{\delta V}{\delta \pi_X} = \ln \pi_X,
\]

since

\[
V(\pi_X + \epsilon \phi) = V(\pi_X) + \epsilon \int_{\mathbb{R}^N} (\phi \ln \pi_X + \phi) dx + \mathcal{O}(\epsilon^2)
\]

\[
= V(\pi_X) + \epsilon \int_{\mathbb{R}^N} \phi \ln \pi_X dx + \mathcal{O}(\epsilon^2),
\]

Hence, we find that the diffusion part of the Fokker-Planck equation is equivalent to

\[
\frac{\partial \pi_X}{\partial t} = \nabla_x \cdot (Q \nabla_x \pi_X) = \nabla_x \cdot \left\{ \pi_X Q \nabla_x \frac{\delta V}{\delta \pi_X} \right\}.
\]

This formulation allows us to treat diffusion in form of a vector field

\[
v(x, t) = -Q \nabla_x \frac{\delta V}{\delta \pi_X}
\]

which, contrary to vector fields arising from the theory of ordinary differential equations, depends on the PDF \( \pi_X \). See the following Section 2.3 for an application.

**Proposition** (Gradient on the manifold of probability densities). Let \( g_\pi \) be a metric tensor defined on \( T_{\pi} \mathcal{M} \) as

\[
g_\pi(\phi_1, \phi_2) = \int_{\mathbb{R}^N} (\nabla_x \psi_1) \cdot (M \nabla_x \psi_2) \pi dx
\]

with potentials \( \psi_i, i = 1, 2 \), determined by the elliptic partial differential equation (PDE)

\[
-\nabla_x \cdot (\pi M \nabla_x \psi_i) = \phi_i,
\]

where \( M \in \mathbb{R}^{N \times N} \) is a symmetric, positive-definite matrix.

Then the gradient of a potential \( F(\pi) \) under \( g_\pi \) satisfies

\[
\nabla_{\pi} F(\pi) = -\nabla_x \cdot \left( \pi M \nabla_x \frac{\delta F}{\delta \pi} \right).
\]

(25)
Proof. Given the metric tensor \( g_\pi \), the gradient is defined by
\[
g_\pi(\text{grad}_\pi F(\pi), \phi) = \int_{\mathbb{R}^N} \frac{\delta F}{\delta \pi} \phi dx
\]  
for all \( \phi \in T_\pi M \). Since any element \( \phi \in T_\pi M \) can be written in the form
\[
\phi = -\nabla_x \cdot (\pi M \nabla_x \psi)
\]
with suitable potential \( \psi \), a potential \( \hat{\psi} \) exists such that
\[
\text{grad}_\pi F(\pi) = -\nabla_x \cdot (\pi M \nabla_x \hat{\psi}) \in T_\pi M
\]
and we need to demonstrate that
\[
\hat{\psi} = \frac{\delta F}{\delta \pi}
\]
is consistent with (26). Indeed, we find that
\[
\int_{\mathbb{R}^N} \frac{\delta F}{\delta \pi} \phi dx = -\int_{\mathbb{R}^N} \frac{\delta F}{\delta \pi} \nabla_x \cdot (\pi M \nabla_x \psi) dx
\]
\[
= \int_{\mathbb{R}^N} \pi \nabla_x \frac{\delta F}{\delta \pi} \cdot (M \nabla_x \psi) dx
\]
\[
= \int_{\mathbb{R}^N} (\nabla_x \hat{\psi}) \cdot (M \nabla_x \psi) \pi dx
\]
\[
= g_\pi(\text{grad}_\pi F(\pi), \phi).
\]

It follows that the diffusion part of the Fokker-Planck equation can be viewed as a gradient flow on the manifold \( M \). More precisely, set \( F(\pi) = V(\pi X) \) and \( M = Q \) to reformulate (24) as a gradient flow
\[
\frac{\partial \pi_X}{\partial t} = -\text{grad}_\pi X V(\pi X)
\]
with potential (23). We will find in Section 3 that related geometric structures arise from Bayes’ formula in the context of filtering. We finally note that
\[
\frac{dV}{dt} = \int_{\mathbb{R}^N} \delta V \frac{\partial \pi_X}{\partial t} dx
\]
\[
= -\int_{\mathbb{R}^N} (\nabla_x \frac{\delta V}{\delta \pi_X}) \cdot (M \nabla_x \frac{\delta V}{\delta \pi_X}) \pi_X dx \leq 0.
\]

2.3 Ensemble prediction and sampling methods

In this section, we extend the Monte Carlo method from Section 1.4 to the approximation of the marginal PDFs \( \pi_X(x, t), t \geq 0 \), evolving under the SDE model (19). Assume that we have a set of independent samples \( x_i(0), i = 1, \ldots, M \), from the initial PDF \( \pi_X(x, 0) \).

Definition (ensemble prediction). A Monte Carlo approximation to the time-evolved marginal PDFs \( \pi_X(x, t) \) can be obtained from solving the SDEs
\[
dx_i = f(x_i)dt + \sqrt{2Q}^{1/2}dW_i(t)
\]
for \( i = 1, \ldots, M \), where \( \{W_i(t)\}_{i=1}^M \) denote realizations of independent standard \( N \)-dimensional Brownian motion and the initial conditions \( \{x_i(0)\}_{i=1}^M \) are realizations of the initial PDF \( \pi_X(x, 0) \). This approximation provides an example for a particle or ensemble prediction method and it can be shown that the estimator
\[
\bar{x}_M(t) = \frac{1}{M} \sum_{i=1}^M x_i(t)
\]
provides a consistent and unbiased approximation to the mean \( E_{X_i}[x] \).
Alternatively, using formulation (24) of the Fokker-Planck equation (20) in the pure diffusion case, we may reformulate the random part in (27) and introduce particle equations

\[
\frac{dx_i}{dt} = f(x_i) - Q\nabla_x \frac{\delta V}{\delta \pi_X}(x_i)
\]

\[
= f(x_i) - \frac{1}{\pi_X(x_i,t)}Q\nabla_x \pi_X(x_i,t),
\]

(i = 1, \ldots, M). Contrary to the SDE (27), this formulation requires the PDF \( \pi_X(x,t) \), which is not explicitly available in general. However, a Gaussian approximation can be obtained from the available ensemble \( x_i(t), i = 1, \ldots, M, \)

with empirical mean (28) and empirical covariance matrix

\[
P = \frac{1}{M-1} \sum_{i=1}^{M} (x_i - \bar{x}_M)(x_i - \bar{x}_M)^T.
\]

Substituting this Gaussian approximation into (29) yields the ensemble evolution equations

\[
\frac{dx_i}{dt} = f(x_i) + QP^{-1}(x_i - \bar{x}_M),
\]

which becomes exact in case the vector field \( f \) is linear, i.e. \( f(x) = Ax + u \), the initial PDF \( \pi_X(x,0) \) is Gaussian and for ensemble sizes \( M \to \infty \).

We finally discuss the application of a particular type of SDEs (19) as a way of generating samples from a given PDF such as the posterior PDF \( \pi \) of Bayesian inference. To do this, consider the SDE (24) with the vector field \( f \) being generated by a potential \( U(x) \), i.e. \( f(x) = -\nabla_x U(x) \), and \( Q = I \). Then it can easily be verified that the PDF

\[
\pi_X^*(x) = Z^{-1}\exp(-U(x)), \quad Z = \int_{\mathbb{R}^N} \exp(-U(x))dx,
\]

is stationary under the associated Fokker-Planck equation (20). Indeed

\[
\nabla_x \cdot (\pi_X^* \nabla_X U) + \nabla_x \cdot \nabla_x \pi_X^* = \nabla_x \cdot (\pi_X^* \nabla_x U + \nabla_x \pi_X^*) = 0.
\]

Furthermore, it can be shown that \( \pi_X^* \) is the unique stationary PDF and that any initial PDF \( \pi_X(t = 0) \) approaches \( \pi_X^* \) at exponential rate under appropriate assumption on the potential \( V \). Hence \( \pi_X \sim \pi_X^* \) for \( t \to \infty \). This allows us to use an ensemble of solutions \( x_i(t) \) of (27) with an arbitrary initial PDF \( \pi_X(x,0) \) as a method for generating ensembles from the prior or posterior Bayesian PDFs provided

\[
U(x) = -\ln \pi_X(x) \quad \text{or} \quad U(x) = -\ln \pi_X(x|y_0),
\]

Note that the temporal dynamics of the associated SDE (19) is not of any physical significance in this context instead the SDE formulation is only taken as a device for generating the desired samples. If the SDE formulation is replaced by the Euler-Maruyama method (17), time-stepping errors lead to sampling errors which can be corrected for by combining (17) with a Metropolis accept-reject criterion. The Metropolis adjusted method gives rise to particular instances of Markov chain Monte Carlo (MCMC) methods such as the Metropolis adjusted Langevin algorithm (MALA) or the hybrid Monte Carlo (HMC) method. The basic idea of MALA (as well as HMC) is to rewrite (17) with \( f(x) = -\nabla_x U(x) \), \( Q = I \) as

\[
p_{n+1/2} = p_n - \frac{1}{2}\sqrt{2\Delta t} \nabla_x U(x_n),
\]

\[
x_{n+1} = x_n + \sqrt{2\Delta t}p_{n+1/2},
\]

\[
p_{n+1} = p_{n+1/2} - \frac{1}{2}\sqrt{2\Delta t} \nabla_x U(p_n)
\]
having introduced a dummy momentum variable $p$ with $p_n$ being a realization of the random variable $Z_n \sim N(0, I)$. Under the Metropolis accept-reject criterion $x_{n+1}$ is accepted with probability

$$\min\{1, \exp(-(E_{n+1} - E_n))\},$$

where

$$E_n = \frac{1}{2} p_n^T p_n + U(x_n), \quad E_{n+1} = \frac{1}{2} p_{n+1}^T p_{n+1} + U(x_{n+1})$$

are the initial and final energies. Upon rejection one continues with $x_n$. The momentum value $p_{n+1}$ is discarded after a completed time-step (regardless of its acceptance or rejection) and a new momentum value is drawn from $N(0, I)$. It should however be noted that $|E_{n+1} - E_n| \to 0$ as the step-size $\Delta t$ goes to zero and in practice the application of the Metropolis accept-rejection step is often not necessary unless $\Delta t$ is chosen too large. The HMC method differs from MALA in that several iterations of (32-34) are applied before the Metropolis accept-reject criterion is being applied.

References

A gentle introduction to stochastic processes can be found in [17] and [10]. A more mathematical treatment can be found in [8, 39] and numerical issues are discussed in [21, 26]. See [11, 49] for a discussion of the gradient flow structure of the Fokker-Planck equation. The ergodic behavior of Markov chains is covered in [33]. Markov chain Monte Carlo methods and the hybrid Monte Carlo method in particular are treated in [32]. See also [44] for the Metropolis adjusted Langevin algorithm (MALA).

3 Recent advances in data assimilation and filtering

In this section, we combine Bayesian inference and stochastic processes to tackle the problem of assimilating observational data into scientific models.

3.1 Preliminaries

We select a model written as a time-discretized SDE, such as (17), with the initial random variable satisfying $X_0 \sim \pi_0$. In addition to the pure prediction problem of computing $\pi_n$, $n \geq 1$, for given $\pi_0$, we assume that model states $x \in X = \mathbb{R}^N$ are partially observed at equally spaced instances in time. These observations are to be assimilated into the model. More generally, intermittent data assimilation is concerned with fixed observation intervals $\Delta t_{\text{obs}} > 0$ and model time-steps $\Delta t$, $L \geq 1$, which allows one to take the limit $L \to \infty$, $\Delta t = \Delta t_{\text{obs}} / L$. For simplicity, we will restrict the discussion to the case where observations $y_n(t_n) = Y_n(\omega) \in \mathbb{R}^N$ are made at every time step $t_n = n \Delta t$, $n \geq 1$ and the limit $\Delta t \to 0$ is not considered here. We will further assume that the observed random variables $Y_n$ satisfy the model (2), i.e.

$$Y_n = h(X_n) + \Xi_n$$

and the measurement errors $\Xi_n \sim N(0, R)$ are mutually independent with common error covariance matrix $R$. We introduce the notation $Y_k = \{y_0(t_i)\}_{i=1, \ldots, k}$ to denote all observations up to and including time $t_k$.

Definition (Data assimilation). Data assimilation is the estimation of marginal PDFs $\pi_n(x|Y_k)$ of the random variable $X_n = X(t_n)$ conditioned on the set of observations $Y_k$. We distinguish three cases: (i) filtering $k = n$, (ii) smoothing $k > n$, and (iii) prediction $k < n$.

The subsequent discussions are restricted to the filtering problem. We have already seen that evolution of the marginal distributions under (17) alone is governed by the Chapman-Kolmogorov equation (15) with transition probability density (18). We denote the associated Frobenius-Perron operator (13) by $\mathcal{P}_{\Delta t}$. Given $X_0 \sim \pi_0$, we first obtain

$$\pi_1 = \mathcal{P}_{\Delta t} \pi_0.$$
This time propagated PDF is used as the prior PDF \( \pi_X = \pi_1 \) in Bayes’ formula (3) at \( t = t_1 \) with \( y_0 = y_0(t_1) \) and likelihood
\[
\pi_Y(y|x) = \frac{1}{(2\pi)^{N/2}|R|^1/2} \exp \left( -\frac{1}{2} (y - h(x))^T R^{-1} (y - h(x)) \right).
\]
Bayes’ formula implies the posterior PDF
\[
\pi_1(x|Y_1) \propto \pi_Y(y_0(t_1)|x) \pi_1(x),
\]
where the constant of proportionality depends on \( y_0(t_1) \) only.

**Proposition** (Sequential filtering). The filtering problem leads to the recursion
\[
\begin{align*}
\pi_{n+1}(\cdot|Y_n) &= \mathcal{P}_{\Delta t} \pi_n(\cdot|Y_n), \\
\pi_{n+1}(x|Y_{n+1}) &\propto \pi_Y(y_0(t_{n+1})|x) \pi_{n+1}(x|Y_n),
\end{align*}
\]
where \( n \geq 0 \), and \( X_n \sim \pi_n(\cdot|Y_n) \) solves the filtering problem at time \( t_n \). The constant of proportionality depends on \( y_0(t_{n+1}) \) only.

**Proof.** The recursion follows by induction. \( \Box \)

Recall that the Frobenius-Perron operator \( \mathcal{P}_{\Delta t} \) is generated by the stochastic difference equation (17). On the other hand, Bayes’ formula only leads to a transition from the predicted \( \pi_{n+1}(x|Y_n) \) to the filtered \( \pi_{n+1}(x|Y_{n+1}) \). Following our discussion on transport maps from Section 1.3, we assume the existence of a transport map \( X' = T_{n+1}(X) \), depending on \( y_0(t_{n+1}) \), that couples the two PDFs. The use of optimal transport maps in the context of Bayesian inference and intermittent data assimilation was first proposed in [12, 36].

**Proposition** (Filtering by transport maps). Assuming the existence of appropriate transport maps \( T_{n+1} \), which couple \( \pi_{n+1}(x|Y_n) \) and \( \pi_{n+1}(x|Y_{n+1}) \), the filtering problem is solved by the following recursion for the random variables \( X_{n+1} \), \( n \geq 0 \):
\[
X_{n+1} = T_{n+1} \left( X_n + \Delta t f(X_n) + \sqrt{2\Delta t} Z_n \right),
\]
which gives rise to a time-dependent Markov process.

**Proof.** Follows trivially from (35). \( \Box \)

The rest of this section is devoted to several Monte Carlo methods for sequential filtering.

### 3.2 Sequential Monte Carlo method

In our framework, a standard sequential Monte Carlo method, also called bootstrap particle filter, may be described as an ensemble of random variables \( X_t \) and associated realizations (referred to as “particles”) \( x_i = X_t(\omega) \), which follow the stochastic difference equation (17), choosing the transport map in (36) to be the identity map. Observational data is taken into account using importance sampling as discussed in Section 1.3, i.e., each particle carries a weight \( w_i(t_n) \), which is updated according to Bayes’ formula
\[
w_i(t_{n+1}) \propto w_i(t_n) \pi(y_0(t_{n+1})|x_i(t_{n+1})).
\]
The constant of proportionality is chosen such that the new weights \( \{w_i(t_{n+1})\}_{i=1}^M \) sum to one.

Whenever the particle weights \( w_i(t_n) \) start to become highly non-uniform (or possibly also after each assimilation step) resampling is necessary in order to generate a new family of random variables with equal weights.

Most available resampling methods start from the weighted empirical measure
\[
\mu_X(dx) = \sum_{i=1}^M w_i \mu_{x_i}(dx)
\]
(37)
associated with a set of weighted samples \( \{x_i, w_i\}_{i=1}^M \). The idea is to replace each of the original samples \( x_i \) by \( \xi_i \geq 0 \) offsprings with equal weights \( \hat{w}_i = 1/M \). The distribution of offsprings is chosen to be equal to the distribution of \( M \) samples (with replacement) drawn at random from the empirical distribution \((37)\). In other words, the offsprings \( \{\xi_i\}_{i=1}^M \) follow a multinomial distribution defined by

\[
P(\xi_i = n_i, i = 1, \ldots, M) = \frac{M!}{\prod_{i=1}^M n_i!} \prod_{i=1}^M (w_i)^{n_i}
\]

with \( n_i \geq 0 \) such that \( \sum_{i=1}^M n_i = M \). In practice, independent resampling is often replaced by residual or systematic resampling. We next summarize residual resampling while we refer the reader to [3] for an algorithmic description of systematic resampling.

**Definition (Residual resampling).** Residual resampling generates

\[
\xi_i = \lfloor M w_i \rfloor + \tilde{\xi}_i,
\]

offsprings of each ensemble member \( x_i \) with weight \( w_i, i = 1, \ldots, M \). Here \( \lfloor x \rfloor \) denotes the integer part of \( x \) and \( \tilde{\xi}_i \) follows the multinomial distribution \((38)\) with weights \( w_i \) being replaced by

\[
\hat{w}_i = \frac{M w_i - \lfloor M w_i \rfloor}{\sum_{j=1}^M (M w_j - \lfloor M w_j \rfloor)}
\]

and with a total of

\[
\sum_{i=1}^M n_i = \overline{M} := M - \sum_{i=1}^M \lfloor M w_i \rfloor
\]

independent trials.

In generalization of \((38)\), we introduce the notation \( \text{Mult}(L; \omega_1, \ldots, \omega_M) \) to denote the multinomial distribution of \( L \) independent trials, where the outcome of each trial is distributed among \( M \) possible outcomes according to probabilities \( \{\omega_i\}_{i=1}^M \). The following algorithm draws random samples from \( \text{Mult}(L; \omega_1, \ldots, \omega_M) \). We first introduce the generalized inverse cumulative distribution function \( F^{-1}_{\text{emp}} : [0, 1] \rightarrow \{1, \ldots, M\} \) for the empirical measure \((37)\), which is defined by

\[
F^{-1}_{\text{emp}}(u) = i \iff \sum_{j=1}^{i-1} \omega_j \leq u < \sum_{j=1}^i \omega_j.
\]

We next draw \( L \) independent samples \( u_l \in [0, 1] \) from the uniform distribution \( U[0, 1] \) and initially set the number of copies \( \xi_i, i = 1, \ldots, M \), equal to zero. For \( l = 1, \ldots, L \), we now increment \( \xi_{I_l} \) by one for indices \( I_l \in \{1, \ldots, M\} \), \( l = 1, \ldots, L \), defined by

\[
I_l = F^{-1}_{\text{emp}}(u_l) = \arg\min_{i \geq 1} \sum_{j=1}^i \omega_j \geq u_l.
\]

Both independent and residual resampling can be viewed as providing a coupling between the empirical measure \((37)\) will all weights being equal to \( w_i = 1/M \) and the target measure \((37)\) with identical samples \( \{x_i\} \) but non-uniform weights. Clearly residual resampling provides a coupling with a smaller transport cost. This can already be concluded from the trivial case of equal weights in the target measure in which case residual resampling reduces to the identity map with zero transport cost while independent resampling remains non-deterministic and produces a non-zero transport cost. The following example outlines the optimal transportation perspective on resampling more precisely for two discrete, univariate random variables.

**Example (Coupling discrete random variables).** Let us consider two discrete, univariate random variables \( X_i : \Omega \rightarrow \mathcal{X}, i = 1, 2 \), with target set

\[
\mathcal{X} = \{x_1, x_2, \ldots, x_M\} \in \mathbb{R}^M.
\]
We furthermore assume that
\[ P(X_1(\omega) = x_i) = 1/M, \quad P(X_2(\omega) = x_i) = w_i \]
for given probabilities/weights \( w_i \geq 0, i = 1, \ldots, M \). Any coupling of \( X_1 \) and \( X_2 \) is characterized by a matrix \( T \in \mathbb{R}^{M \times M} \) such that \( t_{ij} = (T)_{ij} \geq 0 \) and
\[
\sum_{i=1}^{M} t_{ij} = 1/M, \quad \sum_{j=1}^{M} t_{ij} = w_i
\]
Given a coupling \( T \) and the mean values \( \bar{x}_1 = \frac{1}{M} \sum_i x_i \), \( \bar{x}_2 = \sum_i w_i x_i \)
the covariance between \( X_1 \) and \( X_2 \) is defined by
\[
\operatorname{cov}(X_1, X_2) = \sum_{i,j} (x_i - \bar{x}_2) t_{ij} (x_j - \bar{x}_1).
\]
The induced Markov transition matrix from \( X_1 \) to \( X_2 \) is simply given by \( M T \). Independent resampling corresponds to \( t_{ij} = w_i/M \) and leads to a zero correlation between \( X_1 \) and \( X_2 \). On the other hand, maximizing the correlation results in a linear programming problem for the \( M^2 \) unknowns \( \{t_{ij}\} \). Its solution then also defines the solution to the associated optimal transportation problem \( \mathbb{Q} \).

More generally, sequential Monte Carlo methods differ by the way resampling is implemented and also in the choice of proposal step which in our context amounts to choosing transport maps \( T_{n+1} \) in \( (36) \) which are different from the identity map. See also the discussion in Section 3.5 below.

### 3.3 Ensemble Kalman filter (EnKF)

We now introduce an alternative to sequential Monte Carlo methods which has become hugely popular in the geophysical community in recent years. The idea is to construct a simple but robust transport map \( T'_{n+1} \) which replaces \( T_{n+1} \) in \( (36) \). This transport map is based on the Kalman update equations for linear SDEs and Gaussian prior and posterior distributions. We recall the standard Kalman filter update equations.

**Proposition (Kalman update for Gaussian distributions).** Let the prior distribution \( \pi_X \) be Gaussian with mean \( \bar{x}^f \) and covariance matrix \( P^f \). Observations \( y_0 \) are assumed to follow the linear model
\[
Y = H X + \Xi,
\]
where \( \Xi \sim \mathcal{N}(0, R) \) and \( R \) is a symmetric, positive-definite matrix. Then the posterior distribution \( \pi_X(x|y_0) \) is also Gaussian with mean
\[
\bar{x}^a = \bar{x}^f - P^f H^T (HP^f H^T + R)^{-1} (H \bar{x}^f - y_0)
\]
and covariance matrix
\[
P^a = P^f - P^f H^T (HP^f H^T + R)^{-1} HP^f.
\]
Here we adopt the standard meteorological notation with superscript \( f \) (forecast) denoting prior statistics, and superscript \( a \) (analysis) denoting posterior statistics.

**Proof.** By straightforward generalization to vector-valued observations of the case of a scalar observation already discussed in Section 1.2.

EnKFs rely on the assumption that the predicted PDF \( \pi_{n+1}(x|Y_n) \) is approximately Gaussian. The ensemble \( \{x_i\}_{i=1}^{M} \) of model states is used to estimate the mean and the covariance matrix using the empirical estimates \( (28) \) and \( (30) \), respectively. The key novel idea of EnKFs is to then interpret the posterior mean and covariance matrix in terms of appropriately adjusted ensemble positions. This adjustment can be thought of as a coupling of the underlying prior and posterior random variables of which the ensembles are realizations. The original EnKF \( [9] \) uses perturbed observations to achieve the desired coupling.
Definition (Ensemble Kalman Filter). The EnKF with perturbed observations for a linear observation operator \( h(x) = Hx \) is given by

\[
\begin{align*}
X_{n+1}^f &= X_n + \Delta t f(X_n) + \sqrt{2\Delta t} Z_n, \\
X_{n+1} &= X_{n+1}^f - P_{n+1}^f H^T (HP_{n+1}^f H^T + R)^{-1} (HX_{n+1}^f - y_0 + \Sigma_{n+1}),
\end{align*}
\]

where the random variables \( Z_n \sim N(0, Q), \Sigma_{n+1} \sim N(0, R) \) are the mutually independent perturbations to the observations, \( y_0 = y_0(t_{n+1}) \), \( x_{n+1}^f = E_{X_{n+1}}[x] \), and \( P_{n+1}^f = E_{X_{n+1}^f}[(x - x_{n+1}^f)(x - x_{n+1}^f)^T] \).

Next, we investigate the properties of the assimilation step [12].

Proposition (EnKF consistency). The EnKF update step (42) propagates the mean and covariance matrix of \( X \) in accordance with the Kalman filter equations for Gaussian PDFs.

Proof. It is easy to verify that the ensemble mean satisfies

\[
x_{n+1} = x_{n+1}^f - P_{n+1}^f H^T (HP_{n+1}^f H^T + R)^{-1} (HX_{n+1}^f - y_0),
\]

which is consistent with the Kalman filter update for the ensemble mean. Furthermore, the deviation \( \delta X = X - \bar{x} \) satisfies

\[
\delta X_{n+1} = \delta X_{n+1}^f - P_{n+1}^f H^T (HP_{n+1}^f H^T + R)^{-1} (H \delta X_{n+1}^f + \Sigma_{n+1}),
\]

which implies

\[
P_{n+1} = P_{n+1}^f - 2P_{n+1}^f H^T (HP_{n+1}^f H^T + R)^{-1} HP_{n+1}^f +
\]

\[
H P_{n+1} H^T (HP_{n+1}^f H^T + R)^{-1} R (HP_{n+1}^f H^T + R)^{-1} H P_{n+1}^f +
\]

\[
(HP_{n+1} H^T + R)^{-1} H P_{n+1}^f H^T (HP_{n+1}^f H^T + R)^{-1} H P_{n+1}^f
\]

\[
= P_{n+1}^f - P_{n+1}^f H^T (HP_{n+1} H^T + R)^{-1} H P_{n+1}^f
\]

for the update of the covariance matrix, which is also consistent with the Kalman update step for Gaussian random variables.

Practical implementations of the EnKF with perturbed observations replace the exact mean and covariance matrix by ensemble based empirical estimates [28] and [30], respectively.

Alternatively, we can derive a transport map \( T \) under the assumption of Gaussian prior and posterior distributions as follows. Using the empirical ensemble mean \( \bar{x} \) we define ensemble deviations by \( \delta x_i = x_i - \bar{x} \in \mathbb{R}^N \) and an associated ensemble deviation matrix \( \delta X = (\delta x_1, \ldots, \delta x_M) \in \mathbb{R}^{N \times M} \). Using the notation, the empirical covariance matrix of the prior ensemble at \( t_{n+1} \) is then given by

\[
P_{n+1}^f = \frac{1}{M-1} \delta X_{n+1}^f (\delta X_{n+1}^f)^T
\]

We next seek a matrix \( S \in \mathbb{R}^{M \times M} \) such that

\[
P_{n+1} = \frac{1}{M-1} \delta X_{n+1} S S^T (\delta X_{n+1}^f)^T,
\]

where the rows of \( S \) sum to zero in order to preserve the zero mean property of \( \delta X_{n+1} = \delta X_{n+1}^f S \). Such matrices do exist (see e.g. [15]) and give rise the ensemble square root filters. More specifically, Kalman’s update formula [40] for the posterior covariance matrix implies

\[
P^n = \frac{1}{M-1} \delta X_f \left \{ I - \frac{1}{M-1} (\delta Y_f)^T (HP_f H^T + R)^{-1} \delta Y_f \right \} (\delta X_f)^T
\]

\[
= \frac{1}{M-1} \delta X_f S S^T (\delta X_f)^T,
\]

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where we have dropped the time index subscript and introduced the ensemble perturbations $\delta Y^f = H \delta X^f$ in observation space $\mathcal{Y}$. Recalling now the definition of a matrix square root from Section 1.3 and making use of the Sherman-Morrison-Woodbury formula [18], we find that

$$S = \left\{ I - \frac{1}{M-1} (\delta Y^f)^T (HP^f H^T + R)^{-1} \delta Y^f \right\}^{1/2}$$

$$= \left\{ I + \frac{1}{M-1} (\delta Y^f)^T R^{-1} \delta Y^f \right\}^{-1/2}. \quad (43)$$

The complete ensemble update of an ensemble square root filter is then given by

$$x_i(t_{n+1}) = \bar{x}_{n+1} + \delta X^f_{n+1} S e_i,$$  \quad (44)

where $e_i$ denotes the $i$th basis vector in $\mathbb{R}^M$ and

$$\bar{x}_{n+1} = \bar{x}_{n+1}^f - P^f_{n+1} H^T (HP^f_{n+1} H^T + R)^{-1} (H \bar{x}^f_{n+1} - y_0(t_{n+1}))$$

denotes the updated ensemble mean.

We now discuss the update [14] from the perspective of optimal transportation which in our context reduces to finding a matrix $S_{OT} \in \mathbb{R}^{M \times M}$ such that the trace of

$$\text{cov}(\delta X^f_{n+1}, \delta X_{n+1}) = \mathbb{E}[\delta X^f_{n+1} S_{OT}^T (\delta X^f_{n+1})^T]$$

is maximized.

**Proposition** (Optimal update for ensemble square root filter). The trace of the covariance matrix $\text{cov}(\delta X^f_{n+1}, \delta X_{n+1})$ is maximized for

$$\delta X_{n+1} = \delta X^f_{n+1} S_{OT}$$

with transform matrix

$$S_{OT} = \frac{1}{\sqrt{M-1}} S \left[ (\delta X^f_{n+1})^T P^f_{n+1} \delta X^f_{n+1} S \right]^{-1/2} S (\delta X^f_{n+1})^T \delta X^f_{n+1}$$

and $S \in \mathbb{R}^{M \times M}$ given by (43).

Proof. Follows from (9) with $A = \delta X^f_{n+1} S / \sqrt{M-1}$ and $\Sigma_1 = P^f$. The left multiplication in (8) is finally rewritten as a right multiplication by $S_{OT} \in \mathbb{R}^{M \times M}$ in terms of ensemble deviations $\delta X^f_{n+1}$. \qed

We finish this section by brief discussions on a couple of practical issues. It is important to recall that the Kalman filter can be viewed as a linear minimum variance estimator [14]. At the same time it has been noted [52, 30] that the updated ensemble mean $\bar{x}_{n+1}$ is biased in case the prior distribution is not Gaussian. Hence the associated mean squared error (10) does not vanish as $M \to \infty$ even though the variance of the estimator goes to zero. If desired the bias can be removed by replacing $\bar{x}_{n+1}$ in (44) by (11) with weights (12), where $y_0 = y_0(t_{n+1})$ and $x_i^{\text{prior}} = x_i(t_{n+1})$. Higher-order moment corrections can also be implemented [52, 30]. However, the filter performance only improves for sufficiently large ensemble sizes.

We mention the unscented Kalman filter [23] as an alternative extension of the Kalman filter to nonlinear dynamical systems. We also mention the rank histogram filter [2], which is based on first constructing an approximative coupling in the observed variable $y$ along a linear regression of the updates in $y$ onto the state space variable $x$.

Practical implementations of EnKFs for high-dimensional problem rely on additional modifications, in particular inflation and localization. While localization modifies the covariance matrix $P^f$ in the Kalman update (12) in order to increase its rank and to localize the spatial impact of observations in physical space, inflation increases the ensemble spread $\delta x_i = x_i - \bar{x}$ by replacing $x_i$ by $\bar{x} + \alpha (x_i - \bar{x})$ with $\alpha > 1$. Note that the second term on the righthand side of (31) achieves a similar effect and ensemble inflation can be viewed as simple parametrization of (stochastic) model errors. See [15] for more details on inflation and localization techniques.
3.4 Ensemble transform Kalman-Bucy filter

In this section, we describe an alternative implementation of ensemble square root filters based on the Kalman-Bucy filter. We first describe the Kalman-Bucy formulation of the linear filtering problem for Gaussian PDFs.

**Proposition (Kalman-Bucy equations).** The Kalman update step \((39)-(40)\) can be formulated as a differential equation in artificial time \(s \in [0, 1]\). The Kalman-Bucy equations are

\[
\frac{d\bar{x}}{ds} = -PH^T R^{-1} (H\bar{x} - y_0)
\]

and

\[
\frac{dP}{ds} = -PH^T R^{-1} HP.
\]

The initial conditions are \(\bar{x}(0) = \bar{x}^f\) and \(P(0) = P^f\) and the Kalman update is obtained from the final conditions \(\bar{x} = \bar{x}(1)\) and \(P = P(1)\).

**Proof.** We present the proof for \(N = 1\) (one dimensional state space) and \(K = 1\) (a single observation). Under this assumption, the standard Kalman analysis step \((39)-(40)\) gives rise to

\[
P^a = \frac{P^f R}{P^f + R}, \quad \bar{x}^a = \frac{\bar{x}^f R + y_0 P^f}{P^f + R},
\]

for a given observation value \(y_0\).

We now demonstrate that this update is equivalent to twice the application of a Kalman analysis step with \(R\) replaced by \(2R\). Specifically, we obtain

\[
\hat{P}^a = \frac{2P_m R}{P_m + 2R}, \quad P_m = \frac{2P^f R}{P^f + 2R},
\]

for the resulting covariance matrix \(\hat{P}^a\) with intermediate value \(P_m\). The analyzed mean \(\hat{x}^a\) is provided by

\[
\hat{x}^a = \frac{2\bar{x}_m R + y_0 P_m}{P_m + 2R}, \quad \bar{x}_m = \frac{2\bar{x}^f R + y_0 P^f}{P^f + 2R}.
\]

We need to demonstrate that \(P^a = \hat{P}^a\) and \(\bar{x}^a = \hat{x}^a\). We start with the covariance matrix and obtain

\[
\hat{P}^a = \frac{4P^f R}{P^f + 2R} = \frac{4P^f R^2}{4P^f R + 4R^2} = \frac{P^f R}{P^f + R} = P^a.
\]

A similar calculation for \(\hat{x}^a\) yields

\[
\hat{x}^a = \frac{2\bar{x}^f R + y_0 P^f}{2R + \frac{2P^f R}{P^f + 2R}} = \frac{4\bar{x}^f R^2 + 4y_0 P^f R}{4R^2 + 4RP^f} = \bar{x}^a.
\]

Hence, by induction, we can replace the standard Kalman analysis step by \(D > 2\) iterative applications of a Kalman analysis with \(R\) replaced by \(DR\). We set \(P_0 = P^f\), \(\bar{x}_0 = \bar{x}^f\), and iteratively compute \(P_{j+1}\) from

\[
P_{j+1} = \frac{DP_j R}{P_j + DR}, \quad \bar{x}_{j+1} = \frac{D\bar{x}_j R + y_0 P_j}{P_j + DR},
\]

for \(j = 0, \ldots, D - 1\). We finally set \(P^a = P_D\) and \(\bar{x}^a = \bar{x}_D\). Next we introduce a step-size \(\Delta s = 1/D\) and assume \(D \gg 1\). Then

\[
\bar{x}_{j+1} = \frac{\bar{x}_j R + \Delta s y_0 P_j}{R + \Delta s P_j} = \bar{x}_j - \Delta s P_j R^{-1} (\bar{x}_j - y_0) + O(\Delta s^2)
\]

as well as

\[
P_{j+1} = \frac{P_j R}{R + \Delta s P_j} = P_j - \Delta s P_j R^{-1} P_j + O(\Delta s^2).
\]

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Taking the limit $\Delta s \rightarrow 0$, we obtain the two differential equations
\[ \frac{dP}{ds} = -PR^{-1}P, \quad \frac{d\pi}{ds} = -PR^{-1}(\bar{x} - y_0) \]
for the covariance and mean, respectively. The equation for $P$ can be rewritten in terms of its square root $Y$ (i.e., $P = Y^2$) as
\[ \frac{dY}{ds} = -\frac{1}{2}PR^{-1}Y. \] (45)

Upon formally setting $Y = \delta X/\sqrt{M - 1}$ in (45), the Kalman-Bucy filter equations give rise to a particular implementation of ensemble square root filters in terms of evolution equations in artificial time $s \in [0, 1]$.

**Definition (Ensemble transform Kalman-Bucy filter equations).** The ensemble transform Kalman-Bucy filter equations [5, 6, 1] for the assimilation of an observation $y_0 = y_0(t_n)$ at $t_n$ are given by
\[ \frac{dx_i}{ds} = \frac{1}{2}PH^TR^{-1}(HX + H\bar{x} - 2y_0(t_n)) \]
in terms of the ensemble members $x_i, i = 1, \ldots, M$ and are solved over a unit time interval in artificial time $s \in [0, 1]$. Here $P$ denotes the empirical covariance matrix (30) and $\bar{x}$ the empirical mean (28) of the ensemble.

The Kalman-Bucy equations are realizations of an underlying differential equation
\[ \frac{dX}{ds} = -\frac{1}{2}PH^TR^{-1}(HX + H\bar{x} - 2y_0(t_n)) \] (46)
in the random variable $X$ with mean
\[ \bar{x} = E_X[x] = \int_{\mathbb{R}^N} x\pi_X dx \]
and covariance matrix
\[ P = E_X[(x - \bar{x})(x - \bar{x})^T]. \]

The associated evolution of the PDF $\pi_X$ (here assumed to be absolutely continuous) is given by Liouville’s equation
\[ \frac{\partial \pi_X}{\partial s} = -\nabla_x \cdot (\pi_X v) \] (47)
with vector field
\[ v(x) = -\frac{1}{2}PH^TR^{-1}(HX + H\bar{x} - 2y_0(t_n)). \] (48)

Recalling the earlier discussion of the Fokker-Planck equation in Section (2.2), we note that (47) with vector field (48) also has an interesting geometric structure.

**Proposition (Ensemble transform Kalman-Bucy equations as a gradient flow).** The vector field (48) is equivalent to
\[ v(x) = -P\nabla_x \frac{\delta F}{\delta \pi_X} \]
with potential
\[ F(\pi_X) = \frac{1}{4}\int_{\mathbb{R}^N} (Hx - y_0(t_n))^TR^{-1}(Hx - y_0(t_n))\pi_X dx + \frac{1}{4}(H\bar{x} - y_0(t_n))^TR^{-1}(H\bar{x} - y_0(t_n)). \] (49)
Liouville’s equation (47) can be stated as
\[ \frac{\partial \pi_X}{\partial s} = -\nabla_x \cdot (\pi_X v) = -\nabla_{\pi_X} F(\pi_X), \]
where we have used $M = P$ in the definition of the gradient (22).
Proof. The result can be verified by direct calculation.

Nonlinear forward operators can be treated in this framework by replacing the potential (49) by, for example,

$$F(\pi_X) = \frac{1}{4} \int_{R^N} (h(x) - y_0(t_n))^T R^{-1} (h(x) - y_0(t_n)) \pi_X dx +$$

$$\frac{1}{4} (h(\bar{x}) - y_0(t_n))^T R^{-1} (H\bar{x} - y_0(t_n)).$$

Efficient time-stepping methods for the ensemble transform Kalman–Bucy filter equations are discussed in [1] and an application to continuous data assimilation can be found in [6].

3.5 Guided sequential Monte Carlo methods

EnKF techniques are limited by the fact that the empirical PDFs do not converge to the filter solution in the limit of ensemble sizes $M \to \infty$ unless the involved PDFs are Gaussian. Sequential Monte Carlo methods, on the other hand, lead to unbiased estimators for the mean and can be shown to converge under fairly general assumptions, but they do not work well in high-dimensional phase spaces since importance sampling is not sufficient to guarantee good performance of a particle filter for finite ensemble sizes. In particular, the variance in the associated mean squared error (10) can be very large for ensemble sizes typically used in geophysical applications.

The combination of modified particle positions and appropriately adjusted particle weights appears therefore as a promising area for research and might achieve a better bias-variance tradeoff than either the EnKF or traditional sequential Monte Carlo methods. In particular, combining ensemble transform techniques, such as EnKF, with sequential Monte Carlo methods appears as a natural research direction. Indeed, in the framework of Monte Carlo methods discussed in Section 1.4, the standard sequential Monte Carlo approach consists of importance sampling using proposal PDF $\tilde{\pi}_X(x) = \pi_{n+1}(x|Y_{n+1})$ and subsequent reweighting of particles according to (12). As also already discussed in Section 1.4, the performance of importance sampling can be improved by applying modified proposal densities $\pi_{n+1}(x|Y_{n+1})$ with the aim of pushing the updated ensemble members $x_i(t_{n+1})$ to regions of high and nearly equal probability in the targeted posterior PDF $\pi_{n+1}(x|Y_{n+1})$ (compare with eq. (13)). We call the resulting filter algorithms guided sequential Monte Carlo methods.

More precisely, a guided sequential Monte Carlo method is defined by a conditional proposal PDF $\tilde{\pi}_{n+1}(x'|x, y_0(t_{n+1}))$ and an associated joint PDF

$$\tilde{\pi}_{X',X}(x', x|Y_{n+1}) = \tilde{\pi}_{n+1}(x'|x, y_0(t_{n+1})) \pi_n(x|Y_n). \quad (50)$$

An ideal proposal density (in the sense of coupling) would lead to a marginal distribution $\tilde{\pi}_{X'}(x|Y_{n+1})$, which is identical to the posterior PDF $\pi_{n+1}(x|Y_{n+1})$. In guided sequential Monte Carlo methods, a mismatch between $\pi_X(x|Y_{n+1})$ and $\tilde{\pi}_{n+1}(x|Y_{n+1})$ is treated by adjusted particle weights $w_i(t_{n+1})$.

Following the general methodology of importance sampling one obtains the recursion

$$w_i(t_{n+1}) \propto \frac{\pi_Y(y_0(t_{n+1})|x'_i)\pi(x'_i|x_i)}{\tilde{\pi}_{n+1}(x'_i|x_i, y_0(t_{n+1}))} w_i(t_n).$$

Here $\pi(x'|x)$ denotes the conditional PDF (12) describing the model dynamics, $(x'_i, x_i), i = 1, \ldots, M$, are realizations from the joint PDF (50) with weights $w_i(t_n), x_i = x_i(t_n)$, and the approximation

$$E_{X_{n+1}}[g] = \frac{1}{\pi_Y(y_0(t_{n+1}))} \int_{R^N} \int_{R^N} f(x', x) \tilde{\pi}_{X',X}(x', x|Y_{n+1}) dx' dx$$

$$\approx \frac{1}{\pi_Y(y_0(t_{n+1}))} \sum_{i=1}^{M} w_i(t_n) f(x'_i, x_i)$$

$$\propto \sum_{i=1}^{M} w_i(t_{n+1}) g(x'_i).$$

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with
\[ f(x', x) = g(x') \frac{\pi_y(y_0(t_{n+1})|x') \pi(x| x)}{\pi_{n+1}(x'| x, y_0(t_{n+1}))} \]
has been used. The guided sequential Monte Carlo method is continued with \( x_i(t_{n+1}) = x'_i \) and new weights \( w_i(t_{n+1}) \).

Numerical implementations of guided sequential Monte Carlo methods have been discussed, for example, in [28] [4] [11] [35]. More specifically, a combined particle and Kalman filter is proposed in [28] to achieve almost equal particle weights (see also the discussion in [28]), while in [11] [35], new particle positions \( x_i(t_{n+1}) \) are defined by means of implicit equations. We emphasize that both implementation approaches give up the requirement of unbiased estimation in hope for reduced variance at finite ensemble sizes and hence for an overall reduction of the associated mean squared error [10].

Another broad class of methods is based on Gaussian mixture approximations to the prior PDF \( \pi_{n+1}(x|Y_n) \). Provided that the forward operator \( h \) is linear, the posterior PDF \( \pi_{n+1}(x|Y_{n+1}) \) is then also a Gaussian mixture and several procedures have been proposed to adjust the proposals \( x'_i(t_{n+1}) \) such that the adjusted \( x_i(t_{n+1}) \) approximately follow the posterior Gaussian mixture PDF. See, for example, [46] [46] [17]. Broadly speaking, these methods can be understood as providing approximate transport maps \( T_{n+1} \) instead of an exact transport map \( T_{n+1} \). However, none of these methods avoid the need for particle reweighting and resampling. Recall that resampling can be implemented such that it corresponds to a non-deterministic optimal transference plan.

The following section is devoted to an embedding technique for constructing accurate approximations to the transport map \( T_{n+1} \) in [35].

### 3.6 Continuous ensemble transform filter formulations

The implementation of [35] requires the computation of a transport map \( T \). Optimal transportation (i.e., maximising the covariance of the transference plan), leads to \( T = \nabla_x \psi \) and the potential satisfies the highly nonlinear, elliptic Monge-Ampere equation
\[
\pi_X(x) \nabla \psi = \pi_X(x).
\]
A direct numerical implementation for high-dimensional state spaces \( X = \mathbb{R}^N \) seems at present out of reach. Instead, in this section we utilize an embedding method due to Moser [37], replacing the optimal transport map by a suboptimal transport map which is defined as the time-one flow map of a differential equation in artificial time \( s \in [0, 1] \). At each time instant, determining the right hand side of the differential equation requires the solution of a linear elliptic PDE; nonlinearity is exchanged for linearity at the cost of suboptimality. In some cases, such as Gaussian PDFs and mixtures of Gaussian, the linear PDE can be solved analytically. In other cases, further approximations, such as a mean field approach discussed later in this section, are necessary.

Inspired by the embedding method of Moser [37], we first summarize a dynamical systems formulation [12] of Bayes’ formula which generalizes the continuous EnKF formulation from Section 3.3. We first note that a single application of Bayes’ formula [3] can be replaced by an \( \mathcal{D} \)-fold recursive application of the incremental likelihood \( \tilde{\pi} \):
\[
\tilde{\pi}(y|x) = \frac{1}{(2\pi)^{K/2}|R|^{1/2}} \exp \left( -\frac{1}{2D} \left( h(x) - y \right)^\top R^{-1} \left( h(x) - y \right) \right), \tag{51}
\]
i.e., we first write Bayes formula as
\[
\pi_X(x|y_0) \propto \pi_X(x) \prod_{j=1}^{\mathcal{D}} \tilde{\pi}(y_0|x),
\]
where the constant of proportionality depends only on \( y_0 \), and then consider the implied iteration
\[
\pi_{j+1}(x) = \frac{\pi_j(x) \tilde{\pi}(y_0|x)}{\int_{\mathbb{R}^N} dx \pi_j(x) \tilde{\pi}(y_0|x)}
\]

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with \( \pi_0 = \pi_X \) and \( \pi_X(y_0) = \pi_D \). We may now expand the exponential function in (51) in the small parameter \( \Delta s = 1/D \), in the limit \( D \to \infty \) obtaining the evolution equation

\[
\frac{\partial \pi}{\partial s} = -\frac{1}{2} (h(x) - y_0)^T R^{-1} (h(x) - y_0) \pi + \mu \pi
\]  

(52)

in the fictitious time \( s \in [0, 1] \). The scalar Lagrange multiplier \( \mu \) is equal to the expectation value of the negative log likelihood function

\[
L(x; y_0) = \frac{1}{2} (h(x) - y_0)^T R^{-1} (h(x) - y_0)
\]  

(53)

with respect to \( \pi \) and ensures that \( \int_{\mathbb{R}^N} (\partial \pi/\partial s) dx = 0 \). We also set \( \pi(x, 0) = \pi_X(x) \) and obtain \( \pi_X(x|y_0) = \pi(x, 1) \).

We now rewrite (52) in the equivalent, but more compact, form

\[
\frac{\partial \pi}{\partial s} = -\pi (L - \bar{L}), \quad \text{where} \quad \bar{L} = E_X[L].
\]  

(54)

Here \( E_X \) denotes expectation with respect to the PDF \( \pi_X = \pi(\cdot, s) \). It should be noted that the continuous embedding defined by (54) is not unique. Moser [37], for example, used the linear interpolation

\[
\pi(x, s) = (1-s)\pi_X(x) + s\pi(X|y_0),
\]

(55)

Yet another interpolation is given by the displacement interpolation of McCann which is based on the optimal transportation map and which has an attractive “fluid dynamics” interpretation [49, 50].

Eq. (54) (or, alternatively, (55)) defines the change (or transport) of the PDF \( \pi \) in fictitious time \( s \in [0, 1] \). Alternatively, following Moser’s work [37, 49], we can view this change as being induced by a continuity (Liouville) equation

\[
\frac{\partial \pi}{\partial s} = -\nabla_x \cdot (\pi g)
\]  

(56)

for an appropriate vector field \( g(x, s) \in \mathbb{R}^N \).

At any time \( s \in [0, 1] \) the vector field \( g(\cdot, s) \) is not uniquely determined by (54) and (56) unless we also require that it is the minimizer of the kinetic energy

\[
\mathcal{T}(v) = \frac{1}{2} \int_{\mathbb{R}^N} \pi v^T M^{-1} v \, dx
\]

over all admissible vector fields \( v : \mathbb{R}^N \to \mathbb{R}^N \) (i.e. \( g \) satisfies (56) for given \( \pi \) and \( \partial \pi/\partial s \)), where \( M \in \mathbb{R}^{N \times N} \) is a positive definite matrix. Under these assumptions, minimization of the functional

\[
\mathcal{L}[v, \phi] = \frac{1}{2} \int_{\mathbb{R}^N} \pi v^T M^{-1} v \, dx + \int_{\mathbb{R}^N} \phi \left( \frac{\partial \pi}{\partial s} + \nabla_x \cdot (\pi v) \right) dx
\]

for given \( \pi \) and \( \partial \pi/\partial s \) leads to the Euler-Lagrange equations

\[
\pi M^{-1} g - \pi \nabla_x \psi = 0, \quad \frac{\partial \pi}{\partial s} + \nabla_x \cdot (\pi g) = 0
\]

in the velocity field \( g \) and the potential \( \psi \). Hence, provided that \( \pi > 0 \), the desired vector field is given by \( g = \nabla_x \psi \), and we have shown the following result.

**Proposition** (Transport map from gradient flow). *If the potential \( \psi(x, s) \) is the solution of the elliptic PDE*

\[
\nabla_x \cdot (\pi_X M \nabla_x \psi) = \pi_X (L - \bar{L}),
\]

(57)

in the velocity field \( g \) and the potential \( \psi \). Hence, provided that \( \pi > 0 \), the desired vector field is given by \( g = \nabla_x \psi \), and we have shown the following result.
then the desired transport map $x' = T(x)$ for the random variable $X$ with PDF $\pi_X(x, s)$ is defined by the time-one-flow map of the differential equations

$$\frac{dx}{ds} = -M \nabla_x \psi.$$  

The continuous Kalman-Bucy filter equations correspond to the special case $M = P$ and $\psi = \delta F/\delta \pi_X$ with the functional $F$ given by [12].

The elliptic PDE (57) can be solved analytically for Gaussian approximations to the PDF $\pi_X$ and the resulting differential equations are equivalent to the ensemble transform Kalman-Bucy equations (46). Appropriate analytic expressions can also be found in case where $\pi_X$ can be approximated by a Gaussian mixture and the forward operator $h(x)$ is linear (see [43] for details).

Gaussian mixtures are contained in the class of kernel smoothers. It should however be noted that approximating a PDF $\pi_X$ over high-dimensional phase spaces $X = \mathbb{R}^N$ using kernel smoothers is a challenging task, especially if only a relatively small number of realizations $x_i, i = 1, \ldots, M$, from the associated random variable $X$ are available.

In order to overcome this curse of dimensionality, we outline a modification to the above continuous formulation, which is inspired by the rank histogram filter of Anderson [2]. For simplicity of exposition, consider a single observation $y \in \mathbb{R}$ with forward operator $h : \mathbb{R}^N \to \mathbb{R}$. We augment the state vector $x \in \mathbb{R}^N$ by $y = h(x)$, i.e. we consider $(x, y)$ and introduce the associated joint PDF

$$\pi_{XY}(x, y) = \pi_X(x|y)\pi_Y(y).$$  

We apply the embedding technique first to $y$ alone resulting in

$$\frac{dy}{ds} = f_y(y, s)$$

with

$$\partial_y(\pi_Y(y)f_y(y)) = \pi_Y(y)(L - \bar{L}).$$

One then finds an equation in the state variable $x \in \mathbb{R}^N$ from

$$\nabla_x \cdot (\pi_X(x|y)f_x(x, y, s)) + f_y(y, s)\partial_y \pi_X(x|y) = 0$$

and

$$\frac{dx}{ds} = f_x(x, y, s).$$

Next we introduce the mean field approximation

$$\pi_1(x^1|y)\pi_2(x^2|y) \cdots \pi_N(x^N|y)$$

for the conditional PDF $\pi_X(x|y)$ with the components of the state vector written as $x = (x^1, x^2, \ldots, x^N)^T \in \mathbb{R}^N$. Under the mean field approximation the vector field $f_x = (f_{x^1}, f_{x^2}, \ldots, f_{x^N})^T$ can be obtained component-wise by solving scalar equations

$$\partial_z(\pi_k(z|y)f_{x^k}(z, y)) + f_y(y)\partial_y \pi_k(z|y) = 0,$$

$k = 1, \ldots, N$, for $f_{x^k}(z, y)$ with $z = x^k \in \mathbb{R}$. The (two-dimensional) conditional PDFs $\pi_k(x^k|y)$ need to be estimated from the available ensemble members $x_i \in \mathbb{R}^N$ by either using parametric or non-parametric statistics.

We first discuss the case for which both the prior and the posterior distributions are assumed to be Gaussian. In this case, the resulting update equations in $x \in \mathbb{R}^N$ become equivalent to the ensemble transform Kalman-Bucy filter. This can be seen by first noting that the update in a scalar observable $y \in \mathbb{R}$ is

$$\frac{dy}{ds} = -\frac{1}{2}\sigma^2_{yy}R^{-1}(y + \bar{y} - 2y_0).$$
Furthermore, if the condition PDF $\pi_k(z|y)$, $z = x^k \in \mathbb{R}$, is of the form (1), then (59) leads to
\[ f_{x^k}(x^k, y) = \sigma_{xy}^2 \sigma_{yy}^{-2} f_y(y), \]
which, combined with the approximation (58), results in the continuous ensemble transform Kalman-Bucy filter formulation discussed previously.

The rank histogram filter of Anderson [2] corresponds in this continuous embedding formulation to choosing a general PDF $\pi_Y(y)$ while a Gaussian approximation is used for the conditional PDFs $\pi_k(x^k|y)$.

Other ensemble transform filters can be derived by using appropriate approximations to the marginal PDF $\pi_Y$ and the conditional PDFs $\pi_k(x^k|y)$, $k = 1, \ldots, N$, from the available ensemble members $x_i$, $i = 1, \ldots, M$.

References
An excellent introduction to filtering and Bayesian data assimilation is [22]. The linear filter theory (Kalman filter) can, for example, be found in [45]. Fundamental issues of data assimilation in a meteorological context are covered in [25]. Ensemble filter techniques and the ensemble Kalman filter are treated in depth in [15]. Sequential Monte Carlo methods are discussed in [13, 4, 3] and by [27, 7] in a geophysical context. See also the recent monograph [19]. The transport view has been proposed in [12] for continuous filter problems and in [42] for intermittent data assimilation. Gaussian mixtures are a special class of non-parametric kernel smoothing techniques which are discussed, for example, in [51].

4 Concluding remarks
We have summarized the Bayesian perspective on sequential data assimilation and filtering in particular. Special emphasize has been put on discussing Bayes’ formula in the context of coupling of random variables, which allows for a dynamical system’s interpretation of the data assimilation step. Within a Bayesian framework all variables are treated as random. While this implies an elegant mathematical treatment of data assimilation problems, any Bayesian approach should be treated with caution in the presence of sparse data, high-dimensional model problems, and limited sample sizes. It should be noted in this context that successful assimilation techniques such as 4DVar (not covered in this survey) and the EnKF lead to biased approximations to the state estimation problem. In both cases the bias is due to the fact that the algorithms are derived under the assumption that the prior distributions are Gaussian. Nevertheless 4DVar and EnKF work often well in terms of the observed mean squared error (10) since the variance of the estimator remains small even for relatively small ensemble sizes $M$. On the contrary, asymptotically unbiased Bayesian approaches such as sequential Monte Carlo methods suffer from the curse of dimensionality, lead generally to large variances in the estimators for small $M$ and have therefore not yet found systematic applications in operational forecasting, for example. To overcome this limitation, one could consider more suitable proposal steps such as guided sequential Monte Carlo methods and/or impose certain independence assumptions such as mean field approximations which lead to an improved balance between bias and variance in the mean squared error (10). See also the discussion of [20] on the bias-variance tradeoff in the context of supervised learning. Promising results for guided particle filters have been reported very recently in [34, 29]. Alternatively, non-Bayesian approaches to data assimilation could be explored in the future such as: (i) shadowing for partially observed reference solutions, (ii) a nonlinear control approach with transport maps as dynamic feedback laws, (iii) derivation and analysis of ensemble filter techniques within the framework of stochastic interacting particle systems.
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