On-line estimation of atmospheric dispersion model parameters using sequential Monte Carlo methods

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Abstract—Exploitation of the data assimilation methodology in the field of radiation protection is studied. When radioactive pollutants are released into the atmosphere, a radioactive plume is passing over the terrain. The released radioactive material causes pathway-specific irradiation which has detrimental effects on population health. In order to ensure efficiency of introduced countermeasures, it is necessary to predict spatial and temporal distribution of radioactive pollution. The predictions are made by the means of numerical dispersion models with many inputs. A group of the most significant input parameters affecting the dispersion process was selected using available sensitivity and uncertainty studies performed on dispersion models. Exact values of these parameters are uncertain due to the stochastic nature of atmospheric dispersion, hence the parameters are modeled as random quantities. Data assimilation algorithm based on the sequential Monte Carlo methods for online estimation of these parameters is presented. Performance is demonstrated on artificial release scenario.

I. INTRODUCTION

Potential failures occurred in man-made processes can cause dangerous phenomena resulting in an accidental release of harmful substances into the living environment. Hazard evaluation and the decision-making focused on the early warning and population protection has the highest priority. Reliable and up to date information represents the basic inevitable conditions for effective management of the intervention operations targeted on consequence mitigation during the emergency situations. Former accidents on nuclear facilities revealed unsatisfactory level of the decision support, both in hardware equipment (reliable communication channels, computation techniques) and the lack of advanced decision support software tools. During the last years, there have arisen demands of responsible authorities for improvement of the safety preparedness for case of a reactor accident in a nuclear power plant. Great attention to this topic is paid since the Chernobyl disaster. It revealed, that the basic requirements given by the law could not be satisfied and there are tendencies for their further improvement. Various decision support systems (DSS) have become part of the crisis management. Their task is to be launched in case of an accident and predict possible consequences with regards to the introduced countermeasures. Predictions can help to avert radiation exposure and decrease the population radiation burden [10], [13], [14]. Substantial improvement of these predictions in both the early and the late phase of a radiation accident can be achieved by involving of the data assimilation.

Data assimilation results from the methods of objective analysis and it is widely applied in the different branches of the “earth sciences” like meteorology and oceanography [1], [8]. In the early phase of a radiation accident (when a radioactive cloud is passing over the terrain), the data assimilation can improve predictions and thus better identify the affected areas. Predictions of further evolution of the deposited material on terrain in the late phase can be made more reliable using objective analysis [5]. This paper studies exploitation of data assimilation in the early phase. Data assimilation is the optimal way how to exploit information from both the measured data and expert-selected prior knowledge to obtain reliable estimates of the inputs to dispersion models. Early identification (estimation) of the input parameters is essential for reduction of uncertainty of the radiation situation predictions. In presented approach, sampling-importance-resampling algorithm (particle filter) is used to evaluate posterior distribution of estimated parameters and improve their estimates online as the plume is passing over the stationary measuring sites. The algorithm is tested on an artificial scenario with simulated measurements. These measurements are simulated by the means of so called twin experiment – the measurements are simulated via the same model (simple Gaussian puff model) as is used for predictions. Topology of the simulated measurements is identical to the real topology of the Czech National radiation protection network maintained by the responsible authorities.

The outline of this paper is as follows. Section II briefly discusses particle filter and puts it in the scope of the Bayesian filtering. Sampling-importance-resampling algorithm is described here. In Section III, the solved assimilation scenario is presented and the applied approach is described. Gaussian puff model is also briefly described here. Numerical experiment with simulated measurements is demonstrated in Section IV. In Section V, experimental results are discussed and the conclusion is given in Section VI.

II. SEQUENTIAL MONTE CARLO ASSIMILATION METHODS

Let the Markovian dynamic model describing our system is defined by discrete-time state-space transition equation (1) and observation equation (2).

\[
x_t = g(x_{t-1}) + b_t \quad (1)
\]

\[
y_t = h(x_t) + \epsilon_t \quad (2)
\]
Here, $t$ is the time index, $x_t$ is unobservable system state vector, $b_t$ is additive dynamic noise vector. Vector $y_t$ is a vector of sequentially observed data which provides us indirect information about the system state and $e_t$ is its noise. Both the densities of noise terms are assumed to be independent and known. Functions $g(\cdot)$ and $h(\cdot)$ are generally non-linear. State transition function $g(\cdot)$ propagates the prior state to the current one. Forward observation operator $h(\cdot)$ transforms vectors from the state–space to the measurement space, thus constitutes relation of the actual measurements to the current system state. The model formulated above covers a broad class of real life problems.

The goal of the data assimilation is to produce so called analysis – an estimate of the future state taking into account available data [6]. Advanced assimilation algorithms are based on methods of the Bayesian filtering [4], [7]. Bayesian approach to filtering is applicable to all linear and non–linear stochastic systems. In Bayesian context, the model given by (1) and (2) defines at each time $t$ the state transition probability density function (pdf)

$$p(x_t|x_{t-1})$$

and the observation pdf

$$p(y_t|x_t).$$

Hence, the analysis is represented by the means of the marginal posterior pdf

$$p(x_t|Y_t),$$

where $Y_t = \{Y_{t-1}, y_t\}$ are available data.

The procedure of Bayesian filtering consists of two recursively repeated steps. The first step evaluates (3). This step is called the time update (6). In the second step called data update (7), the information provided by actual measurements $y_t$ is included into the current state estimate given by the pdf $p(x_t|Y_{t-1}).$

$$p(x_t|Y_{t-1}) = \int p(x_t|x_{t-1})p(x_{t-1}|Y_{t-1})dx_{t-1}$$  \hspace{1cm} (6)

$$p(x_t|Y_t) = \frac{p(y_t|x_t)p(x_t|Y_{t-1})}{p(y_t|x_{t-1})p(x_{t-1}|Y_{t-1})dx_t}.$$  \hspace{1cm} (7)

The assimilation process is initialized by a pdf $p(x_0|Y_{-1}) = p(x_0)$ representing all the prior information related to the problem. This density is often called background–field or just the prior.

Our aim is to recursively in time estimate posterior pdf and the expectations

$$I(f) := E_{p(x_t|Y_t)}[f(x_t)] = \int f(x_t)p(x_t|Y_t)dx_t$$

for some functions $f(\cdot)$ of random variables $x_t$ integrable with respect to $p(x_t|Y_t).$

Evaluation of (6) and (7) generally involves integration over complex spaces and often it is computationally infeasible. Analytical solution is permitted only very limited class of problems (e.g. Gaussian–linear). Sequential Monte Carlo methods (SMCM), also known as particle filters, provide an efficient way how find good approximation of the integrals. SMCM sequentially update Monte Carlo approximation of the posterior (5). This posterior is represented by a discrete sample of points and weights [3].

Let $\{x_t^{(i)}; i = 1, \ldots, M\}$ is a set of samples from posterior density $p(x_t|Y_t).$ An empirical estimate of this distribution is given by

$$p_M(x_t|Y_t) = \frac{1}{M} \sum_{i=1}^{M} \delta(x_t - x_t^{(i)}),$$  \hspace{1cm} (9)

where $\delta(\cdot)$ is the Dirac $\delta$–function. Function (8) can be then approximated as

$$I_M(f) = \int f(x_t)p_M(x_t|Y_t)dx_t = \frac{1}{M} \sum_{i=1}^{M} f(x_t^{(i)}).$$  \hspace{1cm} (10)

This estimate is unbiased. From the strong law of large numbers follows that

$$I_M(f) \xrightarrow{a.s.} I(f), \text{ as } M \to +\infty,$$

where $a.s.$ denotes almost sure convergence [3].

The advantage of this perfect sampling Monte Carlo method is that from the random samples $\{x_t^{(i)}; i = 1, \ldots, M\}$ can be easily estimated any quantity $I(f)$ and the rate of convergence of this estimate is independent of the dimension of the integrand. Nevertheless, in real problems we are not usually able to sample directly from $p(x_t|Y_t).$ To overcome this obstacle we use a method called importance sampling. Provided that the support of $p(x_t|Y_t)$ is included in support of a pdf $q(x_t|Y_t),$ we can draw independent samples $x_t^{(i)}$ from $q(x_t|Y_t)$ and use them for approximating of $p(x_t|Y_t).$

The known pdf $q(x_t|Y_t)$ we choose is called importance sampling pdf.

The function $I(f)$ can be evaluated as

$$I(f) = \frac{\int \frac{f(x_t)w(x_t)}{q(x_t|Y_t)}dx_t}{\int \frac{w(x_t)}{q(x_t|Y_t)}dx_t},$$  \hspace{1cm} (12)

where $w(x_t)$ is called importance weight defined as

$$w(x_t) = \frac{p(x_t|Y_t)}{q(x_t|Y_t)}.$$  \hspace{1cm} (13)

Assuming the set of $M$ i.i.d. particles $\{x_t^{(i)}; i = 1, \ldots, M\}$ from $q(x_t|Y_t),$ substitution of (10) into (12) yields Monte Carlo estimate $I_M(f)$ of $I(f)$

$$\hat{I}_M(f) = \frac{1}{M} \sum_{i=1}^{M} f(x_t^{(i)})\tilde{w}(x_t^{(i)}),$$

where $\tilde{w}(x_t^{(i)})$ is normalized importance weight given by

$$\tilde{w}(x_t^{(i)}) = \frac{w(x_t^{(i)})}{\sum_{j=1}^{M} w(x_t^{(j)}).}$$  \hspace{1cm} (15)

For $M$ finite, $\hat{I}_M(f)$ is biased but asymptotically holds true

$$\hat{I}_M(f) \xrightarrow{a.s.} I(f), \text{ as } M \to +\infty.$$  \hspace{1cm} (16)
Recursive formula for evaluation of importance weights is an algorithm called sampling–importance–sampling (SIS).

It simplifies to

\[ w_t^{(i)} = w_t^{(i)} \frac{p(y_t|x_t^{(i)}) p(x_t^{(i)}|x_{t-1}^{(i)})}{q(x_t^{(i)}|x_{t-1}^{(i)}, Y_t)}. \]

It is beneficial to choose prior pdf from the current step as an importance function. Recursive formula (19) then simplifies to

\[ \tilde{w}_t^{(i)} \propto \tilde{w}_{t-1}^{(i)} p(y_t|x_t^{(i)}). \]

The SIS algorithm suffers from degeneracy problem, so we have to implement a resampling algorithm. Degeneracy of the sample means, that the algorithm becomes unstable as \( t \) increase due to the growing discrepancy between the weights. The most of particles will have negligible weights. Resampling should eliminate particles with small weights and multiply particles with large weights. After resampling, all the weights are equally set to \( \frac{1}{M} \). If we perform resampling in each step, the weights can be computed as \( \tilde{w}_t^{(i)} = p(y_t|x_t^{(i)}) \). To stabilize the algorithm it is necessary to perform resampling sufficiently often. A suitable measure of degeneracy of the algorithm is the effective sample size \( N_{eff} \). Its estimate \( \tilde{N}_{eff} \) can be obtained as

\[ \tilde{N}_{eff,t} = \frac{1}{\sum_{i=1}^{M} (\tilde{w}_t^{(i)})^2}. \]

Estimate of effective sample size can be evaluated each step. Resampling is performed if \( \tilde{N}_{eff,t} \) exceeds an a priori given threshold \( N_{th,r} \). The modification of SIS algorithm with resampling is known sampling–importance–resampling (SIR), see the box ALGORITHM. More on resampling can be found in [2].

A. Combined filtering on parameters and state variables

Depending on the physical background of the solved problem, some elements of the state vector \( x_t \) can be constant in time. These states can be viewed as fixed model parameters. The original state vector \( x_t \) is then factorized as

\[ x_t = \{ x_t, \theta \}, \]

where \( \theta \) are fixed model parameters and \( x_t \) is a vector of dynamic states. The state transition pdf (3) becomes

\[ p(x_t|x_{t-1}, \theta) \]

and the observation density (4) has the form

\[ p(y_t|x_t, \theta). \]

Measurement vectors \( y_t \) are assumed to be conditionally independent of past states and measurements given the current state \( x_t \) and the parameter vector \( \theta \). The goal becomes to get posterior density \( p(x_t, \theta|Y_t) \) given as

\[ p(x_t, \theta|Y_t) \propto p(Y_t|x_t, \theta)p(x_t, \theta) \]

The problem is solved as combined filtering on parameters and state variables. A zero–mean normal noise is added to parameters during each resampling. This step constitutes the time evolution of parameters.

\[ \theta_{t+1} = \theta_t + \epsilon_{t+1}, \quad \epsilon_{t+1} \sim N(0, \Sigma), \]

where \( N(0, \Sigma) \) is multidimensional normal distribution with zero mean and a covariance matrix \( \Sigma \). The “artificial” evolution prevents degeneracy because of the reduction of the sample diversity [3]. It simply increases the variance of the sample. The algorithm can be then considered as an algorithm for simultaneous estimation of both the fixed model parameters and the state variables.
III. ASSIMILATION SCENARIO

Assimilation scenario studied in this paper is as follows. Assume a reactor accident in a nuclear power plant. After some time, there is a radioactive cloud passing over the terrain. The evolution and the movement of the cloud is usually modeled by the means of numerical dispersion models. Physical effects taking place in the dispersion process are in these models parametrize via semi-empirical formulas having tuning parameters. A group of the most significant parameters affecting the dispersion process (including parametrization of meteorological forecast) was selected using available sensitivity and uncertainty studies performed on dispersion models [12]. Exact values of these parameters are uncertain due to the stochastic nature of atmospheric dispersion, hence the parameters are modeled as random quantities. Wrong initial setting of these parameters can introduce huge errors into the predictions of radiation situation and thus forbid to introduce effective countermeasures in the actually affected areas. Reliability of predictions can be significantly improved using data assimilation. The task is to on-line estimate parameters \( \theta \) in order to increase correspondence of modeled prediction with the physical reality. These parameters are consequently used for prediction of future radiation situation (in terms of a radiological quantity).

Due to the deposition processes is the radioactive puff depleted. Time integrated deposition is the radiological quantity modeled in this scenario.

The problems fits into the family of Markovian models described in Section II. Realization of the process at time \( t \) contains all the information about the past, which is necessary in order to calculate the prediction of future evolution.

A. Dispersion Model

Gaussian puff model is an approximative solution of three dimensional advection–diffusion equation. Since it is a basic statistical approximation of the solution of the three dimensional advection–diffusion equation, its simplicity and transparency allow for better insight. Equation (27) is the basic equation describing concentration of the pollutant released from an instantaneous source in an arbitrary spatial location and time \( t > 0 \) given the appropriate inputs.

\[
C(r, t) = \frac{Q}{(2\pi)^{\frac{3}{2}} \sigma_x \sigma_y \sigma_z} \exp \left\{ -\frac{1}{2} \left( \frac{x-ut}{\sigma_x} \right)^2 + \frac{y^2}{\sigma_y^2} + \frac{z^2}{\sigma_z^2} \right\},
\]  

(27)

where \( r = (x, y, z) \) is a vector of spatial coordinates and \( t \) is time index. The parameter \( \sigma_{xy} \) stands for the horizontal dispersion which is assumed to be identical in both the x-axis and y-axis direction.

The model is able to take into account meteorological forecast provided by the Czech Hydrometeorological Institute. From the concentration given by (27) can be evaluated time integrated concentration (TIC). TIC is the fundamental radiological quantity in these types of emergency calculations and it can be used for evaluation of radiological quantities being subject to the regulatory guides. From near ground TIC can be easily calculated time integrated deposition (TID) [11] which is the output of the developed model.

As the radioactive cloud is passing over the stationary measuring sites on terrain

IV. NUMERICAL EXPERIMENT

Performance of the algorithm is demonstrated on simulated release of I-131 from a nuclear facility. The time horizon assumed in the example was from the release start up to the 120 minutes. As the half–time of decay of the I-131 is approximately 8.1 days, it can be on chosen time horizon neglected. TID is modeled on a rectangular grid \( 21 \times 21 \) with the grid step 1km, where the source of pollution is placed in the centre. Measurements are simulated via the same dispersion model used for calculation of predictions and perturbed with normal noise with the zero mean value. The dispersion of this noise is proportional to the magnitude of “measurement” plus, there is a additive dispersion avoiding production of absolute zeros causing singularities in calculations. Assumed stationary measuring sites are subset of the Radiation monitoring network of the Czech Republic. The topology of measuring sites depicted in the figure 1 is identical to the real topology of radiation monitoring network in the surroundings of the nuclear power plant Temelin. Parameters treated as random in this example and their parameterizations are:

\[
\theta = (\theta_1, \theta_2)
\]  

(28)

- **Magnitude of the released activity** \( Q \) is parametrizes as

\[
Q = \theta_1 \times Q_0,
\]  

(29)

where \( Q_0 \) is initial activity given by responsible authorities and \( \theta_1 \) is multiplicative scaling factor with given prior probability distribution.
• **Wind direction (advection direction)** $\phi$ is parametrized as

$$\phi = \phi_0 + \Delta \phi,$$

where $\phi$ is initial wind direction given by the meteorological forecast and $\Delta \phi = \theta_2 \times (2\pi/80)$ rad is additive factor with given prior probability distribution.

Both the parameters are regarded as time–global. It means, that their values are constant during the release. This has the physical meaning, for example, the Time–global parameters can be viewed as a fixed model parameters. Particle attrition in resampling methods and weight degeneracy in reweighting. It causes degradacy of approximation accuracy. This issues are acute when we deal with fixed model parameters (cite West 1993a,b). Using approach called artificial evolution of particles we can overcome this problem. Its principle consists in adding of random disturbances (“roughening penalties”) to sampled state vectors in an attempt to deal with sample degeneracy.

Prior probability distributions assigned to unknown random parameters are described in the table I. The priors are chosen according to the expert studies performed in [9].

<table>
<thead>
<tr>
<th>Parameter, $\theta$</th>
<th>PDF type</th>
<th>PDF parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\theta_1$</td>
<td>LogNormal</td>
<td>$\alpha_{0.05} = 1.0; \alpha_{0.95} = 10.0, 3\sigma$ truncated</td>
</tr>
<tr>
<td>$\theta_2$</td>
<td>Uniform</td>
<td>$\text{min} = -5.0; \text{max} = 5.0$</td>
</tr>
</tbody>
</table>

The model developed for purposes of algorithm testing allows for direct evaluation of the modeled radiological quantity in a set of a priori given spatial locations, not just in the points of the grid. Advantage of this approach is that we don’t need to evaluate model in all the grid points. Evaluation of TIC is the most “expensive” operation of the algorithm. The time demands grows approximately liner with the number of such a points.

**V. Results**

In the figure 2 are prior distribution of $\theta$ given by the table I. In the figure 3 are empirical distributions of parameters $\theta$ produced by the algorithm after 11 data updates. The estimates of parameters 11 data updates are $\hat{\theta} = (\hat{\theta}_1, \hat{\theta}_2) = (1.6801, -2.1781)$. The values used in the twin experiment for purposes of generating of perturbed measurements are $\Theta = (1.7, -2.1)$. The values found “on-line” during the puff movement over the measuring sites are good approximations of the values used for simulation of measurements. The variance of both the estimated parameters stabilized after some and remains approximately constant, it is the variance artificially introduce in the resampling step by the particle filter to maintain the diversity of the sample.

**VI. Conclusion and Future Works**

Algorithm demonstrated a good performance in this artificial scenario with measurements simulated via identical model. As the experiment is pure theoretical, it is difficult
to learn some details even about the availability of measurements in case of the real reactor accident in a nuclear power plant. The formulation of scenario used in the example has arisen from consultation with experts from National Radiation Protection Institute (NRPI) of the Czech Republic. The chosen methodology consisting in exploitation of sequential Monte Carlo methods for combined filtering on parameters and state variables gives good results in this simple scenario. Its performance in more complicated Primary objective of the future work is testing of the assimilation algorithm on more complex models (plume models or Lagrangian particle models) and evaluate its performance on scenarios with more estimated parameters. The limiting factor in these experiments can be computational demands. The fact that in the experiments is included the real topology of the radiation monitoring network is valuable with respect to the future cooperation with the NRPI.

REFERENCES