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Source Term Estimation based on Invertible Neural Network

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1. Introduction

In the case of severe accident, exposure of radioactive nuclides is the ultimate element of harm on human and environment. Therefore, it is important to estimate source term information based on given information near plant. Among them, method of estimating source term using gamma dose rate has recently made significant progress[1]. Inverse estimation technologies incorporating artificial intelligence (AI) techniques [2, 3], ensemble-based methodologies [4], and others have emerged. However, these studies have drawbacks such as inadequate consideration of observation uncertainties or high computation time.

In this paper, we proposed source term estimation method based on invertible neural network, inspired by structure of generative AI. The results showed that it is possible to provide a mathematically feasible estimation range for the problem of inaccurate conditions induced by the uncertainty in gamma dose measurements. This has the advantage of being more scalable than existing optimization-based inverse problem solutions, as it does not require extensive forward computation or differentiation. Moreover, by pre-training neural networks, it is possible to achieve rapid estimation with lower computational time in emergency situations. Additionally, unlike other AI methods, the approach using this technique facilitates decision-making by offering an accessible and accurate estimation range for measurement uncertainty.

2. Methodology

Estimating source term is kind of inverse problem. In this section, our Bayesian viewpoint about source term estimation and invertible neural network, AI model to solve this problem are introduced. Lastly, to validate invertible neural network (INN), approximate Bayesian computation (ABC) algorithm is introduced.

2.1. Bayesian Inverse Problem of Source Term Estimation

Inverse problem is aiming to find $\boldsymbol{x}$ for a given $\boldsymbol{y}$ in the equation $f(\boldsymbol{x}) = \boldsymbol{y}$. In this study, the atmospheric dispersion process corresponds to the forward function f, consequence of dispersion process corresponds to $\boldsymbol{y}$, and emissions of radionuclides correspond to $\boldsymbol{x}$. In addition, meteorological information plays a different role than $\boldsymbol{x}$ and $\boldsymbol{y}$, serving as *auxiliary input* $\boldsymbol{a}$ provided in both the atmospheric dispersion process and the source term estimation process. This can be expressed in the following equation.

$$\begin{aligned} \text{Forward process } &: f\ \ (\boldsymbol{x};\boldsymbol{a}) = \boldsymbol{y} \\ \text{Inverse problem } &: f^{-1}(\boldsymbol{y};\boldsymbol{a}) = \boldsymbol{x} \end{aligned} \qquad (1)$$

This kind of inverse problem setting is widely adopted by previous studies about source term estimation, and it is valid approach when the forward process f is bijective function. However, in the process of estimating the source term, there is often an incomplete determination of x due to the lack of data for the measured data y_{obs}, and uncertainty of measuring $\boldsymbol{y_{obs}} = \boldsymbol{y} + \boldsymbol{\epsilon}$. In such cases, function f is not bijective thus it becomes an ill-posed inverse problem. Accordingly, the goal should not be to accurately determine $\boldsymbol{x}$ as a specific value, but rather to represent it as a probability distribution.

This probability is referred to as Bayesian probability, where the prior distribution $p(\cdot)$ calculated based on prior information is updated for the given data y_{obs} to infer the posterior probability distribution $p(\cdot\ |\boldsymbol{y_{obs}})$.

$$\underset{\substack{\text{prior}\\\text{distribution}}}{p(\cdot)} \quad \underset{\substack{\text{Update}\\\text{with data } y_{obs}\\\text{and condition a}}}{\rightarrow} \quad \underset{\substack{\text{posterior}\\\text{distribution}}}{p(\cdot\,|\,\boldsymbol{y_{obs}},\boldsymbol{a})} \qquad (2)$$

Therefore, on this paper we treated source term estimation problem as Bayesian Inverse Problem.

2.2. Invertible Neural Network

Invertible Neural Networks (INN) are neural networks designed based on the generative AI to solve the inverse function problem[5]. Generative AI aims to generate new forms of data, such as text or images, by learning vast amounts of identical type of data to emulate their distribution. Subsequently, by sampling based on the emulated distribution, it is possible to generate data of the same form. Applying this approach to the Bayesian Inverse Problem (2) can be described as follows.

$$\begin{gathered} \text{Given training data} \\ [\,\boldsymbol{x_i},\boldsymbol{a_i},\boldsymbol{y_i}\,] \text{ with } y_i = f(\boldsymbol{x_i};\boldsymbol{a_i})\,, \\ \underset{\theta}{\text{minimize}}\, D\{\, p_{NN_\theta}(\,\cdot\,;\boldsymbol{y_i},\boldsymbol{a_i}), p(\,\cdot\,|\boldsymbol{y_i},\boldsymbol{a_i})\} \end{gathered} \qquad (3)$$

Here, the function D represents a statistical distance, and a smaller value indicates that the two distributions are more similar. Next, the subscript i corresponds to the indices of the training data, and the statistical distance is calculated based on the distribution generated by these multiple training data. $p_{NN_\theta}(\cdot\,;\boldsymbol{y_i},\boldsymbol{a_i})$ represents the distribution generated by the neural network NN_θ conditioned with $\boldsymbol{y_i}$ and auxiliary input $\boldsymbol{a_i}$. $\boldsymbol{\theta}$ is parameter of NN_θ those changes over training process. Finally, the minimizing process, which is referred as training process is finding $\boldsymbol{\theta}$ that best aligns the distribution $p_{NN_\theta}(\cdot\,;\boldsymbol{y_i},\boldsymbol{a_i})$ generated by the neural network with $p(\cdot\,|\boldsymbol{y_i},\boldsymbol{a_i})$, the actual posterior probability distribution.

For the neural network to produce such a distribution as its output, the structure should be designed to allow the switching of input and output directions. INN also has a forward mode NN^F and an inverse mode NN^I, satisfying the following relationship.

$$NN^F(\boldsymbol{x};\boldsymbol{y},\boldsymbol{a})=\boldsymbol{z} \qquad NN^I(\boldsymbol{z};\boldsymbol{y},\boldsymbol{a})=\boldsymbol{x} \tag{4}$$

Using this, it is possible to emulate a specific distribution when training as following manner.

$$\begin{aligned}&\text{with}\quad \boldsymbol{x}\sim p(\cdot),\ \ \boldsymbol{y}=f(\boldsymbol{x};\boldsymbol{a})\\ &\text{if}\ \ NN^F(\boldsymbol{x};\ \boldsymbol{y},\boldsymbol{a})\sim N(0,1),\\ &\text{then with sampled,}\ \ \boldsymbol{z}\sim N(0,1),\\ &NN^I(\boldsymbol{z};\ \boldsymbol{y},\boldsymbol{a})\sim p(\boldsymbol{x}\mid \boldsymbol{y},\boldsymbol{a})\end{aligned} \tag{5}$$

In conclusion, whole training process of INN for inverse problem is summarized as followed.

$$\underset{\theta}{\text{minimize}}\, D\{\,p_{NN_\theta^F(x_i\,;y_i\,,a_i)}(\cdot),N(0,1)\} \tag{6}$$

Here, $p_{NN_\theta^F(x_i\,;y_i\,,a_i)}$ represents the distribution generated by the output $NN_\theta^F(\boldsymbol{x_i}\,;\boldsymbol{y_i}\,,\boldsymbol{a_i})$ over data $\boldsymbol{i}$.

2.3. Approximate Bayesian Computation

To validate the results generated by INN, it is important to know the actual posterior distribution. However, in cases where the inverse problem cannot be analytically solved, it is impossible to know such a posterior distribution. Therefore, in this study, we used Approximate Bayesian Computation (ABC)[6] as a method to emulate such posterior probability distributions.

ABC is a kind of Monte Carlo technique that can sample very similarly to the posterior distribution. About inverse problem represented as (2), to a sample $\boldsymbol{x}$ sampled from the prior probability distribution $p(\boldsymbol{x})$, if only $\boldsymbol{x}$ satisfying $f(\boldsymbol{x};\boldsymbol{a})=\boldsymbol{y}$ is accepted, it becomes equivalent to sampling from the posterior probability distribution $p(x|y)$. However, in the actual source term estimation process, what is given is not the exact value $\boldsymbol{y}$ but an observed value that added error, $\boldsymbol{y_{obs}}=\boldsymbol{y}+\boldsymbol{\epsilon}$; as mentioned before that's one of the reasons why it becomes ill-posed and Bayesian Inverse Problem (2). Thus, we can sample from posterior distribution $p(\boldsymbol{x}|\boldsymbol{y_{obs}},\boldsymbol{a})$ considering the relative error $\boldsymbol{\sigma}$ of the observation by following acceptance condition.

$$\left|\frac{f(\boldsymbol{x};\boldsymbol{a})-\boldsymbol{y_{obs}}}{f(\boldsymbol{x};\boldsymbol{a})}\right|<\sigma \tag{8}$$

Following table is Pseudo code represents sampling number of n_{sample} samples with observation $\boldsymbol{y_{obs}}$, observation relative error $\boldsymbol{\sigma}$, and meteorological condition $\boldsymbol{a}$. The sampled $\boldsymbol{x}$ is stored on the list $posterior\_list$ and this is output at last stage.

Table 1: Pseudo code of ABC

```
(Input the state and initialization)
Set n_sample and σ
Input a and y_obs
Initialize posterior_list= [ ]

(Sampling)
While (size of posterior_list) <n_sample :
      Sample x from prior distribution p(x)
      Calculate y_cal = f(x; a)

        (Accept condition)
        If |(f(x;a)−y_obs)/f(x;a)| < σ :
            Stack y on posterior_list
Output posterior_list
```

3. Problem settings

In this study, the forward process f of the inverse problem consists mainly of the atmospheric dispersion of the source term and the measurement of environmental radiation exposure resulting from it. Among these processes, the atmospheric dispersion process is modeled using the Gaussian Plume Model. This is the most basic model and is a widely used model in the Nuclear Regulatory Commission (NRC) for the probabilistic safety assessment in level 3 [7].

Additionally, in the estimation problem of the source term, it is necessary to consider how the distributed point source manifests at a given location as a measured value. In this case, the environmental gamma dose has been set as the measurement factor. The impact of the radioactive source is manifested in indicators such as surface deposition quantity and the concentration of radionuclides in the air. However, obtaining such information in a short period is impractical for emergency response. On the other hand, gamma dose can be obtained in real-time from existing environmental radiation measurement stations, making it relatively suitable for emergency response.

Lastly, since we set Bayesian Inverse Problem caused by observation error $\boldsymbol{\sigma}$, it should be added on gamma dose measurement. In conclusion, the whole process to make $\boldsymbol{x}$ and $\boldsymbol{y}$ can be summarized as followed.

$$\underset{\substack{\text{Souce term}\\ \text{emission rate}}}{\boldsymbol{x}} \rightarrow \underset{\substack{\text{Gaussian plum}\\ \text{model}}}{g(x;\, a)} \rightarrow \underset{\substack{\text{Environmental}\\ \text{gamma dose}\\ \text{measurement}}}{\gamma\big(g(x)\big)} \rightarrow \underset{\substack{\text{Adding}\\ \text{observation}\\ \text{error}}}{\mathbf{y} = \gamma\big(g(x)\big) + \epsilon} \quad (9)$$

Therefore, the function f for inverse problem can be represented as $\boldsymbol{f}(\boldsymbol{x}) = \boldsymbol{\gamma}\big(\boldsymbol{g}(\boldsymbol{x})\big) + \boldsymbol{\epsilon}$.

4. Results and discussion

We generated 800,000 datasets based on section 3. Among them, 700,000 is for training, and 100,000 is for testing. Each data on dataset consists of source term emission rate $\boldsymbol{x}$, meteorological condition $\boldsymbol{a}$, and observed gamma dose rate y_{obs}. Since these datasets are generated for inverse problem, prior distribution $p(\boldsymbol{x})$ and are set as table 2.

Table 2: Input and output range of estimation model

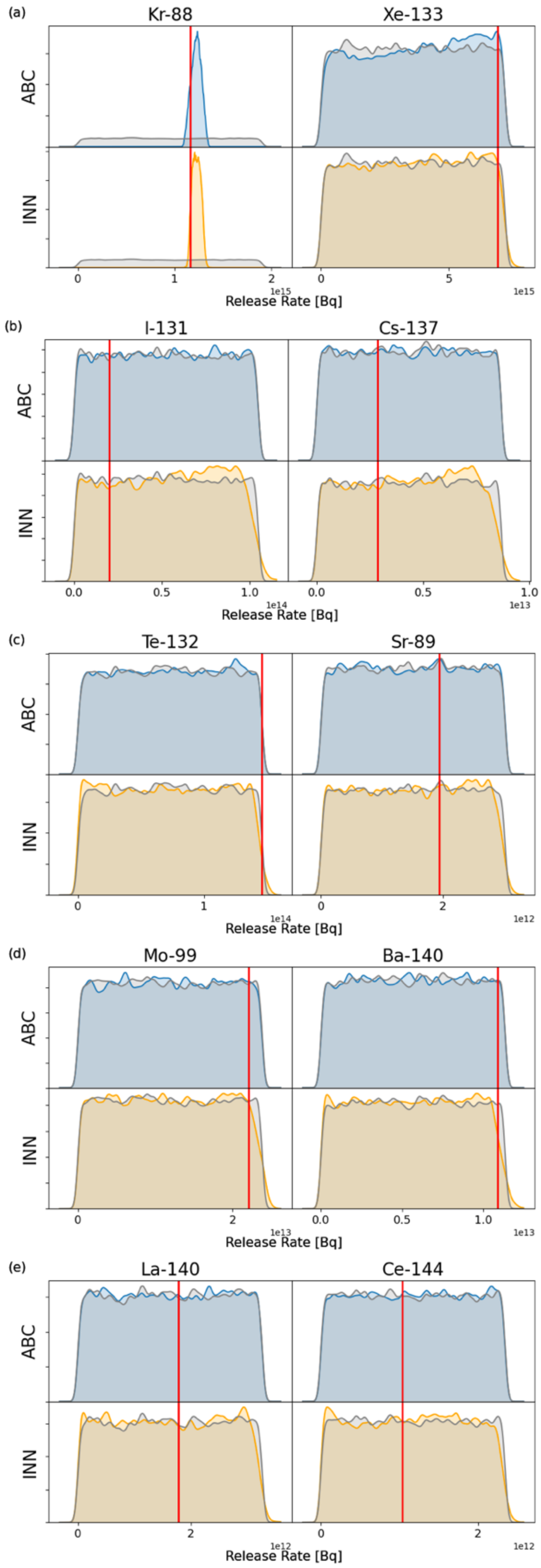
Input $\boldsymbol{x}$	Emission rate of each nuclide $r(1\sim11)$	$Q_r \sim U\big(0, 100q_{r,\text{stc3}}\big)$ [bq]
Auxiliary input $\boldsymbol{a}$	Wind speed	$v \sim U(1, 12)$ [m/s]
	Gustiness atmospheric stability	$Gclass\ (B, C, D, E)$ $\in$ {[1,0,0,0], [0,1,0,0], [0,0,1,0], [0,0,0,1]}
	Effective emit height	$h \sim U(0{,}60)$ [m]
	Observation location of each station $s(1\sim40)$	$\begin{cases} x \sim U(2000{,}10000) \\ y \sim U(0{,}1000) \\ z \sim U(0{,}100) \end{cases}$
Output $\boldsymbol{y}$	Observed gamma dose rate of each station $s(1\sim40)$	$[y_{obs}]_s = \gamma\text{Dose}_s \times (1+\epsilon)$ with $\boldsymbol{\epsilon} \sim U(-\sigma, \sigma)$

Here, $q_{r,\text{stc3}}$. It is emission rate value based on level 3 PSA in case of source term category (STC) 3 [8]. $U(a, b)$ denotes a uniform distribution between a and b.

Gustiness atmospheric stability is categorized by B, C, D, E and one-hot encoded to each elementary vector in 4-diminsional space. Wind direction is set as $+x$ direction. Lastly, observation relative error ϵ has range from $-\sigma$ to σ, is set as 5%.

About 1 random data in 100,000 test data, we depicted in Fig. 1 the posterior distribution simulated using ABC and the one calculated by the proposed INN-based model in this study. Since The proposed estimation model does not represent the source term to be estimated as a single value, but rather presents it as a posterior probability distribution corresponding to a predetermined gamma dose rate observation error. Therefore, it is most appropriate to compare ABC with the shape.

One notable aspect is the impact of measurement relative errors, making it challenging to predict isotopes other than the main isotope Kr-88. Even with a 5% error, the range of Xe-133 was slightly reduced under certain conditions, but the uncertainty was significantly high. This is applicable not only to artificial intelligence models but also to the output of the posterior distribution sampled by ABC. It implies that the influence of measurement uncertainty on defective conditions for the inverse problem of source term estimation is indeed substantial, and this uncertainty represents the unique mathematical characteristics of the inverse problem of source term estimation.



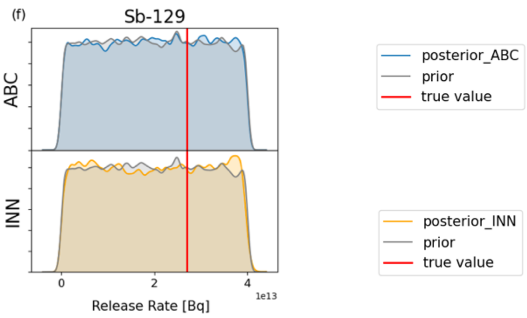


Fig. 1. Prior(grey) and observation updated posterior(colored) distribution calculated by ABC(blue) and INN(orange) of 11 radionuclides.

Simultaneously, it is observed that the posterior probability distribution provided by the INN-based model closely resembles the posterior probability distribution calculated by ABC. Considering the similarity of the results of ABC to mathematical solutions for the given ill-posed inverse problem, it can be inferred that the model operates effectively. Furthermore, while ABC required computations for tens of billions of randomly generated samples to draw the posterior distribution, the INN-based model performed only the necessary operations for precisely 20000 samples extracted from a standard normal distribution.

5. Conclusions

In this study, source term estimating problem was formulated as a Bayesian Inverse Problem considering measurement errors. An approach based on INN was employed to solve such problems. The results showed that the posterior distribution obtained through INNs closely matched the accessible estimation range corresponding to the specified gamma dose rate observation errors.

This source term estimation method based on INN, unlike optimization-based methods, includes no forward operations in the solving process, making it applicable to advanced atmospheric dispersion models. Expectations include rapid operation during emergencies through pre-training. Furthermore, compared to existing artificial intelligence-based techniques, it offers an advantage in understanding emergency situations and responding effectively due to considering realistic measurement errors in the accessible estimation range.

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