Bayesian inference of preferential seepage path by gradient-based Markov Chain Monte Carlo

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ABSTRACT

The region or the path of preferential seepage flow is inversely identified by a gradient-based Markov Chain Monte Carlo method called Hamiltonian Monte Carlo (HMC). Observing hydraulic head and discharge rate of seepage water, HMC method estimates the domain or the path of preferential seepage flow by changing the shapes of finite elements over which the seepage flow is numerically solved by the finite element method. One simple synthetic example is solved in this article, and the numerical result shows that HMC method with a moving mesh performs well for this geometric inverse problem.

Keywords: preferential seepage flow, inverse problem, Hamiltonian Monte Carlo method, moving mesh

1 INTRODUCTION

Piping is a common problem for embankments, such as levees and irrigation tanks, which leads to leakage of reservoir water and unknowingly develops in these soil structures or under the ground. Detection of the piping path or the region of the preferential seepage flow is quite difficult at present even if several types of geophysical exploration methods, such as elastic wave exploration and electrical resistivity survey, are applied. Since these exploration methods estimate the physical properties of elastic wave velocity and electrical resistivity of embankment materials, the exploration result does not provide the clear interface between the highly permeable region and the intact domain (Usually the interface becomes blurred). When the highly permeable region possesses a thin and long or a complex configuration, its detection becomes more difficult.

This article proposes a method which enables the clear interface of the piping region to be estimated by observation data of hydraulic head and discharge rate of seepage water. The method does not estimate a material parameter, such as hydraulic conductivity, but directly identify the shape of the piping region. Hence, the identification of the piping region is regarded as a geometric inverse problem in this study. In order to solve the inverse problem through Bayesian inference, a variant of Markov Chain Monte Carlo method (Duane et al., 1987; Neal, 2011; Betancourt, 2017), called Hamiltonian Monte Carlo method (HMC), is used for generating the posterior probability of parameters characterizing the shape of the piping region. HMC enables efficient sampling of the parameters obeying their posterior probability with the gradient of likelihood. To calculate the gradient of likelihood with respect to the parameters, finite element mesh for forward analysis is continuously deformed. A simple numerical example for detecting a thin and long piping region is shown herein after the above-mentioned methodology is detailed.

2 SEEPAGE FLOW AND OBSERVATION

In this article, the configuration of the piping region is parametrized by $\theta$, which is a vector including geometrical parameters, such width or length, in its components. In order to estimate the geometrical parameters by Bayesian inference, the following observation equation is commonly assumed.

$$y = Hx + w$$

where $y$, $H$, $x$, and $w$, denote the observation vector indicating observed quantities, the observation matrix composed of zero or one component, the state vector describing the state of a system and the observation noise, respectively. The observation noise is assumed to follow the normal distribution with the average of zero and the covariance matrix of $R$. The subscript of $t$ in the above-mentioned vectors implies the time step.

Since the hydraulic head and the seepage flow rate around the piping region are assumed to be observed, the well-known saturated seepage flow problem is solved for the forward analysis for simplicity, which results in the following linear system equation by finite element formulation.
where \( K, \ h_i \) and \( q_i \) denote the matrix indicating global hydraulic conductivity, nodal hydraulic head vector and nodal flux vector, respectively. It should be noted that the matrix \( K \) is constructed as a function of the geometric parameters \( \Theta \). The state vector \( x \) in this study consists of the vectors \( h_i \) and \( q_i \), as shown below.

\[
x_T = (q_i^T, h_i^T)
\]

### 3 HAMILTONIAN MONTE CARLO METHOD

#### 3.1 Basic procedures

Hamiltonian Monte Carlo method (HMC) can be regarded as a gradient-based Markov Chain Monte Carlo method. It can efficiently generate samples following the posterior probability distribution function \( P(\theta | y_{1:T}) \) in which \( T \) denotes the total number of observation time steps. HMC defines Hamiltonian \( \mathcal{H} \), kinetic energy \( K \) and potential energy \( \phi \) as functions of \( \theta \) and momentum vector \( p \).

\[
\mathcal{H}(\theta, p) \equiv K(p) + \phi(\theta)
\]

The potential energy \( \phi \) of Eq. (6) is obtained by taking negative logarithm of the numerator in the posterior probability.

\[
P(\theta | y_{1:T}) \equiv \frac{P(y_{1:T} | \theta) P(\theta)}{\text{const}}
\]

Commonly a Gaussian distribution is given to \( P(p) \). Then, Eq. (5) is rewritten into

\[
K(p) = \frac{1}{2} p^T M^{-1} p
\]

where \( M \) is a mass matrix, which plays the role of scaling and rotating the parameter space, though a diagonal matrix \( M \) is given herein.

Assuming the prior distribution of \( \theta, P(\theta) \) to be Gaussian, the potential energy \( \phi \) has the following form with the aid of Eq. (1), neglecting resultant constants.

\[
\phi(\theta) = \frac{1}{2} \sum_{i=1}^{T} \left[ \theta_i - Hx_i \right]^T R^{-1} \left[ \theta_i - Hx_i \right] + \frac{1}{2} \theta^T \Sigma^{-1}_0 \theta
\]

where \( \Sigma_0 \) is the covariance matrix of the prior distribution of \( \theta \). Sampling process by HMC solves the following equations to give the chain of \( \theta \) through the Hamiltonian dynamics.

\[
\frac{d\theta}{dt} = \frac{\partial \mathcal{H}}{\partial p} = M^{-1} p
\]

\[
\frac{dp}{dt} = -\frac{\partial \mathcal{H}}{\partial \theta} = - \partial \phi \partial \theta
\]

Unless analytical solutions to Eqs. (10) and (11) are available, these equations are numerically integrated. The Leapfrog integrator is a commonly used numerical integrator for sampling by HMC.

This Leapfrog step calculate the following equations iteratively \( L \) times with a step-size of \( \epsilon \).

\[
p_i(t + \epsilon/2) = p_i(t) - \frac{\epsilon \cdot \partial \mathcal{H}}{2 \partial \theta_i}|_{t}
\]

\[
\theta_i(t + \epsilon) = \theta_i(t) + \frac{p_i(t + \epsilon/2)}{m_i}
\]

\[
p_i(t + \epsilon) = p_i(t + \epsilon/2) - \frac{\epsilon \partial \phi}{2 \partial \theta_i}|_{t}
\]

where \( \theta \) and \( p_i \) are the components of the geometric parameter and momentum vectors, respectively, and \( m_i \) denotes the diagonal component of the mass matrix \( M \).

#### 3.2 Gradient of potential energy

As seen in Eqs. (11), (12) and (14), the gradient \( \partial \phi / \partial \theta \) is needed for HMC. Differentiating Eq. (9), it is given as follows.

\[
\frac{\partial \phi}{\partial \theta} = \sum_{i=1}^{T} \left[ \theta_i - Hx_i \right]^T R^{-1} \left( -H \frac{\partial Hx_i}{\partial \theta} \right) + \theta^T \Sigma^{-1}_0 \theta
\]

Eq. (15) includes \( \partial Hx_i / \partial \theta \), which is composed by \( \partial q_i / \partial \theta \) and \( \partial h_i / \partial \theta \) (See Eq. (3)). These two quantities can be computed by solving the following equation.

\[
\frac{\partial K}{\partial \theta} \mathbf{b} + K \frac{\partial h_i}{\partial \theta} = \frac{\partial q_i}{\partial \theta}
\]

Eq. (16) is obtained by differentiating Eq. (2) with respect to \( \theta \). Even though Eq. (16) has two unknown vectors of \( \partial q_i / \partial \theta \) and \( \partial h_i / \partial \theta \), the boundary conditions for Eq. (2) reduce unknown components of the two vectors and make Eq. (16) solvable for the unknowns.

In order to make \( \partial K / \partial \theta \) in the left-hand side of Eq. (16) available, the finite element mesh need to be smoothly changed or moved as the parameter vector \( \theta \) changes. For the calculation of \( \partial K / \partial \theta \), the literatures of shape optimization are helpful (e.g., Haslinger & Mákinen, 2003; Christensen & Klarbring, 2008).

#### 3.3 Algorithm

Let \( N \) be the number of samples generated by HMC. The algorithm of HMC is written as below.

I. Give initial parameter, \( \theta^1 \) and \( n=1 \)

II. Change \( n \) into \( n+1 \) and sample a value of \( p \) following the normal distribution \( N(0, M) \).

III. \( \theta^\text{new} \rightarrow \theta^\text{old} \) and \( p \rightarrow p^\text{old} \)

IV. Leapfrog integration updating \( \theta^\text{old} \) and \( p \):

Eqs. (12) to (14) are repeated \( L \) times \( (j=1, \ldots, L) \)

\[
p_i(j \epsilon/2) = p_i((j-1) \epsilon) - \frac{\epsilon \partial \phi}{2 \partial \theta_i}|_{j \epsilon/2}
\]

\[
\theta_i(j \epsilon) = \theta_i((j-1) \epsilon) + \frac{p_i(j \epsilon/2)}{m_i}
\]

\[
p_i(j \epsilon) = p_i(j \epsilon/2) - \frac{\epsilon \partial \phi}{2 \partial \theta_i}|_{j \epsilon}
\]

V. \( \tilde{\theta}(L \epsilon) \rightarrow \tilde{\theta}^\text{new} , \tilde{p}(L \epsilon) \rightarrow \tilde{p}^\text{new} \) and calculate \( \alpha_n \)

\[
\alpha_n = \min \left\{ 1, \frac{\exp[-\left( \phi(\tilde{\theta}^\text{new}) + K(\tilde{p}^\text{new}) \right)]}{\exp[-\left( \phi(\tilde{\theta}^\text{old}) + K(\tilde{p}^\text{old}) \right)]} \right\}
\]

VI. Metropolis accept step:

Sample a value of \( u \) following the uniform distribution \( U(0,1) \).

\[ \tilde{\theta}^\text{new} = \tilde{\theta}^\text{new} \text{ when } u \leq \alpha_n \]

\[ \tilde{\theta}^\text{old} = \tilde{\theta}^\text{old} \text{ when } u > \alpha_n \]

VII. Return to II unless \( n = N \)
The values of $L$ and $\epsilon$ needed for the Leapfrog integration is a set of tuning parameters for HMC. Dual averaging method (Nesterov, 2009) was used for determining these tuning parameters.

4 ESTIMATION OF PIPING REGION

A simple example estimating a thin piping region is considered in this section. Fig. 1 shows the computational domain and the observation points of this example. The tilted thin piping region is placed in the right side of the rectangular computational domain. The prescribed hydraulic head changing with time was imposed on the left side and the right side had the free outflow boundary condition, where the hydraulic head was assumed to be zero. The boundary condition of zero flux was imposed on the top and bottom impermeable sides.

The shape of the piping region was parametrized by three quantities of $l$, $w$, and $y_d$ which denote the horizontal length, the width and the vertical position of its entrance. The hydraulic head denoted by $h_1$ and $h_2$ was measured at the two observation points indicated by the black circles in Fig.1, and the flow rate at the exit of the piping region was also used as observation data. The observation data was numerically prepared by conducting seepage flow analysis with the above-mentioned boundary conditions over the computational domain.

Table 1. HMC parameters and hydraulic conductivity.

| Parameter                              | Value          |
|----------------------------------------|----------------|
| Number of Observation steps $T$        | 30             |
| Hydraulic conductivity $k$ (m/s)       | $1.0 \times 10^{-5}$ |
| Number of sampling $N$                 | 2000           |
| Number of Leapfrog steps $L$           | 30             |
| Range of $l$ (m)                       | $0.50 \leq l \leq 9.50$ |
| Range of $w$ (m)                       | $0 \leq w \leq 0.50$ |
| Range of $y_d$ (m)                     | $0.50 \leq y_d \leq 4.00$ |
| Initial parameters $\mathbf{p}$        | $\begin{pmatrix} 5.00 & 0.30 & 1.00 \end{pmatrix}^T$ |
| Covariance matrix of observation error $\mathbf{R}$ | $\begin{bmatrix} 1.0 \times 10^{-12} & 0 & 0 \\ 0 & 1.0 \times 10^{-4} & 0 \\ 0 & 0 & 1.0 \times 10^{-4} \end{bmatrix}$ |
| Covariance matrix of target parameter $\Sigma_\theta$ | $\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1.0 \times 10^{-2} & 0 \\ 0 & 0 & 1 \end{bmatrix}$ |

![Fig. 2. Observation data: (a) Discharge rate $Q$, (b) Hydraulic head $h_1$, (c) Hydraulic head $h_2$.](image)

![Fig. 3. Estimated parameters generated by HMC: (a) $l$, (b) $w$, (c) $y_d$.](image)
domain shown by Fig. 1. For this purpose, \( l = 1.0 \) m, \( w = 0.2 \) m and \( y_d = 2.5 \) m were given and the hydraulic head on the left side \( h \) was linearly increased with time steps as follows.

\[
\overline{h} = 2 + (t - 1) \frac{20}{T} \text{ (Unit: m)} \quad (17)
\]

Fig. 2 shows the observation data created by the above procedure.

The geometric inverse analysis for detecting the configuration of the piping region was conducted with HMC parameters listed in Table 1, and the uniform hydraulic conductivity was given to the computational domain. Starting from the initial value of \( l = 5.0 \) m, \( w = 0.3 \) m and \( y_d = 1.0 \) m, HMC generated 2,000 samples following the posterior distribution, as explained in the previous section.

Fig. 3 shows the samples of \( l \), \( w \) and \( y_d \), which were sequentially generated by HMC and correspond to the identified values of the parameters. Approximately, the first 100 samples exhibit the drastic change of their values. This stage is called ‘burn-in’ or ‘warm-up’. Fig. 4 shows the histograms of the estimated three parameters after the warm-up stage. The variance of \( l \) and \( y_d \) is smaller than that of \( w \) (The histograms of \( l \) and \( y_d \) have a steeper distribution). This fact can be also seen in Fig. 3, in which the samples of \( w \) has a greater variance.

This fact implies that the width of the piping region \( w \) was more difficult to be identified than \( l \) and \( y_d \). In other words, \( w \) is not as sensitive to the observation data as \( l \) and \( y_d \). For example, the discharge rate at the exit of the piping region is significantly affected by its surface area because seepage water discharges into the piping region from the soil-void interface. The piping region is thin and long, so that its surface area is dominantly determined by its length. Hence, the width \( w \) can be less sensitive than other parameters.

Table 3 shows the estimated and the target (true) values of the parameters. The estimated values in the table is corresponding to the average of each set of the HMC samples. All the parameters are well-estimated. The identified values of \( l \) and \( y_d \) are approximately the same as the target values, while \( w \) has a relatively large discrepancy between the estimated and target values. The reason for this result is the same as mentioned above.

### 5 CONCLUSIONS

This article has proposed a method to identify the configuration of the region or the path affected by piping phenomenon by observing hydraulic head and flow rate around the piping region. The geometric inverse problem was solved by Bayesian inference, in which the shape of the piping domain was parametrized by geometric quantities, such as length and width, and Hamiltonian Monte Carlo method (HMC) was employed to obtain
sample sets of the posterior probabilistic distribution on the parameter space. Since HMC needs the gradient of the likelihood, the finite element mesh was smoothly deformed, i.e., moved, which enabled the gradient to be computed.

A synthetic example which identify the shape of a thin and long piping region was demonstrated in order to examine the performance of the proposed method. The result has revealed that all the geometric parameters were successfully identified and their probabilistic distribution showed the sensitivity to the observation data.

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