Bayesian Inference Forgetting

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Abstract

The right to be forgotten has been legislated in many countries but the enforcement in machine learning would cause unbearable costs: companies may need to delete whole models trained from massive resources because of single individual requests. Existing works propose to remove the influence of the requested datums on the learned models via its influence function which is no longer naturally well-defined in Bayesian inference. To address this problem, this paper proposes a Bayesian inference forgetting (BIF) framework to extend the applicable domain to Bayesian inference. In the BIF framework, we develop forgetting algorithms for variational inference and Markov chain Monte Carlo. We show that our algorithms can provably remove the influence of single datums on the learned models. Theoretical analysis demonstrates that our algorithms have guaranteed generalizability. Experiments of Gaussian mixture models on the synthetic dataset and Bayesian neural networks on the Fashion-MNIST dataset verify the feasibility of our methods. The source code package is available at https://github.com/fshp971/BIF.

Keywords: Certified knowledge removal, Bayesian inference, variational inference, and Markov chain Monte Carlo.

1 Introduction

The right to be forgotten refers to the right that individuals can ask data controllers to delete their personal information. It has been recognized in many countries through legislation, including the European Union’s General Data Protection Regulation (GDPR) [2] and the California Consumer Privacy Act (CCPA) [1]. However, the enforcement may cause unbearable costs to AI industries. When a single datums deletion request comes, data controllers would need to delete the whole machine learning model which might have cost massive amounts of resources to train, including datums, energy, and time.

To address this issue, recent works [27, 26] propose to forget the influence of some specific datums on the learned models via the influence function [16, 34, 40], which is defined as follows,

\[
\mathcal{I}(x) = -\nabla_\theta^2 L(\theta, S) \nabla_\theta^T \ell(\theta, x),
\]

where \( L(\theta, S) = \frac{1}{n} \sum_{i=1}^{n} \ell(\theta, x_i) \) is the loss function in optimization. This approach can provably remove knowledge of some datums for optimization-based machine learning subject to some conditions on convexity and smoothness.

However, the loss function \( L \) is not always naturally well-defined. In Bayesian inference, one aims to inference the posterior of some probabilistic models, where the loss functions are usually in different forms or even not

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existing. In these cases, the influence function is no longer well-defined, and therefore, the existing forgetting method becomes invalid. The applications of Bayesian inference in machine learning cover a wide spectrum of machine learning algorithms, including probabilistic matrix factorization [48, 64, 74], topic models [32, 10, 76], probabilistic graphic models [41, 8, 73] and Bayesian neural networks [12, 39, 54, 68, 60, 63]. Overlooking Bayesian inference in developing forgetting algorithms leaves a considerable proportion of machine learning algorithms costly to comply with the regulations.

In this paper, we design an energy-based Bayesian inference forgetting (BIF) framework to extend the forgetting algorithms to Bayesian inference. In this framework, we develop certified knowledge removal algorithms for two canonical algorithms in Bayesian inference, variational inference [36, 9] and Markov chain Monte Carlo (MCMC) [24, 47].

- We define new Bayesian inference influence functions based on the pre-defined energy functions, which help provably characterize the influence of some specific datums on the learned posteriors. We prove that these characterizations are rigorous in first-order approximation subject to some mild assumptions on the local convexity and smoothness around the convergence point. Specifically, the approximation error is not larger than the order $O(1/n^2)$ in all cases, and thus can be negligible when the training sample set is sufficiently large.

- We then design the Bayesian inference forgetting (BIF) framework based on the Bayesian inference influence functions. We prove that BIF can realize $\epsilon$-certified knowledge removal, a new notion defined to evaluate performance of knowledge removal.

- We show that the evidence lower bound function (ELBO) [9] plays as an energy function in variational inference. Based on ELBO, a variational inference influence function is design to characterize the influence of a specific datum on the learned model. We then propose a provable variational inference forgetting algorithm. The $\epsilon$-certified knowledge removal is guaranteed on the mean-field Gaussian variational family.

- We design an MCMC influence function for MCMC. The designing procedure is assisted by optimization. We prove that MCMC influence function rigorously characterize the influence induced by a single datum. Based on the MCMC influence function, an MCMC forgetting algorithm is developed. We prove that the $\epsilon$-certified knowledge removal is achieved when the datasets are sufficiently large. Our MCMC forgetting algorithm also applies to stochastic gradient MCMC, including stochastic gradient Langevin dynamics (SGLD) and stochastic gradient Hamiltonian Monte Carlo (SGHMC).

We then investigate whether our forgetting algorithms would affect the generalizabilities of Bayesian models. Based on the PAC-Bayesian theory [49, 50, 51], we prove $O(\sqrt{\log n}/n)$ generalization bounds for the Bayesian models processed by the forgetting algorithms. The results also show that little affect would be introduced by our forgetting algorithms.

From the empirical aspect, we conduct systematic experiments to verify our forgetting algorithms. We first apply the forgetting algorithms to Gaussian mixture models for clustering on a synthetic two-dimensional real-valued dataset. Visualization shows clear movements of the cluster centers caused by forgetting. We then apply the forgetting algorithms to Bayesian neural networks for classification on the Fashion-MNIST dataset. The forgetting performance is analyzed based on the classification errors. Every scenario involves variational inference, SGLD, and SGHMC. All experiments suggest that our forgetting algorithms can effectively remove the influence of specified datums from the learned models and remain other information intact, which are in full agreement with our theoretical results. To secure reproducibility, the generated synthetic data, our code, obtained models, and collected data are available at https://github.com/fshp971/BIF.

The rest of this paper is organized as follows. Section 2 reviews the related works. Section 3 provides the
necessary preliminaries of Bayesian inference. Section 4 presents our main result, the energy-based BIF framework. Section 5 provides the forgetting algorithms developed under the BIF framework for variational inference and MCMC. Section 6 studies the generalization abilities of the proposed algorithms. Section 7 presents the experiment results, and Section 8 concludes the paper.

2 Related Works

Forgetting. The concept “make AI forget you” is first proposed by Ginart et al. [25], which also designs forgetting algorithms for k-means. Bourtoule et al. [13] then propose a “sharded, isolated, sliced, and aggregated” (SISA) framework to approach low-cost knowledge removal via the following three steps: (1) divide the whole training sample set into multiple disjoint shards; (2) train models in isolation on each of these shards; (3) retain the affected model when a request to unlearn a training point arrives. The main challenge of this strategy is that (1) the cost of knowledge removal would still be high if the number of shards is limited; and (2) the learning performance would be undermined when the number of shards goes large. Sommer et al. [65] design a verification algorithm to verify if a machine learning system really processes data deletion requests by poisoning parts of users’ data as backdoor triggers. Guo et al. [27] and Golatkar et al. [26] propose a certified removal based on the influence function [16, 34, 40] of the requested data. Specifically, influence function characterizes the influence of a single datum on the learned model in the empirical risk minimization (ERM) regime. The definition of influence function relies on the gradient and Hessian of the objective function which does not naturally exist in Bayesian inference. Other advances include that Garg et al. [22], Baumhauer et al. [7], and Izzo et al. [35].

We acknowledge that a concurrent work by Nguyen et al. [55] has been proposed on unlearning some data’s influence in Bayesian models. The authors design a variational Bayesian unlearning algorithm that employs variational inference to minimize the KL-divergence between the approximate posterior after unlearning and the posterior of the model retrained on the remaining data. However, no theoretical guarantee has been established, which would be necessary to meet the legal requirements. Moreover, our approach also covers non-parametric models, while variational Bayesian unlearning only applies to parametric models, such as those obtained by variational inference.

Markov chain Monte Carlo (MCMC). Hastings [28] introduces a two-step sampling method named MCMC, which first construct a Markov chain and then draw samples according to the state of the Markov chain. It is proved that the drawn samples will converge to that from the desired distribution. Since that, many improvements have been made on MCMC, including the Gibbs sampling method [24] and hybrid Monte Carlo [18]. Welling and Teh [71] propose a new framework named stochastic gradient Langevin dynamics (SGLD) that by adding a proper noise to a standard stochastic gradient optimization algorithm [61], the iterates will converge to samples from the true posterior distribution as the stepsize annealed. Ahn et al. [5] extend the algorithm based on the SGLD by leveraging the Bayesian Central Limit Theorem, to improve the slow mixing rate of SGLD. Inspired by the idea of a thermostat in statistical physics, Ding et al. [17] leverage a small number of additional variables to stabilize momentum fluctuations caused by the unknown noise. Chen et al. [15] extend the Hamiltonian Monte Carlo (HMC) to Stochastic gradient HMC (SGHMC) by adding a friction term, which enables SGHMC sample from the desired distributions without applying the MH rule. Based on Langevin Monte Carlo methods, Patterson and Teh [59] propose Stochastic gradient Riemannian Langevin dynamics by updating parameters according to both the stochastic gradients and additional noise which forces it to explore the full posterior. Ma et al. [47] introduce a general recipe for creating stochastic gradient MCMC samplers (SGMCMC), which is based on continuous Markov processes specified via two matrices and proved to be complete.

Variational inference. Jordan et al. [36] introduce the use of variational inference in graphical models
Bayesian networks and Markov random fields, in which variational inference is employed to approximate the target posterior with families of parameterized distributions. Blei et al. [10] apply variational inference to local Dirichlet allocation (LDA), which is used to modeling the text corpora. Sung et al. [66] propose a general variational inference framework for conjugate-exponential family models, in which the model parameters except latent variables are integrated in an exact manner, while the latent variables are approximated by a first-order algorithm. By using stochastic optimization [61], a technique that follows noisy estimates of the gradient of the objective, Hoffman et al. [33] derive stochastic variational inference which iterates between subsampling the data and adjusting the hidden structure based only on the subsample. Paisley et al. [57] propose an algorithm that reduces the variance of the stochastic search gradient by using control variates based on stochastic optimization and allows for direct optimization of variational lower bound. Titsias and Lázaro-Gredilla [67] propose local expectation gradients, in which the stochastic gradient estimation problem over multiple variational parameters is decomposed into smaller subtasks, and each sub-task focus on the most relevant part of the variational distribution. Zhang et al. [75] reviews recent advances of variational inference, from four aspects, scalable, generic, accurate, and amortized variational inference.

**Bayesian Neural Networks (BNNs).** Bayesian inference is first applied to neural networks by Neal [54], in which Hybrid Monte Carlo is employed to inference the posteriors of neural networks’ parameters. Blundell et al. [12] propose an efficient backpropagation-compatible algorithm to calculate the gradient of the variational neural networks, which expands the applicable domain of variational inference to deep learning. Based on that, Kingma et al. [39] further propose a local reparameterization technique to reduce the variance of stochastic gradients of variational neural networks. They also develop the variational dropout that can automatically learn the dropout rates. Pearce et al. [60] introduce a procedures family termed randomized MAP sampling (RMS), which includes randomize-then optimize and ensemble sampling, and then realize Bayesian inference for neural networks via ensembling under the RMS family. Roth and Pernkopf [63] successfully apply the Dirichlet process prior to BNNs, which enforces the sharing of the network weights and reduces the number of parameters.

### 3 Preliminaries

Suppose a training sample set is $S = \{ z_1, z_2, \cdots, z_n \}$, where $z_i \in \mathcal{Z}$ is a datum and $n$ is the training sample size. A parametric probabilistic model $p(z|\theta)$ is employed to fit the training sample set $S$, where $\theta \in \Theta \subset \mathbb{R}^d$ is the parameter of model $p(z|\theta)$.

**Bayesian inference** [71, 9, 24] is designed to infer the posterior of the probabilistic model,

$$p(\theta|S) = \frac{p(\theta) \prod_{i=1}^{n} p(z_i|\theta)}{p(S)},$$

where $p(\theta)$ is the prior of model parameter $\theta$ and

$$p(S) = \int p(\theta) \prod_{i=1}^{n} p(z_i|\theta) d\theta$$

is the normalization factor. In most cases, we do not know the closed form of the normalization factor $p(S)$. To address this problem, two canonical solutions are variational inference and MCMC.

**Variational inference** [33, 9] employs a two-step process to inference the posterior:
1. We define a family of distributions, termed variational family, as follows,

$$Q = \{ q_\lambda | \lambda \in \Lambda \},$$

where $\lambda$ is the variational distribution parameter.

2. We search in the variational family $Q$ for the distribution closest to the posterior $p(\theta | S)$ measured by KL divergence, i.e.,

$$\min_\lambda \text{KL}(q_\lambda(\theta) \| p(\theta | S)).$$

Minimizing the KL divergence is equivalent to maximizing the evidence lower bound (ELBO [9]) defined as below,

$$\text{ELBO}(\lambda, S) = \mathbb{E}_{q_\lambda} \log p(\theta, S) - \mathbb{E}_{q_\lambda} \log q_\lambda(\theta).$$

A popular variational family is the mean-field Gaussian family [9]. It has been successfully applied to a variety of tasks, including variational autoencoders (VAEs [38]) and variational neural networks [12, 39]. A mean-field Gaussian variational distribution $q_\lambda$ has the following structure,

$$q_\lambda = \mathcal{N}(\mu, \sigma^2 I),$$

where $\lambda = (\mu_1, \ldots, \mu_d, \sigma_1, \ldots, \sigma_d)$.

**MCMC** [47, 28] constructs a Markov chain whose stationary distribution is the targeted posterior. The Markov chain performs a Monte Carlo procedure to sample the posterior. However, MCMC can be prohibitively time-consuming in large-scale models and large-scale data. To address the issue, stochastic gradient MCMC (SGMCMC [47]) introduces stochastic gradient estimation on mini-batches [61] into Bayesian learning to enable scalable inference. Two major SGMCMC methods are stochastic gradient Langevin dynamics (SGLD [71]) and stochastic gradient Hamiltonian Monte Carlo (SGHMC [15]).

In SGLD, the weight $\theta_t$ is updated as below,

$$\theta_{t+1} = \theta_t + \varepsilon_t \nabla \tilde{U}(\theta) + \mathcal{N}(0, 2\varepsilon_t),$$

where

$$\tilde{U}(\theta) = -\frac{|S|}{|S|} \sum_{z \in \tilde{S}} \log p(z | \theta) - \log p(\theta),$$

$\varepsilon_t \in \mathbb{R}^+$ is the learning rate, and $\tilde{S} \subset S$ is the mini-batch. Usually, one needs to anneal $\varepsilon_t$ to small values.

SGHMC introduces the momentum $v_t$ to improve the convergence speed of SGLD. The weight $\theta_t$ and the momentum $v_t$ are updated as follows,

$$\theta_{t+1} = \theta_t + v_t,$$

$$v_{t+1} = (1 - \alpha_t)v_t - \eta_t \nabla \tilde{U}(\theta) + \mathcal{N}(0, 2\alpha_t \eta_t),$$

where the term $\tilde{U}(\theta)$ is as same as that in SGLD, $\eta_t \in \mathbb{R}^+$ is the learning rate and needs to be annealed to small values, $\alpha_t \in \mathbb{R}^+$ is a factor that satisfies $\alpha_t \propto \sqrt{\eta_t}$ (see eqs. (14), (15) in [15]), and the momentum $v_t$ is initialized as $v_0 \sim \mathcal{N}(0, \eta_0)$. It is worth noting that if we decay $\eta_t$ with a factor of $c$, we also need to decay $\alpha_t$ with a factor of $\sqrt{c}$. 

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5
4 Bayesian Inference Forgetting

This section presents our energy-based Bayesian inference forgetting (BIF) framework. We first define $\varepsilon$-certified knowledge removal in Bayesian inference, which quantitates the knowledge removal performance. Then, we study the energy functions in Bayesian inference. The forgetting algorithm for Bayesian inference is designed based on the energy functions.

4.1 $\varepsilon$-Certified Knowledge Removal

Suppose a Bayesian inference method learns a probabilistic model $\hat{p}_S$ on the training sample set $S$. A client request to remove her/his datums $S' \subset S$. A trivial and costly approach is re-training the model on the datums $S - S'$. Suppose the re-learned probabilistic model is $\hat{p}_{S - S'}$.

A knowledge removal algorithm $\mathcal{M}$ is designed to process the distribution $\hat{p}_S$ to estimate the distribution $\hat{p}_{S - S'}$ as follows

$$\hat{p}_{S - S'} = A(\hat{p}_S, S').$$

We term the distribution $\hat{p}_{S - S'}$ as the processed model.

In order to meet the regulation requirements, we need the algorithm can achieve $\varepsilon$-certified knowledge removal which is defined as follows.

**Definition 4.1** ($\varepsilon$-certified knowledge removal in Bayesian inference). For any subset $S' \subset S$ and $\varepsilon > 0$, if we have,

$$\text{KL}(\hat{p}_{S - S'}, \hat{p}_{S - S'}) \leq \varepsilon,$$

we call the algorithm $A$ performs $\varepsilon$-certified knowledge removal.

4.2 Energy Functions in Bayesian Inference

Bayesian inference can be formulated as minimizing an energy function, echoes the free-energy principle in physics. This section studies the energy functions in Bayesian inference.

Suppose $F(\gamma, S)$ is the energy function of a probabilistic distribution $\chi(\gamma)$ parametrized by $\gamma \in \Gamma \subset \mathbb{R}^K$ over the model parameter space $\Theta$ on the training sample set $S$. It is worth noting that the energy $F(\gamma, S)$ can measure the difference between the distribution $\chi(\gamma)$ and the target posterior $p(\theta|S)$. A low energy corresponds to a small difference between the two distributions. Usually, the energy function $F(\gamma, S)$ has the following structure,

$$F(\gamma, S) = \sum_{i=1}^{n} h(\gamma, z_i) + f(\gamma),$$

(1)

where $h(\gamma, z)$ is a function defined on $\Gamma \times Z$ that characterizes the influence from individual datums, $f(\gamma)$ is a function defined on $\Gamma$ that characterizes the influence from the prior of $\gamma$. In variational inference, ELBO plays as an energy function. In MCMC, we construct an energy function. Please see more details in Sections 5.1 and 5.2.
Similarly, the energy function for $S - S'$ is $F(\gamma, S - S')$. It can be re-arranged as follows,

$$F(\gamma, S - S') = \sum_{z \in S - S'} h(\gamma, z) + f(\gamma)$$

$$= \sum_{i=1}^{n} h(\gamma, z_i) + f(\gamma) - \sum_{z \in S'} h(\gamma, z)$$

$$= F(\gamma, S) - \sum_{z \in S'} h(\gamma, z). \quad (2)$$

### 4.3 Forgetting Algorithm for Bayesian inference

Based on the energy function, the forgetting algorithm for Bayesian inference is designed, shown as the following figure.

Figure 1: The workflow of Bayesian inference forgetting framework that removes the influence of datum $z_j \in S$ from the distribution $\hat{p}_S$. $\hat{p}_S$ is the distribution learned on the training sample set $S$ and is parameterized by $\gamma_S$. $\hat{p}_S^{-z_j}$ is the processed distribution and is parameterized by $\gamma_S^{-z_j}$. $\gamma_S^{-z_j} = \gamma_S - \frac{\partial h(\gamma, z_j)}{\partial \tau}$.

Suppose that the probabilistic model $\hat{p}_S$ learned on the training sample set $S$ is parameterized by $\gamma_S$. Then, $\gamma_S$ is a local minimizer of the energy function $F(\gamma, S)$. Similarly, suppose that the model $\hat{p}_S^{-z_j}$ learned on $S - S'$ is parameterized by $\gamma_S^{-z_j}$. Then $\gamma_S^{-z_j}$ is a local minimizer of the energy function $F(\gamma, S - S')$. Also, we suppose the processed model $\hat{p}_S^{-z_j}$ is parameterized by $\gamma_S^{-z_j}$.

Mathematically, the forgetting in Bayesian inference can be realized by approaching the local minimizer $\gamma_S$ of the energy function $F(\gamma, S)$ to the local minimizer $\gamma_S^{-z_j}$ of the energy function $F(\gamma, S - S')$.

We start with a simple case that remove the influence learned from a single datum $z_j \in S$. The energy function for the posterior $p(\theta|S - \{z_j\})$ is as follows,

$$F(\gamma, S - \{z_j\}) = \sum_{i=1}^{n} h(\gamma, z_i) + f(\gamma) - h(\gamma, z_j). \quad (3)$$
Let \( \gamma_{S-\{z_j\}} \) be a local minimizer of \( F(\gamma, S - \{z_j\}) \). Then,

\[
\nabla_\gamma F(\gamma_S, S) = \sum_{i=1}^{n} \nabla_\gamma h(\gamma_S, z_i) + \nabla_\gamma f(\gamma_S) = 0,
\]

\[
\nabla_\gamma F(\gamma_{S-\{z_j\}}, S - \{z_j\}) = \nabla_\gamma F(\gamma_{S-\{z_j\}}, S) - \nabla_\gamma h(\gamma_{S-\{z_j\}}, z_j) = 0.
\]

Notice that the structures of the above two equations only differ in the term \( \nabla_\gamma h(\gamma, z_j) \). They are two special cases of the following equation,

\[
\nabla_\gamma F(\gamma, S) + \tau \cdot \nabla_\gamma h(\gamma, z_j) = 0,
\]

where \( \tau \in [-1, 0] \). Eq. (4) induces an implicit mapping \( \hat{\gamma}^{-z_j} \) : \([-1, 0] \to \Gamma \) such that \( \hat{\gamma}^{-z_j}(0) = \gamma_S \). For any \( \tau \in [-1, 0] \), \( \hat{\gamma}^{-z_j}(\tau) \) is a solution of eq. (4). Thus, \( \hat{\gamma}^{-z_j}(\tau) \) is also a critical point of the following function,

\[
F_{-z_j, \tau}(\gamma, S) = F(\gamma, S) + \tau \cdot h(\gamma, z_j).
\]

When \( \tau = -1 \), \( F_{-z_j, -1}(\gamma, S) \) is exactly \( F(\gamma, S - \{z_j\}) \), which indicates that \( \hat{\gamma}^{-z_j}(-1) \) is a critical point of \( F(\gamma, S - \{z_j\}) \), and is possible to be a local minimizer. We assume that \( \hat{\gamma}^{-z_j}(-1) \) is really a local minimizer of \( F(\gamma, S - \{z_j\}) \). We also let \( \gamma_{S-\{z_j\}} = \hat{\gamma}^{-z_j}(-1) \). Then, \( \gamma_{S-\{z_j\}} \) can be approached based on \( \gamma_S \) in a first-order approximation manner,

\[
\gamma_{S-\{z_j\}} = \hat{\gamma}^{-z_j}(-1) \approx \hat{\gamma}^{-z_j}(0) - \frac{\partial \hat{\gamma}^{-z_j}(0)}{\partial \tau} = \gamma_S - \frac{\partial \hat{\gamma}^{-z_j}(0)}{\partial \tau}.
\]

Therefore, when a request of removing a datum \( z_j \) comes, our forgetting algorithm will process the request via first calculating \( \frac{\partial \hat{\gamma}^{-z_j}(0)}{\partial \tau} \) from eq. (4) and then subtracting it from \( \gamma_S \). Denote that

\[
\gamma^{-z_j} = \gamma_S - \frac{\partial \hat{\gamma}^{-z_j}(0)}{\partial \tau}.
\]

Then, \( \gamma^{-z_j} \) is the output parameter of our forgetting algorithm.

### 4.4 Theoretical Guarantee

In this section, we give theoretical guarantees for our forgetting algorithms. Under some mild assumptions, we prove that (1) the mapping \( \hat{\gamma}^{-z_j} \) uniquely exists; (2) \( \gamma_{S-\{z_j\}} = \hat{\gamma}_S(-1) \) is the global minimizer of \( F(\gamma, S - \{z_j\}) \); and (3) the approximation error between \( \gamma^{-z_j} \) and \( \gamma_{S-\{z_j\}} \) is not larger than order \( O(1/n^2) \), where \( n \) is the training set size.

We first introduce two definitions.

**Definition 4.2** (compact set). A set is called compact if and only if it is closed and bounded.

**Definition 4.3** (strong convexity). A differentiable function \( f \) is called \( c \)-strongly convex, if and only if there exists a constant real \( c > 0 \), such that for any two points \( z \) and \( z' \) in the domain of the function \( f \), the following inequality holds,

\[
(\nabla f(z) - \nabla f(z'))^T(z - z') \geq \frac{c}{2} \|z - z'\|_2^2.
\]
When $f$ is second-order continuously differentiable, for any $c > 0$, the following three propositions are equivalent:

1. $f$ is $c$-strongly convex;

2. for any $z$ from the domain of the function $f$, the smallest eigenvalue of the Hessian matrix $\nabla^2 f(z)$ is at least $c$, i.e., $\lambda_{\min}(\nabla^2 f(z)) \geq c$;

3. for any $z$ from the domain of $f$, the matrix $(\nabla^2 f(z) - cI)$ is positive semi-definite, i.e., $\nabla^2 f(z) \succeq cI$.

The theoretical guarantees rely on the following two assumptions.

**Assumption 4.1.** Both of the supports $\Gamma$ and $Z$ are compact.

Usually, the energy functions $F(\gamma, S)$ and $F(\gamma, S - \{z_j\})$ are close to each other. Thus, it is reasonable to assume that the local minimizer $\gamma_{S-\{z_j\}}$ falls in the local region around the local minimizer $\gamma_S$. Hence, we only need to analyze in the local region around $\gamma_S$, which justifies Assumption 4.1.

**Assumption 4.2.** Suppose $f(\gamma)$ and $h(\gamma, z)$ are the two inputs of the energy functions $F(\gamma, S)$. We assume that

1. $f(\gamma)$ is 3rd-order continuously differentiable and $c_f$-strongly convex on $\Gamma$,

2. $h(\gamma, z)$ is 3rd-order continuously differentiable with respect to $\gamma$ in $\Gamma \times Z$. Besides, $\forall z \in Z$, $h(\gamma, z)$ is $c_h(z)$-strongly convex with respect to $\gamma$, where $c_h : Z \to \mathbb{R}$ is a continuous function.

Assumption 4.2 is mild in gradient-based optimization. Together with Assumption 4.1, they assume the local strong convexity and smoothness of the energy functions.

We then prove that the energy function $F_{-z_j, \tau}$ is strongly convex, as the following lemma.

**Lemma 4.1.** Suppose Assumption 4.2 holds. For any $\tau \in [-1, 0]$, $F_{-z_j, \tau}(\gamma, S)$ (eq. (5)) is strongly convex with respect to the parameter $\gamma$.

**Proof.** We rewrite the energy function $F_{-z_j, \tau}$ as follows,

$$F_{-z_j, \tau}(\gamma, S) = F(\gamma, S - \{z_j\}) + (1 + \tau)h(\gamma, z_j).$$

Apparently, $F(\gamma, S - \{z_j\})$ is strongly convex. Since $\tau \in [-1, 0]$, we have that $1 + \tau \geq 0$. Thus, $(1 + \tau)h(\gamma, z_j)$ is either strongly convex or equal to zero. Hence, we have that $F_{-z_j, \tau}(\gamma, S)$ is strongly convex with respect to $\gamma$.

The proof is completed. $\square$

We are now able to prove that eq. (4) induces a continuous mapping $\hat{\gamma}_S^{-z_j}$, and $\hat{\gamma}_S^{-z_j}(-1)$ is really a global minimizer of $F(\gamma, S - \{z_j\})$.

**Theorem 4.1.** Suppose assumption 4.2 holds. Then, eq. (4) induces a unique continuous function $\hat{\gamma}_S^{-z_j} : [-1, 0] \to \Gamma$ such that for any $\tau \in [-1, 0]$, $\hat{\gamma}_S^{-z_j}(\tau)$ is (1) the solution of eq. (4) and (2) the global minimizer of eq. (5) with respect to $\gamma$.

**Proof.** According to Lemma 4.1, for any $\tau \in [-1, 0]$, the energy function $F_{-z_j, \tau}(\gamma, S)$ is strongly convex with respect to $\gamma$. Thus, the global minimizer of the energy function $F_{-z_j, \tau}(\gamma, S)$ is unique with respect to
\( \gamma \). Therefore, we can define the mapping \( \hat{\gamma}_S^{-z_j} \) as follows,

\[
\hat{\gamma}_S^{-z_j}(\tau) = \arg \min_{\gamma} F_{-z_j,\tau}(\gamma, S),
\]

where \( \tau \in [-1, 0] \).

Besides, The strong convexity of \( F_{-z_j,\tau}(\gamma, S) \) indicates that when \( \tau \) is fixed, a parameter \( \gamma^* \in \Gamma \) satisfies \( \nabla_\gamma F_{-z_j,\tau}(\gamma^*, S) = 0 \) (eq. (4)), if and only if \( \gamma^* \) is the global minimizer of \( F_{-z_j,\tau}(\gamma, S) \). Thus, \( \forall \tau \in [-1, 0] \), \( \hat{\gamma}_S^{-z_j}(\tau) \) is the only solution of eq. (4).

Eventually, according to Definition 4.3, the strong convexity of \( F_{-z_j,\tau}(\gamma, S) \) implies that the Hessian matrix \( \nabla^2_\gamma F_{-z_j,\tau}(\hat{\gamma}_S^{-z_j}(\tau), S) \) is invertible. Combining with the implicit function theorem, we have that \( \hat{\gamma}_S^{-z_j}(\tau) \) is continuous everywhere on \([-1, 0]\).

The proof is completed. \( \square \)

Theorem 4.1 demonstrates that our algorithm can obtain the \( \hat{\gamma}_S^{-z_j}(-1) \). This ensures that our algorithm can remove the learned influence from the probabilistic model \( \hat{p}_S \).

We then analyze the error introduced by our algorithm. Assume that \( \hat{\gamma}_S^{-z_j} \) is second-order continuously differentiable, then \( \hat{\gamma}_S^{-z_j}(-1) \) can be expanded by the Taylor’s series as follows,

\[
\hat{\gamma}_S^{-z_j}(-1) = \hat{\gamma}_S^{-z_j}(0) + (-1) \cdot \frac{\partial \hat{\gamma}_S^{-z_j}(0)}{\partial \tau} + \frac{(-1)^2}{2} \cdot \frac{\partial^2 \hat{\gamma}_S^{-z_j}(\xi)}{\partial \tau^2},
\]

where \( \xi \in [-1, 0] \), \( \frac{\partial^2 \hat{\gamma}_S^{-z_j}(\xi)}{\partial \tau^2} \) is the Cauchy form of the remainder. Under the following assumption, we prove that the Cauchy remainder term becomes negligible as the training set size \( n \) goes to infinity.

**Theorem 4.2.** Suppose Assumptions 4.2 and 4.1 hold. The induced mapping \( \hat{\gamma}_S^{-z_j} \) is as defined in Theorem 4.1. Then, for any \( \tau \in [-1, 0] \), we have that

\[
\frac{\partial \hat{\gamma}_S^{-z_j}(\tau)}{\partial \tau} = - \left( \nabla^2_\gamma F(\hat{\gamma}_S^{-z_j}(\tau), S) + \tau \cdot \nabla^2 h(\hat{\gamma}_S^{-z_j}(\tau), z_j) \right)^{-1} \cdot \nabla_\gamma h(\hat{\gamma}_S^{-z_j}(\tau), z_j)^T,
\]

and

\[
\left\| \frac{\partial \hat{\gamma}_S^{-z_j}(\tau)}{\partial \tau} \right\|_2 \leq O \left( \frac{1}{n} \right).
\]

The proof of Theorem 4.2 is presented in Appendix A. We first calculate \( \frac{\partial \hat{\gamma}_S^{-z_j}(\tau)}{\partial \tau} \) based on eq. (4). We then upper bound the norm of \( \frac{\partial \hat{\gamma}_S^{-z_j}(\tau)}{\partial \tau} \) by upper bounding the norm of an inverse matrix

\[
\left( \nabla^2_\gamma F(\hat{\gamma}_S^{-z_j}(\tau), S) + \tau \cdot \nabla^2 h(\hat{\gamma}_S^{-z_j}(\tau), z_j) \right)^{-1}
\]

and a vector \( \nabla_\gamma h(\hat{\gamma}_S^{-z_j}(\tau), z_j) \). The norm of the inverse matrix is bounded based on the strong convexity of \( \hat{\gamma}_S^{-z_j}(\tau) \), while the norm of the vector is bounded based on its continuity in a compact domain.
Based on Theorem 4.2, we then prove that the norm of $\frac{\partial^2 \gamma_{S-\{z_j\}}}{\partial \tau^2}(\tau)$ is no larger than order $O(1/n^2)$. Thus, a sufficiently large training sample size ensures that, the second and high order terms in the Taylor’s series are negligible.

**Theorem 4.3.** Suppose Assumptions 4.2 and 4.1 hold. The induced mapping $\gamma_{S-\{z_j\}}$ is as defined in Theorem 4.1. Then, for any $\tau \in [-1, 0]$, we have that

$$\left\| \frac{\partial^2 \gamma_{S-\{z_j\}}}{\partial \tau^2}(\tau) \right\|_2 \leq O\left(\frac{1}{n^2}\right).$$

The proof routine of Theorem 4.3 is similar to Theorem 4.2, while the calculation is more difficult. We leave the details in Appendix A.

**Corollary 4.1.** When Assumptions 4.2 and 4.1 hold, the difference between $\gamma_S$ and $\gamma_{S-\{z_j\}}$ is as follows,

$$\gamma_{S-\{z_j\}} - \gamma_S = \nabla_\gamma^{-2} F(\gamma_S, S) \cdot \nabla_\gamma h(\gamma_S, z_j)^T + O\left(\frac{1}{n^2}\right),$$

where $\gamma_S$ is the global minimizer of the energy function $F(\gamma, S)$ and $\gamma_{S-\{z_j\}}$ is the global minimizer of the energy function $F(\gamma, S - \{z_j\})$.

Eventually, we consider removing a subset $S'$ from $S$. From the previous derivations, we prove that the approximation error of approaching $\gamma_{S-S'}$ based on $\gamma_S$ is also not larger than order $O(1/n^2)$, as stated below,

**Corollary 4.2.** When Assumptions 4.2 and 4.1 hold, the difference between $\gamma_S$ and $\gamma_{S-S'}$ is as follows,

$$\gamma_{S-S'} - \gamma_S = \nabla_\gamma^{-2} F(\gamma_S, S) \cdot \sum_{z_j \in S'} \nabla_\gamma h(\gamma_S, z_j)^T + O\left(\frac{1}{n^2}\right),$$

where $\gamma_S$ is the global minimizer of the energy function $F(\gamma, S)$ and $\gamma_{S-S'}$ is the global minimizer of the energy function $F(\gamma, S - S')$.

### 5 Forgetting Algorithms for Bayesian Inference

In this section, we develop provably certified forgetting algorithms for variational inference and MCMC under the BIF framework.
5.1 Variational Inference Forgetting

As introduced in Section 3, variational inference aims to minimize the following negative ELBO function,

\[-\text{ELBO}(\lambda, S) = -E_{q_\lambda} \log p(\theta, S) + E_{q_\lambda} \log q_\lambda(\theta)\]

\[= -E_{q_\lambda} \log \left( p(\theta) \prod_{i=1}^{n} p(z_i|\theta) \right) + E_{q_\lambda} \log q_\lambda(\theta)\]

\[= \sum_{i=1}^{n} -E_{q_\lambda} \log p(z_i|\theta) + \text{KL}(q_\lambda(\theta)||p(\theta)). \tag{7}\]

Notice that the structure of eq. (7) is similar as that of the energy function (eq. (1)). Thus, we employ the negative ELBO function as the energy function.

Based on the energy function, we define the following variational inference influence function to characterize the influence of single datums on the learned model.

**Definition 5.1** (Variational inference influence function). For any example \(z_j \in S\), its variational inference influence function \(I_{VI}(z_j)\) is defined to be

\[I_{VI}(z_j) := -\nabla_\lambda^{-2} \text{ELBO}(\hat{\lambda}_S, S) \cdot \nabla_\lambda^T E_{q_{\hat{\lambda}_S}} \log p(z_j|\theta), \tag{8}\]

where \(\hat{\lambda}_S\) is the variational parameter that learned on the training sample set \(S\) and \(\nabla_\lambda^2 \text{ELBO}(\lambda, S)\) is assumed to be positive definite.

We then design the **variational inference forgetting** algorithm, to remove the influences of single datums from the learned variational parameter \(\hat{\lambda}_S\),

\[\hat{\lambda}_{S-z_j} = A_{VI}(\hat{\lambda}_S, z_j) = \hat{\lambda}_S - I_{VI}(z_j).\]

We prove that variational inference forgetting can provably remove the influences of datums from the learned model.

**Theorem 5.1.** Let \(\gamma := \lambda, \Gamma := \Lambda, h(\gamma, z) := -E_{q_\lambda} \log p(z|\theta)\) and \(f(\gamma) := \text{KL}(q_\lambda(\theta)||p(\theta))\). Suppose Assumptions 4.2 and 4.1 hold. Then, we have that

\[\hat{\lambda}_{S-z_j} = \hat{\lambda}_S - I_{VI}(z_j) + O\left(\frac{1}{n^2}\right) \approx \hat{\lambda}_S - I_{VI}(z_j),\]

where \(\hat{\lambda}_S\) and \(\hat{\lambda}_{S-z_j}\) are the global minimizers of \(-\text{ELBO}(\lambda, S)\) and \(-\text{ELBO}(\lambda, S - \{z_j\})\), respectively.

**Proof.** It is straightforward from Corollary 4.1. \(\square\)

**Remark 5.1.** When Assumptions 4.2 and 4.1 do not hold, performing variational inference forgetting approaches some critical point of \(-\text{ELBO}(\lambda, S - \{z_j\})\) based on \(\hat{\lambda}_S\).

Beyond single datums removal, Corollary 4.2 further shows that the influence of a sample set \(S'\) can also be
characterized by the variational inference influence function \( I_{\mathcal{V}1}(S') \), as follows,

\[
I_{\mathcal{V}1}(S') = \sum_{z_j \in S'} I_{\mathcal{V}1}(z_j).
\]

This guarantees that one can remove a group of datums at one time. It can significantly speed up and simplify the forgetting process of large amounts of datums.

We next study the \( \varepsilon \)-certified knowledge removal guarantee for the variational inference forgetting algorithm \( \mathcal{A}_{\mathcal{V}1} \). Here, we take the mean-field Gaussian family as an example. Proofs for other variational families are similar.

**Theorem 5.2** (\( \varepsilon \)-certified knowledge removal of mean-field Gaussian variational distribution). Let \( Q \) be a mean-field Gaussian family where the variance of every variational distributions are bounded, i.e., \( \exists M_1, M_2 \in \mathbb{R} \) such that for any \( q_\lambda = \mathcal{N}(\mu, \sigma^2 I) \in Q \), we have \( 0 < M_1 \leq \sigma_i \leq M_2 \) holds for \( i = 1, \ldots, d \). Let \( \hat{\lambda}_S \) and \( \hat{\lambda}_{S-\{z_j\}} \) be the variational parameters that learned on sample sets \( S \) and \( S - \{z_j\} \), respectively. Suppose \( \hat{\lambda}_S^{z_j} = \mathcal{A}_{\mathcal{V}1}(\hat{\lambda}_S, z_j) \) is the processed variational parameter. Then, \( \mathcal{A}_{\mathcal{V}1}(\hat{\lambda}_S, z_j) \) performs \( \varepsilon_{\lambda_S, z_j} \)-certified knowledge removal, where

\[
\varepsilon_{\lambda_S, z_j} = \frac{1}{2M_1^2} \left( 2(M_1 + M_2)\|\hat{\lambda}_S^{z_j} - \hat{\lambda}_{S-\{z_j\}}\|_1 + \|\hat{\lambda}_S^{z_j} - \hat{\lambda}_{S-\{z_j\}}\|_2^2 \right).
\]

The proof of Theorem 5.2 is omitted here and presented in Appendix B. When all the conditions in Theorem 5.1 hold, we have that \( \|\hat{\lambda}^{z_j} - \hat{\lambda}_{S-\{z_j\}}\|_1 \leq O(1/n^2) \) and \( \|\hat{\lambda}_S^{z_j} - \hat{\lambda}_{S-\{z_j\}}\|_2^2 \leq O(1/n^4) \). Thus, \( \varepsilon_{\lambda_S, z_j} \leq O(1/n^2) \). Therefore, \( \mathcal{A}_{\mathcal{V}1} \) performs \( O(1/n^2) \)-certified knowledge removal for mean-field Gaussian variational distribution \( q_{\lambda_S} \).

### 5.2 MCMC Forgetting Algorithm

In MCMC, there is no explicit objective function. In this work, we transport \( p(\theta|S) \) to approximate \( p(\theta|S') \). Specifically, we want to find a “drift” \( \hat{\Delta}_S^{z'} \) to minimize the following KL divergence,

\[
\hat{\Delta}_S^{z'} = \arg \min_{\Delta} \text{KL}(p(\theta|S)||p(\theta + \Delta|S - S')).
\]

This “drift” is named as drifting influence.

The KL term in eq. (9) can be expanded as follows,

\[
\text{KL}(p(\theta|S)||p(\theta + \Delta|S - S')) = \mathbb{E}_{p(\theta|S)} \log p(\theta|S) - \mathbb{E}_{p(\theta|S)} \log p(\theta + \Delta|S - S')
\]

\[
\quad = -\mathbb{E}_{p(\theta|S)} \log \left( \frac{p(\theta + \Delta) \prod_{z \in S} p(z|\theta + \Delta)}{p(S - S') \prod_{z \in S'} p(z|\theta + \Delta)} \right) + \mathbb{E}_{p(\theta|S)} \log p(\theta|S)
\]

\[
\quad = \sum_{i=1}^{n} -\mathbb{E}_{p(\theta|S)} \log p(z_i|\theta + \Delta) - \mathbb{E}_{p(\theta|S)} \log p(\theta + \Delta)
\]

\[
\quad - \sum_{z \in S'} -\mathbb{E}_{p(\theta|S)} \log p(z|\theta + \Delta) + \text{Constant}.
\]

Despite of the constant term, the remaining has the similar structure with \( F(\gamma, S - S') \) (eq. (2)). Therefore,
we define the energy function for MCMC by replacing $h(\gamma, z)$ and $f(\gamma)$ with $-\mathbb{E}_{p(\theta|S)} \log p(z|\theta + \Delta)$ and $-\mathbb{E}_{p(\theta|S)} \log p(\theta + \Delta)$, respectively.

Based on the energy function, we define an MCMC influence function to characterize the drifting influences induced by single datums as follows.

**Definition 5.2** (MCMC influence function). For any example $z_j \in S$, its MCMC influence function $I_{\text{MCMC}}(z_j)$ is defined to be

$$I_{\text{MCMC}}(z_j) := -\left(\mathbb{E}_{p(\theta|S)} \nabla^2_\theta \log p(\theta, S)\right)^{-1} \left(\mathbb{E}_{p(\theta|S)} \nabla_\theta \log p(z_j|\theta)\right)^T.$$ (11)

Then, the MCMC forgetting algorithm is as follows,

$$p^{-z_j}_S(\theta) = A_{\text{MCMC}}(p(\theta|S), z_j) = p(\theta + I_{\text{MCMC}}(z_j)|S).$$

In practice, we do not have the posterior $p(\theta|S)$, but only some samples drawn from $p(\theta|S)$. Thus, we are not able to transform the posterior $p(\theta|S)$ to the processed distribution $p^{-z_j}_S(\theta)$. However, the probability of drawing a sample $\theta_t$ from $p(\theta|S)$ equals that of drawing a sample $\theta_t - I_{\text{MCMC}}(z_j)$ from $p^{-z_j}_S(\theta)$. Therefore, when performing MCMC forgetting, we will replace any drawn sample $\theta_t$ by a new sample $\theta_t - I_{\text{MCMC}}(z_j)$.

We prove that the MCMC forgetting algorithm can provably remove the drifting influence induced by single datums from the learned model.

**Theorem 5.3.** Let $\gamma := \Delta$, $\Gamma := \text{supp}(\Delta)$, $h(\gamma, z) := -\mathbb{E}_{p(\theta|S)} \log p(z|\theta + \Delta)$ and $f(\gamma) := -\mathbb{E}_{p(\theta|S)} \log p(\theta + \Delta)$. Suppose that Assumptions 4.2 and 4.1 hold. Then, we have that

$$\hat{\Delta}^{-z_j}_S = -I_{\text{MCMC}}(z_j) + O\left(\frac{1}{n^2}\right) \approx -I_{\text{MCMC}}(z_j),$$

where $\hat{\Delta}^{-z_j}_S$ is the global minimizer of $\text{KL}(p(\theta|S)\|p(\theta + \Delta|S - \{z_j\}))$.

**Remark 5.2.** When Assumptions 4.2 and 4.1 not hold, performing MCMC forgetting has the following two stages: (1) finding a critical point $\hat{\Delta}^{-z_j}_S$ of the KL divergence $\text{KL}(p(\theta - \Delta|S)\|p(\theta|S - \{z_j\}))$; and (2) replacing the original posterior $p(\theta|S)$ by $p(\theta - \hat{\Delta}^{-z_j}_S|S)$.

**Proof.** When all the conditions hold, the global minimizer of $\text{KL}(p(\theta|S)\|p(\theta + \Delta|S))$ is exactly 0. Meanwhile, $\hat{\Delta}^{-z_j}_S$ is the global minimizer of $\text{KL}(p(\theta|S)\|p(\theta + \Delta|S - \{z_j\}))$. Combining Corollary 4.1, we have
that

\[ \Delta^{-z_j}_S \Delta^{-z_j} = 0 \]

\[ = \left( \nabla^2 \left[ -\mathbb{E}_{p(\theta|S)} \log p(\theta + \Delta, S) \right] \Delta = 0 \right)^{-1} \]

\[ \cdot \left( \nabla \left[ -\mathbb{E}_{p(\theta|S)} \log p(z_j|\theta + \Delta) \right] \Delta = 0 \right)^T + O \left( \frac{1}{n^2} \right) \]

\[ = \left( \mathbb{E}_{p(\theta|S)} \nabla^2 \log p(\theta, S) \right)^{-1} \cdot \left( \mathbb{E}_{p(\theta|S)} \nabla \log p(z_j|\theta) \right)^T + O \left( \frac{1}{n^2} \right) \]

\[ = -I_{\text{MCMC}}(z_j) + O \left( \frac{1}{n^2} \right) \]

\[ \approx -I_{\text{MCMC}}(z_j), \]

The proof is completed. \[ \square \]

Similarly, by applying Corollary 4.2, the MCMC influence function of a sample set \( S' \) is as follows,

\[ I_{\text{MCMC}}(S') = \sum_{z_j \in S'} I_{\text{MCMC}}(z_j). \]

It guarantees that one can adopt MCMC forgetting algorithm to remove a group of datums at one time. This improves the efficiency of removing large amounts of datums.

The MCMC forgetting algorithm also applies to SGMCMC, because SGMCMC draws samples from some target posterior \( p(\theta|S) \) [15, 71, 47], the same as MCMC. We then give the \( \varepsilon \)-certified knowledge removal guarantee for MCMC forgetting.

**Theorem 5.4.** Suppose that

\[ p(\theta|S) = \mathcal{N}(\theta_1, (nJ(\theta_1))^{-1}), \]

\[ p(\theta|S - \{z_j\}) = \mathcal{N}(\theta_2, ((n - 1)J(\theta_2))^{-1}). \]

Let \( p^{-z_j}_S(\theta) = A_{\text{MCMC}}(p(\theta|S), z_j) = p(\theta + I_{\text{MCMC}}(z_j)|S) \) be the processed model. Then, \( A_{\text{MCMC}}(p(\theta|S), z_j) \) performs \( O(\varepsilon_{\theta_1,z_j}) \)-certified knowledge removal, where

\[ \varepsilon_{\theta_1,z_j} = (n - 1)(\theta'_1 - \theta_2)^T J(\theta_2)(\theta'_1 - \theta_2) + \text{tr} \left( J^{-1}(\theta_1)(J(\theta_2) - J(\theta_1)) \right) + \log \left( \frac{|J(\theta_1)|}{|J(\theta_2)|} \right) \]

and \( \theta'_1 = \theta_1 - I_{\text{MCMC}}(z_j). \)

This theorem relies on the following assumption.

**Assumption 5.1.** We assume that the posteriors \( p(\theta|S) \) and \( p(\theta|S - \{z_j\}) \) are Gaussian distributions.

This assumption is from the Bayesian asymptotic theory [23, 44]. Suppose the training set \( S \) is drawn from distribution \( f_1(z) \), while \( S - \{z_j\} \) is drawn from distribution \( f_2(z) \). Then, under some mild assumptions, when the training sample size \( n \) is sufficiently large, the posteriors \( p(\theta|S) \) and \( p(\theta|S - \{z_j\}) \) approach
Gaussian distributions as below,

\[
p(\theta|S) \sim \mathcal{N}(\theta_1, (nJ(\theta_1))^{-1}), \quad p(\theta|S - \{z_j\}) \sim \mathcal{N}(\theta_2, ((n - 1)J(\theta_2))^{-1}),
\]

where \( \theta_i = \arg\min_{\theta} \text{KL}(f_i(z)||p(z|\theta)), \ i = \{1, 2\} \), \( J(\theta) = \mathbb{E}_{p(z|\theta)} \left[ -\frac{\partial^2}{\partial\theta^2} \log p(z|\theta) \right] \) is the Fisher information.

The detailed proof of Theorem 5.4 is omitted here and given in appendix B.

Combining the conditions of Theorem 5.3, we have that \( \|\theta_1' - \theta_2\|_2 \leq O(1/n^2) \). Thus, as \( n \to \infty, \varepsilon_{\theta_1,z} \) will eventually converge to \( \text{tr} \left( J^{-1}(\theta_1)(J(\theta_2) - J(\theta_1)) \right) + \log \frac{|J(\theta_1)|}{|J(\theta_2)|} \).

### 5.3 Efficient Implementation

A major computing burden in both variational inference forgetting and MCMC forgetting algorithms is calculating the product of \( H^{-1}v \), where \( H \) is the Hessian matrix of some vector-valued function \( f(x) \) and \( v \) is a constant vector. The calculation above would have a considerably high computational cost. We follow Agarwal et al. [4] and Koh and Liang [40] to apply a divide-and-conquer strategy to address the issue. This strategy relies on calculating the Hessian-vector product \( Hv \).

**Hessian-vector product (HVP).** We first discuss how to efficiently calculate \( Hv \). The calculation of \( Hv \) can be decomposed into two steps: (1) calculate \( \frac{\partial f(x)}{\partial x} \) and then (2) calculate \( \frac{\partial}{\partial x} \left( \frac{\partial f(x)}{\partial x} \cdot v \right) \). It is worth noting that \( \frac{\partial f(x)}{\partial x} \in \mathbb{R}^{1 \times d} \) and \( v \in \mathbb{R}^{d \times 1} \), where \( d > 0 \) is the dimension of data. Thus, \( \left( \frac{\partial f(x)}{\partial x} \cdot v \right) \) is a scalar value. Calculating its gradient \( \frac{\partial}{\partial x} \left( \frac{\partial f(x)}{\partial x} \cdot v \right) \) has a very low computational cost on platform PyTorch [58] or TensorFlow [3].

**Calculating \( H^{-1}v \).** When the norm \( \|H\| \leq 1 \), the matrix \( H^{-1} \) can be expanded by the Taylor’s series as \( H^{-1} = \sum_{i=0}^{\infty} (I - H)^i \). Define that \( H_j^{-1} = \sum_{i=0}^{j} (I - H)^i \). Then, we have the following recursive equation,

\[
H_j^{-1}v = v + (I - H)H_{j-1}^{-1}v.
\]

Agarwal et al. [4] prove that when \( j \to \infty \), we have \( \mathbb{E}[H_j^{-1}] \to H^{-1} \). Therefore, we employ \( H_j^{-1}v \) to approximate \( H^{-1}v \).

Moreover, to secure the condition \( \|H\| \leq 1 \) stands, we scale \( H \) to \( cH \) by a scale \( c \in \mathbb{R}^+ \), such that \( \|cH\| \leq 1 \). Then, we approximate \( (cH)^{-1} \). Eventually, we have that \( H^{-1} = c(cH)^{-1} \). We can plug it to the applicable equations above.

### 6 Generalization Analysis

In this section, we study the generalization ability of the models that processed by forgetting algorithms. We derive generalization bounds for a mean-field Gaussian variational model and a specified Gaussian MCMC model. Based on PAC-Bayes framework. All the proofs in this section are presented in Appendix C.

Generalization ability is important to machine learning algorithms, which refers to the ability to make accurate predictions on unseen data. A standard measurement of the generalization ability is the generalization bound, i.e., the upper bound of the difference between expected risk and empirical risk [53, 70, 52]. An algorithm with a small generalization bound is expected to generalize well. Existing generalization bound can be
roughly divided into three categories: (1) generalization bounds based on the hypothesis complexity, such as VC dimension [11, 69], Rademacher complexity [43, 42, 6], and covering number [19, 29], which suggest implementations control the hypothesis complexity to help model generalize well; (2) generalization bounds based on the algorithmic stability [62, 14], which follow the intuition that an algorithm with good generalization ability is robust to the interference of single data points; (3) generalization bounds established under the PAC-Bayesian framework [50, 49]; and (4) generalization guarantees from differential privacy [20, 56, 31]. The excellent generalization ability of the over-parameterized model, including Bayesian neural network and others in deep learning, is somehow beyond the explanation of the conventional learning theory. Establishing theoretical foundations has been attracted wide attention [21, 30].

Let $Q$ be a probabilistic model. Then, the expected risk of $Q$ is defined to be

$$\mathcal{R}(Q) = \mathbb{E}_{h \sim Q}\mathbb{E}_z \ell(h, z),$$

where $h$ is a hypothesis drawn from $Q$, and $\ell$ is a loss function with a range of $[0, 1]$. Moreover, suppose $S$ is the training sample set. Then, the empirical risk of $Q$ is defined to be

$$\hat{\mathcal{R}}(Q, S) = \mathbb{E}_{h \sim Q}\frac{1}{n} \sum_{i=1}^{n} \ell(h, z_i).$$

The difference of expected risk $\mathcal{R}(Q)$ and empirical risk $\hat{\mathcal{R}}(Q, S)$ is the generalization error. Its magnitude characterizes the generalizability of the algorithm.

We then prove a generalization bound for mean-field Gaussian variational distributions.

**Theorem 6.1.** Suppose all the conditions in Theorems 5.1 and 5.2 hold. Let $q_\lambda = \mathcal{N}(\mu, \sigma^2 I)$ denotes the mean-field Gaussian distribution learned on the training set $S$. Let $\lambda^- = \mathcal{A}_{\lambda}(\lambda, z_j)$ denotes the processed variational distribution parameter, where $z_j \in S$. Also, let $\Delta_\lambda = \mathcal{I}_{\lambda}(z_j) = (\Delta_{\mu}, \Delta_{\sigma})$ denotes the variational inference influence function. Then, for any real $\delta \in (0, 1)$, with probability at least $1 - \delta$, the following inequality holds for the processed variational distribution $q_{\lambda^-}$:

$$\mathcal{R}(q_{\lambda^-}) \leq \hat{\mathcal{R}}(q_{\lambda^-}, S) + \sqrt{\frac{C_{\lambda, \Delta_{\lambda}} + 2 \log \frac{1}{\delta} + 2 \log n - d + 4}{4n - 2}},$$

(12)

where

$$C_{\lambda, \Delta_{\lambda}} = \|\Delta_{\lambda}\|^2 + 2\|\lambda\| \cdot \|\Delta_{\lambda}\| + \|\lambda\|^2 - 2 \sum_{k=1}^{d} \log (\sigma_k - \Delta_{\sigma_k}) \leq O(1),$$

and $\|\Delta_{\lambda}\| \leq O\left(\frac{1}{n}\right)$.

**Remark 6.1.** This generalization bound is of order $O(\sqrt{(\log n)/n})$.

**Corollary 6.1.** Variational inference forgetting increases the generalization bound by a value not larger than $O(1/n)$.

**Proof.** Variational inference forgetting introduces the term $\|\Delta_{\lambda}\|$ into the generalization bound. Thus, the
generalization bound is increased by the following value:

\[
O \left( \sqrt{\|\Delta \lambda\|^2 + 2\|\lambda\| \cdot \|\Delta \lambda\| - 2 \sum_{k=1}^{d} \log \left( \frac{\sigma_k - \Delta \sigma_k}{\sigma_k} \right)} \right) \leq O \left( \sqrt{\frac{O(1/n^2) + O(1/n) + O(1/n)}{4n - 2}} \right) = O \left( \frac{1}{n} \right). 
\]

The proof is completed.

This corollary secures that variational inference forgetting would not compromise the generalizability.

In Section 5.2, we have shown that when the training sample size is sufficiently large, the posterior distribution \(p(\theta|S)\) is asymptotically Gaussian. Here, we again assume that \(p(\theta|S) = \mathcal{N}(\theta_1,(nJ(\theta_1))^{-1})\), where \(J(\theta)\) is the Fisher information matrix. Then, a generalization bound is obtained as follows.

**Theorem 6.2.** Suppose all the conditions in Theorem 5.3 hold. Suppose that \(p(\theta|S) = \mathcal{N}(\theta_1,(nJ(\theta_1))^{-1})\). Let \(p^* = \mathcal{A}_{\text{MCMC}}(p(\theta|S), z_j)\) denotes the processed distribution, where \(z_j \in S\). Let \(\Delta \theta = \mathcal{I}_{\text{MCMC}}(z_j)\) denotes the MCMC influence function. Then, for any \(\delta \in (0,1)\), with probability at least \(1 - \delta\), the following inequality holds for the processed distribution \(p^*\):

\[
\mathcal{R}(p^*) \leq \mathcal{R}(p^*,S) + \sqrt{\frac{C_{p,\Delta \theta_1} + 2 \log \frac{1}{\delta} + (d + 2) \log n - d + 4}{4n - 2}},
\]

where

\[
C_{p,\Delta \theta_1} = \|\Delta \theta_1\|^2 + 2\|\theta_1\| \cdot \|\Delta \theta_1\| + \|\theta_1\|^2 + \frac{1}{n} \text{tr}(J^{-1}(\theta_1)) + \log |J(\theta_1)| = O(1),
\]

and \(\|\Delta \theta_1\| \leq O \left( \frac{1}{n^{1/4}} \right)\).

**Remark 6.2.** This generalization bound is of order \(O(\sqrt{(\log n)/n})\).

**Corollary 6.2.** MCMC forgetting increases the generalization bound by a value not larger than \(O(1/n)\).

**Proof.** MCMC forgetting introduces the term \(\|\Delta \theta_1\|\) into the generalization bound. Thus, the generalization bound is increased by the following value:

\[
O \left( \sqrt{\|\Delta \theta_1\|^2 + 2\|\theta_1\| \cdot \|\Delta \theta_1\|} \right) \leq O \left( \sqrt{\frac{O(1/n^2) + O(1/n)}{4n - 2}} \right) = O \left( \frac{1}{n} \right).
\]

The proof is completed.

This corollary secures that MCMC forgetting would not compromise the generalizability.
7 Experiments

We conduct comprehensive experiments to investigate the feasibility of our algorithms. In Section 7.1, we apply the forgetting algorithms to Gaussian mixture model (GMM) on a synthetic dataset for the clustering problem. In Section 7.2, we apply the forgetting algorithms to Bayesian neural network on the Fashion-MNIST dataset for classification problem. In every scenario, we employ variational inference and two SGMCMC methods, SGLD and SGHMC. The empirical results are in full agreement with our methods. To secure reproducibility, the generated synthetic data, our code, obtained models, and collected data are available at https://github.com/fshp971/BIF.

7.1 Experiments for Gaussian Mixture Model

We first conduct experiments with GMM on Synthetic data to evaluate our methods.

7.1.1 Implementation Details

The implementation details are given below.

**Synthetic dataset.** We generate a dataset $S$ of size 2,000 for evaluating our algorithms. Every datum is two-dimensional and is possibly from $K$ classes. In this experiment, we set $K$ as 4. The raw data is visualized in the left of fig. 2a, in which four different colors represent four different classes.

**Gaussian mixture model (GMM).** GMMs are usually employed to inference the cluster centers. GMM assumes data is drawn from $K$ Gaussian distributions centered at $\mu_1, \cdots, \mu_K$, respectively. The hierarchical structure of GMM is as follows: (1) draw a clustering center from the uniform distribution over $\{\mu_{c_1}, \cdots, \mu_{c_K}\}$; and (2) sample $z_i$ from a Gaussian distribution centering at $\mu_{c_i}$.

$$
\begin{align*}
\mu_k &\sim \mathcal{N}(0, \sigma^2 I), \\
c_i &\sim \text{categorical} \left( \frac{1}{K}, \cdots, \frac{1}{K} \right), \\
Z_i &\sim \mathcal{N}(\mu_{c_i}, I),
\end{align*}
$$

where $1 \leq k \leq K$, $1 \leq i \leq n$, $\mu_k \in \mathbb{R}^d$, $c_i \in \{1, \cdots, K\}$, $Z_i \in \mathbb{R}^d$, and the hyperparameter $\sigma \in \mathbb{R}$ is the prior standard deviation. We set $\sigma$ as 1 in our experiments.

Applying SGLD and SGHMC to GMM is straightforward. Besides, for variational inference, we utilize the following mean-field variational family [9],

$$
q(\mu, c) = \prod_{k=1}^{K} q(\mu_k) \prod_{i=1}^{n} q(c_i|\mu), \\
\mu_k \sim \mathcal{N}(m_k, s_k^2), \\
q(c_i = k|\mu) \propto \exp \left( \mathbb{E}_{q-c_i} \log p(x_i|\mu, c_i) \right) \\
= \exp \sum_j \left( x_{ij} m_{kj} - \frac{m_{kj}^2 + s_{kj}^2}{2} \right),
$$

where $x_i, m_k, s_k \in \mathbb{R}^d$, and $\lambda = (m_1, \cdots, m_K, s_1, \cdots, s_K)$ is the variational distribution parameter. Thus,
the ELBO function is calculated as follows,

$$ \text{ELBO}(\lambda, S) = - \sum_{k,j} \frac{m_{kj}^2 + s_{kj}^2}{2\sigma^2} + \sum_{k,j} \log s_{kj} - \sum_{i,k,j} \varphi_{ik} \frac{-2 x_{ij} m_{kj} + m_{kj}^2 + s_{kj}^2}{2} $$

$$ - \sum_{i,k} \varphi_{ik} \log \varphi_{ik} - \frac{1}{2} \sum_{i,j} x_{ij}^2 + \text{Constant}, $$

where $1 \leq i \leq n$, $1 \leq k \leq K$, $1 \leq j \leq d$, and

$$ \varphi_{ik} = q(c_i = k|\mu) \propto \exp \sum_{j} \left( x_{ij} m_{kj} - \frac{m_{kj}^2 + s_{kj}^2}{2} \right). $$

**Experiment design.** We employ variational inference, SGLD, and SGHMC to inference GMM on the synthetic datums. Then, we remove 400 points from each of the pink parts and yellow parts, around 40% of the whole dataset at all, by the proposed BIF algorithms. The remaining datums are shown in the right of fig. 2a. We also trained models on only the remaining set with the same Bayesian inference settings in order to show the targets of the forgetting task. The experiments have two main phrases:

1) **Training phase.** Every GMM is trained for 2,000 iterations. The batch size is set as 64. For variational inference, the learning rate is fixed to $2/n$, where $n$ is the training sample set size. For SGLD, the learning rate schedule is set as $4 \cdot t^{-0.15}/n$, where $t$ is the training iteration step. For SGHMC, the learning rate schedule is set as $2 \cdot t^{-0.15}/n$, and the initial $\alpha$ factor is set as 0.4.
(2) **Forgetting phase.** We remove a batch of 4 datums each time. When calculating the inversed-Hessian-vector product $H^{-1}v$ in the influence functions (see Section 5.3), the recursive calculation number $j$ is set as 32, and the scaling factor $c$ is set as $1/n'$, where $n'$ is the number of the current remaining training datums. Notice that $n'$ will gradually decrease as the forgetting process continuing. Moreover, for SGLD and SGHMC, we employ Monte Carlo method to calculate the expectations in MCMC influence functions. Specifically, we repeatedly sample model parameter $\theta$ for 5 times, calculate the matrix or vector in MCMC influence functions, and average the results to approach the expectations.

### 7.1.2 Results Analysis

The empirical results are presented in figs. 2b, 2c, 2d respectively. In figures for variational inference, we draw the learned clustering centers as black points. In every figure for SGLD and SGHMC, (1) we draw the point drawn in the terminated iteration as a black point; and (2) we draw the points drawn in the last 500 iterations in blue, orange, red, or green. The results obtained on the remaining parts (target) are also shown in these figures. This visualization shows that after forgetting, (1) the learned models are close to the target models; and (2) the learned cluster centers of the pink parts and yellow parts significantly moved, while the other centers remained in almost no change. These phenomena demonstrate that our forgetting algorithms can selectively remove specified datums while keeping others intact.

### 7.2 Experiments for Bayesian Neural Network

We then conduct experiments with Bayesian neural networks on real data.

#### 7.2.1 Implementation Details

The implementation details are given below.

**Dataset.** We employ Fashion-MNIST [72] dataset in our experiments. It consists of $28 \times 28$ gray-scale images from 10 different classes, where each class consists of 6,000 training examples and 1,000 test examples. For the data argumentation, we first resize each image to $32 \times 32$ and then normalize each pixel value to $[-0.5, 0.5]$ before feeding them into BNN. For the forgetting experiments, we divide the training set of Fashion-MNIST into two parts, the removed part $S_f$ and the remaining part $S_r$. Apparently, $S_f \cup S_r = S$. For the selection of the removed training set $S_f$, we randomly choose 1,000, 2,000, 3,000, 4,000, 5,000 and 6,000 examples from the class “T-shirt” (i.e., examples that labeled with number 0) in the training set to form $S_f$. For the brevity, we denote the test set by $S_{test}$.

**Bayesian neural network (BNN).** BNNs employ Bayesian inference to inference the posterior of the neural networks parameters. Two major Bayesian inference methods employed wherein are variational inference and SGMC.

For variational inference, one usually utilizes the mean-field Gaussian variational family [12, 39] to train BNNs. The *Bayes by Backprop* technique [12] is utilized to calculate the derivative of ELBO function. Specifically, for the random variable $\theta$ subject to the mean-field variational distribution $q_\lambda = \mathcal{N}(\mu, \sigma^2 I)$, we have that $(\theta - \mu)/\sigma \sim \mathcal{N}(0, I)$. Let $\varepsilon = (\theta - \mu)/\sigma$, then the derivative of the ELBO function can be varied as follows,

$$
\nabla_\lambda \text{ELBO}(\lambda, S) = \nabla_\lambda \mathbb{E}_{q_\lambda} (\log p(\theta, S) - q_\lambda(\theta)) = \nabla_\lambda \mathbb{E}_\varepsilon (\log p(\theta, S) - q_\lambda(\theta)) = \mathbb{E}_\varepsilon \nabla_\lambda (\log p(\theta, S) - q_\lambda(\theta)),
$$
Figure 3: Curves of classification error to the number of the removed training datums. The results of variational inference, SGLD, and SGHMC are presented from left to right, respectively. For each setting, three classification error curves on the forgotten set $S_f$, remained set $S_r$, and test set $S_{test}$ are plotted. The models are trained for 5 times with different random seeds. The darker lines show the average over seeds and the shaded area shows the standard deviations.

Hence, we can calculate the derivative $\nabla_\lambda \text{ELBO}(\lambda, S)$ in two steps: (1) repeatedly sample $\varepsilon$ from $\mathcal{N}(0, I)$ and calculate $\nabla_\lambda (\log p(\theta, S) - q_\lambda(\theta))$ based on $\theta = \mu + \varepsilon \cdot \sigma$; and (2) average the obtained derivatives to approximate $\nabla_\lambda \text{ELBO}(\lambda, S)$. Moreover, we also adopt the local reparameterization trick [39] to further eliminate the covariances between the gradients of examples in a batch.

Bayesian LeNet-5 [45] is employed in our experiments, which consists of two convolutional layers and three fully-connected layers. We follow Liu et al. [46] to use an isotropic Gaussian distribution $\mathcal{N}(0, \sigma^2 I)$ as the prior of BNN, where the standard deviation $\sigma$ is set as 0.15.

**Experiment design.** We employ variational inference, SGLD, and SGHMC to train the BNN on the complete training set $S$. Then, we remove the subset $S_f$ by the proposed BIF algorithms. We also trained models on only the remaining set $S_r$ in order to show the targets of the forgetting task. The experiments have two main phrases:

1. **Training phase.** Every BNN is trained for 10,000 iterations. The batch size is set as 128. For variational inference, the learning rate is initialized as $0.5/n$, where $n$ is the training set size, and decay by 0.1 every 4,000 iterations. Additionally, the sampling times to perform Bayes by Backprop procedure is set as 5. For SGLD, the step-size schedule is set as $0.5 \cdot t^{-0.5}/n$, where $t$ is the training iteration step. For SGHMC, the step-size schedule is set as $0.5 \cdot t^{-0.5}/n$, and the initial $\alpha$ factor is set as 0.4.

2. **Forgetting phase.** We remove a batch of 64 datums each time. When calculating the inverted-Hessian-vector product $H^{-1}v$ in influence functions (see Section 5.3), the recursive calculation number $j$ is set as 64. For variational inference, the scaling factor $c$ is set as $0.1/n'$, where $n'$ is the number of the current remaining datums. Notice that $n'$ will gradually decrease as the forgetting process continuing. For SGLD and SGHMC, the scaling factors $c$ are set as $0.005/n'$ and $0.05/n'$, respectively. Besides, we employ the Monte Carlo method to calculate the expectations in MCMC influence functions. Specifically, we repeatedly sample model parameter $\theta$ for 5 times, calculate the matrix and vector in MCMC influence function based on these sampled parameters, and average the results to approach the desired expectation.

**7.2.2 Results Analysis**

For each of the obtained processed models and target models, we evaluate its classification errors on the sets $S_f$, $S_r$ and $S_{test}$, respectively. The results are collected and plotted in fig. 3. We also collect and present the
Table 1: Time of the training phase and the forgetting phase in the experiments for BNNs. The acceleration rate is calculated by dividing “training time” with “forgetting time”. Our forgetting algorithms is significantly faster than re-training from scratch.

|                  | Variational Inference | SGLD   | SGHMC  |
|------------------|-----------------------|--------|--------|
| Training Time    | 337.77s               | 39.36s | 39.90s |
| Removal Time     | 4.97s                 | 4.04s  | 4.04s  |
| Acceleration Rate| 67.90                 | 9.75   | 9.88   |

training and forgetting times in Table 1.

From fig. 3 and Table 1, we have the following three observations: (1) the processed models are similar to the target models in terms of the classification errors on all the three sample sets $S_f$, $S_r$, and $S_{test}$; (2) as the number of the removed datums increases, for the processed models, the errors on the removed set $S_f$ significantly increase, the errors on the remaining set $S_r$ slightly drop, and the errors on the test set $S_{test}$ slightly increase; and (3) our forgetting algorithms are significantly faster than simply training models from scratch. These phenomena demonstrate that our forgetting algorithms can effectively and efficiently remove influences of datums from BNNs without hurting other remaining information.

8 Conclusion

The right to be forgotten imposes a considerable compliance burden to AI companies that a company may need to delete the whole model learned from massive resources due to a request to delete a single datum. To address this problem, this work designs a Bayesian inference forgetting (BIF) that removes the influence of some specific datum on the learned model without completely deleting the whole model. The BIF framework is established on an energy-based Bayesian inference influence function, which characterizes the influence of some datums on the learned models. We prove that BIF has an $\varepsilon$-certified knowledge removal guarantee, which is a new term on characterizing the forgetting performance. Under the BIF framework, forgetting algorithms are developed for two canonical Bayesian inference algorithms, variational inference and Markov chain Monte Carlo. Theoretical analysis provides guarantees on the generalizability of the proposed methods: performing the proposed BIF has little affect on them. Comprehensive experiments demonstrate that the proposed methods can remove the influence of specified datums without compromising the knowledge learned on the remained data. The source code package is available at https://github.com/fshp971/BIF.

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A Proofs in Section 4

This section provides the missing proofs in Section 4.

Proof of Theorem 4.2. We first calculate $\frac{\partial \tilde{\gamma}_S^{-z_j}(\tau)}{\partial \tau}$ based on eq. (4), i.e., the following equation,

$$\nabla_\gamma F(\gamma, S) + \tau \cdot \nabla_\gamma h(\gamma, z_j) = 0.$$ 

Calculate the derivatives of the both sides of the above equation with respect to $\tau$, we have that

$$\nabla^2_\gamma F(\tilde{\gamma}_S^{-z_j}(\tau), S) \cdot \frac{\partial \tilde{\gamma}_S^{-z_j}(\tau)}{\partial \tau} + \nabla_\gamma h(\tilde{\gamma}_S^{-z_j}(\tau), z_j)^T + \tau \cdot \nabla^2_\gamma h(\tilde{\gamma}_S^{-z_j}(\tau), z_j) \cdot \frac{\partial \tilde{\gamma}_S^{-z_j}(\tau)}{\partial \tau} = 0. \quad (14)$$

By lemma 4.1, $F_{-z_j, \tau}(\gamma, S)$ is strongly convex with respect to $\gamma$. Thus, the following Hessian matrix

$$\nabla^2_\gamma F_{-z_j, \tau}(\tilde{\gamma}_S^{-z_j}(\tau), S) = \nabla^2_\gamma F(\tilde{\gamma}_S^{-z_j}(\tau), S) + \tau \cdot \nabla^2_\gamma h(\tilde{\gamma}_S^{-z_j}(\tau), z_j)$$

is positive definite, hence invertible. Combining with eq. (14), we have that

$$\frac{\partial \tilde{\gamma}_S^{-z_j}(\tau)}{\partial \tau} = -\left(\nabla^2_\gamma F(\tilde{\gamma}_S^{-z_j}(\tau), S) + \tau \cdot \nabla^2_\gamma h(\tilde{\gamma}_S^{-z_j}(\tau), z_j)\right)^{-1} \cdot \nabla_\gamma h(\tilde{\gamma}_S^{-z_j}(\tau), z_j)^T. \quad (15)$$

We then upper bound the norm of $\frac{\partial \tilde{\gamma}_S^{-z_j}(\tau)}{\partial \tau}$. Based on eq. (15), we have that

$$\left\| \frac{\partial \tilde{\gamma}_S^{-z_j}(\tau)}{\partial \tau} \right\|^2_2 \leq \left\| \frac{1}{n} \nabla^2_\gamma F(\tilde{\gamma}_S^{-z_j}(\tau), S) + \frac{\tau}{n} \nabla^2_\gamma h(\tilde{\gamma}_S^{-z_j}(\tau), z_j) \right\|^{-1} \cdot \left\| \frac{1}{n} \nabla_\gamma h(\tilde{\gamma}_S^{-z_j}(\tau), z_j) \right\|_2. \quad (16)$$

We first consider the first term of the right-hand side of eq. (16). By assumption 4.2, $f(\gamma)$ is $c_f$-strongly convex and $h(\gamma, z)$ is $c_h(z)$-strongly convex, where $c_f$ is a positive real number, $c_h(z)$ is a positive continuous
real function on $\mathcal{Z}$. Thus we have that
\[
\frac{1}{n} \nabla^2_{\gamma} F(\hat{\gamma}_S^{-z_j}(\tau), S) + \frac{\tau}{n} \nabla^2_{\gamma} h(\hat{\gamma}_S^{-z_j}(\tau), z_j)
= \frac{1}{n} \sum_{i=1}^{n} \nabla^2_{\gamma} h(\hat{\gamma}_S^{-z_j}(\tau), z_i) + \frac{1}{n} \nabla^2_{\gamma} f(\hat{\gamma}_S^{-z_j}(\tau)) + \frac{\tau}{n} \nabla^2_{\gamma} h(\hat{\gamma}_S^{-z_j}(\tau), z_j)
= \frac{1}{n} \sum_{z \in S - \{z_j\}} \nabla^2_{\gamma} h(\hat{\gamma}_S^{-z_j}(\tau), z) + \frac{1 + \tau}{n} \nabla^2_{\gamma} h(\hat{\gamma}_S^{-z_j}(\tau), z_j) + \frac{1}{n} \nabla^2_{\gamma} f(\hat{\gamma}_S^{-z_j}(\tau))
\geq \left( \frac{1}{n} \sum_{z \in S - \{z_j\}} c_h(z) + \frac{1 + \tau}{n} c_h(z_j) + \frac{c_f}{n} \right) I
\geq \left( \frac{1}{n} \sum_{z \in S - \{z_j\}} c_h(z) \right) I.
\]

Applying Assumption 4.1, we have that $c_h(z)$ is continuous on the compact set $\mathcal{Z}$. This suggests that there exists a real constant $\hat{c}_h > 0$ such that $\forall z \in \mathcal{Z}, c_h(z) \geq \hat{c}_h$. Therefore, we further have that
\[
\frac{1}{n} \nabla^2_{\gamma} F(\hat{\gamma}_S^{-z_j}(\tau), S) + \frac{\tau}{n} \nabla^2_{\gamma} h(\hat{\gamma}_S^{-z_j}(\tau), z_j) \geq \left( \frac{1}{n} \sum_{z \in S - \{z_j\}} c_h(z) \right) I \geq \left( \frac{n - 1}{n} \hat{c}_h \right) I.
\]

Let $\lambda_{\min}$ denote the smallest eigenvalue of the matrix $\left( \frac{1}{n} \nabla^2_{\gamma} F(\hat{\gamma}_S^{-z_j}(\tau), S) + \frac{\tau}{n} \nabla^2_{\gamma} h(\hat{\gamma}_S^{-z_j}(\tau), z_j) \right)$. Then, the above inequality implies that $\lambda_{\min} \geq \frac{n - 1}{n} \hat{c}_h$. Hence, we have the following,
\[
\left\| \left( \frac{1}{n} \nabla^2_{\gamma} F(\hat{\gamma}_S(\tau), S) + \frac{\tau}{n} \nabla^2_{\gamma} h(\hat{\gamma}_S(\tau), z_j) \right)^{-1} \right\|_2 = \frac{1}{\lambda_{\min}} \leq \frac{n}{(n - 1) \hat{c}_h} = O(1).
\]

We then upper bound the second term of the right-hand side of eq. (16). Applying Assumptions 4.2 and 4.1, we have that $\nabla^2_{\gamma} h(\gamma, z)$ is continuous on compact support $\Gamma \times \mathcal{Z}$. This demonstrates that both $\nabla^2_{\gamma} h(\gamma, z)$ and $\left\| \nabla^2_{\gamma} h(\gamma, z) \right\|_2$ are bounded. Therefore, as $n \to \infty$, we have
\[
\left\| \frac{1}{n} \sum_{i=1}^{n} \nabla^2_{\gamma} h(\hat{\gamma}_S(\tau), z_i) \right\|_2 = \frac{1}{n} \left\| \sum_{i=1}^{n} \nabla^2_{\gamma} h(\hat{\gamma}_S(\tau), z_i) \right\|_2 \leq O \left( \frac{1}{n} \right).
\]

Finally, inserting eqs. (17) (18) into eq. (16), we eventually have that
\[
\left\| \frac{\partial \hat{\gamma}_S(\tau)}{\partial \tau} \right\|_2 \leq O(1) \cdot O \left( \frac{1}{n} \right) = O \left( \frac{1}{n} \right).
\]

The proof is completed. □

**Proof of Theorem 4.3.** We first calculate $\frac{\partial^2 \hat{\gamma}_S^{-z_j}(\tau)}{\partial \tau^2}$ based on eq. (4). Similar to the proof of Theorem 4.2,
we calculate the second-order derivatives of the both sides of eq. (4) with respect to $\tau$ and have that

$$
\sum_{i=1}^{n} B(\tau, z_i) + A(\tau) + \left( \sum_{i=1}^{n} \nabla^2_\tau h(\hat{\gamma}^{-z_j}_S(\tau), z_i) + \nabla^2_\gamma f(\hat{\gamma}^{-z_j}_S(\tau)) \right) \cdot \frac{\partial^2 \hat{\gamma}^{-z_j}_S(\tau)}{\partial \tau^2} \\
+ 2 \cdot \nabla^2_\tau h(\hat{\gamma}^{-z_j}_S(\tau), z_j) \cdot \frac{\partial \hat{\gamma}^{-z_j}_S(\tau)}{\partial \tau} + \tau \cdot B(\tau, z_j) + \tau \cdot \nabla^2_\gamma h(\hat{\gamma}^{-z_j}_S(\tau), z_j) \cdot \frac{\partial^2 \hat{\gamma}^{-z_j}_S(\tau)}{\partial \tau^2} = 0,
$$

which means

$$
\frac{\partial^2 \hat{\gamma}^{-z_j}_S(\tau)}{\partial \tau^2} = - \left( \frac{1}{n} \sum_{i=1}^{n} \nabla^2_\gamma F(\hat{\gamma}^{-z_j}_S(\tau), S) + \frac{n}{n} \nabla^2_\gamma h(\hat{\gamma}^{-z_j}_S(\tau), z_j) \right)^{-1} \\
\cdot \left( \frac{1}{n} \sum_{i=1}^{n} B(\tau, z_i) + \frac{n}{n} B(\tau, z_j) + \frac{1}{n} A(\tau) + \frac{2}{n} \nabla^2_\gamma h(\hat{\gamma}^{-z_j}_S(\tau), z_j) \cdot \frac{\partial \hat{\gamma}^{-z_j}_S(\tau)}{\partial \tau} \right),
$$

(19)

where the invertibility of \( \left( \frac{1}{n} \sum_{i=1}^{n} \nabla^2_\gamma F(\hat{\gamma}^{-z_j}_S(\tau), S) + \frac{n}{n} \nabla^2_\gamma h(\hat{\gamma}^{-z_j}_S(\tau), z_j) \right) \) is guaranteed by Lemma 4.1, $A(\tau), B(\tau, z) \in \mathbb{R}^{K \times 1}$, and for $i = 1, \ldots, K$, we have the following,

$$
A(\tau)_i = \frac{\partial \hat{\gamma}^{-z_j}_S(\tau)}{\partial \tau}^T \cdot \nabla^2_\gamma \left( \frac{\partial f(\hat{\gamma}^{-z_j}_S(\tau))}{\partial \gamma_i} \right) \cdot \frac{\partial \hat{\gamma}^{-z_j}_S(\tau)}{\partial \tau},
$$

(20)

$$
B(\tau, z)_i = \frac{\partial \hat{\gamma}^{-z_j}_S(\tau)}{\partial \tau}^T \cdot \nabla^2_\gamma \left( \frac{\partial h(\hat{\gamma}^{-z_j}_S(\tau), z)}{\partial \gamma_i} \right) \cdot \frac{\partial \hat{\gamma}^{-z_j}_S(\tau)}{\partial \tau}.
$$

(21)

We then upper bound the norm of $\frac{\partial^2 \hat{\gamma}^{-z_j}_S(\tau)}{\partial \tau^2}$. Based on eq. (19), we have that

$$
\left\| \frac{\partial^2 \hat{\gamma}^{-z_j}_S(\tau)}{\partial \tau^2} \right\|_2 \\
\leq \left\| \left( \frac{1}{n} \sum_{i=1}^{n} \nabla^2_\gamma F(\hat{\gamma}^{-z_j}_S(\tau), S) + \frac{n}{n} \nabla^2_\gamma h(\hat{\gamma}^{-z_j}_S(\tau), z_j) \right)^{-1} \\
\cdot \frac{1}{n} \left( \sum_{i=1}^{n} \| B(\tau, z_i) \|_2 + \tau \cdot B(\tau, z_j) \|_2 + \| A(\tau) \|_2 + 2 \cdot \nabla^2_\gamma h(\hat{\gamma}^{-z_j}_S(\tau), z_j) \cdot \frac{\partial \hat{\gamma}^{-z_j}_S(\tau)}{\partial \tau} \right) \right\|_2
$$

(22)

$$
\leq O \left( \frac{1}{n} \left( \sum_{i=1}^{n} \| B(\tau, z_i) \|_2 + \tau \cdot B(\tau, z_j) \|_2 + \| A(\tau) \|_2 + 2 \cdot \nabla^2_\gamma h(\hat{\gamma}^{-z_j}_S(\tau), z_j) \cdot \frac{\partial \hat{\gamma}^{-z_j}_S(\tau)}{\partial \tau} \right) \right) .
$$

(23)

where eq. (23) is obtained by inserting eq. (17) (in the proof of Theorem 4.2) into eq. (22). Thus, the remaining is to upper bound the norms of $A(\tau), B(\tau, z)$ and $\nabla^2_\gamma h(\hat{\gamma}^{-z_j}_S(\tau), z_j) \cdot \frac{\partial \hat{\gamma}^{-z_j}_S(\tau)}{\partial \tau}$.

We first upper bound $A(\tau)$. Applying Theorem 4.2, we have that $\left\| \frac{\partial \hat{\gamma}^{-z_j}_S(\tau)}{\partial \tau} \right\|_2 \leq O \left( \frac{1}{n} \right)$. Applying Assumptions 4.2 and 4.1, we have that $\nabla^2_\gamma \left( \frac{\partial f(\hat{\gamma}^{-z_j}_S(\tau))}{\partial \gamma_i} \right)$ is bounded on its support $\Gamma$. As a result, the norm
of \( \left\| \nabla^2_{\gamma} \left( \frac{\partial f(\hat{\gamma}^{-z_j}_S(\tau))}{\partial \gamma_i} \right) \right\|_2 \) is also bounded. Therefore, we have that

\[
\|A(\tau)\|_2 \leq \sum_{i=1}^K \left\| \nabla^2_{\gamma} \left( \frac{\partial f(\hat{\gamma}^{-z_j}_S(\tau))}{\partial \gamma_i} \right) \right\|_2 \cdot \left\| \frac{\partial^2 \hat{\gamma}^{-z_j}_S(\tau)}{\partial \tau^2} \right\|_2 \leq \sum_{i=1}^K O(1) \cdot O \left( \frac{1}{n^2} \right) = O \left( \frac{1}{n^2} \right). \tag{24}
\]

For \( B(\tau, z) \), we similarly have that

\[
\|B(\tau, z)\|_2 \leq O \left( \frac{1}{n^2} \right). \tag{25}
\]

To upper bound the norm of \( \nabla^2_{\gamma} h(\hat{\gamma}^{-z_j}_S(\tau), z_j) \cdot \frac{\partial \hat{\gamma}^{-z_j}_S(\tau)}{\partial \tau} \), we apply Theorem 4.2, Assumptions 4.2 and 4.1, and have that

\[
\left\| \nabla^2_{\gamma} h(\hat{\gamma}^{-z_j}_S(\tau), z_j) \cdot \frac{\partial \hat{\gamma}^{-z_j}_S(\tau)}{\partial \tau} \right\|_2 \leq \left\| \nabla^2_{\gamma} h(\hat{\gamma}^{-z_j}_S(\tau), z_j) \right\|_2 \cdot \left\| \frac{\partial \hat{\gamma}^{-z_j}_S(\tau)}{\partial \tau} \right\|_2 \leq O(1) \cdot O \left( \frac{1}{n} \right) = O \left( \frac{1}{n} \right). \tag{26}
\]

Inserting eqs. (24), (25) and (26), into eq. (23), we eventually have that

\[
\left\| \frac{\partial^2 \hat{\gamma}^{-z_j}_S(\tau)}{\partial \tau^2} \right\|_2 \leq O \left( \frac{1}{n} \left( \sum_{i=1}^n O \left( \frac{1}{n^2} \right) + \tau \cdot O \left( \frac{1}{n^2} \right) + O \left( \frac{1}{n^2} \right) + 2 \cdot O \left( \frac{1}{n} \right) \right) \right) = O \left( \frac{1}{n^2} \right).
\]

The proof is completed. \( \square \)

**B Proofs in Section 5**

This section provides the detailed proofs in Section 5.

**Proof of Theorem 5.2.** Let \( \hat{\lambda}_S, \hat{\lambda}_{S-\{z_j\}} \) be the variational parameters learned on \( S \) and \( S - \{z_j\} \), respectively. Let \( \hat{\lambda}^{-z_j}_S = A_{VT}(\hat{\lambda}_S, z_j) = \hat{\lambda}_S - I_{VT}(z_j) \) be the processed variational parameter. Then, to establish a certified knowledge removal guarantee for \( A_{VT}(\hat{\lambda}_S, z_j) \), we need to bound the KL divergence \( \text{KL}(p_{\hat{\lambda}^{-z_j}_S(\theta)} || p_{\hat{\lambda}_{S-(z_j)}(\theta)}) \).

For the brevity, we denote that

\[
p_{\hat{\lambda}^{-z_j}_S} = \mathcal{N}(\mu_1, \sigma_1^2 I),
\]

where \( \hat{\lambda}^{-z_j}_S = (\mu_{11}, \ldots, \mu_{1d}, \sigma_{11}, \ldots, \sigma_{1d}) \), \( 0 < M_1 \leq \sigma_{11}, \ldots, \sigma_{1d} \leq M_2 \), and

\[
p_{\hat{\lambda}_{S-(z_j)}} = \mathcal{N}(\mu_2, \sigma_2^2 I),
\]

where \( \hat{\lambda}_{S-(z_j)} = (\mu_{21}, \ldots, \mu_{2d}, \sigma_{21}, \ldots, \sigma_{2d}) \), \( 0 < M_1 \leq \sigma_{21}, \ldots, \sigma_{2d} \leq M_2 \).
We then have the following (we assume that $\Theta = \mathbb{R}^d$),

$$
\text{KL}(p_{\lambda_{-z_j}}(\theta)\| p_{\lambda_{S-\{z_j\}}}(\theta))
= \int_{\Theta} \log \left( \frac{p_{\lambda_{-z_j}}(\theta)}{p_{\lambda_{S-\{z_j\}}}(\theta)} \right) p_{\lambda_{S-\{z_j\}}}(\theta) d\theta 
= -\frac{1}{2} \sum_{k=1}^{d} \int \left( \frac{(\theta_k - \mu_k)^2}{\sigma_{1k}^2} - \frac{(\theta_k - \mu_{2k})^2}{\sigma_{2k}^2} \right) p_{\lambda_{S-\{z_j\}}}(\theta_k) d\theta_k - \sum_{k=1}^{d} \log \frac{\sigma_{1k}}{\sigma_{2k}} 
= -\frac{1}{2} \sum_{k=1}^{d} \left( 1 - \frac{\sigma_{1k}^2}{\sigma_{2k}^2} - \frac{(\mu_{1k} - \mu_{2k})^2}{\sigma_{2k}^2} \right) - \sum_{k=1}^{d} \log \frac{\sigma_{1k}}{\sigma_{2k}} 
= \frac{1}{2} \sum_{k=1}^{d} \left( \frac{\sigma_{2k}^2 - \sigma_{1k}^2}{\sigma_{2k}^2} + \frac{(\mu_{1k} - \mu_{2k})^2}{\sigma_{2k}^2} \right) + 2 \log \left( 1 + \frac{\sigma_{2k}^2 - \sigma_{1k}^2}{\sigma_{2k}^2} \right) 
\leq \frac{1}{2} \sum_{k=1}^{d} \left( \frac{2M_2 |\sigma_{1k} - \sigma_{2k}|}{M_1^2} + \frac{(\mu_{1k} - \mu_{2k})^2}{M_1^2} \right) + \frac{2 |\sigma_{1k} - \sigma_{2k}|}{M_1} 
= \frac{1}{2M_1^2} \sum_{k=1}^{d} \left( 2(M_1 + M_2)|\sigma_{1k} - \sigma_{2k}| + (\mu_{1k} - \mu_{2k})^2 \right) 
\leq \frac{1}{2M_1^2} \left( 2(M_1 + M_2)||\hat{\lambda}_{S-\{z_j\}}^{\mu_{-z_j}} - \hat{\lambda}_{S-\{z_j\}}||_1 + ||\hat{\lambda}_{S-\{z_j\}}^{\mu_{-z_j}} - \hat{\lambda}_{S-\{z_j\}}||_2^2 \right) = \varepsilon_{\lambda_{S-\{z_j\}}}. 
$$

Therefore, $\mathcal{A}_{\text{VT}}(\lambda_{S, z_j})$ performs $\varepsilon_{\lambda_{S-\{z_j\}}}$-certified knowledge removal.

The proof is completed. 

**Proof of Theorem 5.4.** Let the processed model be $p^{-z_j}(\theta) = \mathcal{A}_{\text{MCMC}}(p(\theta|S), z_j)$. For the brevity, we denote that

$$
p_1(\theta) = p^{-z_j}(\theta) = \mathcal{N}(\theta'_1, (nJ(\theta_1))^{-1}),
$$

where $\theta'_1 = \theta_1 - \mathcal{I}_{\text{MCMC}}(z_j)$, and

$$
p_2(\theta) = p(\theta|S - \{z_j\}) = \mathcal{N}(\theta_2, ((n-1)J(\theta_2))^{-1}).
$$

Then, to establish the certified removal guarantee, we need to calculate the KL divergence $\text{KL}(p_1(\theta)\|p_2(\theta))$.

Since

$$
p_1(\theta) = \frac{1}{\sqrt{(2\pi)^d|nJ(\theta_1)|^{-1}}} \exp \left( -\frac{1}{2} (\theta - \theta'_1)^T (nJ(\theta_1))(\theta - \theta'_1) \right),
$$

$$
p_2(\theta) = \frac{1}{\sqrt{(2\pi)^d|(n-1)J(\theta_2)|^{-1}}} \exp \left( -\frac{1}{2} (\theta - \theta_2)^T ((n-1)J(\theta_2))(\theta - \theta_2) \right),
$$

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we have that (we assume that $\Theta = \mathbb{R}^d$)

$$
\text{KL}(p_1(\theta) \| p_2(\theta)) \\
= \int_{\Theta} \log \left( \frac{p_1(\theta)}{p_2(\theta)} \right) p_1(\theta) d\theta \\
= -\frac{1}{2} \int_{\Theta} ((\theta - \theta')^T (nJ(\theta_1))(\theta - \theta') - (\theta - \theta_2)^T ((n - 1)J(\theta_2))(\theta - \theta_2)) p_1(\theta) d\theta \\
- \frac{1}{2} \log \frac{|nJ(\theta_1)|^{-1}}{|(n - 1)J(\theta_2)|^{-1}} \\
= -\frac{1}{2} \left( \text{tr}(nJ(\theta_1)(nJ(\theta_1))^{-1}) - \text{tr}((n - 1)J(\theta_2)(nJ(\theta_1))^{-1}) \right) \\
- (\theta_1 - \theta_2)^T ((n - 1)J(\theta_2))(\theta_1 - \theta_2) + \frac{1}{2} \left( \frac{n}{n - 1} \right)^d \log \frac{|J(\theta_1)|}{|J(\theta_2)|} \\
= \frac{1}{2} \left( (n - 1)(\theta_1 - \theta_2)^T J(\theta_2)(\theta_1 - \theta_2) + \frac{n - 1}{n} \text{tr}(J(\theta_2)J^{-1}(\theta_1)) - d + \left( \frac{n}{n - 1} \right)^d \log \frac{|J(\theta_1)|}{|J(\theta_2)|} \right) \\
= O \left( (n - 1)(\theta_1 - \theta_2)^T J(\theta_2)(\theta_1 - \theta_2) + \text{tr}(J^{-1}(\theta_1)(J(\theta_2) - J(\theta_1))) + \log \frac{|J(\theta_1)|}{|J(\theta_2)|} \right) \\
= O(\varepsilon_{\theta_1,z_j}).
$$

which means that $\text{KL}(p^{\varepsilon_{z_j}}(\theta) \| p(\theta|S - \{z_j\})) = O(\varepsilon_{\theta_1,z_j})$. Therefore, $A_{\text{MCMC}}(p(\theta|S), z_j)$ performs $O(\varepsilon_{\theta_1,z_j})$-certified knowledge removal.

The proof is completed.  

\[ \square \]

## C  Proofs in Section 6

This section provides the detailed proofs in Section 6.

We derive generalization bounds for BIF under the PAC-Bayesian framework [49, 50, 51]. The framework can provide guarantees for randomized predictors (e.g. Bayesian predictors).

Specifically, let $Q$ a distribution on the parameter space $\Theta$, $P$ denotes the prior distribution over the parameter space $\Theta$. Then, the expected risks $R(Q)$ is bounded in terms of the empirical risk $\hat{R}(Q, S)$ and KL-divergence $\text{KL}(Q \| P)$ by the following result from PAC-Bayes.

**Lemma C.1** (cf. [51], Theorem 1). For any real $\delta \in (0, 1)$, with probability at least $1 - \delta$, we have the following inequality for all distributions $Q$:

$$
R(Q) \leq \hat{R}(Q, S) + \sqrt{\frac{\text{KL}(Q \| P) + \log \frac{1}{\delta} + \log n + 2}{2n - 1}}.  \tag{28}
$$

Based on Lemma C.1, we prove the generalization bounds in Theorem 6.1 and Theorem 6.2.

**Proof of Theorem 6.1.** Let the prior distribution $P$ be the standard Gaussian distribution $\mathcal{N}(0, I)$, $Q$ be the distribution that obtained after conducting variational inference BIF. Suppose the density functions of $P, Q$...
are \( p(\theta) \), \( q(\theta) \) respectively, then we have

\[
p(\theta) = \frac{1}{\sqrt{(2\pi)^d}} \exp \left( -\frac{||\theta||^2}{2} \right),
\]

\[
q(\theta) = \frac{1}{\sqrt{(2\pi)^d} \prod_{k=1}^{d} \sigma'_{k}} \exp \left( -\frac{\sum_{k=1}^{d} (\theta_k - \mu'_k)^2}{2\sigma'^2_{k}} \right),
\]

where \( \mu'_k = \mu_k - \Delta \mu_k \) and \( \sigma'_k = \sigma_k - \Delta \sigma_k \).

Therefore, we can calculate the KL-divergence \( \text{KL}(Q\|P) \) as follows (where we assume that \( \Theta = \mathbb{R}^d \)),

\[
\text{KL}(Q\|P) = \int_{\Theta} \log \left( \frac{q(\theta)}{p(\theta)} \right) q(\theta) d\theta
\]

\[
= -\frac{1}{2} \sum_{k=1}^{d} \int_{\Theta} \left( \frac{(\theta_k - \mu'_k)^2}{\sigma'_{k}^2} - \theta_k^2 \right) q(\theta) d\theta - \sum_{k=1}^{d} \log \sigma'_{k}
\]

\[
= -\frac{1}{2} \sum_{k=1}^{d} \left( 1 - \mu'_k^2 - \sigma'^2_{k} \right) - \sum_{k=1}^{d} \log \sigma'_{k}
\]

\[
= \frac{1}{2} \left( \|\lambda - \Delta \lambda\|^2 - d - 2 \sum_{k=1}^{d} \log \sigma'_{k} \right)
\]

\[
\leq \frac{1}{2} \left( \|\Delta \lambda\|^2 + 2\|\lambda\| \cdot \|\Delta \lambda\| + \|\lambda\|^2 - 2 \sum_{k=1}^{d} \log (\sigma_k - \Delta \sigma_k) - d \right)
\]

\[
= \frac{1}{2} (C_{\lambda,\Delta \lambda} - d),
\]

where

\[
C_{\lambda,\Delta \lambda} = \|\Delta \lambda\|^2 + 2\|\lambda\| \cdot \|\Delta \lambda\| + \|\lambda\|^2 - 2 \sum_{k=1}^{d} \log (\sigma_k - \Delta \sigma_k).
\]

Eq. (29) gives an upper bound of the KL-divergence between the obtained distribution after BIF and the prior distribution. Inserting eq. (29) into eq. (28) in Lemma C.1, we obtain the PAC-Bayesian generalization bound.

Furthermore, since all the conditions in Theorem 5.1 hold, we can apply Theorem 4.2 and have that \(|\Delta \sigma_k| \leq \|\Delta \lambda\| \leq O(1/n)\). Besides, by applying the conditions in Theorem 5.2, we have that for any \(1 \leq k \leq d, \sigma_k \geq M_1 > 0\), where \(M_1\) is a constant. Therefore, we have that

\[
C_{\lambda,\Delta \lambda} \leq \|\Delta \lambda\|^2 + 2\|\lambda\| \cdot \|\Delta \lambda\| + \|\lambda\|^2 - 2d \log (M_1 - \|\Delta \lambda\|)
\]

\[
= O \left( \log (M_1 - \|\Delta \lambda\|) \right)
\]

\[
\leq O(1).
\]

The proof is completed. \(\square\)
proof of Theorem 6.2. Let the prior distribution $P$ be the standard Gaussian distribution $\mathcal{N}(0, I)$, $Q$ be the processed distribution that obtained after conducting MCMC BIF. Suppose the density functions of $P$, $Q$ are $p(\theta)$, $q(\theta)$ respectively, then we have

$$
p(\theta) = \frac{1}{\sqrt{(2\pi)^d}} \exp \left( -\frac{\|\theta\|^2}{2} \right),
q(\theta) = \frac{1}{\sqrt{(2\pi)^d|nJ(\theta_1)|^{-1}}} \exp \left( -\frac{1}{2}(\theta - \theta_1')^T(nJ(\theta_1))(\theta - \theta_1') \right),$$

where $\theta_1' = \theta_1 - \Delta_{\theta_1}$.

Thus, we can calculate the KL-divergence $KL(Q\|P)$ as follows (where we assume that $\Theta = \mathbb{R}^d$),

$$
KL(Q\|P) = \int_{\Theta} \log \left( \frac{q(\theta)}{p(\theta)} \right) q(\theta) d\theta
= -\frac{1}{2} \left( \int_{\Theta} ((\theta - \theta_1')^T(nJ(\theta_1))(\theta - \theta_1') - \|\theta\|^2) q(\theta) d\theta - \log |nJ(\theta_1)| \right)
= -\frac{1}{2} \left( \text{tr}(I) - \text{tr} \left( (nJ(\theta_1))^{-1} \right) - \|\theta_1'\|^2 - \log |nJ(\theta_1)| \right)
= \frac{1}{2} \left( \|\theta_1'\|^2 + \frac{1}{n} \text{tr}(J^{-1}(\theta_1)) - d + \log \left( \frac{\text{det}(J(\theta_1))}{\text{det}(nJ(\theta_1))} \right) \right)
\leq \frac{1}{2} \left( \|\Delta_{\theta_1}\|^2 + 2\|\theta_1\| \cdot \|\Delta_{\theta_1}\| + \|\theta_1\|^2 + \frac{1}{n} \text{tr}(J^{-1}(\theta_1)) + \log |J(\theta_1)| + d \log n - 1 \right)
= \frac{1}{2} \left( C_{p,\Delta_{\theta_1}} + d \log n - 1 \right),
$$

where

$$C_{p,\Delta_{\theta_1}} = \|\Delta_{\theta_1}\|^2 + 2\|\theta_1\| \cdot \|\Delta_{\theta_1}\| + \|\theta_1\|^2 + \frac{1}{n} \text{tr}(J^{-1}(\theta_1)) + \log |J(\theta_1)|.$$

Eq. (30) bounds the KL-divergence between the processed distribution after conducting BIF and the prior distribution. Inserting eq. (30) into eq. (28) in Lemma C.1, we then obtain the PAC-Bayesian generalization bound.

Eventually, since all the conditions in Theorem 5.3 hold, we can apply Theorem 4.2 and have that $\|\Delta_{\theta_1}\| \leq O(1/n)$. Therefore, we have the following,

$$C_{p,\Delta_{\theta_1}} = O \left( \|\theta_1\|^2 + \frac{1}{n} \text{tr}(J^{-1}(\theta_1)) + \log |J(\theta_1)| \right) = O(1).$$

The proof is completed. \qed