

**SUPPLEMENTARY MATERIAL OF “VARIATIONAL BAYES’  
METHOD FOR FUNCTIONS WITH APPLICATIONS TO  
INVERSE PROBLEMS”**

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ABSTRACT. In this supplementary material, we provide all of the proof details for the lemmas and theorems presented in the main text.

**Proof of Lemma 2**

*Proof.* Let  $\{\nu_n\}_{n=1}^\infty = \{\prod_{i=1}^M \nu_n^i\}_{n=1}^\infty$  be a sequence of measures in  $\mathcal{C}$  that converges weakly to a probability measure  $\nu_*$ . We want to show that  $\nu_* \in \mathcal{C}$ . Define

$$(0.1) \quad \nu_*^i := \int_{\prod_{j \neq i} \mathcal{H}_j} d\nu_*, \quad \text{for } i = 1, 2, \dots, M.$$

Obviously, each  $\nu_*^i$  is a probability measure. Let  $f_i$  be some bounded continuous function defined on  $\mathcal{H}_i$  with  $i = 1, 2, \dots, M$ . Based on the definition of weak convergence, we obtain

$$(0.2) \quad \int_{\prod_{j=1}^M \mathcal{H}_j} f_i d\nu_n \rightarrow \int_{\mathcal{H}_i} f_i d\nu_*^i, \quad \text{as } n \rightarrow \infty.$$

It should be noted that the left hand side of (0.2) is equal to

$$(0.3) \quad \int_{\mathcal{H}_i} f_i d\nu_n^i,$$

and we find that each  $\nu_n^i$  converges weakly to  $\nu_*^i$ . Therefore, we find that  $\nu_*^i$  belongs to  $\mathcal{A}_i$ . Let  $f$  be a bounded continuous function defined on  $\prod_{j=1}^M \mathcal{H}_j$ . Then, it is a bounded continuous function for each variable. Based on the definition of weak convergence, we find that

$$(0.4) \quad \int_{\prod_{j=1}^M \mathcal{H}_j} f d\nu_n \rightarrow \int_{\prod_{j=1}^M \mathcal{H}_j} f d\nu_*,$$

and

$$(0.5) \quad \int_{\prod_{j=1}^M \mathcal{H}_j} f d\nu_n = \int_{\prod_{j=1}^M \mathcal{H}_j} f d\nu_n^1 \cdots d\nu_n^M \rightarrow \int_{\prod_{j=1}^M \mathcal{H}_j} f d\nu_*^1 \cdots d\nu_*^M,$$

when  $n \rightarrow \infty$ . Relying on the arbitrariness of  $f$ , we conclude that  $\nu_* = \prod_{j=1}^M \nu_*^j$ , which completes the proof.  $\square$

**Proof of Theorem 5**

*Proof.* From the proof of Lemma 2, we know that  $\nu_n^j$  converges weakly to  $\nu_*^j$  for every  $j = 1, 2, \dots, M$ . According to  $\nu_n^j \ll \nu_*^j$  for  $j = 1, 2, \dots, M$ , we have

$$(0.6) \quad \begin{aligned} D_{\text{KL}}(\nu_n || \nu_*) &= \int \frac{d\nu_n}{d\nu_*} \log \left( \frac{d\nu_n}{d\nu_*} \right) d\nu_* = \sum_{j=1}^M \int \log \left( \frac{d\nu_n^j}{d\nu_*^j} \right) d\nu_n^j \\ &= \sum_{j=1}^M D_{\text{KL}}(\nu_n^j || \nu_*^j). \end{aligned}$$

Using Lemma 2.4 proved in [2] and Lemma 22 shown in [1], we find that  $\nu_n$  converges to  $\nu_*$  in the total-variation norm. Combined with the above equality (0.6), the proof is completed.  $\square$

### Proof of Theorem 9

*Proof.* For a fixed  $j$ , let  $B \in \mathcal{M}(\mathcal{H}_j)$ , and  $\nu_n^j \in \mathcal{A}_j$  be a sequence that converges weakly to  $\nu_*^j$  and

$$(0.7) \quad \frac{d\nu_n^j}{d\mu_r^j} = \frac{1}{Z_{nr}^j} \exp(-\Phi_j^{nr}(x_j)).$$

Assuming that  $\mu_r^j(B) = 0$  and by assumption (16) in the main text, we have

$$\nu_n^j(B) = \int_B \frac{1}{Z_{nr}^j} \exp(-\Phi_j^{nr}(x_j)) \mu_r^j(dx_j) = 0.$$

Define

$$(0.8) \quad B_m = \{x \in B \mid \text{dist}(x, B^c) \geq 1/m\},$$

and let  $f_m > 0$  be a positive continuous function that satisfies

$$f_m(x) = \begin{cases} 1, & x \in B_m, \\ 0, & x \in B^c. \end{cases}$$

Then, we have

$$(0.9) \quad \nu_*^j(B_m) \leq \int_{\mathcal{H}_j} f_m d\nu_*^j = \lim_{n \rightarrow \infty} \int_{\mathcal{H}_j} f_m d\nu_n^j \leq \lim_{n \rightarrow \infty} \nu_n^j(B) = 0,$$

and

$$(0.10) \quad \nu_*^j(B) = \sup_m \nu_*^j(B_m) = 0,$$

based on the inner regular property of finite Borel measures. Therefore, there exists a constant and a continuous function denoted by  $Z_r^j$  and  $\Phi_j^r(\cdot)$  such that

$$(0.11) \quad \frac{d\nu_*^j}{d\mu_r^j}(x_j) = \frac{1}{Z_r^j} \exp(-\Phi_j^r(x_j)).$$

To complete the proof, we should verify the almost surely positiveness of the right-hand side of the above equality. Assume that  $\frac{1}{Z_r^j} \exp(-\Phi_j^r(x_j)) = 0$  on a set  $B \subset \mathcal{H}_j$  with  $\mu_r^j(B) > 0$ . If  $B \subset \mathcal{H}_j \setminus \text{sup}_N T_N^j$ , then it holds that  $\mu_r^j(B) = 0$  by our assumption. Therefore,  $B \cap \text{sup}_N T_N^j$  is not empty, and there exists a constant  $\tilde{N}$  such that for all  $N \geq \tilde{N}$ ,  $B \cap T_N^j$  is not empty. Denote  $B_N = B \cap T_N^j$ , and then for a sufficiently large  $N$ , we have  $\mu_r^j(B_N) \geq \frac{1}{2} \mu_r^j(B)$ . Let

$$B_N^m = \{x \in B_N \mid \text{dist}(x, B_N^c) \geq 1/m\},$$

and define a function  $g_m$  similar to  $f_m$  with  $B_m$  replaced by  $B_N^m$ . Given that  $\mu_r^j(B_N) = \sup_m \mu_r^j(B_N^m)$ , for a large enough  $m$ , we find that

$$\mu_r^j(B_N^m) \geq \frac{1}{2} \mu_r^j(B_N) \geq \frac{1}{4} \mu_r^j(B) > 0.$$

By the definition of weak convergence, we have

(0.12)

$$\lim_{n \rightarrow \infty} \int_{\mathcal{H}_j} g_m(x) \frac{1}{Z_{nr}^j} \exp(-\Phi_j^{nr}(x)) d\mu_r^j = \int_{\mathcal{H}_j} g_m(x) \frac{1}{Z_r^j} \exp(-\Phi_j^r(x)) d\mu_r^j.$$

The right hand side of the above equation is equal to 0, but for a large enough  $m$ , the left hand side is positive and the lower bound is

$$(0.13) \quad \frac{1}{4} \exp(-C_N) \mu_r^j(B).$$

This is a contradiction, and thereby the closedness of  $\mathcal{A}_j (j = 1, \dots, M)$  have been proved. Combining the obtained results with the statements in Theorem 3, we obviously obtain the existence of a solution which completes the proof.  $\square$

### Proof of Theorem 10

*Proof.* Here, we focus on the deduction of formula (21) presented in the main text. By inserting the prior probability measure into the Kullback-Leibler divergence between  $\nu$  and  $\mu$ , for each  $i$  ( $i = 1, 2, \dots, M$ ) we find that

$$\begin{aligned} D_{\text{KL}}(\nu || \mu) &= \int_{\mathcal{H}} \log \left( \frac{d\nu}{d\mu_r} \right) - \log \left( \frac{d\mu_0}{d\mu_r} \right) - \log \left( \frac{d\mu}{d\mu_0} \right) d\nu \\ &= \int_{\mathcal{H}} \left( - \sum_{j=1}^M \Phi_j^r(x_j) + \Phi^0(x) + \Phi(x) \right) d\nu + \text{Const} \\ &= \int_{\mathcal{H}_i} \left[ \int_{\prod_{j \neq i} \mathcal{H}_j} \left( \Phi^0(x) + \Phi(x) \right) \prod_{j \neq i} \nu^j(dx_j) \right] \nu^i(dx_i) \\ &\quad - \int_{\mathcal{H}_i} \Phi_i^r(x_i) \nu^i(dx_i) + \text{terms not related to } \Phi_i(x_i). \end{aligned}$$

For  $i = 1, 2, \dots, M$ , let  $\tilde{\nu}^i$  be a probability measure defined as follows:

$$(0.14) \quad \frac{d\tilde{\nu}^i}{d\mu_r^i} \propto \exp \left( - \int_{\prod_{j \neq i} \mathcal{H}_j} \left( \Phi^0(x) + \Phi(x) \right) \prod_{j \neq i} \nu^j(dx_j) \right).$$

By assumption (19) and (20) shown in the main text, we know that the right-hand side of (0.14) is positive almost surely. Then, we easily know that the measures  $\tilde{\nu}^i$  and  $\mu_r^i$  are equivalent with each other. Therefore, we obtain

$$(0.15) \quad \begin{aligned} D_{\text{KL}}(\nu || \mu) &= - \int_{\mathcal{H}_i} \log \left( \frac{d\tilde{\nu}^i}{d\mu_r^i} \right) d\nu^i + \int_{\mathcal{H}_i} \log \left( \frac{d\nu^i}{d\mu_r^i} \right) d\nu^i + \text{Const} \\ &= D_{\text{KL}}(\nu^i || \tilde{\nu}^i) + \text{terms not related to } \nu^i. \end{aligned}$$

Obviously, in order to attain the infimum of the Kullback-Leibler divergence, we should take  $\nu^i = \tilde{\nu}^i$ . Comparing formula (0.14) with definition (14) in the main

text, we notice that the condition  $\nu^i = \tilde{\nu}^i$  implies the following equality:

$$\Phi_i^r(x_i) = \int_{\prod_{j \neq i} \mathcal{H}_j} \left( \Phi^0(x) + \Phi(x) \right) \prod_{j \neq i} \nu^j(dx_j) + \text{Const},$$

which completes the proof.  $\square$

### Verify conditions in Theorem 10 for the linear inverse problem introduced in Subsection 3.1

At last, we provide a detailed verification of the conditions in Theorem 10 for the example employed in Subsection 3.1. As stated in Remark 14, we consider  $\lambda' = \log \lambda$  and  $\tau' = \log \tau$  as hyper-parameters. For a sufficiently small  $\epsilon > 0$ , taking  $a_u(\epsilon, u) := \|u\|_{\mathcal{H}_u}^2$ ,  $a_{\lambda'}(\epsilon, \lambda') := \max \{ -\lambda', \exp(\epsilon \exp(\lambda')) \}$  and  $a_{\tau'}(\epsilon, \tau') := \max \{ -\tau', \exp(\epsilon \exp(\tau')) \}$ , then we try to verify conditions (19) and (20). In the following, the notation  $C$  is a constant that may be different from line to line. In this example, we take  $x_1 = u$ ,  $x_2 = \lambda'$ , and  $x_3 = \tau'$ . As shown in the main text, we have

$$\begin{aligned} \Phi^0(u, \lambda', \tau') &= \frac{1}{2} \sum_{j=1}^K (u_j - u_{0j})^2 (e^{\lambda'} - 1) \alpha_j^{-1} - \frac{K}{2} \lambda', \\ \Phi(u, \lambda', \tau') &= \frac{e^{\tau'}}{2} \|Hu - d\|^2 - \frac{N_d}{2} \tau'. \end{aligned}$$

With these preparations, we firstly verify

$$(0.16) \quad T^1 := \sup_{u \in T_N^u} \sup_{\substack{\nu^{\lambda'} \in \mathcal{A}_{\lambda'} \\ \nu^{\tau'} \in \mathcal{A}_{\tau'}}} \int_{\mathbb{R}} \int_{\mathbb{R}} (\Phi^0 + \Phi) 1_A(u, \lambda', \tau') \nu^{\lambda'}(d\lambda') \nu^{\tau'}(d\tau') < \infty.$$

Taking the specific expressions of  $\Phi^0$  and  $\Phi$  into (0.16), we have

$$(0.17) \quad T^1 \leq C \sup_{u \in T_N^u} \sup_{\substack{\nu^{\lambda'} \in \mathcal{A}_{\lambda'} \\ \nu^{\tau'} \in \mathcal{A}_{\tau'}}} (T^{11} + T^{12} + T^{13} + T^{14}),$$

where

$$\begin{aligned} T^{11} &= \int_{\mathbb{R}^+} \int_{\mathbb{R}} \frac{1}{2} \sum_{j=1}^K (u_j - u_{0j})^2 (e^{\lambda'} - 1) \alpha_j^{-1} e^{-\Phi_{\tau'}^r(\tau')} e^{-\Phi_{\lambda'}^r(\lambda')} \mu_{\tau'}^{\tau'}(d\tau') \mu_{\lambda'}^{\lambda'}(d\lambda'), \\ T^{12} &= \int_{\mathbb{R}^-} -\frac{K}{2} \lambda' e^{-\Phi_{\lambda'}^r(\lambda')} \mu_{\lambda'}^{\lambda'}(d\lambda'), \\ T^{13} &= \int_{\mathbb{R}} \frac{e^{\tau'}}{2} \|Hu - d\|^2 e^{-\Phi_{\tau'}^r(\tau')} \mu_{\tau'}^{\tau'}(d\tau'), \\ T^{14} &= \int_{\mathbb{R}^-} -\frac{N_d}{2} \tau' e^{-\Phi_{\tau'}^r(\tau')} \mu_{\tau'}^{\tau'}(d\tau'). \end{aligned}$$

Because the techniques used for estimating these terms are similar, we provide the estimates of  $T^{13}$  as an example and omit the details for other terms. Because  $H$  is

assumed to be a linear bounded operator, we have

$$(0.18) \quad \begin{aligned} T^{13} &\leq C \int_{\mathbb{R}} (e^{\epsilon e^{\tau'}} + 1) e^{-\Phi_{\tau'}^r(\tau')} \mu_{\tau'}^{\tau'}(d\tau') \\ &\leq C \int_{\mathbb{R}} \max(1, a_{\tau'}(\epsilon, \tau')) e^{-\Phi_{\tau'}^r(\tau')} \mu_{\tau'}^{\tau'}(d\tau') < \infty. \end{aligned}$$

Next, we need to estimate

$$(0.19) \quad T^2 := \sup_{\lambda' \in T_N^{\lambda'}} \sup_{\substack{\nu^u \in \mathcal{A}_u \\ \nu^{\tau'} \in \mathcal{A}_{\tau'}}} \int_{\mathcal{H}_u} \int_{\mathbb{R}} (\Phi^0 + \Phi) 1_A(u, \lambda', \tau') \nu^{\tau'}(d\tau') \nu^u(du) < \infty.$$

Taking the specific expressions of  $\Phi^0$  and  $\Phi$  into (0.19), we have

$$(0.20) \quad T^2 \leq C \sup_{\lambda' \in T_N^{\lambda'}} \sup_{\substack{\nu^u \in \mathcal{A}_u \\ \nu^{\tau'} \in \mathcal{A}_{\tau'}}} (T^{21} + T^{22} + T^{23} + T^{24}),$$

where

$$\begin{aligned} T^{21} &= e^{\lambda'} \int_{\mathcal{H}_u} \frac{1}{2} \sum_{j=1}^K (u_j - u_{0j})^2 \alpha_j^{-1} e^{-\Phi_u^r(u)} \mu_r^u(du), \\ T^{22} &= \frac{K}{2} |\lambda'|, \\ T^{23} &= \int_{\mathcal{H}_u} \|Hu - d\|^2 e^{-\Phi_u^r(u)} \mu_r^u(du) \int_{\mathbb{R}} \frac{1}{2} e^{\tau'} e^{-\Phi_{\tau'}^r(\tau')} \mu_{\tau'}^{\tau'}(d\tau'), \\ T^{24} &= \frac{Nd}{2} \int_{\mathbb{R}} |\tau'| e^{-\Phi_{\tau'}^r(\tau')} \mu_{\tau'}^{\tau'}(d\tau'). \end{aligned}$$

Remembering that the operator  $H$  is bounded and the specific forms of  $a_{\tau'}(\epsilon, \tau')$  and  $a_u(\epsilon, u)$ , we can obtain that the above four terms are all bounded. The following inequality

$$(0.21) \quad T^3 := \sup_{\tau' \in T_N^{\tau'}} \sup_{\substack{\nu^u \in \mathcal{A}_u \\ \nu^{\lambda'} \in \mathcal{A}_{\lambda'}}} \int_{\mathcal{H}_u} \int_{\mathbb{R}} (\Phi^0 + \Phi) 1_A(u, \lambda', \tau') \nu^{\lambda'}(d\lambda') \nu^u(du) < \infty$$

can be proved similarly, we omit the details. With the above calculations, we verified conditions (19) with  $i = 1, 2, 3$ . Now, we turn to verify conditions (20). For conditions (20) with  $i = 2, 3$ , the inequalities could be verified similarly as for the case of  $i = 1$ . Hence, we only provide details when  $i = 1$  that is to prove

$$T^4 := \sup_{\substack{\nu^{\lambda'} \in \mathcal{A}_{\lambda'} \\ \nu^{\tau'} \in \mathcal{A}_{\tau'}}} \int_{\mathcal{H}_u} \exp\left(-\int_{\mathbb{R}^2} (\Phi^0 + \Phi) 1_{A^c} \nu^{\lambda'}(d\lambda') \nu^{\tau'}(d\tau')\right) \max(1, \|u\|_{\mathcal{H}_u}^2) \mu_r^u(du) < \infty.$$

Through a direct calculation, we find that

$$\begin{aligned} -\int_{\mathbb{R}^2} (\Phi^0 + \Phi) 1_{A^c} \nu^{\lambda'}(d\lambda') \nu^{\tau'}(d\tau') &\leq \frac{1}{2} \sum_{j=1}^K \alpha_j^{-1} (u_j - u_{0j})^2 \int_{\mathbb{R}^-} (1 - e^{\lambda'}) \nu^{\lambda'}(d\lambda') \\ &\quad + \frac{K}{2} \int_{\mathbb{R}} |\lambda'| e^{-\Phi_{\lambda'}^r(\lambda')} \mu_r^{\lambda'}(d\lambda') \\ &\quad + \frac{Nd}{2} \int_{\mathbb{R}} |\tau'| e^{-\Phi_{\tau'}^r(\tau')} \mu_r^{\tau'}(d\tau'). \end{aligned}$$

Then we have

$$T^4 \leq C \int_{\mathcal{H}_u} \exp\left(\frac{1}{2} \sum_{j=1}^K \alpha_j^{-1} (u_j - u_{0j})^2 \int_{\mathbb{R}^-} (1 - e^{\lambda'}) \nu^{\lambda'}(d\lambda')\right) \max(1, \|u\|_{\mathcal{H}_u}^2) \mu_r^u(du).$$

Considering  $\int_{\mathbb{R}^-} (1 - e^{\lambda'}) \nu^{\lambda'}(d\lambda') < 1$  and the definition of  $\mu_r^u$ , we know that the right hand side of the above inequality is bounded which completes the proof.

#### REFERENCES

- [1] M. Dashti and A. M. Stuart. The Bayesian approach to inverse problems. *Handbook of Uncertainty Quantification*, pages 311–428, 2017.
- [2] F. J. Pinski, G. Simpson, A. M. Stuart, and H. Weber. Kullback-Leibler approximation for probability measures on infinite dimensional space. *SIAM J. Math. Anal.*, 47(6):4091–4122, 2015.

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