

# Supplementary material for the manuscript titled

## *Unique reconstruction for discretized inverse problems: a random sketching approach via subsampling*

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### Extended discussion on theoretical inverse problems

In this supplementary material, we introduce the foundation of theoretical inverse problems, complementing the discussion of discretized inverse problems in the paper's main body. Theoretical inverse problems are often studied in an ideal infinite-dimensional setting. The well-posedness theory provides a unique reconstruction of the parameter function, when an infinite amount of data is given. In the following, we will set up the rigorous formulation for the infinite-dimensional reconstruction and justify the uniqueness identification via the positivity of Hessian.

Under the constraint that the PDE model is honored, we formulate the theoretical inverse problem through the lens of PDE-constrained optimization:

$$\begin{aligned} \min_{\sigma \in L^2(\Omega)} \text{Loss}[\sigma] &= \frac{1}{2} \|\mathcal{M}[\sigma] - d\|_{L^2(\mathcal{D})}^2, \quad \text{where } d = \mathcal{M}[\sigma_*] \in L^2(\mathcal{D}), \\ \text{where } \mathcal{M}[\sigma] &= \omega[u_\sigma] = \omega \circ \mathcal{L}_\sigma^{-1}[S], \end{aligned} \tag{1}$$

where  $\sigma(x) \in L^2(\Omega)$  is the parameter function to be inferred with  $x$  supported in  $\Omega$  (typically assumed to be compactly supported and with  $C^1$  boundary). The mismatch is quantified by the functional  $\text{Loss} : L^2(\Omega) \rightarrow \mathbb{R}^+$ . The parameter-to-observation map is  $\mathcal{M} : L^2(\Omega) \rightarrow L^2(\mathcal{D})$ , where the measured location is denoted by the set  $\mathcal{D}$  and is not necessarily the same as  $\Omega$ . This map  $\mathcal{M}$  is read as follows. The PDE solution is  $u_\sigma(x)$ , as a function of  $x$ , for PDE operator  $\mathcal{L}_\sigma$  that is parameterized by  $\sigma(x)$  using the source term

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$S(x)$ , and  $\omega[u_\sigma]$  takes the measurement of the solution  $u_\sigma$ , and returns another function. Note that only a single source  $S(x)$  is denoted in (1) for notational simplicity, but the formulation can easily incorporate situations where multiple sources present. We are to compare this measured PDE-simulated solution with the true measurement data  $d(x)$  in  $L^2(\mathcal{D})$  norm, assuming the data has no noise pollution, i.e.  $d = \mathcal{M}[\sigma_*]$ . Since both the to-be-reconstructed parameter  $\sigma : \Omega \rightarrow \mathbb{R}$ , and the available data  $d : \mathcal{D} \rightarrow \mathbb{R}$  are functions, the problem is posed in the infinite-to-infinite dimensional setting.

Next we demonstrate that the parameter function  $\sigma(x)$  is guaranteed to be uniquely recovered due to the positive Hessian functional around the ground-truth  $\sigma_*$ . For any given function  $\sigma \in L^2(\Omega)$ , formally we denote  $\mathcal{H} \text{Loss}[\sigma] : L^2(\Omega) \times L^2(\Omega) \rightarrow \mathbb{R}$ , then for every pair of  $(\tilde{\sigma}_1, \tilde{\sigma}_2)$ , the Hessian is a bilinear map defined as

$$\mathcal{H} \text{Loss}[\sigma](\tilde{\sigma}_1, \tilde{\sigma}_2) = \lim_{\delta \rightarrow 0} \frac{\text{Loss}[\sigma + \delta \tilde{\sigma}_1 + \delta \tilde{\sigma}_2] + \text{Loss}[\sigma] - \text{Loss}[\sigma + \delta \tilde{\sigma}_1] - \text{Loss}[\sigma + \delta \tilde{\sigma}_2]}{\delta^2}.$$

We give the proof details below to show that the Hessian operator  $\mathcal{H} \text{Loss}[\cdot]$  is strictly positive-definite in the neighbourhood of  $\sigma_*$ , i.e.

$$\mathcal{H} \text{Loss}[\sigma_*] \succ 0, \quad \text{or equivalently, for any } \tilde{\sigma} \neq 0 \in L^2(\Omega), \quad \mathcal{H} \text{Loss}[\sigma_*](\tilde{\sigma}, \tilde{\sigma}) > 0.$$

Consequently  $\sigma_*$  is a local unique optimum to the mismatch (1).

**Proposition 1.** *Assuming that 1. the Hessian operator  $\mathcal{H} \text{Loss}[\cdot]$  is continuous in the neighborhood of  $\sigma_*$ ; 2. the function set  $\{\frac{\delta \mathcal{M}[\sigma_*](x)}{\delta \sigma} : \Omega \rightarrow \mathbb{R} | x \in \mathcal{D}\}$  spans the entire  $L^2(\Omega)$ . Then  $\mathcal{H} \text{Loss}[\cdot]$  is strictly positive-definite at  $\sigma_*$  and in the neighbourhood of  $\sigma_*$ .*

*Proof.* We first prove that the Hessian operator  $\mathcal{H} \text{Loss}[\cdot]$  is positive-definite at  $\sigma_*$ . For any  $\tilde{\sigma} \in L^2(\Omega)$ , the Hessian of the optimization in (1) is derived as

$$\begin{aligned} \mathcal{H} \text{Loss}[\sigma_*](\tilde{\sigma}, \tilde{\sigma}) &= 2 \int_{\mathcal{D}} \left\langle \frac{\delta \mathcal{M}[\sigma_*](x)}{\delta \sigma}, \tilde{\sigma} \right\rangle^2 dx + 2 \mathcal{H} \mathcal{M}[\sigma_*](\tilde{\sigma}, \tilde{\sigma})(\mathcal{M}[\sigma_*] - \mathcal{M}[\sigma_*]) \\ &= 2 \int_{\mathcal{D}} \left\langle \frac{\delta \mathcal{M}[\sigma_*](x)}{\delta \sigma}, \tilde{\sigma} \right\rangle_{\Omega}^2 dx. \end{aligned} \tag{2}$$

Suppose there exists a non-zero function  $\tilde{\sigma}_0 \in L^2(\Omega)$  that makes the Hessian value (2) be 0. Then it would also be the case that

$$\left\langle \frac{\delta \mathcal{M}[\sigma_*](x)}{\delta \sigma}, \tilde{\sigma}_0 \right\rangle_{\Omega} = 0, \quad \forall x \in \mathcal{D}.$$

Due to Assumption 2 that

$$\left\{ \frac{\delta \mathcal{M}[\sigma_*](x)}{\delta \sigma} : \Omega \rightarrow \mathbb{R} \mid x \in \mathcal{D} \right\} = L^2(\Omega),$$

it implies that  $\tilde{\sigma}_0$  must be the zero function. This contradicts the above presumption of the Hessian value being 0 for a non-zero function. Therefore, the Hessian value  $\mathcal{H} \text{Loss}[\sigma_*]$  (2) must be strictly above 0 for all non-trivial  $\tilde{\sigma} \in L^2(\Omega)$ .

Moreover, due to Assumption 1 that  $\mathcal{H} \text{loss}[\cdot]$  is continuous around  $\sigma_*$ , we conclude that the Hessian operator is strictly positive-definite in the neighborhood of  $\sigma_*$ .  $\square$