Observability Gramian for Bayesian Inference in Nonlinear Systems With Its Industrial Application

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***Abstract*—In this letter, we present a novel (empirical) observability Gramian for nonlinear stochastic systems in the light of Bayesian inference. First, we define our observability Gramian, which we refer to as the estimability Gramian, based on the relation to the so-called Bayesian Fisher Information Matrix for initial state estimation. Then, we study the fundamental properties of an empirical version of the estimability Gramian. The practical usefulness of the proposed framework is examined through its application to a parameter and initial state estimation in a natural gas engine cylinder.**

***Index Terms*—Bayesian Fisher information, Bayesian state estimation, data-driven oveservability analysis, nonlinear systems, observability Gramian.**

I. Introduction

THE GROWING interest in digital transformation, especially digital twin, has increased the importance of state estimation problems in complex dynamics. In general statistical inference, utilizing *a priori* information based on domain knowledge can reduce the amount of data required. Such a framework is called Bayesian inference, where *a priori* information is formulated as a prior distribution. On the other hand, in the modern control theory for linear deterministic systems, the difficulty of initial state estimation is quantified with a matrix called observability Gramian. It is known that data-driven indirect calculation is possible using the initial state and output trajectory, which is referred to as the empirical observability Gramian [1], [2], [3], [4], [5], [6], [7], [8]; See Section II-B.

Although the empirical observability Gramian is just conceived from the formal similarity to linear systems' observability Gramian, it can be viewed as the Fisher Information Matrix as shown in Proposition 1. *The main contribution of this letter is to provide an observability Gramian-based framework to utilize the a priori information from a statistical inference point of view.* To be more precise, we newly define a matrix (estimability Gramian in Definition 1 below) that quantifies the difficulty of initial state estimation in terms of the Bayesian Fisher Information Matrix and clarify its relationship to the conventional observability Gramian. We also examine the practical usefulness of the proposed framework through its application to a parameter and initial state estimation in a natural gas engine cylinder.

Organization: The remainder of this letter is organized as follows. In Section II, we introduce the Bayesian Fisher Information Matrix and empirical observability Gramian as preliminary. In Section III, we define the estimability Gramian and confirm its consistency with the observability Gramian for the linear system case. In Section IV, we describe the data-driven method of calculating the estimability Gramian. In Section V, a numerical example illustrates the utility of the proposed method. Some concluding remarks are given in Section VI.

Notation: Let $[a]$ denote $\{1, 2, \ldots, a\}$ for a natural number a. Let $\mathbb{R}^n$ denote n-dimensional Euclidean space, and $\mathbf{e}^i$ denote its ith regular basis. Let $\mathbb{E}[\,\cdot\,]$ denote the expected value of a random variable. Let I denote the Identity matrix. Let $A \succeq B$ denote when A and B are both symmetric and $A - B$ is positive semidefinite. Let $\|x\|_A^2$ denote the quadratic form $x^\top Ax$. We represent a random variable in ordinary font and its realization in bold font. For example, the realization of the random variable x is $\mathbf{x}$. When random variable x has a probability density function (p.d.f.), denote it as $\varphi_x(\mathbf{x})$, and let the joint p.d.f. of the random variable x, y be $\varphi_{x,y}(\mathbf{x}, \mathbf{y})$, and the conditional p.d.f. $\varphi_x(\mathbf{x}|y = \mathbf{y})$. When two random variables x and y are independent, we denote $x \perp y$. Let $\sigma_{\min}(A)$ denote the smallest eigenvalue of matrix A.

II. Preliminary

In this section, we describe the Bayesian Fisher Information Matrix and the empirical observability Gramian as preliminary knowledge of our proposed method.

A. Bayesian Fisher Information Matrix

Let (x, y) be a pair of multivariate random variables and consider the point estimation of x using the observation of y.

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The Fisher Information Matrix (FIM) is defined as below:

$$I_y(x = \mathbf{x}) := \int \varphi_y(\mathbf{y}|x = \mathbf{x})\mathrm{Sc}_x(\mathbf{x}|y = \mathbf{y})\mathrm{Sc}_x(\mathbf{x}|y = \mathbf{y})^\top d\mathbf{y} \tag{1}$$

with the likelihood function and score function defined by

$$l_x(\mathbf{x}|y = \mathbf{y}) := \varphi_y(\mathbf{y}|x = \mathbf{x}), \tag{2}$$

$$\mathrm{Sc}_x(\mathbf{x}|y = \mathbf{y}) := \frac{\partial}{\partial \mathbf{x}} \log l_x(\mathbf{x}|y = \mathbf{y}). \tag{3}$$

Note that this matrix can be related to the Hessian:

$$I_y(x = \mathbf{x}) = -\mathbb{E}_y\left[\frac{\partial^2}{\partial \mathbf{x}^2} \log l_x(\mathbf{x}|y = \mathbf{y})\right]. \tag{4}$$

Then, the Cramer-Rao Bound [9] characterizes a fundamental estimation performance limitation: for any unbiased estimator $\hat{x}$ (i.e., $\mathbb{E}[\hat{x}(y)|x = \mathbf{x}] = \mathbf{x}$), the error covariance matrix has the following lower bound:

$$\mathbb{E}[(\hat{x}(y) - \mathbf{x})(\hat{x}(y) - \mathbf{x})^\top|x = \mathbf{x}] \succeq I_y^{-1}(x = \mathbf{x}), \ \forall \mathbf{x}. \tag{5}$$

Note that $I_y(x = \mathbf{x})$ depends on $\mathbf{x}$ and not on the prior distribution of x.

On the other hand, Bayesian FIM (BFIM) is defined by

$$J_{x,y} := -\mathbb{E}_{x,y}\left[\frac{\partial^2}{\partial \mathbf{x}^2} \log \varphi_{x,y}(\mathbf{x}, \mathbf{y})\right]. \tag{6}$$

For this matrix, we have Bayesian Cramer-Rao Bound [10]:

$$\mathbb{E}[(\hat{x}(y) - x)(\hat{x}(y) - x)^\top] \succeq J_{x,y}^{-1} \tag{7}$$

holds for estimator $\hat{x}(y)$ which satisfies weak unbiasedness condition [11]. In contrast to FIM $I_y(x = \mathbf{x})$, BFIM $J_{x,y}$ depends on the prior distribution of x and not on any realization $\mathbf{x}$. Note that the left-hand side of (7) is the average (over realization of x) of error covariance matrices. Therefore, the Bayesian Cramer-Rao Bound implies that the smaller the minimum eigenvalue of BFIM $J_{x,y}$ is, the more difficult it is to estimate x.

B. Empirical Observability Gramian

Consider a linear discrete-time deterministic system

$$\begin{cases} x_{k+1} = Ax_k \\ y_k = Cx_k. \end{cases} \tag{8}$$

When the matrix A is Schur stable, the observability Gramian

$$G^o := \sum_{k=0}^{\infty} (A^k)^\top C^\top C A^k \tag{9}$$

is a well-known measure for the difficulty of the initial state estimation from an output sequence [4], [12].

By the fact that A is Schur stable, G^o can be approximated by $G^o_{\bar{k}}$ which is a finite sum up to a sufficiently large $\bar{k}$ in (9). However, this calculation can be done only after obtaining A, C by system identification. On the other hand, the empirical observability Gramian $\hat{G}^o_{\bar{k}}$, which is proposed in [1] and re-examined in [3], can be used to obtain $G^o_{\bar{k}}$ using output trajectories without system identification:

$$x_0^{(ilm)} := c_m U_l \mathbf{e}^i, \ (U_l)^\top U_l = I$$

$$y_k^{(ilm)} := CA^k x_0^{(ilm)}$$

$$\hat{Y}_k^{(lm)} := [y_k^{(1lm)} \ \cdots \ y_k^{(nlm)}]$$

$$\hat{G}^o_{\bar{k}} := \sum_{l=1}^{r}\sum_{m=1}^{s}\sum_{k=0}^{\bar{k}-1} \frac{1}{rsc_m^2} U_l (\hat{Y}_k^{(lm)})^\top \hat{Y}_k^{(lm)} (U_l)^\top. \tag{10}$$

This empirical observability Gramian $\hat{G}^o_{\bar{k}}$ coincides with $G^o_{\bar{k}}$ for linear systems [3].

Even if the system is nonlinear, the empirical observability Gramian can be defined in the same way by setting $y_k^{(ilm)}$ to be the observation at time step k with the initial state $x_0^{(ilm)}$. The empirical observability Gramian is used in model reduction [2], [3] for nonlinear systems, and sensor placement problem [13], [14], [15].

III. Observability Gramian for Nonlinear Systems

Let us consider the nonlinear discrete-time stochastic system

$$\begin{cases} x_{k+1} = f(x_k) \\ y_k = h(x_k) + w_k \\ x_0 \sim \mathcal{Q}, w_k \sim \mathcal{N}(\mathbf{0}, \Sigma_w), w_k \perp x_0. \end{cases} \tag{11}$$

For mathematical simplicity, we consider the finite terminal time $\bar{k}$. Let $x_k \in \mathbb{R}^n$ ($y_k \in \mathbb{R}^q$) be the state (observation) at time step k, and let $f : \mathbb{R}^n \to \mathbb{R}^n$ and $h : \mathbb{R}^n \to \mathbb{R}^q$ denote a map representing state transitions and observation processes. Let $y_{0:\bar{k}-1}$ denote the output trajectory from time step 0 to $\bar{k} - 1$. The initial state x_0 follows a prior distribution $\mathcal{Q}$ and the observation noise w_k at time step k follows a normal distribution $\mathcal{N}(\mathbf{0}, \Sigma_w)$ with $\Sigma_w \succ 0$. The mean vector $\bar{x}_0$ and covariance matrix Σ_x of $\mathcal{Q}$ are assumed to be known and finite.

Recall that the larger an eigenvalue of the observability Gramian, the more significant the contribution to the observed energy of the initial state in the corresponding eigenvector direction. This fact implies that the state of that direction is easy to estimate [4]. Actually, the observability Gramian and the FIM has a close relationship as follows:

Proposition 1: For the linear system given by

$$\begin{cases} x_{k+1} = Ax_k \\ y_k = Cx_k + w_k \\ x_0 \sim \mathcal{Q}, w_k \sim \mathcal{N}(\mathbf{0}, \Sigma_w), \text{i.i.d.}, w_k \perp x_0, \end{cases} \tag{12}$$

the FIM $I_{y_{0:\bar{k}-1}}(x_0 = \mathbf{x}_0)$ is given by

$$I_{y_{0:\bar{k}-1}}(x_0 = \mathbf{x}_0) = \sum_{k=0}^{\bar{k}-1} (A^k)^\top C^\top \Sigma_w^{-1} C A^k, \tag{13}$$

independently of the initial state $\mathbf{x}_0$. In particular, $I_{y_{0:\bar{k}-1}}(x_0 = \mathbf{x}_0) = G^o_{\bar{k}}$ for $\Sigma_w = I$.

Proof: This result follows from a straightforward calculation. ■

Remark 1: Even if $\Sigma_w \neq I$, by normalizing the observation noise (i.e. by making the covariance matrix of w_k equal to I) using the presence of a matrix M satisfying $M\Sigma_w M^\top = I$ because of $\Sigma_w \succ 0$, it is possible to match $I_{y_{0:\bar{k}-1}}(x_0 =$

$\mathbf{x}_0$) to the observability Gramian $G^o_{\bar{k}}$ of the system where the observation is replaced to $z_k := My_k$ from (12).

This fact motivates us to define the observability Gramian for nonlinear systems as the FIM. Note that $I_{y_{0:\bar{k}-1}}(x_0 = \mathbf{x}_0)$ depends on $\mathbf{x}_0$ for nonlinear system in general. Instead of considering this *initial-state dependent* observability Gramian, we attempt to introduce a novel observability Gramian for nonlinear systems *with prior initial distribution*:

Definition 1: For nonlinear system in (11), the *Estimability Gramian* $\mathcal{G}^o$ is defined by

$$\mathcal{G}^o_{\bar{k}} := J_{x_0, y_{0:\bar{k}-1}}. \tag{14}$$

The following theorem is useful to understand the relation between the observability and estimability Gramians:

Theorem 1: For linear Gaussian system

$$\begin{cases} x_{k+1} = Ax_k \\ y_k = Cx_k + w_k \\ x_0 \sim \mathcal{N}(\bar{x}_0, \Sigma_x),\, w_k \sim \mathcal{N}(\mathbf{0}, \Sigma_w), \text{ i.i.d.}, w_k \perp x_0, \end{cases} \tag{15}$$

the estimability Gramian is given by

$$\mathcal{G}^o_{\bar{k}} = \sum_{k=0}^{\bar{k}-1} (CA^k)^\top \Sigma_w^{-1} CA^k + \Sigma_x^{-1}. \tag{16}$$

In particular, for $\Sigma_w = I$ we have

$$\mathcal{G}^o_{\bar{k}} \to G^o_{\bar{k}} \tag{17}$$

as $\Sigma_x^{-1} \to 0$.

Proof: Let $\mathcal{O}_{\bar{k}} \in \mathbb{R}^{q\bar{k}\times n}$ be a matrix in which CA^k ($k \in [0, \bar{k}-1]$) are arranged vertically, and $\Sigma_{w,\bar{k}}$ a block diagonal matrix in which Σ_w is arranged in $\bar{k}$ diagonal blocks. Then, the random vector $[x_0^\top \; y_{0:\bar{k}-1}^\top]^\top$ is given by

$$\begin{bmatrix} x_0 \\ y_0 \\ \vdots \\ y_{\bar{k}-1} \end{bmatrix} = \begin{bmatrix} x_0 \\ Cx_0 + w_0 \\ \vdots \\ CA^{\bar{k}-1}x_0 + w_{\bar{k}-1} \end{bmatrix} = \begin{bmatrix} I \\ \mathcal{O}_{\bar{k}} \end{bmatrix} x_0 + \begin{bmatrix} 0 \\ w_0 \\ \vdots \\ w_{\bar{k}-1} \end{bmatrix}.$$

Since x_0 and $w_{0:\bar{k}-1}$ follow an independent Gaussian distribution,

$$\begin{bmatrix} x_0 \\ y_{0:\bar{k}-1} \end{bmatrix} \sim \mathcal{N}\left(\begin{bmatrix} I \\ \mathcal{O}_{\bar{k}} \end{bmatrix} \bar{x}_0, \begin{bmatrix} I \\ \mathcal{O}_{\bar{k}} \end{bmatrix} \Sigma_x \begin{bmatrix} I \\ \mathcal{O}_{\bar{k}} \end{bmatrix}^\top + \begin{bmatrix} 0 & 0 \\ 0 & \Sigma_{w,\bar{k}} \end{bmatrix} \right)$$
$$= \mathcal{N}\left(\underbrace{\begin{bmatrix} \bar{x}_0 \\ \mathcal{O}_{\bar{k}}\bar{x}_0 \end{bmatrix}}_{=:\mu_{\bar{k}}}, \underbrace{\begin{bmatrix} \Sigma_x & \Sigma_x \mathcal{O}_{\bar{k}}^\top \\ \mathcal{O}_{\bar{k}}\Sigma_x & \mathcal{O}_{\bar{k}}\Sigma_x\mathcal{O}_{\bar{k}}^\top + \Sigma_{w,\bar{k}} \end{bmatrix}}_{=:\Sigma_{\bar{k}}} \right)$$

holds. Then, the logarithm of joint p.d.f. of $[x_0^\top \; y_{0:\bar{k}-1}^\top]^\top$ can be written as

$$-\frac{1}{2}\left\| \begin{bmatrix} \mathbf{x}_0 \\ \mathbf{y}_{0:\bar{k}-1} \end{bmatrix} - \mu_{\bar{k}} \right\|^2_{\Sigma_{\bar{k}}^{-1}} + \text{const.} \tag{18}$$

This shows

$$-\frac{\partial^2}{\partial \mathbf{x}_0^2} \log \varphi_{x_0, y_{0:\bar{k}-1}}(\mathbf{x}_0, \mathbf{y}_{0:\bar{k}-1}) = \mathbf{H}, \tag{19}$$

where $\mathbf{H}$ denotes $n \times n$ size left upper block matrix of $\Sigma_{\bar{k}}^{-1}$. Since $\mathbf{H}$ does not depend on the value of $\mathbf{x}_0, \mathbf{y}_{0:\bar{k}-1}$, we obtain $J_{x_0, y_{0:\bar{k}-1}} = \mathbf{H}$ from (6). Next,

$$\mathbf{H} = (\Sigma_x - \Sigma_x \mathcal{O}_{\bar{k}}^\top (\mathcal{O}_{\bar{k}}\Sigma_x\mathcal{O}_{\bar{k}}^\top + \Sigma_{w,\bar{k}})^{-1} \mathcal{O}_{\bar{k}}\Sigma_x)^{-1} \tag{20}$$
$$= \Sigma_x^{-1} + \Sigma_x^{-1}(\Sigma_x\mathcal{O}_{\bar{k}}^\top)\{\mathcal{O}_{\bar{k}}\Sigma_x\mathcal{O}_{\bar{k}}^\top + \Sigma_{w,\bar{k}} - (\mathcal{O}_{\bar{k}}\Sigma_x)\Sigma_x^{-1}(\Sigma_x\mathcal{O}_{\bar{k}}^\top)\}^{-1}(\mathcal{O}_{\bar{k}}\Sigma_x)\Sigma_x^{-1} \tag{21}$$
$$= \Sigma_x^{-1} + \mathcal{O}_{\bar{k}}^\top \Sigma_{w,\bar{k}}^{-1} \mathcal{O}_{\bar{k}}, \tag{22}$$

which is equal to the right-hand-side of (16). Here, we used the generalized Schur complement [16] in (20) and the Woodbury matrix identity [17] in (21).

Finally, (17) readily follows from (16). ■

Eq. (16) shows that $\mathcal{G}^o_{\bar{k}}$ is expressed as the sum of the FIM and the precision matrix of the prior distribution of the linear Gaussian system. Eq. (17) indicates that the estimability Gramian is equal to the observability Gramian when no *a priori* information is given.

IV. Data-Driven Calculation of Estimability Gramian

In this section, we propose a data-driven calculation method of the estimability Gramian, which is similar to the conventional empirical observability Gramian.

A. Empirical Estimability Gramian

Let $\sigma_i^2, \mathbf{u}^i$, $i \in [n]$ denote the eigenvalues and normalized eigenvectors of Σ_x, respectively. Let $\Lambda := \text{diag}(\sigma_1, \ldots, \sigma_n)$ be a diagonal matrix with σ_i on its diagonal components, and $U := [\mathbf{u}^1 \; \cdots \; \mathbf{u}^n]$ be the orthogonal matrix with eigenvectors arranged horizontally. Then the singular value decomposition of Σ_x can be written as $\Sigma_x = U\Lambda^2 U^\top$. We are now ready to define an empirical version of $\mathcal{G}^o_{\bar{k}}$:

Definition 2: For nonlinear stochastic system in (11), the *Empirical Estimability Gramian* $\tilde{\mathcal{G}}^o_{\bar{k}}$ is defined by

$$\begin{aligned} \tilde{x}_0 &:= x_0 - \bar{x}_0 \\ \tilde{y}_k &:= y_k - \mathbb{E}[y_k] \\ \tilde{y}_{k,i} &:= n \cdot \mathbb{E}\left[\tilde{y}_k \frac{\sigma_i^{-2}\tilde{x}_0^\top \mathbf{u}^i}{(\tilde{x}_0)^\top \Sigma_x^{-1} \tilde{x}_0} \right] \\ \tilde{Y}_k &:= [\tilde{y}_{k,1} \; \cdots \; \tilde{y}_{k,n}] \\ \tilde{\mathcal{G}}^o_{\bar{k}} &:= U\left(\sum_{k=0}^{\bar{k}-1} (\tilde{Y}_k)^\top \Sigma_w^{-1} \tilde{Y}_k + \Lambda^{-2} \right) U^\top. \end{aligned} \tag{23}$$

The following theorem ensures that $\tilde{\mathcal{G}}^o_{\bar{k}}$ is an *empirical* version of $\mathcal{G}^o_{\bar{k}}$:

Theorem 2: For linear Gaussian system (15),

$$\tilde{\mathcal{G}}^o_{\bar{k}} = \mathcal{G}^o_{\bar{k}} \tag{24}$$

holds.

Proof: Introducing $z := \Lambda^{-1}U^\top \tilde{x}_0 \sim \mathcal{N}(0, I)$, $\tilde{y}_{k,i}$ in (23) can be rewritten as

$$\tilde{y}_{k,i} = n \cdot \mathbb{E}_{\tilde{x}_0}\left[CA^k \tilde{x}_0 \frac{\sigma_i^{-2}\tilde{x}_0^\top \mathbf{u}^i}{(\tilde{x}_0)^\top \Sigma_x^{-1} \tilde{x}_0} \right]$$

$$= n \cdot \mathbb{E}_z\left[CA^k(U\Lambda z)\frac{\sigma_i^{-2}(U\Lambda z)^\top U\mathbf{e}^i}{(U\Lambda z)^\top U\Lambda^{-2}U^\top(U\Lambda z)}\right]$$
$$= n \cdot CA^k U\sigma_i^{-1}\Lambda\mathbb{E}_z\left[\frac{zz^\top}{z^\top z}\right]\mathbf{e}^i$$
$$= CA^k U\mathbf{e}^i, \tag{25}$$

where we used $\Lambda\mathbf{e}^i = \sigma_i\mathbf{e}^i$ and the equality

$$\mathbb{E}_{z\sim\mathcal{N}(\mathbf{0},I_n)}\left[\frac{zz^\top}{z^\top z}\right] = \mathbb{E}_{z\sim\mathrm{Uni}(\mathcal{B})}\left[zz^\top\right] = \frac{1}{n}I, \tag{26}$$

$\mathrm{Uni}(\mathcal{B})$ denotes the uniform distribution on the unit ball in $\mathbb{R}^n$; See [18, Th. 4.3].

We, therefore, have $\tilde{Y}_k = CA^kU$, which completes the proof via comparison between (16) and (23). ■

Similarly to the empirical observability Gramian, the empirical estimability Gramian is justifiable through its consistency for the linear case and is computable for nonlinear systems.

B. Sample Approximation

For the data-driven calculation, we employ sample approximation of the expectation in (23). To this end, let $\{x^{(s)}\}_{s=1}^N$ be i.i.d. samples drawn from the prior distribution $\mathcal{Q}$. Let M the number of output trajectories be generated for each $x^{(s)}$, and let $m \in [M]$ be their indices. Let $y_k^{(sm)}$ be the output value at time step k of the mth output trajectory for the initial state $x^{(s)}$. Then, we can obtain

$$\hat{\mathcal{G}}^o_{\bar{k}} := U\left(\sum_{k=0}^{\bar{k}-1}(\hat{Y}_k)^\top\Sigma_w^{-1}\hat{Y}_k + \Lambda^{-2}\right)U^\top \tag{27}$$

with

$$\hat{x}^{(s)} := x^{(s)} - \bar{x}_0$$
$$\hat{y}_k^{(sm)} := y_k^{(sm)} - \frac{1}{NM}\sum_{s=1}^N\sum_{m=1}^M y_k^{(sm)}$$
$$\hat{y}_{k,i} := \frac{n}{NM}\sum_{s=1}^N\sum_{m=1}^M \hat{y}_k^{(sm)}\frac{\sigma_i^{-2}(\hat{x}^{(s)})^\top\mathbf{u}^i}{(\hat{x}^{(s)})^\top\Sigma_x^{-1}\hat{x}^{(s)}}$$
$$\hat{Y}_k := [\hat{y}_{k,1}\ \cdots\ \hat{y}_{k,n}]. \tag{28}$$

Remark 2: In (10), the initial states for calculating empirical observability Gramian are designated by c_m and U_l, whose valid choice were not discussed in any of existing result, to the best of our knowledge. This shows a clear contrast to (28) that the initial state samples should be generated according to the given prior distribution $\mathcal{Q}$.

Thanks to the law of large numbers $\hat{\mathcal{G}}^o_{\bar{k}}$ converges to $\tilde{\mathcal{G}}^o_{\bar{k}}$ in the large sample size N, M limit. Also, according to Theorem 2, $\hat{\mathcal{G}}^o_{\bar{k}}$ in the linear Gaussian system is valid as a sample approximation of the estimability Gramian $\mathcal{G}^o_{\bar{k}}$.

V. Industrial Application

In this section, we verify the usefulness of our proposed method through its application to an experimental design of a natural gas engine cylinder depicted in Fig. 1.

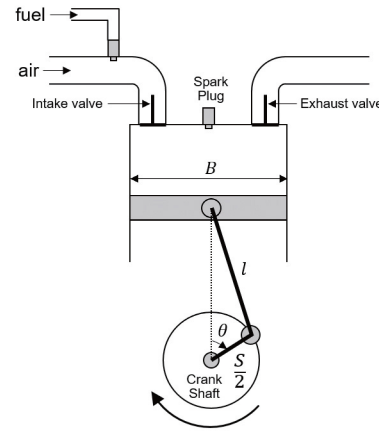


Fig. 1. The engine cylinder model.

A. System Dynamics and Prior Distribution

The dynamics of the mixed gas inside the cylinder during the compression stroke are described as

$$\begin{cases}\dot{\theta} &= \omega\\ \dot{V} &= \frac{\omega\pi B^2}{4}\left(\frac{S}{2}\sin\theta + \frac{S^2\sin 2\theta}{8\sqrt{l^2 - \frac{S^2}{4}\sin^2\theta}}\right)\\ \dot{P} &= -\frac{PC_p}{V(C_p - R)}\dot{V}\\ C_p &:= \frac{\frac{m_{\mathrm{air}}}{M_{\mathrm{air}}}C_{p\mathrm{air}} + \frac{m_{\mathrm{fuel}}}{M_{\mathrm{fuel}}}C_{p\mathrm{fuel}}}{\frac{m_{\mathrm{air}}}{M_{\mathrm{air}}} + \frac{m_{\mathrm{fuel}}}{M_{\mathrm{fuel}}}}\end{cases} \tag{29}$$

where the physical meaning and value of each variable are summarized in Table I. Eq. (29) is derived from the first law of thermodynamics and the ideal gas law. The constant pressure specific heat C_p is expressed by a function of temperature T that can be obtained by

$$T = \frac{10^5 PV}{R(\frac{m_{\mathrm{air}}}{M_{\mathrm{air}}} + \frac{m_{\mathrm{fuel}}}{M_{\mathrm{fuel}}})}. \tag{30}$$

In this letter, we adopted the function in [19]:

$$\begin{bmatrix}C_{p\mathrm{air}}\\ C_{p\mathrm{fuel}}\end{bmatrix} := \begin{bmatrix}a_0 & a_1 & a_2 & a_3 & a_4\\ b_0 & b_1 & b_2 & b_3 & b_4\end{bmatrix}\begin{bmatrix}1\\ T\\ T^2\\ T^3\\ T^4\end{bmatrix}$$
$$\begin{bmatrix}a_0\\ a_1\\ a_2\\ a_3\\ a_4\end{bmatrix} = \begin{bmatrix}27.9\\ 2.94\times10^{-3}\\ 4.56\times10^{-6}\\ -2.9\times10^{-7}\\ 4.7\times10^{-13}\end{bmatrix}, \begin{bmatrix}b_0\\ b_1\\ b_2\\ b_3\\ b_4\end{bmatrix} = \begin{bmatrix}35.9\\ -5.46\times10^{-2}\\ 2.42\times10^{-4}\\ -2.15\times10^{-7}\\ 6.34\times10^{-11}\end{bmatrix}.$$

It is crucial to control the weight of air and fuel (i.e. m_{air} and m_{fuel}) filled in the cylinder to improve combustion efficiency. However, we cannot measure it directly. This motivates us to estimate m_{air} and m_{fuel} by using the noisy measurement of the pressure $P(t)$ and the *a priori* information below.

In our experiment setup,

- the initial values of the crank angle θ and the cylinder volume V are available as $\theta(0) = -\frac{\pi}{3}$, $V(0) = 0.000207$, and

TABLE I
VARIABLE AND PARAMETER LIST IN (29)

Note	Name	Values	Unit
θ	Crank angle	-	rad
V	Cylinder volume	-	m^3
P	Pressure	-	bar
m_{air}	The weight of air	-	g
m_{fuel}	The weight of fuel	-	g
C_p	Constant pressure specific heat	-	J/(molK)
ω	Engine speed	78.53	rad/s
B	Cylinder bore	86/1000	m
S	Piston stroke	86.07/1000	m
l	Connecting rod length	175/1000	m
R	Gas constant	8.3143	J/(molK)
M_{air}	The molecular weight of air	28.85	g/mol
M_{fuel}	The molecular weight of fuel	16.05	g/mol

TABLE II
PRIOR DISTRIBUTION FOR EACH SIMULATION CONDITION

	$P(0)$	m_{air}	m_{fuel}
Case 1	$\mathcal{N}(10, 0.01)$	$\mathrm{Uni}(0, 8.0)$	$\mathrm{Uni}(0, 0.2)$
Case 2	$\mathcal{N}(10, 0.01)$	Eq. (31)	$\mathrm{Uni}(0, 0.2)$
Case 3	$\mathcal{N}(10, 0.01)$	Eq. (32)	$\mathrm{Uni}(0, 0.2)$

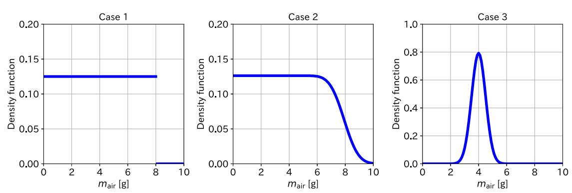


Fig. 2. The prior marginal distribution of m_{air}.

- we have an *a priori information* of $P(0)$ and m_{fuel} represented by the prior distribution $P(0) \sim \mathcal{N}(10, 0.01)$ and $m_{\mathrm{fuel}} \sim \mathrm{Uni}(0, 0.2)$, respectively.

In order to indirectly know the weight of the air that cannot be physically measured, we can prepare the following three experimental conditions shown in Table II:

- In Case 1, we know m_{air} takes a value in the interval $[0, 8.0]$ independent of m_{fuel},
- In Case 2, we have knowledge about the air-fuel ratio represented by

$$\frac{m_{\mathrm{air}}}{m_{\mathrm{fuel}}} \sim \mathcal{N}(40, 16), \tag{31}$$

- In Case 3, we have the knowledge of the total weight of the gas mixture represented by

$$m_{\mathrm{air}} + m_{\mathrm{fuel}} \sim \mathcal{N}(4.1, 0.25). \tag{32}$$

Fig. 2 shows the prior marginal distribution $\varphi_{m_{\mathrm{air}}}$ for each Case. This may indicate that a good estimation would be obtained based on the experimental result for Case 3 because the variance of $\varphi_{m_{\mathrm{air}}}$ under Case 3 is smaller than the others. However, this is incorrect, as we will see below.

B. Proposed Method

The constant parameters m_{air}, m_{fuel} are treated as the initial condition for $\dot{m}_{\mathrm{air}} = 0$, $\dot{m}_{\mathrm{fuel}} = 0$. The difficulty of initial state estimation is then evaluated by calculating the empirical estimability Gramians for each of the three prior distributions. Note that since these Cases differ only in prior distributions, the conventional empirical observability Gramian cannot distinguish them; See Remark 2.

TABLE III
EMPIRICAL ESTIMABILITY GRAMIAN AND MINIMUM EIGENVALUE OF EACH PRIOR DISTRIBUTION

	$\hat{\mathcal{G}}_{\bar{k}}^{o}$	$\sigma_{\min}(\hat{\mathcal{G}}_{\bar{k}}^{o})$
Case 1	$10^4 \begin{bmatrix} 3.8 & 0.6 & -3.2 \\ 0.6 & 0.1 & -0.6 \\ -3.2 & -0.6 & 3.3 \end{bmatrix}$	12.43
Case 2	$10^4 \begin{bmatrix} 7.1 & 0.8 & 6.8 \\ 0.8 & 0.1 & 0.8 \\ 6.8 & 0.8 & 7.4 \end{bmatrix}$	182.88
Case 3	$10^4 \begin{bmatrix} 6.4 & 0.2 & -2 \\ 0.2 & 0.01 & -0.08 \\ -2 & -0.08 & 0.73 \end{bmatrix}$	13.04

The dynamical model is time-discretized with the Runge-Kutta method under the time step size $\Delta t = 0.22$[ms]. Note that $\bar{k}$ (the length of the output trajectories) is 41 and the observation noise follows $\mathcal{N}(0, 0.0025)$. We generated 10,000 output trajectories for each Case by setting $N = 100$ and $M = 100$, and calculated the empirical estimability Gramian $\hat{\mathcal{G}}_{\bar{k}}^{o}$ in (27). Calculation time (including the trajectory generation) is about 0.17s for each Case.

Table III shows the empirical estimability Gramians and their minimum eigenvalue. Recall that the smaller the minimum eigenvalue of BFIM, the more difficult it is to estimate the initial state; See (7). These observations counterintuitively suggest that Case 2, which has the largest minimum eigenvalue, will be the easiest to estimate $P(0)$, m_{air} and m_{fuel}. This trend remained the same for all sample sizes and time horizons tested.

C. Markov Chain Monte Carlo Methods

The empirical Gramian based methods [1], [2], [3], [4], [5], [6], [7], [8] have theoretical underpinnings only for linear systems, but are widely used for nonlinear systems because of their practical usefulness. Since our theoretical results also cover linear systems only, we *virtually* observe what happens in a physical experiment and confirm that Case 2 is preferable for the estimation. To this end, we numerically generate one typical trajectory instead of a physical observation and then calculate the posterior distribution of $P(0)$, m_{air} and m_{fuel} that is the (distributional) estimate under the obtained observation.

As a typical real parameter, we choose $P^*(0) = 10$, $m_{\mathrm{fuel}}^* = 0.1$ and let m_{air}^* be the median of the distribution in Fig. 2, which satisfies $m_{\mathrm{air}}^* \approx 4.0$ for all three Cases. The solution $P^*(t)$ to (29) under these parameters (with additive observation noise following $\mathcal{N}(0, 0.0025)$) is used a typical pressure trajectory; See Fig. 3. Next, using Markov Chain Monte Carlo (MCMC) method [20] implemented by Stan [21], 10,000 posterior samples were calculated. Computation time for MCMC was about 2549s, 973s, 3899s for Case 1, Case 2, and Case 3, respectively.

The simulation resulted in posterior distributions of $P(0)$ and m_{air} with nearly the same variance for all three Cases. In contrast, there was a clear difference for m_{fuel} as shown in

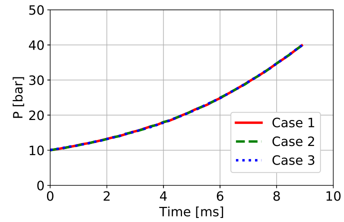
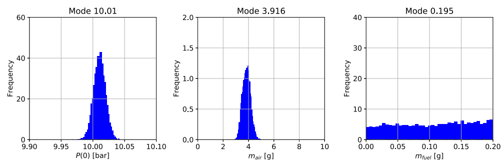
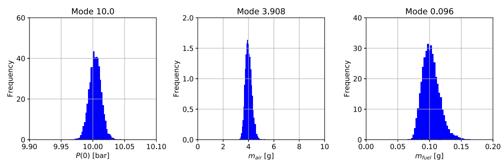


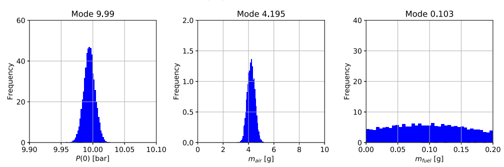
Fig. 3. Time series data $P^*(t)$ used for MCMC.



(a) Case 1



(b) Case 2



(c) Case 3

Fig. 4. Histograms of MCMC samples.

Fig. 4. It can be observed that the posterior distribution in Case 1 and 3 are not so different from the prior distribution (i.e., Uni$(0, 0.2)$), whereas Case 2 has a sharp-shaped distribution. This means that we can obtain a better estimate of m_{fuel} in Case 2 than in the other Cases, which is consistent with the result predicted by using the proposed empirical estimability Gramian.

Remark 3: Calculating the posterior distribution for each of all the trajectories used for the empirical estimability Gramian is overly time-consuming for our purpose.

VI. Conclusion

In this letter, we derived the concept of the estimability Gramian for initial state estimation with nonlinear stochastic systems, which is based on the relation to BFIM. For linear Gaussian systems, we proved that it agrees with the BFIM and the observability Gramian under a certain condition. The practical usefulness of the proposed framework is examined through its application to a parameter and initial state estimation in a natural gas engine cylinder.

We are currently applying the proposed method to a more realistic model of a hydrogen gas engine. From a theoretical point of view, the so-called observability function is revisited for a better understanding of the estimability Gramian; See [22, eq. (2)] for the controllability Gramian. Also, the relationship with existing works [23], [24], [25] needs to be clarified.

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