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General regularization scheme in data-driven learning of Koopman operators

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Анотація. Як відомо, оператор Купмана широко використовується при аналізі складних динамічних систем. У цій статті ми розглядаємо проблему чисельного представлення операторів Купмана на відтворюючих ядерних Гільбертових просторах. Основною ідеєю запропонованого підходу є використання поняття загальної схеми регуляризації для забезпечення стійкості побудованих апроксимацій. Ця концепція дозволяє нам одночасно розглядати кілька добре відомих методів регуляризації, які раніше використовувалися для апроксимації операторів Купмана. Ми також обговорюємо питання вибору параметра регуляризації, яке досі було недостатньо вивченим.

Abstract. As is known, the Koopman operator is widely used in the analysis of complex dynamic systems. In this paper, we consider the problem of numerical representation of the Koopman operators on Reproducing Kernel Hilbert spaces. The main idea of the proposed approach is the use of a concept of general regularization scheme to ensure the stability of the constructed approximations. This concept allows us to simultaneously consider several well-known regularization methods, which have been previously employed for approximating the Koopman operators. We also discuss the issue of the regularization parameter choice, that has been understudied so far.

1 Introduction

The Koopman operator [8] is a tool to predict the values of the so-called observable functions ψ along the trajectories of dynamical systems. The use of the Koopman operator is most effective when studying dynamic systems, information about which has a high degree of uncertainty or is too large in amount. Therefore, the problem of numerical representation of the Koopman operator is of great interest to researchers. There are various approaches to the approximate representation of the Koopman operator, for example, using neural networks [11, 12] and tensor product spaces [7, 13]. Recently, the representation of the Koopman operator for observable functions ψ from reproducing kernel Hilbert spaces (RKHS) has become increasingly popular [20], [4,6,9,10,16,18,21]. Within this approach, the Koopman operator is represented in terms of the inversion of some compact operator. Then such a representation becomes an ill-posed problem that needs to be regularized. In previous studies, the above regularization has been performed by means of the standard Tikhonov technique (see, e.g., [6]) and by the so-called spectral cut-off method (see, e.g., [2, 16]). The first contribution of the present study is that we analyze the general regularization scheme that covers previously used Tikhonov techniques and spectral cut-off method as particular cases. Moreover, the present study sheds light on the choice of a parameter regulating the performance of the regularization. Note that the above choice remained in fact open in [2, 6, 16].

The article is organized as follows. Section 2 contains definitions, concepts and notation which are necessary for the further presentation. Section 3 describes the general regularization scheme that will be used to numerical representation of the Koopman operator. The main result of the study, Theorem 4.1, containing an accuracy estimate of the approximation of the Koopman operator and a suitable choice of regularization parameter, is presented and proven in Section 4.

Key words: Koopman operator, general regularization scheme, reproducing kernel Hilbert space.

2 Definitions, notation and concepts

Let $\mathcal{X} \subset \mathbb{R}^d$ be equipped with the Borel σ-algebra $\mathcal{B}_{\mathcal{X}}$ and the corresponding probability measure μ. Let also $L_{2,\mu} = L_{2,\mu}(\mathcal{X})$ be the Hilbert space of functions that are square-integrable with respect to the measure μ. By $\langle \cdot, \cdot \rangle_{L_{2,\mu}}$ and $\|\cdot\|_{L_{2,\mu}}$, respectively, we will denote the scalar product and norm on $L_{2,\mu}(\mathcal{X})$, such that, for example, $\langle f, g \rangle_{L_{2,\mu}} := \int f(t)g(x)d\mu(x)$.

In this study we will follow very recent publication [16] and consider the semigroup of the Koopman operators $K^t : L_{2,\mu}(\mathcal{X}) \to L_{2,\mu}(\mathcal{X})$ indexed by time $t \in [0, \infty)$ and associated with the Caushy problem for a stochastic differential equation (SDE)

$$dX_t = b(X_t)dt + \sigma(X_t)dW_t, \tag{2.1}$$

$$X_0 = x \in \mathcal{X},$$

such that the image of any observable function $\psi \in L_{2,\mu}(\mathcal{X})$ under the action of K^t is defined by the relation

$$(K^t\psi)(x) = \mathbb{E}[\psi(X_t)|X_0 = x] = \int \psi(y)\rho_t(x, dy),$$

where in the above formulas W_t is d-dimensional Browian motion, $b : \mathcal{X} \to \mathbb{R}^d$, $\sigma : \mathcal{X} \to \mathbb{R}^{d\times d}$ are assumed to be Lipschitz-continuous and for each $A \in \mathcal{B}_{\mathcal{X}}$

$$\rho_t(x, A) = \mathbb{P}(X_t \in A|X_0 = x).$$

Note that the above conditions on b, σ and Theorem 5.2.1 from [14] guarantee the existence and uniqueness of the solution X_t, $t \geq 0$, to SDE (2.1) in $\mathcal{X}$.

Moreover, in the sequel we assume the invariance of μ for the stochastic process described by SDE (2.1), which means that for any $t \geq 0$ and $A \in \mathcal{B}_{\mathcal{X}}$

$$\int \rho_t(x, A)d\mu(x) = \mu(A)$$

and it is equivalent to the identity

$$\int (K^t\psi)(x)d\mu(x) = \int \psi(x)d\mu(x)$$

for all $t \geq 0$ and $\psi \in L_{2,\mu}(\mathcal{X})$.

To study the Koopman operator we will use the concept of Reproduction Kernel Hilbert Space (RKHS). It is known (see, e.g., [19]) that every RKHS can be generated from a symmetric and positive definite function $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ of two variables in $\mathcal{X}$, called the reproducing kernel of $H = H(\mathcal{X}, k)$. Recall that a function $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is called positive definite on $\mathcal{X}$ if for any m and any pairwise distinct $x_1, x_2, \ldots, x_m \in \mathcal{X}$ the quadratic form

$$\langle \mathcal{K}b, b \rangle_{\mathbb{R}^m} = \sum_{i=1}^{m}\sum_{j=1}^{m} b_i b_j k(x_i, x_j)$$

is positive for all m-dimensional vectors $b = (b_1, b_2, \ldots, b_m) \in \mathbb{R}^m \backslash \{0\}$, where $\mathcal{K} = \{k(x_i, x_j)\}_{i,j=1}^m$ is sometimes called the Gram matrix of $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$. It is well known that for any $\psi \in H$ the following reproducing property follows:

$$\psi(x) = \langle \psi, \Phi(x) \rangle_H, \quad x \in \mathcal{X},$$

where $\langle \cdot, \cdot \rangle_H$ is the inner product in H and $\Phi : \mathcal{X} \to H$ denotes the so-called feature map corresponding to the kernel k, i.e.

$$\Phi(x) = k(x, \cdot), \quad x \in \mathcal{X}.$$

The norm on H is defined in the standard way $\|\cdot\|_H^2 := \langle\cdot,\cdot\rangle_H$.

Assumption 2.1. *The kernel $k(x,y)$ is bounded on $\mathcal{X}\times\mathcal{X}$.*

The above assumption is usual in the kernel-based learning, see, e.g., [17]. One needs this assumption to guarantee the bounds for the operator norms (2.7), (2.8) below.

As in [17] we define the linear operator $\mathcal{E} : L_{2,\mu}(\mathcal{X}) \to H$

$$\mathcal{E}\psi := \int \psi(x)\Phi(x)d\mu(x), \quad \psi \in L_{2,\mu}(\mathcal{X}).$$

It is known (see, e.g., [15]) that the adjoint operator $\mathcal{E}^* : H \to L_{2,\mu}(\mathcal{X})$ is the embedding operator from H into $L_{2,\mu}(\mathcal{X})$, i.e.

$$\mathcal{E}^*\xi = \xi, \qquad \xi \in H.$$

Following [16], we consider the covariance operator

$$C_H = \mathcal{E}\mathcal{E}^* \in \mathcal{L}(H)$$

and the cross-covariance operator $C_H^t : H \to H$, which acts as follows on $\psi \in H$

$$C_H^t\psi := \int (K^t\psi)\Phi(x)d\mu(x) = \mathcal{E}K^t\psi = \mathcal{E}K^t\mathcal{E}^*\psi. \tag{2.2}$$

Moreover, as in [16] we also consider the operator

$$K_H^t := C_H^{-1}C_H^t. \tag{2.3}$$

Next proposition relates the above introduced operators.

Proposition 2.1. *[16, Proposition 4.4] For $t > 0$, the following statements are equivalent:*

(i) $K^tH \subset H$.

(ii) $K_H^t \in \mathcal{L}(H)$.

(iii) $\mathrm{rank} C_H^t \subset \mathrm{rank} C_H$.

Observe that if one of (i)–(iii) holds, then $K_H^t = K^t\,|_H$, and for any $\varphi \in H$ we have

$$K^t\varphi = K_H^t\varphi = C_H^{-1}C_H^t\varphi. \tag{2.4}$$

Moreover, according to [16, Equation (4.7)] for any $\varphi \in H$ it holds

$$C_H^{-1}C_H^t\varphi = (\mathcal{E}^*)^{-1}K^t\mathcal{E}^*\varphi. \tag{2.5}$$

Combining (2.4) and (2.5), we get

$$\mathcal{E}^*K_H^t\varphi = \mathcal{E}^*C_H^{-1}C_H^t\varphi = K^t\mathcal{E}^*\varphi. \tag{2.6}$$

At this point we note that the exact Koopman operator K^t is not accessible, and our goal is to mimic its action. For this we can use points x_i, y_i, $i = 0, 1, \ldots, m-1$, sampled from trajectories of the considered dynamical systems.

As an empirical estimator for C_H^t we take

$$C_H^{m,t} = \frac{1}{m}\sum_{j=0}^{m-1} k(x_j,\cdot)\langle k(y_j,\cdot),\cdot\rangle_H, \qquad C_H^{m,t} \in \mathcal{L}(H).$$

Note that in fact the above operator acts in the m-dimensional space spanned by the kernel sections $k(x_j,\cdot)$.

Assumption 2.2. *Assume that* $x_0 = X_0$, $x_1, x_2, \dots, x_{m-1}$ *are drawn i.i.d. from* μ. *Then* y_i, $i = 0, 1, \dots, m-1$, *are obtained from the conditional distribution* $\rho_t(x_k, \cdot)$, *i.e.,* $y_k|(x_k = x) \sim \rho_t(x_k, \cdot)$ *for* μ*-a.e.* $x \in X$.

It follows from Proposition 3.5 [16] that if Assumptions 2.1 and 2.2 are satisfied, then with probably $1-\delta$ it holds

$$\|C_H^t - C_H^{m,t}\|_{HS} \le \frac{\gamma \log^{\frac{1}{2}} \frac{2}{\delta}}{m^{1/2}}, \tag{2.7}$$

where $\|\cdot\|_{HS}$ is the Hilbert-Schmidt operator norm. Here and in the sequel, we adopt the convention that γ denotes a generic positive coefficient, which can vary from inequality to inequality and does not depend on quantities such as δ and m.

Let us also consider the sampling operator

$$\mathcal{E}_m^* : H \to \mathbb{R}^m, \qquad \mathcal{E}_m^* f = (f(x_0), \dots, f(x_{m-1})),$$

which can be seen as an empirical version of the embedding operator $\mathcal{E}^* : H \to L_{2,\mu}$. Then for any $v = (v_0, v_1, \dots, v_{m-1})$ the adjoint operator $\mathcal{E}_m = (\mathcal{E}_m^*)^* : \mathbb{R}^m \to H$ can be defined as

$$\mathcal{E}_m v = (\mathcal{E}_m^*)^* v = \frac{1}{m} \sum_{j=0}^{m-1} k(x_j, \cdot) v_j.$$

If Assumption 2.1 is satisfied then it is well-known (see, e.g., Lemma 4.2 [15]) that with probably $1-\delta$ we have

$$\|\mathcal{E}\mathcal{E}^* - \mathcal{E}_m\mathcal{E}_m^*\|_{H\to H} \le \|\mathcal{E}\mathcal{E}^* - \mathcal{E}_m\mathcal{E}_m^*\|_{HS} \le \frac{\gamma \log^{\frac{1}{2}} \frac{2}{\delta}}{m^{1/2}}. \tag{2.8}$$

3 General regularization scheme

From (2.3) and Proposition 2.1 it follows that the representation of the Koopman operator on H involves the inverse of the covariance operator, which becomes an unbounded operator due to its compactness. Therefore, to ensure a stability in the approximate calculation of the Koopman operator, regularization is required, since such approximation is an ill-posed problem. To this end, we will use a general approach, originated in [1], to solve a wide range of ill-posed problems. More detailed information about this approach can be found in [3, 5].

Recall that the most regularization schemes can also be indexed by families of parameterized functions $g_\alpha(t)$, $0 < t < \infty$, $\alpha > 0$. The only requirement is that there are positive constants γ_0, $\overline{\gamma}$, $\tilde{\gamma}$ such that

$$\sup_{0<t<\infty} |g_\alpha(t)| \le \frac{\gamma_0}{\alpha}, \qquad \sup_{0<t<\infty} \sqrt{t}|g_\alpha(t)| \le \frac{\overline{\gamma}}{\sqrt{\alpha}}, \qquad \sup_{0<t<\infty} t\,|g_\alpha(t)| \le \tilde{\gamma}. \tag{3.1}$$

Further important property of the regularization method indexed by $\{g_\alpha\}$ is its qualification that is the largest positive number p for which it holds

$$\sup_{0<t<\infty} t^p |1 - t g_\alpha(t)| \le \gamma_p \alpha^p, \tag{3.2}$$

where γ_p does not depend on α.

For example, the standard Tikhonov method with $g_\alpha(t) = (\alpha + t)^{-1}$ has the qualification 1. The iterated Tikhonov method with

$$g_\alpha(t) = g_{r,\alpha}(t) = \sum_{i=1}^{r} \alpha^{i-1}(\alpha+t)^{-i} = \frac{1}{t}\Big(1 - \frac{\alpha^r}{(\alpha+t)^r}\Big), \quad \lambda \ne 0, \quad r = 1, 2, \dots$$

has the qualification r. The spectral cut-off method, in which

$$g_\alpha(t) = \begin{cases} t^{-1}, & \alpha^{-1} \le t < \infty \\ 0, & 0 \le t < \alpha^{-1} \end{cases}, \tag{3.3}$$

has infinite qualification.

We will look for an approximate representation of (2.3) in the form

$$\hat{K}_\alpha^{m,t} f = g_\alpha(\mathcal{E}_m \mathcal{E}^*) C_H^{m,t} f.$$

At this point we note that when using the Koopman operator $K^t : L_{2,\mu} \to L_{2,\mu}$ for predicting the values of observable functions $\psi \in H$, it is natural to consider and approximate K^t as an operator from H to $L_{2,\mu}$, such that the approximation accuracy will be evaluated in terms of the operator norm $\|\cdot\|_{H\to L_{2,\mu}}$. Our main result, presented in the next section consists in estimating that accuracy. For this we need the following statement.

Proposition 3.1. *It holds true*

$$\|K^t - \hat{K}_\alpha^{m,t}\|_{H\to L_{2,\mu}} = \|(\mathcal{E}\mathcal{E}^*)^{1/2}(K^t - \hat{K}_\alpha^{m,t})\|_{H\to H}.$$

Proof. For any $h \in H$ we have

$$\|h\|_{L_{2,\mu}} = \|\mathcal{E}^* h\|_{L_{2,\mu}} = \langle \mathcal{E}^* h, \mathcal{E}^* h\rangle_{L_{2,\mu}}^{1/2} = \langle \mathcal{E}\mathcal{E}^* h, h\rangle_H^{1/2}$$

$$= \left\langle (\mathcal{E}\mathcal{E}^*)^{1/2}(\mathcal{E}\mathcal{E}^*)^{1/2} h, h\right\rangle_H^{1/2} = \left\langle (\mathcal{E}\mathcal{E}^*)^{1/2} h, (\mathcal{E}\mathcal{E}^*)^{1/2} h\right\rangle_H^{1/2} = \|(\mathcal{E}\mathcal{E}^*)^{1/2} h\|_H.$$

Substituting $h = (K^t - \hat{K}_\alpha^{m,t})f$, $f \in H$, into the relation above, we obtain the statement of Proposition. □

4 Main result

Now we are in a position to prove the following statement.

Theorem 4.1. *Let Assumptions 2.1 and 2.2 be satisfied. Then with probably $1-\delta$ it holds*

$$\|K^t - \hat{K}_\alpha^{m,t}\|_{H\to L_{2,\mu}} \le \gamma\left(\sqrt{\alpha} + \frac{\log^{3/4}\frac{2}{\delta}}{m^{1/4}} + \frac{\log^{1/2}\frac{2}{\delta}}{\sqrt{\alpha m}} + \frac{\log^{3/4}\frac{2}{\delta}}{\alpha m^{3/4}}\right)$$

and for $\alpha \asymp m^{-1/2}$ we have

$$\|K^t - \hat{K}_\alpha^{m,t}\|_{H\to L_{2,\mu}} \le \gamma m^{-1/4}\log^{3/4}\frac{2}{\delta}.$$

Proof. Let us write the following representation for the error

$$K^t f - \hat{K}_\alpha^{m,t} f = K^t f - g_\alpha(\mathcal{E}_m\mathcal{E}_m^*) C_H^{m,t} = \triangle_1 f + \triangle_2 f,$$

where

$$\triangle_1 := K^t f - g_\alpha(\mathcal{E}_m\mathcal{E}_m^*) C_H^t,$$
$$\triangle_2 := g_\alpha(\mathcal{E}_m\mathcal{E}_m^*)(C_H^t - C_H^{m,t}).$$

Using relations (2.2) and (2.6) we obtain

$$C_H^t = \mathcal{E}K^t\mathcal{E}^* = \mathcal{E}\mathcal{E}^* K_H^t.$$

Then

$$\triangle_1 f = K^t f - g_\alpha(\mathcal{E}_m\mathcal{E}_m^*)\mathcal{E}K^t\mathcal{E}^* f = (I - g_\alpha(\mathcal{E}_m\mathcal{E}_m^*)\mathcal{E}\mathcal{E}^*)\, K_H^t f.$$

We consider the operator

$$\bar{\triangle}_1 = (\mathcal{E}\mathcal{E}^*)^{1/2}\left(I - g_\alpha(\mathcal{E}_m\mathcal{E}_m^*)\mathcal{E}\mathcal{E}^*\right).$$

It is easy to see that

$$\bar{\triangle}_1 = \sum_{i=1}^{5} \bar{\triangle}_{1,i},$$

where

$$\bar{\triangle}_{1,1} = (\mathcal{E}\mathcal{E}^*)^{1/2} - (\mathcal{E}_m\mathcal{E}_m^*)^{1/2},$$

$$\bar{\triangle}_{1,2} = (\mathcal{E}_m\mathcal{E}_m^*)^{1/2}\left(I - g_\alpha(\mathcal{E}_m\mathcal{E}_m^*)\mathcal{E}_m\mathcal{E}_m^*\right),$$

$$\bar{\triangle}_{1,3} = \left((\mathcal{E}_m\mathcal{E}_m^*)^{1/2} - (\mathcal{E}\mathcal{E}^*)^{1/2}\right) g_\alpha(\mathcal{E}_m\mathcal{E}_m^*)\mathcal{E}_m\mathcal{E}_m^*,$$

$$\bar{\triangle}_{1,4} = \left((\mathcal{E}\mathcal{E}^*)^{1/2} - (\mathcal{E}_m\mathcal{E}_m^*)^{1/2}\right) g_\alpha(\mathcal{E}_m\mathcal{E}_m^*)\left(\mathcal{E}_m\mathcal{E}_m^* - \mathcal{E}\mathcal{E}^*\right),$$

$$\bar{\triangle}_{1,5} = (\mathcal{E}_m\mathcal{E}_m^*)^{1/2} g_\alpha(\mathcal{E}_m\mathcal{E}_m^*)\left(\mathcal{E}_m\mathcal{E}_m^* - \mathcal{E}\mathcal{E}^*\right).$$

By means of (3.1), (3.2) and (2.8) we obtain

$$\|\bar{\triangle}_{1,1}\|_{H\to H} \le \frac{\gamma \log^{\frac{1}{4}}\frac{2}{\delta}}{m^{1/4}}, \qquad \|\bar{\triangle}_{1,2}\|_{H\to H} \le \gamma_{1/2}\sqrt{\alpha},$$

$$\|\bar{\triangle}_{1,3}\|_{H\to H} \le \frac{\gamma \log^{\frac{1}{4}}\frac{2}{\delta}}{m^{1/4}}\tilde{\gamma}, \qquad \|\bar{\triangle}_{1,4}\|_{H\to H} \le \frac{\gamma \log^{\frac{3}{4}}\frac{2}{\delta}}{m^{3/4}}\frac{\gamma_0}{\alpha},$$

$$\|\bar{\triangle}_{1,5}\|_{H\to H} \le \frac{\gamma \log^{\frac{1}{2}}\frac{2}{\delta}}{m^{1/2}}\frac{\bar{\gamma}}{\sqrt{\alpha}}.$$

Then

$$\|\bar{\triangle}_1\|_{H\to H} \le \gamma\left(\sqrt{\alpha} + \frac{\log^{3/4}\frac{2}{\delta}}{m^{1/4}} + \frac{\log^{1/2}\frac{2}{\delta}}{\sqrt{\alpha m}} + \frac{\log^{3/4}\frac{2}{\delta}}{\alpha m^{3/4}}\right)$$

and taking into account Proposition 3.1, for $\alpha \asymp m^{-1/2}$ we have

$$\|\triangle_1 f\|_{L_{2,\mu}} = \|(\mathcal{E}\mathcal{E}^*)^{1/2}\bar{\triangle}_1 K_H^t f\|_H \le \gamma m^{-1/4}\log^{3/4}\frac{2}{\delta}\|K_H^t f\|_H.$$

Using (2.7) we find

$$\|\triangle_2 f\|_{L_{2,\mu}} = \|(\mathcal{E}\mathcal{E}^*)^{1/2} g_\alpha(\mathcal{E}_m\mathcal{E}_m^*)(C_H^t - C_H^{m,t})f\|_H$$

$$\le \|(\mathcal{E}_m\mathcal{E}_m^*)^{1/2} g_\alpha(\mathcal{E}_m\mathcal{E}_m^*)(C_H^t - C_H^{m,t})f\|_H$$

$$+\|((\mathcal{E}\mathcal{E}^*)^{1/2} - (\mathcal{E}_m\mathcal{E}_m^*)^{1/2}) g_\alpha(\mathcal{E}_m\mathcal{E}_m^*)(C_H^t - C_H^{m,t})f\|_H$$

$$\le \frac{\gamma \log^{\frac{1}{2}}\frac{2}{\delta}}{m^{1/2}}\frac{\bar{\gamma}}{\sqrt{\alpha}}\|f\|_H + \frac{\gamma \log^{\frac{3}{4}}\frac{2}{\delta}}{m^{3/4}}\frac{\gamma_0}{\alpha}\|f\|_H.$$

Hence, for $\alpha \asymp m^{-1/2}$ it holds

$$\|\triangle_2 f\|_{L_{2,\mu}} \le \gamma m^{-1/4}\log^{3/4}\frac{2}{\delta}.$$

Summing up the estimates for $\|\triangle_1 f\|_{L_{2,\mu}}$, $\|\triangle_2 f\|_{L_{2,\mu}}$ we get the assertion of Theorem. □

Remark 4.1. *As it has been already mentioned in the introduction, some particular cases of the general regularization scheme (3.1) have been studied in the context of approximate representation of the Koopman operators in RKHS. For example, in [6] the accuracy of an approximate representation of the Koopman operators by means of the Tikhonov regularization corresponding to* $g_\alpha = (\alpha + t)^{-1}$ *has been proven to be of the order* $O(m^{-1/2}\alpha^{-2})$ *that is worse than the bound given by Theorem 4.1. Note also that in our terms the accuracy of an approximate representation of the Koopman operators by means of the spectral cut-off regularization (2.6) has been proven to be of order not better than* $O(\sqrt{\alpha} + m^{-1/2}\alpha^{-1})$, *which is still worse than the bound of Theorem 4.1. Thus, if no additional assumptions are made concerning the spectrum of the Koopman operators, such as the ones in [9], then the order of accuracy obtained in Theorem 4.1 is the best among the reported in literature.*

Declarations

Conflict of Interest.

The authors declare that there is no conflict of interest.

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Author Contributions.

All authors contributed equally to the research and preparation of this article.

Additional information

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