Simulator Calibration under Covariate Shift with Kernels

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Contents of This Talk

- Keiichi Kisamori, Motonobu Kanagawa and Keisuke Yamazaki
- Simulator Calibration under Covariate Shift with Kernels
- *AISTATS 2020*, to appear
- arXiv:1809.08159

Outline

Computer Simulators are Everywhere

- Computer Simulator: computer program for modeling a real-world phenomenon.

- e.g., climate, epidemics, natural disasters, cardiology, industrial manufacturing process, etc, etc...

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- Computer Simulator: computer program for modeling a real-world phenomenon.

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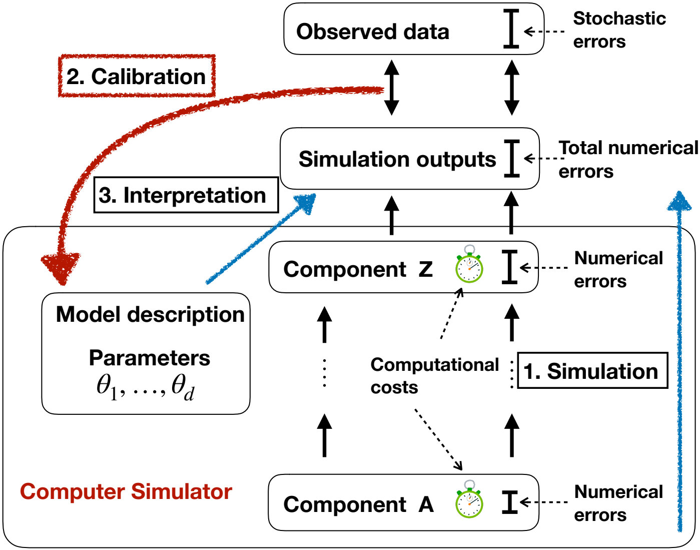
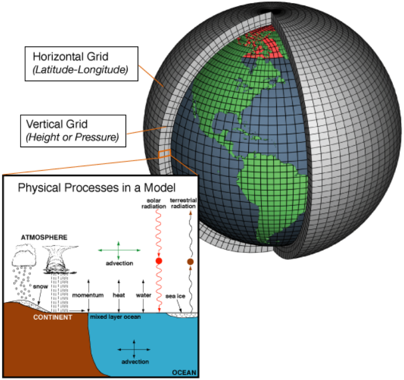
- Simulation provides insights/understanding about the system of interest.

- Enables prediction about the phenomenon in the future / under a hypothetical condition.

Computer Simulation and Related Tasks



Example: Climate Simulator



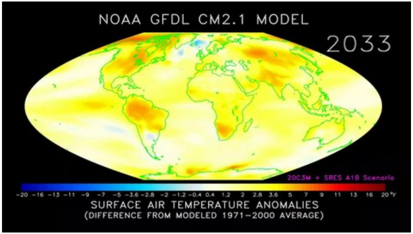


Figure 1: From Wikipedia "General circulation model"

Example: Industrial Manufacturing Process Simulator

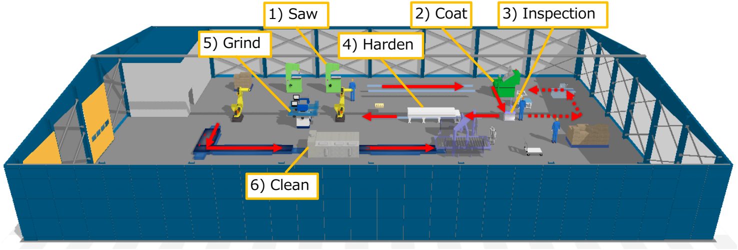


Figure 2: Simulator constructed with *WITNESS*, a popular software package for production simulation (`https://www.lanner.com/en-us/`).

Target System: Formulation as a Regression Model

- We consider a system takes $x \in \mathcal{X} \subset \mathbb{R}^{d_\mathcal{X}}$ as a input, and outputs $y(x) \in \mathbb{R}$.

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$$y(x) := R(x) + e(x), \quad x \in \mathcal{X}$$

where

- $R : \mathcal{X} \to \mathbb{R}$: an (unknown) deterministic regression function.

- $e : \mathcal{X} \to \mathbb{R}$: an (unknown) zero-mean stochastic process (representing stochastic error).

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Climate simulation (How global temperature changes?):

- Input x: time point.

- Output $R(x)$: the global temperature.

Manufacturing process simulation (How production efficiency changes?):

- Input x: the number of products to be manufactured in one day.

- Output $R(x)$: the total time required to manufacture all the products.

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$$X_1, \ldots, X_n \sim q_0 \quad \text{(i.i.d.)}$$
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- The input density q_0 may be known, if it is designed by the user (experimental design).

Simulator

- Let $\Theta \subset \mathbb{R}^{d_\Theta}$ be a parameter space, and $r : \mathcal{X} \times \Theta \to \mathbb{R}$ be a deterministic function.

- For a fixed $\theta \in \Theta$, we define a "simulation model" as the mapping

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- The "user" designs $r(x, \theta)$ so that it resembles the regression function $R(x)$ of the target system.

- By design, the user can produce the output $r(x, \theta)$ given $(x, \theta) \in \mathcal{X} \times \Theta$.

- However, simulating one output $r(x, \theta)$ for given (x, θ) may be computationally very expensive.

Calibration: Parameter Tuning of a Simulation Model

- The question is how to find a "good" parameter θ in the simulation model $r(x, \theta)$.

- To this end we can use data $D_n := \{(X_i, Y_i)\}_{i=1}^n$ from the target system $y(x) = R(x) + e(x)$.

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- "Good" θ should be such that $r(x, \theta)$ "approximates well" the true (unknown) function $R(x)$.

- But in what sense should $r(x, \theta)$ "approximate well" $R(x)$?

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Examples:

- **Climate Simulation**: Prediction is required for the future, but data are only available from the past.

- **Manufacturing Process Simulation**: Prediction is required for mass production (when the factory is deployed), while data are only available from a trial period.

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- Training inputs locations are generated $X_1, \ldots, X_n \sim q_0$;

- But test (or prediction) is required for locations $\tilde{X}_1, \ldots, \tilde{X}_m \sim q_1$.

Calibration for Extrapolation: Covariate Shift

- Therefore the generalization error should be defined in terms of the test input density $q_1(x)$.

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\begin{aligned}
L(\theta) &:= \int (y(x) - r(x,\theta))^2 \, q_1(x) dx \\
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- One needs to tune the parameter $\theta \in \Theta$ so that this generalization error will be small.

- The generalization error can be approximated by weighted squares:

$$L_n(\theta) := \frac{1}{n} \sum_{i=1}^{n} \beta(X_i) \left(Y_i - r(X_i, \theta)\right)^2.$$

because $X_1, \ldots, X_n \sim q_0$.

Why One Needs to Care About Covariate Shift?

- Simulator $r(x, \theta)$ is a **parametric** model, with a finite degree of freedom.

- As such, $r(x, \theta)$ cannot capture all aspects of the unknown target system $R(x)$ ("All models are wrong").

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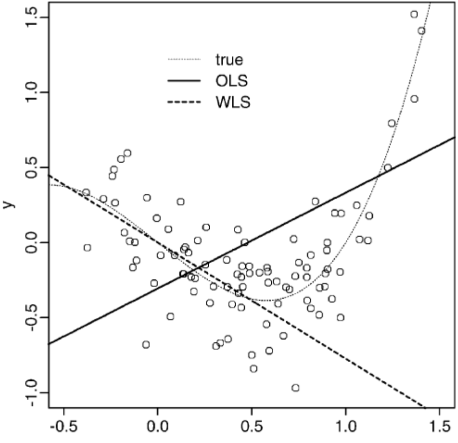
- Under such a model misspecification, the optimal model under covariate shift can be **drastically different** from the one without covariate shift.

Effect of Covariate Shift under Model Misspecification

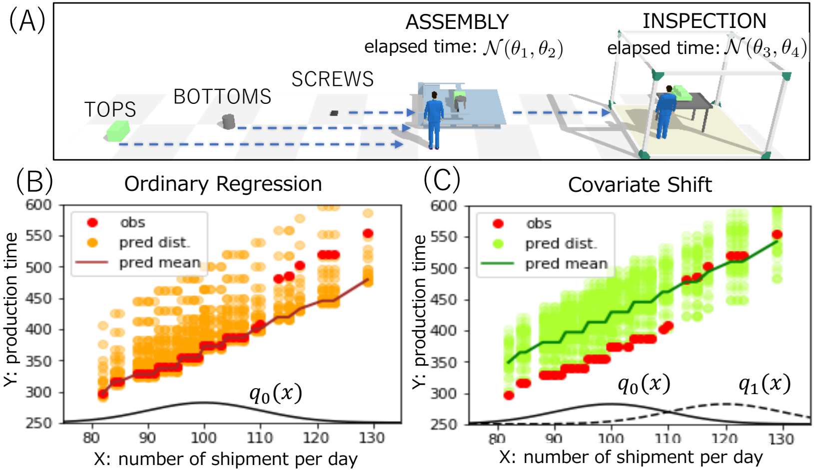
- **True** = 3rd order polynomial (curve); **OLS** = standard linear fit (solid line); **WLS** = linear with importance weighting (dotted line).

- $q_0 = \mathcal{N}(0.5, 2.5^2)$, $q_1 = \mathcal{N}(0.0, 0.3^2)$. [Shimodaira, 2000]



(a)

Covariate Shift in Manufacturing Process Simulation



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- One can only generate an output $y = r(x, \theta)$, but one such simulation may be **computationally very expensive**.

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- Experiments on **manufacturing process simulators**.

Outline

Kernels and Reproducing Kernel Hilbert Spaces (RKHS)

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Examples of positive definite kernels on $\mathcal{X} = \mathbb{R}^d$:

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In this talk, I will simply call k a kernel.

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- - $\mathcal{H}$ can be written as

$$\mathcal{H} = \overline{\text{span}\, \{k(\cdot, x) \mid x \in \mathcal{X}\}}$$

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A key concept: Characteristic kernels [Fukumizu et al., 2008].

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- In other words, k is characteristic if

$$\text{the mapping} \quad P \in \mathcal{P} \to \mu_P \in \mathcal{H} \quad \text{is } \textbf{injective}.$$

Kernel Mean Embeddings [Smola et al., 2007]

Intuitively, k being **characteristic** implies that $\mathcal{H}$ **is large enough.**

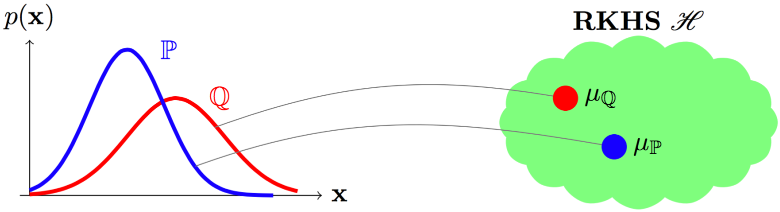

Figure 3: Injective embedding [Muandet et al., 2017, Figure 2.3]

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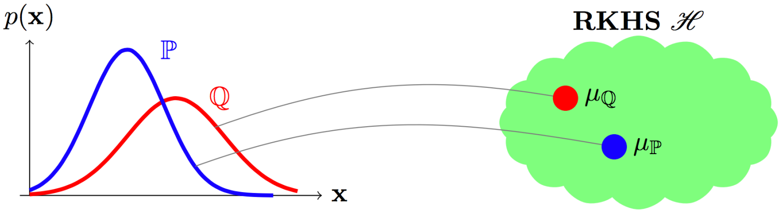

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- Gaussian and Matérn kernels [Sriperumbudur et al., 2010].

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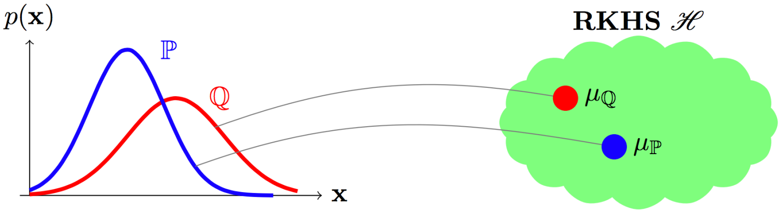

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Examples of **non**-characteristic kernels on $\mathcal{X} = \mathbb{R}^d$:
- Linear and polynomial kernels.

Outline

Vector-valued Function Defined with the Simulator

- We define a vector-valued function $r^n : \Theta \to \mathbb{R}^n$ by

$$r^n(\theta) := (r(X_1, \theta), \ldots, r(X_n, \theta))^\top \in \mathbb{R}^n, \quad \theta \in \Theta.$$

where $r(x, \theta)$ is the simulation model.

Vector-valued Function Defined with the Simulator

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$$r^n(\theta) := (r(X_1, \theta), \dots, r(X_n, \theta))^\top \in \mathbb{R}^n, \quad \theta \in \Theta.$$

where $r(x, \theta)$ is the simulation model.

- We assume that input points $X_1, \dots, X_n \in \mathcal{X}$ are **given and fixed** (throughout the talk).

Optimal Parameters and Predictions under Covariate Shift

- Define $\Theta^* \subset \Theta$ as the set of optimal parameters minimizing the weighted squares.

- i.e., for all $\theta^* \in \Theta^*$, we have

$$\sum_{i=1}^{n} \beta(X_i)(Y_i - r(X_i, \theta^*))^2 = \min_{\theta \in \mathrm{supp}(\pi)} \sum_{i=1}^{n} \beta(X_i)(Y_i - r(X_i, \theta))^2.$$

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- Θ^* may contain multiple (or even infinitely meany) elements.

- We assume that the resulting simulator outputs are unique, i.e.,

$$r^* := r^n(\theta^*) = r^n(\tilde{\theta^*}), \quad \forall \theta^*, \tilde{\theta^*} \in \Theta^*.$$

- r^* is "optimal" predictions under covariate shift.

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- The support of the push-forward measure $r^n\pi$ is given by

$$\operatorname{supp}(r^n\pi) = \{r^n(\theta) \mid \theta \in \operatorname{supp}(\pi)\}.$$

"Target" Poster Distribution

- For the joint random variables

$$(\vartheta, r^n(\vartheta)) \in \Theta \times \mathbb{R}^n.$$

consider the **conditioning** $r^n(\vartheta) = \boldsymbol{y} \in \mathrm{supp}(r^n \pi)$.

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- It will turn out that our approach aims at estimating

$$P_\pi(\theta|r^*)$$

the "posterior" distribution of ϑ, provided that $r^* = r^n(\vartheta)$ is "observed".

Outline

Overview of the Proposed Approach

- Let $k_\Theta(\theta, \theta')$ be a characteristic kernel on Θ, with $\mathcal{H}_\Theta$ its the RKHS.

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2) Sampling parameters from the estimate of $\mu_{\Theta|r^*}$, using **Kernel Herding**.

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- $\sigma^2 > 0$: constant.

Kernel ABC with the Importance-weighted Kernel

- To estimate the kernel mean of the target posterior $P_\pi(\theta|r^*)$,

$$\mu_{\Theta|r^*} := \int k_\Theta(\cdot, \theta) dP_\pi(\theta|r^*) \in \mathcal{H}_\Theta,$$

we use Kernel ABC (**A**pproximate **B**ayesian **C**omputation) [Nakagome et al., 2013].

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- For this we use the importance-weighted kernel.

Kernel ABC with the Importance-weighted Kernel

Step 1: Simulate **parameter-data pairs**

$$(\bar{\theta}_1, \bar{Y}_1^n), \ldots, (\bar{\theta}_m, \bar{Y}_m^n) \in \Theta \times \mathbb{R}^n$$

as follows:

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- Generate pseudo data $\bar{Y}_j^n$ by running the simulator $r(\cdot, \theta)$ with $\theta = \bar{\theta}_j$ for $j = 1, \ldots, m$:

$$\bar{Y}_j^n := r^n(\bar{\theta}_j) = \left(r(X_1, \bar{\theta}_j), \ldots, r(X_n, \bar{\theta}_j)\right)^\top \in \mathbb{R}^n,$$

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- Step 2: Regard $(k_\Theta(\cdot, \bar{\theta}_1), \bar{Y}_1^n), \ldots, (k_\Theta(\cdot, \bar{\theta}_m), \bar{Y}_m^n)$ as "training data" for **regression from $\mathbb{R}^n$ to $\mathcal{H}_\Theta$.**

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- Perform **Kernel Ridge Regression** using observed data Y^n as an "input":

$$\hat{\mu}_{\Theta|r^*} := \sum_{j=1}^{m} w_j k_\Theta(\cdot, \bar{\theta}_j) \ \in \mathcal{H}_\Theta,$$

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Posterior Sampling from the Estimate of Kernel ABC

- We generate parameters $\check{\theta}_1, \ldots, \check{\theta}_m \in \Theta$ from the posterior embedding $\hat{\mu}_{\Theta|r^*} \in \mathcal{H}_\Theta$.

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- To this end, we apply Kernel Herding [Chen et al., 2010], a **deterministic, sequential** sampling method:

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\check{\theta}_1 &:= \arg\max_{\theta \in \Theta} \hat{\mu}_{\Theta|r^*}(\theta) \\
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- Convergence guarantee under a mild condition [Bach et al., 2012].

$$\left\| \hat{\mu}_{\Theta|r^*} - \frac{1}{t}\sum_{j=1}^{t} k_\Theta(\cdot, \check{\theta}_j) \right\|_{\mathcal{H}_\Theta} = O(t^{-1/2}) \quad (t \to \infty).$$

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- Kernel Herding is a version of Quasi Monte Carlo [Dick et al., 2013].

Predictions with the Posterior-sampled Parameters

- For any test input $x \in \mathcal{X}$, we define the predictive output distribution as

$$P_\pi(y|x, r^*) = \int \delta\left(y = r(x, \theta)\right) dP_\pi(\theta|r^*)$$

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We approximate $P_\pi(y|x, r^*)$ in the following way:

- For each sampled parameter $\check{\theta}_j$, run the simulator $r(x, \check{\theta}_j)$, and obtain a set of predictive outputs

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- Then approximate $P_\pi(y|x, r^*)$ as an empirical distribution

$$\hat{P}_\pi(y|x, r^*) := \frac{1}{m} \sum_{j=1}^{m} \delta(y - r(x, \check{\theta}_j)).$$

Why Should It Work?

We present a theoretical justification after describing experimental results.

Outline

Common Setting for All Experiments (Evaluation Metric)

-Training data $(X_1, Y_1), \ldots, (X_n, Y_n)$ are generated as

$$X_1, \ldots, X_n \sim q_0 \quad \text{(i.i.d.)}$$
$$Y_i = R(X_i) + \varepsilon_i, \quad i = 1, \ldots, n,$$

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- We evaluate the quality of the sampled parameters $\check{\theta}_1, \ldots, \check{\theta}_m$, in **predictions at test input locations**

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$$\tilde{X}_1, \ldots, \tilde{X}_n \sim q_1 \quad \text{(i.i.d.)}.$$

- To this end, we compute Root Mean Square Errors (RMSE) defined as

$$\sqrt{\frac{1}{n} \sum_{i=1}^{n} \left(R(\tilde{X}_i) - \frac{1}{m} \sum_{j=1}^{m} r(\tilde{X}_i, \check{\theta}_j) \right)^2}.$$

Common Setting for All Experiments (Proposed Method)

We use the following kernels for all the experiments:

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k_{\mathbb{R}^n}(Y_a^n, Y_b^n) &= \exp\left(-\frac{1}{2\sigma^2}\sum_{i=1}^{n}\beta(X_i)(Y_{ai}-Y_{bi})^2\right), \\
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- Importance weights $\beta(X_i) = q_1(X_i)/q_0(X_i)$ are assumed to be known.

- Constants $\sigma^2, \sigma_\Theta^2 > 0$ are determined by the median heuristic using the simulated pairs $(\bar{\theta}_j, \bar{Y}_j^n)_{j=1}^m$.

Common Setting for All Experiments (Baseline)

- For comparison, we used the Metropolis-Hastings (MH) algorithm for sampling from the posterior

$$\Pr\left(\theta \mid |(X_i, Y_i)_{i=1}^n\right) \propto \pi(\theta) \prod_{i=1}^{n} \Pr(Y_i | X_i, \theta).$$

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where

$$\Pr(Y_i | X_i, \theta) \propto \exp\left(-\frac{1}{2{\sigma_{\text{noise}}}^2} \sum_{i=1}^n \beta(X_i)(Y_i - r(X_i, \theta))^2\right).$$

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- For comparison, we used the Metropolis-Hastings (MH) algorithm for sampling from the posterior

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where

$$\mathrm{Pr}(Y_i|X_i, \theta) \propto \exp\left(-\frac{1}{2{\sigma_{\mathrm{noise}}}^2} \sum_{i=1}^{n} \beta(X_i)(Y_i - r(X_i, \theta))^2\right).$$

- For MH, we assume that the **perfect knowledge** of the likelihood $\mathrm{Pr}(Y_i|X_i)$ is available, including its noise distribution

$$\varepsilon_i \sim N(0, \sigma^2_{\mathrm{noise}}).$$

- This is an unfair advantage over the proposed method.

Simple Synthetic Experiment: Setting

- The input space is $\mathcal{X} = \mathbb{R}$.

- True (unknown) regression function: **Third order polynomial**

$$R(x) = -x + x^3.$$

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$$q_0(x) = N(0.5, 0.5), \quad q_1(x) = N(0, 0.3).$$

- Prior on the parameter space: $\pi(\theta) = N(\mathbf{0}, 5I_2)$.

- Training data $(X_i, Y_i)_{i=1}^n$ with $n = 100$.

Simple Synthetic Experiment: Setting

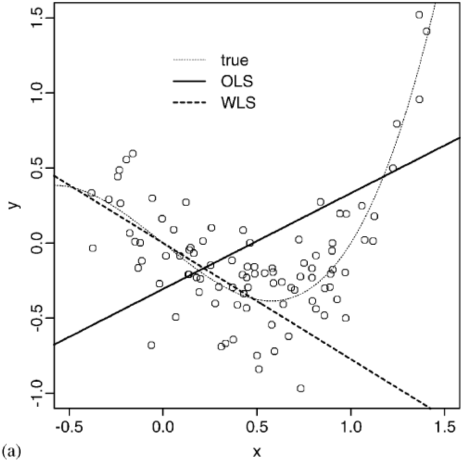


Figure 4: Fig.1(a) from [Shimodaira, 2000].

Simple Synthetic Experiments: Setting

- For the proposed method, we set the regularization constant to be $\varepsilon = 1.0$.

- We set the proposal distribution of MH to be Gaussian, whose variance is tuned so as to make the acceptance ratios to be about 20%, 40%, and 60%.

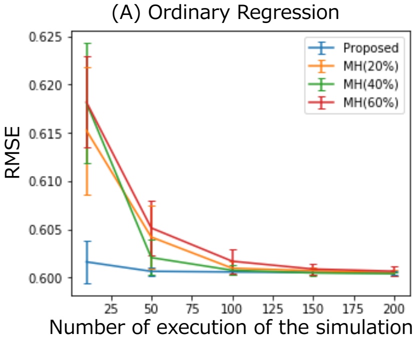
Simple Synthetic Experiments: Results

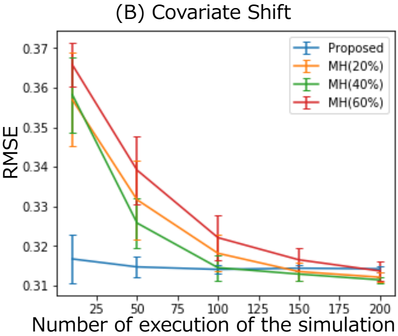
- (A) Ordinary regression ($q_1 = q_0$); (B) Covariate shift ($q_1 \neq q_0$).

- Horizontal axis: the number of simulations m.

- The proposed method performs better for smaller m.

- Promising result, since often simulations are computationally expensive.





Manufacturing Process Simulator (WITNESS Software)

- Computer simulator for a factory assembling certain products.

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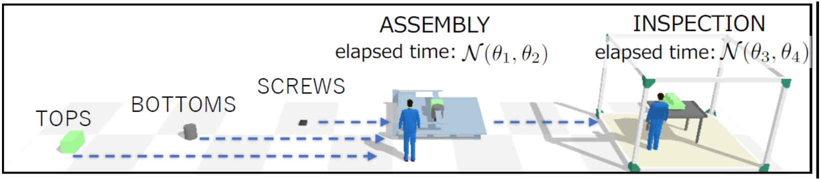
- There are 4 parameters $\theta = (\theta_1, \theta_2, \theta_3, \theta_4)^\top \in \mathbb{R}^n$ to be specified.

- θ_1 is the mean time spent in ASSEMBLY, and θ_3 in INSPECTION.



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- The data generating process $y(x) = R(x) + \varepsilon$ is defined as

$$R(x) = \begin{cases} r(x, (2, 0.5, 5, 1)^\top) & \text{if } x < 110 \\ r(x, (3.5, 0.5, 7, 1)^\top) & \text{if } x \geq 110. \end{cases}$$

- When $x > 110$, the production efficiency decreases because of overload of the workers.

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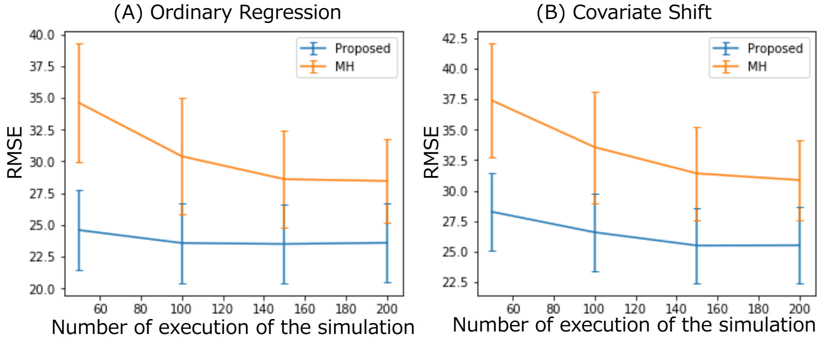
- Prior $\pi(\theta)$ is uniform over $\Theta := [0, 5] \times [0, 2] \times [0, 10] \times [0, 2] \subset \mathbb{R}^4$.

Manufacturing Process Simulator: Results

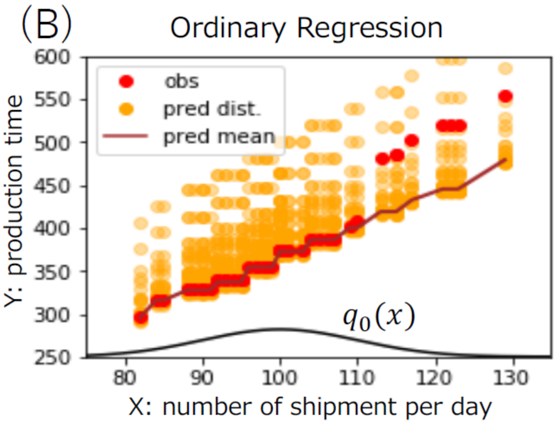
- The size of training data $(X_i, Y_i)_{i=1}^n$ is $n = 50$.
- (A) Ordinary regression ($q_1 = q_0$); (B) Covariate shift ($q_1 \neq q_0$).
- Horizontal axis: the number of simulations m.



Manufacturing Process Simulator: Results

- Results of our method *without* covariate shift adaptation ($q_1 = q_0$).

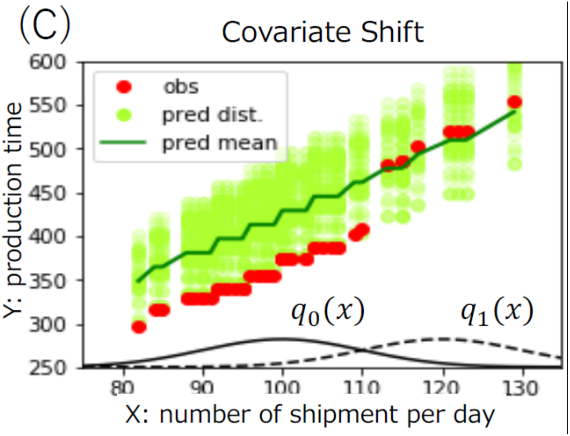
- Training data (red points), generated predictive outputs (orange) and their means (brown curve).



Manufacturing Process Simulator: Results

- Results of our method **with** covariate shift adaptation ($q_1 \neq q_0$).

- Training data (red points), generated predictive outputs (light green) and their means (green curve).

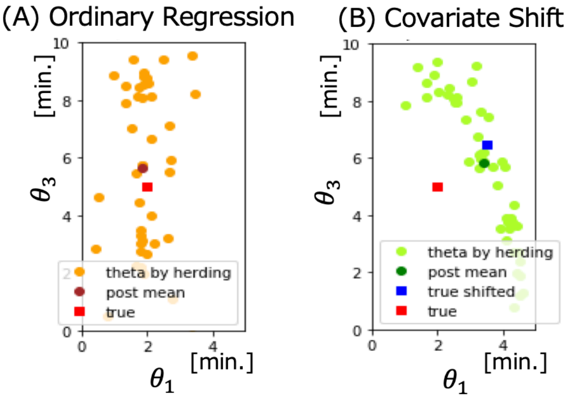


Manufacturing Process Simulator: Sensitivity Analysis

- Parameters generated from the posterior with the proposed method.

- (A) Ordinary regression ($q_1 = q_0$); (B) Covariate shift ($q_1 \neq q_0$).

- θ_1 (mean time for ASSEMBLY) is more sensitive than θ_3 (mean time for INSPECTION) for the outputs (total processing time).



Outline

Goal of the Theoretical Analysis

- We show that the estimate $\hat{\mu}_{\Theta|r^*}$ obtained from Kernel ABC and the importance-weighted kernel is an estimator of

$$\mu_{\Theta|r^*} := \int k_\Theta(\cdot, \theta) dP_\pi(\theta|r^*) \in \mathcal{H}_\Theta,$$

where $P_\pi(\theta|r^*)$ is the "target" posterior under prior $\pi(\theta)$.

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where Θ^* is the set of "optimal parameters" such that for all $\theta^* \in \Theta^*$:

$$\sum_{i=1}^n \beta(X_i)(Y_i - r(X_i, \theta^*))^2 = \min_{\theta \in \mathrm{supp}(\pi)} \sum_{i=1}^n \beta(X_i)(Y_i - r(X_i, \theta))^2.$$

Preliminaries: Covariance Operators

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$$\begin{aligned} C_{\vartheta \boldsymbol{y}} f &:= \mathbb{E}[k_\Theta(\cdot, \vartheta) f(\boldsymbol{y})] \in \mathcal{H}_\Theta \quad (f \in \mathcal{H}_{\mathbb{R}^n}). \\ C_{\boldsymbol{y}\boldsymbol{y}} f &:= \mathbb{E}[k_{\mathbb{R}^n}(\cdot, \boldsymbol{y}) f(\boldsymbol{y})] \in \mathcal{H}_{\mathbb{R}^n} \quad (f \in \mathcal{H}_{\mathbb{R}^n}). \end{aligned}$$

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- $C_{\vartheta \boldsymbol{y}}$ encodes the joint distribution of $(\vartheta, \boldsymbol{y})$.

- $C_{\boldsymbol{y}\boldsymbol{y}}$ encodes the marginal distribution of $\boldsymbol{y}$.

Preliminaries: Empirical Covariance Operators

- Parameter-data pairs generated in Kernel ABC

$$(\bar{\theta}_j, \bar{Y}_j^n)_{j=1}^m = (\bar{\theta}_j, r^n(\bar{\theta}_j))_{j=1}^m \subset \Theta \times \mathbb{R}^n$$

are i.i.d. copies of $(\vartheta, \boldsymbol{y})$.

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- Thus empirical covariance operators $\hat{C}_{\vartheta \boldsymbol{y}} : \mathcal{H}_{\mathbb{R}^n} \to \mathcal{H}_\Theta$ and $\hat{C}_{\boldsymbol{yy}} : \mathcal{H}_{\mathbb{R}^n} \to \mathcal{H}_{\mathbb{R}^n}$ are defined as

$$\hat{C}_{\vartheta \boldsymbol{y}} f := \frac{1}{m} \sum_{j=1}^m k_\Theta(\cdot, \bar{\theta}_j) f(\bar{Y}_j^n) \quad (f \in \mathcal{H}_{\mathbb{R}^n}).$$

$$\hat{C}_{\boldsymbol{yy}} f := \frac{1}{m} \sum_{j=1}^m k_{\mathbb{R}^n}(\cdot, \bar{Y}_j^n) f(\bar{Y}_j^n) \quad (f \in \mathcal{H}_{\mathbb{R}^n}).$$

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- $\hat{C}_{\vartheta \boldsymbol{y}}$ is an empirical approximation of $C_{\vartheta \boldsymbol{y}}$.

- $\hat{C}_{\boldsymbol{yy}}$ is an empirical approximation of $C_{\boldsymbol{yy}}$.

Kernel ABC via Empirical Covariance Operators

- Using the empirical covariance operators, the estimator $\hat{\mu}_{\Theta|r^*}$ can be written as

$$\hat{\mu}_{\Theta|r^*} = \hat{C}_{\vartheta \boldsymbol{y}}(\hat{C}_{\boldsymbol{yy}} + \varepsilon I)^{-1} k_{\mathbb{R}^n}(\cdot, Y^n).$$

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- This is how the estimator was originally proposed [Song et al., 2009, Nakagome et al., 2013].

- The estimator is known as conditional mean embedding, and has been studied extensively [Grünewälder et al., 2012, Fukumizu, 2015, Singh et al., 2019].

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- This is because observed data $Y^n = (Y_1, \ldots, Y_n)^\top$ may not lie in the support of the distribution of $\boldsymbol{y} = r^n(\vartheta)$:

$$Y^n \notin \{(r(X_1, \theta), \ldots, r(X_n, \theta)^\top \mid \theta \in \mathrm{supp}(\pi)\},$$

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- Existing theoretical results on conditional mean embeddings do not cover this situation.

- We provide a novel theoretical analysis of conditional mean embedding in this regard.

Subspace Spanned by the Simulator

- Consider a subset in $\mathbb{R}^n$ given by the simulator $r(x, \theta)$ and prior $\pi(\theta)$:

$$\begin{aligned}\mathrm{supp}(r^n\pi) &= \{r^n(\theta) \mid \theta \in \mathrm{supp}(\pi)\} \\ &= \{(r(X_1, \theta), \ldots, r(X_n, \theta)) \mid \theta \in \mathrm{supp}(\pi)\} \subset \mathbb{R}^n,\end{aligned}$$

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- Then define a Hilbert subspace of the RKHS $\mathcal{H}_{\mathbb{R}^n}$ by

$$\mathcal{H}_{\boldsymbol{y}} := \overline{\mathrm{span} \left\{ k_{\mathbb{R}^n}(\cdot, \tilde{Y}^n) \mid \tilde{Y}^n \in \mathrm{supp}(r^n \pi) \right\}} \subset \mathcal{H}_{\mathbb{R}^n},$$

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- We will call this the "subspace spanned by the simulator $r(x, \theta)$ (and the prior $\pi(\theta)$)."

Orthogonal Projection onto the Subspace

- For the observed data Y^n, consider the orthogonal projection of the feature vector $k_{\mathbb{R}^n}(\cdot, Y^n) \in \mathcal{H}_{\mathbb{R}^n}$ onto $\mathcal{H}_{\boldsymbol{y}}$:

$$h^* := \arg\min_{h \in \mathcal{H}_{\boldsymbol{y}}} \|h - k_{\mathbb{R}^n}(\cdot, Y^n)\|_{\mathcal{H}_{\mathbb{R}^n}}.$$

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- Then $k_{\mathbb{R}^n}(\cdot, Y^n)$ can be written as

$$k_{\mathbb{R}^n}(\cdot, Y^n) = h^* + h_\perp,$$

where $h_\perp \in \mathcal{H}_{\mathbb{R}^n}$ is orthogonal to $\mathcal{H}_{\boldsymbol{y}}$.

Population Conditional Mean Embedding via Projection

- Note that the Kernel ABC estimator

$$\hat{\mu}_{\Theta|r^*} = \hat{C}_{\vartheta \boldsymbol{y}}(\hat{C}_{\boldsymbol{yy}} + \varepsilon I)^{-1} k_{\mathbb{R}^n}(\cdot, Y^n).$$

is an approximation of the corresponding population expression

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Lemma (Population Expression via Projection)

- *Assume k_Θ is bounded and continuous, and $0 < \beta(X_i) < \infty$ for $i = 1, \ldots, n$.*

- *Let h^* be the orthogonal projection of $k_{\mathbb{R}^n}(\cdot, Y^n)$ onto the subspace $\mathcal{H}_{\boldsymbol{y}}$ spanned by the simulator $r(x, \theta)$.*

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- Then we have

$$C_{\vartheta \boldsymbol{y}}(C_{\boldsymbol{y}\boldsymbol{y}} + \varepsilon I)^{-1} k_{\mathbb{R}^n}(\cdot, Y^n) = C_{\vartheta \boldsymbol{y}}(C_{\boldsymbol{y}\boldsymbol{y}} + \varepsilon I)^{-1} h^*.$$

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- We assume there exists

$$\tilde{Y}^n \in \mathrm{supp}(r^n \pi) = \left\{ (r(X_1, \theta), \ldots, r(X_n, \theta))^\top \mid \theta \in \mathrm{supp}(\pi) \right\}$$

such that

$$k_{\mathbb{R}^n}(\cdot, \tilde{Y}^n) = h^*.$$

Conditional Mean Embedding under Misspecification

- Recall that $r^* \in \mathbb{R}^n$ are "optimal predictions" defined by

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Theorem (Population Expression via Optimal Predictions)

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- *Then we have*

$$C_{\vartheta \boldsymbol{y}}(C_{\boldsymbol{yy}} + \varepsilon I)^{-1} k_{\mathbb{R}^n}(\cdot, Y^n) = C_{\vartheta \boldsymbol{y}}(C_{\boldsymbol{yy}} + \varepsilon I)^{-1} k_{\mathbb{R}^n}(\cdot, r^*).$$

Convergence Result

- As $m \to \infty$ (num. of simulations), the Kernel ABC estimator

$$\hat{\mu}_{\Theta|r^*} = \hat{C}_{\vartheta \boldsymbol{y}}(\hat{C}_{\boldsymbol{yy}} + \varepsilon I)^{-1} k_{\mathbb{R}^n}(\cdot, Y^n)$$

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On the other hand, as $\varepsilon \to 0$, this expression converges to

$$\mu_{\Theta|r^*} := \int k_{\Theta}(\cdot, \theta) dP_{\pi}(\theta | r^*),$$

where $P_{\pi}(\theta|r^*)$ is the "target" posterior under prior $\pi(\theta)$.

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- *For any fixed* $C > 0$, *set the regularization constant of of* $\hat{\mu}_{\Theta|r^*}$ *as* $\varepsilon := \varepsilon_m := Cm^{-\frac{b}{1+4b}}$.
- *Then, under an additional technical condition, we have*

$$\left\|\hat{\mu}_{\Theta|r^*} - \mu_{\Theta|r^*}\right\|_{\mathcal{H}_\Theta} = O_p\left(m^{-\frac{b}{1+4b}}\right) \ (m \to \infty).$$

Outline

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- Future work includes a formal analysis of the identifiability assumption.

Collaborators

- Keiichi Kisamori (NEC/AIST, Japan)
- Keisuke Yamazaki (AIST, Japan)

Bach, F., Lacoste-Julien, S., and Obozinski, G. (2012).
On the equivalence between herding and conditional gradient algorithms.
In *Proceedings of the 29th International Conference on Machine Learning (ICML2012)*, pages 1359–1366.

Chang, J. T. and Pollard, D. (1997).
Conditioning as disintegration.
Statistica Neerlandica, 51:287–317.

Chen, Y., Welling, M., and Smola, A. (2010).
Supersamples from kernel-herding.
In *Proceedings of the 26th Conference on Uncertainty in Artificial Intelligence (UAI 2010)*, pages 109–116.

Dick, J., Kuo, F. Y., and Sloan, I. H. (2013).
High dimensional numerical integration - the Quasi-Monte Carlo way.
Acta Numerica, 22(133-288).

Fukumizu, K. (2015).

Nonparametric Bayesian Inference with Kernel Mean Embedding.

In *Modern Methodology and Applications in Spatial-Temporal Modeling*, Springer Briefs in Statistics. Springer, Tokyo.

Fukumizu, K., Gretton, A., Sun, X., and Schölkopf, B. (2008).
Kernel measures of conditional dependence.
In *Advances in Neural Information Processing Systems 20*, pages 489–496.

Grünewälder, S., Lever, G., Baldassarre, L., Patterson, S., Gretton, A., and Pontil, M. (2012).
Conditional mean embeddings as regressors.
In *Proceedings of the 29th International Conference on Machine Learning (ICML2012)*, pages 1823–1830.

Muandet, K., Fukumizu, K., Sriperumbudur, B. K., and Schölkopf, B. (2017).
Kernel mean embedding of distributions : A review and beyond.
Foundations and Trends in Machine Learning, 10(1–2):1–141.

Nakagome, S., Fukumizu, K., and Mano, S. (2013).
Kernel approximate Bayesian computation in population genetic inferences.
Statistical Applications in Genetics and Molecular Biology, 12(6):667–678.

Shimodaira, H. (2000).
Improving predictive inference under covariate shift by weighting the log-likelihood function.
Journal of Statistical Planning and Inference, 90(2):227–244.

Singh, R., Sahani, M., and Gretton, A. (2019).
Kernel instrumental variable regression.
In *NeurIPS*.

Smola, A., Gretton, A., Song, L., and Schölkopf, B. (2007).
A Hilbert space embedding for distributions.
In *Proceedings of the International Conference on Algorithmic Learning Theory*, volume 4754, pages 13–31. Springer.

Song, L., Huang, J., Smola, A., and Fukumizu, K. (2009).

Hilbert space embeddings of conditional distributions with applications to dynamical systems.
In *Proceedings of the 26th International Conference on Machine Learning (ICML2009)*, pages 961–968.

Sriperumbudur, B. K., Gretton, A., Fukumizu, K., Schölkopf, B., and Lanckriet, G. R. (2010).
Hilbert space embeddings and metrics on probability measures.
Jounal of Machine Learning Research, 11:1517–1561.