Kernel Recursive ABC: Point Estimation with Intractable Likelihood

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Contents of This Talk

1. **Kernel Recursive ABC: Point Estimation with Intractable Likelihood** (ICML 2018)
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Outline

Machine Learning for Computer Simulation

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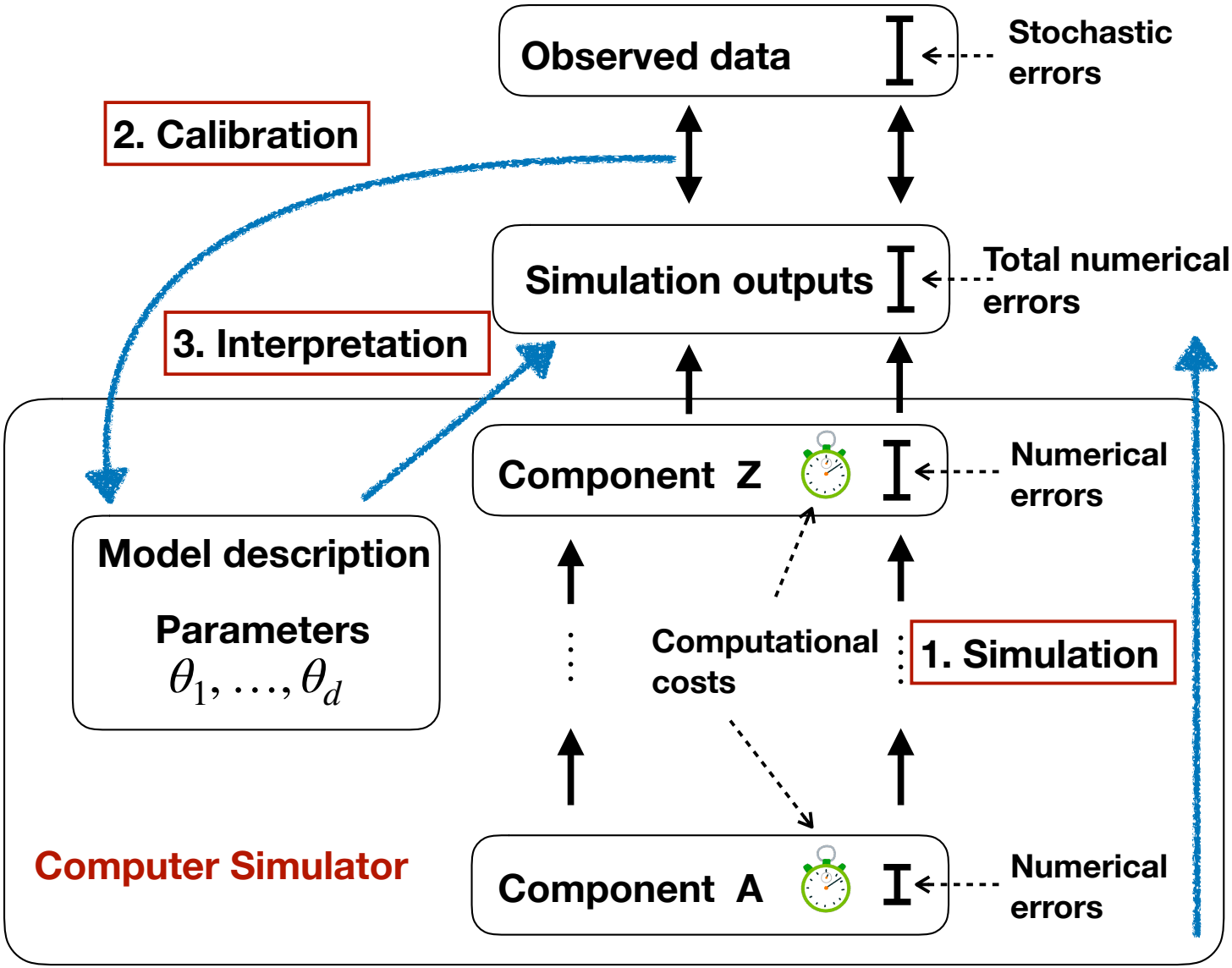
The power of computer simulation is extrapolation, which enables

- predictions of quantities/phenomena in the future.
- gaining understanding of the phenomena of interest.

Machine Learning for Computer Simulation



Example: Tsunami Simulation [Saito, 2019, p.211]

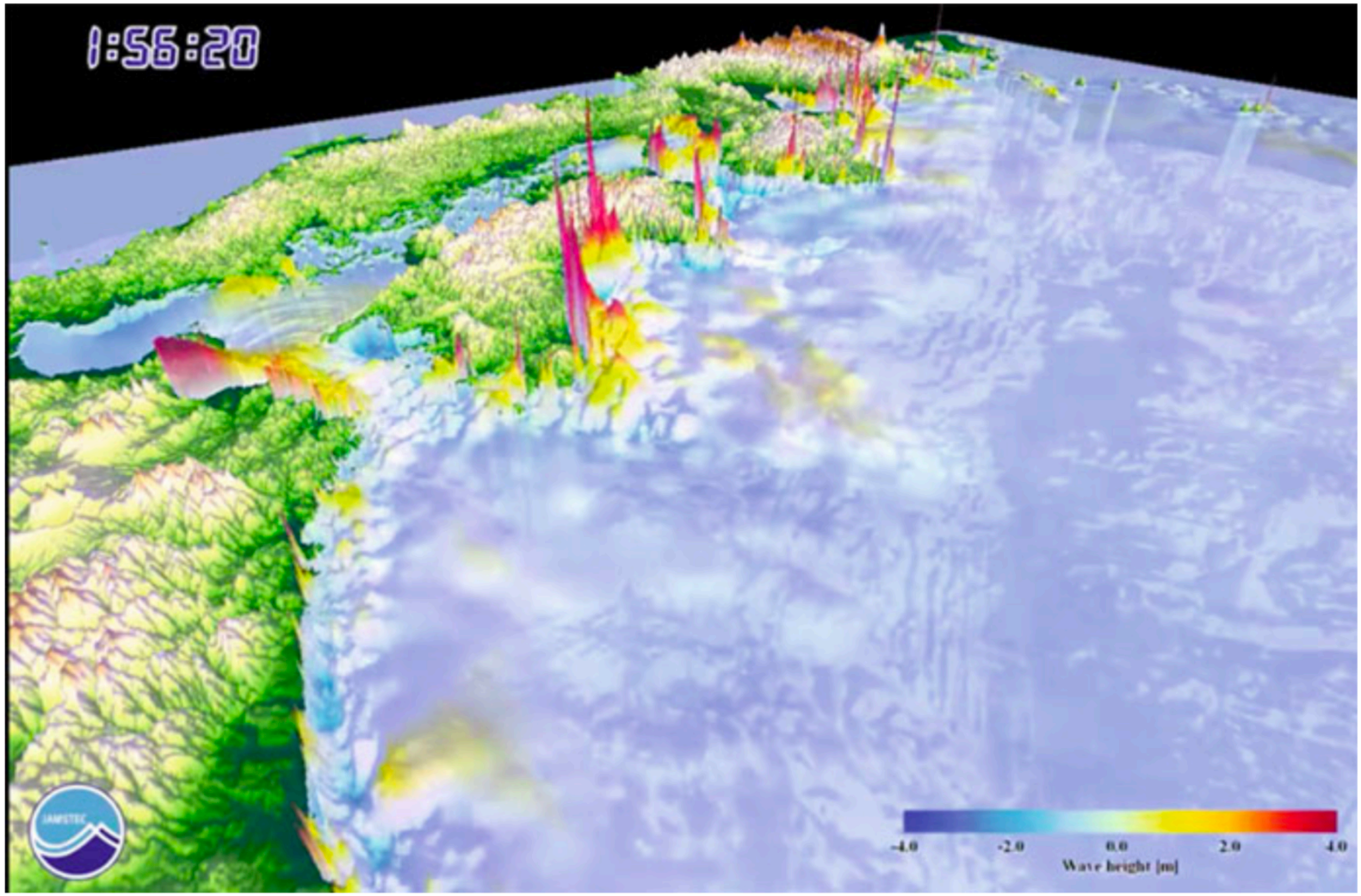


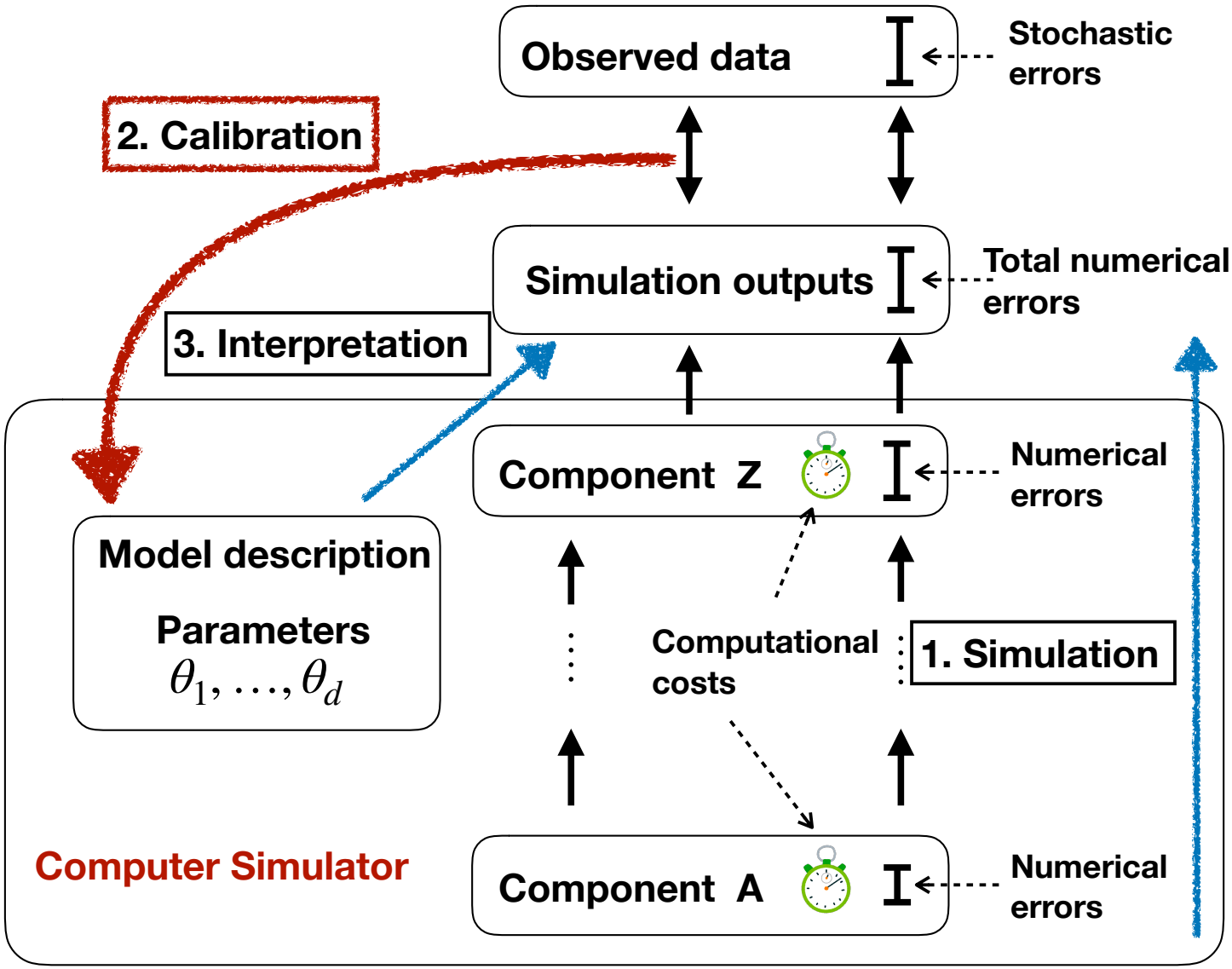
Fig. 6.5 An example of a tsunami simulation (JAGURS code) in the Nankai subduction zone, southwestern Japan. (Courtesy of T. Baba)

Example: Pedestrian Flow Simulation [Yamashita et al., 2010]

Multi-agent systems for pedestrians walking in Ginza.

Figure 1: Points representing individual pedestrians. (red = slow)

Calibration: Parameter Estimation and Model Selection



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In the language of statistics, computer simulation can be defined as sampling from a probabilistic model $p(\boldsymbol{y}|\theta)$.

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Approaches to likelihood-free inference include

- Approximate Bayesian Computation (ABC) [Sisson et al., 2018].
- Bayesian optimization [Gutmann and Corander, 2016].

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– For $j = 1, \ldots, n$, set

$$J \leftarrow J \cup \{j\} \quad \text{if} \quad \mathrm{dist}(\boldsymbol{y}_i, \boldsymbol{y}^*) \leq \varepsilon,$$

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– Monte Carlo approximation of the posterior:

$$p(\theta|\boldsymbol{y}^*) \approx \hat{p}_\varepsilon(\theta|\boldsymbol{y}^*) := \frac{1}{|J|} \sum_{j \in J} \underbrace{\delta_{\theta_j}}_{\text{Dirac at } \theta_j}$$

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- when one simulation is computationally very expensive, and
- when your purpose is on predictions based on simulations.

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Kernels and Reproducing Kernel Hilbert Spaces (RKHS)

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The function $k(x, x')$ is called a **positive definite kernel**, if

$$\sum_{i=1}^{n} \sum_{j=1}^{n} c_i c_j k(x_i, x_j) \geq 0 \quad \text{holds}$$

for all $\quad n \in \mathbb{N}, \quad c_1, \ldots, c_n \in \mathbb{R}, \quad x_1, \ldots, x_n \in \mathcal{X}.$

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

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\text{Gaussian} \quad & k(x, x') &&= \exp(-\|x - x'\|^2/\gamma^2). \\
\text{Laplace (Matérn)} \quad & k(x, x') &&= \exp(-\|x - x'\|/\gamma). \\
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In this talk, I will simply call k a kernel.

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– $\mathcal{H}$ can be written as

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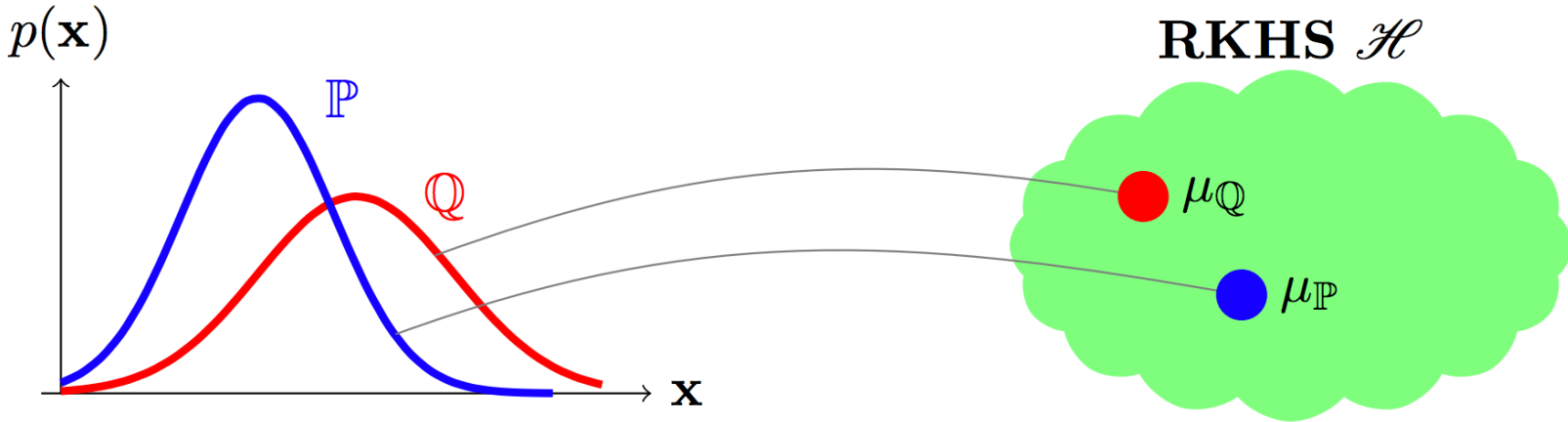
– In other words, k is characteristic if

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

Kernel Mean Embeddings [Smola et al., 2007]

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



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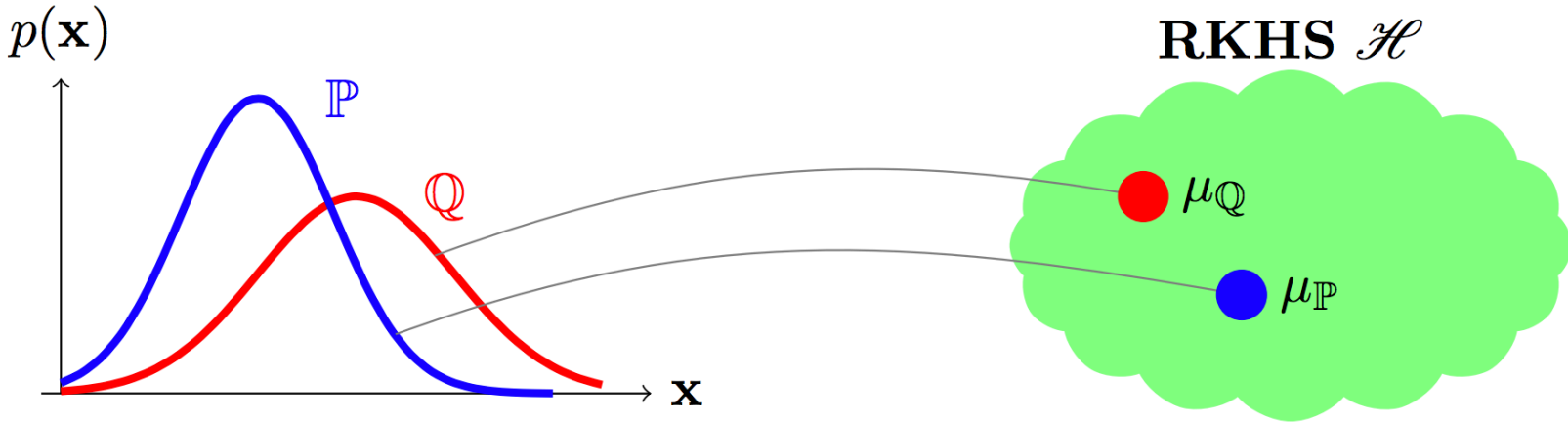

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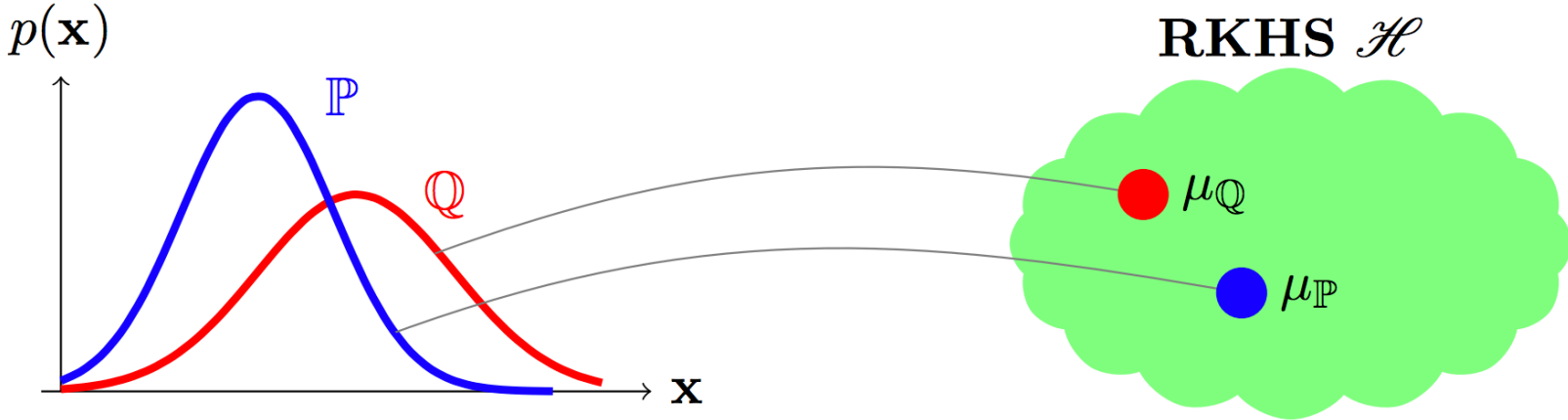

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Examples of **non**-characteristic kernels on $\mathcal{X} = \mathbb{R}^d$:
– Linear and polynomial kernels.

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Recursive Bayes Updates and Power Posteriors

Given observed data $\boldsymbol{y}^*$, **Bayes' rule** yields a posterior distribution:

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\end{aligned}$$

Recursive Bayes Updates and Power Posteriors

Given observed data $\boldsymbol{y}^*$, **Bayes' rule** yields a posterior distribution:

$$\underbrace{p(\theta|\boldsymbol{y}^*)}_{\text{Posterior}} \propto \underbrace{p(\boldsymbol{y}^*|\theta)}_{\text{Likelihood}} \underbrace{\pi(\theta)}_{\text{Prior}}.$$

Recursive Bayes updates: Apply **Bayes' rule recursively** to the **same observed data $\boldsymbol{y}^*$**.

$$\begin{aligned}
\textbf{1st recursion} \quad \pi_1(\theta) := p_1(\theta|\boldsymbol{y}^*) &\propto p(\boldsymbol{y}^*|\theta)\pi(\theta). \\
\textbf{2nd recursion} \quad \pi_2(\theta) := p_2(\theta|\boldsymbol{y}^*) &\propto p(\boldsymbol{y}^*|\theta)\pi_1(\theta) \\
&= p(\boldsymbol{y}^*|\theta)^2\pi(\theta). \\
\textbf{3rd recursion} \quad \pi_3(\theta) := p_3(\theta|\boldsymbol{y}^*) &\propto p(\boldsymbol{y}^*|\theta)\pi_2(\theta) \\
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This implies that recursive Bayes updates provide a way of Maximum Likelihood Estimation.

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$$\mu_{P_N} := \int \underbrace{k_\Theta(\cdot, \theta)}_{\text{Kernel on } \Theta} p_N(\theta|\boldsymbol{y}^*) d\theta \tag{1}$$

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Kernel ABC [Nakagome et al., 2013]

– Define

- a kernel $k_{\mathcal{Y}}(\boldsymbol{y}, \boldsymbol{y}')$ on the data space $\mathcal{Y}$,
- a kernel $k_{\Theta}(\theta, \theta')$ on the parameter space Θ, and
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$$\begin{aligned} \boldsymbol{k}_Y(\boldsymbol{y}^*) &:= (k_{\mathcal{Y}}(\boldsymbol{y}^*, \boldsymbol{y}_1), \ldots, k_{\mathcal{Y}}(\boldsymbol{y}^*, \boldsymbol{y}_n))^\top \in \mathbb{R}^n. \\ (w_1(\boldsymbol{y}^*), \ldots, w_n(\boldsymbol{y}^*))^\top &:= (G_Y + n\lambda I_n)^{-1} \boldsymbol{k}_Y(\boldsymbol{y}^*) \in \mathbb{R}^n, \end{aligned}$$

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Output: An estimate of the posterior kernel mean:

$$\begin{aligned} \int k_{\Theta}(\cdot, \theta) p(\theta|\boldsymbol{y}^*) d\theta &\approx \sum_{i=1}^{n} w_i(\boldsymbol{y}^*) k_{\Theta}(\cdot, \theta_i), \\ p(\theta|\boldsymbol{y}^*) &\propto p(\boldsymbol{y}^*|\theta)\pi(\theta). \end{aligned}$$

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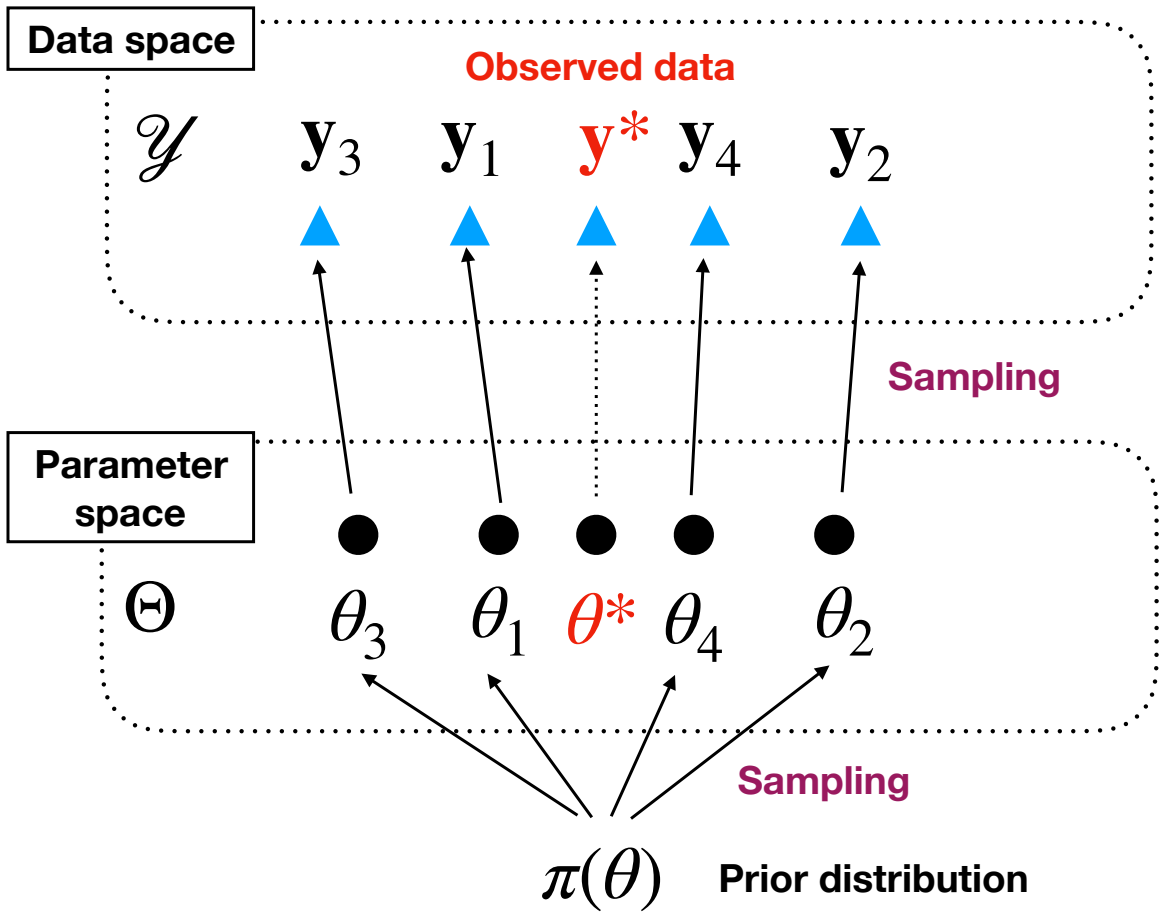

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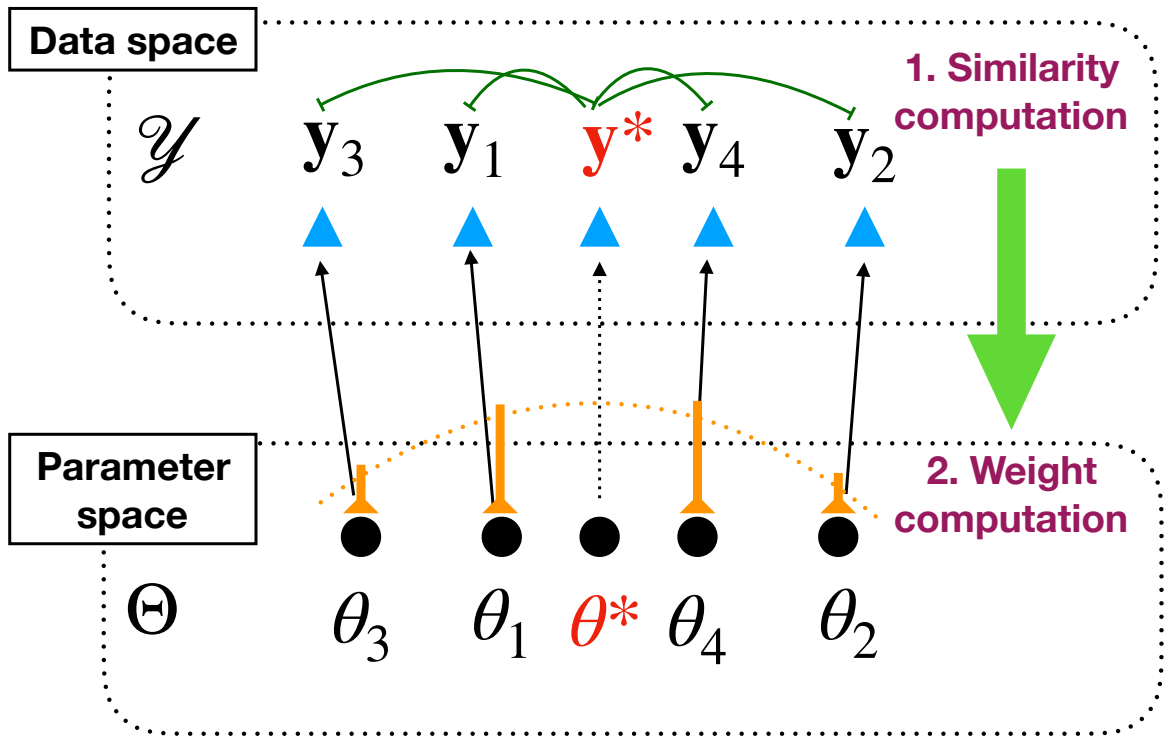

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Kernel Herding [Chen et al., 2010]

Let

– P be a known probability distribution on Θ; and

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– is equivalent to greedily approximating the kernel mean μ_P:

$$\theta'_T = \arg\min_{\theta \in \Theta} \left\| \mu_P - \frac{1}{T} \left(k_\Theta(\cdot, \theta) + \sum_{i=1}^{T-1} k_\Theta(\cdot, \theta'_i) \right) \right\|_{\mathcal{H}_\Theta},$$

if k_Θ is shift-invariant. ($\mathcal{H}_\Theta$ is the RKHS of k_Θ.)

Kernel Herding [Chen et al., 2010]

Red squares: Sample points generated from kernel herding

Purple circles: Randomly generated i.i.d. sample points.

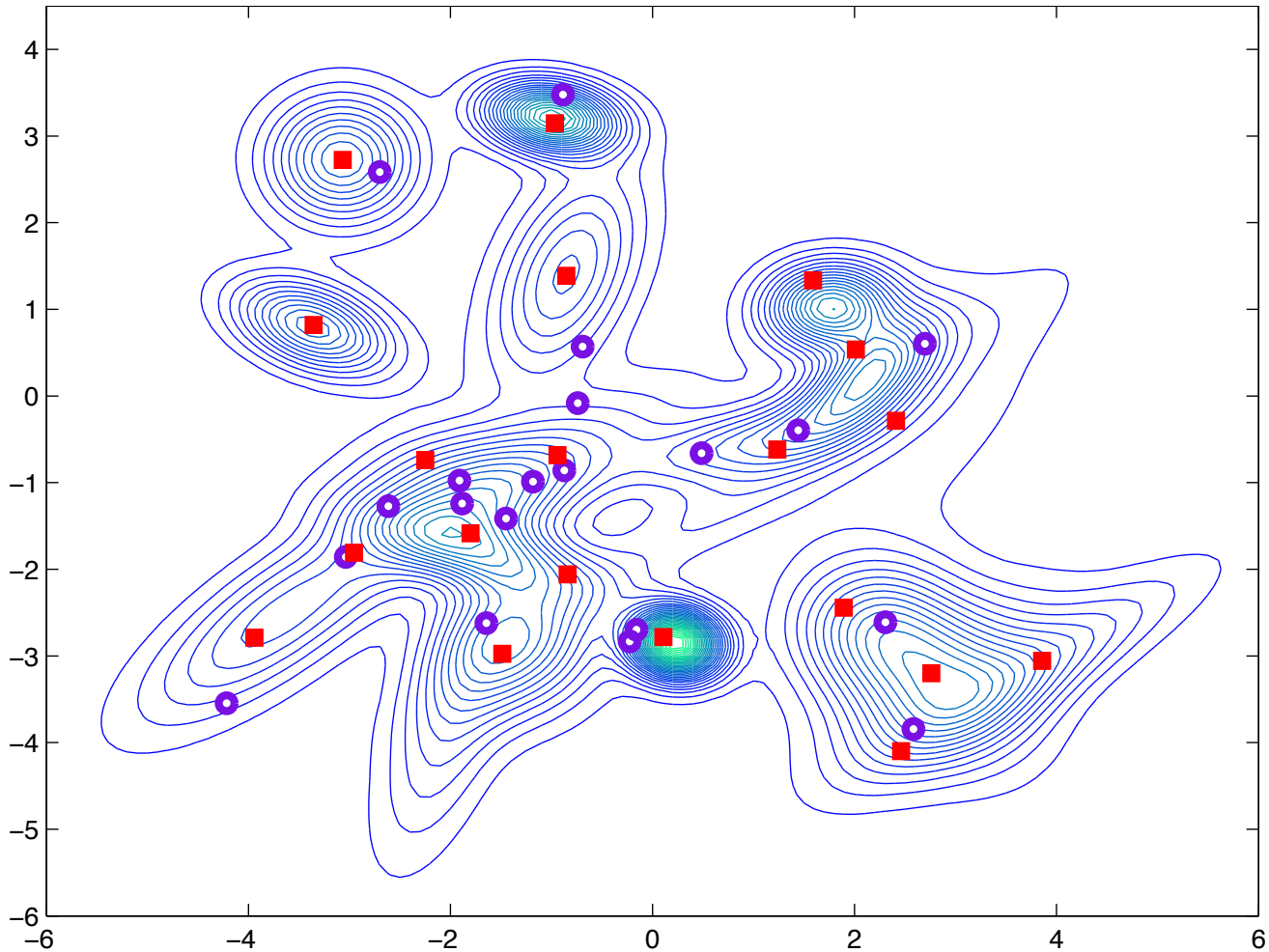

Figure 3: [Chen et al., 2010, Fig 1]

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Why Kernels?

– The combination of Kernel ABC and Kernel Herding leads to robustness against misspecfication of the prior $\pi(\theta)$.

Outline

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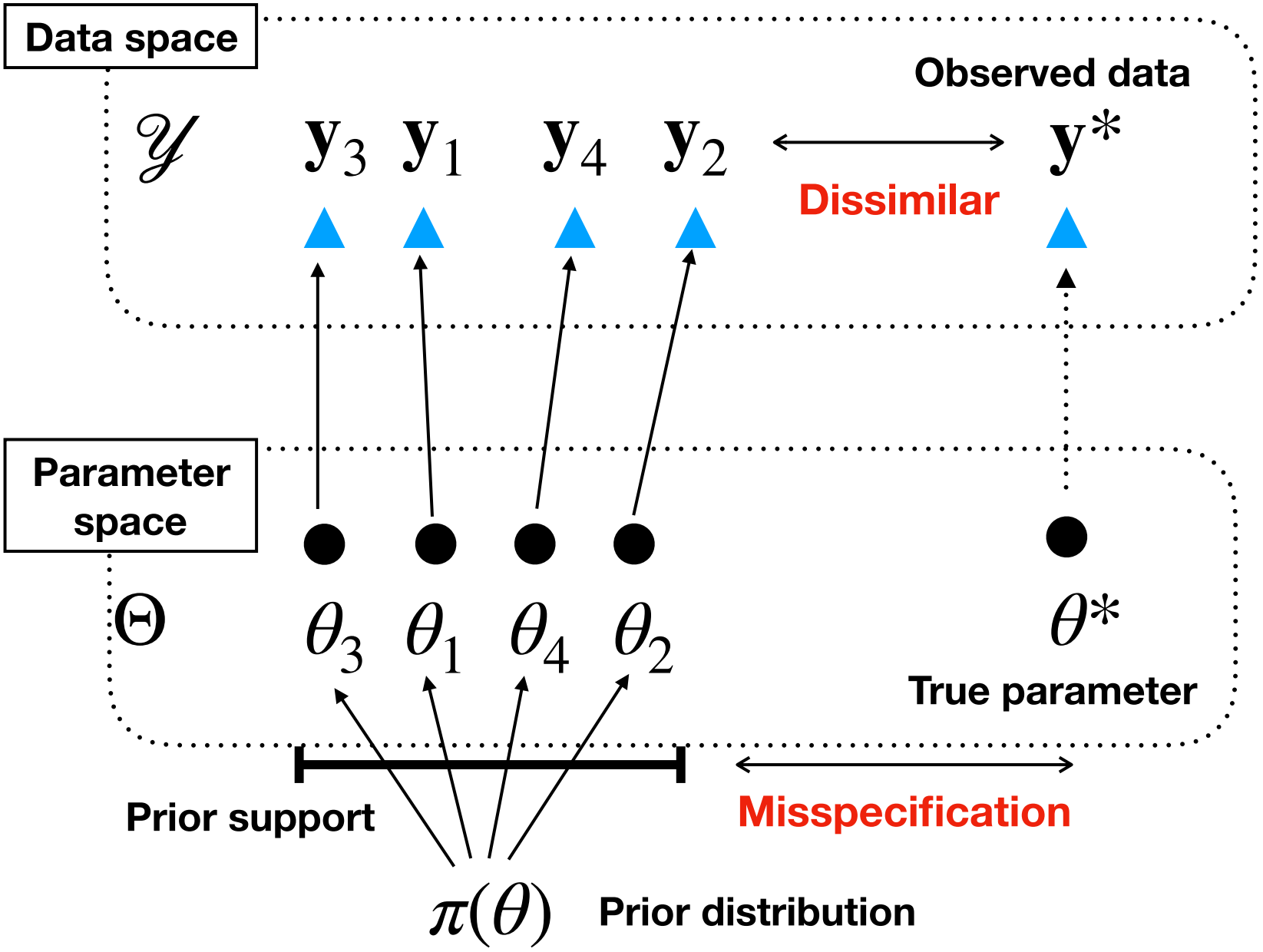
As a result, simulated data

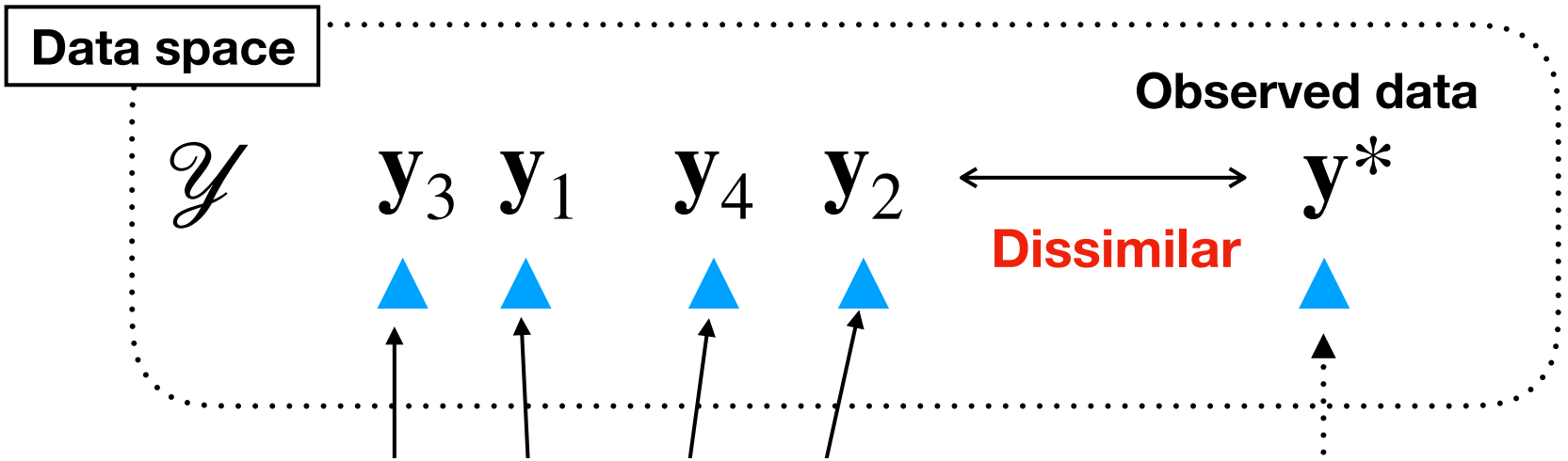
$$\boldsymbol{y}_i \sim p(\boldsymbol{y}|\theta_i), \quad \theta_i \sim \pi(\theta) \quad (i = 1, \ldots, n).$$

may become **far apart** from observed data $\boldsymbol{y}^*$.

Prior Misspecification



Auto-Correction Mechanism: The Kernel ABC Step



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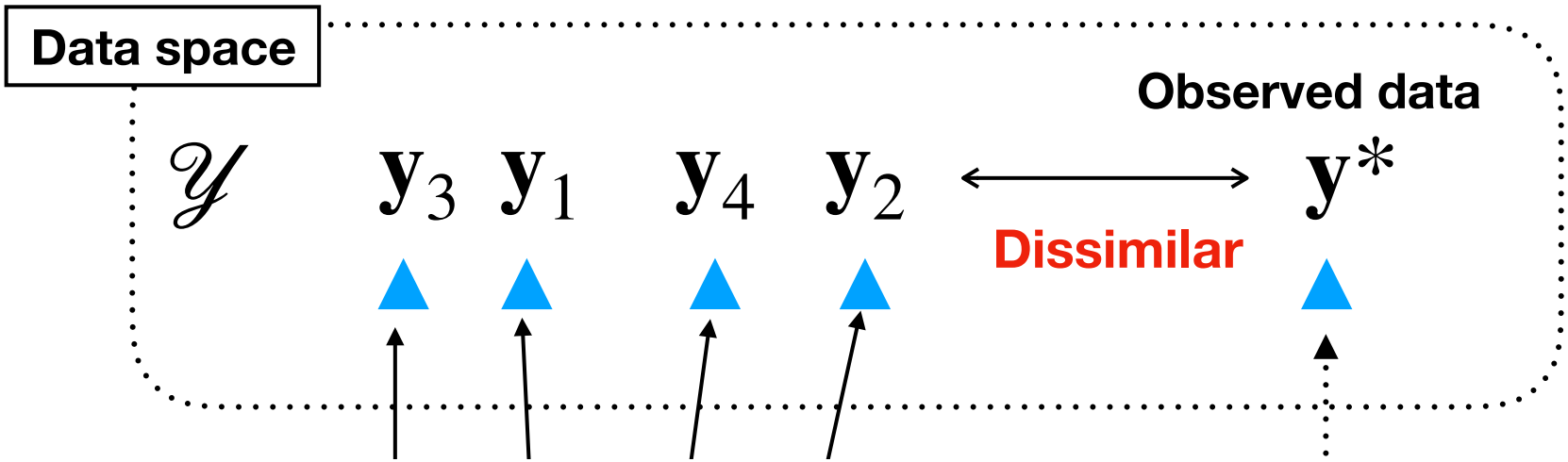

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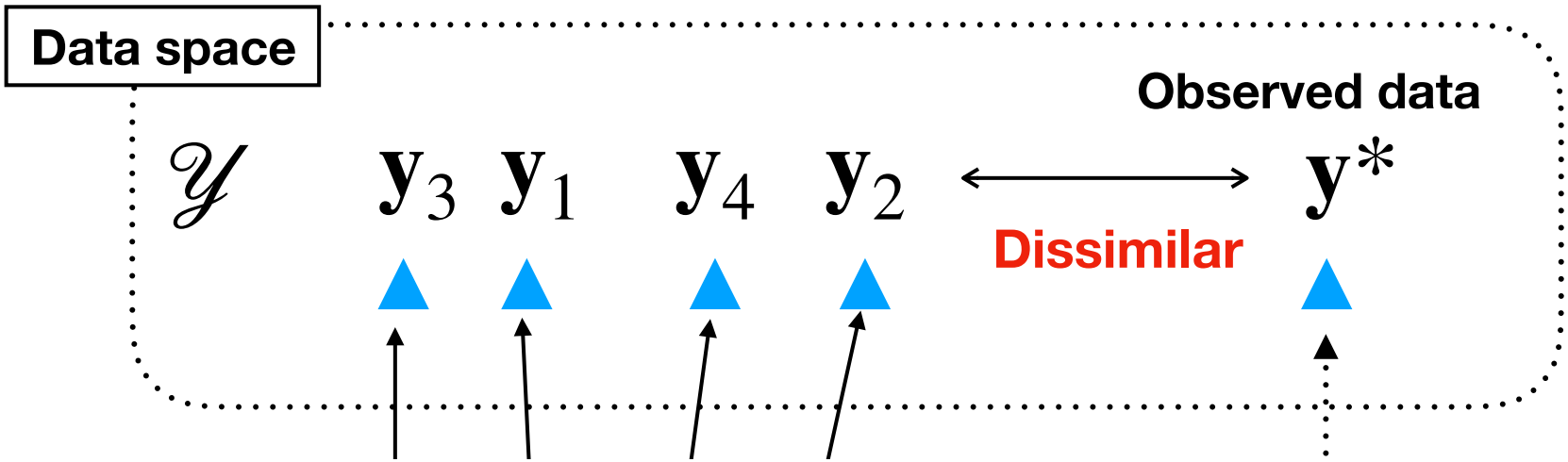

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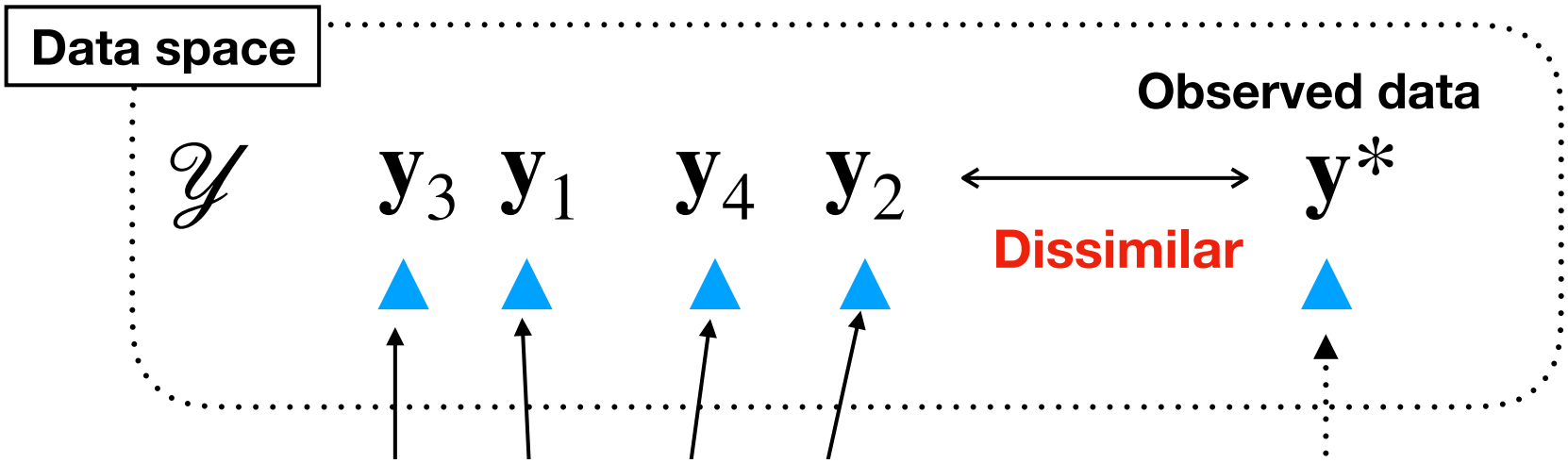

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Auto-Correction Mechanism: The Kernel Herding Step

Deterministically sample $\theta'_1, \ldots, \theta'_n$

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Therefore, θ'_T is chosen to be distant from $\theta'_1, \ldots, \theta'_{T-1}$.

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In each iteration, 300 $(\theta_i, \boldsymbol{y}_i)$-pairs are simulated.

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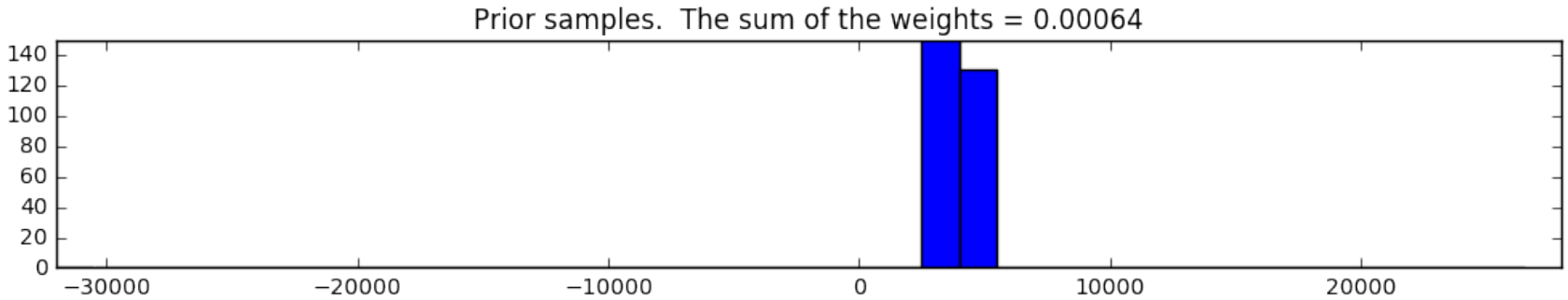
Initial sampling from the prior $\pi(\theta) = \text{uniform}[2000, 3000]$:
(Recall $\theta^* = 0$.)



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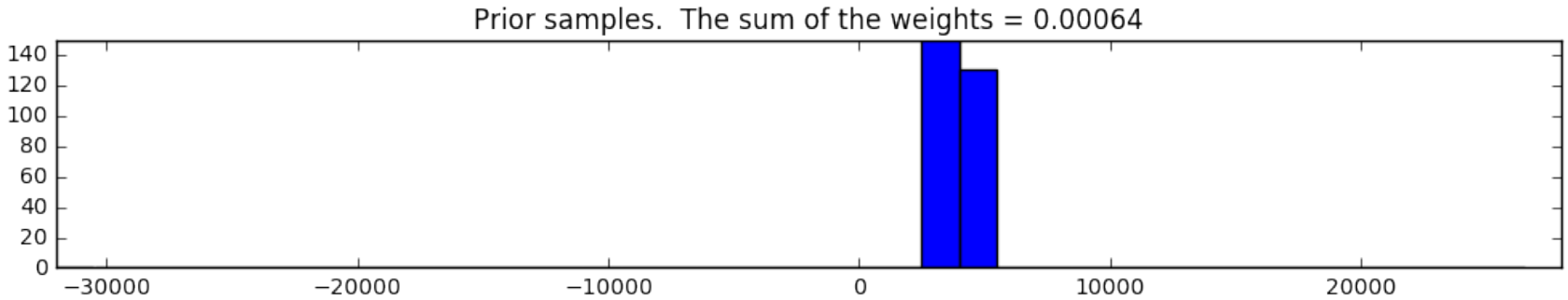
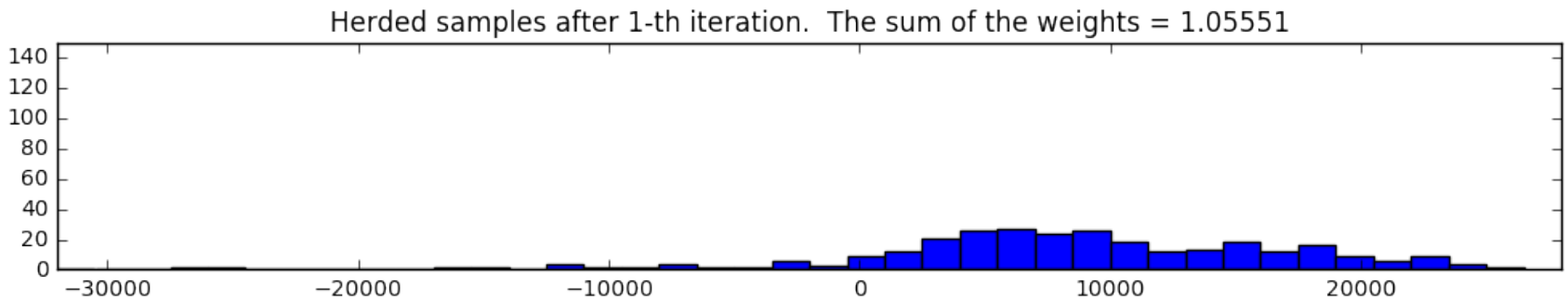
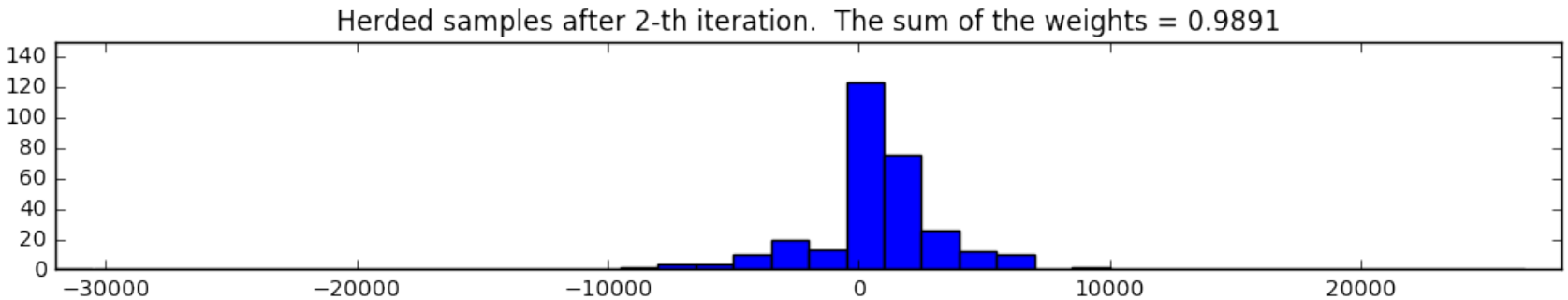


After **1 recursion** of Kernel ABC + Kernel Herding:



Auto-Correction Mechanism: A Nummerical Illustration

After **2 recursions** of Kernel ABC + Kernel Herding:



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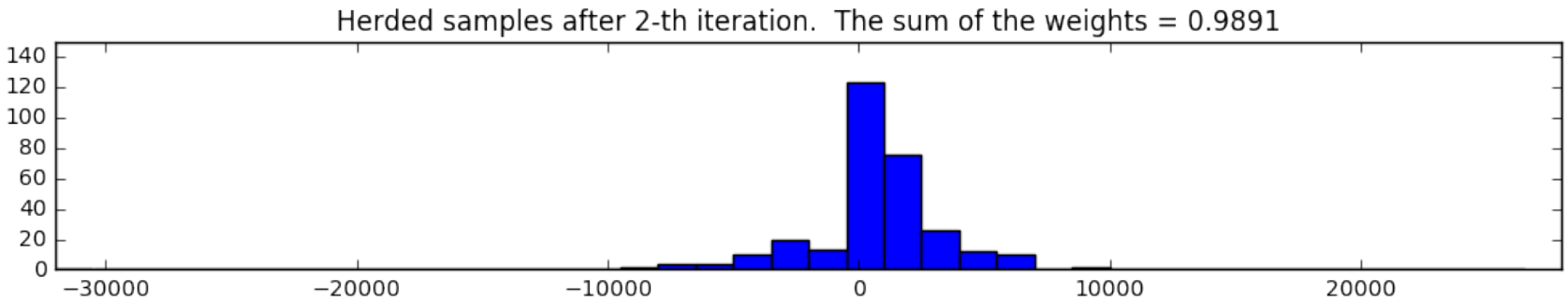

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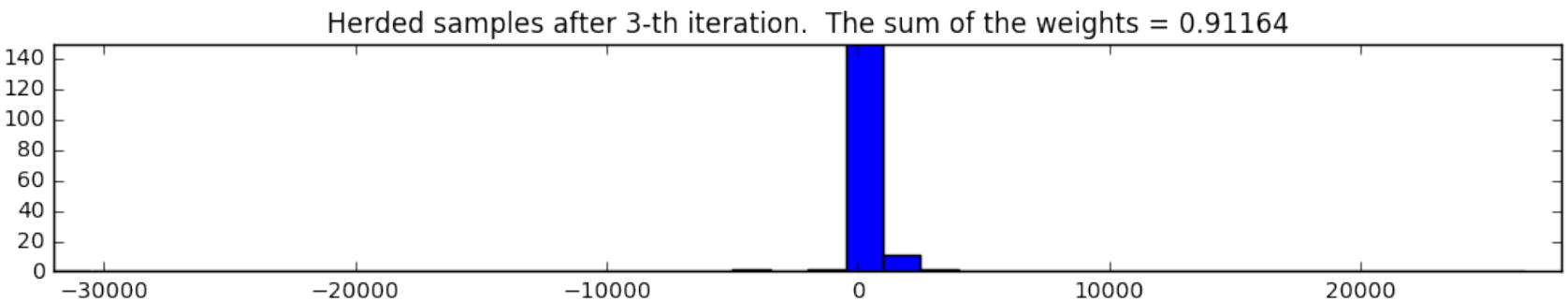

Outline

Summary

The proposed method outperformed competitors in most cases ...

Please look at the paper for details!!

Point Estimation with a Misspecified Prior Distribution

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Algorithm	parameter error	data error	cputime
KR-ABC	0.70(0.29)	0.008(0.004)	866.02(26.12)
KR-ABC (less samples)	7.22(3.28)	0.02(0.24)	353.498(23.05)
K2-ABC	>1e+6 (>1e+3)	>1e+5 (>1e+3)	209.51(11.49)
K-ABC	>1e+6 (>1e+3)	>1e+5 (>1e+3))	403.93(24.97)
SMC-ABC (mean)	>1e+6 (>1e+3)	>1e+5 (>1e+3)	590.41(29.54)
SMC-ABC (MAP)	>1e+6 (>1e+3)	>1e+5 (>1e+3)	590.41(29.54)
ABC-DC	>1e+6 (>1e+3)	>1e+5 (>1e+3)	313.99(16.85)
BO	>1e+5(>1e+4)	>1e+5 (>1e+4)	25940.86(936.40)
MSM	>1e+5(>1e+4)	>1e+5(>1e+4)	307.42(67.94)

Parameter Estimation of a Pedestrian Flow Simulator [Yamashita et al., 2010]

Estimate certain parameters characterising groups of pedestrians.

Figure 4: Points representing individual pedestrians. (red = slow)

Parameter Estimation of a Pedestrian Flow Simulator

Algorithm	$\theta^{(N)}$ error	$\theta^{(T)}$ error	data error	cputime
KR-ABC	61.58(74.42)	70.93(102.08)	0.008(0.009)	2233.45(97.54)
KR-ABC (less samples)	82.46(75.05)	134.00(161.85)	0.014(0.014)	1875.32(147.16)
K2-ABC	298.94(120.71)	308.95(109.43)	0.10(0.10)	1547.32(56.31)
K-ABC	354.72(145.76)	389.52(140.91)	0.12(0.09)	1773.74(84.91)
SMC-ABC (mean)	271.51(104.64)	363.12(91.28)	0.09(0.07)	2017.89(110.02)
SMC-ABC (MAP)	255.15(139.33)	348.43(104.74)	0.09(0.1)	2017.89(110.02)
ABC-DC	273.93(136.14)	327.48(98.12)	0.09(0.14)	1984.43(59.12)
BO	194.57(65.83)	291.73(105.33)	0.04(0.06)	37541.23(3047.46)
MSM	453.58(89.43)	510.04(55.10)	0.24(0.17)	1869.83(49.51)

Outline

Conclusions

We proposed the **Kernel Recursive ABC**, a method for point estimation of simulator-based statistical models that is **robust to misspecification of a prior distribution**.

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– Perform model selection by mixture modelling, using the Kernel Recursive ABC.

Future Work:
– Statistical convergence analysis.
– Scalability to large scale problems.

Collaborators

- Takafumi Kajihara (NEC/AIST/RIKEN)
- Keisuke Yamazaki (AIST)
- Kenji Fukumizu (ISM)
- Yuuki Nakaguchi (NEC)
- Kanishk Khandelwal (NEC)

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