# K2-ABC: Approximate Bayesian Computation with Kernel Embeddings

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# Approximate Bayesian Computation (ABC)

- Given: prior $p(\boldsymbol{\theta})$, intractable likelihood $p(\mathbf{Y}|\boldsymbol{\theta})$, observations $\mathbf{Y}$.
- Goal: Sample from $p(\boldsymbol{\theta}|\mathbf{Y}) \propto p(\boldsymbol{\theta})p(\mathbf{Y}|\boldsymbol{\theta})$.
- Problem: Cannot evaluate $p(\mathbf{Y}|\boldsymbol{\theta})$. But, can sample $\mathbf{X} \sim p(\cdot|\boldsymbol{\theta})$.

**Example**: a complicated dynamical system for blow fly population

$$N_{t+1} = PN_{t-\tau} \exp\left(-\frac{N_{t-\tau}}{N_0}\right) e_t + N_t \exp(-\delta\epsilon_t)$$

where $e_t \sim \text{Gamma}\left(\frac{1}{\sigma_P^2}, \sigma_P^2\right)$ and $\epsilon_t \sim \text{Gamma}\left(\frac{1}{\sigma_d^2}, \sigma_d^2\right)$.

- $\boldsymbol{\theta} := \{P, N_0, \sigma_d, \sigma_p, \tau, \delta\}$
- Given $\mathbf{Y} = \{N_1, \ldots, N_T\}$, want to sample from $p(\boldsymbol{\theta}|\mathbf{Y})$.

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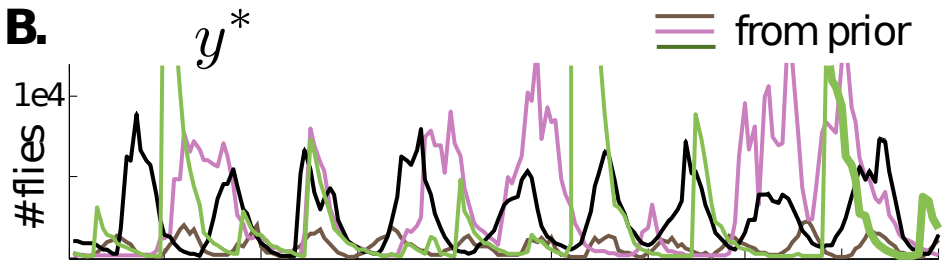

# ABC Likelihood $p_\epsilon(\mathbf{Y}|\boldsymbol{\theta})$

- Observe a dataset $\mathbf{Y}$,

$$p(\mathbf{Y}|\boldsymbol{\theta}) = \int p(\mathbf{X}|\boldsymbol{\theta})\delta(\mathbf{X}-\mathbf{Y})\,\mathrm{d}\mathbf{X}$$

$$\text{(ABC likelihood)} \approx \int p(\mathbf{X}|\boldsymbol{\theta})\kappa_\epsilon(\mathbf{X},\mathbf{Y})\,\mathrm{d}\mathbf{X} := p_\epsilon(\mathbf{Y}|\boldsymbol{\theta})$$

$$\approx \kappa_\epsilon(\mathbf{X}^{\boldsymbol{\theta}},\mathbf{Y}) \text{ where } \mathbf{X}^{\boldsymbol{\theta}} \sim p(\cdot|\boldsymbol{\theta}),$$

  where $\kappa_\epsilon(\mathbf{X},\mathbf{Y})$ defines similarity between $\mathbf{X}$ and $\mathbf{Y}$.
- ABC algorithms sample from $p_\epsilon(\boldsymbol{\theta}|\mathbf{Y}) \propto p(\boldsymbol{\theta})p_\epsilon(\mathbf{Y}|\boldsymbol{\theta})$
- Rejection ABC sets

$$\kappa_\epsilon(\mathbf{X},\mathbf{Y}) := \mathbf{1}[\|s(\mathbf{X})-s(\mathbf{Y})\|_2 < \epsilon],$$

  - $s$ : function to compute summary statistics
  - $\mathbf{1}[\cdot] \in \{0,1\}$: indicator function

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- Difficult to choose $s(\cdot)$.
  - More statistics give high sufficiency.
  - But, higher rejection rate.
- Insufficient will $s(\cdot)$ lead to an incorrect posterior.

Contribution:

- Use a kernel-based distance to define $\kappa_\epsilon$. No need to design $s(\cdot)$.

Rejection ABC:

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K2-ABC (proposed):

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# Maximum Mean Discrepancy (MMD) [Gretton et al., 2006]

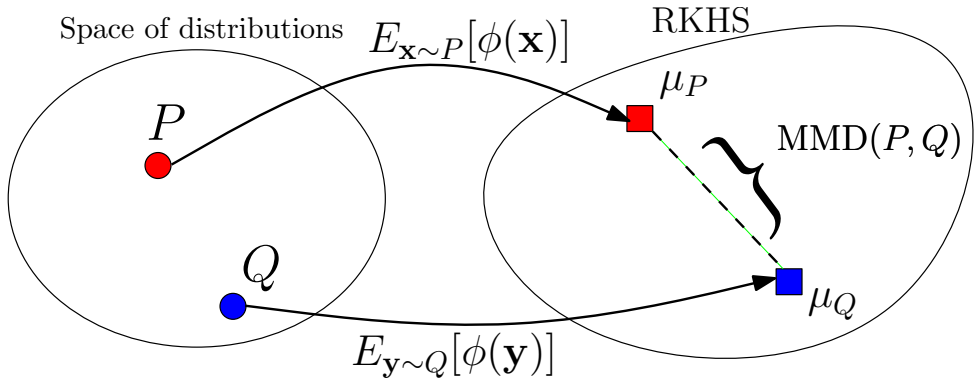
$$\widehat{\mathrm{MMD}}^2(\mathbf{X},\mathbf{Y}) = \Big\| \overbrace{\frac{1}{n}\sum_{i=1}^{n}\phi(\mathbf{x}_i)}^{\hat{\mu}_P} - \overbrace{\frac{1}{n}\sum_{j=1}^{n}\phi(\mathbf{y}_j)}^{\hat{\mu}_Q} \Big\|^2_{\mathrm{RKHS}}$$

$$\overset{\text{(unbiased)}}{\equiv} \frac{1}{n(n-1)}\sum_{i\neq j} k(\mathbf{x}_i,\mathbf{x}_j) + \frac{1}{n(n-1)}\sum_{i\neq j} k(\mathbf{y}_i,\mathbf{y}_j) - \frac{2}{n^2}\sum_{i,j=1}^{n} k(\mathbf{x}_i,\mathbf{y}_j)$$

- If kernel $k$ is characteristic (e.g., Gaussian kernel), MMD defines a distance i.e.,

$$\mathrm{MMD}(P,Q) = 0 \iff P = Q.$$

- $k(\mathbf{x},\mathbf{y}) = \langle \phi(\mathbf{x}), \phi(\mathbf{y}) \rangle_{\mathrm{RKHS}}$
- Intuitively, $\mu_P$ contains all moments of $P$.



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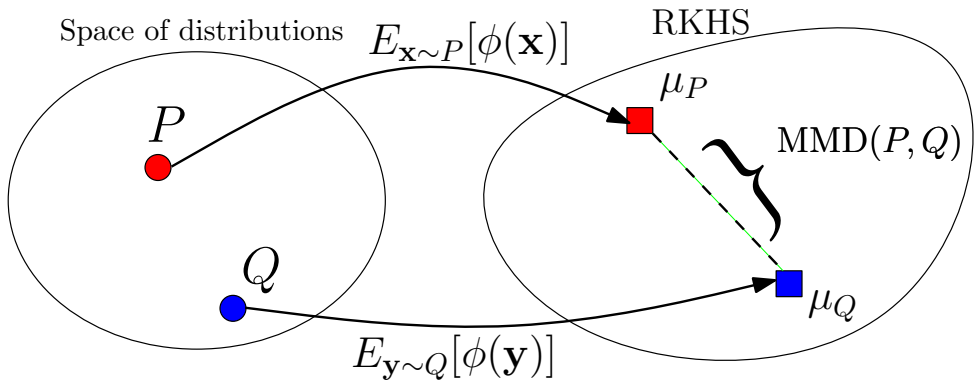

# K2-ABC (Proposed Method)

- Recall ABC likelihood: $p_\epsilon(\mathbf{Y}|\boldsymbol{\theta}) := \int p(\mathbf{X}|\boldsymbol{\theta})\kappa_\epsilon(\mathbf{X},\mathbf{Y})\,\mathrm{d}\mathbf{X}$.
- Use $\kappa_\epsilon(\mathbf{X},\mathbf{Y}) = \exp\left(-\frac{\widehat{\mathrm{MMD}}^2(\mathbf{X},\mathbf{Y})}{\epsilon}\right)$. No rejection.

1: **for** $i = 1,\ldots,M$ **do**
2: Sample $\boldsymbol{\theta}_i \sim p(\boldsymbol{\theta})$
3: Sample pseudo dataset $\mathbf{X}_i \sim p(\cdot|\boldsymbol{\theta}_i)$
4: $\widetilde{w}_i = \kappa_\epsilon(\mathbf{X}_i,\mathbf{Y}) = \exp\left(-\frac{\widehat{\mathrm{MMD}}^2(\mathbf{X}_i,\mathbf{Y})}{\epsilon}\right)$
5: **end for**
6: $w_i = \widetilde{w}_i / \sum_{j=1}^M \widetilde{w}_j$ for $i = 1,\ldots,M$
7: **return** $\{\boldsymbol{\theta}_i\}_{i=1}^M$ with weights $\{w_i\}_{i=1}^M$

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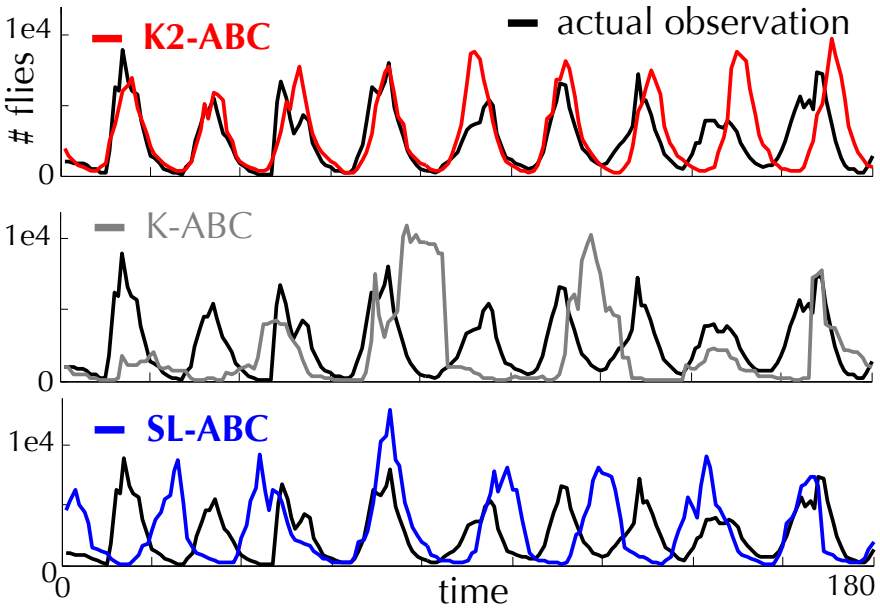
# Blow Fly Population Modelling

Number of blow flies over time

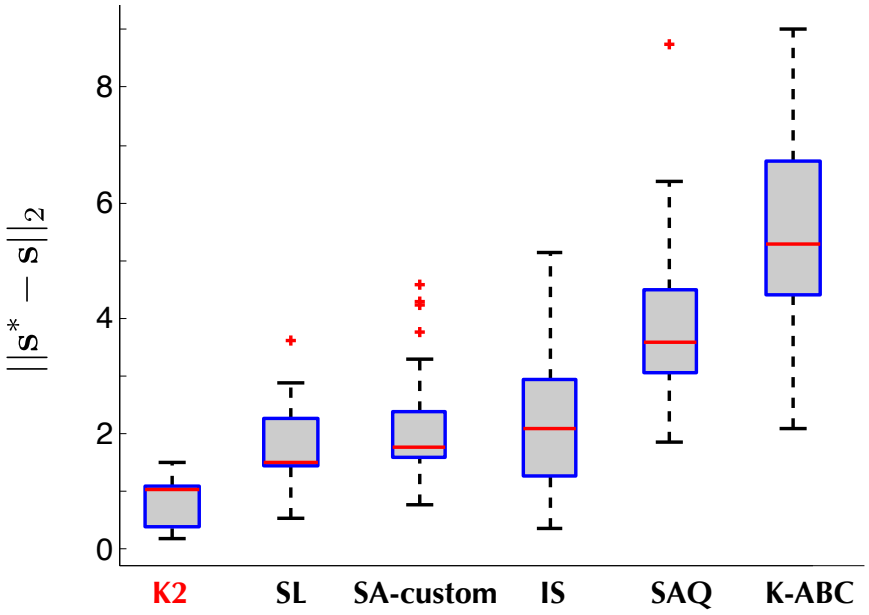
$$N_{t+1} = PN_{t-\tau} \exp\left(-\frac{N_{t-\tau}}{N_0}\right) e_t + N_t \exp(-\delta\epsilon_t)$$

- $e_t \sim \text{Gam}\left(\frac{1}{\sigma_P^2}, \sigma_P^2\right)$ and $\epsilon_t \sim \text{Gam}\left(\frac{1}{\sigma_d^2}, \sigma_d^2\right)$.
- Want $\boldsymbol{\theta} := \{P, N_0, \sigma_d, \sigma_p, \tau, \delta\}$.




- ← Simulated trajectories with inferred posterior mean of $\boldsymbol{\theta}$
  - Observed sample of size 180.
  - Other methods use handcrafted 10-dim. summary statistics.
- $s(\mathbf{X}) \in \mathbb{R}^{10}$ are as in [Meeds and Welling, 2014]
  - quantiles of the marginal distribution
  - quantiles of first-order differences
  - maximal peaks

# Errors on Summary Statistics




- $\tilde{\boldsymbol{\theta}} :=$ posterior mean.
- Simulate $\mathbf{X} \sim p(\cdot|\tilde{\boldsymbol{\theta}})$ 100 times.
- $\mathbf{s} = s(\mathbf{X})$ and $\mathbf{s}^* = s(\mathbf{Y})$.

- $\tilde{\boldsymbol{\theta}}$ inferred by K2-ABC gives lowest error on $\mathbf{s}$.
- Recall that K2-ABC does not use $\mathbf{s}$, unlike others.

K2-ABC can infer the generative parameters without the need of summary statistics.

# Linear-Time K2-ABC

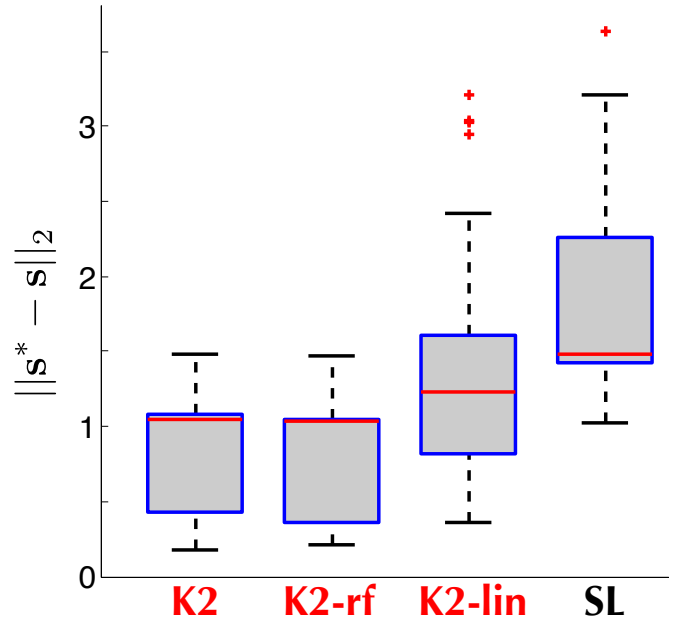
- $\widehat{\mathrm{MMD}}^2(\mathbf{X}, \mathbf{Y})$ costs $O(n^2)$ where $n =$ sample size.

1. Linear-time unbiased estimator. Costs $O(n)$.

$$\widehat{\mathrm{MMD}}^2_{\mathrm{lin}}(\mathbf{X}, \mathbf{Y}) = \frac{1}{n-1}\sum_{i=1}^{n-1} k(\mathbf{x}_i, \mathbf{x}_{i+1}) + \frac{1}{n-1}\sum_{i=1}^{n-1} k(\mathbf{y}_i, \mathbf{y}_{i+1}) - \frac{2}{n}\sum_{i=1}^{n} k(\mathbf{x}_i, \mathbf{y}_i)$$

2. Random Fourier features $\hat{\phi}(\mathbf{x}) \in \mathbb{R}^D$ such that $k(\mathbf{x}, \mathbf{y}) \approx \hat{\phi}(\mathbf{x})^\top \hat{\phi}(\mathbf{y})$. Costs $O(Dn)$. We set $D = 50$.

$$\widehat{\mathrm{MMD}}^2_{\mathrm{rf}}(\mathbf{X}, \mathbf{Y}) = \left\| \frac{1}{n}\sum_{i=1}^{n} \hat{\phi}(\mathbf{x}_i) - \frac{1}{n}\sum_{j=1}^{n} \hat{\phi}(\mathbf{y}_j) \right\|_2^2$$



# Summary

ABC problem:

- Goal: Sample from $p(\boldsymbol{\theta}|\mathbf{Y})$ where the likelihood is intractable.
- Can only sample from the likelihood.

Solution:

- Idea: Keep $\boldsymbol{\theta}$ such that $\mathbf{X} \sim p(\cdot|\boldsymbol{\theta})$ is "*similar*" to $\mathbf{Y}$.
- **Contribution**: K2-ABC uses kernel MMD to define the similarity.
  - No need to design summary statistics.
  - Capture all information of $p(\cdot|\boldsymbol{\theta})$.
- Code/Paper: `https://github.com/wittawatj/k2abc`

# Questions?

Thank you

# References I

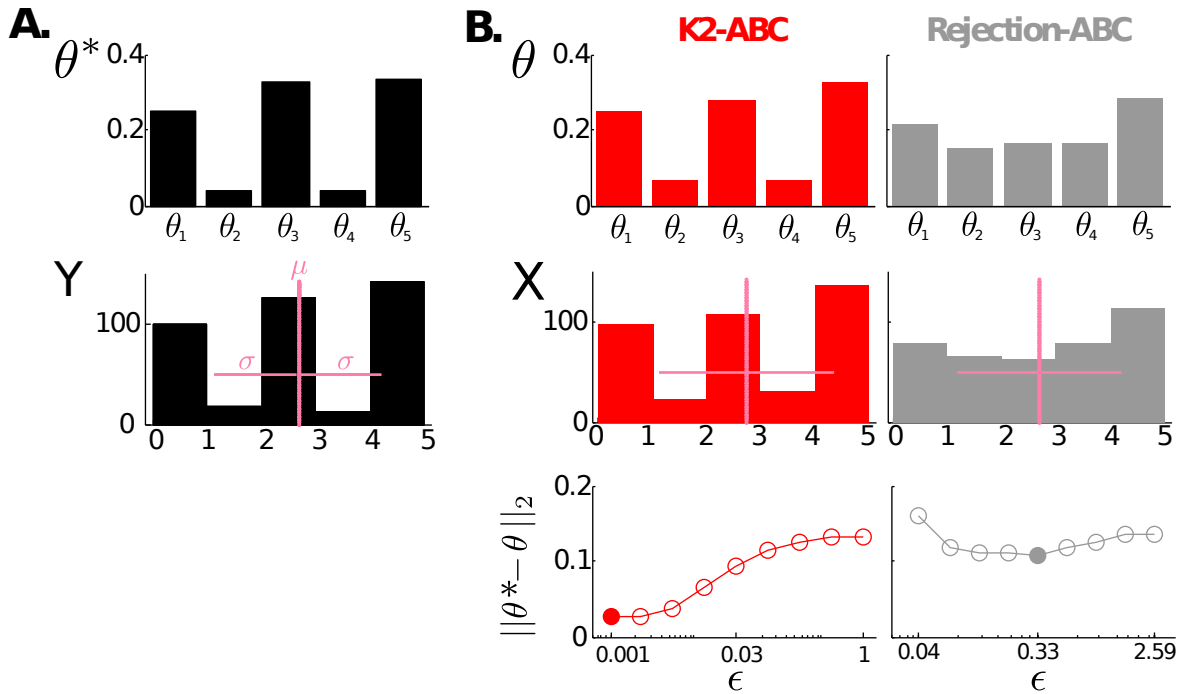
- K2-ABC on Arxiv: http://arxiv.org/abs/1502.02558


Gretton, A., Borgwardt, K. M., Rasch, M., Schölkopf, B., and Smola, A. J. (2006).
A kernel method for the two-sample-problem.
In *Advances in neural information processing systems*, pages 513–520.

Meeds, E. and Welling, M. (2014).
GPS-ABC: Gaussian Process Surrogate Approximate Bayesian Computation.
In *UAI*, volume 30, pages 593–601.

# Toy Problem: Failure of Insufficient Statistics

$$
\begin{aligned}
p(y|\boldsymbol{\theta}) &= \sum_{i=1}^{5} \theta_i \text{Uniform}(y; [i-1, i]) \\
\pi(\boldsymbol{\theta}) &= \text{Dirichlet}(\boldsymbol{\theta}; \mathbf{1}) \\
\boldsymbol{\theta}^* &= \text{(see figure A)}
\end{aligned}
$$




- $s(\mathbf{X}) = (\hat{\mathbb{E}}[x], \hat{\mathbb{V}}[x])^\top$ for Rejection and Soft ABC.
- Insufficient to represent $p(y|\theta)$.

# Rejection ABC Algorithm

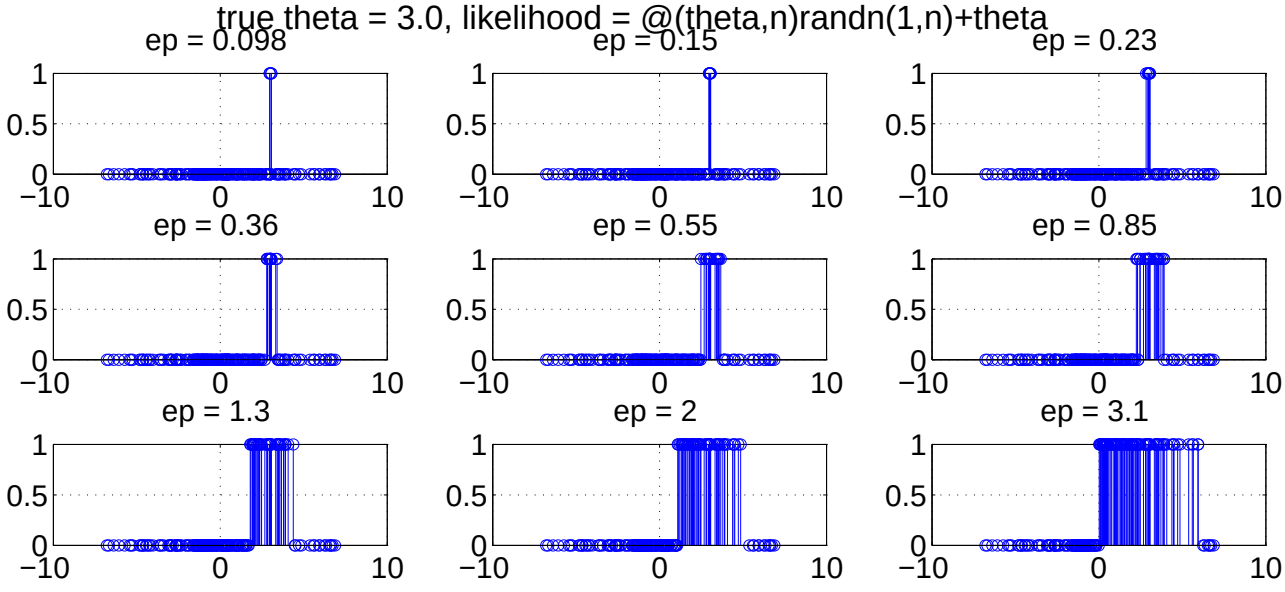
- **Input:** observed dataset $\mathbf{Y}$, distance $\rho$, threshold $\epsilon$
- **Output:** posterior sample $\{\boldsymbol{\theta}_i\}_{i=1}^{M}$ from approximate posterior $p_\epsilon(\boldsymbol{\theta}|\mathbf{Y}) \propto p(\boldsymbol{\theta})p_\epsilon(\mathbf{Y}|\boldsymbol{\theta})$

1: **repeat**
2: Sample $\boldsymbol{\theta} \sim p(\boldsymbol{\theta})$
3: Sample a pseudo dataset $\mathbf{X} \sim p(\cdot|\boldsymbol{\theta})$
4: **if** $\rho(\mathbf{X}, \mathbf{Y}) < \epsilon$ **then**
5: Keep $\boldsymbol{\theta}$
6: **end if**
7: **until** we have $M$ points

- **Notation**: $\mathbf{Y} =$ observed set. $\mathbf{X} =$ pseudo (generated) dataset.

# Rejection ABC Example

$$
\begin{aligned}
p(y|\theta) &= \mathcal{N}(y;\theta,1) \\
p(\theta) &= \mathcal{N}(\theta,0,8) \\
\theta^* &= 3.0 \\
\rho(\mathbf{X},\mathbf{Y}) &= \left|\hat{\mathbb{E}}_{\mathbf{X}}[x] - \hat{\mathbb{E}}_{\mathbf{Y}}[y]\right|
\end{aligned}
$$




- Low $\epsilon \Rightarrow$ sample closely follows true posterior. High rejection rate.
- High $\epsilon \Rightarrow$ get $\theta$ sample from prior.

# 1D Gaussian Example with K2-ABC

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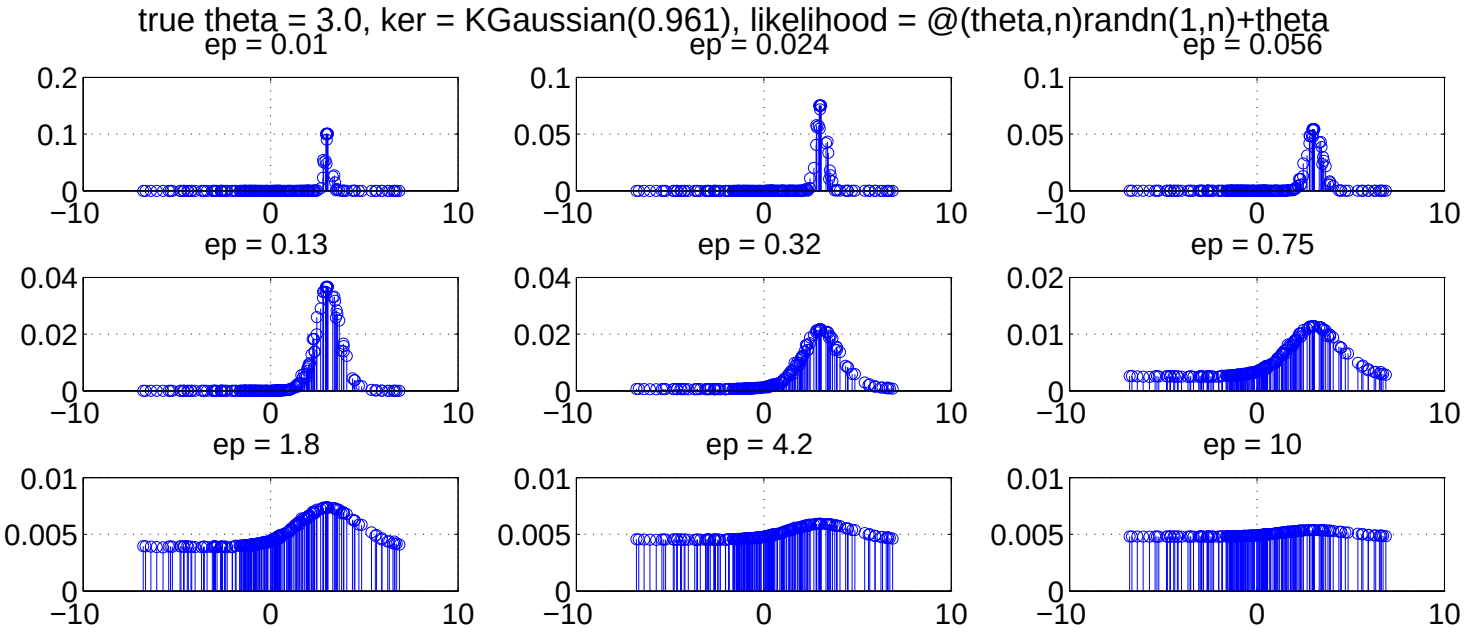


- High $\epsilon \Rightarrow$ get $\theta$ sample from prior
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