Bayesian Machine Learning

May 2022 - François HU
https://curiousml.github.io/

Outline

1 Bayesian statistics

2 Latent variable models

3 Variational Inference

4 **Markov Chain Monte Carlo**
- Monte Carlo Estimation
- MCMC and differences with VI

5 Extensions and oral presentations

1 Monte Carlo estimation

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Classic estimation methods

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$$\mathbb{E}[h(X)]$$

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$$\mathbb{P}(X > 2)$$

$$\pi = 4 \times \mathbb{P}[U^2 + V^2 \leq 1]$$

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Yes with usual simulations or MCMC

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Usual simulations : the power of uniform distribution

Starting point : we know how to simulate a pseudo-random uniform $U \sim \mathscr{U}(0,1)$

For « usual » distributions : both **discrete** and **continuous r.v.** can be sampled thanks to the uniform distribution

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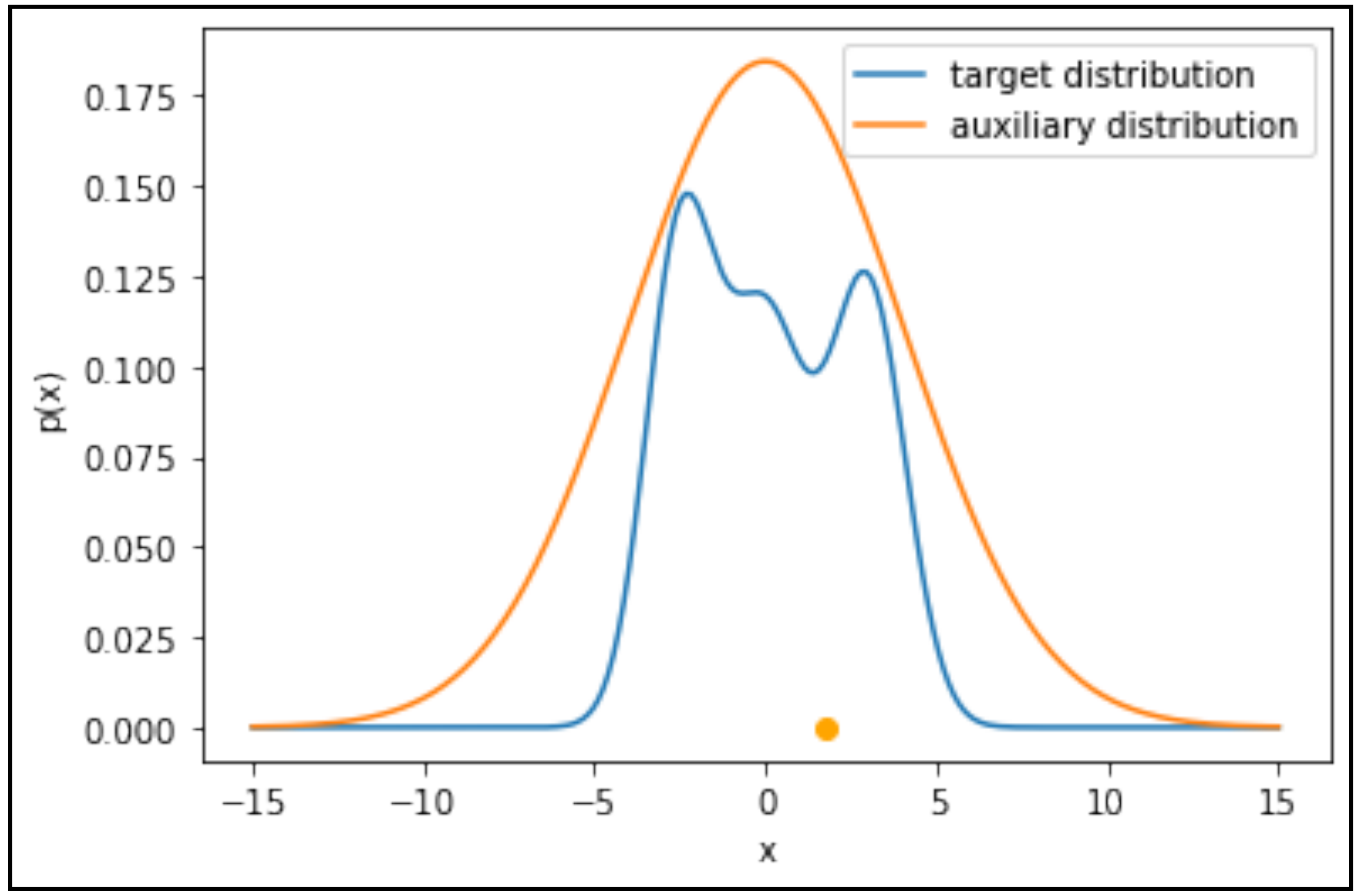

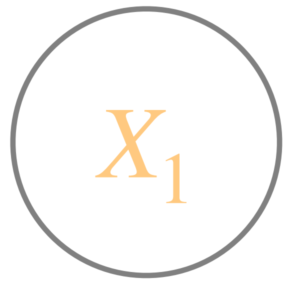

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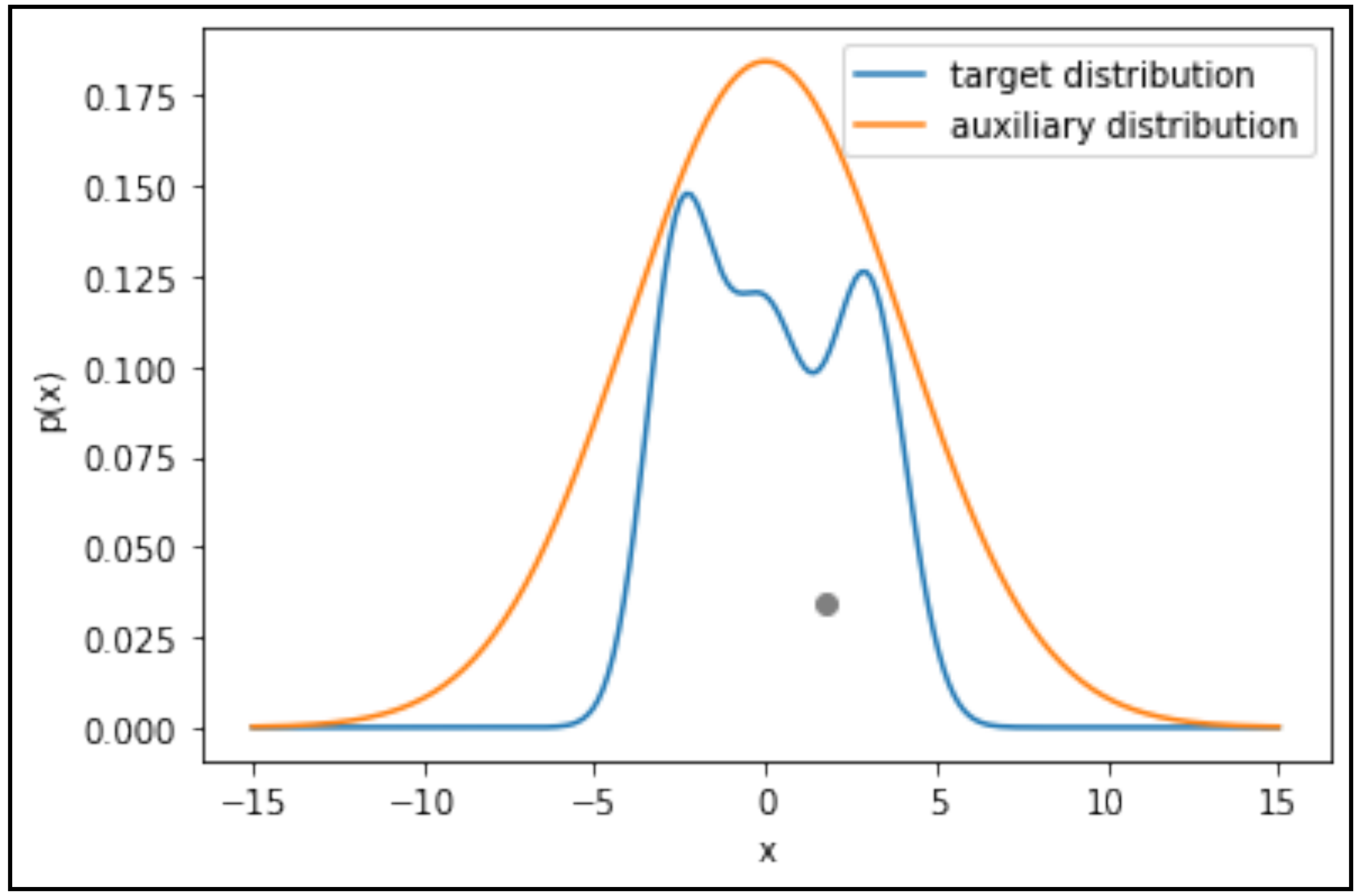

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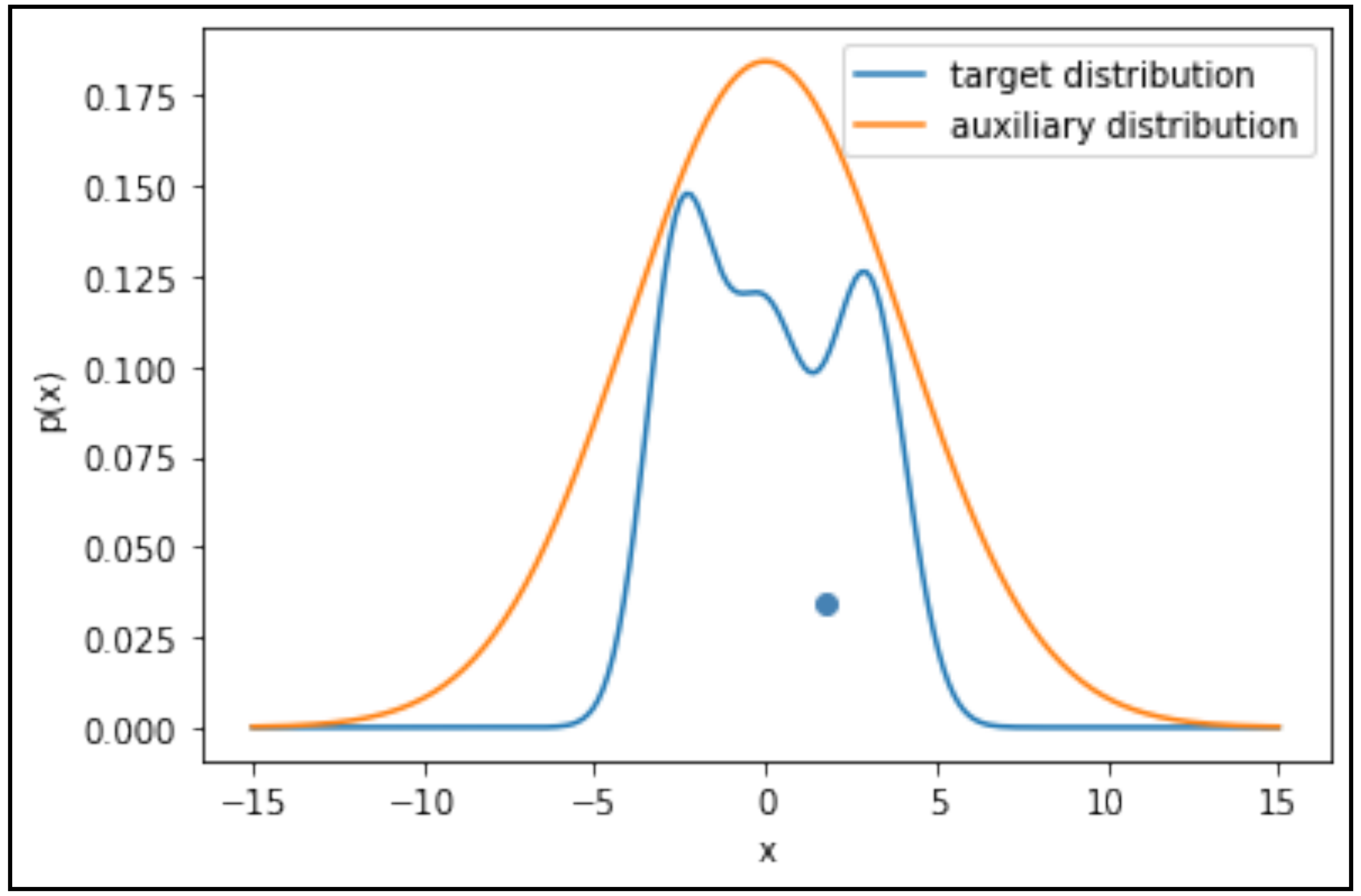

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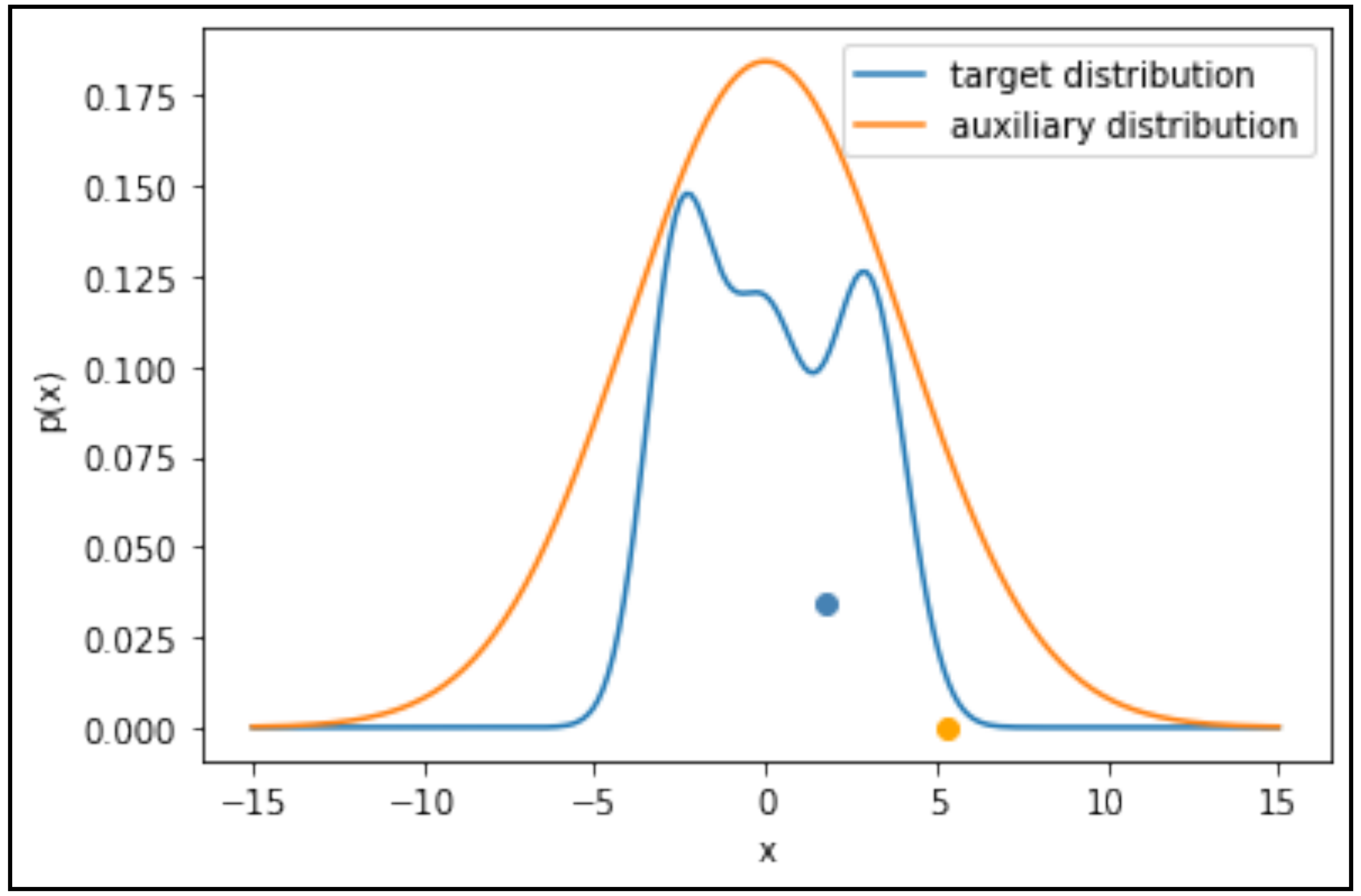

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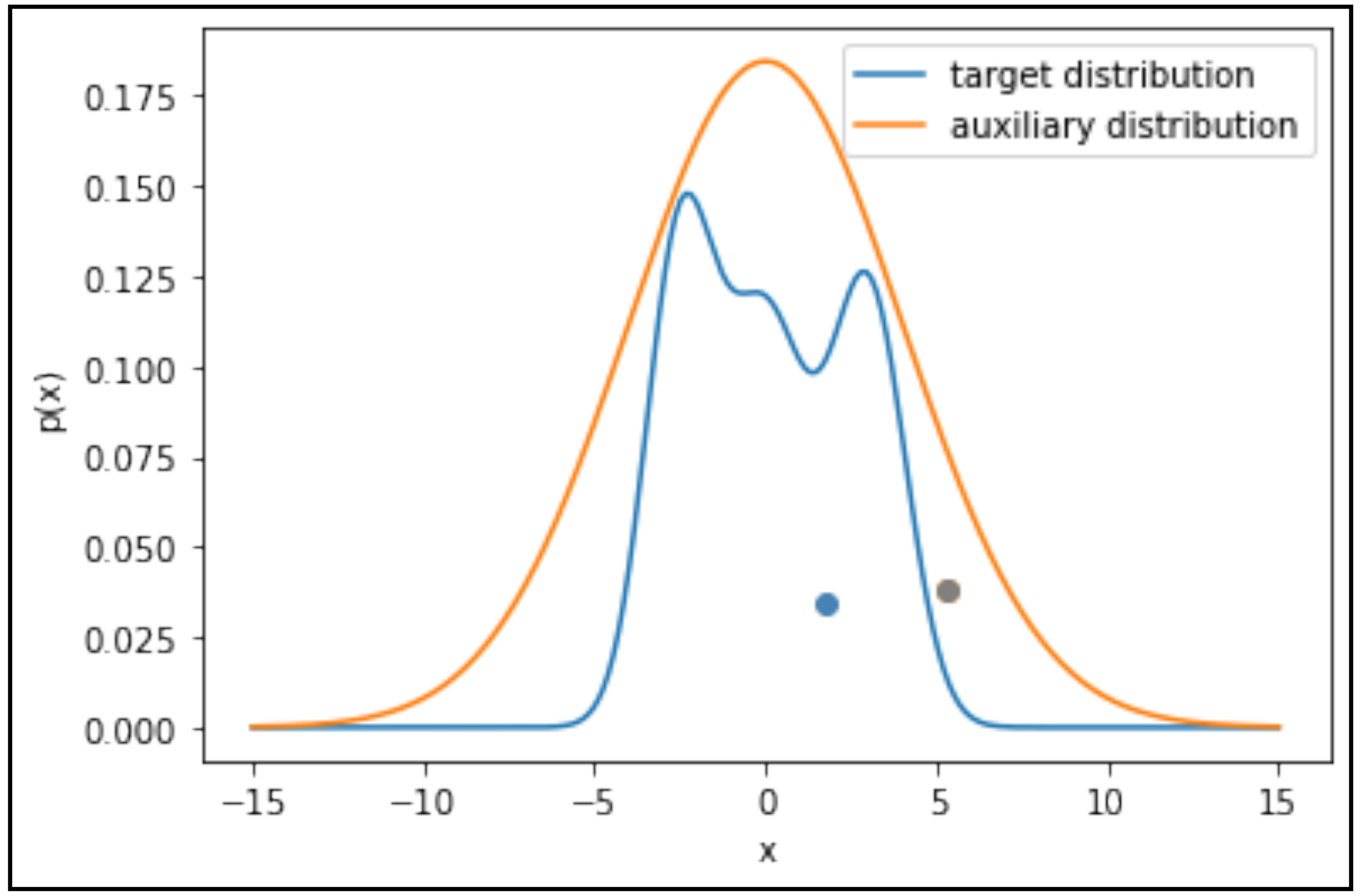

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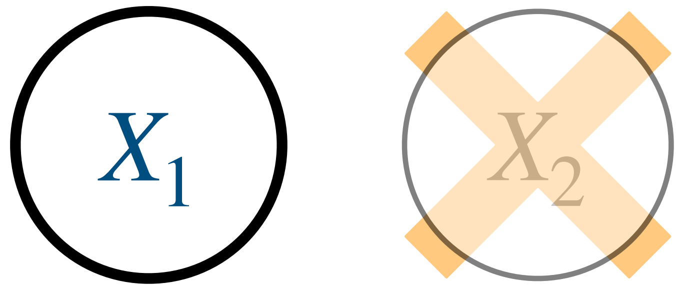

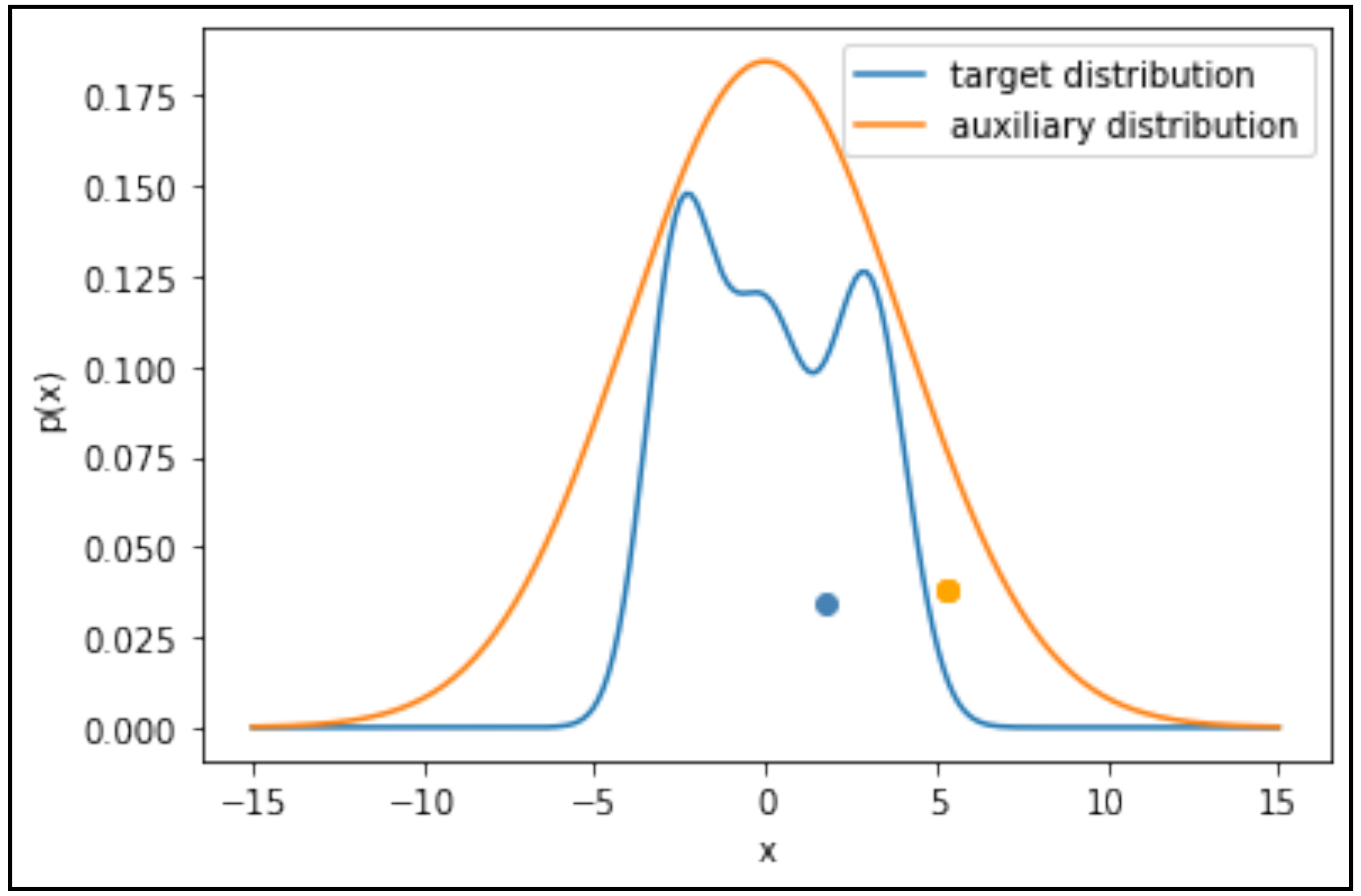

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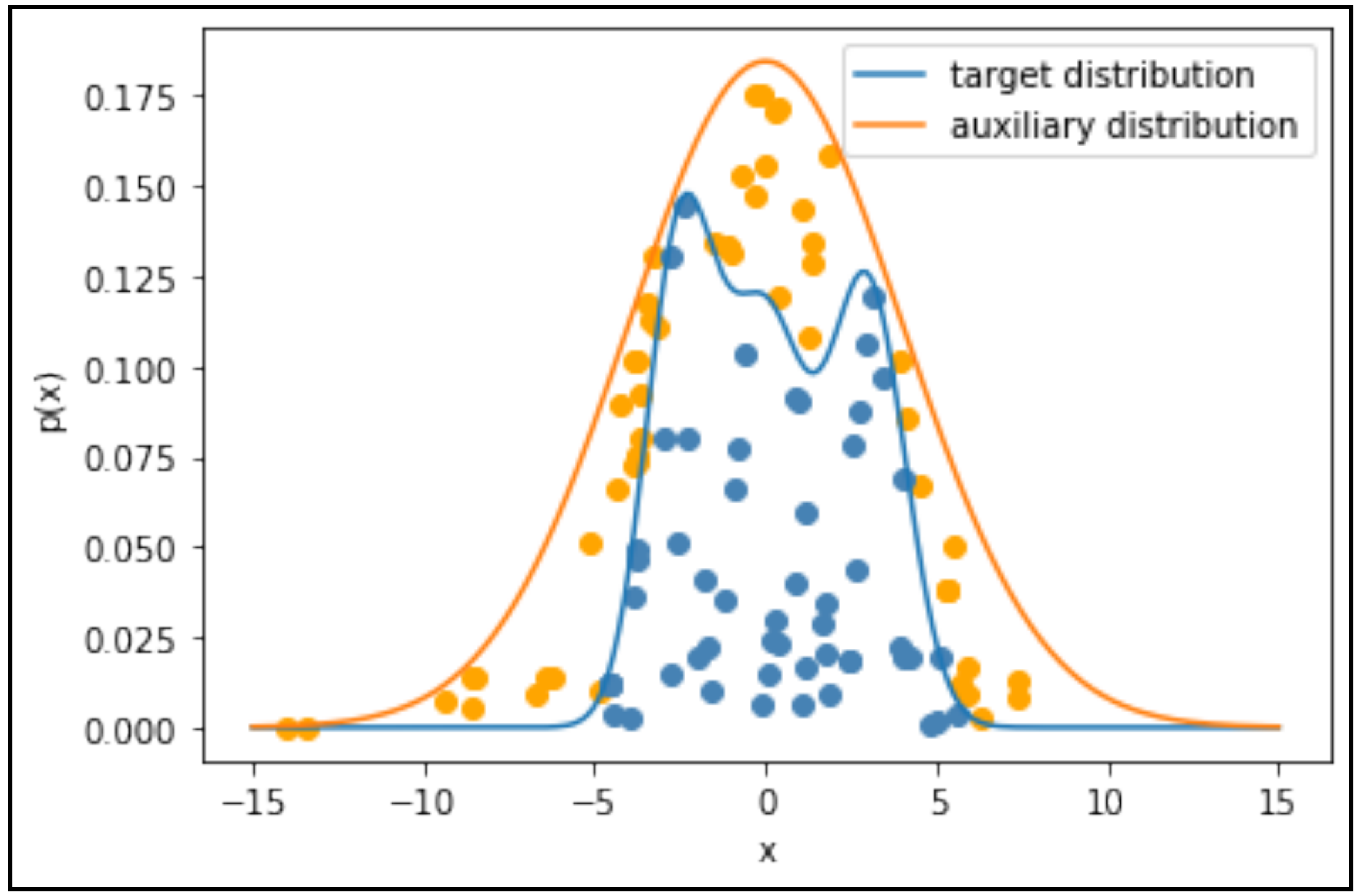

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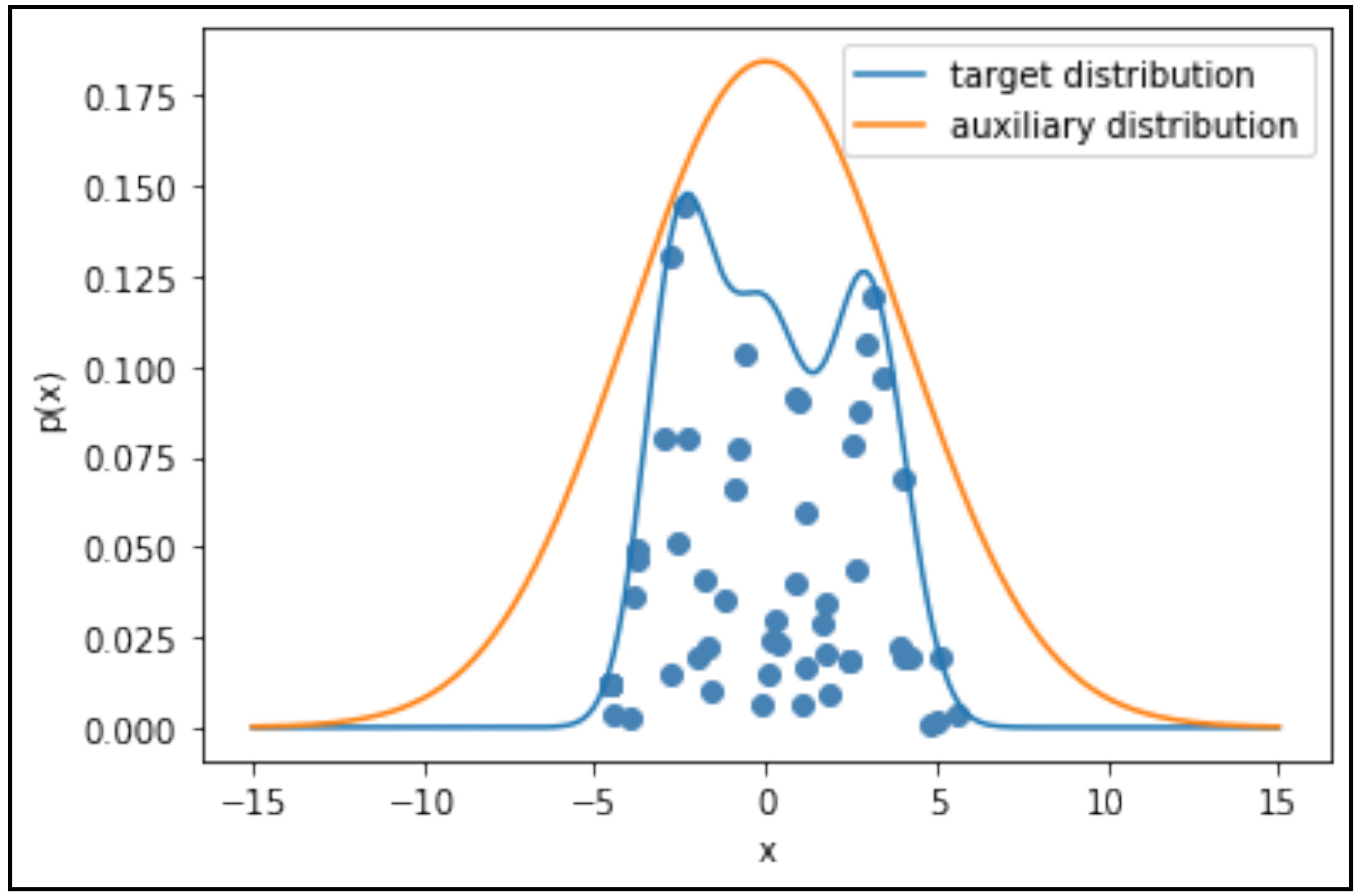

X_1 X_2 ... X_n

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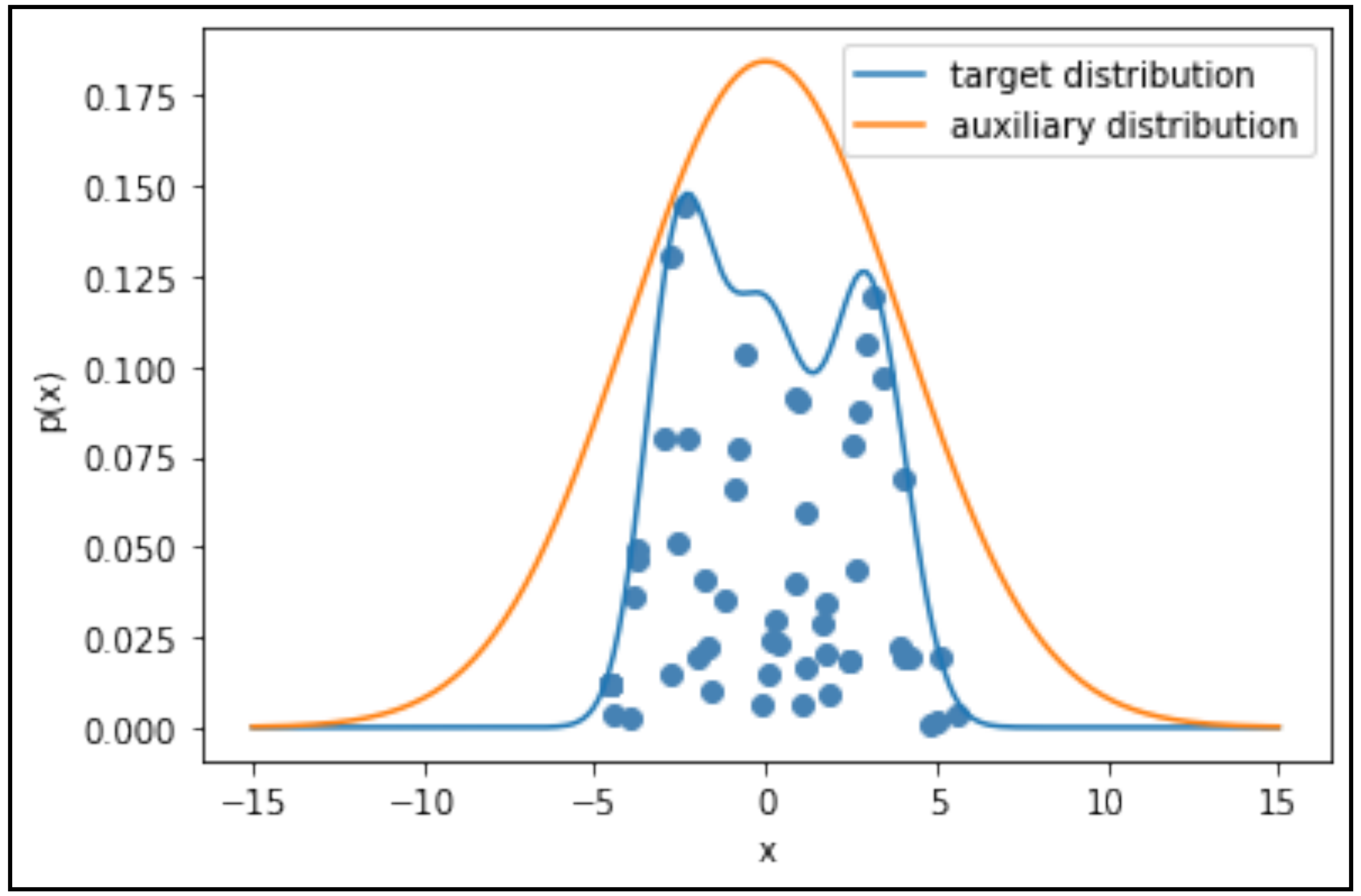


X_1

X_2

...

X_n

✓ works for most distribution

✗ if the « **gaps** » between P and Q are too large, we reject most of the sample

1. Monte Carlo estimation

Usual simulations : the power of uniform distribution

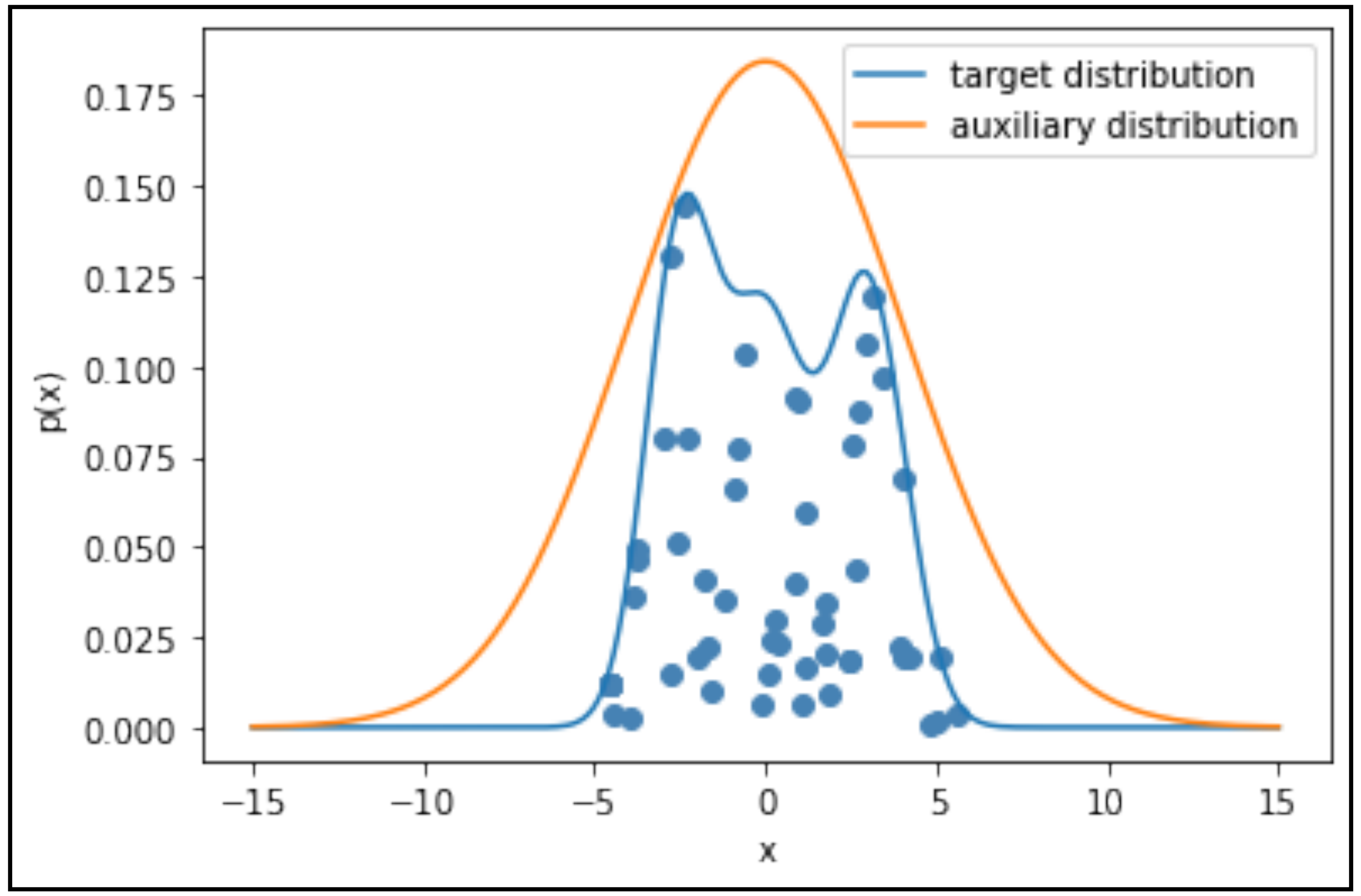
Starting point : we know how to simulate a pseudo-random uniform $U \sim \mathcal{U}(0,1)$

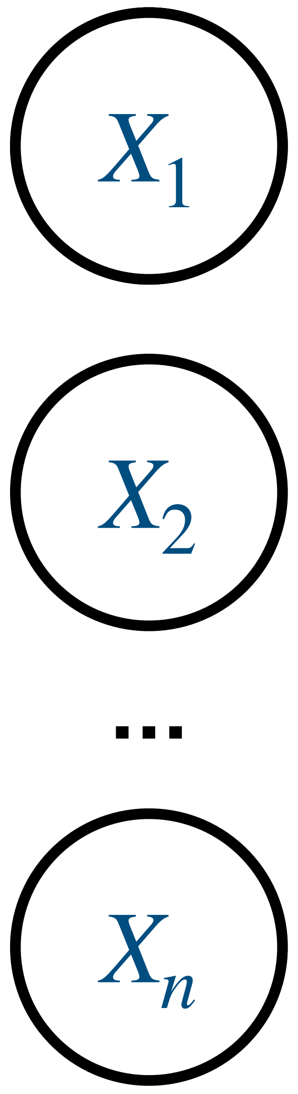
For « usual » distributions : both **discrete** and **continuous r.v.** can be sampled thanks to the uniform distribution

> **In practice (with python)** we can easily sample them (via **scipy** and **numpy** for example)

Otherwise : if there isn't an analytical way to sample it then

> **Rejection sampling** algorithm.
> Assumption : we can compute **distribution's pdf** P and sample from an **auxiliary distribution** Q s.t. $P \leq \text{const} \times \mathrm{Q}$
>
> **Algorithm**
> 1. generate sample $x_i \sim Q$ (**auxiliary distribution**)
> 2. generate sample $u \sim \mathcal{U}(0, \text{const} \cdot \mathrm{Q}(\mathrm{x_i}))$
> 3. if $u \leq P(x_i)$ then **accept** x_i else **reject**.





✓ works for most distribution

✗ if the « **gaps** » between P and Q are too large,
we reject most of the sample

use MCMC

2 Markov Chain Monte Carlo : Definition

2. Markov Chain Monte Carlo

Definition : Monte Carlo sampling

Monte Carlo sampling : generates independent samples from the probability distribution in order to estimate an expected value

X_1 X_2 … X_n where $X_1, \ldots, X_n \sim P$ i.i.d

2. Markov Chain Monte Carlo

Definition : Markov Chain

Monte Carlo sampling : generates independent samples from the probability distribution in order to estimate an expected value

X_1 X_2 ... X_n where $X_1, \ldots, X_n \sim P$ i.i.d

Markov Chain : generates a sequence of r.v. where the *next* variable is probabilistically dependent upon the *current* variable.

P is called **stationary** if $P(x') = \sum_{x \in \mathrm{supp(X)}} T(x, x') \cdot P(x)$

$T(x, x')$ the transition probability of being in the state x' given the current state x

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Markov Chain Monte Carlo sampling : a sequence of *Monte Carlo Samples* where the *next* sample is dependent upon the *current* sample

$$X_1 \xrightarrow{T} X_2 \xrightarrow{T} \cdots \xrightarrow{T} X_b \xrightarrow{T} X_{b+1} \xrightarrow{T} \cdots \xrightarrow{T} X_{n+b}$$

Burn-in samples

$X_{b+1}, \ldots, X_{b+n} \sim P$ **with some possible correlations**

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Objective : Build a Markov Chain that converges to the target distribution P no matter the starting point

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$$X_1 \quad X_2 \quad \dots \quad X_n$$

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Burn-in samples

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Objective : Build a Markov Chain that converges to the target distribution P no matter the starting point

Theorem : if $T(x, x') > 0$ for all x, x' then there *exists* an *unique* **stationary** and **convergent** distribution

3 Markov Chain Monte Carlo : Algorithms

3. Markov Chain Monte Carlo

Algorithm : Gibbs sampling

Reminder : we want to sample $x^{(1)}, \ldots, x^{(n)} \sim P\left(x_1, x_2, \ldots, x_d\right)$

Remark : we denote $x^{(i)} := \left(x_1^{(i)}, \ldots, x_d^{(i)}\right)$; $x_{-j} = \left(x_1, \ldots, x_{j-1}, x_{j+1}, \ldots, x_d\right)$; $x_{m:n} = \left(x_m, x_{m+1}, \ldots, x_n\right)$

Gibbs Sampling Algorithm

- **Hypothesis** : The conditional $P(x_j \mid x_{-j})$ can be sampled
- **Initialisation** : $x^{(0)} = (0,\ldots,0)$ or random values
- **Repeat** :

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$$x_2^{(i)} \sim P(\, x_2 \,|\, x_1^{(i)}, x_3^{(i-1)}, \ldots,\; x_d^{(i-1)}\,)$$

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…

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for each position, $x_k^{(i)} \sim P(\, x_1 \mid x_{1:k-1}^{(i)}, x_{k+1:d}^{(i-1)}\,)$

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sometimes it can converge slowly to the desired distribution

sometimes Gibbs samples can be too correlated

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Use a variant Gibbs sampling : Metropolis-Hastings

3. Markov Chain Monte Carlo

Algorithm : Metropolis-Hastings

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Metropolis-Hastings Algorithm

- **Hypothesis** : Let $P = \hat{P}/\mathrm{const}$ where $\hat{P}$ can be calculated and let Q be an auxiliary distribution we can sample from

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- **Repeat** :

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- **Repeat** :

  sample a **candidate** $x^{(i)} \sim Q(\, x^{(i)} \mid x^{(i-1)}\,) =$ (example of auxiliary distribution) $\mathcal{N}(x^{(i-1)}, \sigma^2 I)$

3. Markov Chain Monte Carlo

Algorithm : Metropolis-Hastings

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  with **acceptance probability** : $\min\left(1, \dfrac{Q(x^{(i-1)} \mid x^{(i)}) \times \hat{P}(x^{(i)})}{Q(x^{(i)} \mid x^{(i-1)}) \times \hat{P}(x^{(i-1)})}\right)$ accept $x^{(i)}$ **as an sample from** P

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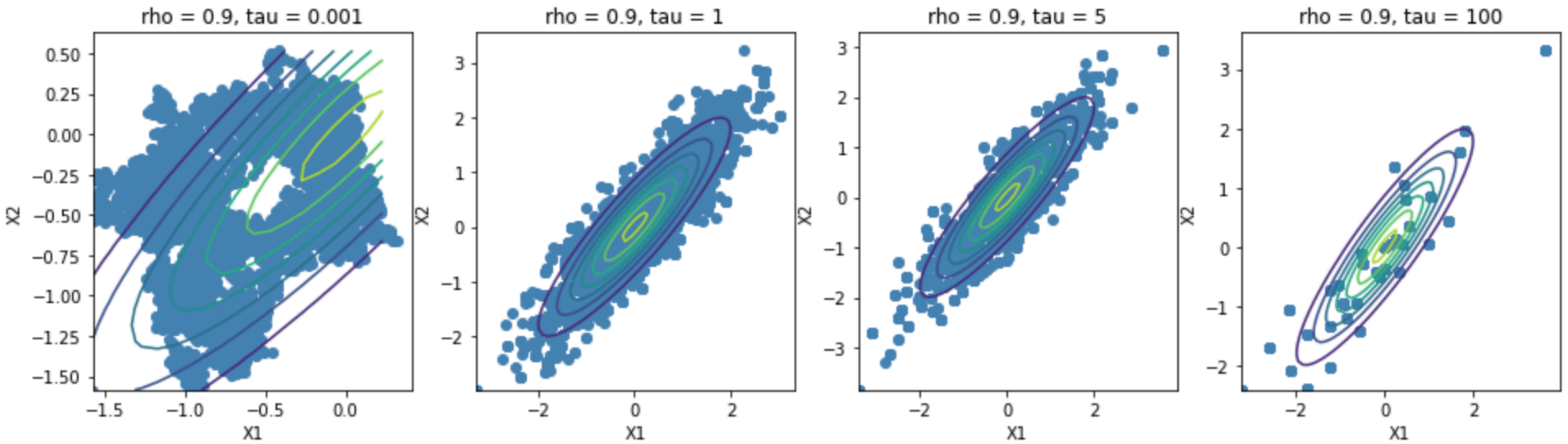

$\tau = \sigma^2$ **and** ρ **the correlation between two gaussians** X_1 **and** X_2

3.b. MCMC vs VI

3.b. **MCMC vs VI**

pros and cons

MCMC

Pros :
- Useful when the posterior is intractable
- Asymptotically exact
- Suited to small / medium dataset

Cons :
- Usually slower than alternatives (VI)
- Can generates dependant samples from the distribution

VI (see lecture 3)

Pros :
- Useful when the posterior is intractable
- Suited to large dataset

Cons :
- Can never generate exact result

4 Applications : notebook

! Road map

1. Bayesian statistics

Bayesian perspective :

$$P(\theta|X) = \frac{P(X,\theta)}{P(X)} = \frac{P(X|\theta)\cdot P(\theta)}{P(X)}$$

Likelihood: $P(X|\theta)$ — Prior distribution: $P(\theta)$ — Posterior distribution: $P(\theta|X)$

Evidence: $P(X)$

Hard to compute !

θ parameters

X observations

MAP : $\arg\max_{\theta} P(X|\theta)\cdot P(\theta)$

Conjugate distribution

Exemple :
Naive Bayes classifier,
Linear regression, ….

Pros :	Cons :
- exact posterior	- conjugate prior maybe inadequate

2. Latent variable models

Hidden variable models :

$$P(X|\theta) = \sum_{t\in T_{indexes}} P(X, T=t|\theta)$$

$$P(X,T|\theta) = P(X|T,\theta)P(T|\theta)$$

Exemple :
GMM, K-means, PCA/PPCA

Pros :	Cons :
- fewer parameters / simpler models - hidden variable sometimes meaningful - clustering / dimensionality reduction	- harder to work with - requires math - only local maximum or saddle point - EM : the posterior of T could be intractable

3. Variational Inference

Deterministic approximation of posterior :

$$p(Z|X) = \frac{P(X|Z)\cdot P(Z)}{P(X)}$$

Mean Field Approximation !

Exemple :
Topic modelling, LDA trained by VI

Pros :	Cons :
- Useful when the posterior is intractable - Suited to large dataset	- can never generate exact result

4. Markov Chain Monte Carlo

Sampling techniques for estimate expected values :

$$\mathbb{E}_{p(x)}[h(x)] \approx \frac{1}{M}\sum_{s=1}^{M} f(x_s)$$

$f(x_s) \sim p(x)$ Gibbs sampling / Metropolis-Hastings !

Exemple :
Topic modelling, LDA trained by MCMC

Pros :	Cons :
- train / inference almost every probabilistic model - asymptotically exact - suited to small / medium dataset	- Usually slower than alternatives (VI) - can generates dependant samples from the distribution

5. Extensions

Oral presentations (20 points)

+

Exercice 1 of lecture 1 : 1 bonus point
Notebook 1 : 1 bonus point
Notebook 2 : 2 bonus points
Notebook 3 : 0.5 bonus point
Notebook 4 : 0.5 bonus point
Notebook 5 : 1 bonus point