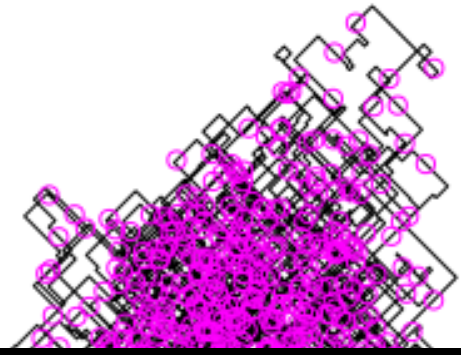
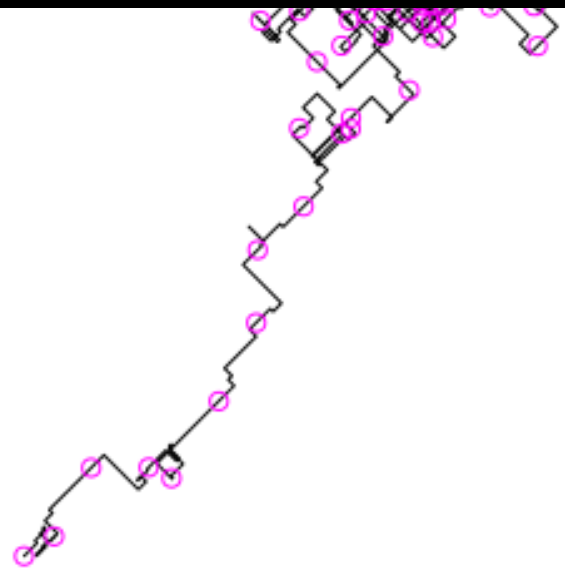


Developments in Piecewise Deterministic Monte Carlo

Athens University of Economics and Business

Joris Bierkens

2 December 2022



Acknowledgements

Collaborators

Andrew Duncan

Paul Fearnhead

Kengo Kamatani

Gareth Roberts

Financial support

NWO

Outline

Next Section

One-dimensional Zig-Zag process

(B., Roberts, **Ann. Appl. Prob. 2017**, https://arxiv.org/abs/1509.00302)

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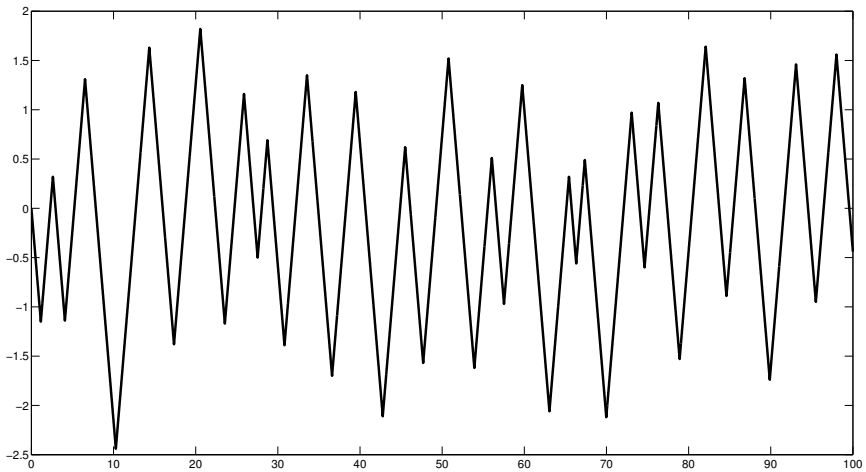

Relation between switching rate and potential

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Example: Gaussian distribution $\mathcal{N}(0, \sigma^2)$

- Density $\pi(x) \propto \exp(-x^2/(2\sigma^2))$
- Potential $U(x) = x^2/(2\sigma^2)$
- Derivative $U'(x) = x/\sigma^2$
- Switching rates $\lambda(x, v) = (vx/\sigma^2)_+ + \gamma(x)$

Multi-dimensional Zig-Zag process

(B., Fearnhead, Roberts, https://arxiv.org/abs/1607.03188)

- Target $\pi(x) = \exp(-U(x))$ on $\mathbb{R}^d$.
- Set of directions $v \in \{-1, +1\}^d$.
- Switching rates $\lambda_i(x, v) = (v_i \partial_i U(x))_+ + \gamma_i(x, v)$, for $i = 1, \ldots, d$.

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- The excess switching rate $\gamma_i(x, v)$ should not depend on the i-th component of v.

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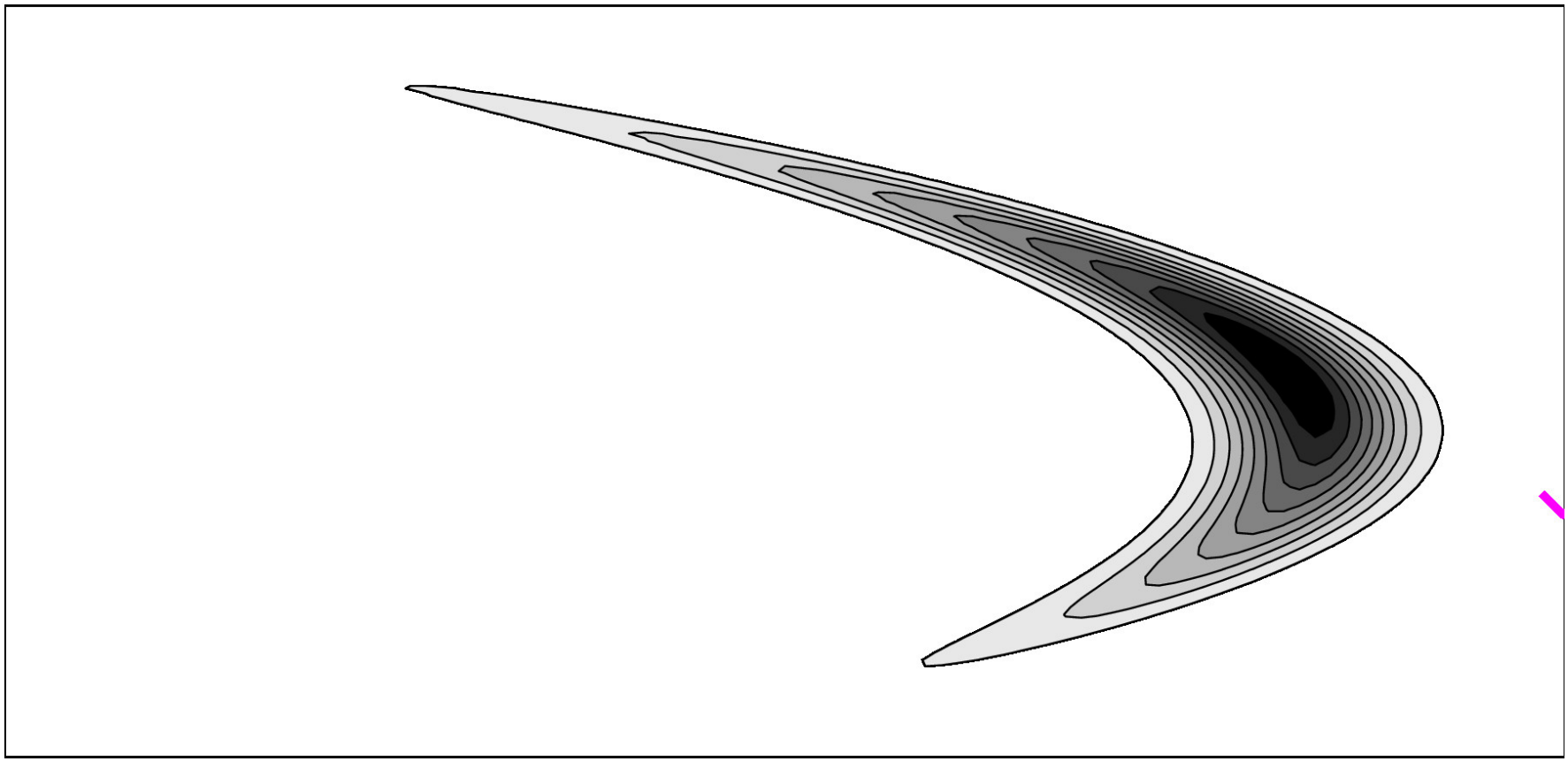

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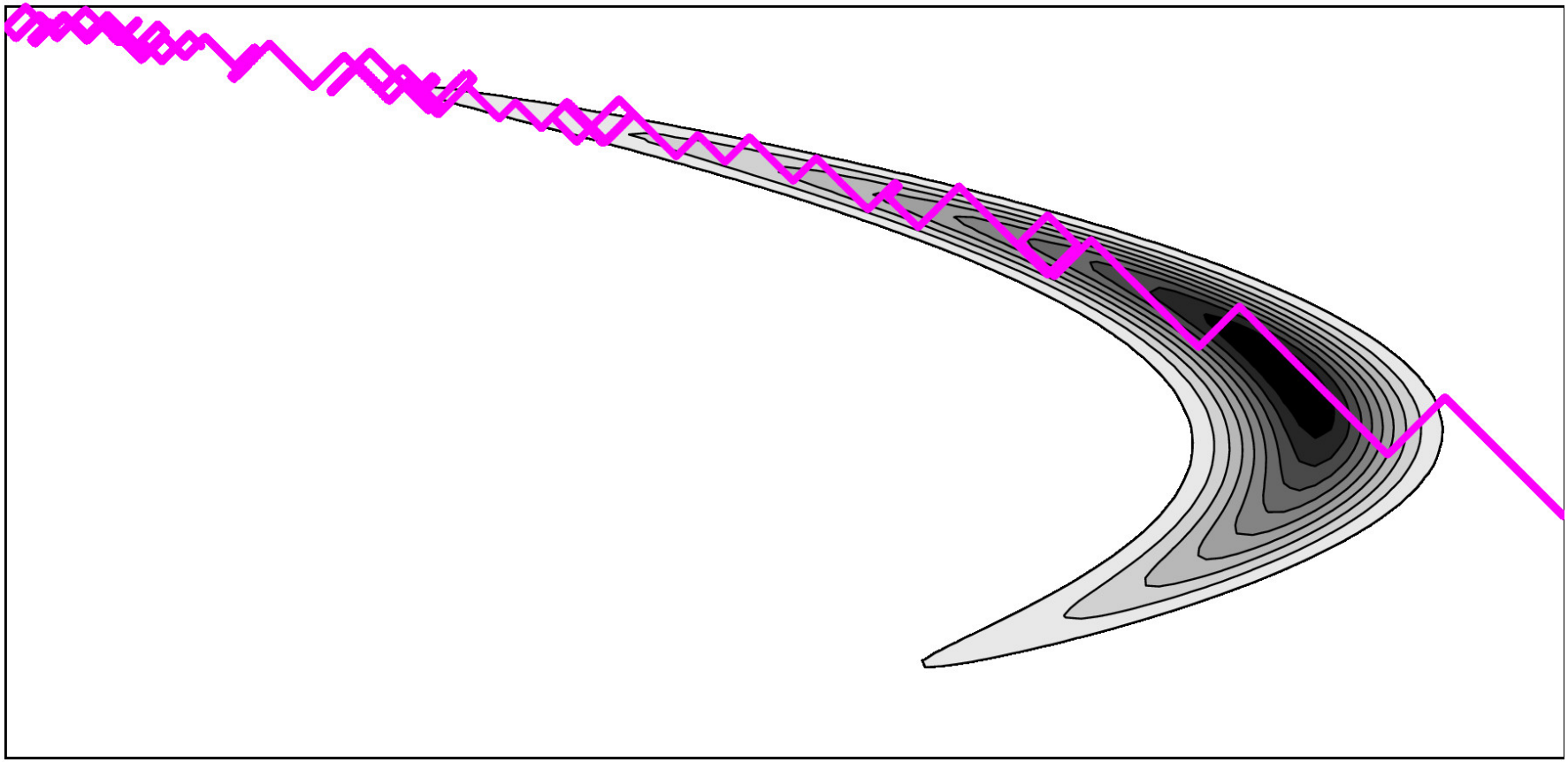

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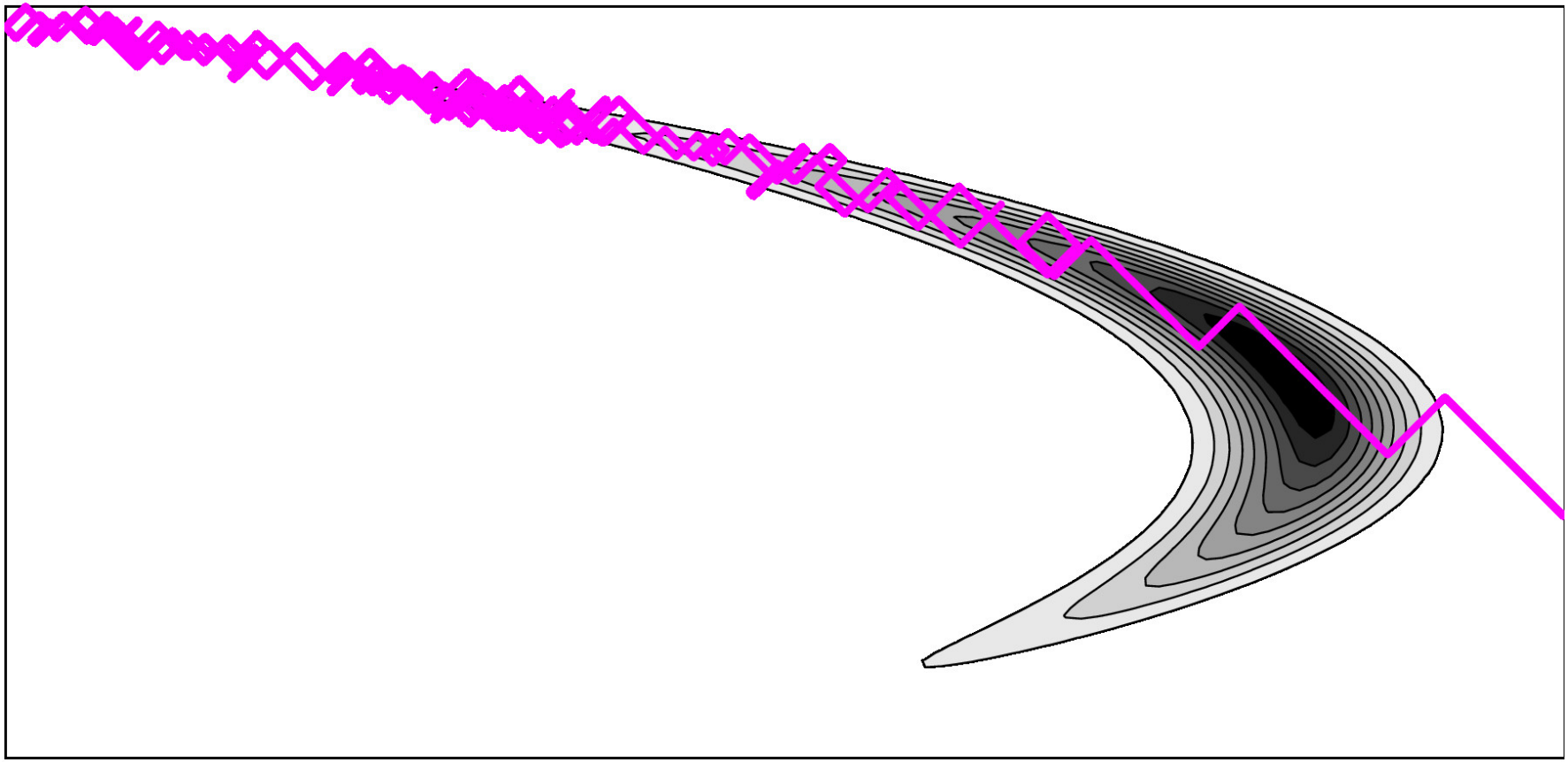

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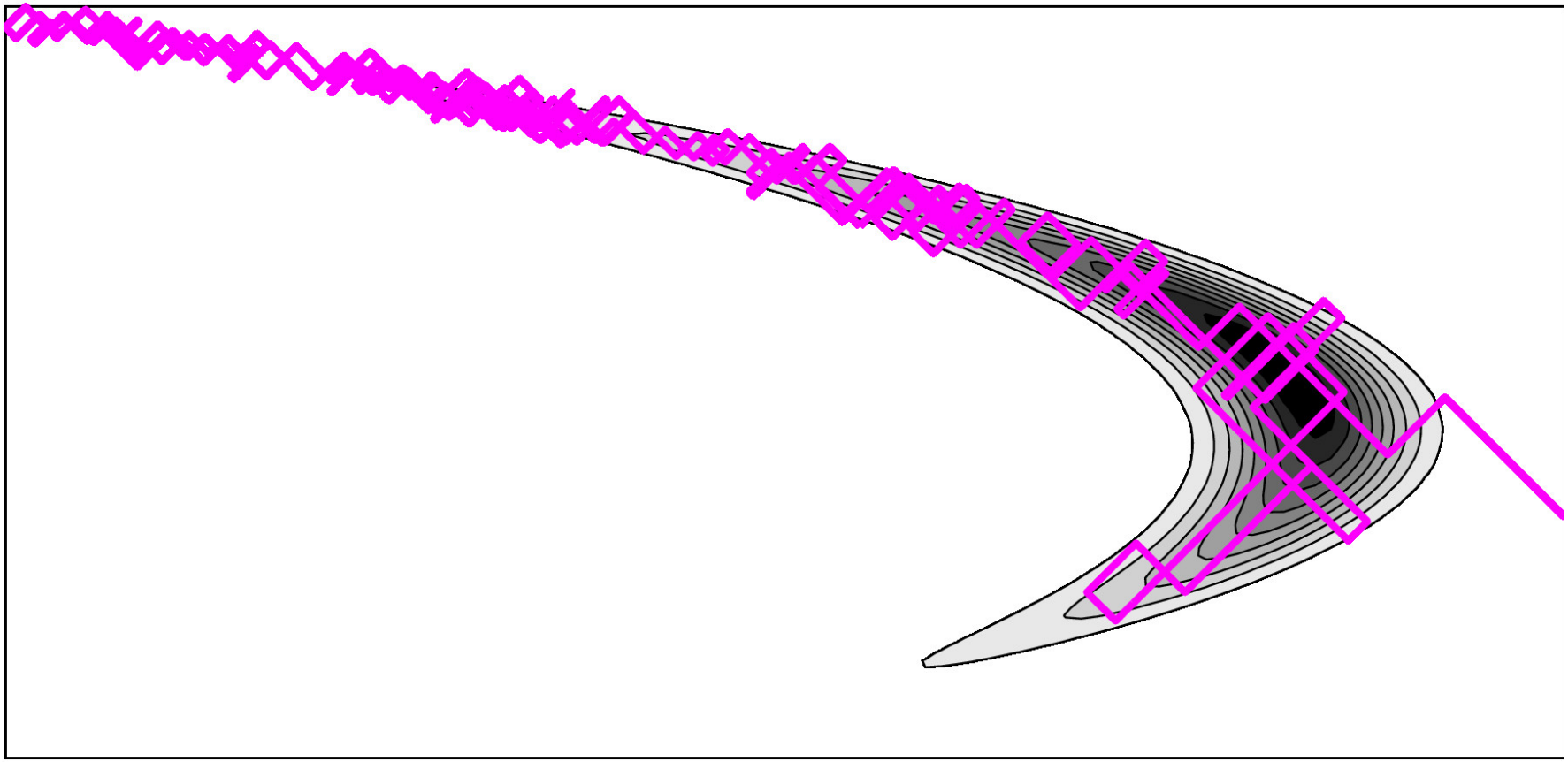

Use in Monte Carlo

(B., Fearnhead, Roberts, https://arxiv.org/abs/1607.03188)

$(X(t), V(t))_{t\geq 0}$ has stationary distribution proportional to $\pi(x)$.
If ergodic,

$$\lim_{T\to\infty} \frac{1}{T}\int_0^T h(X(s))\,ds = \int_{\mathbb{R}^d} h(x)\pi(x)\,dx.$$

Usage in computations

Two possibilities:

- Integrate $\frac{1}{T}\int_0^T h(X(s))\,ds$ for some finite $T > 0$ (numerically/analytically), or
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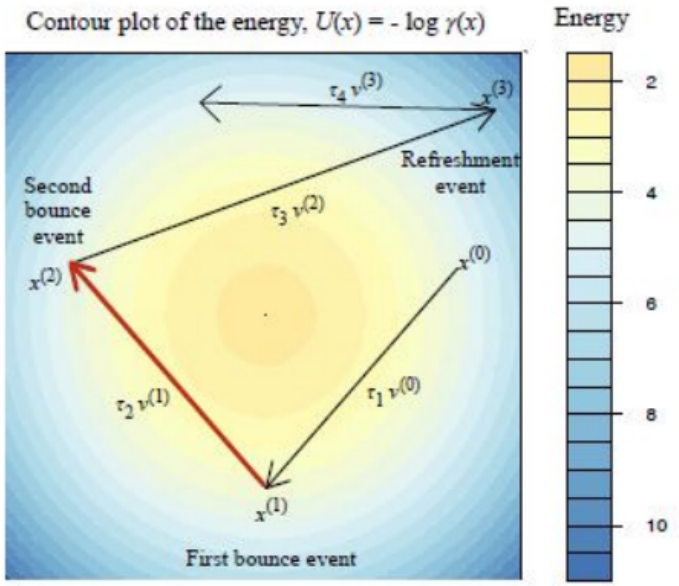
Be careful: the switching locations ('skeleton points') are biased towards the tail of the target distribution and cannot be used as samples

The Bouncy Particle Sampler

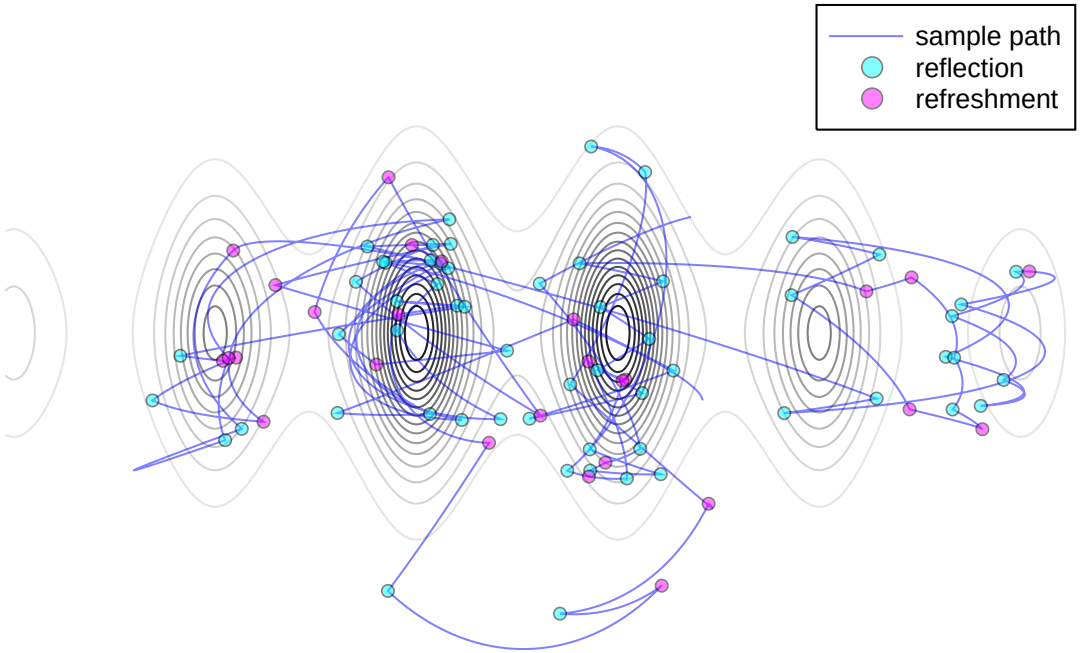
(Bouchard-Côté, Vollmer, Doucet, JASA, 2017, https://arxiv.org/abs/1510.02451**)**

The Bouncy Particle Sampler (BPS) is a second canonical example of a PDMP which can be used for sampling.
State space is $\mathbb{R}^d \times \mathbb{R}^d$ with stationary distribution $\pi(x)\,dx \otimes \mathcal{N}(0, \sigma^2 I_n)$.
The BPS bounces off at random contours of π, through specular reflection.
Additionally, the momentum gets refreshed after at rate λ_{ref}.



The Boomerang Sampler

[B., Grazzi, Kamatani. Roberts. ICML. 2020]

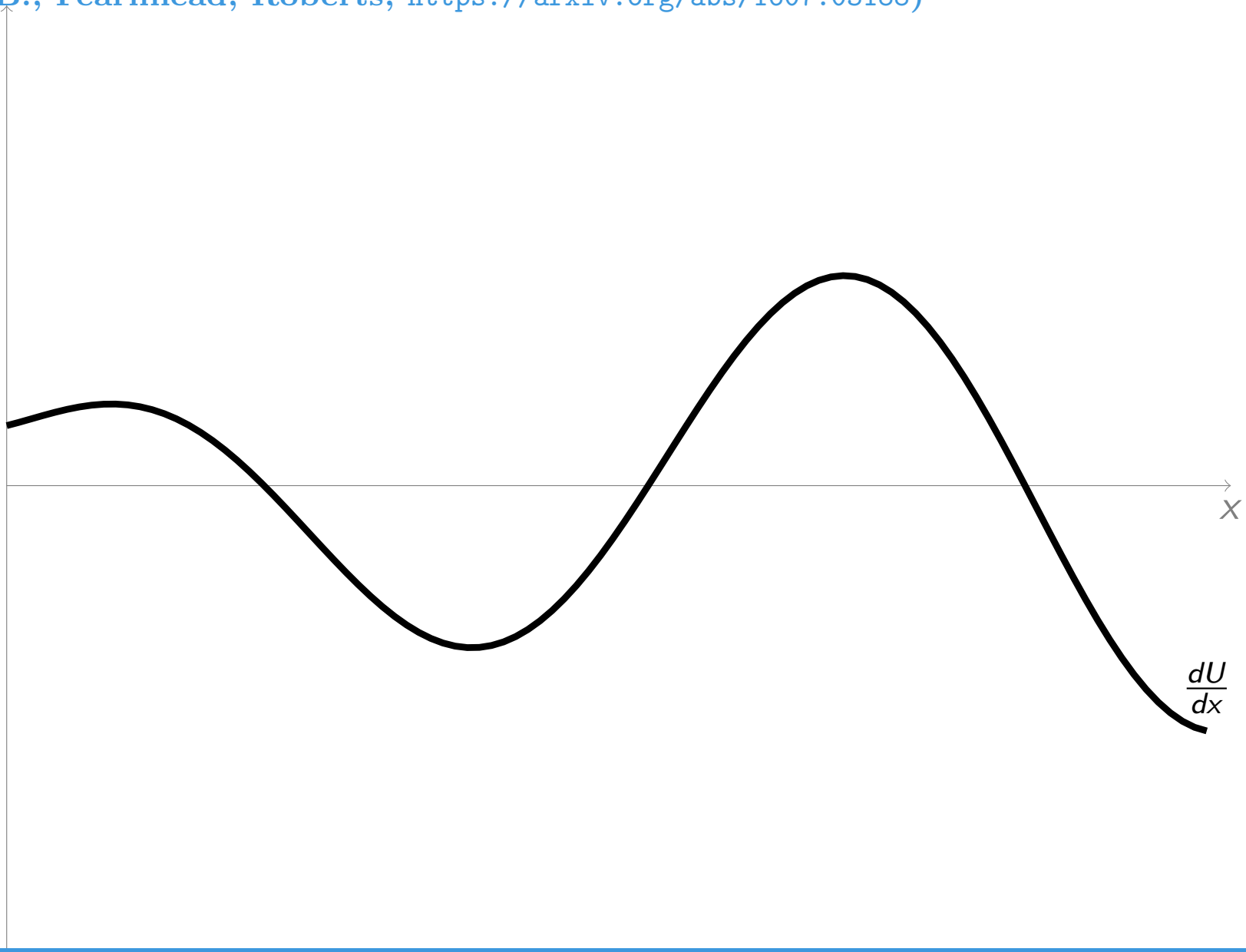


- Position $\boldsymbol{x} \in \mathbb{R}^d$, velocity $\boldsymbol{v} \in \mathbb{R}^d$
- Target distribution $\exp(-U(\boldsymbol{x}))\,\mu_0(d\boldsymbol{x}) \otimes \mu_0(d\boldsymbol{v})$ with $\mu_0 = \mathcal{N}(\mathbf{0}, \boldsymbol{\Sigma})$
- Hamiltonian dynamics for μ_0: $\dot{\boldsymbol{x}} = \boldsymbol{v}$, $\dot{\boldsymbol{v}} = -\boldsymbol{x}$
- Refreshment rate $\lambda_{\text{refr}} > 0$
- Reflection rate $\lambda(\boldsymbol{x}, \boldsymbol{v}) = \max(0, \langle \boldsymbol{v}, \nabla U(\boldsymbol{x}) \rangle)$
- U relative to Gaussian, so potentially fewer reflections than BPS, ZZ.

Next Section

Sampling

(B., Fearnhead, Roberts, https://arxiv.org/abs/1607.03188)



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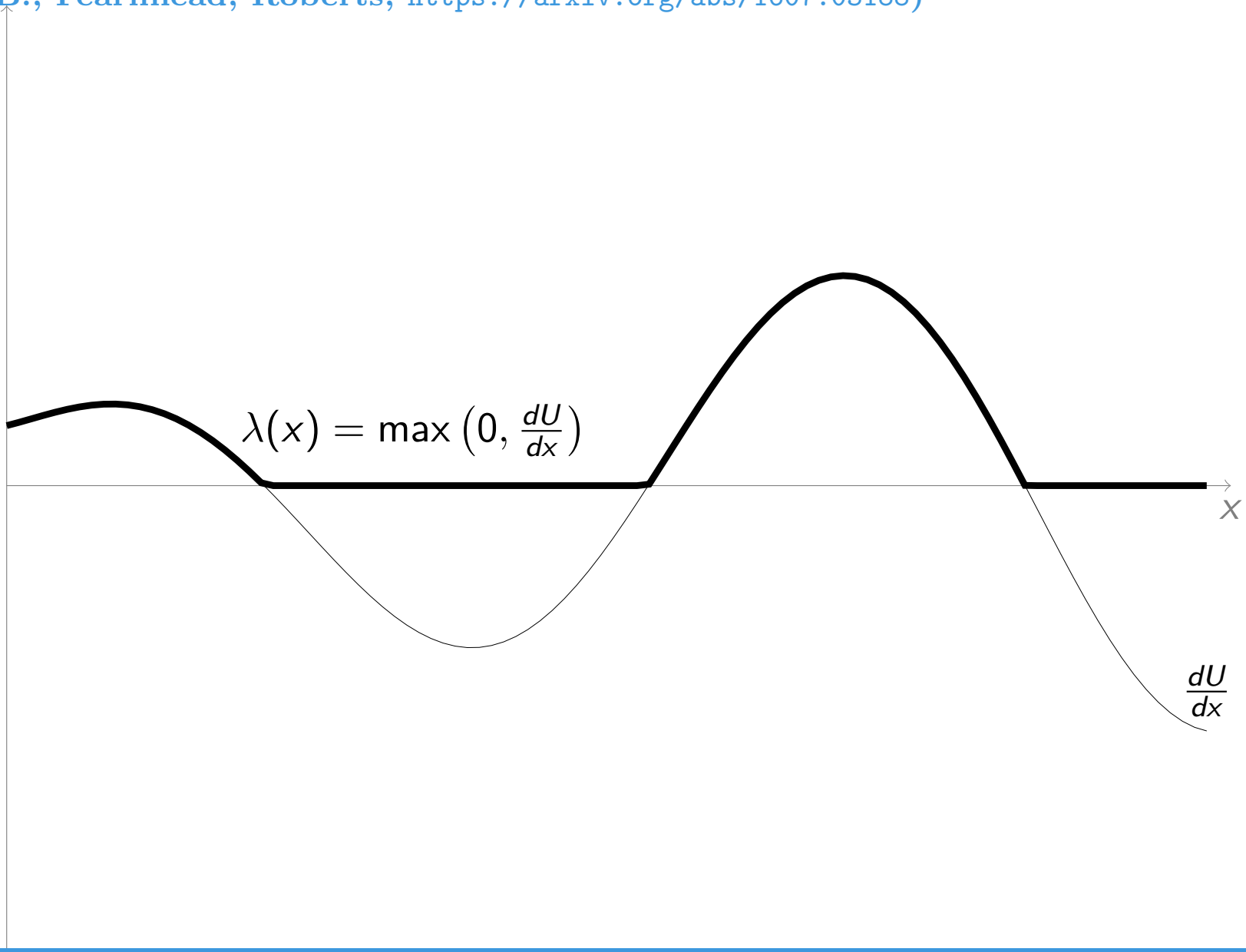

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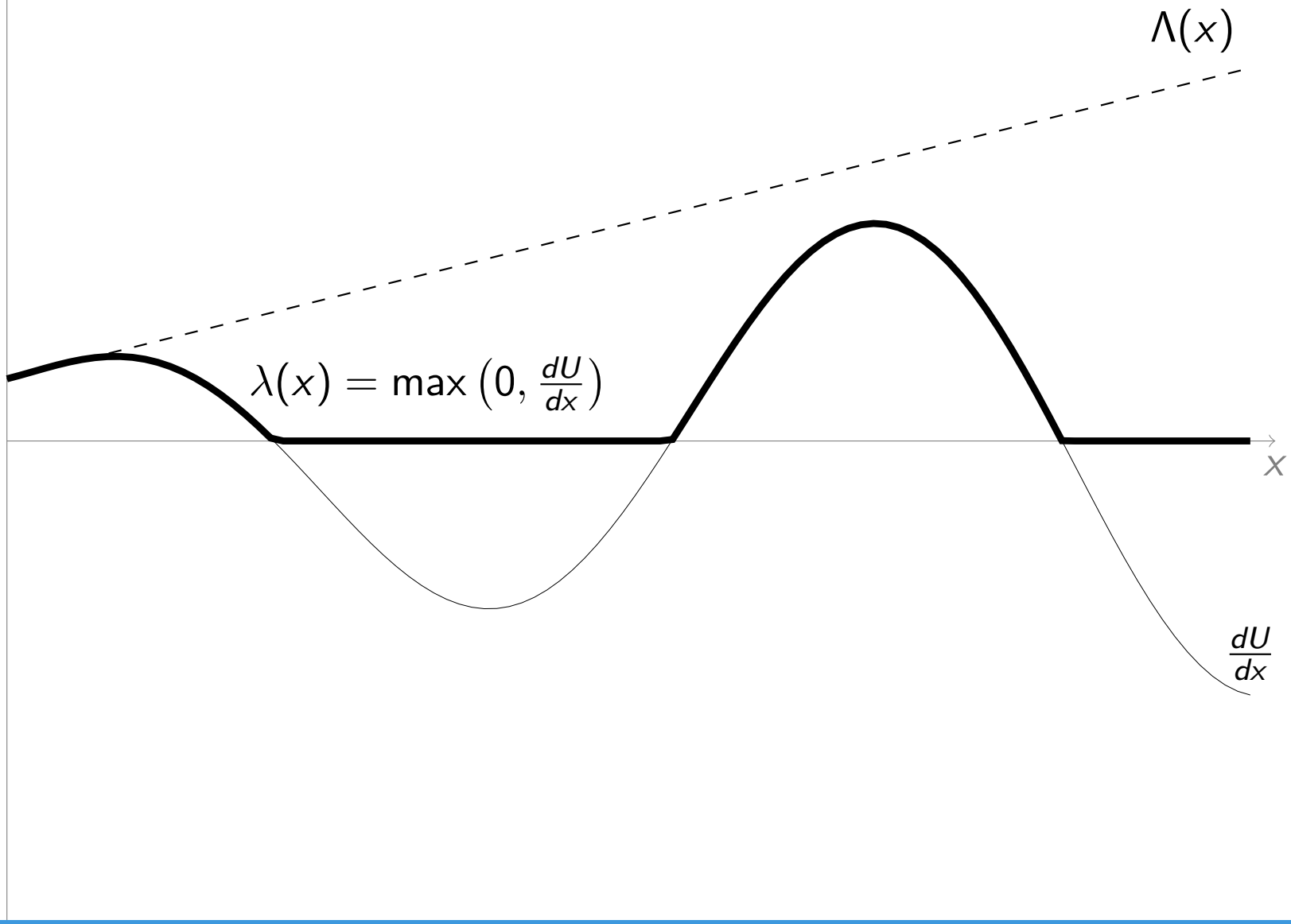

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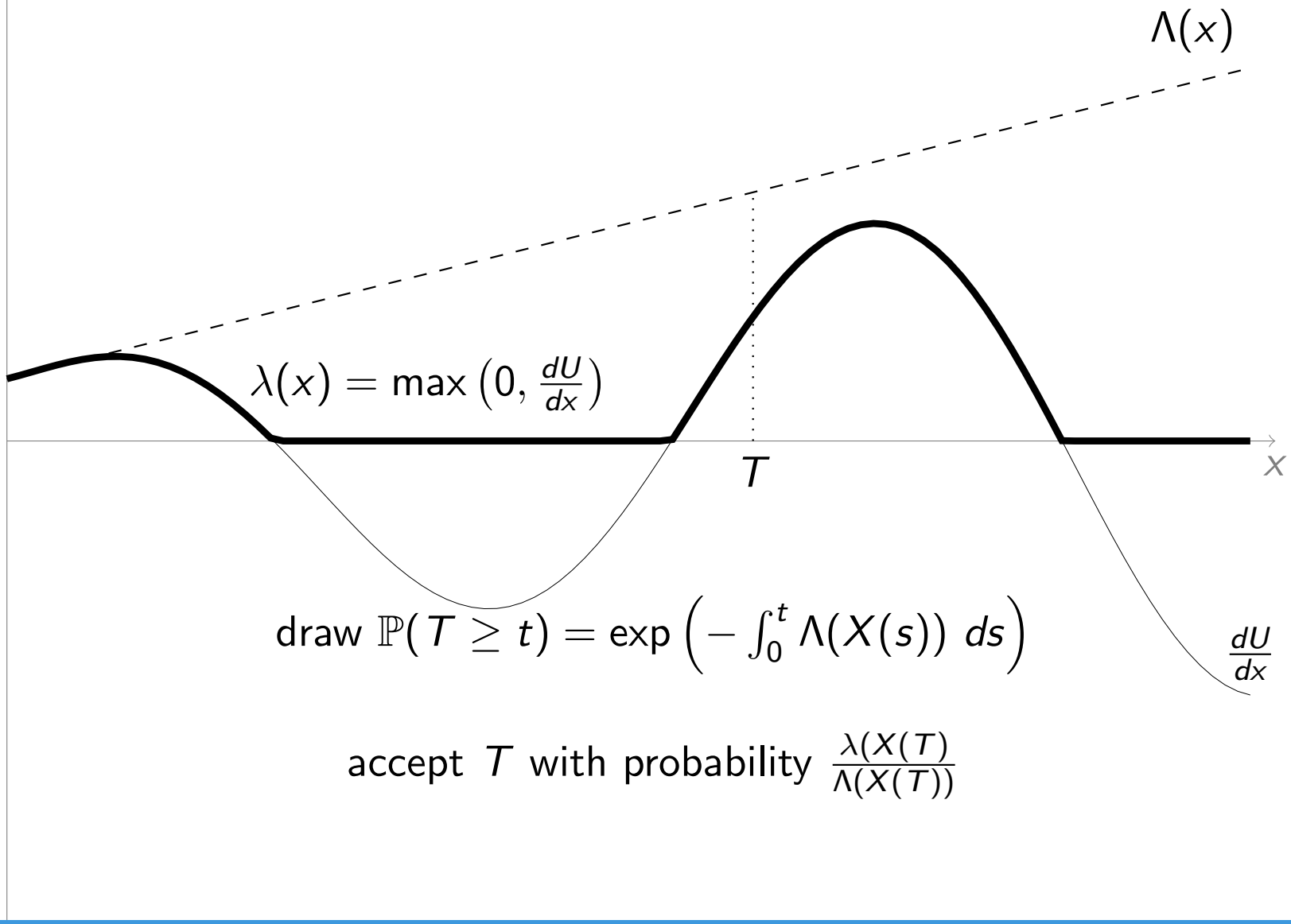
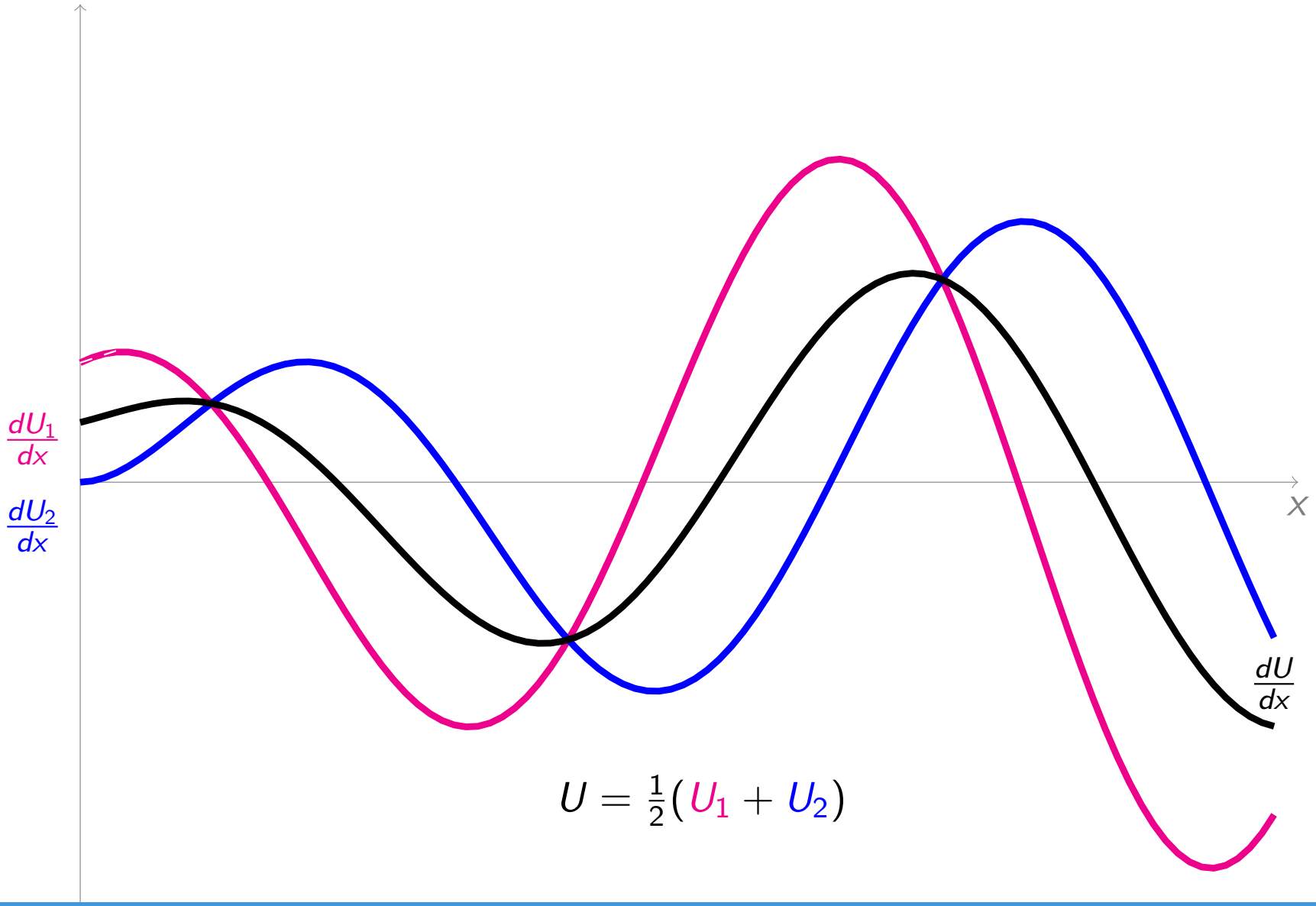


draw $\mathbb{P}(T \geq t) = \exp\left(-\int_0^t \Lambda(X(s))\, ds\right)$

accept T with probability $\frac{\lambda(X(T))}{\Lambda(X(T))}$

Subsampling

(B., Fearnhead, Roberts, https://arxiv.org/abs/1607.03188)



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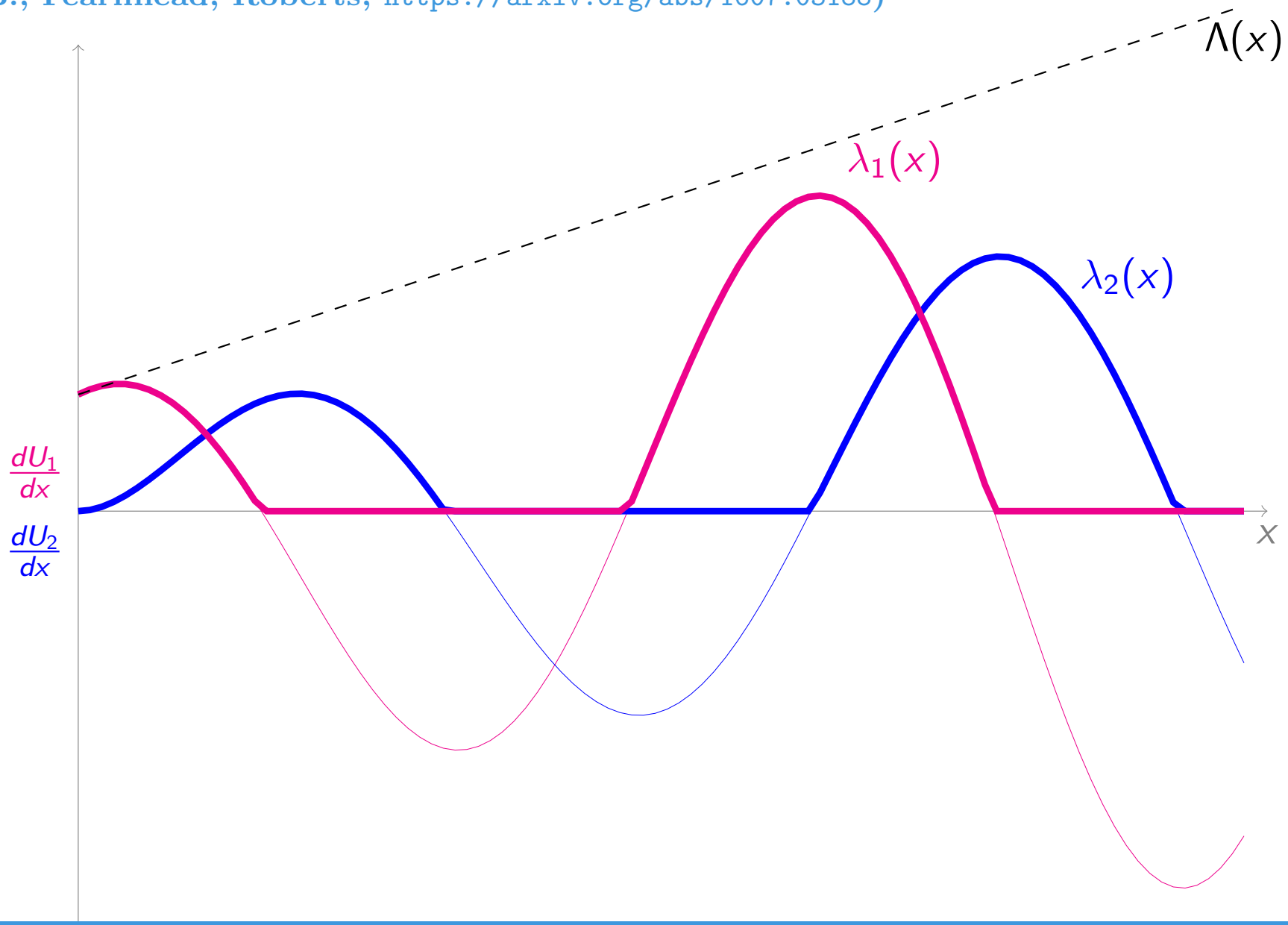

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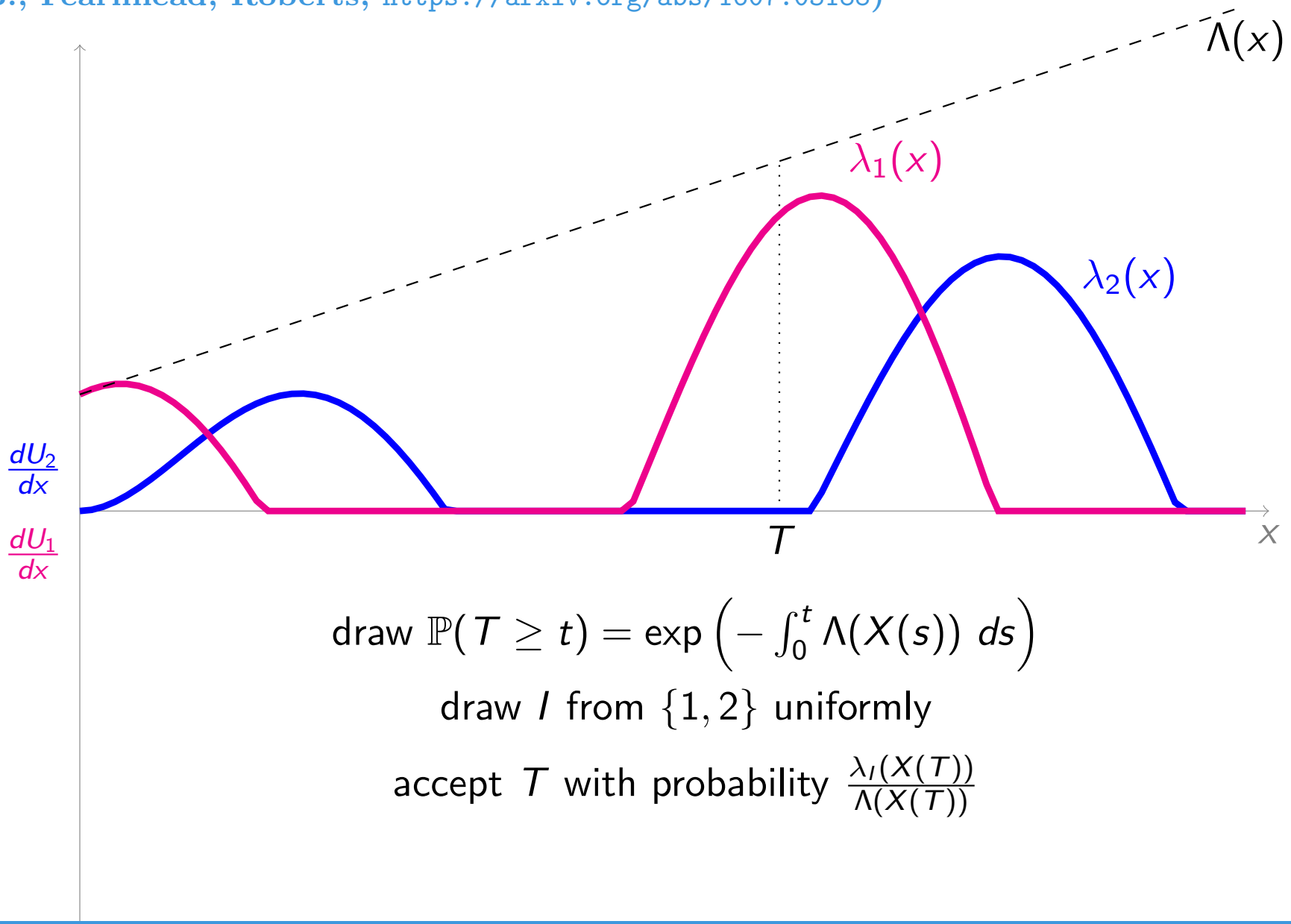


draw $\mathbb{P}(T \geq t) = \exp\left(-\int_0^t \Lambda(X(s))\, ds\right)$

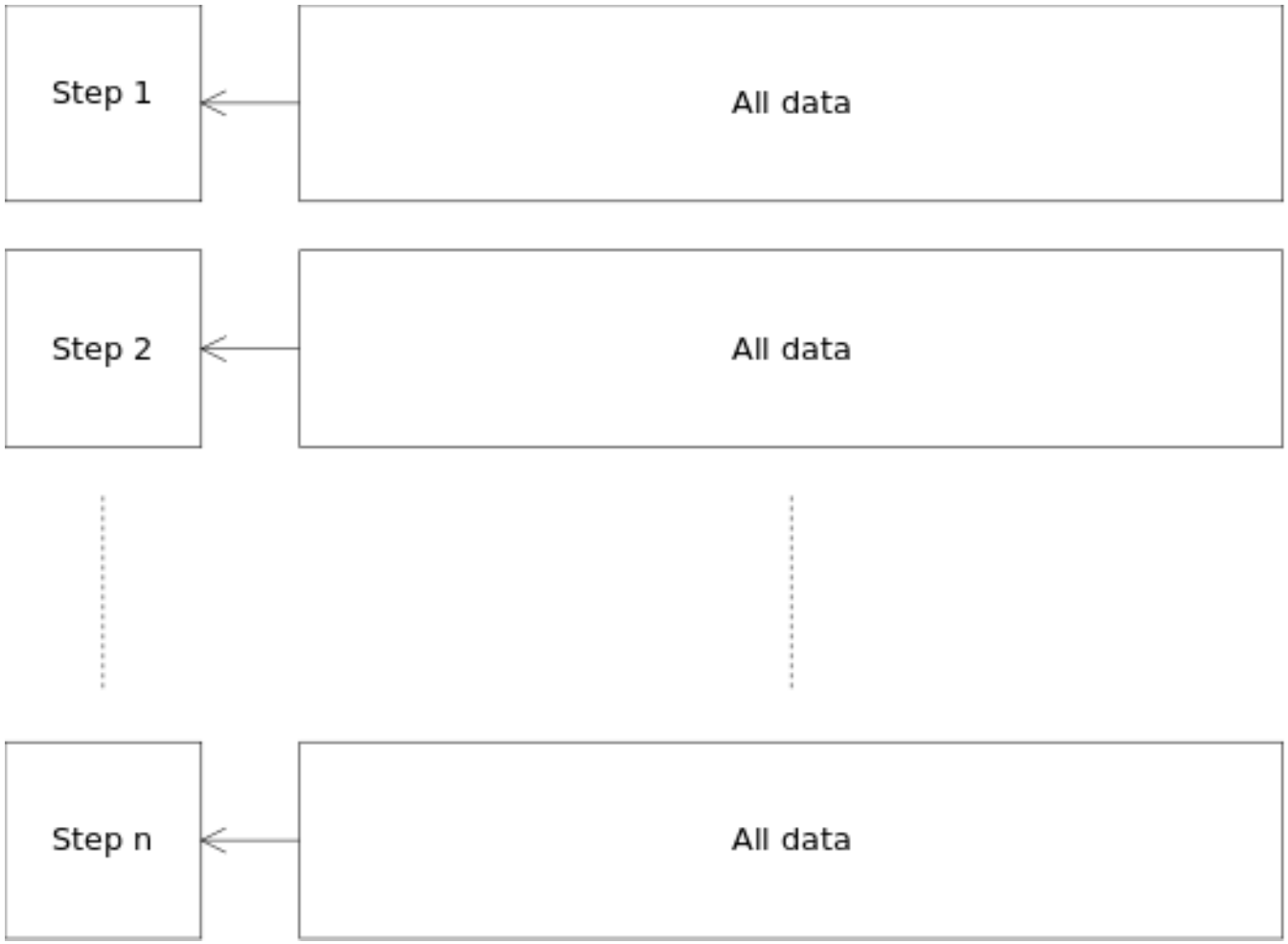
draw I from $\{1, 2\}$ uniformly

accept T with probability $\frac{\lambda_I(X(T))}{\Lambda(X(T))}$

Subsampling

$\pi(x) \propto \exp\left(-\sum_{i=1}^{n} U_i(x)\right)$

[B., Fearnhead, Roberts, 2016]



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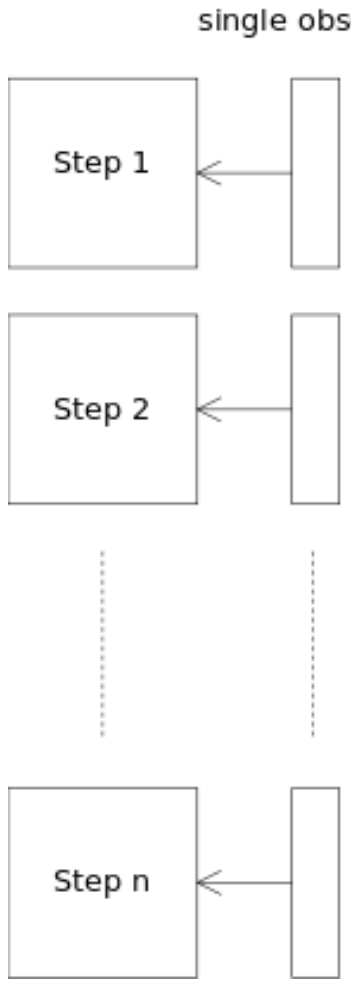


Improve efficiency by a factor n – without losing correctness

Control variates

(B., Fearnhead, Roberts, https://arxiv.org/abs/1607.03188)

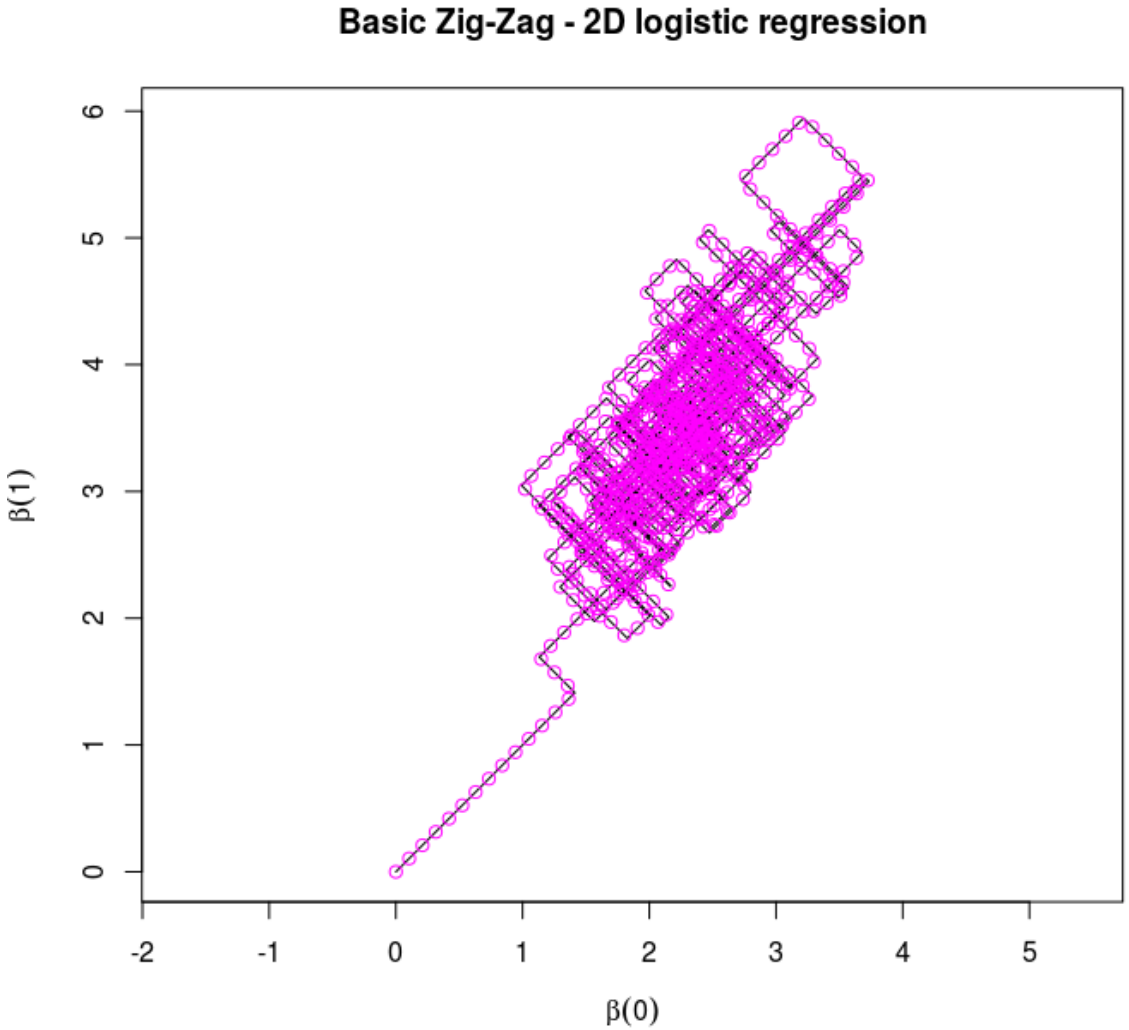
- $U(x) = \frac{1}{n} \sum_{i=1}^{n} U_i(x)$
- Let $x^\star$ denote (a point 'close' to) the mode of the posterior distribution.
- Naive subsampling: $\lambda_i(x, v) = (vU_i'(x))_+$.
- Control variates:

$$\lambda_i(x, v) = \left(v \left\{U_i'(x) + U'(x^\star) - U_i'(x^\star)\right\}\right)_+ .$$

- If x is close to the mode then $U_i'(x) - U_i'(x^\star)$ is small (under assumptions on U)
- So each $\lambda_i(x, v)$ is close to the 'ideal' switching rate $(vU'(x))_+$.

100 observations

(B., Fearnhead, Roberts, https://arxiv.org/abs/1607.03188)



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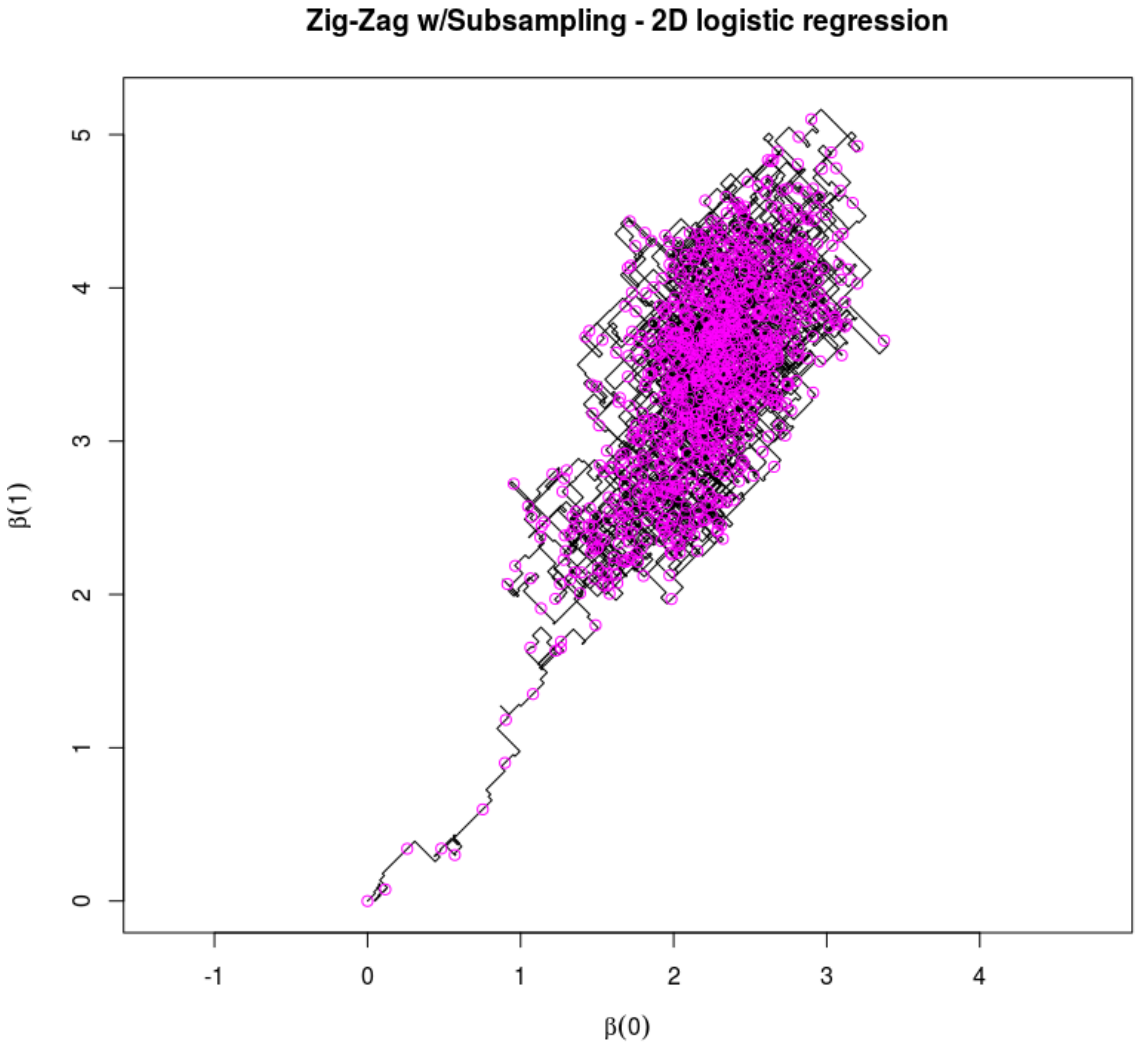

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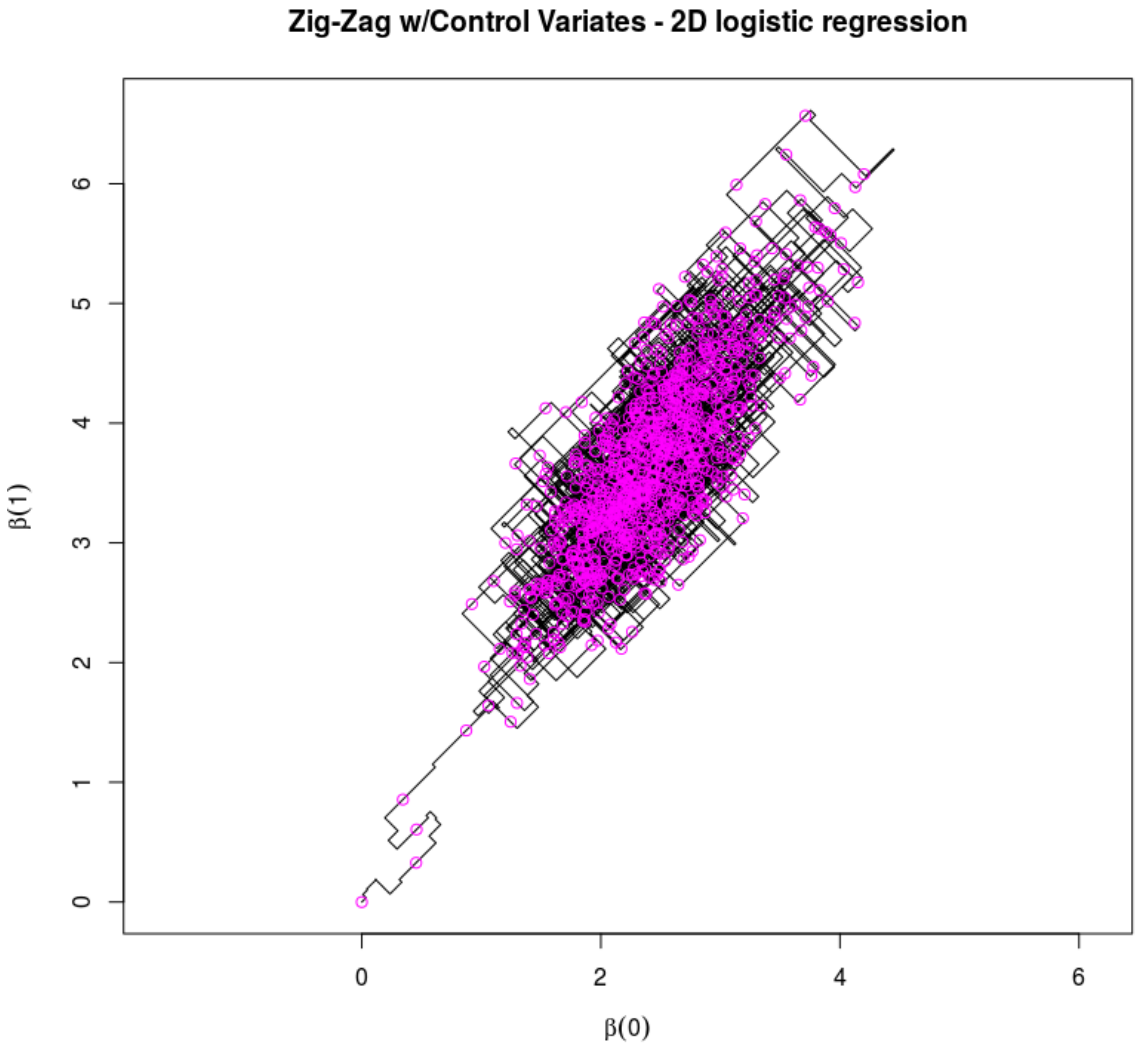
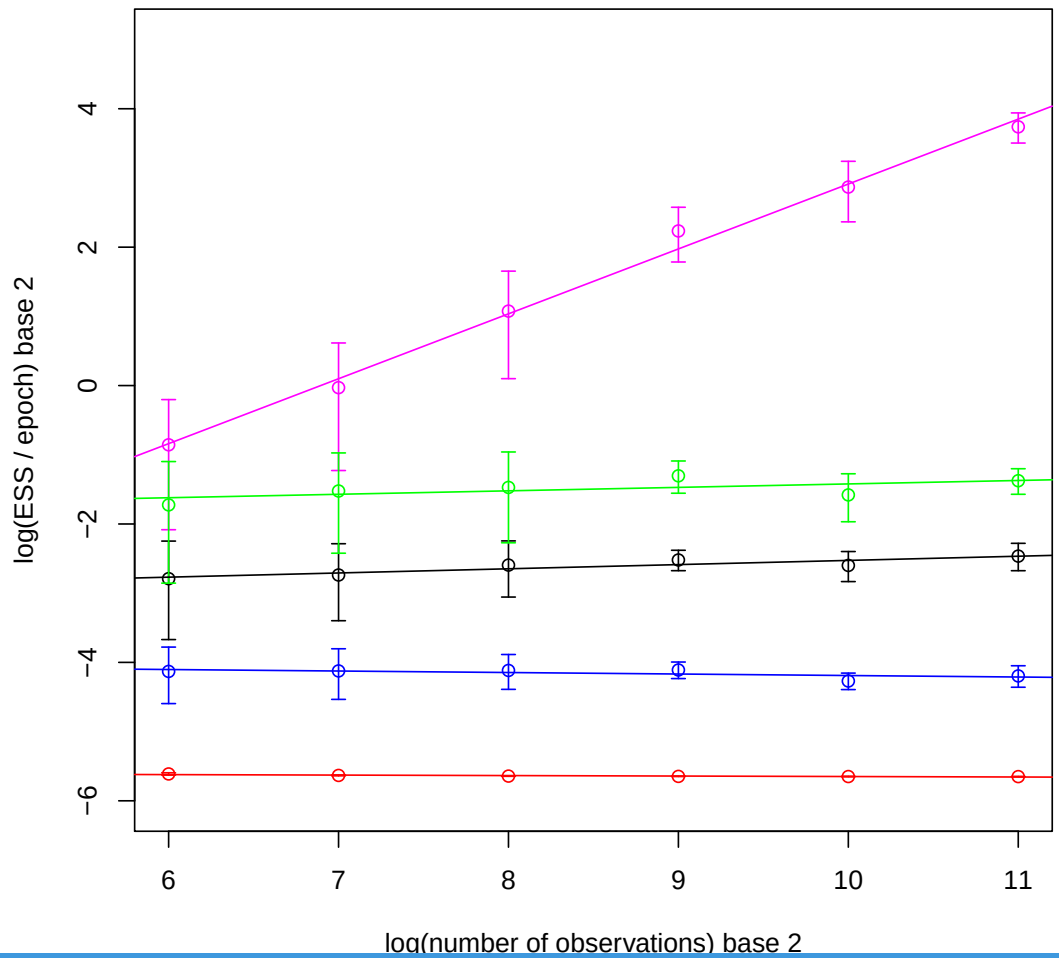


Scaling in number of observations

(B., Fearnhead, Roberts, https://arxiv.org/abs/1607.03188)

Zig-Zag, Zig-Zag w/Subsampling, Zig-Zag w/Control Variates, Zig-Zag with sub-optimal bound, MALA



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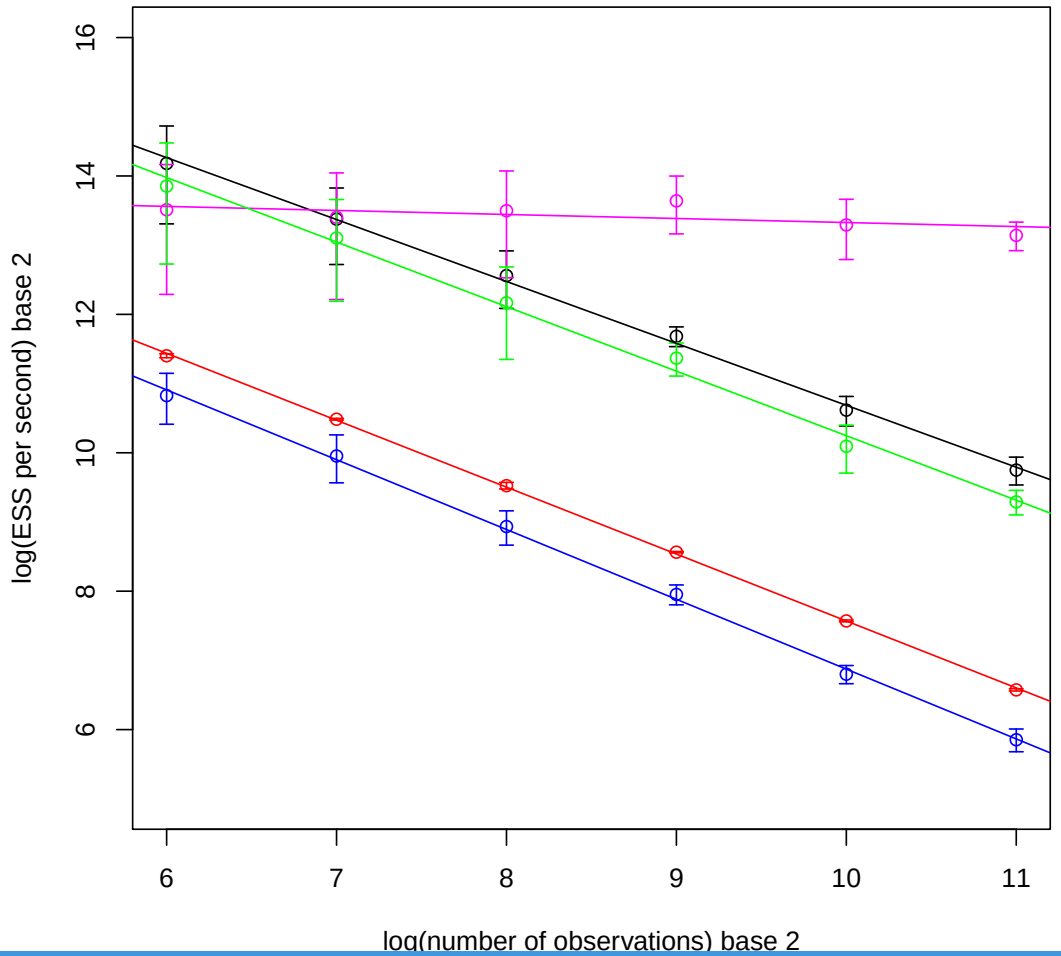
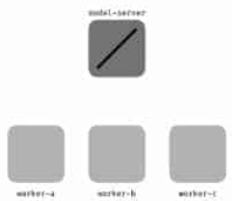
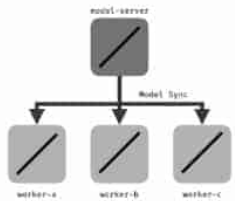
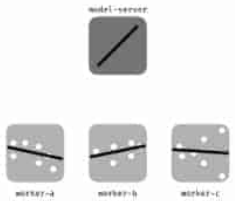
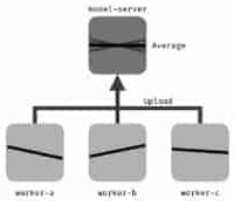


Next Section

Federated learning

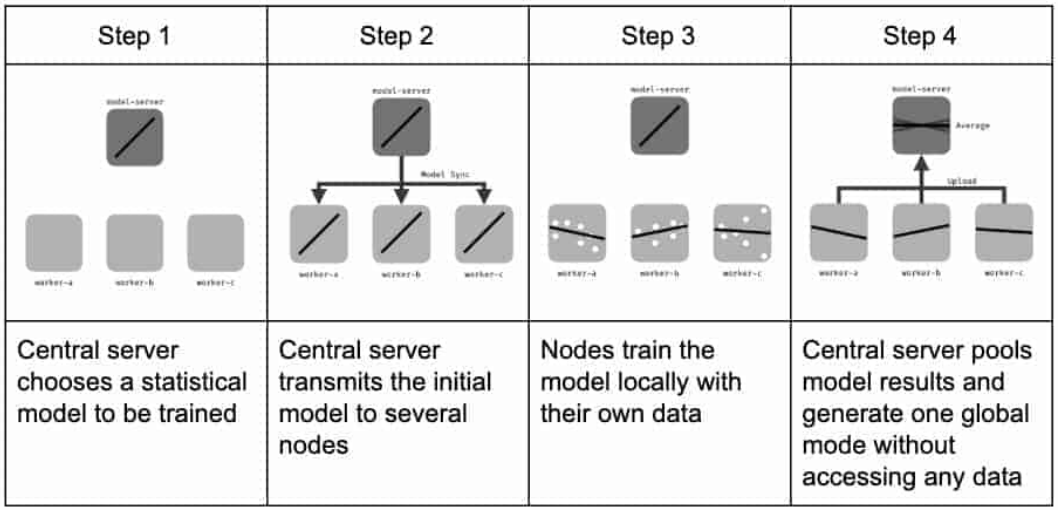
Federated learning (also known as *collaborative learning*) is a machine learning technique that trains an algorithm across multiple decentralized (...) servers holding local data samples, without exchanging them.

Step 1	Step 2	Step 3	Step 4
			
Central server chooses a statistical model to be trained	Central server transmits the initial model to several nodes	Nodes train the model locally with their own data	Central server pools model results and generate one global mode without accessing any data

Source: Wikipedia

Federated learning

Federated learning (also known as collaborative learning) is a machine learning technique that trains an algorithm across multiple decentralized (...) servers holding local data samples, without exchanging them.



Source: Wikipedia

Motivation

- Privacy
- Efficiency gains by distributed computation

Goal: Federated MCMC

Can we design a federated MCMC method?

The mth worker has access to local likelihood $f_m(y_m \mid x) = \exp(-U_m(x))$

Posterior $\pi(x) \propto \pi_0(x) \prod_{m=1}^{M} \exp(-U_m(x))$.

Wishlist

Our method should:

- Generate samples from π
- Workers do not (directly) communicate their local data (y_m)

Tool: Piecewise Deterministic Monte Carlo

Piecewise Deterministic Monte Carlo (PDMC) is a MCMC method based on continuous time, piecewise deterministic Markov processes.

Ingredients:

- Deterministic dynamics $t \mapsto \phi(t; z_0)$ from any initial position z_0.
- Jumping intensity $\lambda(z)$.
- Jump transition kernel $Q(z, dz')$.

Example: one-dimensional Zig-Zag

- $z = (x, v) \in \mathbb{R} \times \{-1, +1\}$
- $\phi(t; z_0) = (x_0 + v_0 t, v_0)$: linear motion in direction v_0
- $\lambda(z) = \lambda(x, v)$ satisfies $\lambda(x, +1) - \lambda(x, -1) = U'(x)$.
- $Q(z, dz') = \delta_x(dx') \otimes \delta_{-v}(dv')$: flip velocity

The switching intensity

Write $U(x) = \sum_{m=1}^{M} U_m(x)$.

Say $\pi(x) \propto \exp\left(-\sum_{m=1}^{M} U_m(x)\right) = \exp(-U(x))$ (flat prior).

Switching intensity condition

$$\lambda(x, +1) - \lambda(x, -1) = U'(x)$$

guarantees that the continuous time process (X_t, V_t) has marginal stationary density $\pi(x)$ for (X_t).

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Possible choices

- $\lambda_{\text{std}}(x, v) = \max(vU'(x), 0) = (vU'(x))_+$, then

$$\lambda_{\text{std}}(x, +1) - \lambda_{\text{std}}(x, -1) = (U'(x))_+ - (U'(x))_- = U'(x).$$

- By similar logic, may take

$$\lambda_{\text{fed}}(x, v) = \sum_{m=1}^{M} \lambda_m(x, v) = \sum_{m=1}^{M} (vU_m'(x))_+.$$

The switching intensity

We have seen that a valid switching intensity is

$$\lambda_{\text{fed}}(x, v) = \sum_{m=1}^{M} \lambda_m(x, v)$$

where $\lambda_m(x, v) = (vU_m'(x))_+$.

To simulate the first switching time τ, we have

$$\mathbb{P}(\tau \geq t) = \exp\left(-\int_0^t \sum_{m=1}^{M} \lambda_m(x + vs, v)\, ds\right)$$

Equivalent:

- simulate τ_m such that

$$\mathbb{P}(\tau_m \geq t) = \exp\left(-\int_0^t \lambda_m(x + vs, v)\, ds\right)$$

- set $\tau = \min\{\tau_1, \ldots, \tau_M\}$.

Federated Piecewise Deterministic Monte Carlo

Input: Initial condition $(x, v) \in \mathbb{R} \times \{-1, +1\}$.
Output: The sequence of skeleton points $(T_k, X_k, V_k)_{k=0}^{\infty}$.

1: Set $(T_0, X_0, V_0) = (0, x, v)$.
2: **for** $k = 0, 1, 2, \ldots$ **do**
3: Every machine simulates τ_m such that

$$\mathbb{P}(\tau_m \geq t) = \exp\left(-\int_0^t \lambda_m(X_k + sV_k, V_k)\, ds\right)$$

4: Set

$$\begin{aligned} \tau &= \min\{\tau_1, \ldots, \tau_M\}, \\ T_{k+1} &= T_k + \tau, \\ X_{k+1} &= X_k + \tau V_k, \\ V_{k+1} &= -V_k. \end{aligned}$$

5: **end for**

Efficiency

The computational efficiency of the algorithm is influenced by the switching intensity.

Large intensity $\Longrightarrow$ Many switches $\Longrightarrow$ Large computational overhead

Consider N 'data points' distributed equally over M machines,

$$U_m(x) = -\sum_{i=1}^{N/M} \log \underbrace{f(y_{m,i} \mid x)}_{\text{single observation likelihood}}.$$

For the standard rate λ_{std}, we have

$$\mathbb{E}_\pi \lambda_{\text{std}}(x,v) = \mathbb{E}_\pi \left(vU'(x)\right) \leq \tfrac{1}{2}\mathbb{E}_\pi |U'(x)| \leq \frac{1}{2}\left(\mathbb{E}_\pi |U'(x)|^2\right)^{1/2} = \mathcal{O}(N^{1/2}).$$

For the federated rate λ_{fed}, it turns out that 'typically' (Gaussian case)

$$\mathbb{E}_\pi \lambda_{\text{fed}}(x,v) = \mathcal{O}(M^{1/2}N^{1/2})$$

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Differential Privacy

Does the computation of switching times not give away too much information?

Differential privacy

Consider a random algorithm with output X based on data $y_1, \ldots, y_N$ and the same algorithm with 'one datum' y_i changed, with output $\tilde{X}$.
The algorithm is (ε, δ) differentially private if, for all sets S,

$$\mathbb{P}(X \in S) \leq \exp(\varepsilon)\mathbb{P}(\tilde{X} \in S) + \delta.$$

Differential Privacy

Theorem

Suppose $\lambda(t) \geq \rho$ *and* $|\lambda(t) - \tilde{\lambda}(t)| \leq K$ *for* $t \geq 0$ *and some constants* $\rho > 0$ *and* $K > 1$. *Then for any* $S \subset [0, \infty)$ *we have*

$$\mathbb{P}(\tau \in S) \leq \exp(\varepsilon)\mathbb{P}(\tilde{\tau} \in S) + \delta. \tag{1}$$

where $\varepsilon > \log\left(1 + \frac{K}{\rho}\right)$ *and*

$$\delta = \exp\left(-\frac{\rho}{K}\left[\varepsilon - \log\left(1 + \frac{K}{\rho}\right)\right]\right).$$

In particular, for $\varepsilon > 0$ *and* $\delta > 0$, *if*

$$\rho \geq K\left(\frac{1 + \log(1/\delta)}{\varepsilon}\right), \tag{2}$$

we have that (1) *holds.*

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Thank you!