

# Current developments in MCMC II: Comparison of Markov chains via weak Poincaré inequalities

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**CoSInES**



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  - Two examples of pseudo-marginal MCMC
- 2 Weak Poincaré inequalities
- 3 Application to pseudo-marginal MCMC
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  - Application to PMMH
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Can our results be extended into these settings?

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Given  $\pi$ -invariant Markov kernel  $P$ , it follows that  $P : L^2(\pi) \rightarrow L^2(\pi)$  given by

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Interested to study for  $f \in L^2(\pi)$ , how fast do we have

$$\|P^2 f - \pi(f)\|_2 \rightarrow 0.$$

# Exponential convergence and spectral gap

In many cases the convergence is exponential: for any  $f \in L^2(\pi)$ ,

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**Theorem** ([Andrieu, Lee, Power, Wang (2022a)], *c.f.* [Roberts, Gelman, Gilks (1997)])

*When the target  $\pi$  has a strongly concave and  $L$ -smooth potential, the **spectral gap** of RWM with proposal variance of  $d^{-1}$  on  $\mathbb{R}^d$  scales like*

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This is nice when applicable, but many chains actually converge at a **subgeometric rate** and have **0 spectral gap**.

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**Algorithm 1** (Marginal) Metropolis–Hastings (MH)

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1: initialise:  $X_0 = x_0, i = 0$ 
2: while  $i < N$  do
3:    $i \leftarrow i + 1$ 
4:   simulate  $Y_i \sim q(X_{i-1}, \cdot)$ 
5:    $\alpha(X_{i-1}, Y_i) = 1 \wedge \frac{q(Y_i, X_{i-1})\pi(Y_i)}{q(X_{i-1}, Y_i)\pi(X_{i-1})}$ 
6:   with probability  $\alpha(X_{i-1}, Y_i)$ 
7:      $X_i \leftarrow Y_i$ 
8:   else
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10: return  $(X_i)_{i=1, \dots, n}$ 
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# MH example



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$$\ell_y(x) = \prod_{i=1}^N f_x(y_i), \quad \text{or } \ell_y(x) = \int \int \cdots \int g(x, z, y) dz_1 dz_2 \cdots dz_N,$$

corresponding to ‘**big data**’ or **latent variable models**.

## Pseudo-marginal MH [Andrieu and Roberts (2009)]

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(One subtlety: need to ‘carry around’ the previous estimator  $\hat{\pi}(X_{n-1})$  in the next step rather than generating it again.)

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**Algorithm 2** Pseudo-marginal Metropolis–Hastings

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- 1: *initialise*:  $X_0 = x_0, i = 0$
  - 2: **while**  $i < N$  **do**
  - 3:      $i \leftarrow i + 1$
  - 4:     simulate  $Y_i \sim q(X_{i-1}, \cdot)$
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A miracle: with an unbiased estimator, this is still a valid algorithm which targets  $\pi$ .

# Pseudo-marginal RWM example

## Two examples of pseudo-marginal MH

We have replaced  $\pi(x)$  with a **stochastic estimator**  $\hat{\pi}(x)$  (which in practice could have a **large variance**), so we expect the performance of **pseudo-marginal MH** to be **worse** than the original **marginal MH**.

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Will consider two particular examples.

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- **Particle Marginal Metropolis–Hastings** (PMMH) [Andrieu et. al. (2010)] for inference with **time series** in **State Space Models** (SMMs), also known as **Hidden Markov Models** (HMMs).



# Example 1: Approximate Bayesian Computation (ABC)

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So instead we use an **approximate likelihood**:

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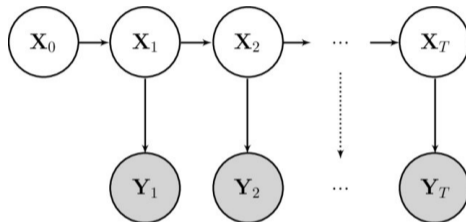
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N.B. the chain is almost always **subgeometric** [Lee and Łatuszyński (2014)].

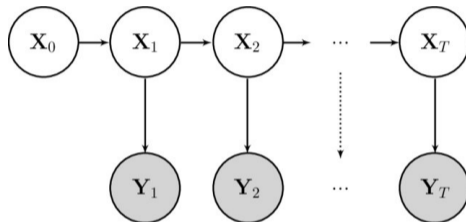
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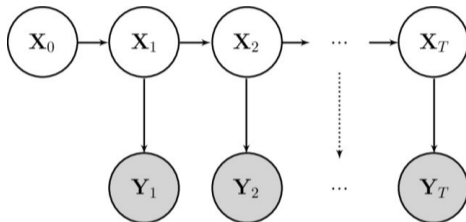


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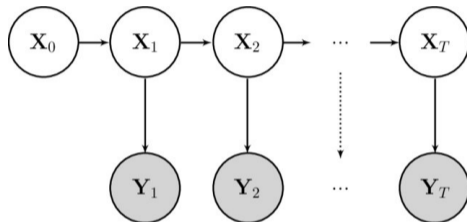


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Natural questions: **(subgeometric) convergence rate, how to tune the particle filter?**

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A first answer was given in [Andrieu and Vihola (2015)]: model  $\hat{\pi}(x) = W_x \cdot \pi(x)$ , with  $W_x \sim Q_x$  nonnegative and  $\mathbb{E}[W_x] = 1$ .

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Theorem ([Andrieu and Vihola (2015)])

*If the marginal MH is geometric, and the  $W_x$  are uniformly bounded, then the pseudo-marginal chain is geometric. If the  $W_x$  have unbounded support, then the chain is subgeometric.*

# Summary

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# Standard Poincaré inequalities

We work on  $L^2(\mu) = \{f : \mathcal{X} \rightarrow \mathbb{R} : \|f\|_2^2 < \infty\}$ ,  $\langle f, g \rangle := \int fg \, d\mu$ ,  
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For a  $\mu$ -invariant Markov transition kernel  $P$  with  $L^2(\mu)$ -adjoint  $P^*$ , define the **Dirichlet form**  $\mathcal{E}(P^*P, f)$ , for  $f \in L_0^2(\mu)$ :

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## Standard Poincaré inequality (SPI)

A **SPI** holds if there exists a constant  $C_P > 0$  such that for all  $f \in L_0^2(\mu)$ ,

$$C_P \|f\|_2^2 \leq \mathcal{E}(P^*P, f).$$



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## Theorem (Geometric convergence)

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*Proof.* Rewriting the SPI, see  $\mathcal{E}(P^*P, f)$  behaves like a *discrete derivative*:

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$$\begin{aligned} C_P \|f\|_2^2 &\leq \mathcal{E}(P^*P, f) = \|f\|_2^2 - \langle P^*P f, f \rangle \\ &= \|f\|_2^2 - \|P f\|_2^2 \\ \Rightarrow \|P f\|_2^2 &\leq (1 - C_P) \|f\|_2^2. \end{aligned}$$

$$C_P \|f\|_2^2 \leq \mathcal{E}(P^*P, f).$$

## Theorem (Geometric convergence)

Under a *standard Poincaré inequality*, we have for all  $f \in L_0^2(\mu)$ ,  $n \in \mathbb{N}_0$ ,

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The rest is by induction.  $\square$

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A **WPI** holds if: for some such  $\beta, \Phi, \forall s > 0, f \in L_0^2(\mu)$ ,

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E.g.  $\beta(s) = c_0 s^{-c_1}$ .

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Call this final inequality optimized WPI (**oWPI**).

## Proof of convergence bound (II)

Now define

$$F(x) := \int_x^1 \frac{dv}{K^*(v)}, \quad x \in (0, a], \quad h_n := \frac{\|P^n f\|_2^2}{\Phi(f)}.$$

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So we invert this to obtain

$$\|P^n f\|_2^2 \leq \Phi(f) F^{-1}(n). \quad \square$$

Theorem ([Andrieu, Lee, Power, Wang (2022)])

Under a *weak Poincaré inequality*, we have,  $\forall n \in \mathbb{N}_0$ ,  $f \in L_0^2(\mu)$ ,

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Intuition: the **faster**  $\beta$  decays, the **faster** the rate of convergence.



- 1 Introduction: Bayesian inference on modern datasets
- 2 Weak Poincaré inequalities
- 3 Application to pseudo-marginal MCMC**
  - Application to ABC
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# Application to pseudo-marginal MCMC

Recall our goal was to precisely characterise the degradation in convergence when using a pseudo-marginal chain with  $\hat{\pi}(x) = W_x \cdot \pi(x)$  compared to the marginal MH chain with  $\pi(x)$ .

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Have  $W_x \sim Q_x$  nonnegative with  $\mathbb{E}[W_x] = 1$ , and set  $\tilde{\pi}_x(dw) := Q_x(dw)w$ .

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**Theorem ([Andrieu, Lee, Power, Wang (2022)])**

*We have for any  $s > 0$ ,  $f \in L_0^2(\mu)$  bounded,*

$$\mathcal{E}(P, f) \leq s \mathcal{E}(\tilde{P}, f) + \beta(s) \|f\|_{\text{osc}}^2,$$

*where*

$$\beta(s) := \int_{\mathcal{X}} \tilde{\pi}_x(w \geq s) \pi(dx), \quad s > 0.$$

# Application 1: Approximate Bayesian Computation (ABC)

We run an MCMC chain targeting the ABC posterior, true likelihood  $\ell_y(x) = f_x(y)$ ,

$$\pi_{\text{ABC}}(x) \propto \nu(x)\ell_{\text{ABC}}(x),$$

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This is further approximated using a pseudo-marginal approach:  $\mathcal{W}_M := \frac{1}{M} \sum_{j=1}^M W_j$ ,

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Theorem ([Andrieu, Lee, Power, Wang (2022)])

Suppose that  $\int_{\mathcal{X}} \nu(x) \ell_{\text{ABC}}^{-(p-1)}(x) dx < \infty$ . Then there is  $C_{M,p} > 0$  such that for all  $s > 0$ ,

$$\beta(s) = \int_{\mathcal{X}} \pi(dx) \tilde{\pi}_x(\mathcal{W}_M \geq s) \leq C_{M,p} s^{-p},$$

and as  $M \rightarrow \infty$ ,  $C_{M,p} = 1 + O(1/M)$ . The convergence rate for the chain is  $O(n^{-p})$ .



## Application 2: Particle Marginal Metropolis–Hastings (PMMH)

PMMH is a well-established algorithm to perform MCMC, e.g. for state space models [Andrieu et. al. (2010)].

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Theorem ([Andrieu, Lee, Power, Wang (2022)])

Assume the marginal chain satisfies a *SPI*. Then we have the convergence bound,  $\forall n \in \mathbb{N}$ ,

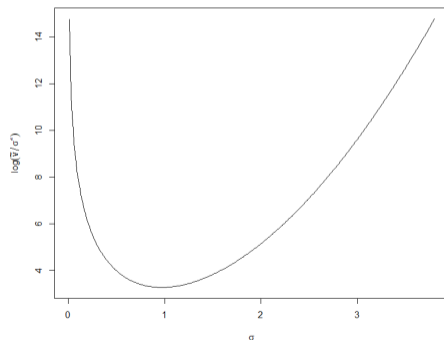
$$F_{\text{PMMH}}^{-1}(n) \leq \frac{2}{C_P} \exp \left\{ -\frac{1}{2\sigma^2} W^2 \left( \frac{C_P \sigma^2}{2 \exp(\sigma^2/2)} \cdot n \right) \right\},$$

$W$  is the Lambert function (inverse of  $x \mapsto xe^x$ ).

## Application to Particle Marginal Metropolis–Hastings (PMMH) II

To minimize the **asymptotic variance** taking into account the **computational cost**, (*c.f.* our results for **convergence bounds** and **mixing times**), tune algorithm so that

$$\sigma \approx 0.973.$$



# Summary

I introduced the framework of [Andrieu, Lee, Power, Wang (2022)]: weak Poincaré inequalities for Markov chains, as a new tool to compare convergence of Markov chains, which covers subgeometric convergence.

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Combined with our results for this morning for RWM, this enables us to give complete convergence bounds for **psuedo-marginal RWM**.

Further fundamental theory in our follow-up report [Andrieu, Lee, Power, Wang (2022b)].

Later today: comparisons for **slice sampling**.

- 1 Introduction: Bayesian inference on modern datasets
- 2 Weak Poincaré inequalities
- 3 Application to pseudo-marginal MCMC
- 4 References**

# Thanks for listening! I



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# Thanks for listening! II



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# Thanks for listening! III



Röckner, M., Wang, F.-Y. (2001). Weak Poincare Inequalities and  $L^2$  Convergence Rates of Markov Semigroups. *J. Funct. Anal.*, 185, 564-603.



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Posit a model (density function)  $f_x(y)$  which generated  $y$ , which depends upon **parameters**  $x \in \mathcal{X} = \mathbb{R}^d$ .

Seek **learn** or **infer** values of the **parameter**  $x$  which are **commensurate** with the observed dataset  $y$ .



# The Bayesian approach

Encode prior beliefs into a **prior distribution**  $\nu(x)$ , and define **likelihood**  $\ell_y(x) := f_x(y)$ .

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We are then interested in quantities of the form

$$I = \pi(f) = \int_{\mathcal{X}} f(x)\pi(x) dx,$$

e.g.  $f(x) = \|x\|^p$  (**posterior moments**),  $f(x) = 1_A(x)$  (**credible sets / posterior tail probabilities**), etc.

# Sampling

So we wish to **evaluate integrals**

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Will not be discussing optimization-based approaches such as **Variational Inference, INLA, ...**

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We simulate a  $\pi$ -reversible ergodic Markov chain,

$$X_1, X_2, \dots$$

where  $X_n \rightarrow \pi$  in distribution and considering

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We will focus on **random walk Metropolis–Hastings** (RWM):  $q(X_{i-1}, \cdot) = \mathcal{N}(X_{i-1}, \Sigma)$ .

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Theorem ([Roberts and Tweedie (1996), Jarner and Hansen (2000)])

*RWM converges to equilibrium **exponentially** fast if\* and only if  $\pi$  has an **exponential moment** (e.g.  $\pi(x) \propto \exp(-\|x - \mu\|^\alpha)$ ,  $\alpha \geq 1$ ). Otherwise, the chain converges at a **subgeometric** (e.g. **polynomial**) rate.*



## Reversibility and positivity

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The following MCMC chains are **positive**: **Random Walk Metropolis** with Gaussian proposals, the **Independence Sampler**, and **pseudo-marginal MH** built from any of these chains.

Theorem [Andrieu, Lee, Power, Wang (2022)]

For a **positive** kernel  $P$ , we have for all  $f \in L^2(\mu)$ ,

$$\mathcal{E}(P, f) \leq \mathcal{E}(P^2, f).$$

Therefore a **WPI for  $P$**  implies a **WPI for  $P^*P = P^2$** .

## WPIs

We have discussed **WPIs** of the form:

$$\|f\|_2^2 \leq s\mathcal{E}(P, f) + \beta(s)\Phi(f), \quad \forall s > 0, \quad \forall f \in L_0^2(\mu). \quad (1)$$

# Comparison of Markov chains

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In order to **compare Markov chains**, we will consider a more general form of inequalities.

## General comparison inequality

For two (reversible) Markov kernels  $P, P_2$ :

$$\mathcal{E}(P_1, f) \leq s\mathcal{E}(P_2, f) + \beta(s)\Phi(f), \quad \forall s > 0, \quad \forall f \in L_0^2(\mu). \quad (2)$$

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Intuition: (2) gives a bound on the convergence of  $P_2$  relative to the convergence rate of  $P_1$ .



# General comparison result

Theorem ([Andrieu, Lee, Power, Wang (2022)])

Let  $P_1, P_2$  be two  $\mu$ -invariant Markov kernels on  $E \times \mathcal{F}$ . Assume that for any  $(x, B) \subset E \times \mathcal{F}$ ,

$$P_2(x, B \setminus \{x\}) \geq \int_{B \setminus \{x\}} \epsilon(x, y) P_1(x, dy),$$

for some  $\epsilon : E^2 \rightarrow (0, \infty)$ .

Then for any  $s > 0$ ,  $f \in L_0^\infty(\mu) \subset L_0^2(\mu)$ ,

$$\mathcal{E}(P_1, f) \leq s \mathcal{E}(P_2, f) + \frac{1}{2} \mu \otimes P_1(A(s)^c \cap \{X \neq Y\}) \Phi(f),$$

where  $A(s) := \{(x, y) \in E^2 : s \epsilon(x, y) > 1\}$ , and

$$\Phi(f) := \|f\|_{\text{osc}}^2.$$

## General comparison result - remarks

What we need to show is

$$P_2(x, B \setminus \{x\}) \geq \int_{B \setminus \{x\}} \epsilon(x, y) P_1(x, dy),$$

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If  $\inf_{x,y} \epsilon(x, y) > 0$ , then we will get a **SPI / geometric convergence**.

If we aren't interested in comparisons, but want an (absolute) **WPI**, note that if  $P(x, dy) = \pi(dy)$  represents **perfect sampling**, then  $\mathcal{E}(P, f) = \|f\|_2^2$ , and there is the useful representation (exercise!)

$$\|f\|_2^2 = \frac{1}{2} \int \pi(x)\pi(y)[f(y) - f(x)]^2 dx dy.$$

# Independence Sampler: geometric case

The **Independence Sampler** (IS) is one the simplest MCMC methods: given target  $\pi$ , at each step sample **proposal**  $Y_i \sim q$ , and accept with probability

$$\alpha(X_{i-1}, Y_i) = 1 \wedge \frac{q(X_{i-1})\pi(Y_i)}{\pi(X_{i-1})q(Y_i)} = 1 \wedge \frac{w(Y_i)}{w(X_{i-1})}.$$

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Well-known that there is a **spectral gap** if and only if the **weights are bounded**:

$$w(x) := \frac{\pi(x)}{q(x)} \leq M, \quad \forall x \in \mathcal{X}.$$

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(E.g. if so, then you can just do rejection sampling.) The kernel is

$$P(x, dy) = q(y) \cdot 1 \wedge \frac{w(y)}{w(x)} dy + (1 - \alpha(x))\delta_x(dy).$$



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- 1 Use the general comparison theorem to establish a WPI for the Independence Sampler (i.e. show that  $P(x, y) \geq \epsilon(x, y)\pi(y)$  for an appropriate function  $\epsilon(x, y)$ ).
- 2 Directly deduce a WPI for the Independence Sampler using the useful representations below.

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Useful representations (exercise!):

$$\|f\|_2^2 = \frac{1}{2} \int \pi(x)\pi(y)[f(y) - f(x)]^2 dx dy,$$

$$\mathcal{E}(P, f) = \frac{1}{2} \int \pi(x)\pi(y) \left( w^{-1}(x) \wedge w^{-1}(y) \right) [f(x) - f(y)]^2 dx dy.$$

# Independence Sampler: subgeometric case

Suppose the weights are unbounded, namely

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The previous representation of  $\mathcal{E}(P, f)$  immediately gives us a WPI for the subgeometric IS: take

$$\epsilon(x, y) = \left( w^{-1}(x) \wedge w^{-1}(y) \right),$$

then

$$A(s) = \left\{ (x, y) \in E \times E : \left( w^{-1}(x) \wedge w^{-1}(y) \right) \geq 1/2 \right\}.$$

# Pseudo-marginal derivation

The WPI for pseudo-marginal is derived in almost the same way as for the **Independence Sampler!**

We work on the augmented state space  $\mathcal{X} \times [0, \infty)$ .

The pseudo-marginal kernel  $\tilde{P}$  is given by:  $\tau(x, y)$  is the standard MH acceptance ratio,

$$\tilde{P}(x, w; dy, du) = \left[ 1 \wedge \left\{ \tau(x, y) \frac{u}{w} \right\} \right] q(x, dy) Q_y(du) + \delta_{x,w}(dy, du) \tilde{\rho}(x, w),$$

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which we compare to the standard MH, on the extended state space:

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The problematic region is when  $w$  gets large. We take

$$\epsilon(x, w; y, u) = w^{-1} \wedge u^{-1}.$$