EPSRC

Engineering and Physical Sciences
Research Council





SPECIAL

CASES

OUR APPROACH

REFERENC

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We want to sample from some target distribution

$$\pi(\boldsymbol{\theta}) = \frac{f(\boldsymbol{\theta})}{C}$$

but only have a noisy unbiased estimator for $f(\theta)$

$$\hat{f}\left(oldsymbol{ heta};\,oldsymbol{u}
ight)\;:\;\;\mathbb{E}_{q\left(oldsymbol{u}
ight)}\left[\hat{f}\left(oldsymbol{ heta};\,oldsymbol{u}
ight)
ight]=f\left(oldsymbol{ heta}
ight)$$

 \boldsymbol{u} random variates used in estimator $\sim q(\cdot)$

Marginal likelihood $p(\boldsymbol{y} \mid \boldsymbol{\theta}) = \int p(\boldsymbol{y} \mid \boldsymbol{z}, \boldsymbol{\theta}) p(\boldsymbol{z} \mid \boldsymbol{\theta}) d\boldsymbol{z}$

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$$f(\boldsymbol{\theta}) = p(\boldsymbol{y} \mid \boldsymbol{\theta}) p(\boldsymbol{\theta}) \quad \hat{f}(\boldsymbol{\theta}; \, \boldsymbol{u}) = \frac{p(\boldsymbol{y} \mid \mathsf{z}(\boldsymbol{u}), \boldsymbol{\theta}) p(\mathsf{z}(\boldsymbol{u}) \mid \boldsymbol{\theta}) p(\boldsymbol{\theta})}{\mathcal{N}(\mathsf{z}(\boldsymbol{u}); \, \boldsymbol{\mu}, \, \boldsymbol{\Sigma})} \quad q(\boldsymbol{u}) = \mathcal{N}(\boldsymbol{u}; \, \boldsymbol{0}, \, \boldsymbol{I})$$

z deterministic function $\mathbf{z}(\boldsymbol{u}) = \boldsymbol{\mu} + \operatorname{chol}(\boldsymbol{\Sigma}) \mathbf{u}$ $\boldsymbol{\mu}, \boldsymbol{\Sigma}$ Gaussian approximation $\mathcal{N}(\boldsymbol{z}; \boldsymbol{\mu}, \boldsymbol{\Sigma}) \approx p(\boldsymbol{z} \mid \boldsymbol{y}, \boldsymbol{\theta})$

Likelihood
$$p(\boldsymbol{y} | \boldsymbol{\theta}) = \frac{g(\boldsymbol{y}; \boldsymbol{\theta})}{Z(\boldsymbol{\theta})}$$
 with $Z(\boldsymbol{\theta})$ intractable

$$f(\boldsymbol{\theta}) = g(\boldsymbol{y}; \boldsymbol{\theta}) p(\boldsymbol{\theta}) \frac{Z(\hat{\boldsymbol{\theta}})}{Z(\boldsymbol{\theta})} \quad \hat{f}(\boldsymbol{\theta}; \boldsymbol{u}) = g(\boldsymbol{y}; \boldsymbol{\theta}) p(\boldsymbol{\theta}) \frac{g(\mathbf{y}(\boldsymbol{u}); \hat{\boldsymbol{\theta}})}{g(\mathbf{y}(\boldsymbol{u}); \boldsymbol{\theta})} \quad \boldsymbol{q}(\boldsymbol{u}) = \mathcal{U}(\boldsymbol{u})$$

- y deterministic function $\boldsymbol{u} \sim \mathcal{U}(\cdot) \Rightarrow y(\boldsymbol{u}) \sim p(\cdot \mid \boldsymbol{\theta})$
- $\hat{\boldsymbol{\theta}}$ fixed set of reference parameters

Pseudo-Marginal (PM) MCMC, as analysed in Andrieu and Roberts (2009):

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Inputs: current parameters $\boldsymbol{\theta}$, previous estimate of unnormalized target probability \hat{f} , proposal dist. $r(\boldsymbol{\theta}'; \boldsymbol{\theta})$, unbiased estimator : $\mathbb{E}_{\epsilon(\hat{f}; \boldsymbol{\theta})} \left[\hat{f} \right] = f(\boldsymbol{\theta}) \ \forall \ \boldsymbol{\theta}$,

Output: new state-estimate pair (θ, \hat{f}) .

1. Propose new state and estimate its probability:

$$m{ heta}' \sim r(\,\cdot\,;\,m{ heta})$$
 $\hat{f}' \sim \epsilon(\,\cdot\,;\,m{ heta}')$

2. Metropolis-Hastings style acceptance rule,

with probability min
$$\left(1, \frac{\hat{f}'}{\hat{f}} \frac{r(\boldsymbol{\theta}; \boldsymbol{\theta}')}{r(\boldsymbol{\theta}'; \boldsymbol{\theta})}\right)$$
:

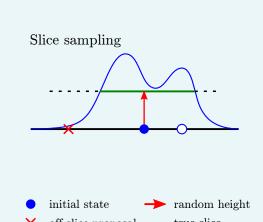
Accept: **return** $(\boldsymbol{\theta}', \hat{f}')$

else: Reject: return $(\boldsymbol{\theta}, \hat{f})$

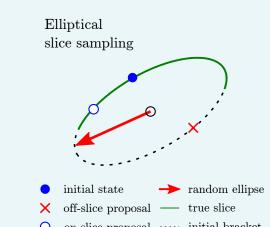
If estimator distribution is heavy-tailed, moves to large \hat{f} are occasionally accepted which it is hard to move away from.

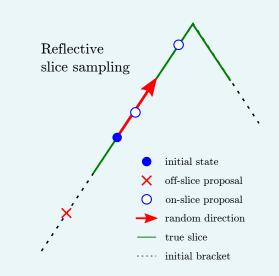
PM methods notorious for this 'sticking' behaviour.

Slice sampling (Neal, 2003) - family of MCMC algorithms with updates that locally adapt to the target density.



initial bracket





Slice sampling algorithms always move the state being updated: can we apply them in the pseudo-marginal setting?

• Optimal efficiency at step size giving acceptance rate

• Not applicable to PM approach - in Gaussian test case

 \bullet Using APM with independent proposals for u update

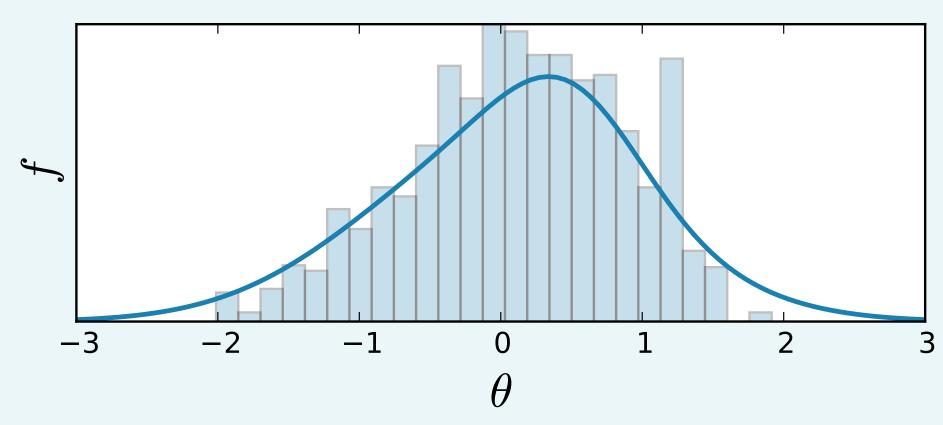
and Gaussian proposals for θ update, optimal

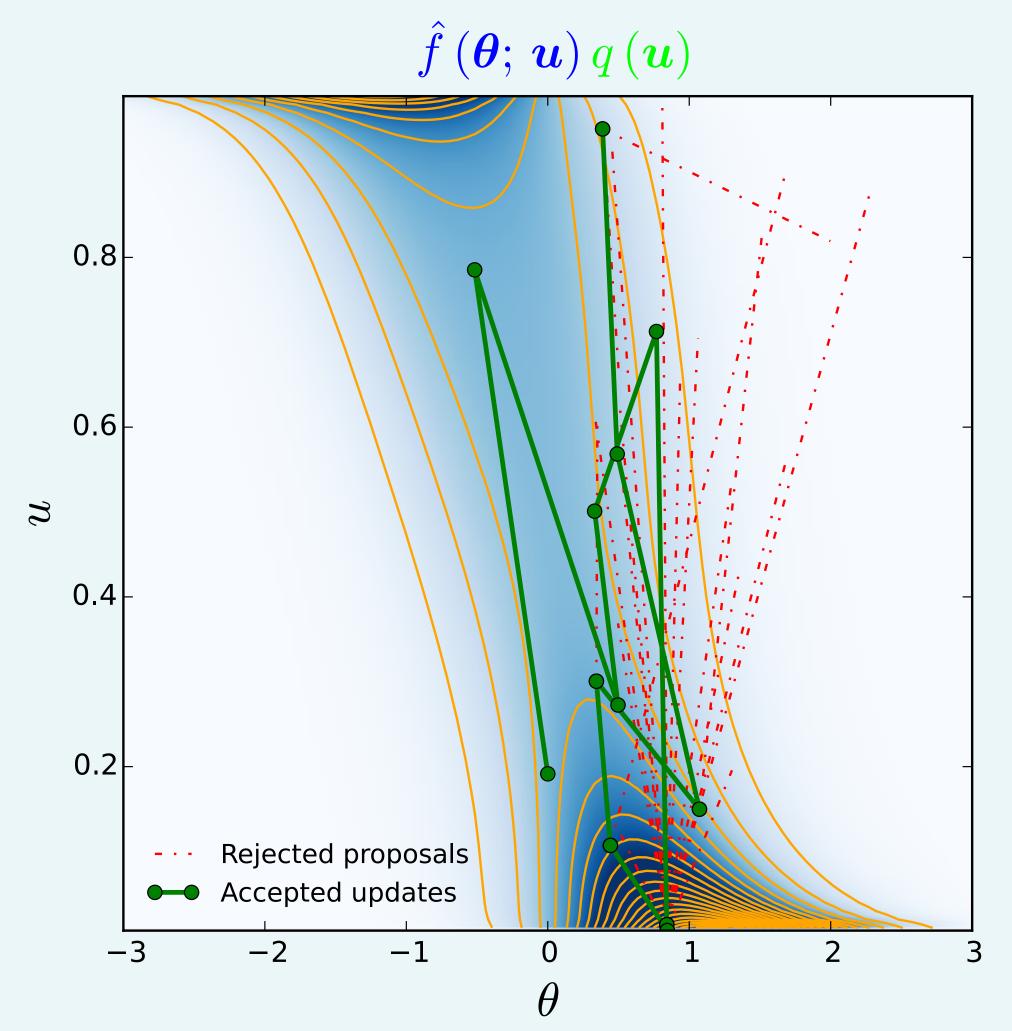
0.234 for standard Metropolis proposals in high

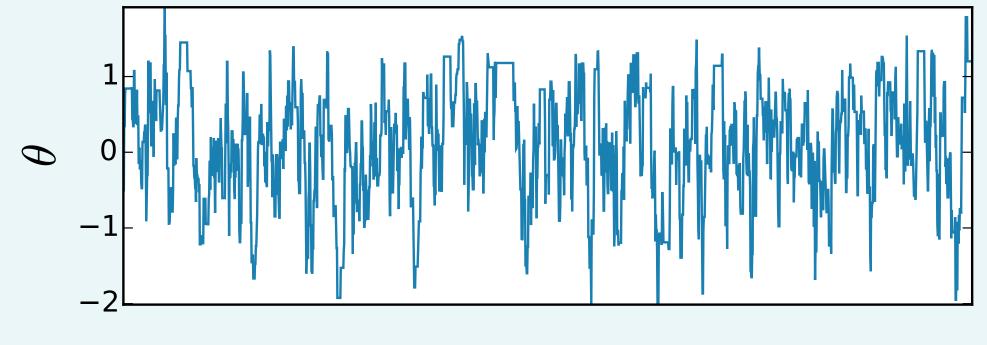
dimensions (Roberts et al. 1997).

0.234 acceptance not even achievable.

acceptance rate now close to 0.234.







Consider u as auxiliary variables as in Chopin and Singh (2015). This gives a new state (θ, u) with joint target density

$$\pi(\boldsymbol{\theta}, \boldsymbol{u}) = \hat{f}(\boldsymbol{\theta}; \boldsymbol{u}) q(\boldsymbol{u})/C$$

$$\int \pi(\boldsymbol{\theta}, \boldsymbol{u}) d\boldsymbol{u} = \int \hat{\boldsymbol{f}}(\boldsymbol{\theta}; \boldsymbol{u}) q(\boldsymbol{u}) / C d\boldsymbol{u} = \boldsymbol{f}(\boldsymbol{\theta}) / C$$

Standard PM MCMC: Metropolis—Hastings update on the joint target with proposal

$$\tilde{r}[(\boldsymbol{\theta}', \boldsymbol{u}') | (\boldsymbol{\theta}, \boldsymbol{u})] = r(\boldsymbol{\theta}'; \boldsymbol{\theta}) q(\boldsymbol{u}')$$

Our Auxiliary Pseudo-Marginal (APM) framework:

Inputs: current state: parameters $\boldsymbol{\theta}$, randomness \boldsymbol{u} ; unbiased estimator : $\mathbb{E}_{q(\boldsymbol{u})}\left[\hat{f}\left(\boldsymbol{\theta};\,\boldsymbol{u}\right)\right] = f\left(\boldsymbol{\theta}\right)\;\forall\;\boldsymbol{\theta}$,

Output: new state (θ, u) .

1. Update \boldsymbol{u} leaving invariant its target conditional:

$$\pi(\boldsymbol{u} \mid \boldsymbol{\theta}) \propto \hat{f}(\boldsymbol{\theta}; \boldsymbol{u}) q(\boldsymbol{u})$$

2. Update $\boldsymbol{\theta}$ leaving invariant its target conditional:

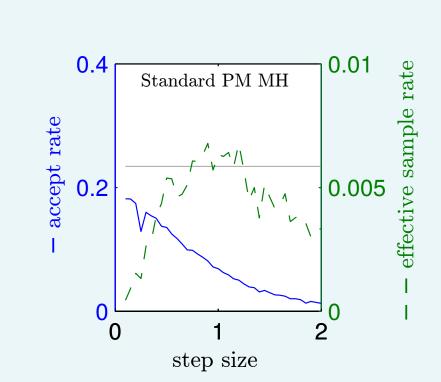
$$\pi(\boldsymbol{\theta} \mid \boldsymbol{u}) \propto \hat{f}(\boldsymbol{\theta}; \boldsymbol{u}) q(\boldsymbol{u})$$

Free to mix and match any standard MCMC operators for the two updates.

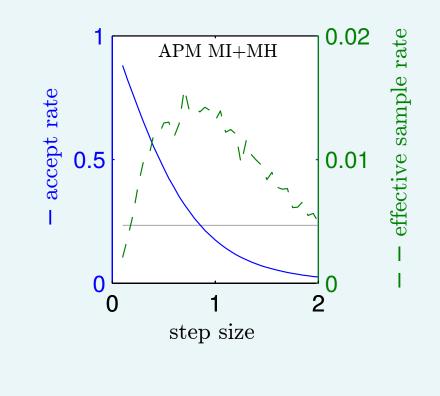
With \boldsymbol{u} now clamped during the $\boldsymbol{\theta}$ updates, usual case of a conditional distribution proportional to a deterministic function.

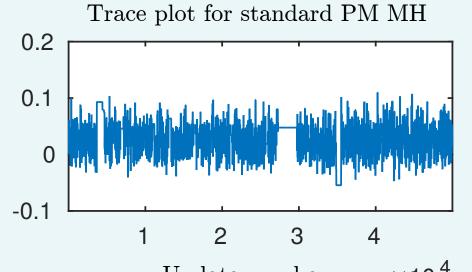
Slice sampling will move θ if $\hat{f}(\theta; u)$ is continuous almost everywhere.

Equally can make perturbative moves to the random variates \boldsymbol{u} with slice sampling or other adaptive methods.

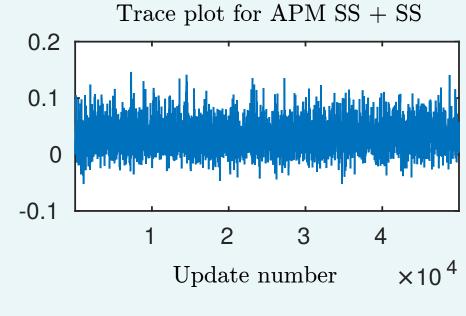


Clearer step-size selection



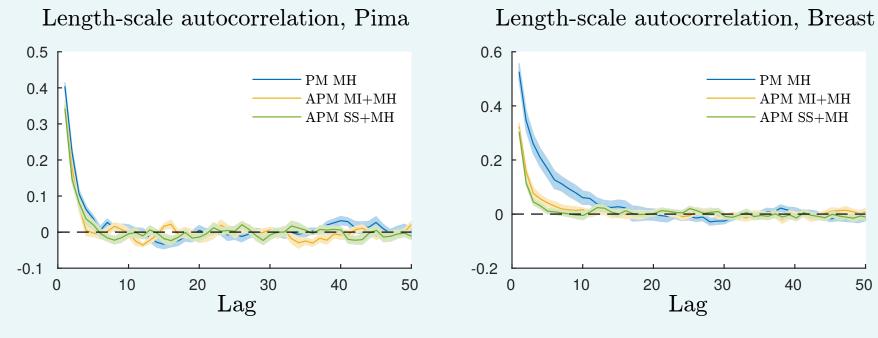


Parameter inference in Ising model



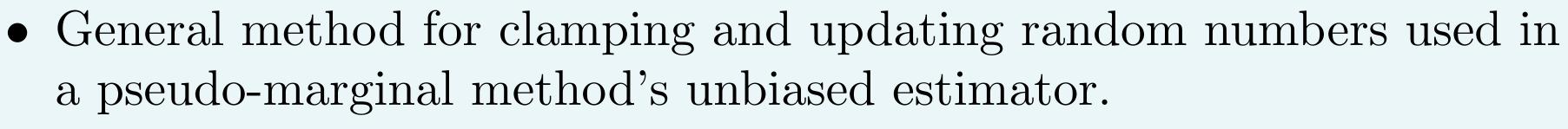


- Doubly-intractable distribution 30 × 10 lattice.
 Data generated using exact sampler.
 Using standard PM approach chains stick for long periods.
- Using APM framework with slice sampling updates for u and θ eliminates sticking and gives much improved cost-scaled autocorrelations.
- With lower-variance estimator using annealed importance sampling, standard PM performs better than APM.



Parameter inference in Gaussian process classifier

- Two UCI datasets, Pima and Breast, modelled following Filippone and Girolami, (2014).
- Estimator for marginal likelihood importance sampler with using Gaussian latent posterior approximation as importance distribution.
- Adaptive tuning of step size significantly more consistent with APM approaches.
- Cost-normalised effective sample size when using APM updates significantly better than standard PM approach.



- Within this framework it is possible to use slice sampling and other adaptive methods.
- Resulting Markov chains are most robust and often mix more quickly.

Andrieu & Roberts. The pseudo-marginal approach for efficient Monte Carlo computations. *Annals of Statistics*, 2009. Chopin & Singh. On particle Gibbs sampling. *Bernoulli*, 2015 Filippone & Girolami. Pseudo-marginal Bayesian inference for Gaussian Processes. *IEEE TPAMI*, 2014. Neal. Slice Sampling. *Annals of Statistics*, 2003.

Roberts, Gelman & Wilks. Weak convergence and optimal scaling of random walk Metropolis algorithms. Annals of Applied Probability, 1997.