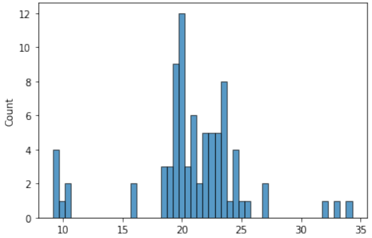
Nonparametric Involutive Markov Chain Monte Carlo

Carol Mak Fabian Zaiser Luke Ong
University of Oxford
ICML 2022

Probabilistic Programming



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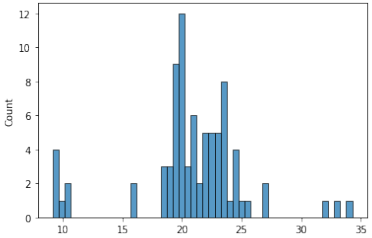
How many Gaussian mixtures there are?



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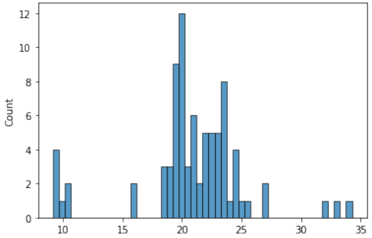

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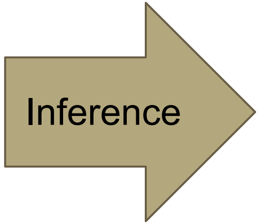

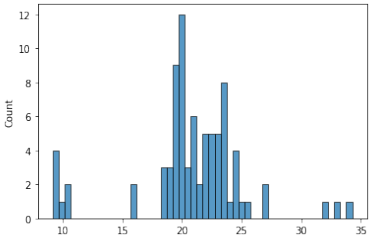

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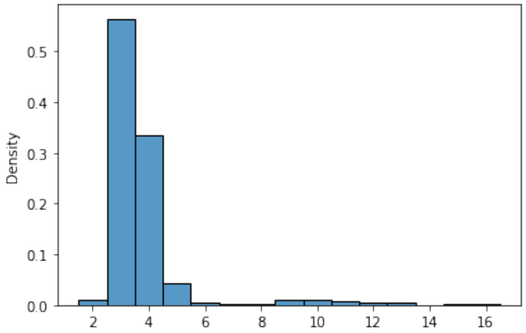

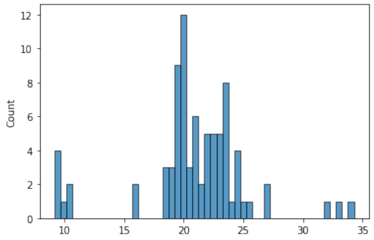

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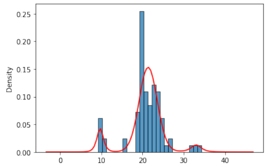

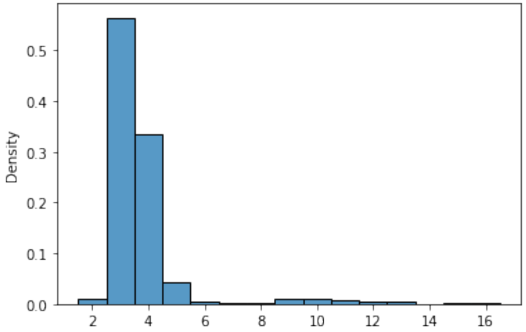

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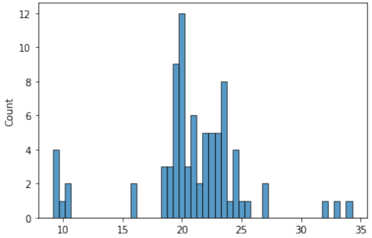

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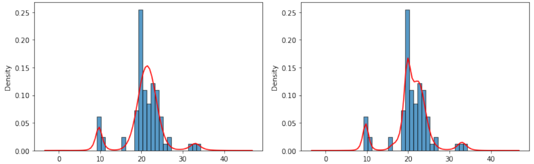

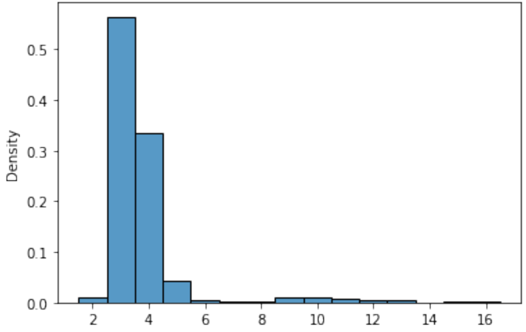

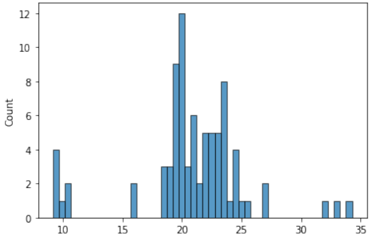

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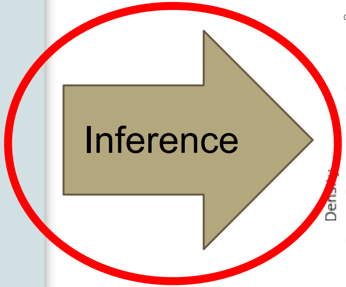

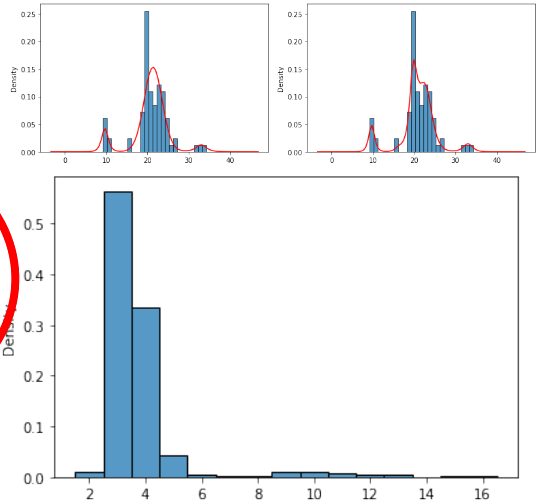

Inference for probabilistic programs in a Turing-complete language (Infinite GMM, Dirichlet process etc)

MCMC Inference for Probabilistic Programming

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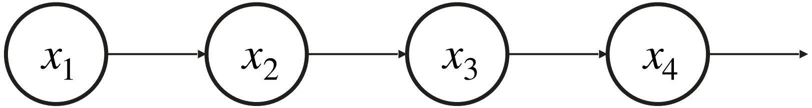
Simulate posterior by **updating states** in such a way that preserves the target distribution



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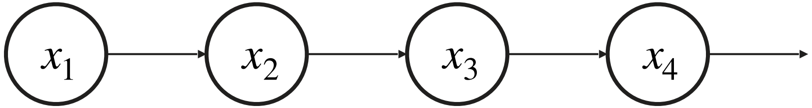

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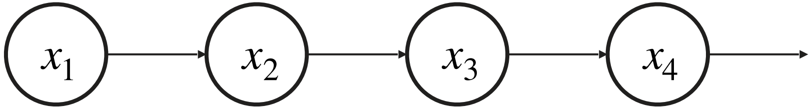

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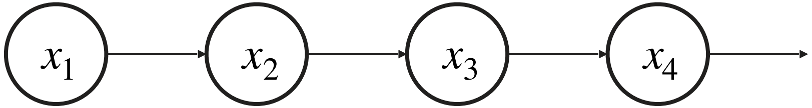

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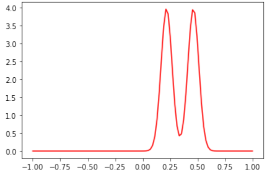

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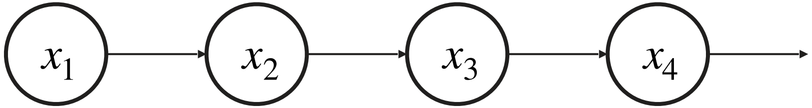

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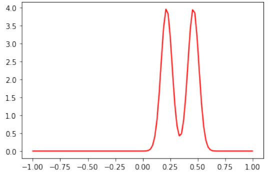

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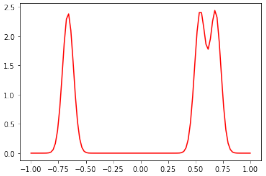

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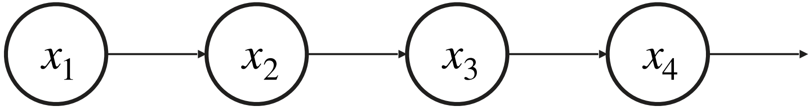

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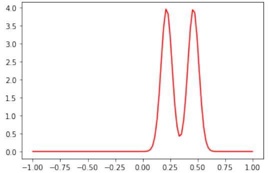

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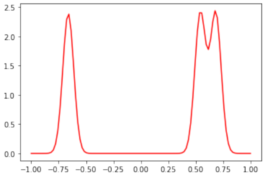

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    v0 ~ Normal(0,1)
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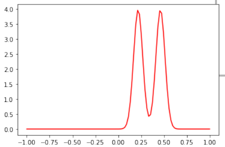

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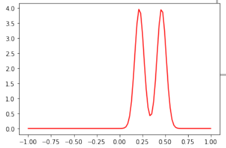

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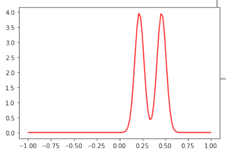

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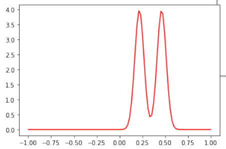

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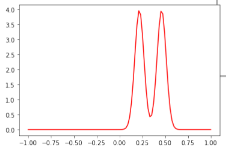

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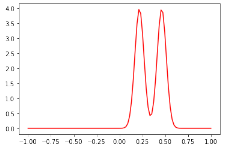

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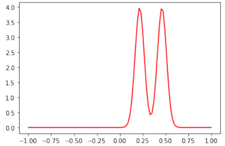

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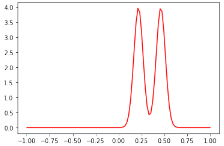

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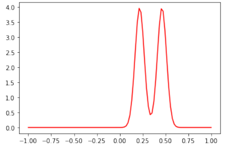
    (x,v) = (v0,x0)
    Return x with probability
```

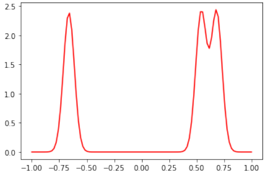
```
While w(x[1:k]) == 0 for all k
    append!(x0, Normal(0,1))
    append!(v0, Normal(0,1))
    (x,v) = (v0,x0)
```

```
Return x[1:k] with prob min{1, w(x[1:k])/w(x0[1:k0])*
                               pdfnormal(x,v)/pdfnormal(x0,v0)}
Else Return x0[1:k0]
```



	x0	v0
K	2.847	3.514
μs	0.218 0.462	0.542 -0.662
	0.105	0.683

	x	v
K	3.514	2.847
μs	0.542 -0.662	0.218 0.462
	0.683	0.105



Nonparametric Metropolis-Hastings (NP-MH)

```
function NPMHstep(x0)
    v0 ~ Normal(0,1)
    (x,v) = (v0,x0)
    Return x with probability
```

```
While w(x[1:k]) == 0 for all k
    append!(x0, Normal(0,1))
    append!(v0, Normal(0,1))
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```

```
Return x[1:k] with prob min{1, w(x[1:k])/w(x0[1:k0])*
                               pdfnormal(x,v)/pdfnormal(x0,v0)}
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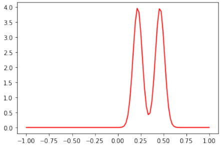
```



	x0	v0
K	2.847	3.514
µs	0.218 0.462	0.542 -0.662
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	x	v
K	3.514	2.847
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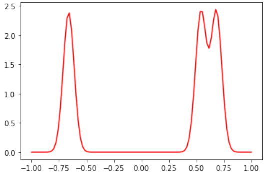

`Return x with some prob > 0`

Does such extension work for other MCMC inferences?

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Involutive MCMC (Neklyudov et al. ICML 2020) provides a unified view of many known MCMC algorithms

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```
Inputs: target density w
        auxiliary kernel k
        involution f
function iMCMCstep(x0)
    v0 ~ k(x0,-)
    (x,v) = f(x0,v0)
    Return x with probability
        min{1,(w(x)*k(x,v))/
              (w(x0)*k(x0,v0))*
              absdetjac(f(x,v))}
    Else Return x0
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Name & Citation	Appendix
Metropolis-Hastings (Hastings, 1970)	B.1
Mixture Proposal (Habib & Barber, 2018)	B.2
Multiple-Try Metropolis (Liu et al., 2000)	B.3
Sample-Adaptive MCMC (Zhu, 2019)	B.4
Reversible-Jump MCMC (Green, 1995)	B.5
Hybrid Monte Carlo (Duane et al., 1987)	B.6
RMHMC (Girolami & Calderhead, 2011)	B.7
NeuTra (Hoffman et al., 2019)	B.8
A-NICE-MC (Song et al., 2017)	B.9
L2HMC (Levy et al., 2017)	B.10
Persistent HMC (Horowitz, 1991)	B.11
Gibbs (Geman & Geman, 1984)	B.12
Look Ahead (Sohl-Dickstein et al., 2014)	B.13
NRJ (Gagnon & Doucet, 2019)	B.14
Lifted MH (Turitsyn et al., 2011)	B.15

Table 1: List of algorithms that we describe by the Involutive MCMC framework. See their descriptions and formulations in terms of iMCMC in corresponding appendices.

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    Else Return x0
```

Name & Citation	Appendix
Metropolis-Hastings (Hastings, 1970)	B.1
Mixture Proposal (Habib & Barber, 2018)	B.2

```
Inputs: target density w
        k(x,v) := Normal(0,1)(v)
        f(x,v) := (v,x)
function MHstep(x0)
    v0 ~ Normal(0,1)
    (x,v) = (v0,x0)
    Return x with probability
      min{1,w(x)/w(x0)*
      pdfnormal(x,v)/pdfnormal(x0,v0)}
    Else Return x0
```

Table 1: List of algorithms that we describe by the Involutive MCMC framework. See their descriptions and formulations in terms of iMCMC in corresponding appendices.

Nonparametric Involutive MCMC (NP-iMCMC)

Nonparametric Involutive MCMC (NP-iMCMC)

```
target density w
auxiliary kernel K[n] for each n
involution f[n] for each n
function NPiMCMCstep(x0)
    k0 = len(x0)
    v0 ~ K[k0](x0,-)
    (x,v) = f[k0](x0,v0)
    while w(x[1:k]) == 0 for all k
        append!(x0, Normal(0,1));
        append!(v0, Normal(0,1));
        (x,v) = f[len(x0)](x0,v0)
    Return x[1:k] with prob min{1,P}
    Else Return x0[1:k0]
```

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        (x,v) = f[len(x0)](x0,v0)
    Return x[1:k] with prob min{1,P}
    Else Return x0[1:k0]
```

$$P := \frac{w(x^{1\dots k})\cdot \mathrm{pdf}K^{(k)}(x^{1\dots k},v^{1\dots k})\cdot\varphi(x,v)}{w(x^{1\dots k_0})\cdot \mathrm{pdf}K^{(k_0)}(x^{1\dots k_0},v^{1\dots k_0})\cdot\varphi(x_0,v_0)}\left|\det \nabla\Phi^{(n)}(x_0,v_0)\right|$$

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        (x,v) = f[len(x0)](x0,v0)
    Return x[1:k] with prob min{1,P}
    Else Return x0[1:k0]
```

- **Target density** w is (A1) integrable and (A2) almost surely terminating
- **Auxiliary kernel** $K^{(n)}$ for each dim. n
- **Involution** $\Phi^{(n)}$ for each dim. n satisfying the (A3) projection commutation property:

For all (x, v) where |x| = m, if $w(x^{1..n}) > 0$ for some n, then for all k = n, …, m, $\text{take}_k(\Phi^{(m)}(x, v)) = \Phi^{(k)}(\text{take}_k(x, v))$

$$P := \frac{w(x^{1\dots k})\cdot \text{pdf}K^{(k)}(x^{1\dots k},v^{1\dots k})\cdot\varphi(x,v)}{w(x^{1\dots k_0})\cdot \text{pdf}K^{(k_0)}(x^{1\dots k_0},v^{1\dots k_0})\cdot\varphi(x_0,v_0)}\left|\det \nabla\Phi^{(n)}(x_0,v_0)\right|$$

Generalisations of NP-iMCMC

Generalisations of NP-iMCMC

Hybrid NP-iMCMC

for discrete and continuous samplers

```
Sum = 0;
while Bern(0.5): count += Normal(0,1)
```

Generalisations of NP-iMCMC

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Sum = 0;
while Bern(0.5): count += Normal(0,1)
```

Multiple Step NP-iMCMC

for complex involutions

```
function leapfrog(q0,p0)
     q = q0; p = p0
     for i in 1:L
          p = p - ep/2 * grad(U)(q)
          q = q + ep * grad(K)(p)
          p = p - ep/2 * grad(U)(q)
     return (q,-p)
```

Generalisations of NP-iMCMC

Hybrid NP-iMCMC

for discrete and continuous samplers

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Sum = 0;
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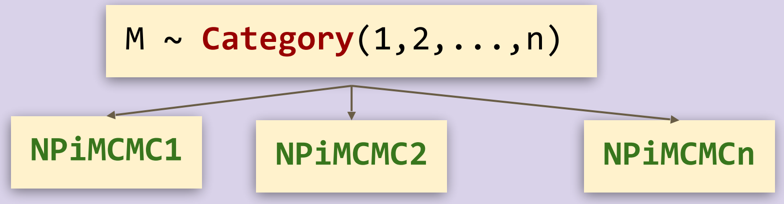
          p = p - ep/2 * grad(U)(q)
     return (q,-p)
```

State-dependent Mixtures of NP-iMCMC



Generalisations of NP-iMCMC

Hybrid NP-iMCMC

for discrete and continuous samplers

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Sum = 0;
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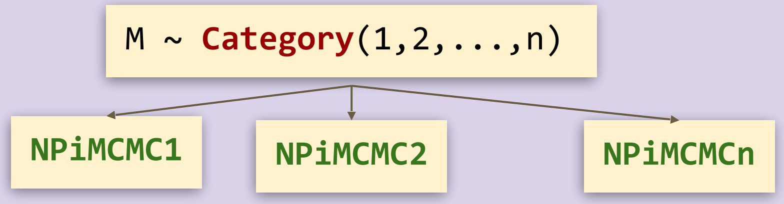
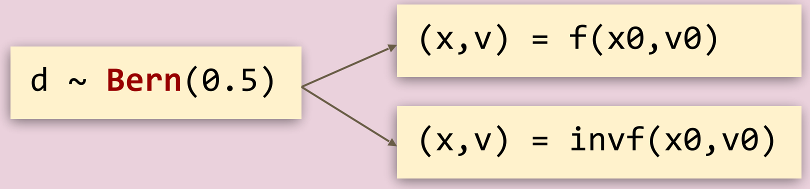
State-dependent Mixtures of NP-iMCMC



Direction NP-iMCMC



Generalisations of NP-iMCMC

Hybrid NP-iMCMC

for discrete and continuous samplers

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Sum = 0;
while Bern(0.5): count += Normal(0,1)
```

Multiple Step NP-iMCMC

for complex involutions

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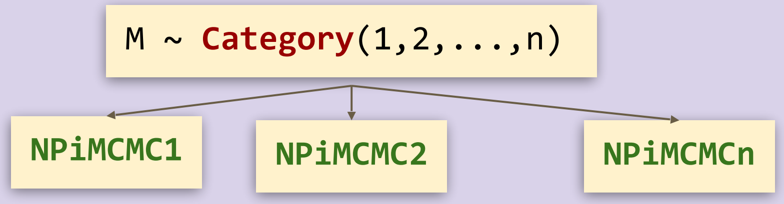
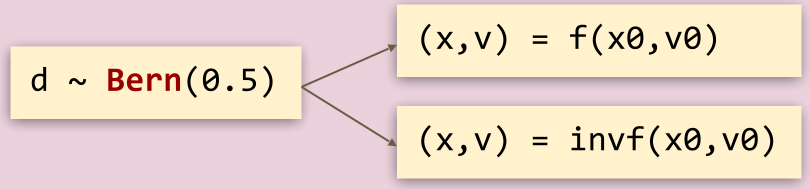
function leapfrog(q0,p0)
     q = q0; p = p0
     for i in 1:L
          p = p - ep/2 * grad(U)(q)
          q = q + ep * grad(K)(p)
          p = p - ep/2 * grad(U)(q)
     return (q,-p)
```

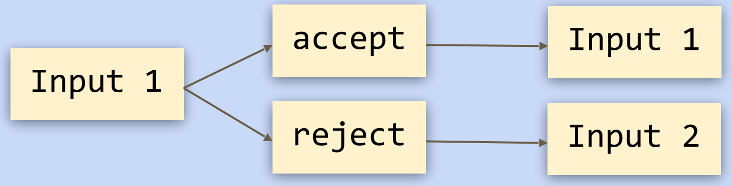
State-dependent Mixtures of NP-iMCMC



Direction NP-iMCMC



Persistent NP-iMCMC



NP-HMC on Infinite GMM

NP-HMC on Infinite GMM

HMC ⟶ NP-HMC (Mak et al 2021)

NP-HMC on Infinite GMM

HMC ⟶ NP-HMC (Mak et al 2021)

Generalised HMC (Horowitz 1991)

Look Ahead HMC
(Sohl-Dickstein et al., 2014;
Campos & Sanz-Serna, 2015)

NP-HMC on Infinite GMM

HMC → NP-HMC (Mak et al 2021)

Generalised HMC (Horowitz 1991) → NP-HMC with persistence

Look Ahead HMC (Sohl-Dickstein et al., 2014; Campos & Sanz-Serna, 2015) → NP-Look Ahead HMC

NP-HMC on Infinite GMM

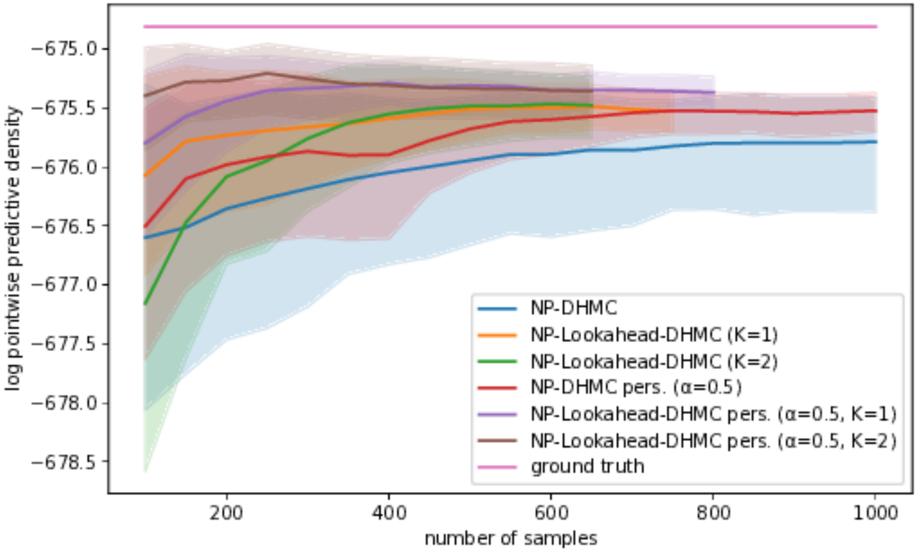
HMC → NP-HMC (Mak et al 2021)

Generalised HMC (Horowitz 1991) → NP-HMC with persistence

Look Ahead HMC (Sohl-Dickstein et al., 2014; Campos & Sanz-Serna, 2015) → NP-Look Ahead HMC

Infinite GMM

- 200 training data points generated from a mixture of 9 components
- Compute LPPD on 50 data points



Summary

- **NP-iMCMC** transform many existing MCMC inference to **work on probabilistic programs**
- NP-iMCMC is **theoretically correct**
- Existing strengths of iMCMC algorithms **carry over to their nonparametric extensions**