Probabilistic Programming and AI: Lecture 3

Markov Chain Monte Carlo Inference

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Independent versus Dependent Sampling

Why sampling?

Prior $P(\Theta)$

- chosen by modeller
- **computable**

Likelihood $P(X|\Theta)$

- encodes generative process from latents Θ to observes X
- **computable**

Marginal / Evidence $P(X)$

- can be **approximated** with sampling methods

Posterior $P(\Theta|X) = \frac{P(X|\Theta) \times P(\Theta)}{P(X)}$

- what we want to know
- can be **approximated** with sampling methods

Limitations of Independent Samples

Rejection Sampling:

Curse of dimensionality / continuous variables

Importance Sampling:

How to specify reference distribution?

Rejection Sampling

Coin model:

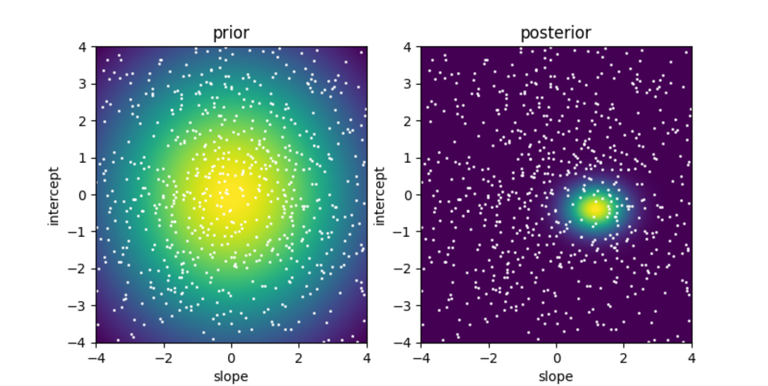
$$p \sim \text{Uniform}(0, 1)$$
$$x_i \sim \text{Bernoulli}(p)$$

```python
def rejection_sampling(xs_observed):
    while True:
        p = dist.Uniform(0,1).sample()
        xs = dist.Bernoulli(p).sample(xs_observed.shape)
        if (xs == xs_observed).all():
            return p # accept
        # reject
```

```
Rejected 50.54% of iterations for 1 number of observations.
Rejected 83.78% of iterations for 2 number of observations.
Rejected 91.76% of iterations for 3 number of observations.
Rejected 96.68% of iterations for 4 number of observations.
Rejected 98.26% of iterations for 5 number of observations.
```

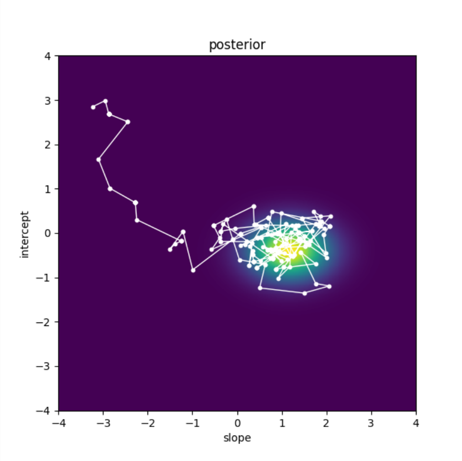
Likelihood Weighting

Sample from prior, reweigh to approximate posterior.



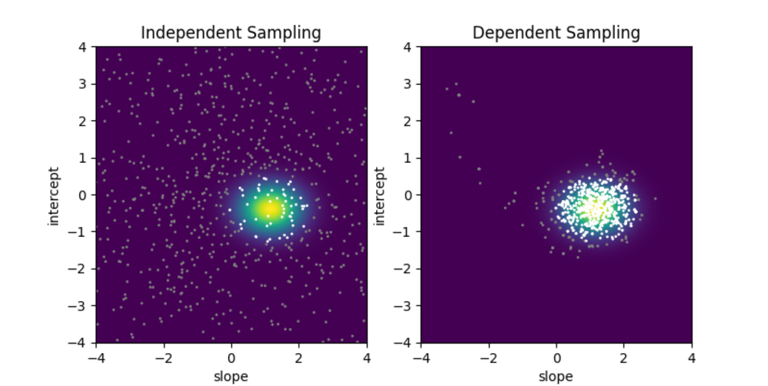
Most samples from reference distribution are of low probability.

Dependent Sampling Idea



Perturb the current sample to generate new sample.

Independent versus Dependent Sampling



Dependent Sampling Idea

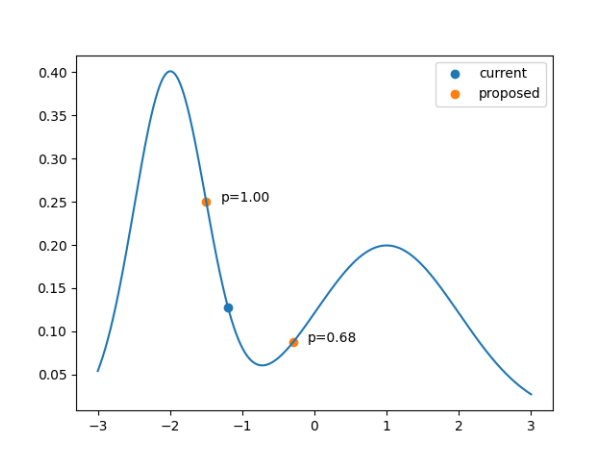
$$P(\Theta|X) = \frac{P(X|\Theta) \times P(\Theta)}{P(X)} \propto P(X|\Theta) \times P(\Theta)$$

As we will see, we can generate dependent samples of the posterior by only evaluating the joint.

Metropolis Hastings Algorithm

Metropolis Hastings Algorithm

"Hill climbing with the possibility of stepping down."



$$p = \min\left(\frac{f(x_{proposed})}{f(x_{current})}, 1\right)$$

Metropolis Hastings Algorithm

Let $P(x)$ be the target distribution and $Q(x'|x)$ be a proposal distribution.

1. Initialise x_0.
2. For each $i = 1, \ldots, n$
    - Propose a new value according to the proposal $x' \sim Q(.|x_i)$
    - Calculate the acceptance probability

$$A = \min\left(1, \frac{P(x')Q(x_i|x')}{P(x_i)Q(x'|x_i)}\right)$$

    - Draw a random number $0 \leq p \leq 1$ and let

$$x_{i+1} = \begin{cases} x' & p \leq A \quad \text{(accept)} \\ x_i & p > A \quad \text{(reject)} \end{cases}$$

Metropolis Hastings Algorithm

The Metropolis Hastings algorithm produces a so-called **Markov Chain**, where each value only depends on its predecessor (and not multiple predecessors).

Soundness:

It can be shown that for sensible Q and $n \to \infty$, the resulting chain is indistinguishable from a sample from the target distribution P.

Metropolis Hastings Algorithm

Proposal Distributions

- Should propose values that are accepted frequently, but also explore the entire state space.
- Random walk (Gaussian drift) proposals:

$$x' \sim \text{Normal}(x_i, \sigma)$$

- Unconditional proposals:

$$x' \sim Q(.) \quad \text{(no dependence on } x_i\text{)}$$

- Example nonsensical proposal:

$$x' \sim \text{Uniform}(x_i, x_i + 1)$$

- Best proposal distribution would be the target itself $Q(x'|x_i) = P(x')$ (not available)

Metropolis Hastings Algorithm

Ad Soundness:

Let $x_{i+1} \sim T(x_{i+1}|x_i)$ be the transition kernel, as defined by the algorithm ($x_{i+1} = x'$ with probability A, ...).

This kernel satisfies the detailed-balance condition

$$P(x_i)T(x_{i+1}|x_i) = P(x_{i+1})T(x_i|x_{i+1}),$$

the probability of being in state x_i and transitioning to state x_{i+1} must be equal to the probability of being in state x_{i+1} and transitioning to state x_i.

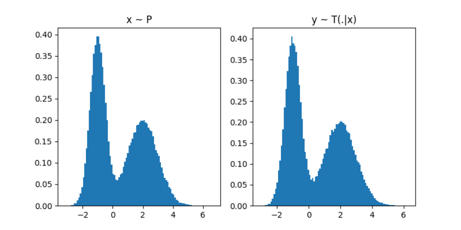
Also, if the proposal distribution is chosen such that the resulting Markov chain is ergodic, then the stationary distribution of the Markov chain is P.

Informally, any state should be reachable from any other state in any number of steps less or equal to a number N.

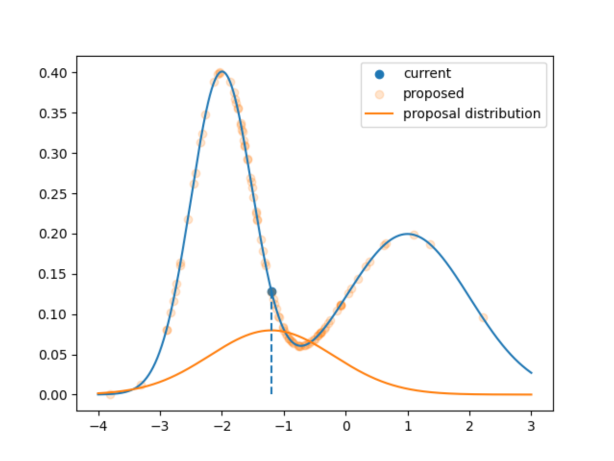
Ad Soundness: Stationary distribution

$$\int T(y|x)P(x)dx = \int T(x|y)P(y)dx = P(y)$$

```python
def T(x, P, sigma):
    P_current = P(x)
    proposed = dist.Normal(x, sigma).sample()
    P_proposed = P(proposed)

    A = P_proposed/P_current

    if torch.rand(()) < A:
        y = proposed
    else:
        y = x

    return y

X = sample_P(-1,2,100000)
Y = torch.tensor([T(x, P, 0.5) for x in X])
```

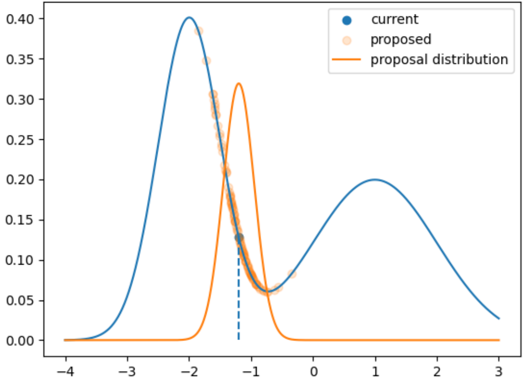


Random walk proposal $x' \sim \text{Normal}(x_i, \sigma)$

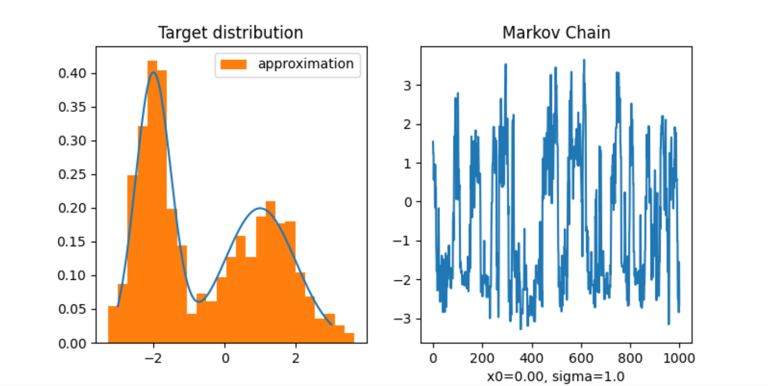


Metropolis Hastings Algorithm

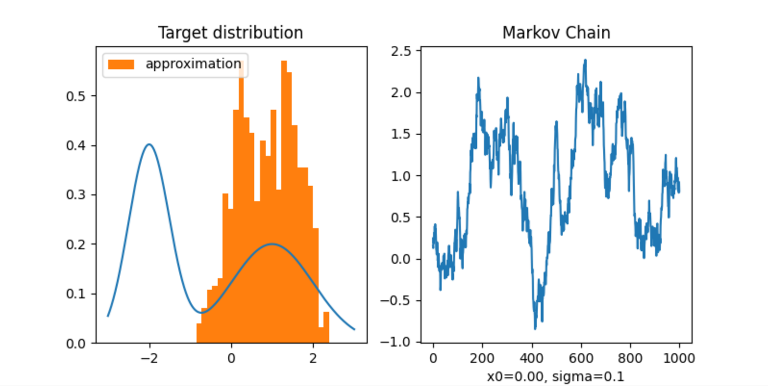
Random walk proposal $x' \sim \mathrm{Normal}(x_i, \sigma)$



Example Markov Chain generated by random walk proposal
$x' \sim \mathrm{Normal}(x_i, \sigma)$

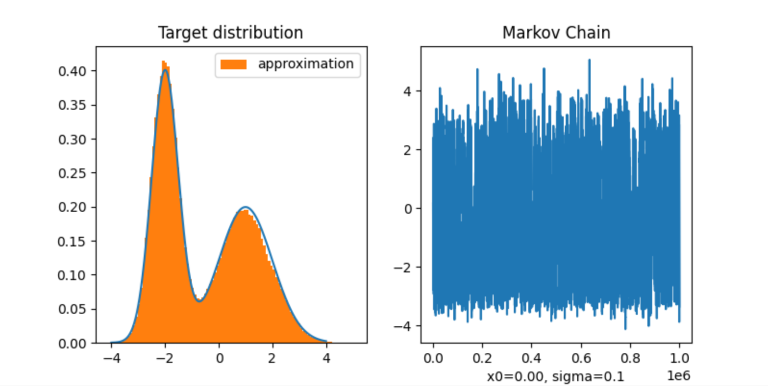


Example Markov Chain generated by random walk proposal $x' \sim \mathrm{Normal}(x_i, \sigma)$: step-size too small

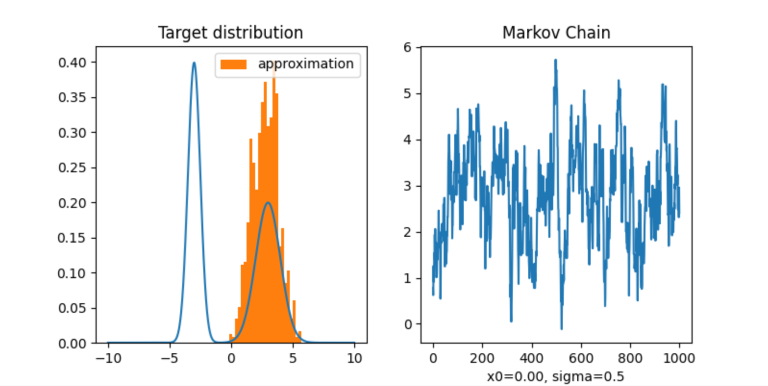


Metropolis Hastings Algorithm

Example Markov Chain generated by random walk proposal $x' \sim \text{Normal}(x_i, \sigma)$: large number of iterations

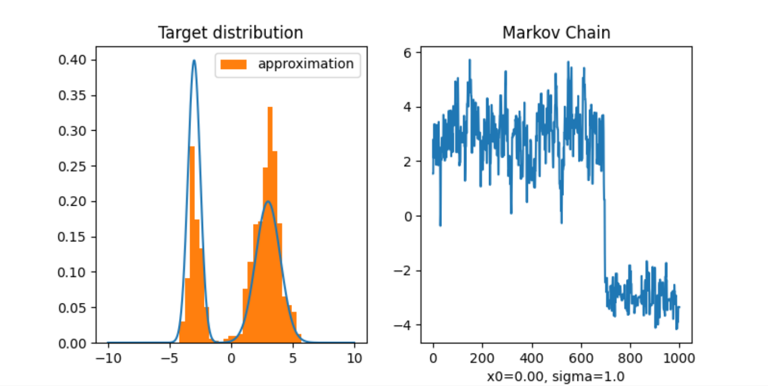


Example Markov Chain generated by random walk proposal $x' \sim \text{Normal}(x_i, \sigma)$: cannot bridge gaps in target density

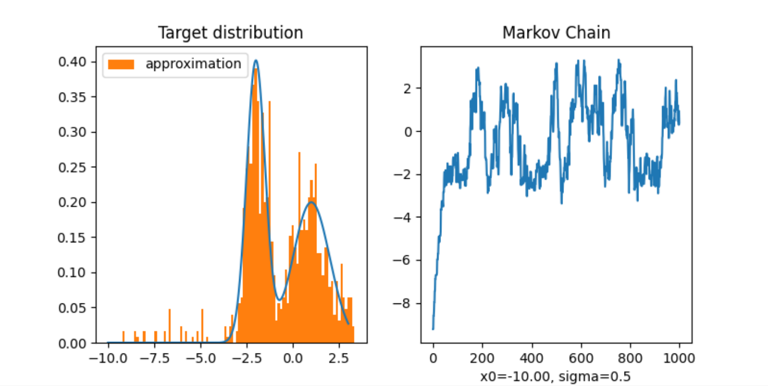


Metropolis Hastings Algorithm

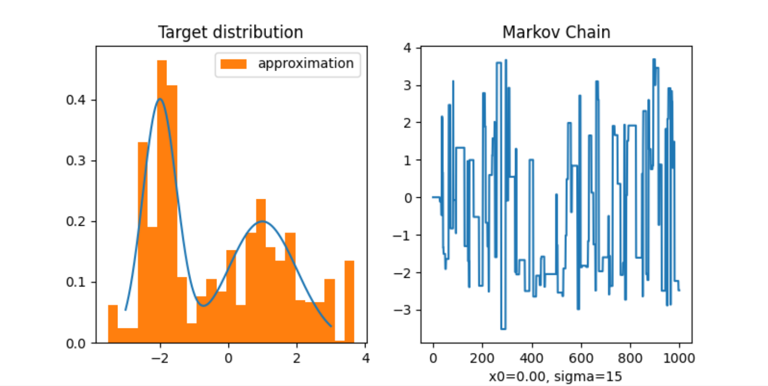
Example Markov Chain generated by random walk proposal $x' \sim \text{Normal}(x_i, \sigma)$: increased step-size



Example Markov Chain generated by random walk proposal $x' \sim \text{Normal}(x_i, \sigma)$: bad initial state, "burn-in" phase



Example Markov Chain generated by random walk proposal $x' \sim \text{Normal}(x_i, \sigma)$: step-size too large



Metropolis Hastings Algorithm

Why does it work for Bayesian Inference?

Target is $\tilde{P}(\Theta) = P(\Theta|X)$ which we cannot evaluate.

But, with Bayes Theorem:

$$\begin{aligned}
\frac{\tilde{P}(\theta') \times Q(\theta_i|\theta')}{\tilde{P}(\theta_i) \times Q(\theta'|\theta_i)} &= \frac{\frac{P(X|\theta')P(\theta')}{P(X)} \times Q(\theta_i|\theta')}{\frac{P(X|\theta)P(\theta)}{P(X)} \times Q(\theta'|\theta_i)} \\
&= \frac{P(X|\theta')P(\theta') \times Q(\theta_i|\theta')}{P(X|\theta)P(\theta) \times Q(\theta'|\theta_i)}
\end{aligned}$$

The normalisation constant, the marginal $P(X)$, cancels!

We only need to be able to evaluate the joint to apply the Metropolis Hastings algorithm to the posterior!

Metropolis Hastings Algorithm For PPLs

Metropolis Hastings Algorithm For PPLs

```python
def noisy_geometric(p):
    x = 0
    while True:
        b = sample(f"b_{x}", dist.Bernoulli(p))
        if b:
            break
        x += 1
    y = sample("y", dist.Normal(x,1), observed=torch.tensor(3))
    return x
```

Metropolis Hastings Algorithm For PPLs

```
torch.manual_seed(0)
ctx = Trace()
with ctx:
    x = noisy_geometric(0.25)
ctx.trace
```

Returns:

```
{'b_0': {'value': tensor(0.),
  'distribution': Bernoulli(probs: 0.25),
  'is_observed': False,
  'log_prob': tensor(-0.2877)},
 'b_1': {'value': tensor(0.),
  'distribution': Bernoulli(probs: 0.25),
  'is_observed': False,
  'log_prob': tensor(-0.2877)},
 'b_2': {'value': tensor(1.),
  'distribution': Bernoulli(probs: 0.25),
  'is_observed': False,
  'log_prob': tensor(-1.3863)},
 'y': {'value': tensor(3),
  'distribution': Normal(loc: 2.0, scale: 1.0),
  'is_observed': True,
  'log_prob': tensor(-1.4189)}}
```

How to propose from left to right and vice-versa?

```
torch.manual_seed(1)
ctx = Trace()
with ctx:
    x = noisy_geometric(0.25)
ctx.trace
```

Returns:

```
{'b_0': {'value': tensor(0.),
  'distribution': Bernoulli(probs: 0.25),
  'is_observed': False,
  'log_prob': tensor(-0.2877)},
 'b_1': {'value': tensor(0.),
  'distribution': Bernoulli(probs: 0.25),
  'is_observed': False,
  'log_prob': tensor(-0.2877)},
 'b_2': {'value': tensor(0.),
  'distribution': Bernoulli(probs: 0.25),
  'is_observed': False,
  'log_prob': tensor(-0.2877)},
 'b_3': {'value': tensor(0.),
  'distribution': Bernoulli(probs: 0.25),
  'is_observed': False,
  'log_prob': tensor(-0.2877)},
 'b_4': {'value': tensor(1.),
  'distribution': Bernoulli(probs: 0.25),
  'is_observed': False,
  'log_prob': tensor(-1.3863)},
 'y': {'value': tensor(3),
  'distribution': Normal(loc: 4.0, scale: 1.0),
  'is_observed': True,
  'log_prob': tensor(-1.4189)}}
```

Single-Site Metropolis Hastings Algorithm For PPls

- Choose a single variable X_0 at random, for which we make a conditional proposal.
- For all new variables, propose from prior.
- For all other variables, reuse value from current trace.
- The proposal probability can be calculated as follows

$$Q(\mathit{prop.}|\mathit{curr.}) = \underbrace{\frac{1}{|\mathit{curr.}|}}_{\text{Pr. of choosing } X_0} \times \underbrace{Q(X_0'|X_0)}_{\text{Conditional proposal for } X_0} \times \underbrace{\prod_{X \in \mathit{sampled}} P(X)}_{\text{Pr. of proposing new variables from priors}}$$

- New variables can be determined with

$$\mathit{sampled} = \mathit{prop.} \setminus \mathit{curr.},$$

i.e. all variables that are in proposed trace but not in current trace.

Metropolis Hastings Algorithm For PPLs

```python
torch.manual_seed(0)
ctx = Trace()
with ctx:
    x = noisy_geometric(0.25)
ctx.trace
```

Returns:

```python
{'b_0': {'value': tensor(0.),
  'distribution': Bernoulli(probs: 0.25),
  'is_observed': False,
  'log_prob': tensor(-0.2877)},
 'b_1': {'value': tensor(0.),
  'distribution': Bernoulli(probs: 0.25),
  'is_observed': False,
  'log_prob': tensor(-0.2877)},
 'b_2': {'value': tensor(1.),
  'distribution': Bernoulli(probs: 0.25),
  'is_observed': False,
  'log_prob': tensor(-1.3863)},
 'y': {'value': tensor(3),
  'distribution': Normal(loc: 2.0, scale: 1.0),
  'is_observed': True,
  'log_prob': tensor(-1.4189)}}
```

- Chosen address is *b_2*.
- *b_0* and *b_1* are reused.
- *b_3* and *b_4* are sampled from prior (left to right) or forgotten (right to left).
- *y* is observed.

```python
torch.manual_seed(1)
ctx = Trace()
with ctx:
    x = noisy_geometric(0.25)
ctx.trace
```

Returns:

```python
{'b_0': {'value': tensor(0.),
  'distribution': Bernoulli(probs: 0.25),
  'is_observed': False,
  'log_prob': tensor(-0.2877)},
 'b_1': {'value': tensor(0.),
  'distribution': Bernoulli(probs: 0.25),
  'is_observed': False,
  'log_prob': tensor(-0.2877)},
 'b_2': {'value': tensor(0.),
  'distribution': Bernoulli(probs: 0.25),
  'is_observed': False,
  'log_prob': tensor(-0.2877)},
 'b_3': {'value': tensor(0.),
  'distribution': Bernoulli(probs: 0.25),
  'is_observed': False,
  'log_prob': tensor(-0.2877)},
 'b_4': {'value': tensor(1.),
  'distribution': Bernoulli(probs: 0.25),
  'is_observed': False,
  'log_prob': tensor(-1.3863)},
 'y': {'value': tensor(3),
  'distribution': Normal(loc: 4.0, scale: 1.0),
  'is_observed': True,
  'log_prob': tensor(-1.4189)}}
```

Metropolis Hastings Algorithm For PPLs

```python
def linear_regression(x, y):
    slope = sample("slope", dist.Normal(0,3))
    intercept = sample("intercept", dist.Normal(0,3))
    for i in range(len(x)):
        sample(f"y_{i}",dist.Normal(slope*x[i]+intercept, 1.),observed=y[i])
```

Chosen address: `slope`

$Q(\mathit{prop.}|\mathit{curr.}) = \frac{1}{2}Q(\mathit{slope}'|\mathit{slope}), \quad Q(\mathit{curr.}|\mathit{prop.}) = \frac{1}{2}Q(\mathit{slope}|\mathit{slope}')$

Current:

```python
{'slope': {'value': tensor(4.6230), # changes
  'distribution': Normal(loc: 0.0, scale: 3.0),
  'is_observed': False,
  'log_prob': tensor(-3.2049)}, # changes
 'intercept': {'value': tensor(-0.8803),
  'distribution': Normal(loc: 0.0, scale: 3.0),
  'is_observed': False,
  'log_prob': tensor(-2.0606)},
 'y_0': {'value': tensor(-1.2000),
  'distribution': Normal(loc:-5.5032,scale:1.0), # changes
  'is_observed': True,
  'log_prob': tensor(-10.1780)}, # changes
  ...
}
```

Proposed:

```python
{'slope': {'value': tensor(1.9841), # changes
  'distribution': Normal(loc: 0.0, scale: 3.0),
  'is_observed': False,
  'log_prob': tensor(-2.2362)}, # changes
 'intercept': {'value': tensor(-0.8803),
  'distribution': Normal(loc: 0.0, scale: 3.0),
  'is_observed': False,
  'log_prob': tensor(-2.0606)},
 'y_0': {'value': tensor(-1.2000),
  'distribution': Normal(loc:-2.8643,scale:1.0), # changes
  'is_observed': True,
  'log_prob': tensor(-2.3041)}, # changes
  ...
}
```

Metropolis Hastings Algorithm For PPLs

```
def linear_regression(x, y):
    slope = sample("slope", dist.Normal(0,3))
    intercept = sample("intercept", dist.Normal(0,3))
    for i in range(len(x)):
        sample(f"y_{i}",dist.Normal(slope*x[i]+intercept, 1.),observed=y[i])
```

Chosen address: `intercept`

$Q(prop.|curr.) = \frac{1}{2}Q(intercept'|intercept), Q(curr.|prop.) = \frac{1}{2}Q(inter.|inter.')$

Current:

```
{'slope': {'value': tensor(4.6230),
  'distribution': Normal(loc: 0.0, scale: 3.0),
  'is_observed': False,
  'log_prob': tensor(-3.2049)},
 'intercept': {'value': tensor(-0.8803), # changes
  'distribution': Normal(loc: 0.0, scale: 3.0),
  'is_observed': False,
  'log_prob': tensor(-2.0606)}, # changes
 'y_0': {'value': tensor(-1.2000),
  'distribution':Normal(loc:-5.5032,scale:1.0), # changes
  'is_observed': True,
  'log_prob': tensor(-10.1780)}, # changes
  ...
}
```

Proposed:

```
{'slope': {'value': tensor(4.6230),
  'distribution': Normal(loc: 0.0, scale: 3.0),
  'is_observed': False,
  'log_prob': tensor(-3.2049)},
 'intercept': {'value': tensor(-0.4119), # changes
  'distribution': Normal(loc: 0.0, scale: 3.0),
  'is_observed': False,
  'log_prob': tensor(-2.0270)}, # changes
 'y_0': {'value': tensor(-1.2000),
  'distribution':Normal(loc:-5.0349,scale:1.0), # changes
  'is_observed': True,
  'log_prob': tensor(-8.2722)}, # changes
  ...
}
```

Metropolis Hastings Algorithm For PPLs

```python
def model():
    X = sample("X", dist.Normal(0,1))
    Y = sample("Y", dist.Normal(X,1))
    if Y < 0:
        sample("A", dist.Normal(0,1), observed=torch.tensor(1.))
    else:
        sample("B", dist.Normal(0,1))
```

Chosen address: X

$$Q(prop.|curr.) = \frac{1}{3}Q(X'|X), \quad Q(curr.|prop.) = \frac{1}{3}Q(X|X')$$

Current:

```
{'X': {'value': tensor(1.5410), # changes
  'distribution': Normal(loc: 0.0, scale: 1.0),
  'is_observed': False,
  'log_prob': tensor(-2.1063)}, # changes
 'Y': {'value': tensor(1.2476),
  'distribution': Normal(loc: 1.5410, scale: 1.0),
  'is_observed': False,
  'log_prob': tensor(-0.9620)}, # changes
 'B': {'value': tensor(-2.1788),
  'distribution': Normal(loc: 0.0, scale: 1.0),
  'is_observed': False,
  'log_prob': tensor(-3.2925)}}
```

Proposed:

```
{'X': {'value': tensor(1.3281), # changes
  'distribution': Normal(loc: 0.0, scale: 1.0),
  'is_observed': False,
  'log_prob': tensor(-1.8009)}, # changes
 'Y': {'value': tensor(1.2476),
  'distribution': Normal(loc: 1.3281, scale: 1.0),
  'is_observed': False,
  'log_prob': tensor(-0.9222)}, # changes
 'B': {'value': tensor(-2.1788),
  'distribution': Normal(loc: 0.0, scale: 1.0),
  'is_observed': False,
  'log_prob': tensor(-3.2925)}}
```

Metropolis Hastings Algorithm For PPLs

```
def model():
    X = sample("X", dist.Normal(0,1))
    Y = sample("Y", dist.Normal(X,1))
    if Y < 0:
        sample("A", dist.Normal(0,1), observed=torch.tensor(1.))
    else:
        sample("B", dist.Normal(0,1))
```

Chosen address: Y

$$Q(\boldsymbol{prop.}|\boldsymbol{curr.}) = \frac{1}{3}Q(Y'|Y), \quad Q(\boldsymbol{curr.}|\boldsymbol{prop.}) = \frac{1}{2}Q(Y|Y')P(B),$$

Current:

```
{'X': {'value': tensor(1.5410),
  'distribution': Normal(loc: 0.0, scale: 1.0),
  'is_observed': False,
  'log_prob': tensor(-2.1063)},
 'Y': {'value': tensor(1.2476), # changes
  'distribution': Normal(loc: 1.5410, scale: 1.0),
  'is_observed': False,
  'log_prob': tensor(-0.9620)}, # changes
 'B': {'value': tensor(-2.1788), # changes
  'distribution': Normal(loc: 0.0, scale: 1.0),
  'is_observed': False, # changes
  'log_prob': tensor(-3.2925)}} # changes
```

Proposed:

```
{'X': {'value': tensor(1.5410),
  'distribution': Normal(loc: 0.0, scale: 1.0),
  'is_observed': False,
  'log_prob': tensor(-2.1063)},
 'Y': {'value': tensor(-0.1596), # changes
  'distribution': Normal(loc: 1.5410, scale: 1.0),
  'is_observed': False,
  'log_prob': tensor(-2.3650)}, # changes
 'A': {'value': tensor(1.0000), # changes
  'distribution': Normal(loc: 0.0, scale: 1.0),
  'is_observed': True, # changes
  'log_prob': tensor(-1.4189)}} # changes
```

Metropolis Hastings Algorithm For PPLs

```
def model():
    X = sample("X", dist.Normal(0,1))
    Y = sample("Y", dist.Normal(X,1))
    if Y < 0:
        sample("A", dist.Normal(0,1), observed=torch.tensor(1.))
    else:
        sample("B", dist.Normal(0,1))
```

Chosen address: **B**

$$Q(\boldsymbol{prop.}|\boldsymbol{curr.}) = \frac{1}{3}Q(B'|B), \quad Q(\boldsymbol{curr.}|\boldsymbol{prop.}) = \frac{1}{3}Q(B|B'),$$

Current:

```
{'X': {'value': tensor(1.5410),
  'distribution': Normal(loc: 0.0, scale: 1.0),
  'is_observed': False,
  'log_prob': tensor(-2.1063)},
 'Y': {'value': tensor(1.2476),
  'distribution': Normal(loc: 1.5410, scale: 1.0),
  'is_observed': False,
  'log_prob': tensor(-0.9620)},
 'B': {'value': tensor(-2.1788), # changes
  'distribution': Normal(loc: 0.0, scale: 1.0),
  'is_observed': False,
  'log_prob': tensor(-3.2925)}} # changes
```

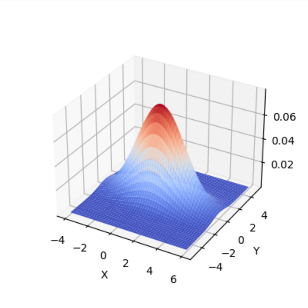
Proposed:

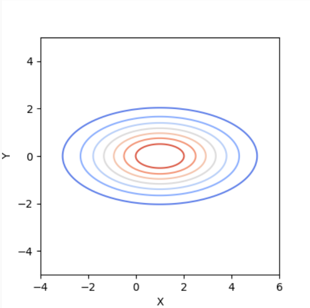
```
{'X': {'value': tensor(1.5410),
  'distribution': Normal(loc: 0.0, scale: 1.0),
  'is_observed': False,
  'log_prob': tensor(-2.1063)},
 'Y': {'value': tensor(1.2476),
  'distribution': Normal(loc: 1.5410, scale: 1.0),
  'is_observed': False,
  'log_prob': tensor(-0.9620)},
 'B': {'value': tensor(-1.2213), # changes
  'distribution': Normal(loc: 0.0, scale: 1.0),
  'is_observed': False,
  'log_prob': tensor(-1.6647)}} # changes
```

Hamiltonian Monte Carlo

Hamiltonian Monte Carlo

- Assumptions: Finite number of continuous (unconstrained) random variables
- Makes the program density essentially differentiable
- Idea: Interpret density as energy potential and samples as particles in the potential
- The improved version of HMC called NUTS is state-of-the-art inference algorithm





Hamiltonian Monte Carlo

Hamiltonian Mechanics:

- position vector x, momentum vector p
- Hamiltonian

$$H(x, p) = \underbrace{U(x)}_{\text{potential energy}} + \underbrace{K(p)}_{\text{kinetic energy}}$$

- Mechanics
  - Particle's velocity equals the derivative of kinetic energy with respect to momentum:

$$\frac{dx_i}{dt} = \frac{\partial H}{\partial p_i} = \frac{\partial K}{\partial p_i}$$

  - Force on the particle equals the negative gradient of the potential energy:

$$\frac{dp_i}{dt} = -\frac{\partial H}{\partial x_i} = -\frac{\partial U}{\partial x_i}$$

Hamiltonian Monte Carlo

$$H(x,p) = \underbrace{U(x)}_{\text{potential energy}} + \underbrace{K(p)}_{\text{kinetic energy}}$$

$$U(x) := -\log P(x)$$
$$K(p) := \frac{p^T p}{2}$$

Joint distribution of position and momentum:

$$P(x,p) \propto \exp(-H(x,p)) = \underbrace{P(x)}_{\text{target distribution}} \underbrace{\exp\left(-\frac{p^T p}{2}\right)}_{\text{Normal distribution}}$$

Hamiltonian Monte Carlo

Idea:

- Sample random momentum.
- Simulate Hamiltonian mechanics.

If simulation is reversible and preserves volume, then the resulting Markov chain satisfies detailed balance and produces the correct samples.

This is true because, such a simulation makes the proposals symmetric. The acceptance probability simplifies to

$$\min\left(1, \frac{P(x', p')}{P(x, p)}\right) = \min\left(1, \exp(-H(x', p') + H(x, p))\right)$$

A perfect simulation preserves the Hamiltonian and we would accept with probability 1!

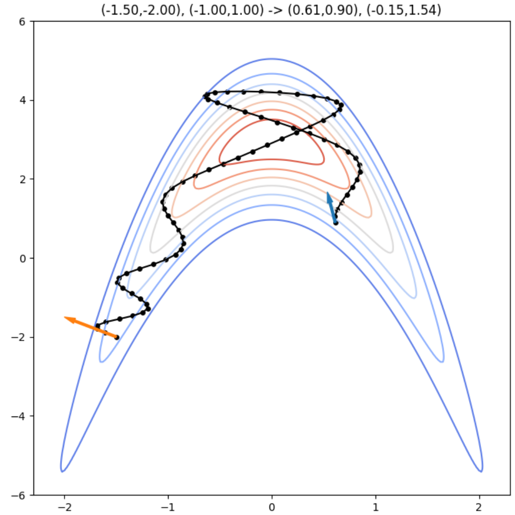
Leap-Frog Integration

$$
\begin{aligned}
p_i\left(t + \frac{\epsilon}{2}\right) &= p_i(t) - \frac{\epsilon}{2} \cdot \frac{\partial U}{\partial x_i}(x(t)) && \text{half-step} \\
x_i(t+\epsilon) &= x_i(t) + \epsilon \cdot p_i\left(t + \frac{\epsilon}{2}\right) && \text{full-step} \\
p_i(t+\epsilon) &= p_i\left(t + \frac{\epsilon}{2}\right) - \frac{\epsilon}{2} \cdot \frac{\partial U}{\partial x_i}(x(t+\epsilon)) && \text{half-step}
\end{aligned}
$$

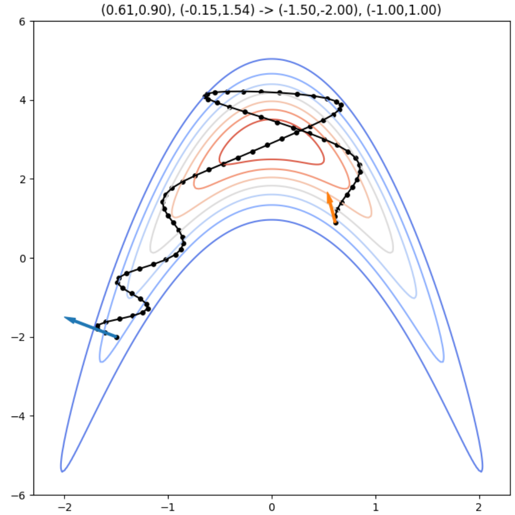
This procedure gets more accurate with $\epsilon \to 0$.

```
P = P - eps/2 * grad_U       # half-step

repeat:
    X = X + eps * P          # full-step
    P = P - eps * grad_U(X)  # full-step

X = X + eps * P              # full-step
P = P - eps/2 * grad_U(X)    # half-step
```

Hamiltonian Monte Carlo: Leap-frog trajectory



Hamiltonian Monte Carlo: Leap-frog trajectory



Hamiltonian Monte Carlo

Let $P(x)$ be the target distribution, set $U(x) = -\log P(x)$, $K(p) = p^T p/2$.

1. Initialise x_0
2. For each $i = 1, \ldots, n$
    - Sample the momentum, $p \sim \text{Normal}(0, 1)$
    - Simulate mechanics

$$x', p' = \text{leapfrog}(x, p)$$

    - Calculate the acceptance probability

$$A = \min\left(1, \exp(-H(x', p') + H(x, p))\right)$$

    - Draw a random number $0 \leq p \leq 1$ and let

$$x_{i+1} = \begin{cases} x' & p \leq A \quad \text{(accept)} \\ x_i & p > A \quad \text{(reject)} \end{cases}$$

Resources

Why we use dependent sampling to sample from the posterior
https://www.youtube.com/watch?v=CfpRdmddVPM

An introduction to the Random Walk Metropolis algorithm
https://www.youtube.com/watch?v=U561HGMWjcw

Paper: Single-Site MH for PPL *http://proceedings.mlr.press/v15/wingate11a/wingate11a.pdf*

Handbook of MCMC: Chapter 5: MCMC Using Hamiltonian Dynamics
http://www.mcmchandbook.net/HandbookChapter5.pdf

The intuition behind the Hamiltonian Monte Carlo algorithm
https://www.youtube.com/watch?v=a-wydhEuAm0

MCMC Interactive Gallery
https://chi-feng.github.io/mcmc-demo/app.html

Paper: No-U-Turn Sampler
https://arxiv.org/abs/1111.4246