Probabilistic Graphical Models

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5. Inference with Monte Carlo methods

- Monte Carlo methods
  Monte Carlo integration
  Sampling from simple distributions
  Rejection sampling
  Importance sampling

- Markov chain Monte Carlo
  Metropolis-Hastings algorithm
  Gibbs sampling
  Hamiltonian Monte Carlo

Outline

- Monte Carlo methods
  - Monte Carlo integration
  - Sampling from simple distributions
  - Rejection sampling
  - Importance sampling
- Markov chain Monte Carlo
  - Metropolis-Hastings algorithm
  - Gibbs sampling
  - Hamiltonian Monte Carlo

Monte Carlo integration

$$\mathbf{E}[f(X)] = \int f(x)p(x)\ dx$$

- $x \in \mathbf{R}^n$
- $f : \mathbf{R}^n \to \mathbf{R}^m$
- $p(x)$: target distribution of X
- target distribution as posterior $p(x \mid y)$
  - use the unnormalized distribution $\tilde{p}(x) = p(x, y)$
  - normalize the result with $Z = \int p(x, y)\ dx = p(y)$

Monte Carlo (MC) integration: draw n random samples $x \sim p(x)$

$$\mathbf{E}[f(X)] = \int f(x)p(x)\ dx \approx \frac{1}{n}\sum_{i=1}^{n} f(x_i)$$

Monte Carlo integration

let $\mu = \mathbf{E}[f(X)]$ be the exact mean, $\hat{\mu}$ be the MC approximation

- with independence samples:

$$(\hat{\mu} - \mu) \to \mathcal{N}\left(0, \frac{\hat{\sigma}^2}{n}\right)$$

  – $\hat{\sigma}^2 = \frac{1}{n}\sum_{i=1}^{n}\left(f(x_i) - \hat{\mu}\right)^2$

- for large enough n:

$$\mathbf{P}\left(\hat{\mu} - 1.96\sqrt{\frac{\hat{\sigma}^2}{n}} \leq \mu \leq \hat{\mu} + 1.96\sqrt{\frac{\hat{\sigma}^2}{n}}\right) \approx 0.95$$

  – $\sqrt{\frac{\hat{\sigma}^2}{n}}$: (numerical) standard error, denotes the uncertainty about our μ estimation
  – standard error of μ estimation is independent of the integration dimensionality

Monte Carlo integration

example: estimating π by MC integration

- given a (Euclidean) ball in $\mathbf{R}^2$: $B(r) = \{x, y \mid x^2 + y^2 \leq r^2\}$
- the area of the ball $S = \pi r^2 = \int_{-r}^{r} \int_{-r}^{r} I_B(x, y)\ dxdy$
  - I_B: indicator function of ball $B(r)$, equals to 1 for points inside the ball, and 0 outside
- let $p(x), p(y) \sim \mathcal{U}(-r, r)$

$$
\begin{aligned}
\pi = \frac{1}{r^2} S &= \frac{1}{r^2}(2r)(2r) \iint I_B(x, y) p(x) p(y)\ dxdy \\
&= \frac{1}{r^2} 4r^2 \iint I_B(x, y) p(x) p(y)\ dxdy \\
&\approx 4 \times \frac{1}{n} \sum_{i=1}^{n} I_B(x_i, y_i)
\end{aligned}
$$

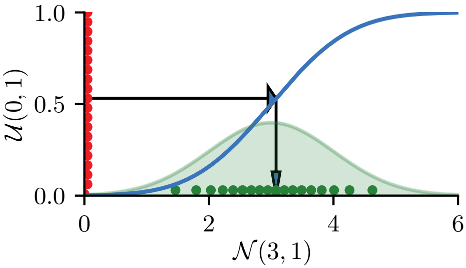
Sampling from simple distributions

inverse probability transform

$$U \sim \mathcal{U}(0,1) \implies F^{-1}(U) \sim F$$

- F: **cumulative density function (CDF)** of target distribution
- F^{-1}: the inverse of CDF F
- proof:

$$\begin{aligned} \mathbf{P}\left(F^{-1}(U) \le x\right) &= \mathbf{P}(U \le F(x)) \\ &= F(x) \end{aligned}$$



Sampling from simple distributions

example: sampling from $\mathrm{Exp}(\lambda)$

$$p_\lambda(x) = \begin{cases} \lambda e^{-\lambda x} & x \geq 0 \\ 0 & x < 0 \end{cases} \implies F_\lambda(x) = \begin{cases} 1 - e^{-\lambda x} & x \geq 0 \\ 0 & x < 0 \end{cases}$$

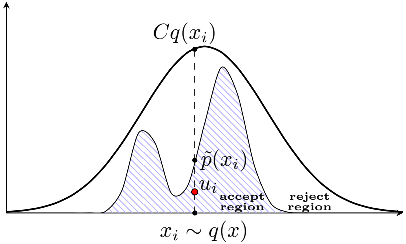
$$\implies F_\lambda^{-1}(u) = -\frac{\log(1-u)}{\lambda}$$

- $\mathbf{dom}(F_\lambda^{-1}) = [0, 1)$
- sample $U \sim \mathcal{U}(0, 1)$, then $F_\lambda^{-1}(U) \sim \mathrm{Exp}(\lambda)$

Rejection sampling

given:

- target distribution $p(x) = \tilde{p}(x)/Z_p$, where $Z_p = \int \tilde{p}(x)\ dx$
- proposal distribution $q(x)$, satisfying $Cq(x) \geq \tilde{p}(x)$ for some $C \in \mathbf{R}$



rejection sampling

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1. Sample $x_i \sim q(x)$.
2. Sample $u_i \sim \mathcal{U}(0, Cq(x_i))$.
3. If $u_i > \tilde{p}(x_i)$, reject the sample, otherwise accept it.

- $q(x_i \mid \text{accept}) = p(x_i)$

Rejection sampling

proof

$$q(\text{accept} \mid x_i) = \int_0^{\tilde{p}(x_i)} \frac{1}{Cq(x_i)}\, du = \frac{\tilde{p}(x_i)}{Cq(x_i)}$$

$$\Longrightarrow q(\text{propose and accept } x_i) = q(x_i)q(\text{accept} \mid x_i) = q(x_i)\frac{\tilde{p}(x_i)}{Cq(x_i)} = \frac{\tilde{p}(x_i)}{C}$$

$$\Longrightarrow \int q(x_i)q(\text{accept} \mid x_i)\, dx_i = q(\text{accept}) = \frac{\int \tilde{p}(x_i)\, dx_i}{C} = \frac{Z_p}{C}$$

$$\Longrightarrow q(x_i \mid \text{accept}) = \frac{q(x_i, \text{accept})}{q(\text{accept})} = \frac{\tilde{p}(x_i)}{C}\frac{C}{Z_p} = \frac{\tilde{p}(x_i)}{Z_p} = p(x_i)$$

Rejection sampling

$$q(\text{accept}) = \frac{Z_p}{C}$$

- $q(\text{accept}) = 1/C$ if $\tilde{p}$ is a normalized target distribution
- example: $p(x) = \mathcal{N}(0, \sigma_p^2 I)$, $q(x) = \mathcal{N}(0, \sigma_q^2 I)$ $(\sigma_q^2 \geq \sigma_p^2)$
  - in n dimensions, optimum $C = (\sigma_q/\sigma_p)^n$
  - acceptance rate decreases exponentially with dimension

Importance sampling

direct importance sampling with normalized target distribution:

$$\mathbf{E}[f(X)] = \int f(x)p(x)\ dx = \int f(x)\frac{p(x)}{q(x)}q(x)\ dx$$

- $q(x)$: proposal distribution
- $\mathbf{supp}(p) \subseteq \mathbf{supp}(q)$: the proposal is non-zero whenever the target is non-zero

draw n samples $x \sim q(x)$

$$\mathbf{E}[f(X)] \approx \frac{1}{n}\sum_{i=1}^{n}\frac{p(x_i)}{q(x_i)}f(x_i) = \frac{1}{n}\sum_{i=1}^{n} w_i f(x_i)$$

- $w_i = \frac{p(x_i)}{q(x_i)}$: importance weight
- unbiased estimate of the true mean $\mathbf{E}[f(X)]$

Importance sampling

self-normalized importance sampling (SNIS) with unnormalized target distribution $\tilde{p}(x)$:

draw n samples $x \sim q(x)$

$$\mathbf{E}[f(X)] = \int f(x)p(x)\ dx = \frac{\int f(x)\tilde{p}(x)\ dx}{\int \tilde{p}(x)\ dx} = \frac{\int \left[\frac{\tilde{p}(x)}{q(x)} f(x)\right] q(x)\ dx}{\int \left[\frac{\tilde{p}(x)}{q(x)}\right] q(x)\ dx}$$

$$\approx \frac{\frac{1}{n}\sum_{i=1}^{n} \tilde{w}_i f(x_i)}{\frac{1}{n}\sum_{i=1}^{n} \tilde{w}_i} = \sum_{i=1}^{n} W_i f(x_i)$$

- $q(x)$: proposal distribution, $\mathbf{supp}(\tilde{p}) \subseteq \mathbf{supp}(q)$
- $\tilde{w}_i = \frac{\tilde{p}(x_i)}{q(x_i)}$: unnormalized weight
- $W_i = \frac{\tilde{w}_i}{\sum_{i'=1}^{n} \tilde{w}_{i'}}$: normalized weight
- $p(x) \approx \hat{p}(x) = \sum_{i=1}^{n} W_i \delta(x - x_i)$, and $Z_p \approx \hat{Z}_p = \frac{1}{n}\sum_{i=1}^{n} \tilde{w}_i$

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Markov chain Monte Carlo (MCMC)

idea

- construct a Markov chain on state space X, whose stationary distribution is the target density $p^*(x)$
- by drawing (correlated) samples $x_0, x_1, \ldots$ from the Markov chain, we can perform Monte Carlo integration w.r.t. p^*
- the initial samples from the chain do not come from the stationary distribution, and should be discarded (**burn in**)

Metropolis-Hastings (MH) algorithm

idea

at each step:

- propose to move from x to x' with proposal distribution $q(x' \mid x)$
- decide whether to accept this proposal, or to reject it, according to some acceptance probability A
- if the proposal is accepted, the new state is x', otherwise the new state is the same as the current state x

Metropolis-Hastings (MH) algorithm

acceptance probability A

- symmetric proposal $q(x' \mid x) = q(x \mid x')$:

$$A = \min\left\{1, \frac{p^*(x')}{p^*(x)}\right\}$$

  - if x' is more probable than x, we definitely move there (since $\frac{p^*(x')}{p^*(x)} > 1$)
  - if x' is less probable than x, we move there depending on the probability ratio $\frac{p^*(x')}{p^*(x)}$

- asymmetric proposal $q(x' \mid x) \neq q(x \mid x')$: Hastings correction

$$A = \min\{1, \alpha\}, \quad \alpha = \frac{p^*(x')q(x \mid x')}{p^*(x)q(x' \mid x)}$$

Metropolis-Hastings (MH) algorithm

- we should be able to **evaluate** target distribution $p^*(x)$
- valid proposal q: $\mathbf{supp}(p^*) \subseteq \cup_x \mathbf{supp}(q(\cdot \mid x))$
- sampling from unnormalized target distribution $p^*(x) = \frac{1}{Z_p}\tilde{p}(x)$:

$$\alpha = \frac{(\tilde{p}(x')/Z_p)q(x \mid x')}{(\tilde{p}(x)/Z_p)q(x' \mid x)} = \frac{\tilde{p}(x')q(x \mid x')}{\tilde{p}(x)q(x' \mid x)}$$

Metropolis-Hastings (MH) algorithm

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given proposal distribution q.
initialize x.
repeat

- Sample $x' \sim q(x' \mid x)$.
- Compute $\alpha := \frac{p^*(x')q(x|x')}{p^*(x)q(x'|x)}$.
- Compute acceptance probability $A := \min\{1, \alpha\}$.
- Sample $u \sim \mathcal{U}(0,1)$.
- Set new sample to $x := \begin{cases} x' & u \leq A \text{ (accept)} \\ x & u > A \text{ (reject)}. \end{cases}$

until number of iterations reached.

Metropolis-Hastings (MH) algorithm

convergence analysis

- MH defines a Markov chain with transition matrix

$$p(x' \mid x) = \begin{cases} q(x' \mid x)A(x' \mid x) & x' \neq x \\ q(x \mid x) + \sum_{x' \neq x} q(x' \mid x)(1 - A(x' \mid x)) & \text{otherwise} \end{cases}$$

- if the target distribution p^* is the stationary distribution of this Markov chain, then it satisfies the **detailed balance** criterion

$$p(x' \mid x)p^*(x) = p(x \mid x')p^*(x')$$

Metropolis-Hastings (MH) algorithm

proof

- assume that the Markov chain is ergodic and irreducible

- given two states x and x', we have

$$p^*(x)q(x' \mid x) < p^*(x')q(x \mid x') \quad \text{or} \quad p^*(x)q(x' \mid x) \geq p^*(x')q(x \mid x')$$

- without losing generality, we can assume

$$p^*(x)q(x' \mid x) > p^*(x')q(x \mid x')$$

$$\Longrightarrow \alpha(x' \mid x) = \frac{p^*(x')q(x \mid x')}{p^*(x)q(x' \mid x)} < 1$$

$$\Longrightarrow A(x' \mid x) = \alpha(x' \mid x) \quad \text{and} \quad A(x \mid x') = 1$$

Metropolis-Hastings (MH) algorithm

$$\Longrightarrow \begin{cases} p(x' \mid x) = q(x' \mid x)A(x' \mid x) = q(x' \mid x)\dfrac{p^*(x')q(x \mid x')}{p^*(x)q(x' \mid x)} = \dfrac{p^*(x')}{p^*(x)}q(x \mid x') \\ p(x \mid x') = q(x \mid x')A(x \mid x') = q(x \mid x') \end{cases}$$

$$\Longrightarrow p^*(x)p(x' \mid x) = p^*(x')q(x \mid x')$$

$$\Longrightarrow p^*(x)p(x' \mid x) = p^*(x')p(x \mid x')$$

$\Longrightarrow$ detailed balence is satisfied by p^*

Metropolis-Hastings (MH) algorithm

proposal distributions q

- independence sampler: $q(x' \mid x) = q(x')$, e.g., $x' \sim \mathcal{N}(\mu, \Sigma)$
- random walk Metropolis (RWM):

$$x' \sim \mathcal{N}(x, \sigma^2 I) \iff (x' - x) \sim \mathcal{N}(0, \sigma^2 I)$$

- composing proposals:

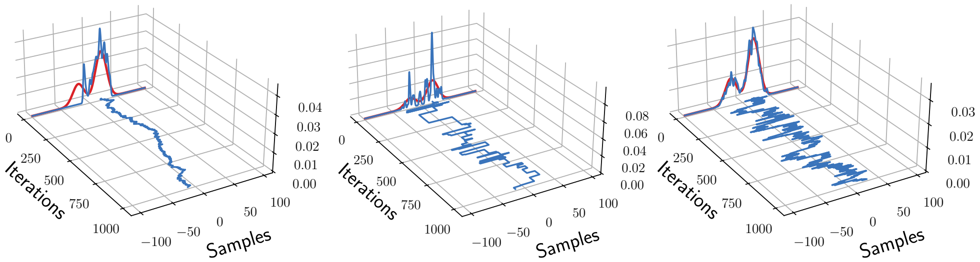
$$q(x' \mid x) = \sum_{i=1}^{m} w_i q_i(x' \mid x)$$

  - w: mixing weights, and $w^T \mathbf{1} = 1$
  - if each q_i is valid individually and $w \succeq 0$, the overall mixture proposal q is also valid

Metropolis-Hastings (MH) algorithm

example: sampling from a mixture of Gaussians with RWM

MH with $\mathcal{N}(0, 1^2)$ proposal   MH with $\mathcal{N}(0, 500^2)$ proposal   MH with $\mathcal{N}(0, 8^2)$ proposal



Gibbs sampling

- a special case of MH algorithm
- exploiting conditional independence properties of a graphical model on X to automatically create a good proposal q, with 100% acceptance probability

idea: sample each variable in turn, conditioned on the values of all the other variables in the distribution

example: sample some variable $X \in \mathbf{R}^3$ according to

$$\begin{aligned} x_1' &\sim p(x_1' \mid x_2, x_3) \\ x_2' &\sim p(x_2' \mid x_1', x_3) \\ x_3' &\sim p(x_3' \mid x_1', x_2') \end{aligned}$$

Gibbs sampling

- $p(x_i' \mid x_{-i})$: **full conditional** for variable X_i

- if X_i is a known variable, we do not sample it, but it may be used as input to the another conditional distributions

- if we represent $p(x)$ as a graphical model,

$$x_i' \sim p(x_i' \mid x_{-i}) = p(x_i' \mid \mathbf{mb}(x_i))$$

- we should have access to the analytical expression of target distribution p to derive the full conditionals for each X_i

Gibbs sampling

connections to MH

- Gibbs sampling is a special case of MH using a sequence of proposals

$$q_i(x' \mid x) = p(x' \mid x_{-i}) I_{x_{-i}}(x'_{-i}), \quad i = 1, \dots, n$$

  - $X \in \mathbf{R}^n$
  - $I_{x_{-i}}$: indicator function

- proof of 100% acceptance probability: for sampling each X_i, we have $x'_{-i} = x_{-i}$, thus

$$\alpha = \frac{p(x') q_i(x \mid x')}{p(x) q_i(x' \mid x)} = \frac{p(x'_i \mid x'_{-i}) p(x'_{-i}) p(x_i \mid x'_{-i})}{p(x_i \mid x_{-i}) p(x_{-i}) p(x'_i \mid x_{-i})}$$
$$= \frac{p(x'_i \mid x_{-i}) p(x_{-i}) p(x_i \mid x_{-i})}{p(x_i \mid x_{-i}) p(x_{-i}) p(x'_i \mid x_{-i})} = 1$$

Gibbs sampling

example: Gibbs sampling for Ising models

for a 2-dimensional lattice $G = (X, E)$:

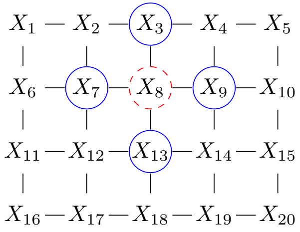
- lattice model:

$$p(x) = \frac{1}{Z_p} \prod_{(X_i, X_j) \in E} \psi_{ij}(x_i, x_j)$$

  - $\psi_{ij}(x_i, x_j)$: potential function of clique $C = \{X_i, X_j\}$

- Ising model:
  - X_i are binary for all $i = 1, \ldots, n$
  - potential function expressed as

$$\psi_{ij}(x_i, x_j) = \begin{cases} e^{J} & x_i = x_j \\ e^{-J} & x_i \neq x_j \end{cases} = \exp(J x_i x_j)$$



Gibbs sampling

to sample for an n-dimensional random vector X following an Ising model,

$$p(x_i \mid x_{-i}) \propto \prod_{X_j \in \mathbf{adj}(X_i)} \psi_{ij}(x_i, x_j), \quad i = 1, \ldots, n$$

$$\begin{aligned}
\implies p(x_i = +1 \mid x_{-i}) &= \frac{\prod_{X_j \in \mathbf{adj}(X_i)} \psi_{ij}(x_i = +1, x_j)}{\prod_{X_j \in \mathbf{adj}(X_i)} \psi_{ij}(x_i = +1, x_j) + \prod_{X_j \in \mathbf{adj}(X_i)} \psi_{ij}(x_i = -1, x_j)} \\
&= \frac{\exp(J \sum_{X_j \in \mathbf{adj}(X_i)} x_j)}{\exp(J \sum_{X_j \in \mathbf{adj}(X_i)} x_j) + \exp(-J \sum_{X_j \in \mathbf{adj}(X_i)} x_j)} \\
&= \frac{\exp(J\eta_i)}{\exp(J\eta_i) + \exp(-J\eta_i)}
\end{aligned}$$

- $\eta_i = \sum_{X_j \in \mathbf{adj}(X_i)} x_j$

Gibbs sampling

Metropolis within Gibbs

- use MH algorithm to sample from the full conditionals

to sample $x'_i \sim p(x'_i \mid x'_{1:i-1}, x_{i+1:n})$:

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1. Propose $x''_i \sim q(x''_i \mid x_i)$.
2. Compute the acceptance probability $A_i = \min\{1, \alpha_i\}$, where

$$\alpha_i = \frac{p(x''_i \mid x'_{1:i-1}, x_{i+1:n}) q(x_i \mid x''_i)}{p(x_i \mid x'_{1:i-1}, x_{i+1:n}) q(x''_i \mid x_i)}.$$

3. Sample $u \sim \mathcal{U}(0, 1)$.
4. Set $x'_i = x''_i$ if $u < A_i$, and $x'_i = x_i$ otherwise.

Hamiltonian Monte Carlo (HMC)

idea: create proposal q based on gradient information

Hamiltonian mechanics
the total energy of a particle rolling around an energy landscape is

$$\mathcal{H}(\theta, v) = \mathcal{E}(\theta) + \mathcal{K}(v)$$

- $\theta \in \mathbf{R}^n$: position
- $v \in \mathbf{R}^n$: momentum
- (θ, v): phase space
- $\mathcal{E}(\theta)$: potential energy
- $\mathcal{K}(v) = \frac{1}{2} v^T \Sigma^{-1} v$: kinetic energy, where $\Sigma \in \mathbf{S}^n_{++}$ is the mass matrix
- $\mathcal{H}(\theta, v)$: total energy (Hamiltonian)

Hamiltonian Monte Carlo (HMC)

- trajectory of the particle can be obtained by solving **Hamilton's equations**:

$$\begin{cases} \frac{d\theta}{dt} = \frac{\partial \mathcal{H}}{\partial v} = \frac{\partial \mathcal{K}}{\partial v} \\ \frac{dv}{dt} = -\frac{\partial \mathcal{H}}{\partial \theta} = -\frac{\partial \mathcal{E}}{\partial \theta} \end{cases}$$

- energy is conserved under Hamiltonian mechanics, since

$$\frac{d\mathcal{H}}{dt} = \sum_{i=1}^{n} \left(\frac{\partial \mathcal{H}}{\partial \theta_i} \frac{d\theta_i}{dt} + \frac{\partial \mathcal{H}}{\partial v_i} \frac{dv_i}{dt} \right) = \sum_{i=1}^{n} \left(\frac{\partial \mathcal{H}}{\partial \theta_i} \frac{\partial \mathcal{H}}{\partial v_i} - \frac{\partial \mathcal{H}}{\partial \theta_i} \frac{\partial \mathcal{H}}{d v_i} \right) = 0$$

Hamiltonian Monte Carlo (HMC)

to solve Hamilton's equations in discrete time:

- **Euler's method**:

$$\begin{cases} v_{t+1} = v_t + \eta \left.\dfrac{dv}{dt}\right|_{\theta=\theta_t, v=v_t} = v_t - \eta \left.\dfrac{\partial \mathcal{E}}{\partial \theta}\right|_{\theta=\theta_t} \\ \theta_{t+1} = \theta_t + \eta \left.\dfrac{d\theta}{dt}\right|_{\theta=\theta_t, v=v_t} = \theta_t + \eta \left.\dfrac{\partial \mathcal{K}}{\partial v}\right|_{v=v_t} \end{cases}.$$

  - η: step size
  - if $\mathcal{K}(v) = \frac{1}{2} v^T \Sigma^{-1} v$, the second term reduces to

$$\theta_{t+1} = \theta_t + \eta \Sigma^{-1} v_t$$

Hamiltonian Monte Carlo (HMC)

- **modified Euler's method**:

$$\begin{cases} v_{t+1} = v_t + \eta \left.\dfrac{dv}{dt}\right|_{\theta=\theta_t, v=v_t} = v_t - \eta \left.\dfrac{\partial \mathcal{E}}{\partial \theta}\right|_{\theta=\theta_t} \\ \theta_{t+1} = \theta_t + \eta \left.\dfrac{d\theta}{dt}\right|_{\theta=\theta_t, v=v_{t+1}} = \theta_t + \eta \left.\dfrac{\partial \mathcal{K}}{\partial v}\right|_{v=v_{t+1}} \end{cases}.$$

  - slightly more accurate than Euler's method
  - asymmetry of this method can cause some theoretical problems

Hamiltonian Monte Carlo (HMC)

- **leapfrog integrator**:

$$\begin{cases} v_{t+1/2} = v_t - \dfrac{\eta}{2} \dfrac{\partial \mathcal{E}}{\partial \theta}\Big|_{\theta=\theta_t} \\ \theta_{t+1} = \theta_t + \eta \dfrac{\partial \mathcal{K}}{\partial v}\Big|_{v=v_{t+1/2}} \\ v_{t+1} = v_{t+1/2} - \dfrac{\eta}{2} \dfrac{\partial \mathcal{E}}{\partial \theta}\Big|_{\theta=\theta_{t+1}} \end{cases}.$$

  - symmetrized version of the modified Euler's method
  - can be extended to multiple leapfrog steps, i.e., performing a half step update of v at the beginning and end of the trajectory, and alternating between full step updates of θ and v in between

Hamiltonian Monte Carlo (HMC)

the HMC algorithm

- establish a new target by introducing an auxiliary variable v to the initial target distribution $p(\theta)$:

$$p(\theta, v) = \frac{1}{Z}\exp(-\mathcal{H}(\theta, v)) = \frac{1}{Z}\exp\left(-\mathcal{E}(\theta) - \frac{1}{2}v^T\Sigma^{-1}v\right)$$

- after sampling w.r.t. $p(\theta, v)$, we just 'throw away' the v's so that

$$p(\theta) = \int p(\theta, v)\ dv = \frac{1}{Z_\theta}e^{-\mathcal{E}(\theta)} \int \frac{1}{Z_v}e^{-\frac{1}{2}v^T\Sigma^{-1}v}\ dv = \frac{1}{Z_\theta}e^{-\mathcal{E}(\theta)}$$

Hamiltonian Monte Carlo (HMC)

suppose the previous state of the Markov chain is (θ_{t-1}, v_{t-1}), to sample the next state,

- set the initial position to $\theta'_0 = \theta_{t-1}$, and sample a new random momentum $v'_0 \sim \mathcal{N}(0, \Sigma)$
- starting from (θ'_0, v'_0), perform L leapfrogs to get the proposed state $(\theta^*, v^*) = (\theta'_L, v'_L)$
- check divergence of the simulated trajectory, if $\mathcal{H}_0 \neq \mathcal{H}_L$, reject the sample
- if the trajectory is not diverged, compute the MH acceptance probability as

$$A = \min\left\{1, \frac{p(\theta^*, v^*)}{p(\theta_{t-1}, v_{t-1})}\right\} = \min\left\{1, \exp\left(-\mathcal{H}(\theta^*, v^*) + \mathcal{H}(\theta_{t-1}, v_{t-1})\right)\right\}$$

  - the transition probabilities cancel since the proposal is reversible

- accept the proposal with probability A by setting $(\theta_t, v_t) = (\theta^*, v^*)$, otherwise reject it $((\theta_t, v_t) = (\theta_{t-1}, v_{t-1}))$

Hamiltonian Monte Carlo (HMC)

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given the number of leapfrog steps L, the step size η, and the covariance matrix Σ.
repeat
  Generate random momentum $v_{t-1} \sim \mathcal{N}(0, \Sigma)$.
  Set $(\theta'_0, v'_0) := (\theta_{t-1}, v_{t-1})$.
  Half step for momentum: $v'_{1/2} := v'_0 - \frac{\eta}{2} \nabla \mathcal{E}(\theta'_0)$.
  for $l = 1, \ldots, L-1$ **do**
    $\theta'_l := \theta'_{l-1} + \eta \Sigma^{-1} v'_{l-1/2}$.
    $v'_{l+1/2} := v'_{l-1/2} - \eta \nabla \mathcal{E}(\theta'_l)$.
  end for
  Full step for location: $\theta'_L := \theta'_{L-1} + \eta \Sigma^{-1} v'_{L-1/2}$.
  Half step for momentum: $v'_L := v'_{L-1/2} - \frac{\eta}{2} \nabla \mathcal{E}(\theta'_L)$.
  Obtain proposal $(\theta^*, v^*) := (\theta'_L, v'_L)$.
  Compute acceptance probability $A := \min\{1, \exp(-\mathcal{H}(\theta^*, v^*) + \mathcal{H}(\theta_{t-1}, v_{t-1}))\}$.
  Set $\theta_t := \theta^*$ with probability A, other wise $\theta_t := \theta_{t-1}$.
until number of iterations reached.

- we must pick a random momentum at the start of each iteration to ensure the sampler explores the full space