3-HMC

August 5, 2019

[2]:
```
import matplotlib.pyplot as plot
import scipy.stats as stats
import numpy
import math

light = "#DCBCBC"
light_highlight = "#C79999"
mid = "#B97C7C"
mid_highlight = "#A25050"
dark = "#8F2727"
dark_highlight = "#7C0000"
green = "#00FF00"
```

To facilitate the computation of Markov chain Monte Carlo estimators, let's define a *Welford accumulator* that computes empirical summaries of a sample in a single pass

[8]:
```
def welford_summary(x, L = 100):
  summary = [0] * (L + 1)
  for n in range(len(x)):
    delta = x[n] - summary[0]
    summary[0] += delta / (n + 1)
    for l in range(L):
      if n > l:
        summary[l + 1] += delta * (x[n - l] - summary[0])

  norm = 1.0 / (len(x) - 1)
  for l in range(L): summary[l + 1] *= norm
  return summary

# We can then use the Welford accumulator output to compute the
# Markov chain Monte Carlo estimators and their properties
def compute_mcmc_stats(x, L = 20):
  summary = welford_summary(x, L)

  mean = summary[0]
  var = summary[1]
  acov = summary[1:(L + 1)]
```

```
  # Compute the effective sample size
  rho_hat_s = [0] * L
  rho_hat_s[1] = acov[1] / var

  # First we transform our autocovariances into Geyer's initial positive␣
↪sequence
  max_s = 1
  for s in [ 2 * i + 1 for i in range((L - 1) // 2) ]:
    rho_hat_even = acov[s + 1] / var
    rho_hat_odd = acov[s + 2] / var;

    max_s = s + 2

    if rho_hat_even + rho_hat_odd > 0:
      rho_hat_s[s + 1] = rho_hat_even
      rho_hat_s[s + 2] = rho_hat_odd
    else:
      break

  # Then we transform this output into Geyer's initial monotone sequence
  for s in [ 2 * i + 3 for i in range((max_s - 2)// 2) ]:
    if rho_hat_s[s + 1] + rho_hat_s[s + 2] > rho_hat_s[s - 1] + rho_hat_s[s]:
      rho_hat_s[s + 1] = 0.5 * (rho_hat_s[s - 1] + rho_hat_s[s])
      rho_hat_s[s + 2] = rho_hat_s[s + 1]

  ess = len(x) / (1.0 + 2 * sum(rho_hat_s))

  return [mean, math.sqrt(var / ess), math.sqrt(var), ess]
```

To generate our samples we'll use numpy's pseudo random number generator which needs to be seeded to achieve reproducible results

[9]:
```
numpy.random.seed(seed=8675309)

# To ensure accurate results let's generate pretty large samples
N = 10000
```

One Hundred-Dimensional Gaussian Target

[10]:
```
D = 100

def target_lpdf(x):
  return - 0.5 * sum([ x_n**2 for x_n in x ]) \
         - 0.5 * len(x) * math.log(6.283185307179586)

def grad_target_lpdf(x):
  return - x
```

1 Random Walk Metropolis

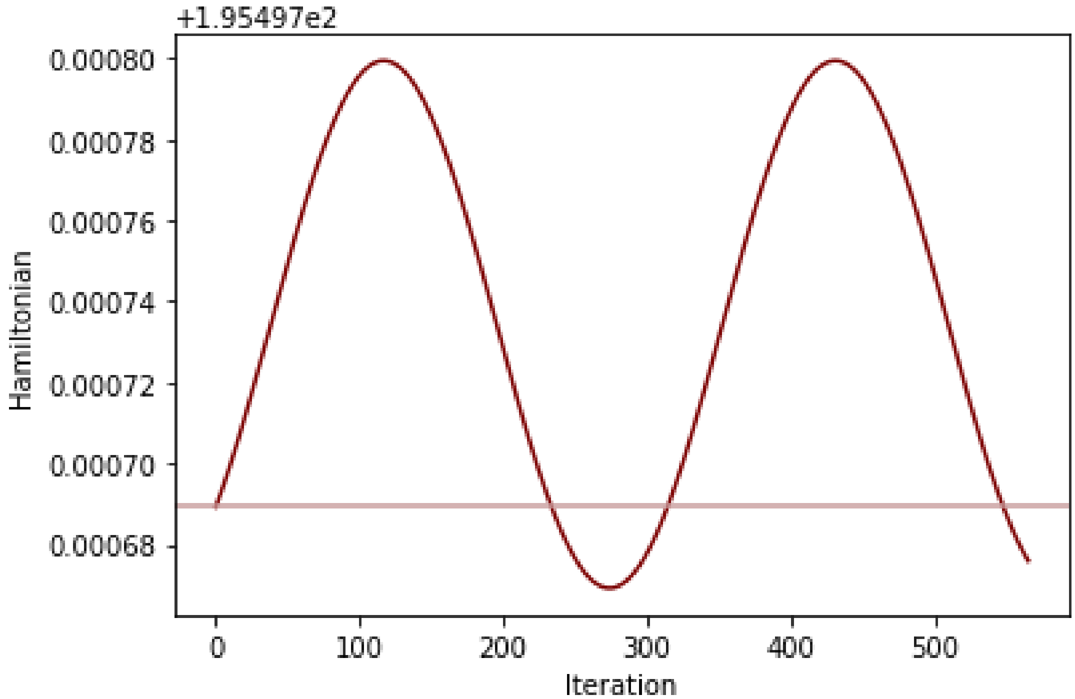
[11]:
```
rwm_accept_prob_mean = 0
rwm_accept_prob_se = 0
rwm_ave_eff_sample_size = 0

# Optimal proposal tuning
opt_sigma = 2.5 / math.sqrt(D)

# A place to store our Markov chain
# D columns for the parameters and one extra column
# for the Metropolis acceptance probability
mcmc_samples = [[0] * (D + 1) for _ in range(N)]

# Seeding the initial state with an exact sample
# from the target distribution ensures that we
# start in the typical set and avoid having to
# worry about warmup.
for d in range(D):
  mcmc_samples[0][d] = stats.norm.rvs(0, 3)
mcmc_samples[0][D] = 1

for n in range(1, N):
  x0 = [ mcmc_samples[n - 1][d] for d in range(D) ]
  xp = [ stats.norm.rvs(x0[d], opt_sigma) for d in range(D) ]

  # Compute acceptance probability
  accept_prob = 1
  if target_lpdf(xp) < target_lpdf(x0):
    accept_prob = math.exp(target_lpdf(xp) - target_lpdf(x0))
  mcmc_samples[n][D] = accept_prob

  # Apply Metropolis correction
  u = stats.uniform.rvs(0, 1)
  if accept_prob > u:
    mcmc_samples[n][0:D] = xp
  else:
    mcmc_samples[n][0:D] = x0

# Compute MCMC estimator statistics
mcmc_stats = compute_mcmc_stats([ s[D] for s in mcmc_samples])

rwm_accept_prob_mean = mcmc_stats[0]
rwm_accept_prob_se = mcmc_stats[1]

# Estimate effective sample size
eff_sample_sizes = [ compute_mcmc_stats([ s[d] for s in mcmc_samples])[3] \
```

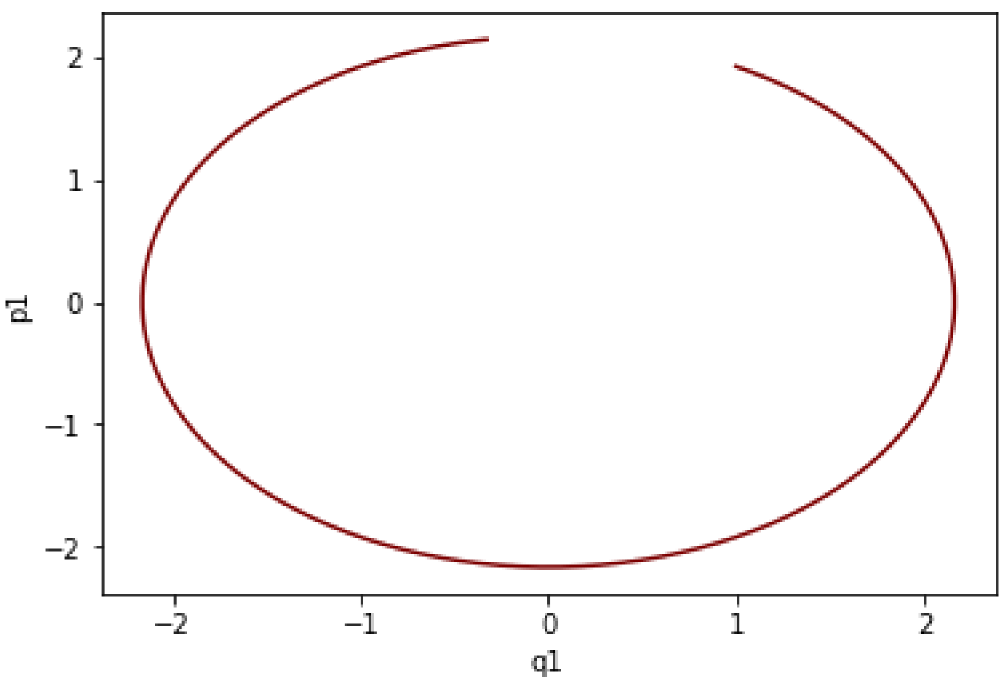
```
                   for d in range(D) ]
rwm_ave_eff_sample_size = sum(eff_sample_sizes) / D
```

2 Hamiltonian Basics

[12]:
```
def leapfrog(q, p, epsilon):
  p += 0.5 * epsilon * grad_target_lpdf(q)
  q += epsilon * p
  p += 0.5 * epsilon * grad_target_lpdf(q)
  return [q, p]

def hamiltonian(q, p):
  return 0.5 * numpy.dot(p, p) - target_lpdf(q)

# Tuning
T = 1.8 * math.pi
epsilon = 0.01
L = int(math.floor(T / epsilon))

# Visualize a single trajectory
q = numpy.asarray([1.0 for _ in range(D)])
p = numpy.asarray([stats.norm.rvs(0, 1) for _ in range(D) ])

Hs = [0] * (L + 1)
q1s = [0] * (L + 1)
p1s = [0] * (L + 1)

Hs[0] = hamiltonian(q, p)
q1s[0] = q[0]
p1s[0] = p[0]

for l in range(L):
  q, p = leapfrog(q, p, epsilon)
  Hs[l + 1] = hamiltonian(q, p)
  q1s[l + 1] = q[0]
  p1s[l + 1] = p[0]

plot.plot(range(L + 1), Hs, color=dark_highlight)
plot.axhline(Hs[0], color=light_highlight)
plot.gca().set_xlabel("Iteration")
plot.gca().set_ylabel("Hamiltonian")
plot.show()

plot.plot(q1s, p1s, color=dark_highlight)
plot.gca().set_xlabel("q1")
plot.gca().set_ylabel("p1")
```

```
plot.show()
```


+1.95497e2
0.00080
0.00078
0.00076
0.00074
0.00072
0.00070
0.00068
Hamiltonian
0
100
200
300
400
500
Iteration


2
1
0
−1
−2
p1
−2
−1
0
1
2
q1

3 Hybrid Monte Carlo

Hamiltonian Monte Carlo with static integration time considering only the final state in each numerical trajectory two which a Metropolis acceptance procedure is applied

[13]:
```
# Tuning
T = 1.8 * math.pi
epsilon = 0.6
L = int(math.floor(T / epsilon))

hybrid_accept_prob_mean = 0
hybrid_accept_prob_se = 0
hybrid_ave_eff_sample_size = 0

# A place to store our Markov chain
# D columns for the parameters and two extra columns,
# one for the Metropolis acceptance probability
# and one for divergent trajectory indicator
mcmc_samples = [[0] * (D + 2) for _ in range(N)]

# Seeding the initial state with an exact sample
# from the target distribution ensures that we
# start in the typical set and avoid having to
# worry about warmup.
for d in range(D):
  mcmc_samples[0][d] = stats.norm.rvs(0, 3)
mcmc_samples[0][D] = 1
mcmc_samples[0][D + 1] = 0

for n in range(1, N):
  q0 = [ mcmc_samples[n - 1][d] for d in range(D) ]

  q = numpy.asarray(x0)
  p = numpy.asarray([stats.norm.rvs(0, 1) for _ in range(D) ])

  H0 = hamiltonian(q, p)

  divergent = 0
  for l in range(L):
    q, p = leapfrog(q, p, epsilon)
    H = hamiltonian(q, p)
    if (H - H0 > 1000):
      divergent = 1
      break

  H = hamiltonian(q, -1 * p)

  mcmc_samples[n][D + 1] = divergent
```

```
  # Compute acceptance probability
  accept_prob = 1
  if H > H0:
    accept_prob = math.exp(H0 - H)
  mcmc_samples[n][D] = accept_prob

  # Apply Metropolis correction
  u = stats.uniform.rvs(0, 1)
  if accept_prob > u:
    mcmc_samples[n][0:D] = q
  else:
    mcmc_samples[n][0:D] = q0

# Compute MCMC estimator statistics
mcmc_stats = compute_mcmc_stats([ s[D] for s in mcmc_samples])

hybrid_accept_prob_mean = mcmc_stats[0]
hybrid_accept_prob_se = mcmc_stats[1]

# Estimate effective sample size
eff_sample_sizes = [ compute_mcmc_stats([ s[d] for s in mcmc_samples])[3] \
                     for d in range(D) ]
hybrid_ave_eff_sample_size = sum(eff_sample_sizes) / D

# Check divergences
sum([ s[D + 1] for s in mcmc_samples])
```

[13]: 0

4 Static Multinomial Hamiltonian Monte Carlo

Hamiltonian Monte Carlo with static integration time but multinomially sampling from all points within a numerical trajectory

[14]:
```
def log_sum_exp(x, y):
  if x > y:
    return x + math.log(1 + math.exp(y - x))
  else:
    return y + math.log(1 + math.exp(x - y))

smhmc_accept_prob_mean = 0
smhmc_accept_prob_se = 0
smhmc_ave_eff_sample_size = 0

# A place to store our Markov chain
# D columns for the parameters and one extra column
```

```
# for the Metropolis acceptance probability
mcmc_samples = [[0] * (D + 2) for _ in range(N)]

# Seeding the initial state with an exact sample
# from the target distribution ensures that we
# start in the typical set and avoid having to
# worry about warmup.
for d in range(D):
  mcmc_samples[0][d] = stats.norm.rvs(0, 3)
mcmc_samples[0][D] = 1
mcmc_samples[0][D + 1] = 0

for n in range(1, N):
  q0 = [ mcmc_samples[n - 1][d] for d in range(D) ]
  q_propose = q0

  q = numpy.asarray(q0)
  p = numpy.asarray([stats.norm.rvs(0, 1) for _ in range(D) ])

  H0 = hamiltonian(q, p)

  divergent = 0
  log_sum_weight = 0
  sum_metro_prob = 1

  Lp = stats.randint.rvs(0, L - 1)

  # Backwards evolution
  for l in range(Lp):
    q, p = leapfrog(q, p, -epsilon)
    H = hamiltonian(q, p)

    if (H - H0 > 1000):
      divergent = 1
      break

    log_weight = H0 - H
    log_sum_weight = log_sum_exp(log_weight, log_sum_weight)
    sum_metro_prob += min(1, math.exp(H0 - H))

    u = stats.uniform.rvs(0, 1)
    if math.exp(log_weight - log_sum_weight):
      q_propose = q

  # Forwards evolution
  q = numpy.asarray(q0)
```

```
  for l in range(L - 1 - Lp):
    q, p = leapfrog(q, p, epsilon)
    H = hamiltonian(q, p)

    if (H - H0 > 1000):
      divergent = 1
      break

    log_weight = H0 - H
    log_sum_weight = log_sum_exp(log_weight, log_sum_weight)
    sum_metro_prob += min(1, math.exp(H0 - H))

    u = stats.uniform.rvs(0, 1)
    if math.exp(log_weight - log_sum_weight):
      q_propose = q

  mcmc_samples[n][0:D] = q_propose

  # Acceptance probability proxy
  accept_prob = sum_metro_prob / L
  mcmc_samples[n][D] = accept_prob

  mcmc_samples[n][D + 1] = divergent

# Compute MCMC estimator statistics
mcmc_stats = compute_mcmc_stats([ s[D] for s in mcmc_samples])

smhmc_accept_prob_mean = mcmc_stats[0]
smhmc_accept_prob_se = mcmc_stats[1]

# Estimate effective sample size
eff_sample_sizes = [ compute_mcmc_stats([ s[d] for s in mcmc_samples])[3] \
                     for d in range(D) ]
smhmc_ave_eff_sample_size = sum(eff_sample_sizes) / D

# Check divergences
sum([ s[D + 1] for s in mcmc_samples])
```

[14]: 0

5 Comparison

[15]:
```
print("Random Walk Metropolis")
print("  Metropolis Accept Probability = "
      + str(rwm_accept_prob_mean) + " +/- " + str(rwm_accept_prob_se))
print("  Average Effective Sample Size = "
```

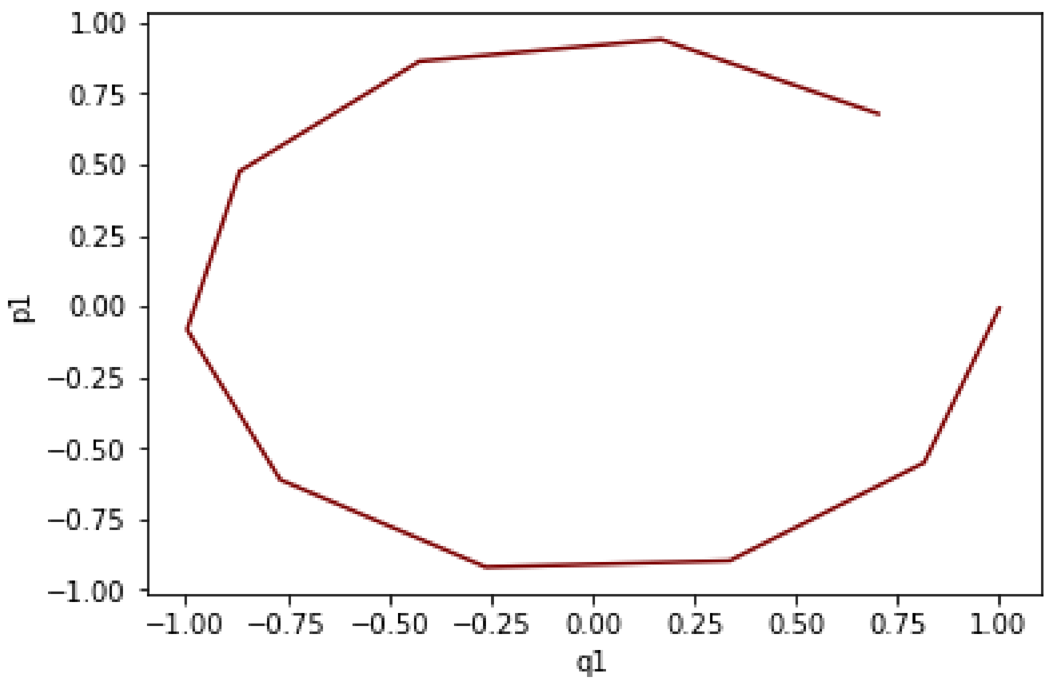
```
      + str(rwm_ave_eff_sample_size))
print("  Average Effective Sample Size Per Comp = "
      + str(rwm_ave_eff_sample_size))
print("")
print("Hybrid Monte Carlo")
print("  Metropolis Accept Probability = "
      + str(hybrid_accept_prob_mean) + " +/- " + str(hybrid_accept_prob_se))
print("  Average Effective Sample Size = "
      + str(hybrid_ave_eff_sample_size))
print("  Average Effective Sample Size Per Comp = "
      + str(hybrid_ave_eff_sample_size / L))
print("")
print("Static Multinomial Hamiltonian Monte Carlo")
print("  Proxy Metropolis Accept Probability = "
      + str(smhmc_accept_prob_mean) + " +/- " + str(smhmc_accept_prob_se))
print("  Average Effective Sample Size = "
      + str(smhmc_ave_eff_sample_size))
print("  Average Effective Sample Size Per Comp = "
      + str(smhmc_ave_eff_sample_size / L))
```

```
Random Walk Metropolis
  Metropolis Accept Probability = 0.21876429946907805 +/- 0.003362724315144871
  Average Effective Sample Size = 274.1377025107051
  Average Effective Sample Size Per Comp = 274.1377025107051

Hybrid Monte Carlo
  Metropolis Accept Probability = 0.5020859807097536 +/- 0.002352870600547754
  Average Effective Sample Size = 3328.5620845935896
  Average Effective Sample Size Per Comp = 369.84023162150993

Static Multinomial Hamiltonian Monte Carlo
  Proxy Metropolis Accept Probability = 0.6844684490061823 +/-
0.0020960658539367384
  Average Effective Sample Size = 24550.04682330573
  Average Effective Sample Size Per Comp = 2727.782980367303
```

Why does Hybrid Monte Carlo perform so poorly here? Bad tuning! The integration time is too long and the numerical trajectories end up back near the initial state, wasting the Hamiltonian flow.

[16]:
```
q = numpy.asarray([1.0 for _ in range(D)])
p = numpy.asarray([stats.norm.rvs(0, 1) for _ in range(D) ])

Hs = [0] * (L + 1)
q1s = [0] * (L + 1)
p1s = [0] * (L + 1)

Hs[0] = hamiltonian(q, p)
```

```
q1s[0] = q[0]
p1s[0] = p[0]

for l in range(L):
  q, p = leapfrog(q, p, epsilon)
  Hs[l + 1] = hamiltonian(q, p)
  q1s[l + 1] = q[0]
  p1s[l + 1] = p[0]

plot.plot(q1s, p1s, color=dark_highlight)
plot.gca().set_xlabel("q1")
plot.gca().set_ylabel("p1")
plot.show()
```



By multinomially sampling we utilize the entire numerial trajectory and become more robust to tuning. The random forward and backwards evolution also sets up dynamic methods that automatically tune the integration time.

[ ]:

```

```