

HW3

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My code lives in the repo https://github.com/geoffwoollard/prob_prog

Acknowledgments

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I gratefully acknowledge helpful code snippets from Masoud Mokhatari, Mohamad Amin Mohamad, and Dylan Green, in particular during the implementation of Hamiltonian Monte Carlo.

Code snippets

```
In [2]: from dill.source import getsource, getsourcelines
```

Importance sampling

- I modified the evaluator from hw2 to also return σ , which gets accumulated from the `log_prob` of evaluating observes

```
In [3]: for line_number, function_line in enumerate(getsourcelines(evaluate)[0]):
        print(line_number, function_line, end='')

0 def evaluate(e, sigma=0, local_env={}, defn_d={}, do_log=False, logger_string=''):
1     # TODO: get local_env to evaluate values to tensors, not regular floats
2     # remember to return evaluate (recursive)
3     # everytime we call evaluate, we have to use local_env, otherwise it gets overwritten with the default {}
4     # if do_log: logger.info('logger_string {}'.format(logger_string))
5     if do_log: logger.info('ls {}'.format(logger_string))
6     if do_log: logger.info('e {}'.format(e), sigma {}.format(e, local_env, sigma))
7
8     # get first expression out of list or list of one
9     if not isinstance(e, list) or len(e) == 1:
10         if isinstance(e, list):
11             e = e[0]
12         if isinstance(e, bool):
13             if do_log: logger.info('match case number: e {}, sigma {}'.format(e, sigma))
14             return torch.tensor(e), sigma
15         if isinstance(e, number):
16             if do_log: logger.info('match case number: e {}, sigma {}'.format(e, sigma))
17             return torch.tensor(float(e)), sigma
18         elif isinstance(e, list):
19             if do_log: logger.info('match case list: e {}, sigma {}'.format(e, sigma))
20             return e, sigma
21         elif e in list(primitives_d.keys()):
22             if do_log: logger.info('match case primitives_d: e {}, sigma {}'.format(e, sigma))
23             return e, sigma
24         elif e in list(distributions_d.keys()):
25             if do_log: logger.info('match case distributions_d: e {}, sigma {}'.format(e, sigma))
26             return e, sigma
27         elif torch.is_tensor(e):
28             if do_log: logger.info('match case is_tensor: e {}, sigma {}'.format(e, sigma))
29             return e, sigma
30         elif e in local_env.keys():
31             if do_log: logger.info('match case local_env: e {}, sigma {}'.format(e, sigma))
32             if do_log: logger.info('match case local_env: local_env[e] {}'.format(local_env[e]))
33             return local_env[e], sigma # TODO return evaluate?
34         elif e in list(defn_d.keys()):
35             if do_log: logger.info('match case defn_d: e {}, sigma {}'.format(e, sigma))
36             return e, sigma
37         elif isinstance(e, distribution_types):
38             if do_log: logger.info('match case distribution: e {}, sigma {}'.format(e, sigma))
39             return e, sigma
40         else:
41             assert False, 'case not matched'
42         elif e[0] == 'sample':
43             if do_log: logger.info('match case sample: e {}, sigma {}'.format(e, sigma))
44             distribution, sigma = evaluate(e[1], sigma, local_env, defn_d, do_log=do_log)
45             return distribution.sample(), sigma # match shape in number base case
46         elif e[0] == 'observe':
47             if do_log: logger.info('match case observe: e {}, sigma {}'.format(e, sigma))
48             e1, e2 = e[1:]
49             d1, sigma = evaluate(e1, sigma, local_env, defn_d, do_log=do_log)
50             c2, sigma = evaluate(e2, sigma, local_env, defn_d, do_log=do_log)
51             log_w = score(d1, c2)
52             if do_log: logger.info('match case observe: d1 {}, c2 {}, log_w {}, sigma {}'.format(e, d1, c2, log_w, sigma))
53             sigma += log_w
54             return c2, sigma
55         elif e[0] == 'let':
56             if do_log: logger.info('match case let: e {}, sigma {}'.format(e, sigma))
57             # let [v1 e1] e0
58             # here
59             # e[0] : "let"
60             # e[1] : [v1, e1]
61             # e[2] : e0
62             # evaluates e1 to c1 and binds this value to e0
63             # this means we update the context with old context plus {v1:c1}
64             c1, sigma = evaluate(e[1][1], sigma, local_env, defn_d, do_log=do_log) # evaluates e1 to c1
65             v1 = e[1][0]
66             return evaluate(e[2], sigma, local_env = (**local_env, v1:c1), defn_d=defn_d, do_log=do_log)
67         elif e[0] == 'if': # if e0 el e2
68             if do_log: logger.info('match case if: e {}, sigma {}'.format(e, sigma))
69             e1 = e[1]
70             e2 = e[2]
71             e3 = e[3]
72             el_prime, sigma = evaluate(e1, sigma, local_env, defn_d, do_log=do_log)
73             if el_prime:
74                 return evaluate(e2, sigma, local_env, defn_d, do_log=do_log)
75             else:
76                 return evaluate(e3, sigma, local_env, defn_d, do_log=do_log)
77
78         else:
79             cs = []
80             for ei in e:
81                 if do_log: logger.info('cycling through expressions: ei {}, sigma {}'.format(ei, sigma))
82                 c, sigma = evaluate(ei, sigma, local_env, defn_d, do_log=do_log)
83                 cs.append(c)
84                 if cs[0] in primitives_d:
85                     if do_log: logger.info('do case primitives_d: cs0 {}'.format(cs[0]))
86                     if do_log: logger.info('do case primitives_d: cs1 {}'.format(cs[1]))
87                     if do_log: logger.info('do case primitives_d: primitives_d[cs[0]] {}'.format(primitives_d[cs[0]]))
88                     return primitives_d[cs[0]](cs[1:]), sigma
89                 elif cs[0] in distributions_d:
90                     if do_log: logger.info('do case distributions_d: cs0 {}'.format(cs[0]))
91                     return distributions_d[cs[0]](cs[1:]), sigma
92                 elif cs[0] in defn_d:
93                     if do_log: logger.info('do case defn: cs0 {}'.format(cs[0]))
94                     defn_function_l1 = defn_d[cs[0]]
95                     defn_function_args, defn_function_body = defn_function_l1
96                     local_env_update = {key:value for key,value in zip(defn_function_args, cs[1:])}
97                     if do_log: logger.info('do case defn: update to local_env from defn_d {}'.format(local_env_update
98 e))
99                     return evaluate(defn_function_body, sigma, local_env = (**local_env, **local_env_update), defn_d=de
100 fn_d, do_log=do_log)
101             else:
102                 assert False, 'not implemented'
```

I also wrote my own score function. It handles boolean cases by converting them to

```
In [4]: from evaluation_based_sampling import score
        for line_number, function_line in enumerate(getsourcelines(score)[0]):
            print(line_number, function_line, end='')

0 def score(distribution, c):
1     """score pytorch distributions with .log_prob, but in a robust way for the type of c
2     """
3     if isinstance(c, bool) or c.type() in ['torch.BoolTensor', 'torch.LongTensor']:
4         log_w = distribution.log_prob(c.double())
5     else:
6         log_w = distribution.log_prob(c)
7     return log_w

I added a few more distributions and boolean operation primitives, for the problems in this assignment
```

```
In [6]: from primitives import distributions_d
        for key in distributions_d.keys():
            print(key, ':')
            for line_number, function_line in enumerate(getsourcelines(distributions_d[key])[0]):
                print(line_number, function_line, end='')
            print()

normal :
0 def normal(mean_std):
1     return two_arg_op_primitive(torch.distributions.Normal, mean_std)

beta :
0 def beta(alpha_beta):
1     return two_arg_op_primitive(torch.distributions.Beta, alpha_beta)

exponential :
0 def exponential(lam):
1     return one_arg_op_primitive(torch.distributions.Exponential, lam)

uniform :
0 def uniform(low_hi):
1     return two_arg_op_primitive(torch.distributions.Uniform, low_hi)

discrete :
0 def discrete(prob_vector):
1     return one_arg_op_primitive(torch.distributions.Categorical, prob_vector)

flip :
0 def flip(prob):
1     return one_arg_op_primitive(torch.distributions.Bernoulli, Bernoulli, prob)

dirichlet :
0 def dirichlet(concentration):
1     return one_arg_op_primitive(torch.distributions.Dirichlet, Dirichlet, concentration)

gamma :
0 def gamma(concentration_rate):
1     return two_arg_op_primitive(torch.distributions.Gamma, Gamma, concentration_rate)

In [7]: from primitives import primitives_d
        for key in ['and', 'or', '>', '<', '>=', '<=', '==']:
            print(key, ':')
            for line_number, function_line in enumerate(getsourcelines(primitives_d[key])[0]):
                print(line_number, function_line, end='')
            print()

and :
0 def and_primitive(arg1_arg2):
1     return two_arg_op_primitive(torch.logical_and, arg1_arg2)

or :
0 def or_primitive(arg1_arg2):
1     return two_arg_op_primitive(torch.logical_or, arg1_arg2)

> :
0 def gt_primitive(consequent_alternative):
1     return two_arg_op_primitive(torch.gt, consequent_alternative)

< :
0 def lt_primitive(consequent_alternative):
1     return two_arg_op_primitive(torch.lt, consequent_alternative)

>= :
0 def ge_primitive(consequent_alternative):
1     return two_arg_op_primitive(torch.ge, consequent_alternative)

<= :
0 def le_primitive(consequent_alternative):
1     return two_arg_op_primitive(torch.le, consequent_alternative)

= :
0 def eq_primitive(consequent_alternative):
1     return two_arg_op_primitive(torch.eq, consequent_alternative)
```

MH within Gibbs

I implmented Metropolis-Hastings within Gibbs in the following manner

- parse the graph in `mh_gibbs_wrapper`
- topologically sort the graph vertices
- sample from the joint (ie prior) to initialize all values of the graph
- cycle through the graph with `gibbs_step`
- accept an update at a specific vertex with `accept`
- collect each state after a Gibbs update (all the vertices)
- return all the fully specified graphs in `gibbs` for `num_steps`
- finally, I evaluate return value (the meaning of the program) for all the sampled graphs with `evaluate_program_return_from_samples_whole_graph`

```
In [207]: from mh_gibbs import mh_gibbs_wrapper, gibbs_step, accept, gibbs, evaluate_program_return_from_samples_whole_graph
        list_of_programs = [mh_gibbs_wrapper, gibbs_step, accept, gibbs, evaluate_program_return_from_samples_whole_graph]

        for program in list_of_programs:
            for line_number, function_line in enumerate(getsourcelines(program)[0]):
                print(line_number, function_line, end='')
            print()

0 def mh_gibbs_wrapper(graph, num_steps, do_log=False):
1     G = graph[1]
2     vertices = G['V']
3     A = G['A']
4     P = G['P']
5     X = set(vertices) - set(G['V'].keys())
6     Y = G['Y']
7     Y = {key:evaluate({Y[key]}, do_log=do_log)[0] for key in Y.keys()}
8
9
10    vertices_topsorted = sample_from_joint_precompute(graph)
11    _, local_env = sample_from_joint(graph, vertices_topsorted=vertices_topsorted)
12    local_env_list = [local_env, *Y]
13    local_env_list0 = [local_env]
14
15    local_env_list = gibbs(num_steps, local_env, P, A, X, do_log=do_log)
16
17    local_env_list = local_env_list0 + local_env_list
18
19    return list, samples_whole_graph = evaluate_program_return_from_samples_whole_graph(graph, local_env_list

20
21
22
23    return local_env_list

0 def gibbs_step(local_env, P, A, X, sample_vertices, do_log):
1     for vertex in X_sample_vertices:
2         link_function = P[vertex]
3         e = link_function[1]
4
5         distribution, sigma = evaluate(e, local_env=local_env, do_log=do_log)
6         local_env_prime = local_env.copy()
7         local_env_prime[vertex] = distribution.sample()
8
9         alpha = accept(vertex, local_env, local_env_prime, A, P, do_log=do_log)
10        u = torch.rand(1)
11        if u < alpha:
12            local_env = local_env_prime
13        return local_env

0 def accept(vertex, local_env, local_env_prime, A, P, do_log):
1     link_function = P[vertex]
2     e = link_function[1]
3     d_q, _ = evaluate(e, local_env=local_env, do_log=do_log)
4     d_q_prime, _ = evaluate(e, local_env=local_env_prime, do_log=do_log)
5     log_a = d_q_prime.log_prob(local_env[vertex]) - d_q.log_prob(local_env_prime[vertex])
6     V_x = A[vertex] + [vertex]
7     for observed_vertex in V_x:
8         d_p_prime = evaluate(P[observed_vertex][1], local_env = local_env_prime, do_log=do_log)[0]
9         if do_log: evaluate(1, do_log=do_log, logger_string='d_p_prime {}'.format(d_p_prime))
10        d_p = evaluate(P[observed_vertex][1], local_env = local_env, do_log=do_log)[0]
11        if do_log: evaluate(1, do_log=do_log, logger_string='d_p {}'.format(d_p))
12        if do_log: evaluate(1, do_log=do_log, logger_string='local_env_prime (1, observed vertex {}, local_env_prime[observed_vertex] {}'.format(local_env_prime, observed_vertex))
13        log_a += score(d_p_prime, local_env_prime[observed_vertex])
14        log_s = d_p_prime.log_prob(local_env_prime[observed_vertex])
15        # log_a = score(d_p_prime, local_env_prime[observed_vertex])
16        log_a = d_q - d_p.log_prob(local_env[observed_vertex])
17        # log_a --> d_p.log_prob(local_env[observed_vertex])
18
19    return torch.exp(log_a)

0 def gibbs(num_steps, local_env, P, A, X, do_log):
1     local_env_list = []
2     for step in range(num_steps):
3         local_env = gibbs_step(local_env, P, A, X, do_log=do_log)
4         local_env_list.append(local_env)
5     return local_env_list

0 def evaluate_program_return_from_samples_whole_graph(graph, samples_whole_graph):
1     # evaluate samples (on whatever function, here the return of the program) as needed
2     e = graph[2]
3     # TODO suggest daphne put return as program, so return is ['sample2'] not 'sample2'
4     if isinstance(e, str):
5         e = [e]
6     return_list = []
7     for X_s in samples_whole_graph:
8         return_s, _ = evaluate(e, local_env = X_s) # TODO: handle defs
9         return_list.append(return_s)
10    return return_list
```

Hamiltonian Monte Carlo

I implemented HMC in the following way

- I parse the graph for the link functions P, and the samples X and observes Y
- I turn on autodiff on the torch.tensor(float): `turn_on_autodiff`
- I run HMC algorithm 20 from the textbook: `hmc_algo20`
 - inside I use the leapfrog algorithm 19 from the textbook: `leapfrog`
 - this relies on computing the gradient of the potential energy with respect to the values of X: `grad_U`. There are important implementation details with pytorch autodiff, avoiding gradient accumulation
 - I also have to add Xt (a dict) and Rt (a vector) with a helper function `add_dict_to_tensor`. I use `X_vertex_names_to_idx_d` to keep track of what key in X corresponds to what index of R. This is important if the keys change order and H is different for different values of X (i.e. not proportional to the Identity matrix)
 - I compute the kinetic and potential energy and the hamiltonian: `compute_K`, `compute_U` (just negative of `compute_log_joint_prob`) and `compute_H`
- After I collect samples from the whole graph, I evaluate the return function on each graph.

```
In [208]: from hmc import hmc_wrapper, turn_on_autodiff, hmc_algo20, leapfrog, grad_U, add_dict_to_tensor, compute_K, compute_U

        list_of_programs = [hmc_wrapper, turn_on_autodiff, hmc_algo20, leapfrog, grad_U, add_dict_to_tensor, compute_K, compute_U]

        for program in list_of_programs:
            for line_number, function_line in enumerate(getsourcelines(program)[0]):
                print(line_number, function_line, end='')
            print()

0 def hmc_wrapper(graph, num_samples, T=10, epsilon=0.1, M=tensor(1.)):
1     #set up X, Y list of tensors
2     G = graph[1]
3     vertices = ['V']
4     Y = G['Y']
5     P = G['P']
6
7     # evaluate to constants
8     Y = {key:evaluate((value)) [0] for key,value in Y.items()}
9
10    #X = set(vertices) - set(Y.keys())
11    #X = sample_from_joint(graph)
12    _, X0 = sample_from_joint(graph) # does not include observes
13
14    # initialize in dict
15    X_vertex_names_to_idx_d = {key:idx for idx, key in enumerate(X0.keys())}
16
17    # set up autograd on tensors
18    turn_on_autodiff(X0)
19    turn_on_autodiff(Y) # TODO: why do we need this?
20
21    # run HMC algorithm 20 from book
22    # inside use leapfrog algorithm 19 from book
23    # include kinetic and potential energy functions
24    # MC acceptance criteria
25    samples_whole_graph = hmc_algo20(X0, num_samples, T, epsilon, M, Y, P, X_vertex_names_to_idx_d)
26
27    # evaluate samples (on whatever function, here the return of the program) as needed
28    e = graph[2]
29    # TODO suggest daphne put return as program, so return is ['sample2'] not 'sample2'
30    if isinstance(e, str):
31        e = [e]
32    return_list = []
33    for X_s in samples_whole_graph:
34        return_s, _ = evaluate(e, local_env = X_s) # TODO: handle defs
35        return_list.append(return_s)
36    return_list.append(return_s)
37
38    return return_list, samples_whole_graph

0 def turn_on_autodiff(dictionary_of_tensors):
1     """
2     cant be integers, ie long tensors, but floats or complex
3     """
4     for x in dictionary_of_tensors.values():
5         if torch.is_tensor(x):
6             x.requires_grad = True

0 def hmc_algo20(X0, num_samples, T, epsilon, M, Y, P, X_vertex_names_to_idx_d):
1     X_s = X0
2     samples = []
3     size = len(X0.keys())
4     normal_R_reuse = torch.distributions.Normal(torch.zeros(size), M)
5
6     for s in range(num_samples):
7         R_s = normal_R_reuse.sample()
8         R_p, X_p = leapfrog(copy.deepcopy(X_s), copy.deepcopy(R_s), T, epsilon, Y, P, X_vertex_names_to_idx_d)
9         # X_p, R_p = leapfrog(X_s, R_s, T, epsilon, X_vertex_names_to_idx_d)
10        # copy X_s?
11        u = torch.rand(1)
12        delta_H = compute_H(X_p, R_p, M, Y, P) - compute_H(X_s, R_p, M, Y, P)
13        boltzmann_ratio = torch.exp(-delta_H)
14        if u < boltzmann_ratio:
15            X_s = X_p
16            #no need to update X_s because should stay the same for next round.
17            #X_s turns into X_s_minus from algo 20 by indexing
18            samples.append(X_s)
19        return samples

0 def leapfrog(X0, R0, T, epsilon, Y, P, X_vertex_names_to_idx_d):
1     """
2     leapfrog as in algo 19 of book
3     Y and P needed for grad calc
4     """
5
6     epsilon_2 = epsilon/2
7     R_t = R0 - epsilon_2 * grad_U(X0, Y, P, X_vertex_names_to_idx_d)
8     X_t = X0
9
10    for t in range(T-1):
11        # TODO: save all in loop instead of overwriting to visualize
12        X_t = add_dict_to_tensor(X_t, epsilon*R_t, X_vertex_names_to_idx_d)
13        R_t = R_t - epsilon*grad_U(X_t, Y, P, X_vertex_names_to_idx_d)
14        X_t = add_dict_to_tensor(X_t, epsilon*R_t, X_vertex_names_to_idx_d)
15        R_t = R_t - epsilon_2*grad_U(X_t, Y, P, X_vertex_names_to_idx_d)
16    return R_t, X_t

0 def grad_U(X, Y, P, X_vertex_names_to_idx_d):
1     """
2     call autodiff backward pass, with constant indexing given by X_vertex_names_to_idx_d
3     return vector of gradients
4     """
5     energy_U = compute_U(X, Y, P)
6
7     # Zero the gradients.
8     # without this running grad_U back to back accumulates the grad (not what we want!)
9     for key in X.keys():
10        if X[key].grad is not None:
11            X[key].grad.zero_()
12
13    energy_U.backward()
14    grads = torch.zeros(len(X.keys()))
15    for key in X.keys():
16        print('key', key)
17        idx = X_vertex_names_to_idx_d[key]
18        # print('idx', idx)
19        # print('X[key]', X[key])
20        # print('X[key].grad', X[key].grad)
21        grads[idx] = X[key].grad
22
23    # Need to have been referenced in linking function.
24    # So key connected to evaluation of energy.
25    # Otherwise key not a part of the computational graph of energy_U,
26    # and grad remains none when run energy_U.backwards()
27
28    return grads

0 def add_dict_to_tensor(X, R, X_vertex_names_to_idx_d):
1     """
2     X:R using mapping from X_vertex_names_to_idx_d
3     TODO: avoid detach?
4     R must be dimension 1, not 0 D
5     similar to using with torch.no_grad() as in https://github.com/MasoudMo/cpsc532w_hw/blob/master/HW3/graph_based_sampling.py#L275
6     """
7     assert R.dim() >= 1
8     X_new = {}
9     for vertex in X.keys():
10        idx = X_vertex_names_to_idx_d[vertex]
11        # overwriting the value, and only want to autograd accumulated gradient to depend on the final value
12        # TODO: would this problem go away if we stored a vector over all leapfrog time steps?
13        X_new[vertex] = X[vertex].detach() + R[idx]
14        X_new[vertex].requires_grad = True
15    return X_new

0 def compute_K(R, M):
1     R_over_2M = R/(2*M) # TODO: generalize for non scalar M, e.g. diagonal M
2     if R.dim() == 0:
3         energy_K = R*R_over_2M
4     elif R.dim() == 1:
5         energy_K = torch.matmul(R, R_over_2M)
6     else:
7         assert False
8     return energy_K

0 def compute_log_joint_prob(X, Y, P):
1     """
2     call link functions under context and score.
3     TODO: remove Y dependence
4     TODO: add in user defs https://github.com/MasoudMo/cpsc532w_hw/blob/master/HW3/graph_based_sampling.py#L
5
6     need to parse link functions like
7     # 'sample2': ['sample*', ['normal', 1, ['sqrt', 5]]]
8     # 'observe3': ['observe*', ['normal', 'sample2', ['sqrt', 2]], 8],
9     """
10    log_prob = tensor(0.0)
11    for X_vertex in X.keys():
12        e = P[X_vertex][1]
13        distribution = evaluate(e, local_env=X)[0]
14        log_prob += score(distribution, X[X_vertex])
15    for Y_vertex in Y.keys():
16        e = P[Y_vertex][1]
17        distribution = evaluate(e, local_env=X)[0]
18        log_prob += score(distribution, Y[Y_vertex])
19
20    return log_prob

0 def compute_U(X, Y, P):
1     energy_U = -compute_log_joint_prob(X, Y, P)
2     return energy_U

0 def compute_H(X, R, M, Y, P):
1     """Compute Hamiltonian.
2     """
3     energy_U = compute_U(X, Y, P)
4     energy_K = compute_K(R, M)
5     energy_H = energy_U + energy_K
6     return energy_H
```



```
In [1]: import torch
import numpy as np
import os, json
import pandas as pd
import matplotlib.pyplot as plt
import seaborn as sns
import importlib

from evaluation_based_sampling import evaluate, evaluate_program
from daphne import daphne

from graph_based_sampling import sample_from_joint
```

Problem 1

```
In [2]: from load_helper import ast_helper, graph_helper
```

Importance sampling

10k in 3.34s implies 1.7e6 in 10 min

```
In [3]: import parse
import importance_sampling
import importlib
importlib.reload(parse)
```

```
Out[3]: <module 'parse' from '/Users/gw/repos/prob_prog/hw/hw3/parse.py'>
```

```
In [35]: fname = '1.daphne'
ast = ast_helper(fname)
ast
```

```
Out[35]: [['let',
['mu', ['sample', ['normal', 1, ['sqrt', 5]]],
['let',
['sigma', ['sqrt', 2]],
['let',
['lik', ['normal', 'mu', 'sigma']],
['let',
['dontcare0', ['observe', 'lik', 8]],
['let', ['dontcare1', ['observe', 'lik', 9]], 'mu']]]]]]
```

```
In [53]: %time
num_samples=1790000
samples, sigmas = parse.take_samples(num_samples,ast)

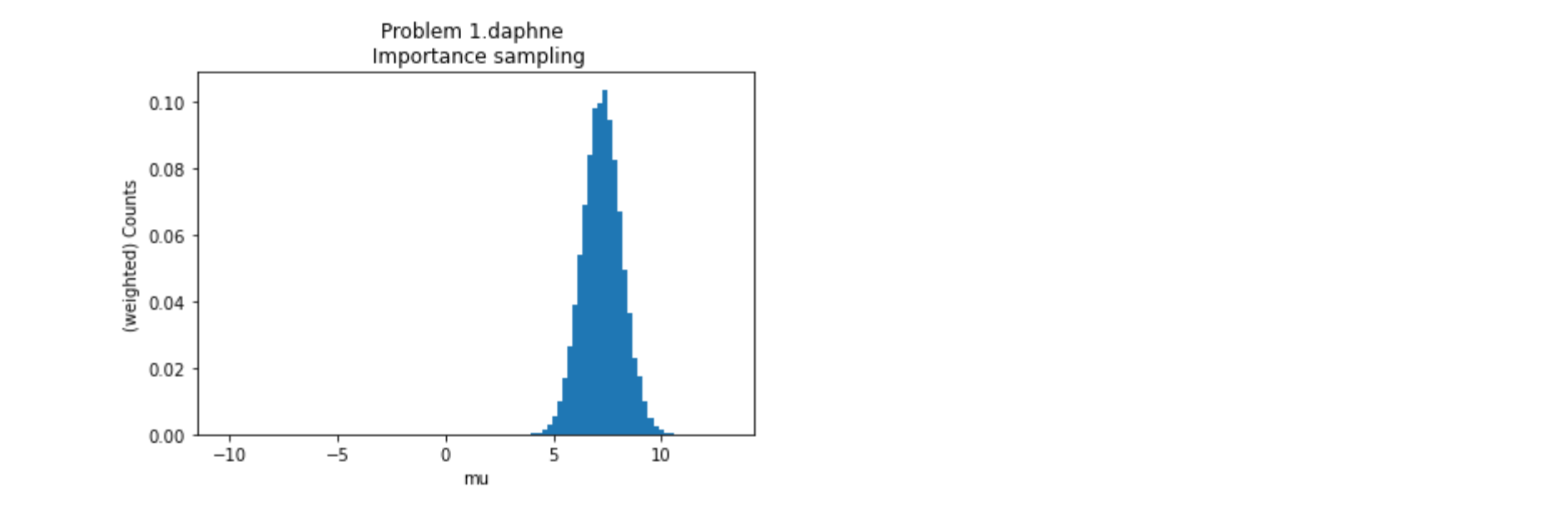
CPU times: user 10min 27s, sys: 3.59 s, total: 10min 31s
Wall time: 10min 32s
```

```
In [54]: samples = np.array([sample.item() for sample in samples])
```

```
In [55]: posterior_mean, probs = importance_sampling.weighted_average(samples,sigmas)
posterior_mean
```

```
Out[55]: 7.2549860583141825
```

```
In [60]: # pd.Series(samples).plot.hist()
_ = plt.hist(samples, weights=probs, bins=100)
plt.title('Problem {} \n Importance sampling \n importance sampling weighted counts from proposal'.format(fname))
plt.xlabel('mu')
plt.ylabel('(weighted) Counts')
```



```
In [57]: expectation_samples_2, probs = importance_sampling.weighted_average(samples**2,sigmas)
posterior_variance = expectation_samples_2 - posterior_mean**2
```

```
In [58]: "Importance sampling: posterior mean of mu {:.3f} | variance {:.3e}".format(posterior_mean,posterior_variance)
```

```
Out[58]: 'Importance sampling: posterior mean of mu 7.255 | variance 8.292e-01'
```

MH within Gibbs

5k in 5.58s implies 537k samples in 10 min

```
In [11]: import mh_gibbs
from hmc import compute_log_joint_prob
importlib.reload(mh_gibbs)
```

```
Out[11]: <module 'mh_gibbs' from '/Users/gw/repos/prob_prog/hw/hw3/mh_gibbs.py'>
```

```
In [12]: fname = '1.daphne'
graph = graph_helper(fname)
graph
```

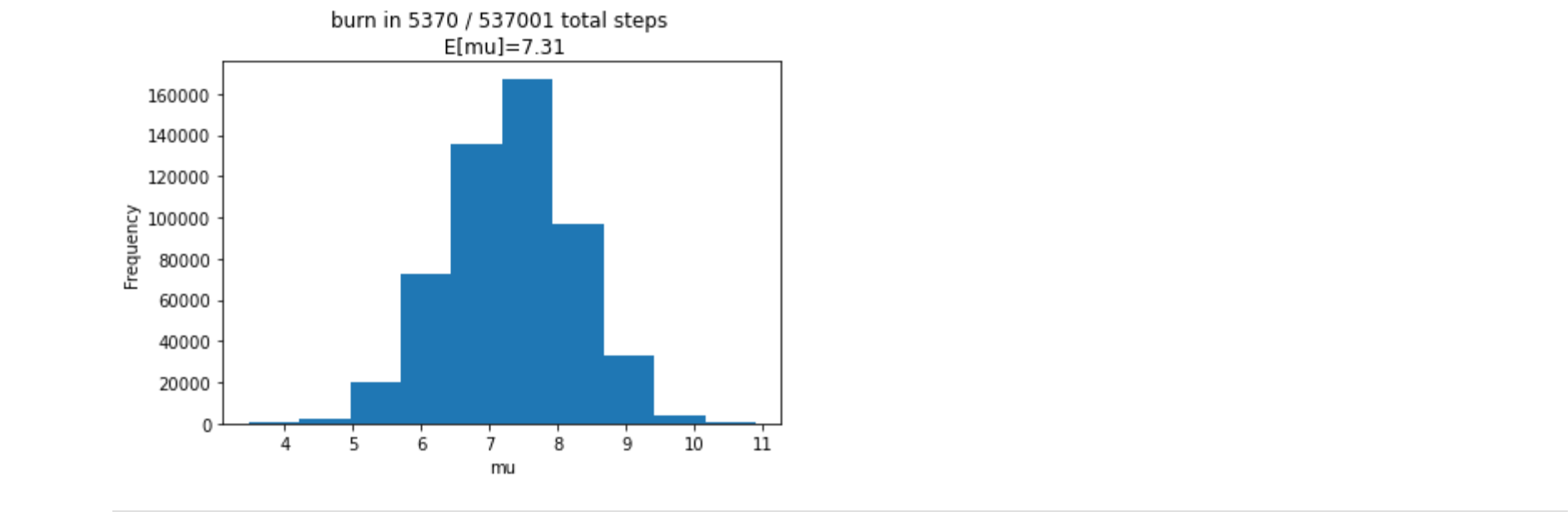
```
Out[12]: {'V': ['observe3', 'observe4', 'sample2'],
'A': {'sample2': ['observe3', 'observe4']},
'P': {'sample2': ['sample*', ['normal', 1, ['sqrt', 5]]],
'observe3': ['observe*', ['normal', 'sample2', ['sqrt', 2]], 8],
'observe4': ['observe*', ['normal', 'sample2', ['sqrt', 2]], 9]},
'Y': {'observe3': 8, 'observe4': 9}},
'sample2'
```

```
In [13]: %time
num_steps=537000
return_list, samples_whole_graph = mh_gibbs.mh_gibbs_wrapper(graph,num_steps=num_steps)

CPU times: user 9min 48s, sys: 2.11 s, total: 9min 51s
Wall time: 9min 54s
```

```
In [14]: samples = np.array([x.item() for x in return_list])
```

```
In [15]: burn_in = int(0.01*num_steps)
sr = pd.Series(samples[burn_in:])
sr.plot.hist()
sr.mean()
plt.title('burn in {} / {} total steps \n E[mu]={:2f}'.format(burn_in, len(samples),sr.mean()))
plt.xlabel('mu')
```

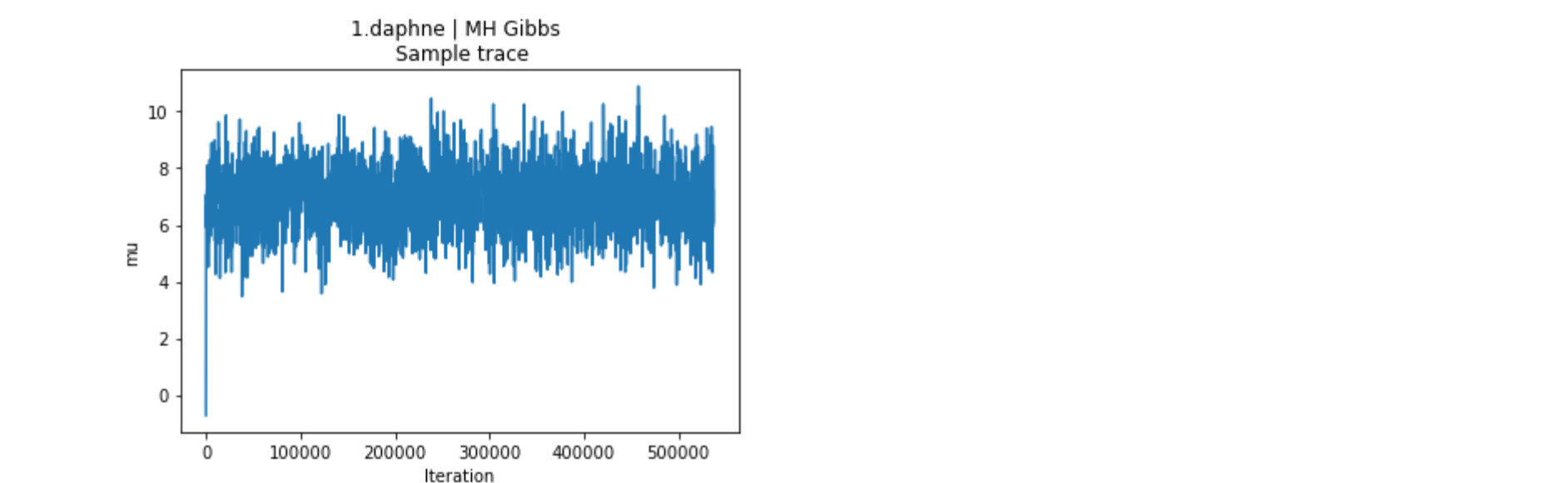


```
In [16]: "MH Gibbs: posterior mean of mu {:.3f} | variance {:.3e}".format(sr.mean(),sr.var())
```

```
Out[16]: 'MH Gibbs: posterior mean of mu 7.310 | variance 8.421e-01'
```

```
In [17]: pd.Series(samples).plot()
plt.xlabel('Iteration')
plt.ylabel('mu')
plt.title('{} | MH Gibbs \n Sample trace'.format(fname))
```

```
Out[17]: Text(0.5, 1.0, '1.daphne | MH Gibbs \n Sample trace')
```

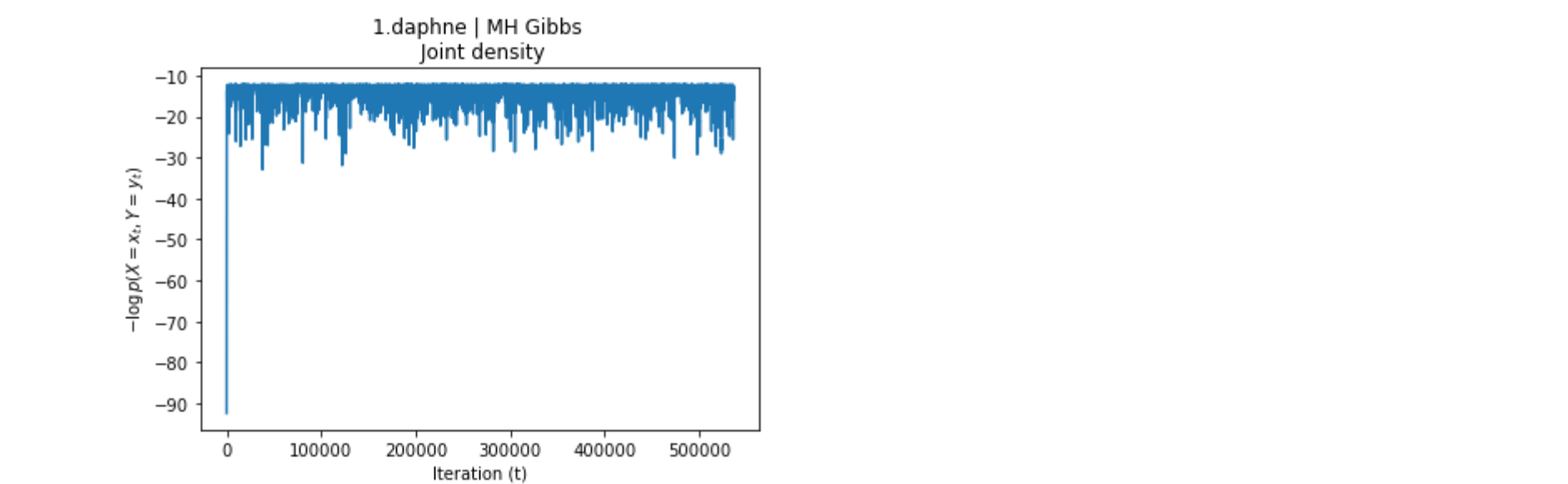


```
In [18]: G = graph[1]
Y = G['Y']
Y = {key:evaluate([value])[0] for key,value in Y.items()}
P = G['P']
```

```
In [19]: size = len(samples_whole_graph)
jll = np.zeros(size)
for idx in range(size):
    jll[idx] = compute_log_joint_prob(samples_whole_graph[idx],Y,P)
```

```
In [20]: pd.Series(jll).plot()
plt.xlabel('Iteration (t)')
plt.ylabel('r'${-}\log p(X=x_t,Y=y_t)$')
plt.title('{} | MH Gibbs \n Joint density'.format(fname))
```

```
Out[20]: Text(0.5, 1.0, '1.daphne | MH Gibbs \n Joint density')
```



HMC

5k samples in 41.4 s implies 72k in 10 min

```
In [61]: fname = '1.daphne'
graph = graph_helper(fname)
```

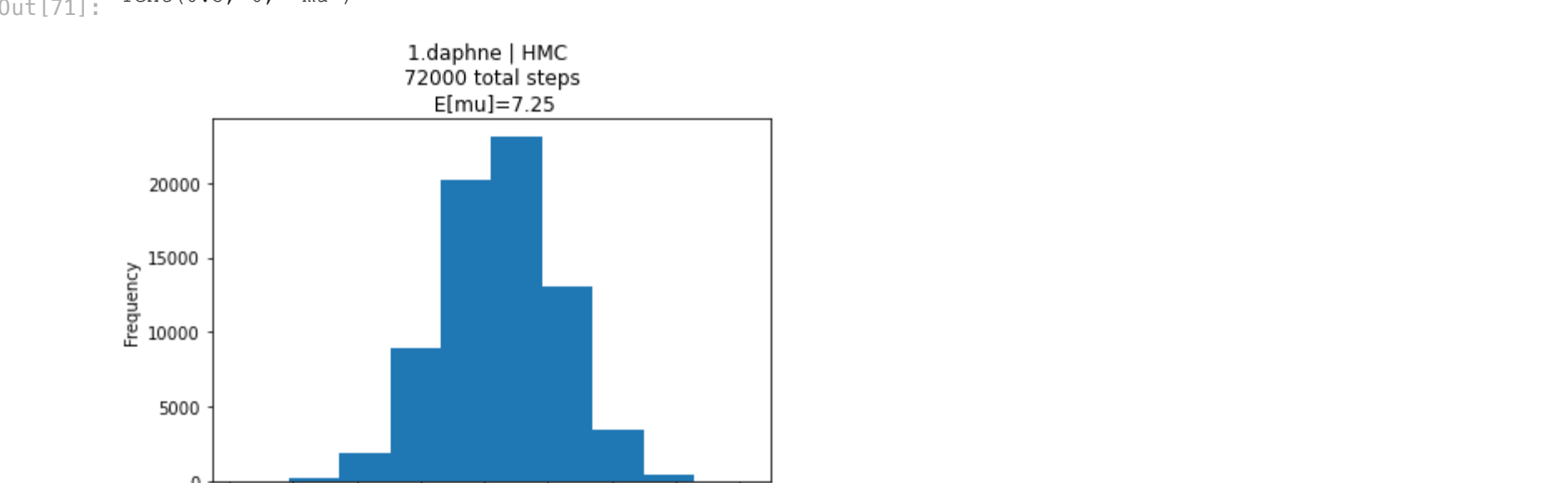
```
In [62]: import hmc
importlib.reload(hmc)
from hmc import hmc_wrapper
```

```
In [ ]: num_samples=72000
return_list, samples_whole_graph = hmc_wrapper(graph,num_samples,T=20,epsilon=0.1)
```

```
In [70]: samples = np.array([x.item() for x in return_list])
```

```
In [71]: burn_in = int(0.01*num_samples) # ~500 from inspecting joint density plot, with given hyper params T, epsilon,
sr = pd.Series(samples[burn_in:])
sr.plot.hist()
sr.mean()
plt.title('{} | HMC \n {} total steps \n E[mu]={:2f}'.format(fname,len(samples),sr.mean()))
plt.xlabel('mu')
```

```
Out[71]: Text(0.5, 0, 'mu')
```

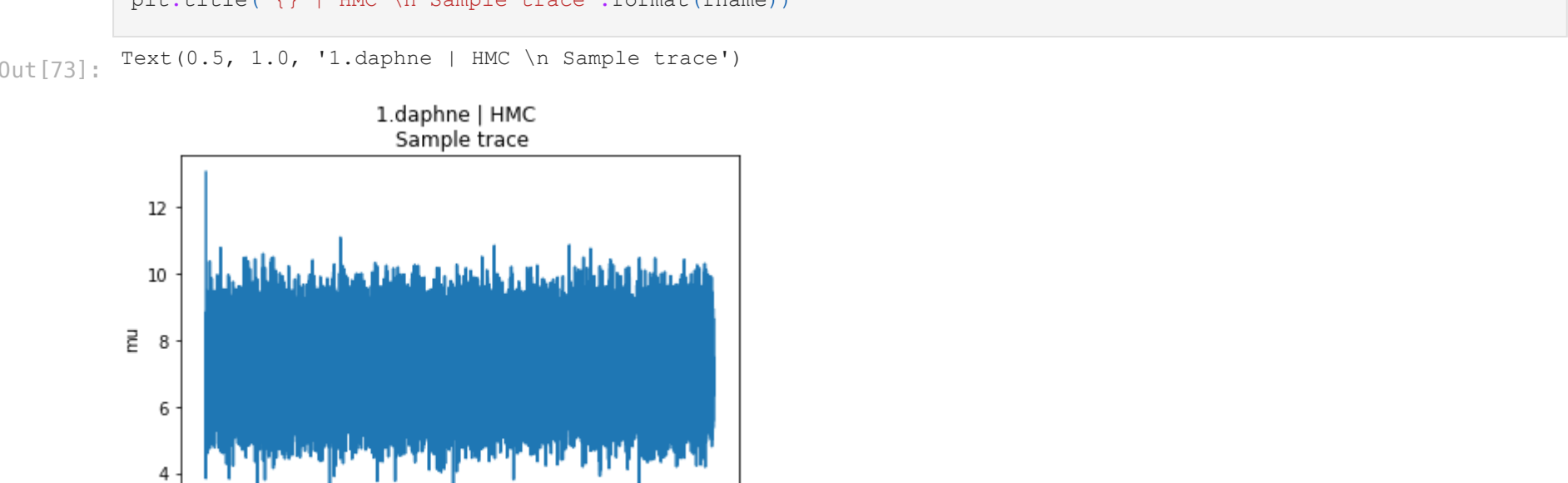


```
In [72]: "HMC: posterior mean of mu {:.3f} | variance {:.3e}".format(sr.mean(),sr.var())
```

```
Out[72]: 'HMC: posterior mean of mu 7.249 | variance 8.324e-01'
```

```
In [73]: pd.Series(samples).plot()
plt.xlabel('Iteration')
plt.ylabel('mu')
plt.title('{} | HMC \n Sample trace'.format(fname))
```

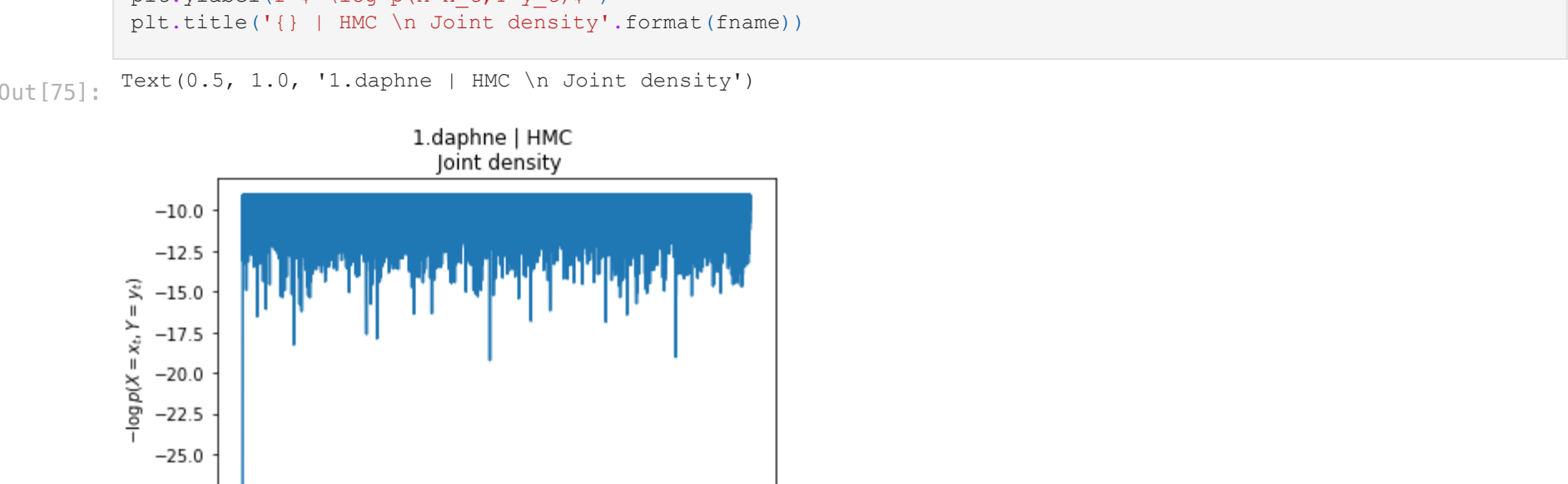
```
Out[73]: Text(0.5, 1.0, '1.daphne | HMC \n Sample trace')
```



```
In [74]: size = len(samples_whole_graph)
jll = np.zeros(size)
for idx in range(size):
    jll[idx] = compute_log_joint_prob(samples_whole_graph[idx],Y,P)
```

```
In [75]: pd.Series(jll).plot()
plt.xlabel('Iteration (t)')
plt.ylabel('r'${-}\log p(X=x_t,Y=y_t)$')
plt.title('{} | HMC \n Joint density'.format(fname))
```

```
Out[75]: Text(0.5, 1.0, '1.daphne | HMC \n Joint density')
```




```
In [1]: import torch
import numpy as np
import os, json
import pandas as pd
import matplotlib.pyplot as plt
import seaborn as sns
import importlib

from evaluation_based_sampling import evaluate, evaluate_program
from daphne import daphne

from graph_based_sampling import sample_from_joint
```

Problem 2

10k samples in 1.59s implies 384k samples

```
In [2]: from load_helper import ast_helper, graph_helper
```

Importance sampling

```
In [3]: import parse
import importance_sampling
import importlib
importlib.reload(parse)
```

```
Out[3]: <module 'parse' from '/Users/gw/repos/prob_prog/hw/hw3/parse.py'>
```

```
In [52]: fname = '2.daphne'
ast = ast_helper(fname)
```

```
In [53]: %%time
num_samples=384000
samples, sigmas = parse.take_samples(num_samples,ast=ast)
```

CPU times: user 10min 28s, sys: 918 ms, total: 10min 29s
Wall time: 10min 29s

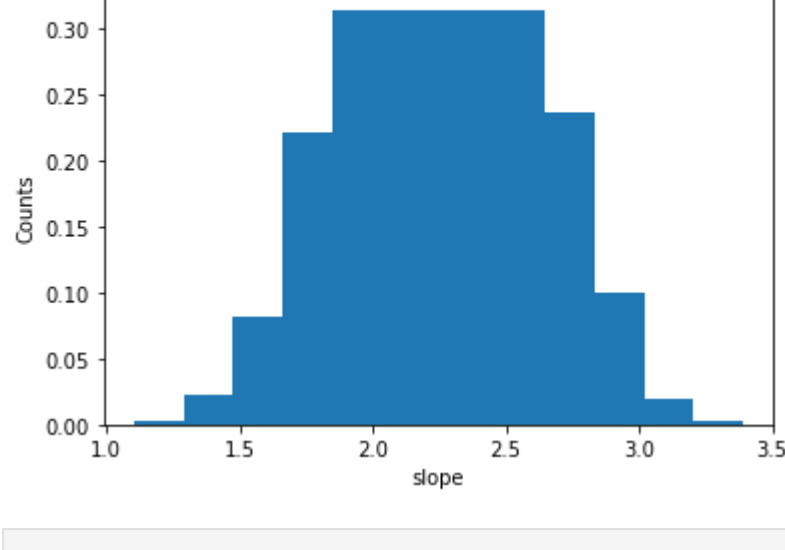
```
In [54]: samples = np.array([sample.tolist() for sample in samples])
```

```
In [55]: posterior_mean, probs = importance_sampling.weighted_average(samples,sigmas,reshape_probs=(-1,1),axis=0)
posterior_mean
```

```
Out[55]: array([ 2.15895652, -0.53834023])
```

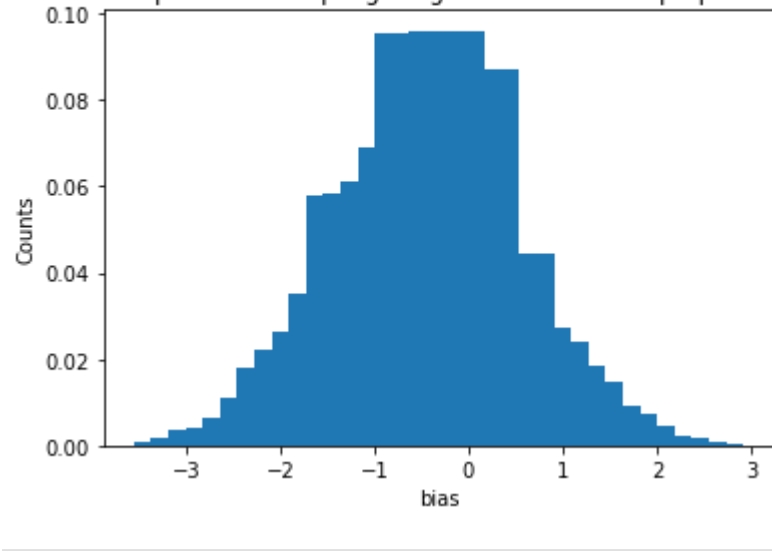
```
In [106... counts_bins = np.histogram(samples[:,0], weights=probs, bins=500)
counts, bins = counts_bins[0], counts_bins[1]
idx = (counts > counts.max()*0.005)
plt.bar(bins[1:][idx],counts[idx])
plt.title('Problem {} \n Importance sampling \n importance sampling weighted counts from proposal'.format(fname))
plt.ylabel('Counts')
plt.xlabel('slope')
```

```
Out[106... Text(0.5, 0, 'slope')
```



```
In [104... counts_bins = np.histogram(samples[:,1], weights=probs, bins=500)
counts, bins = counts_bins[0], counts_bins[1]
idx = (counts > counts.max()*0.005)
plt.bar(bins[1:][idx],counts[idx])
plt.title('Problem {} \n Importance sampling \n importance sampling weighted counts from proposal'.format(fname))
plt.ylabel('Counts')
plt.xlabel('bias')
```

```
Out[104... Text(0.5, 0, 'bias')
```



```
In [58]: expectation_samples_2, probs = importance_sampling.weighted_average(samples**2,sigmas,reshape_probs=(-1,1),axis=0)
posterior_variance = expectation_samples_2 - posterior_mean**2
posterior_variance
```

```
Out[58]: array([0.05376331, 0.79199928])
```

```
In [59]: expectation_samplex_sampley, probs = importance_sampling.weighted_average(samples[:,0]*samples[:,1],sigmas)
covariance = expectation_samplex_sampley - posterior_mean[0]*posterior_mean[1]
covariance
```

```
Out[59]: -0.18463132614140898
```

```
In [60]: for result in [
    "() Importance sampling: posterior mean slope {:.13f} | variance slope {:.13e}".format(fname,posterior_mean[0],posterior_variance[0]),
    "() Importance sampling: posterior mean bias {:.13f} | variance bias {:.13e}".format(fname,posterior_mean[1],posterior_variance[1]),
    "() Importance sampling: posterior covariance of slope and bias variance bias {:.13e}".format(fname,covariance),
]:
    print(result)
```

2.daphne Importance sampling: posterior mean slope 2.159 | variance slope 5.376e-02
2.daphne Importance sampling: posterior mean bias -0.538 | variance bias 7.920e-01
2.daphne Importance sampling: posterior covariance of slope and bias variance bias -1.846e-01

Numpy contains it's own method for computing this, and we can check it agrees with our results (where things are spelt out a bit more for learning purposes).

```
In [61]: np.cov(samples.T,aweights=probs,ddof=0)
```

```
Out[61]: array([[ 0.05376331, -0.18463133],
                [-0.18463133, 0.79199928]])
```

MH Gibbs

5k samples in 21.3s implies 140k samples in 10 min

```
In [12]: import mh_gibbs
from hmc import hmc_wrapper, compute_log_joint_prob
importlib.reload(mh_gibbs)
```

```
Out[12]: <module 'mh_gibbs' from '/Users/gw/repos/prob_prog/hw/hw3/mh_gibbs.py'>
```

```
In [13]: fname = '2.daphne'
graph = graph_helper(fname)
graph
```

```
Out[13]: [{'observe-data': {'fn',
  [' ', 'data', 'slope', 'bias'],
  ['let',
  ['xn', ['first', 'data']],
  ['let',
  ['yn', ['second', 'data']],
  ['let',
  ['zn', ['+', ['*', 'slope', 'xn'], 'bias']],
  ['let',
  ['dontcare9', ['observe', ['normal', 'zn', 1.0], 'yn']],
  ['rest', ['rest', 'data']]]]]],
{'V': ['observe3',
'observe6',
'observe4',
'observe7',
'sample2',
'sample1',
'observe8',
'observe5'],
'A': {'sample2': ['observe3',
'observe6',
'observe4',
'observe7',
'observe8',
'observe5'],
'sample1': ['observe3',
'observe6',
'observe4',
'observe7',
'observe8',
'observe5']},
'P': {'sample1': ['sample*', ['normal', 0.0, 10.0]],
'sample2': ['sample*', ['normal', 0.0, 10.0]],
'observe3': ['observe*',
['normal', ['+', ['*', 'sample1', 1.0], 'sample2'], 1.0],
2.1],
'observe4': ['observe*',
['normal', ['+', ['*', 'sample1', 2.0], 'sample2'], 1.0],
3.9],
'observe5': ['observe*',
['normal', ['+', ['*', 'sample1', 3.0], 'sample2'], 1.0],
5.3],
'observe6': ['observe*',
['normal', ['+', ['*', 'sample1', 4.0], 'sample2'], 1.0],
7.7],
'observe7': ['observe*',
['normal', ['+', ['*', 'sample1', 5.0], 'sample2'], 1.0],
10.2],
'observe8': ['observe*',
['normal', ['+', ['*', 'sample1', 6.0], 'sample2'], 1.0],
12.9]],
'Y': {'observe3': 2.1,
'observe4': 3.9,
'observe5': 5.3,
'observe6': 7.7,
'observe7': 10.2,
'observe8': 12.9]],
['vector', 'sample1', 'sample2']}]
```

```
In [14]: %%time
num_steps=140000
return_list, samples_whole_graph = mh_gibbs.mh_gibbs_wrapper(graph,num_steps)
```

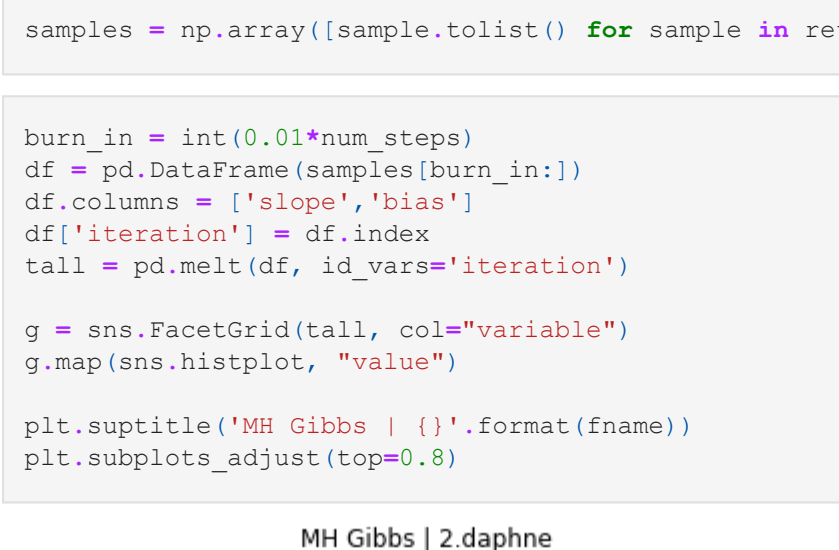
CPU times: user 10min 14s, sys: 2.36 s, total: 10min 16s
Wall time: 10min 20s

```
In [15]: samples = np.array([sample.tolist() for sample in return_list])
```

```
In [16]: burn_in = int(0.01*num_steps)
df = pd.DataFrame(samples[burn_in:])
df.columns = ['slope','bias']
df['iteration'] = df.index
tall = pd.melt(df, id_vars='iteration')

g = sns.FacetGrid(tall, col="variable")
g.map(sns.histplot, "value")

plt.suptitle('MH Gibbs | {}'.format(fname))
plt.subplots_adjust(top=0.8)
```



```
In [17]: posterior_mean = samples[burn_in:].mean(0)
cov_matrix = np.cov(samples[burn_in:].T,ddof=0)
posterior_variance = samples[burn_in:].var(0)
covariance = cov_matrix[0,1]
assert np.isclose(cov_matrix[0,0],posterior_variance[0])
assert np.isclose(cov_matrix[1,1],posterior_variance[1])
```

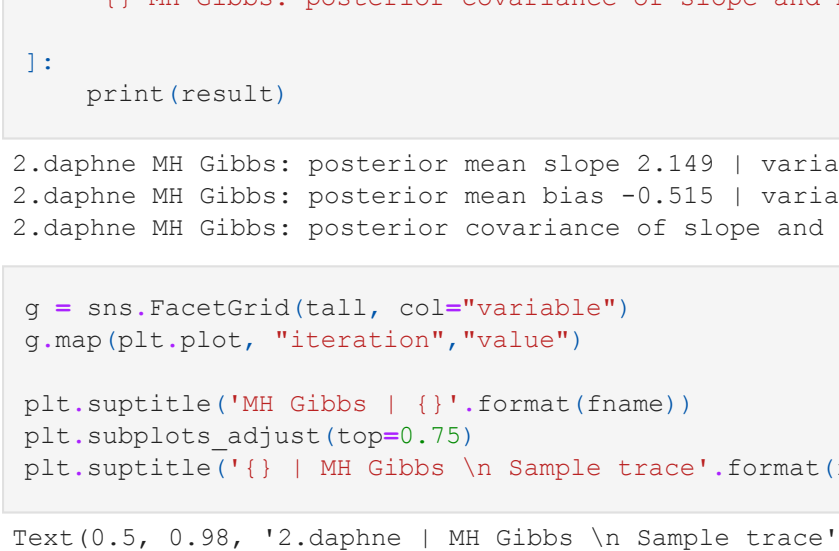
```
In [18]: for result in [
    "() MH Gibbs: posterior mean slope {:.13f} | variance slope {:.13e}".format(fname,posterior_mean[0],posterior_variance[0]),
    "() MH Gibbs: posterior mean bias {:.13f} | variance bias {:.13e}".format(fname,posterior_mean[1],posterior_variance[1]),
    "() MH Gibbs: posterior covariance of slope and bias variance bias {:.13e}".format(fname,covariance),
]:
    print(result)
```

2.daphne MH Gibbs: posterior mean slope 2.149 | variance slope 5.918e-02
2.daphne MH Gibbs: posterior mean bias -0.515 | variance bias 8.965e-01
2.daphne MH Gibbs: posterior covariance of slope and bias variance bias -2.070e-01

```
In [19]: g = sns.FacetGrid(tall, col="variable")
g.map(plt.plot, "iteration", "value")

plt.suptitle('MH Gibbs | {}'.format(fname))
plt.subplots_adjust(top=0.75)
plt.suptitle('{} | MH Gibbs \n Sample trace'.format(fname))
```

```
Out[19]: Text(0.5, 0.98, '2.daphne | MH Gibbs \n Sample trace')
```

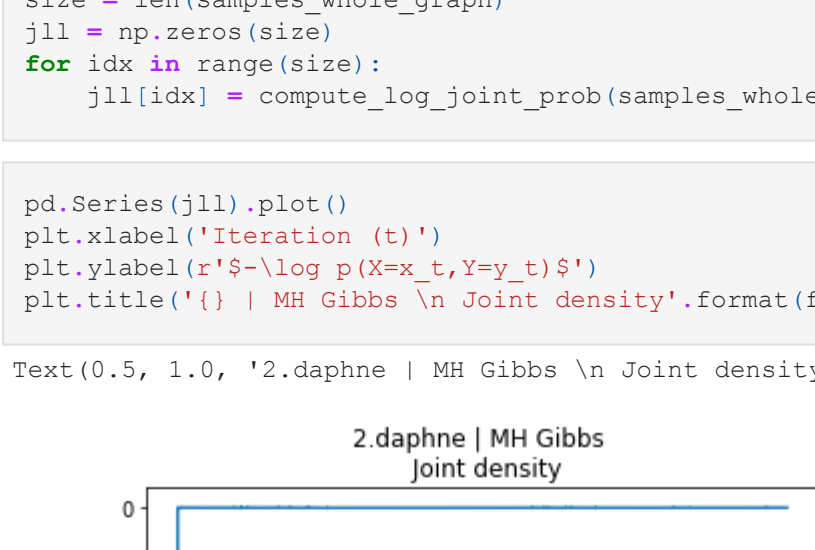


```
In [20]: G = graph[1]
Y = G['Y']
Y = [key:evaluate([value])[0] for key,value in Y.items()]
P = G['P']
```

```
In [21]: size = len(samples_whole_graph)
jll = np.zeros(size)
for idx in range(size):
    jll[idx] = compute_log_joint_prob(samples_whole_graph[idx],Y,P)
```

```
In [22]: pd.Series(jll).plot()
plt.xlabel('Iteration (t)')
plt.ylabel(r'$-\log p(X=x_t,Y=y_t)$')
plt.title('{} | MH Gibbs \n Joint density'.format(fname))
```

```
Out[22]: Text(0.5, 1.0, '2.daphne | MH Gibbs \n Joint density')
```



HMC

4.2s/ 200 samples implies 28.5k samples in 10 min 1k samples in 21.3 s implies 28k samples

```
In [143... fname = '2.daphne'
graph = graph_helper(fname)
```

```
In [144... import hmc
importlib.reload(hmc)
from hmc import hmc_wrapper
```

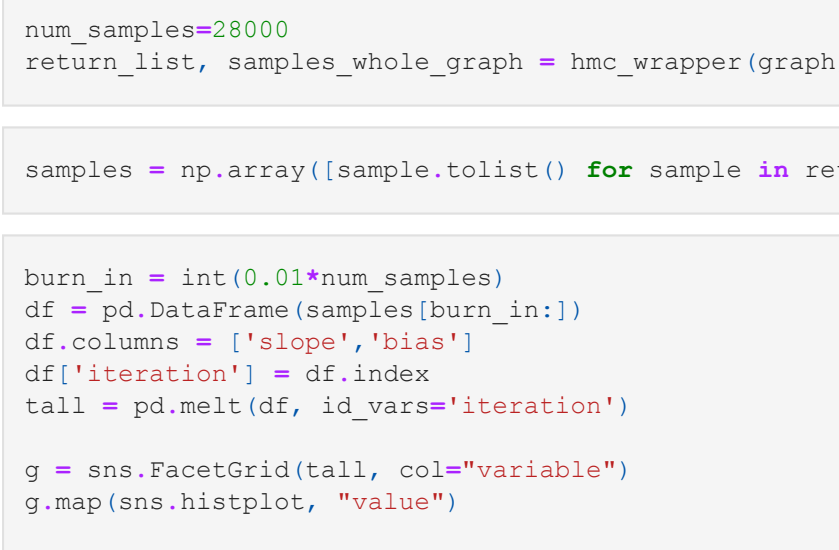
```
In [ ]: num_samples=28000
return_list, samples_whole_graph = hmc_wrapper(graph,num_samples,T=20,epsilon=0.01)
```

```
In [154... samples = np.array([sample.tolist() for sample in return_list])
```

```
In [155... burn_in = int(0.01*num_samples)
df = pd.DataFrame(samples[burn_in:])
df.columns = ['slope','bias']
df['iteration'] = df.index
tall = pd.melt(df, id_vars='iteration')

g = sns.FacetGrid(tall, col="variable")
g.map(sns.histplot, "value")

plt.suptitle('HMC | {}'.format(fname))
plt.subplots_adjust(top=0.8)
```



```
In [156... posterior_mean = samples[burn_in:].mean(0)
cov_matrix = np.cov(samples[burn_in:].T,ddof=0)
posterior_variance = samples[burn_in:].var(0)
covariance = cov_matrix[0,1]
assert np.isclose(cov_matrix[0,0],posterior_variance[0])
assert np.isclose(cov_matrix[1,1],posterior_variance[1])
```

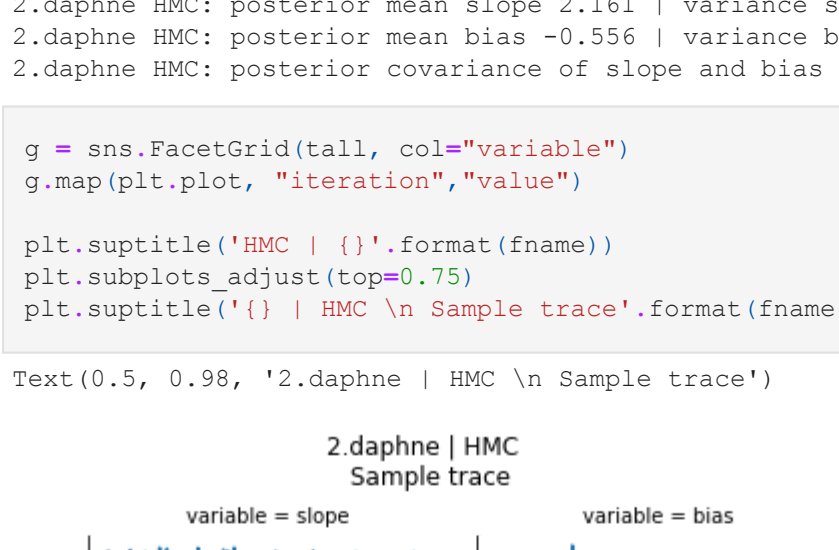
```
In [157... for result in [
    "() HMC: posterior mean slope {:.13f} | variance slope {:.13e}".format(fname,posterior_mean[0],posterior_variance[0]),
    "() HMC: posterior mean bias {:.13f} | variance bias {:.13e}".format(fname,posterior_mean[1],posterior_variance[1]),
    "() HMC: posterior covariance of slope and bias variance bias {:.13e}".format(fname,covariance),
]:
    print(result)
```

2.daphne HMC: posterior mean slope 2.161 | variance slope 5.652e-02
2.daphne HMC: posterior mean bias -0.556 | variance bias 8.609e-01
2.daphne HMC: posterior covariance of slope and bias variance bias -1.984e-01

```
In [158... g = sns.FacetGrid(tall, col="variable")
g.map(plt.plot, "iteration", "value")

plt.suptitle('HMC | {}'.format(fname))
plt.subplots_adjust(top=0.75)
plt.suptitle('{} | HMC \n Sample trace'.format(fname))
```

```
Out[158... Text(0.5, 0.98, '2.daphne | HMC \n Sample trace')
```

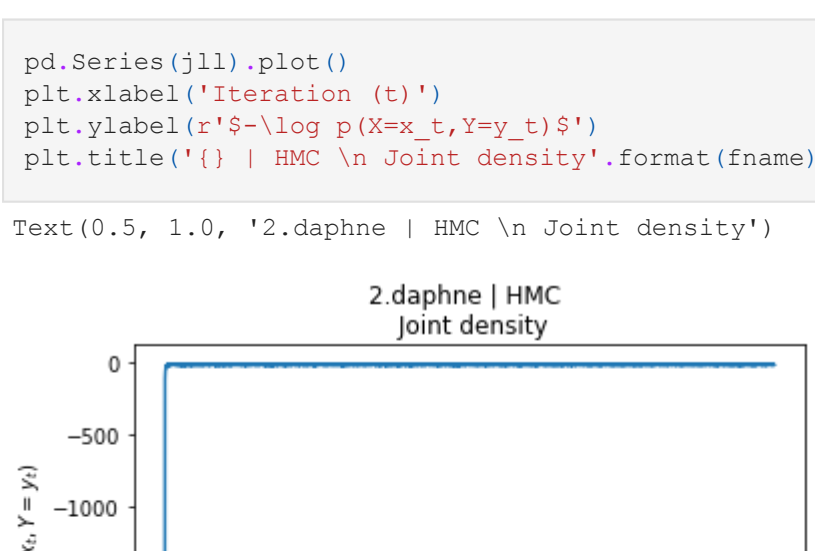


```
In [159... G = graph[1]
Y = G['Y']
Y = [key:evaluate([value])[0] for key,value in Y.items()]
P = G['P']
```

```
In [160... size = len(samples_whole_graph)
jll = np.zeros(size)
for idx in range(size):
    jll[idx] = compute_log_joint_prob(samples_whole_graph[idx],Y,P)
```

```
In [161... pd.Series(jll).plot()
plt.xlabel('Iteration (t)')
plt.ylabel(r'$-\log p(X=x_t,Y=y_t)$')
plt.title('{} | HMC \n Joint density'.format(fname))
```

```
Out[161... Text(0.5, 1.0, '2.daphne | HMC \n Joint density')
```




```
In [1]: import torch
import numpy as np
import os, json
import pandas as pd
import matplotlib.pyplot as plt
import seaborn as sns

from evaluation_based_sampling import evaluate, evaluate_program
from daphne import daphne
```

Problem 4

```

11 [2]: from load_helper import ast_helper, graph_helper

```

Importance sampling

- 10k samples in 6.82s implies 879k samples in 10 min

```
import parse
import importance_sampling
```

```
ast = ast_helper(fname)
ast
```

```
Out[4]: [['let',
['sprinkler', True],
['let',
['wet-grass', True],
['let',
['is-cloudy', ['sample', ['flip', 0.5]]],
['let',
['is-raining',
['if',
['=', 'is-cloudy', True],
['sample', ['flip', 0.8]],
['sample', ['flip', 0.2]]]],
['let',
['sprinkler-dist',
['if', ['=', 'is-cloudy', True], ['flip', 0.1], ['flip', 0.5]]],
['let',
['wet-grass-dist',
['if',
['and', ['=', 'sprinkler', True], ['=', 'is-raining', True]],
['flip', 0.99]],
['if',
['and', ['=', 'sprinkler', False], ['=', 'is-raining', False]],
['flip', 0.0]],
['if',
['or', ['=', 'sprinkler', True], ['=', 'is-raining', True]],
['flip', 0.9],
None]]],
['let',
['dontcare0', ['observe', 'sprinkler-dist', 'sprinkler']],
['let',
['dontcare1', ['observe', 'wet-grass-dist', 'wet-grass']],
```

```
In [26]: %%time
          num_samples=879000
          samples,sigma = parse.take_samples(num_samples,ast=ast)

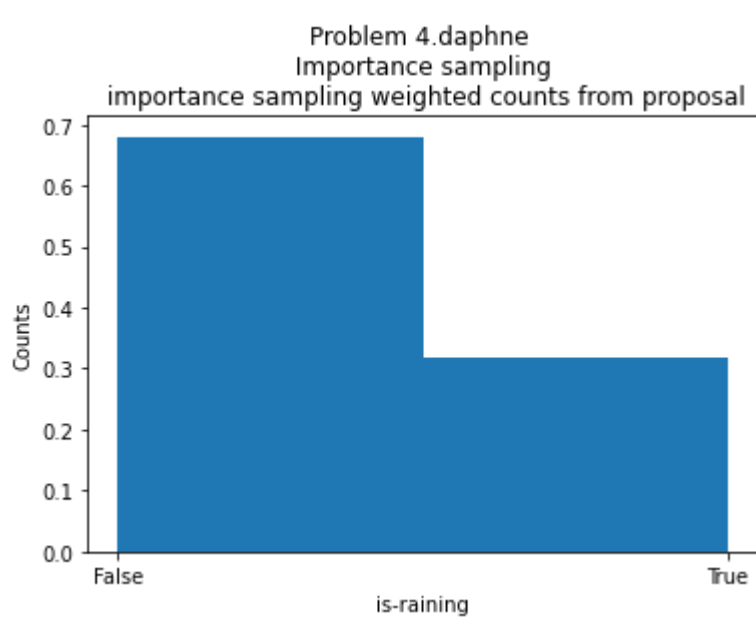
CPU times: user 10min 22s, sys: 2.84 s, total: 10min 25s
Wall time: 10min 27s
```

```
In [27]: samples = np.array([sample.item() for sample in samples])
```

```
In [28]: posterior_mean, probs = importance_sampling_weighted_average(samples, sigmas)
```

```
In [29]: _ = plt.hist(samples.astype(int), weights=probs, bins=2)
plt.xlabel('is-raining')
plt.title('Problem {} \n Importance sampling \n importance sampling weighted counts from proposal'.format(fname))
plt.xticks([0,1],["False","True"])
plt.ylabel('Counts')
```

```
Out[29]: Text(0, 0.5, 'Counts')
```



```
In [30]: """The posterior probability that it is raining, i.e. of "is-raining.": {:.3f}""".format(posterior.mean())
```

```
Out[30]: 'The posterior probability that it is raining, i.e. of "is-raining.": 0.320'
```

MH Gibbs

2k samples in 8.55s implies 140k samples in 10 min

```
In [10]: import graph_based_sampling
import mh_gibbs
from hmc import compute_log_joint_prob
```

```
fname = '4.daphne'
graph = graph_helper(fname)
graph
```

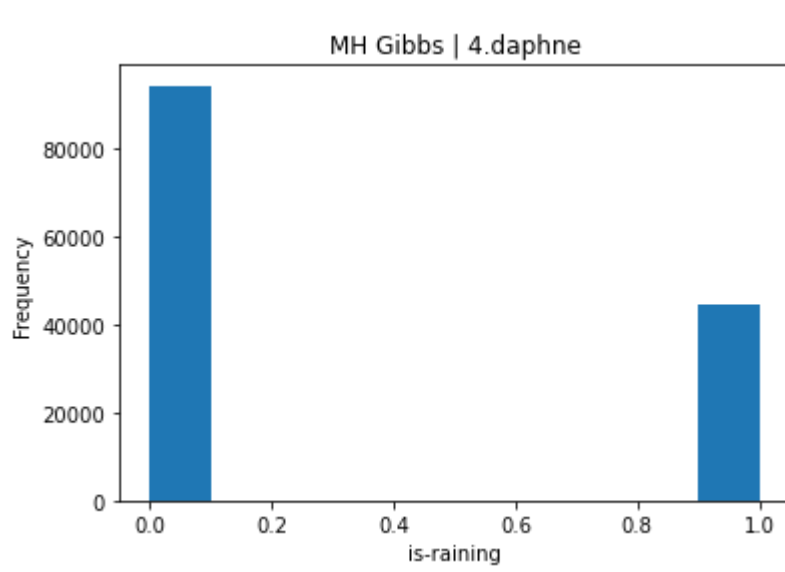
```
{
  'V': ['observe6', 'sample4', 'sample2', 'observe5', 'sample3'],
  'A': {'sample2': ['observe6', 'observe5'],
        'sample4': ['observe6'],
        'sample3': ['observe6']},
  'P': {'sample2': ['sample*', ['flip', 0.5]],
        'sample3': ['sample*', ['flip', 0.8]],
        'sample4': ['sample*', ['flip', 0.2]],
        'observe5': ['observe*',
                      ['if', ['=', 'sample2', True], ['flip', 0.1], ['flip', 0.5]],
                      True],
        'observe6': ['observe*',
                      ['if',
                       ['and',
                        True,
                        ['=', ['if', ['=', 'sample2', True], 'sample3', 'sample4'], True]],
                       ['flip', 0.99]],
                      ['if',
                       ['and',
                        False,
                        ['=', ['if', ['=', 'sample2', True], 'sample3', 'sample4'], False]],
                       ['flip', 0.0]],
                      ['if',
                       ['or',
                        True,
                        ['=', ['if', ['=', 'sample2', True], 'sample3', 'sample4'], True]],
                       ['flip', 0.9],
                        None]]],
                      True]],
        'Y': {'observe5': True, 'observe6': True}},
  ['if', ['=', 'sample2', True], 'sample3', 'sample4']]
}
```

```
num_steps=140000
return_list, samples_whole_graph = mh_gibbs.mh_gibbs_wrapper(graph,num_steps)
```

```
samples = np.array([sample.item() for sample in return_list])
```

```
In [14]: burn_in = int(0.01*num_steps)
pd.Series(samples[burn_in:]).astype(float).plot.hist()
plt.xlabel('is-raining')
plt.title('MH Gibbs | {}'.format(fname))
```

```
Out[14]: Text(0.5, 1.0, 'MH Gibbs | 4.daphne')
```

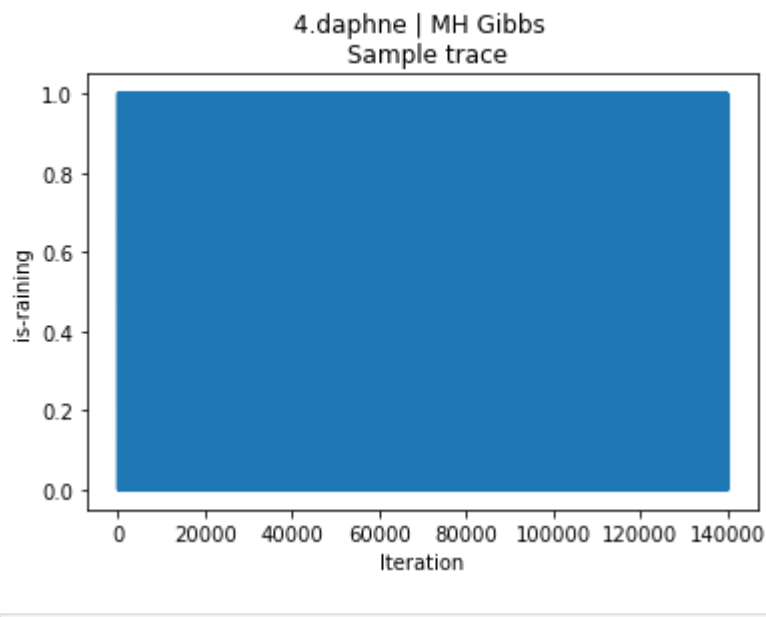


```
In [15]: posterior_mean = samples[burn_in:].mean(0)
```

```
out[16]: 'The posterior probability that it is raining, i.e. of "is-raining.": 0.321'
```

```
In [17]: pd.Series(samples).astype(int).plot()
plt.xlabel('Iteration')
plt.ylabel('is-raining')
plt.title('{} | MH Gibbs \n Sample trace'.format(fname))
```

```
Out[17]: Text(0.5, 1.0, '4.daphne | MH Gibbs \n Sample trace')
```

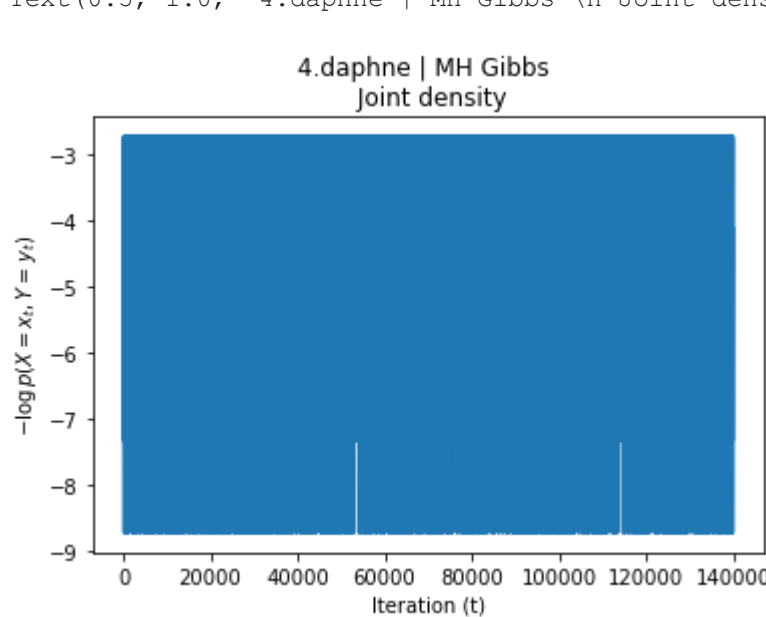


```
Y = G['Y']
Y = {key:evaluate([value])[0] for key,value in Y.items()}
P = G['P']
```

```
In [19]: size = len(samples_whole_graph)
jll = np.zeros(size)
for idx in range(size):
    jll[idx] = compute_log_joint_prob(samples_whole_graph[idx], Y, P)
```

```
In [34]: pd.Series(jll).plot()
plt.xlabel('Iteration (t)')
plt.ylabel('r' + '$-\log p(X=x_t, Y=y_t)$')
```

```
Text(0.5, 1.0, '4 daphne | MH Gibbs \n Joint density!')
```




```
In [1]: import torch
import numpy as np
import os, json
import pandas as pd
import matplotlib.pyplot as plt
import seaborn as sns
import importlib

from evaluation_based_sampling import evaluate, evaluate_program
from daphne import daphne

from graph_based_sampling import sample_from_joint
```

Problem 5

I approach this problem with approximate Bayesian computation. Relaxing the dirac into a normal. This is inspired by the definition of the dirac as a normal pdf in the limit of the variance going to zero.

- Khuri, A. I. (2004). Applications of Dirac's delta function in statistics. International Journal of Mathematical Education in Science and Technology, 35(2), 185–195. <http://doi.org/10.1080/00207390310001638313>

I set the variance of the normal to 0.1^2 more detailed study could be done showing the behaviour as a function of the variance. At $\sigma^2 <= 0.03^2$ I encountered errors in HMC, likely caused by things going to infinity (log_prob scoring was out of distribution, and it is normal...?)

Comments on ABC for this problem

There are really only one degree of freedom for this problem, since when one value is fixed, the other must be seven minus it, to be compatible with the observe statement (`observe (dirac (+ x y)) 7`). So there is only one variance, and no covariance. In the ABC approximation however, we only strictly enforce that $x + y = 7$ and thus we get a covariance of x and y .

Any $x + y = 7$ is compatible with the observe, and this "manifold" is the line. The ABC makes this line have non-zero measure.

Another way to do this problem, would be to incorporate the observe into the program, and replace y with $7-x$ somehow to enforce the constraint.

Comparison of IS, MH Gibbs & HMC

- IS. has high variance, but gets reasonable means of near 3.5
- Gibbs is still and so can't update very well. It is exploring along a very narrow ridge, instead of along the line. x and y should be updated together as a block. The problem is very stiff (the dicar makes it initily stiff).
- HMC has variance near IS. We can see from the joint that it is converging with iterations gradually.

Error trace

for normal that is too narrow (intentionally put below)

```
ValueError                                Traceback (most recent call last)
/var/folders/bg/cb0crr7ls61352lhy50167r0c0000gn/T/ipykernel_58709/4110678344.py in <module>
      1 num_samples=28000//10
----> 2 return_list, samples_whole_graph = hmc_wrapper(graph,num_samples,T=40,epsilon=0.1)

~/repos/prob_prog/hw/hw3/hmc.py in hmc_wrapper(graph, num_samples, T, epsilon, M)
     33     # include kinetic and potential energy functions
     34     # MC acceptance criteria
----> 35     samples_whole_graph = hmc_algo20(X0,num_samples,T,epsilon,M,Y,P,X_vertex_names_to_idx_d)
     36
     37     # evaluate samples (on whatever function, here the return of the program) as needed

~/repos/prob_prog/hw/hw3/hmc.py in hmc_algo20(X0, num_samples, T, epsilon, M, Y, P, X_vertex_names_to_idx_d)
     56     for s in range(num_samples):
     57         R_s = normal_R_reuse.sample()
----> 58         R_p, X_p =
 leapfrog(copy.deepcopy(X_s),copy.deepcopy(R_s),T,epsilon,Y,P,X_vertex_names_to_idx_d)
     59         # X_p, R_p = leapfrog(X_s,R_s,T,epsilon,X_vertex_names_to_idx_d)
     60         # copy X_s?

~/repos/prob_prog/hw/hw3/hmc.py in leapfrog(X0, R0, T, epsilon, Y, P, X_vertex_names_to_idx_d)
     83     # TODO: save all in loop instead of overwriting to visualize
     84     X_t = add_dict_to_tensor(X_t,epsilon*R_t,X_vertex_names_to_idx_d)
----> 85     R_t = R_t - epsilon*grad_U(X_t,Y,P,X_vertex_names_to_idx_d)
     86     X_T = add_dict_to_tensor(X_t,epsilon*R_t,X_vertex_names_to_idx_d)
     87     R_T = R_t - epsilon_2*grad_U(X_T,Y,P,X_vertex_names_to_idx_d)

~/repos/prob_prog/hw/hw3/hmc.py in grad_U(X, Y, P, X_vertex_names_to_idx_d)
    112     return vector of gradients
    113     """
--> 114     energy_U = compute_U(X,Y,P)
    115
    116     # Zero the gradients.

~/repos/prob_prog/hw/hw3/hmc.py in compute_U(X, Y, P)
    177
    178     def compute_U(X,Y,P):
--> 179         energy_U = <compute_log_joint_prob(X,Y,P)
    180         return energy_U
    181

~/repos/prob_prog/hw/hw3/hmc.py in compute_log_joint_prob(X, Y, P)
    167         e = P[X_vertex][1]
    168         distribution = evaluate(e,local_env=X)[0]
--> 169         log_prob += score(distribution,X[X_vertex])
    170         for Y_vertex in Y.keys():
    171             e = P[Y_vertex][1]

~/repos/prob_prog/hw/hw3/evaluation_based_sampling.py in score(distribution, c)
     55     log_w = distribution.log_prob(c.double())
     56     else:
----> 57         log_w = distribution.log_prob(c)
     58     return log_w
     59

~/miniconda2/envs/prob_prog/lib/python3.9/site-packages/torch/distributions/normal.py in log_prob(self, value)
     71     def log_prob(self, value):
     72         if self._validate_args:
----> 73             self._validate_sample(value)
     74         # compute the variance
     75         var = (self.scale ** 2)

~/miniconda2/envs/prob_prog/lib/python3.9/site-packages/torch/distributions/distribution.py in _validate_sample(self, value)
    275         assert support is not None
    276         if not support.check(value).all():
--> 277             raise ValueError('The value argument must be within the support')
    278
    279     def _get_checked_instance(self, cls, _instance=None):

ValueError: The value argument must be within the support
```

```
In [2]: from load_helper import ast_helper, graph_helper
```

Importance sampling

30k in 10s implies 1.698 million

```
In [3]: import parse
import importance_sampling
import importlib
importlib.reload(parse)
```

```
Out[3]: <module 'parse' from '/Users/gw/repos/prob_prog/hw/hw3/parse.py'>
```

```
In [4]: fname = '5_abc.daphne'
ast = ast_helper(fname)
ast
```

```
Out[4]: [{}let',
[{}x', ['sample', ['normal', 0, 10]]],
[{}let',
[{}y', ['sample', ['normal', 0, 10]]],
[{}let',
[{}dotncare0', ['observe', ['normal', ['+', 'x', 'y'], 0.09], 7]]],
[{}vector', 'x', 'y']]]]]
```

```
In [5]: %time
num_samples=int(1.698e6)
samples, sigmas = parse.take_samples(num_samples,ast=ast)
samples = np.array([sample.tolist() for sample in samples])

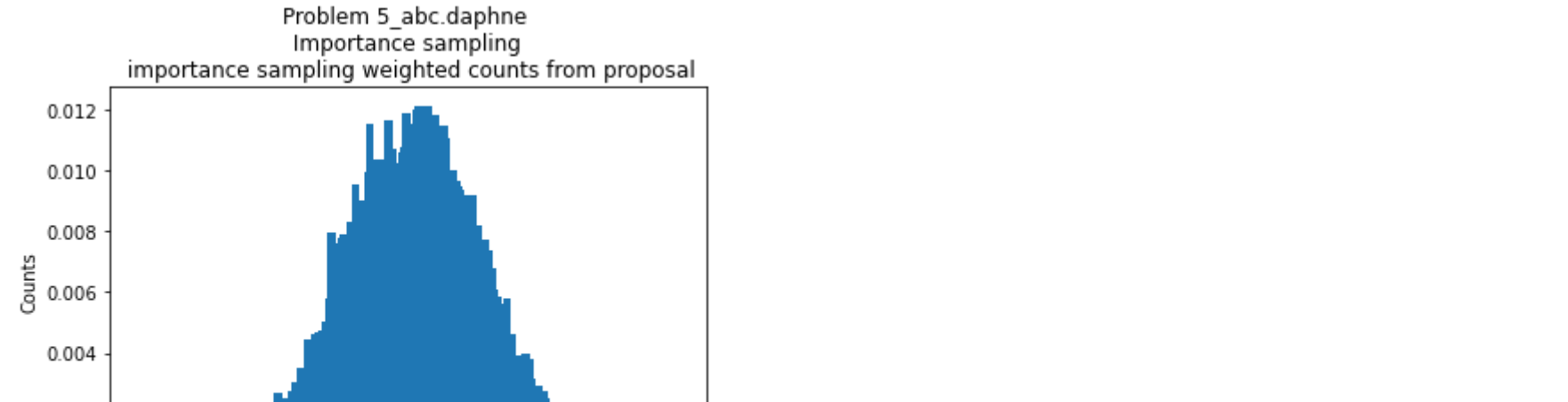
CPU times: user 9min 37s, sys: 2.48 s, total: 9min 40s
Wall time: 9min 40s
```

```
In [6]: posterior_mean, probs = importance_sampling.weighted_average(samples,sigmas,reshape_probs=(-1,1),axis=0)
posterior_mean
```

```
Out[6]: array([3.53386895, 3.46580443])
```

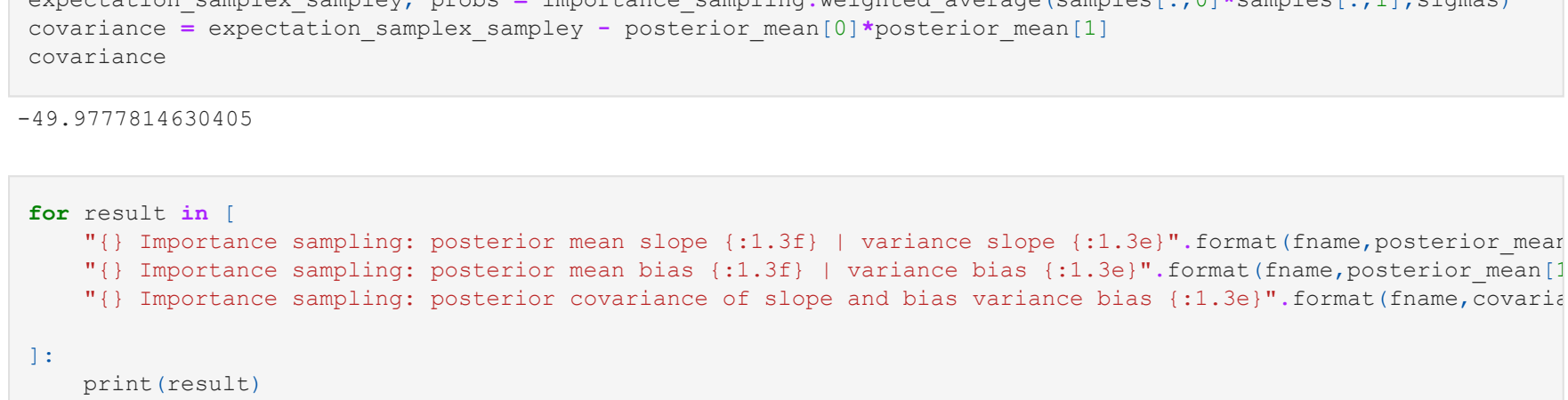
```
In [7]: counts_bins = np.histogram(samples[:,0], weights=probs[:,0], bins=500)
counts, bins = counts_bins[0], counts_bins[1]
idx = (counts > counts.max()*0.005)
plt.bar(bins[1:][idx],counts[idx])
plt.title('Problem {} \n Importance sampling \n importance sampling weighted counts from proposal'.format(fname))
plt.xlabel('slope')
```

```
Out[7]: Text(0.5, 0, 'slope')
```



```
In [8]: counts_bins = np.histogram(samples[:,1], weights=probs[:,0], bins=500)
counts, bins = counts_bins[0], counts_bins[1]
idx = (counts > counts.max()*0.005)
plt.bar(bins[1:][idx],counts[idx])
plt.title('Problem {} \n Importance sampling \n importance sampling weighted counts from proposal'.format(fname))
plt.xlabel('Counts')
```

```
Out[8]: Text(0.5, 0, 'bias')
```



```
In [9]: expectation_samples_2, probs = importance_sampling.weighted_average(samples**2,sigmas,reshape_probs=(-1,1),axis=0)
posterior_variance = expectation_samples_2 - posterior_mean**2
posterior_variance
```

```
Out[9]: array([49.98343282, 49.98004001])
```

```
In [10]: expectation_samplex_sampley, probs = importance_sampling.weighted_average(samples[:,0]*samples[:,1],sigmas)
covariance = expectation_samplex_sampley - posterior_mean[0]*posterior_mean[1]
covariance
```

```
Out[10]: -49.9777814630405
```

```
In [11]: for result in [
    "({} Importance sampling: posterior mean slope {:1.3f} | variance slope {:1.3e})".format(fname,posterior_mean[0],posterior_variance[0]),
    "({} Importance sampling: posterior mean bias {:1.3f} | variance bias {:1.3e})".format(fname,posterior_mean[1],posterior_variance[1]),
    "({} Importance sampling: posterior covariance of slope and bias variance bias {:1.3e})".format(fname,covariance),
]:
    print(result)
```

```
5_abc.daphne Importance sampling: posterior mean slope 3.534 | variance slope 4.998e+01
5_abc.daphne Importance sampling: posterior mean bias 3.466 | variance bias 4.998e+01
5_abc.daphne Importance sampling: posterior covariance of slope and bias variance bias -4.998e+01
```

Numpy contains it's own method for computing this, and we can check it agrees with our results (where things are spelt out a bit more for learning purposes).

```
In [12]: np.cov(samples.T,aweights=probs,ddof=0)
```

```
Out[12]: array([[ 49.98343282, -49.97778146],
 [-49.97778146,  49.98004001])
```

MH Gibbs

14k in 22.8s implies 368k in 10 min

```
In [13]: import mh_gibbs
from hmc import hmc_wrapper, compute_log_joint_prob
importlib.reload(mh_gibbs)
```

```
Out[13]: <module 'mh_gibbs' from '/Users/gw/repos/prob_prog/hw/hw3/mh_gibbs.py'>
```

```
In [14]: fname = '5_abc.daphne'
graph = graph_helper(fname)
graph
```

```
Out[14]: [{}(),
[{}V': ['observe3', 'sample2', 'sample1'],
'A': ['sample2': ['observe3'], 'sample1': ['observe3']],
'P': ['sample1': ['sample', ['normal', 0, 10]],
'sample2': ['sample', ['normal', 0, 10]],
'observe3': ['observe*', ['normal', ['+', 'sample1', 'sample2'], 0.09], 7]],
'Y': ['observe3': 7]],
[{}vector', 'sample1', 'sample2']]]
```

```
In [15]: %time
num_steps=368000
return_list, samples_whole_graph = mh_gibbs.mh_gibbs_wrapper(graph,num_steps)
samples = np.array([sample.tolist() for sample in return_list])

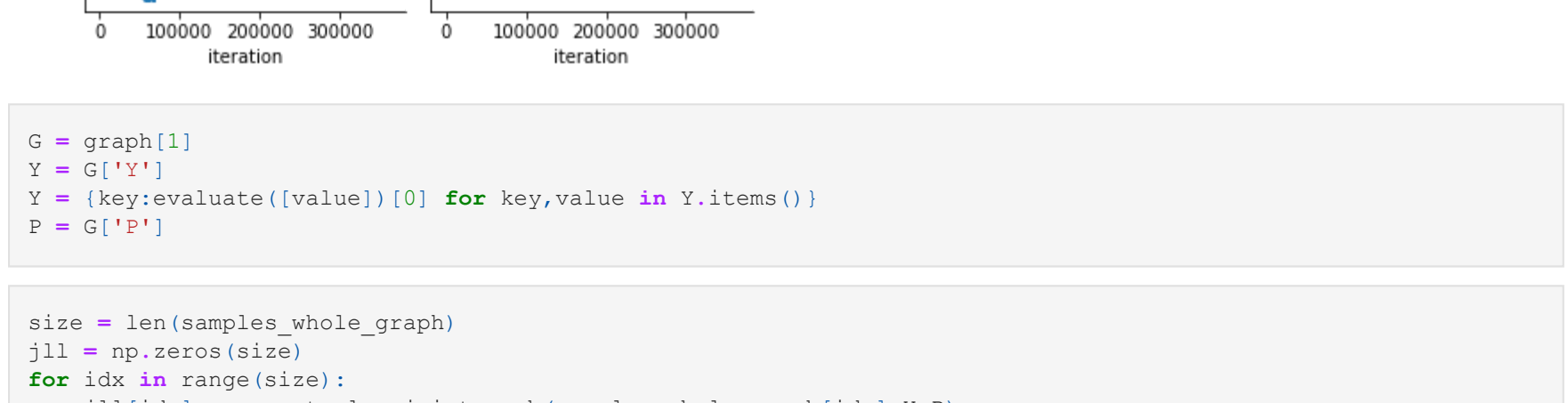
CPU times: user 9min 48s, sys: 1.51 s, total: 9min 49s
Wall time: 9min 50s
```

```
In [16]: samples = np.array([sample.tolist() for sample in return_list])
```

```
In [17]: burn_in = int(0.01*num_steps)
df = pd.DataFrame(samples[burn_in:])
df.columns = ['x','y']
df['iteration'] = df.index
tall = pd.melt(df, id_vars='iteration')

g = sns.FacetGrid(tall, col="variable")
g.map(sns.histplot, "value")

plt.suptitle('MH Gibbs | {}'.format(fname))
plt.subplots_adjust(top=0.8)
```



```
In [18]: posterior_mean = samples[burn_in:].mean(0)
cov_matrix = np.cov(samples[burn_in:].T,ddof=0)
posterior_variance = samples[burn_in:].var(0)
covariance = cov_matrix[0,1]
assert np.isclose(cov_matrix[0,0],posterior_variance[0])
assert np.isclose(cov_matrix[1,1],posterior_variance[1])
```

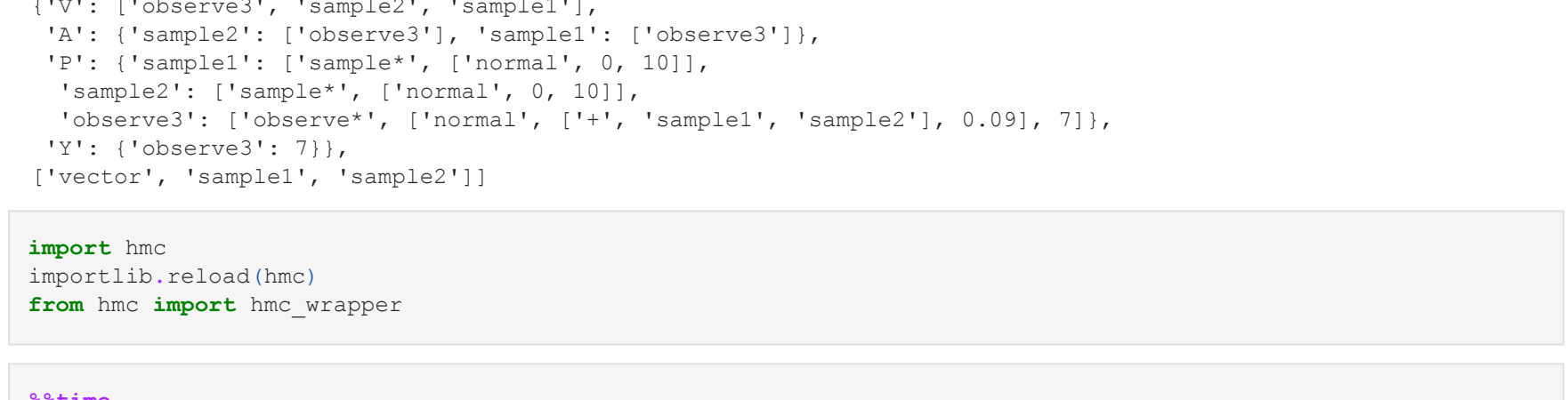
```
In [19]: for result in [
    "({} MH Gibbs: posterior mean slope {:1.3f} | variance slope {:1.3e})".format(fname,posterior_mean[0],posterior_variance[0]),
    "({} MH Gibbs: posterior mean bias {:1.3f} | variance bias {:1.3e})".format(fname,posterior_mean[1],posterior_variance[1]),
    "({} MH Gibbs: posterior covariance of slope and bias variance bias {:1.3e})".format(fname,covariance),
]:
    print(result)
```

```
5_abc.daphne MH Gibbs: posterior mean slope -2.343 | variance slope 3.465e+00
5_abc.daphne MH Gibbs: posterior mean bias 9.342 | variance bias 3.465e+00
5_abc.daphne MH Gibbs: posterior covariance of slope and bias variance bias -3.461e+00
```

```
In [20]: g = sns.FacetGrid(tall, col="variable")
g.map(plt.plot, "iteration","value")

plt.suptitle('MH Gibbs | {}'.format(fname))
plt.subplots_adjust(top=0.75)
plt.suptitle('{} | MH Gibbs \n Sample trace'.format(fname))
```

```
Out[20]: Text(0.5, 0.98, '5_abc.daphne | MH Gibbs \n Sample trace')
```

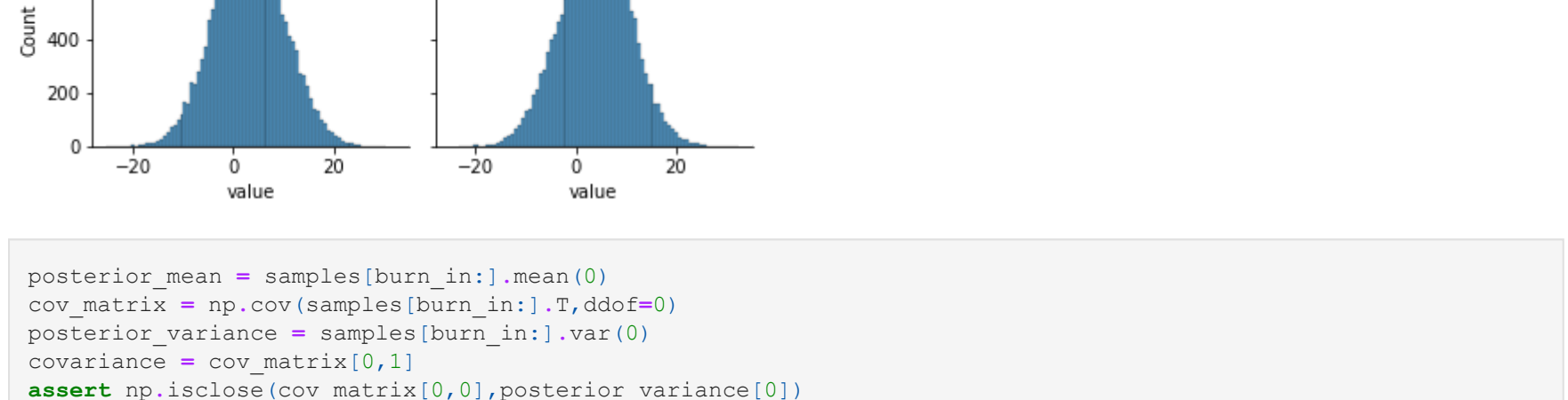


```
In [21]: G = graph[1]
Y = G['Y']
Y = {key:evaluate([value])[0] for key,value in Y.items()}
P = G['P']
```

```
In [22]: size = len(samples_whole_graph)
jll = np.zeros(size)
for idx in range(size):
    jll[idx] = compute_log_joint_prob(samples_whole_graph[idx],Y,P)
```

```
In [23]: pd.Series(jll).plot()
plt.xlabel('Iteration (t)')
plt.ylabel(r'$-\log p(x=y, Y=y_t)$')
plt.title('{} | MH Gibbs \n Joint density'.format(fname))
```

```
Out[23]: Text(0.5, 1.0, '5_abc.daphne | MH Gibbs \n Joint density')
```



HMC

- 0.56k in 16.2s implies 20.7k in 10 min

```
In [24]: fname = '5_abc.daphne'
graph = graph_helper(fname)
graph
```

```
Out[24]: [{}(),
[{}V': ['observe3', 'sample2', 'sample1'],
'A': ['sample2': ['observe3'], 'sample1': ['observe3']],
'P': ['sample1': ['sample', ['normal', 0, 10]],
'sample2': ['sample', ['normal', 0, 10]],
'observe3': ['observe*', ['normal', ['+', 'sample1', 'sample2'], 0.09], 7]],
'Y': ['observe3': 7]],
[{}vector', 'sample1', 'sample2']]]
```

```
In [25]: import hmc
importlib.reload(hmc)
from hmc import hmc_wrapper
```

```
In [26]: %time
num_samples=20700
return_list, samples_whole_graph = hmc_wrapper(graph,num_samples,T=40,epsilon=0.1)

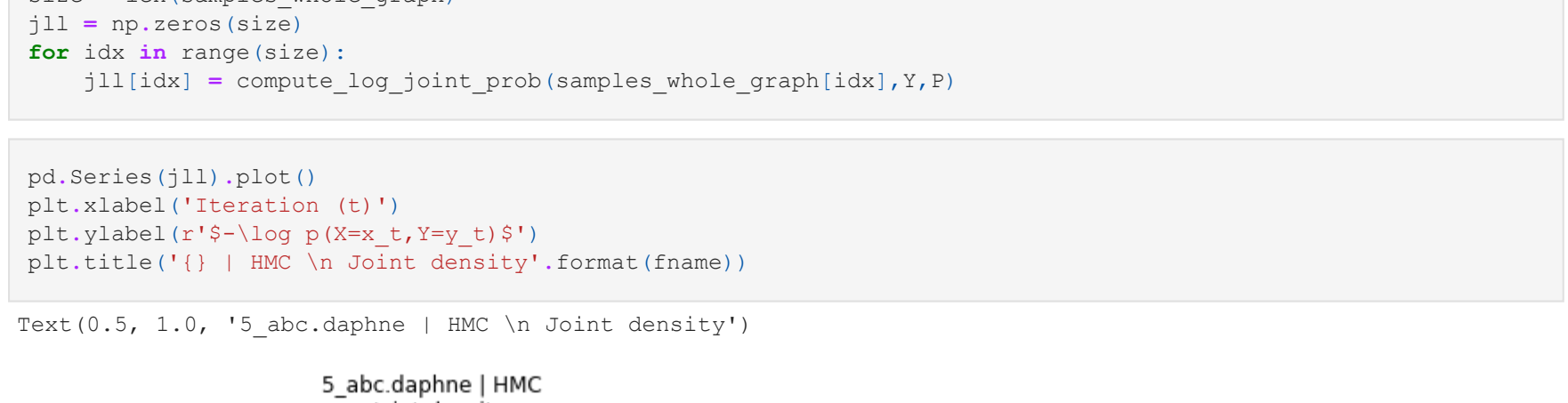
CPU times: user 9min 40s, sys: 1.46 s, total: 9min 42s
Wall time: 9min 43s
```

```
In [27]: samples = np.array([sample.tolist() for sample in return_list])
```

```
In [28]: burn_in = int(0.01*num_samples)
df = pd.DataFrame(samples[burn_in:])
df.columns = ['x','y']
df['iteration'] = df.index
tall = pd.melt(df, id_vars='iteration')

g = sns.FacetGrid(tall, col="variable")
g.map(sns.histplot, "value")

plt.suptitle('HMC | {}'.format(fname))
plt.subplots_adjust(top=0.75)
plt.suptitle('{} | HMC \n Sample trace'.format(fname))
```



```
In [29]: posterior_mean = samples[burn_in:].mean(0)
cov_matrix = np.cov(samples[burn_in:].T,ddof=0)
posterior_variance = samples[burn_in:].var(0)
covariance = cov_matrix[0,1]
assert np.isclose(cov_matrix[0,0],posterior_variance[0])
assert np.isclose(cov_matrix[1,1],posterior_variance[1])
```

```
In [30]: for result in [
    "({} HMC: posterior mean slope {:1.3f} | variance slope {:1.3e})".format(fname,posterior_mean[0],posterior_variance[0]),
    "({} HMC: posterior mean bias {:1.3f} | variance bias {:1.3e})".format(fname,posterior_mean[1],posterior_variance[1]),
    "({} HMC: posterior covariance of slope and bias variance bias {:1.3e})".format(fname,covariance),
]:
    print(result)
```

```
5_abc.daphne HMC: posterior mean slope 3.279 | variance slope 4.787e+01
5_abc.daphne HMC: posterior mean bias 3.721 | variance bias 4.788e+01
5_abc.daphne HMC: posterior covariance of slope and bias variance bias -4.739e+01
```

```
In [31]: g = sns.FacetGrid(tall, col="variable")
g.map(plt.plot, "iteration","value")

plt.suptitle('HMC | {}'.format(fname))
plt.subplots_adjust(top=0.75)
plt.suptitle('{} | HMC \n Sample trace'.format(fname))
```

```
Out[31]: Text(0.5, 0.98, '5_abc.daphne | HMC \n Sample trace')
```



```
In [32]: G = graph[1]
Y = G['Y']
Y = {key:evaluate([value])[0] for key,value in Y.items()}
P = G['P']
```

```
In [33]: size = len(samples_whole_graph)
jll = np.zeros(size)
for idx in range(size):
    jll[idx] = compute_log_joint_prob(samples_whole_graph[idx],Y,P)
```

```
In [34]: pd.Series(jll).plot()
plt.xlabel('Iteration (t)')
plt.ylabel(r'$-\log p(x=y, Y=y_t)$')
plt.title('{} | HMC \n Joint density'.format(fname))
```

```
Out[34]: Text(0.5, 1.0, '5_abc.daphne | HMC \n Joint density')
```

