Tools and Techniques for ML Homework 3

Zian Jiang (zj444)

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1 Derivation of importance-weighted reward imputation

1.1

The training dataset is a fixed dataset that is limited to samples from π_0. We lack knowledge of the reward $\delta(X_i, y)$ for many $y \in \mathcal{Y}$ that π would have chosen differently from π_0), but also that the actions preferred by π_0 are over-represented). Thus there is a covariate shift between π_0 and π.

1.2

Due to the covariate shift, we need to remove the distribution mismatch between π_0 and π by adding an importance weight to each term in the squared loss sum.

$$J_{IW}(r) = \frac{1}{n}\sum_{i=1}^{n} \frac{\pi(A_i|X_i)}{\pi_0(A_i|X_i)}(r(X_i, A_i) - R_i(A_i))^2$$

As we can see, $J_{IW}(r)$ is just $J(r)$ with each term re-weighted, thus by the change of measure theorem it follows naturally that $E(J_{IW}(r)) = E(J(r))$.

2 Optimizing 0/1 loss for binary classification

2.1

We can easily write out a table with the 4 cases and their respective losses and see that

$$El(A, Y) = (1 - p)\pi + p(1 - \pi) = p + \pi - 2p\pi.$$

Take the partial derivative and we can derive that the optimal π is 0.5.

2.2

$$E_{Y\sim Ber(p)}l(\pi, y) = pl(\pi, y = 1) + (1 - p)l(\pi, y = 0) = (1 - p)\pi + p(1 - \pi).$$

Thus, $l(\pi, y = 1) = 1 - \pi$ and $l(\pi, y = 0) = \pi$. According to the hint, we get

$$l(a, y) = a^{1-y}(1 - a)^y.$$

2.3

First, note that we can write $P(Y|X = x; w)$ compactly as

$$P(Y|X = x; w) = (\phi(w^T x))^y (1 - \phi(w^T x))^{1-y}.$$

$$E_{X,Y \sim P, a \sim Ber(\phi(w^T x))} \mathbf{1}[a \neq y] = \sum_{a=0}^{1} \sum_{y=0}^{1} P(A = a|X = x; w) P(Y = y|X = x) P(X = x) \mathbf{1}[a \neq y],$$

and canceling further out, we get

$$E_{X,Y \sim P, a \sim Ber(\phi(w^T x))} \mathbf{1}[a \neq y] = (1 - \phi(w^T x)) P(Y = 1|X = x) P(X) + \phi(w^T x) P(Y = 0|X = x) P(X).$$

2.4

$$J(w) = \sum_{i=1}^{n} (1 - Y_i) \phi(w^T X_i) + Y_i (1 - \phi(w^T X_i)).$$

This is almost equivalent to the negative log likelihood loss; both functions are optimized when for each example we make a correct prediction. However, consider the case of a large dataset and large feature space, where we have to use stochastic gradient descent (SGD) to optimize. SGD would only work on convex functions and the standard logistic function ϕ is not convex. However, $\log \phi$ is convex. Thus in this case only logistic regression with negative log likelihood loss would perform as expected.

Homework 3: Offline Policy Value Estimation (i.e. Counterfactual evaluation)

Introduction

In this lab, we're going to be reproducing a few results from http://proceedings.mlr.press/v97/vlassis19a.html, and extending their results in a few ways. Here's an overview: We start by taking a multiclass classification problem and splitting it into train and test. There are 26 classes, which we'll interpret as 26 possible actions to take for every input context. On the training set, we fit a multinomial logistic regression model to predict the correct label/best action. Following the paper, we create a logging policy based on this model (details supplied in the relevant spot below). We then generate "logged bandit feedback" for this logging policy using the **test** set. Given this logged bandit feedback, we'll try out several different methods for estimating the value of various policies. We'll also estimate the value of each of these policies using the full-feedback (i.e. the full observed rewards), and we'll treat that as the ground truth value for the purpose of performance assessment.

Load and process data

In [1]:
```
%load_ext autoreload
%autoreload 2
```

In [35]:
```
import abc

from sklearn.linear_model import LogisticRegression, LogisticRegressionCV, RidgeCV, Rid
from sklearn.ensemble import RandomForestRegressor, GradientBoostingRegressor
from sklearn.linear_model import LinearRegression
from sklearn.model_selection import train_test_split
import pandas as pd
from pandas.api.types import is_integer_dtype
import numpy as np
from numpy.random import default_rng
from scipy.special import expit
import seaborn as sns
import warnings;
warnings.filterwarnings('ignore');
import sys
```

In [3]:
```
def get_fully_observed_bandit():
    """
    This loads in a multiclass classification problem and reformulates it as a fully ob

    """
    df_l = pd.read_csv('data/letter-recognition.data',
                       names = ['a']+[f'x{i}' for i in range(16)])
    X = df_l.drop(columns=['a'])

    # Convert labels to ints and one-hot
    y = df_l['a']
    # if y is not column of integers (that represent classes), then convert
    if not is_integer_dtype(y.dtype):
        y = y.astype('category').cat.codes
```

```
    ## Full rewards
    n = len(y)
    k = max(y)+1
    full_rewards = np.zeros([n, k])
    full_rewards[np.arange(0,n),y] = 1
    contexts = X
    best_actions = y
    return contexts, full_rewards, best_actions
```

In [4]:

```
contexts, full_rewards, best_actions = get_fully_observed_bandit()
n, k = full_rewards.shape
_, d = contexts.shape
print(f"There are {k} actions, the context space is {d} dimensional, and there are {n}
print(f"For example, the first item has context vector:\n{contexts.iloc[0:1]}.")
print(f"The best action is {best_actions[0]}.  The reward for that action is 1 and all
print(f"The reward information is store in full_rewards as the row\n{full_rewards[0]}."
```

```
There are 26 actions, the context space is 16 dimensional, and there are 20000 examples.
For example, the first item has context vector:
   x0  x1  x2  x3  x4  x5  x6  x7  x8  x9  x10  x11  x12  x13  x14  x15
0   2   8   3   5   1   8  13   0   6   6   10    8    0    8    0    8.
The best action is 19.  The reward for that action is 1 and all other actions get reward
0.
The reward information is store in full_rewards as the row
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 0. 0.
 0. 0.].
```

In [5]:

```
## Choose train/test indices
rng = default_rng(7)
train_frac = 0.5
train_size = round(train_frac * n)
train_idx = rng.choice(n, size = train_size, replace = False)
test_idx = np.setdiff1d(np.arange(n), train_idx, assume_unique=True)
```

Policies

In this section, we'll build out a Policy class, some specific policies, and evaluate policies on full-feedback data.

Problem 1. Complete the Policy class and the UniformActionPolicy classes below. Run the code provided to get an estimate of the value of the uniform action policy using the test set. Explain why the value you get makes sense.

In [6]:

```
class Policy:
    def __init__(self, num_actions=2):
        self.num_actions = num_actions

    @abc.abstractmethod
    def get_action_distribution(self, X):
        """
        This method is intended to be overridden by each implementation of Policy.

        Args:
            X (pd.DataFrame): contexts

        Returns:
            2-dim numpy array with the same number of rows as X and self.num_actions co
                Each rows gives the policy's probability distribution over actions cond
```

```
        """
        raise NotImplementedError("Must override method")

    def get_action_propensities(self, X, actions):
        """
        Args:
            X (pd.DataFrame): contexts, rows correspond to entries of actions
            actions (np.array): actions taken, represented by integers, corresponding t

        Returns:
            1-dim numpy array of probabilities (same size as actions) for taking each a
        """
        ## DONE
        action_distribution = self.get_action_distribution(X)
        return np.take_along_axis(action_distribution, actions.reshape(-1, 1), axis=1).

    def select_actions(self, X, rng=default_rng(1)):
        """
        Args:
            X (pd.DataFrame): contexts, rows correspond to entries of actions and prope

        Returns:
            actions (np.array): 1-dim numpy array of length equal to the number of rows
                The action is selected randomly according to the policy, conditional on
            propensities (np.array): 1-dim numpy array of length equal to the number of

        """
        ## DONE
        action_distribution = self.get_action_distribution(X)
        actions = np.array([np.random.choice(26, 1, p=action_distribution[i]) for i in
        propensities = self.get_action_propensities(X, actions)
        assert len(actions) == len(propensities) == X.shape[0]

        return actions, propensities


    def get_value_estimate(self, X, full_rewards):
        """
        Args:
            X (pd.DataFrame): contexts, rows correspond to entries of full_rewards
            full_rewards (np.array): 2-dim numpy array with the same number of rows as
                each row gives the rewards that would be received for each action for t
                This would only be known in a full-feedback bandit, or estimated in a d

        Returns:
            scalar value giving the expected average reward received for playing the po

        """
        ## DONE
        n = X.shape[0]
        actions, propensities = self.select_actions(X)
        action_distribution = self.get_action_distribution(X)

        return (full_rewards*action_distribution).sum()/n


class UniformActionPolicy(Policy):
    def __init__(self, num_actions=2):
        self.num_actions = num_actions

    def get_action_distribution(self, X):
```

```
        ## DONE
        return np.full((X.shape[0], self.num_actions), 1.0/self.num_actions)
```

In [7]:
```
X_train = contexts.iloc[train_idx].to_numpy()
y_train = best_actions.iloc[train_idx].to_numpy()
X_test = contexts.iloc[test_idx].to_numpy()
y_test = best_actions.iloc[test_idx].to_numpy()
full_rewards_test = full_rewards[test_idx]

uniform_policy = UniformActionPolicy(num_actions=k)
uniform_policy_value = uniform_policy.get_value_estimate(X=X_test, full_rewards=full_re
print(f"The estimate of the value of the uniform action policy using the full-feedback
```

```
The estimate of the value of the uniform action policy using the full-feedback test set
is 0.038461538461538484.
```

This estimate of the value of this uniform action policy is $\frac{1}{26}$. This makes sense because as the formulation of the value estimate suggests,

$$V(\pi) = \frac{1}{n}\sum_{i=1}^{n}\sum_{a=1}^{k}[r(X_i, a)\pi(a|X_i)],$$

in the inner sum every propensity score is $\frac{1}{26}$ and only 1 action out of 26 has the reward 1 while the rest is 0. Thus, the inner sum is essentially $\frac{1}{26}$. We add $\frac{1}{26}$ up for n times and take the average, which results in $\frac{1}{26}$ as value.

Problem 2. Complete the SKLearnPolicy class below and run the code that creates two policies and estimates their values using the full reward information in the test set. You should find that the deterministic policy has a higher value than the stochastic policy. Nevertheless, why might one choose to deploy the stochastic policy rather than the deterministic policy?

In [8]:
```
## Develop more policies

class SKLearnPolicy(Policy):
    """
    An SKLearnPolicy uses a scikit learn model to generate an action distribution.  If
    then the predict distribution for a context x should be whatever predict_proba for
    should be concentrated on whatever predict of the model returns.
    """
    def __init__(self, model, num_actions=2, is_deterministic=False):
        self.is_deterministic = is_deterministic
        self.num_actions = num_actions
        self.model = model

    def get_action_distribution(self, X):
        ## DONE
        if (self.is_deterministic):
            predictions = self.model.predict(X)
            return np.eye(self.num_actions)[predictions.reshape(-1)] # one hot
        else:
            return self.model.predict_proba(X)


    def select_actions(self, X, rng=default_rng(1)):
        ## DONE
        if (self.is_deterministic):
            actions = self.model.predict(X)
```

```
            propensities = np.full(len(actions), 1.0)
            return actions, propensities
        else:
            actions, propensities = Policy.select_actions(self, X)
            return actions, propensities

model = LogisticRegression(multi_class='multinomial')
model.fit(X_train, y_train)
policy_stochastic = SKLearnPolicy(model=model, num_actions=k, is_deterministic=False)
policy_deterministic = SKLearnPolicy(model=model, num_actions=k, is_deterministic=True)

policy_stochastic_true_value = policy_stochastic.get_value_estimate(X_test, full_reward
policy_deterministic_true_value = policy_deterministic.get_value_estimate(X_test, full_
print(f"Stochastic policy true value {policy_stochastic_true_value}.")
print(f"Deterministic policy true value {policy_deterministic_true_value}.")
```

```
Stochastic policy true value 0.6261601174415055.
Deterministic policy true value 0.7631.
```

Since we know our training data is biased towards π_0, the deterministic policy may also be biased and offeres no exploration. On the other hand the stochastic policy offers exploration by randomly selecting actions based on the action distribution trained from data.

Problem 3. Fill in the VlassisLoggingPolicy class below, and evaluate the value of this logging policy using the code provided.

In [9]:
```
class VlassisLoggingPolicy(Policy):
    """
    This policy derives from another deterministic policy following the recipe describe
    For any context x, if the deterministic policy selects action a, then this policy s
    rest of the probability mass uniformly over the other actions.
    """
    def __init__(self, deterministic_target_policy, num_actions=2, eps=0.05):
        self.num_actions = num_actions
        self.target_policy = deterministic_target_policy
        self.eps = eps

    def get_action_distribution(self, X):
        rest = (1.0-self.eps)/(self.num_actions-1)
        actions, propensities = self.target_policy.select_actions(X)
        action_distribution = np.eye(self.num_actions)[actions.reshape(-1)]*self.eps
        action_distribution[action_distribution == 0.0] = rest
        return action_distribution


logging_policy = VlassisLoggingPolicy(policy_deterministic, num_actions=k, eps=0.05)
logging_policy_value = logging_policy.get_value_estimate(X=X_test, full_rewards=full_re
print(f"The estimate of the value of the logging policy using the full-feedback test se
```

```
The estimate of the value of the logging policy using the full-feedback test set is 0.04
715720000000002.
```

Simulate bandit feedback and on-policy evaluation

Problem 4. Take a look at the generate_bandit_feedback function, so you understand how it works. Then generate bandit feedback using the test data -- generate as many rounds are there are contexts in the test data. Use the result to generate an "on-policy" estimate of the value of the logging policy. How does it compare to our "ground truth" estimate you found previously using the full-feedback test set? Repeat using 1/100th, 1/10th, and 10x as much bandit feedback, to see how much the value estimates change.

In [10]:
```
def generate_bandit_feedback(contexts, full_rewards, policy,
                             new_n = None,
                             rng=default_rng(1)):
    """
    Args:
        contexts (np.array): contexts, rows correspond to entries of rewards
        full_rewards (np.array): 2-dim numpy array with the same number of rows as X an
            each row gives the reward that would be received for each action for the co

    Returns:
        new_contexts (np.array): new_n rows and same number of columns as in contexts
        actions (np.array): vector with new_n entries giving actions selected by the pr
        observed_rewards (np.array): vector with new_n entries giving actions selected
    """

    if new_n is None:
        new_n = contexts.shape[0]
    n, k = full_rewards.shape
    num_repeats = np.ceil(new_n / n).astype(int)
    new_contexts = np.tile(contexts, [num_repeats,1])
    new_contexts = new_contexts[0:new_n]
    new_rewards = np.tile(full_rewards, [num_repeats,1])
    new_rewards = new_rewards[0:new_n]
    actions, propensities = policy.select_actions(X=new_contexts, rng=rng)
    observed_rewards = new_rewards[np.arange(new_n), actions]
    return new_contexts, actions, observed_rewards, propensities
```

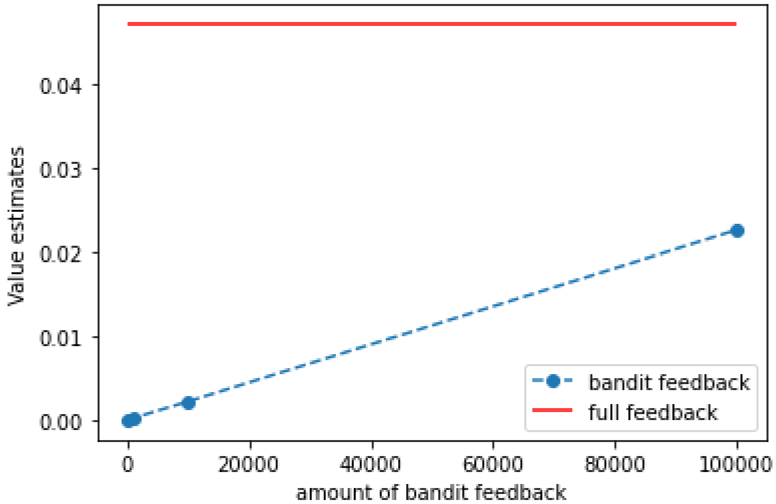
In [11]:
```
n = full_rewards_test.shape[0]
vals = []

for n_ in [n/100, n/10, n, 10*n]:
    new_contexts, actions, observed_rewards, propensities = generate_bandit_feedback(X_
                                                                    logging_policy, new_n=i
    vals.append(sum(observed_rewards*propensities)/n)
```

In [12]:
```
import matplotlib.pyplot as plt

plt.plot([n/100, n/10, n, 10*n], vals, "--o", label="bandit feedback")
plt.xlabel("amount of bandit feedback")
plt.ylabel("Value estimates")
plt.hlines(logging_policy_value, xmin=0, xmax=100000, label="full feedback", color="r")
plt.legend(loc=4)
```

Out[12]: <matplotlib.legend.Legend at 0x203a58179a0>



As we can see, with more bandit feedback, the higher the value estimate will be.

Test out off-policy value estimators

Problem 5. Complete the get_value_estimators function below, per the specification. Include the following estimators

- Unweighted mean (done for you)
- Importance-weighted (IW) value estimator
- Self-normalized IW mean
- Direct method with linear ridge regression reward predictor fit for each action
- Direct method with IW-linear ridge regression reward predictor fit for each action
- [Optional (not for credit)] Direct method with a non-linear reward predictor fit for each action
- [Optional (not for credit)] Direct method with a non-linear reward predictor fit for all actions at once (action becomes part of the input)

Run the code below that will apply your value estimators to a policy on logged bandit feedback. Verify that your results are reasonable. (Don't worry if your numbers are not a very close match for the results in the table.)

In [100…

```
## Build our value estimators

def get_value_estimators(policy, contexts, actions, rewards, propensities, skip_slow_st
    """
    Args:
        policy (Policy): the policy we want to get a value estimate for
        contexts (np.array): contexts from bandit feedback
        actions (np.array): actions chosen for bandit feedback
        rewards (np.array): rewards received in bandit feedback
        propensities (np.array): the propensity for each action selected under the logg
        skip_slow_stuff (boolean): boolean flag which allows you to turn on/off some sl
    Returns:
        est (dict): keys are string describing the value estimator, values are the corr
    """

    est = {}
    est["mean"] = np.mean(rewards)
```

```
    ## DONE
    pi_w = policy.get_action_propensities(contexts, actions)

    assert len(rewards) == len(pi_w) == len(propensities)
    importance_weights = pi_w/propensities

    est["IW"] = np.mean(rewards*importance_weights)
    est["SNIW"] = np.sum(rewards*importance_weights) / np.sum(importance_weights)

    if not skip_slow_stuff:
        models = []
        for i in range(26):
            idx = actions == i
            X = contexts[idx]
            y = rewards[idx]
            model = Ridge()
            model.fit(X, y)
            models.append(model)

        n = len(actions)
        res = 0.0
        for i in range(n):
            X_i = contexts[i].reshape(1, -1)
            all_action_propensities = policy.get_action_propensities(X_i, np.arange(26)
            predicted_rewards = []
            for a in range(26):
                model = models[a]
                predicted_reward = model.predict(X_i)[0]
                predicted_rewards.append(predicted_reward)
            res += sum(all_action_propensities * np.asarray(predicted_rewards))
        est["Ridge"] = res/n


        models = []
        for i in range(26):
            idx = actions == i
            X = contexts[idx]
            y = rewards[idx]
            p_0 = propensities[idx]
            p_w = policy.get_action_propensities(X, np.full(X.shape[0], i, dtype=int))
            sample_weights = p_w/p_0
            model = Ridge()
            model.fit(X, y, sample_weights)
            models.append(model)

        n = len(actions)
        res = 0.0
        for i in range(n):
            X_i = contexts[i].reshape(1, -1)
            propensities = policy.get_action_propensities(X_i, np.arange(26))
            predicted_rewards = []
            for a in range(26):
                model = models[a]
                predicted_reward = model.predict(X_i)[0]
                predicted_rewards.append(predicted_reward)
            res += sum(propensities*np.asarray(predicted_rewards))
        est["Ridge_IW"] = res/n

    return est
```

In [101…
```
def get_estimator_stats(estimates, true_parameter_value=None):
    """

     Args:
        estimates (pd.DataFrame): each row corresponds to collection of estimates for a
            each column corresponds to an estimator
        true_parameter_value (float): the true parameter value that we will be comparin

    Returns:
        pd.Dataframe where each row represents data about a single estimator
    """

    est_stat = []
    for est in estimates.columns:
        pred_means = estimates[est]
        stat = {}
        stat['stat'] = est
        stat['mean'] = np.mean(pred_means)
        stat['SD'] = np.std(pred_means)
        stat['SE'] = np.std(pred_means) / np.sqrt(len(pred_means))
        if true_parameter_value:
            stat['bias'] = stat['mean'] - true_parameter_value
            stat['RMSE'] = np.sqrt(np.mean((pred_means - true_parameter_value) ** 2))
        est_stat.append(stat)

    return pd.DataFrame(est_stat)
```

In [102…
```
contexts_test, actions_test, rewards_test, propensities_test = generate_bandit_feedback
policy = policy_deterministic
est = get_value_estimators(policy, contexts_test, actions_test, rewards_test, propensit
policy_true_value = policy.get_value_estimate(X_test, full_rewards_test)
print(f"policy true value {policy_true_value}.")
df = pd.DataFrame(est, index=[0])
est
```

```
policy true value 0.7631.
```

Out[102…
```
{'mean': 0.0482,
 'IW': 0.816,
 'SNIW': 0.783109404990403,
 'Ridge': 0.27112898219944515,
 'Ridge_IW': 0.7623822729000462}
```

Problem 6. Run the code below to test your value estimators across multiple trials. Write a few sentences about anything you learned from these experiments or that you find interesting.

In [103…
```
trials=20
val_ests = []
policy = policy_deterministic
policy_true_value = policy.get_value_estimate(X_test, full_rewards_test)
rng=default_rng(6)
for i in range(trials):
    contexts, actions, rewards, propensities = generate_bandit_feedback(X_test, full_re
    est = get_value_estimators(policy, contexts, actions, rewards, propensities)
    val_ests.append(est)

df = pd.DataFrame(val_ests)
print(get_estimator_stats(df, true_parameter_value=policy_true_value))
```

```
   stat      mean        SD        SE      bias      RMSE
0  mean  0.046790  0.002009  0.000449 -0.716310  0.716313
1    IW  0.762100  0.030799  0.006887 -0.001000  0.030815
```

```
2      SNIW  0.762522  0.012827  0.002868 -0.000578  0.012841
3     Ridge  0.266487  0.009019  0.002017 -0.496613  0.496695
4  Ridge_IW  0.791159  0.031913  0.007136  0.028059  0.042494
```

In [104…

```
trials=20
val_ests = []
policy = policy_stochastic
policy_true_value = policy.get_value_estimate(X_test, full_rewards_test)
rng=default_rng(6)
for i in range(trials):
    contexts, actions, rewards, propensities = generate_bandit_feedback(X_test, full_re
    est = get_value_estimators(policy, contexts, actions, rewards, propensities)
    val_ests.append(est)

df = pd.DataFrame(val_ests)
print(get_estimator_stats(df, true_parameter_value=policy_true_value))
```

```
       stat      mean        SD        SE      bias      RMSE
0      mean  0.047580  0.001715  0.000384 -0.578580  0.578583
1        IW  0.634605  0.022671  0.005069  0.008445  0.024192
2      SNIW  0.628373  0.012770  0.002856  0.002213  0.012961
3     Ridge  0.254693  0.007423  0.001660 -0.371467  0.371541
4  Ridge_IW  0.610243  0.016766  0.003749 -0.015918  0.023118
```

In [105…

```
trials=20
val_ests = []
policy = uniform_policy
policy_true_value = policy.get_value_estimate(X_test, full_rewards_test)
rng=default_rng(6)
for i in range(trials):
    contexts, actions, rewards, propensities = generate_bandit_feedback(X_test, full_re
    est = get_value_estimators(policy, contexts, actions, rewards, propensities)
    val_ests.append(est)

df = pd.DataFrame(val_ests)
print(get_estimator_stats(df, true_parameter_value=policy_true_value))
```

```
       stat      mean        SD        SE      bias      RMSE
0      mean  0.047705  0.002322  0.000519  0.009243  0.009531
1        IW  0.038915  0.001803  0.000403  0.000454  0.001859
2      SNIW  0.038921  0.001826  0.000408  0.000460  0.001883
3     Ridge  0.044560  0.001578  0.000353  0.006099  0.006299
4  Ridge_IW  0.038709  0.001403  0.000314  0.000247  0.001425
```

As we can see across the 3 policies, uniform policy has a very low value. Stochastic and deterministic policies are more preferable. Also, importance weighting is very important due to the selection bias; this is true in both reward imputation and importance weighting. Of course, they are all better than the naive unweighted mean estimate. Also, using self-normalized weights on top of importance weighting gives the best result generally.