Documentation for Optimization.py

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June 2017

1 Introduction

The purpose of the optimization is to find the mitigation value in every node of the decision tree that maximizes the current utility

$$x^* = \underset{x}{\operatorname{argmax}}U(x) \tag{1}$$

Our approach to solving this problem is to use the genetic algorithm (GA) as well as a gradient search (GS) method. The GA is used to search the state space globally and to find good initial points for the GS, which applies a gradient descent algorithm to multiple initial points.

2 Genetic Algorithm

2.1 Theory

The GA is an evolutionary algorithm, inspired by the evolution of species in nature. The evolution process starts from a population of vectors with random elements uniformly distributed on [0, bound]. For each generation, the evolution steps are:

- 1. Select the individuals to perform cross-over and mutation.
- 2. Cross over among the selected candidate.
- 3. Mutate result as offspring.
- 4. Combine the result of offspring and parent together. And selected the top 80 percent of original population amount.
- 5. Randomly generate 20 percent of original population amount new individuals and combine the above new population.

The mutation and cross-over methods are chosen to fit the optimization problem of the EZ-Climate model.

2.2 GA Class

It is a class that runs the genetic search given right population and fit function.

2.2.1 Inputs and Outputs

Inputs:

- **pop_amount**: (int) number of individuals in the population
- num_feature: (int) number of elements in each individual, i.e. number of nodes in TreeModel. For the base case, the number is 63.
- num_generations : (int) number of generations of the populations to be evaluated
- **bound**: (float) upper bound of mitigation in each node. (the bound of the initial population. In the model, it would be 1 since the mitigation level won't be larger than 1.)
- cx_prob : (float) probability of mating
- mut_prob : (float) probability of mutation.
- utility: ('Utility' object) object of utility class
- fixed_values: (ndarray, optional) nodes to keep fixed
- fixed_indicies : (ndarray, optional) indicies of nodes to keep fixed
- print_progress: (bool, optional) if the progress of the evolution should be printed

In which, the probabilities of mating and mutation could be changed to provide a faster speed.

Outputs:

the main function that will be use in this class is **run** and it returns the optimization result in a tuple :(final population, the fitness for the final population) the results (individuals) with the highest k fitness will be used in the next step (GS)

2.2.2 Attributes

- pop_amount : (int) number of individuals in the population
- num_feature : (int) number of elements in each individual, i.e. number of nodes in tree-model
- num_generations : (int) number of generations of the populations to be evaluated
- **bound**: (float) upper bound of mitigation in each node
- **cx_prob** : (float) probability of mating

- mut_prob : (float) probability of mutation.
- u : ('Utility' object) object of utility class
- fixed_values : (ndarray, optional) nodes to keep fixed
- fixed_indicies : (ndarray, optional) indicies of nodes to keep fixed
- print_progress: (bool, optional) if the progress of the evolution should be printed

2.2.3 Methods

_generate_population: A private function that generates the initial population.

Inputs:

• size: the size of init population

Outputs:

• **pop** (ndarray) An array of random values with 'size' number of lists. And the lists' length are the number of final nodes. For example, if size = 2 and there are four final nodes, the output will be: array[[0.1,0.4,0.4,0.2],[0.2,0.3,0.3,0.3]]

_evaluate: a private function that evaluates the fitness of the individual within a population. In our model, the fitness it defined by utility.

```
def _evaluate(self, indvidual):
    """Returns the utility of given individual."""
    return self.u.utility(indvidual)
```

_select: a private function that returns an array of selected individuals.

Inputs:

- pop: the population that you want to make selection from.
- rate: the probability that a individual is selected

Outputs: an array pf selected individual.

For example:

```
>>> _select([4,5,6,7],0.5)
[4,5,6]
```

```
def _select(self, pop, rate):
                 """Returns a 1D-array of selected individuals.
            Parameters
             _____
            pop : ndarray
                     population given by 2D-array with shape ('pop_amount', 'num_featur
            rate: float
                     the probability of an individual being selected
            Returns
             _____
            ndarray
                     selected individuals
                index = np.random.choice(self.pop_amount, int(rate*self.pop_amount), rep
                return pop[index,:] #return a list of random instance of pop
_random_index: a private function that generates a random index of individuals of given
size (amount \cdot rate). It's is the same with \_select but just returns the index rather than the
item itself. For example:
>>> _random_index([4,5,6,7],0.5)
[1,2,3]
\textbf{Inputs}:
\begin{itemize}
  \item \texfbf{individuals}: (ndarray) target individuals.
  \item \textbf{size}: (ndarray) target size.
\end{itemize}
\textbf{Outputs}:
\begin{itemize}
  \item chosen indexes
\end{itemize}
        def _random_index(self, individuals, size):
                """Generate a random index of individuals of size 'size'.
                 Parameters
                 _____
                 individuals : ndarray or list
                         2D-array of individuals
                 size : int
                         number of indices to generate
                 Returns
```

_selection_tournament: a private function that for given k times, randomly chooses a 'tournsize' number of index and picks up the one with the highest fitness. Work flow is as follows:

- 1. pick a tournsize t
- 2. randomly choose t individuals in the input population
- 3. find the one with highest fitness then store the winner
- 4. repeat for k times

Inputs:

- individuals : (ndarray or list) 2D-array of individuals to select from
- k (int number of individuals to select
- tournsize: (int) number of individuals participating in each tournament
- fitness: utility in out model

Outputs: an array with length k which stores the individual picked for each tournament.

_two_point_cross_over: a private function that does the two-point cross-over. Two-point crossover calls for two points to be selected on the parent organism strings. Everything

between the two points is swapped between the parent organisms, rendering two child organisms. A two-point cross-over is illustrated as following graph:

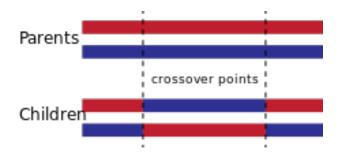


Figure 1: Two Point Crossover

Inputs: Original population

Outputs: population after two point cross over. (returns None but change the input pop)

```
def _two_point_cross_over(self, pop):
```

```
child_group1 = pop[::2] # instance with even index
child_group2 = pop[1::2] # instance with odd index
for child1, child2 in zip(child_group1, child_group2):
        if np.random.random() <= self.cx_prob:</pre>
                #generates 2 random index for the swap, can be done much
                cxpoint1 = np.random.randint(1, self.num_feature)
                cxpoint2 = np.random.randint(1, self.num_feature - 1)
                if cxpoint2 >= cxpoint1:
                        cxpoint2 += 1
                else: # Swap the two cx points
                        cxpoint1, cxpoint2 = cxpoint2, cxpoint1
                child1[cxpoint1:cxpoint2], child2[cxpoint1:cxpoint2] \
                = child2[cxpoint1:cxpoint2].copy(), child1[cxpoint1:cxpo
                if self.fixed_values is not None:
                        child1[self.fixed_indicies] = self.fixed_values
                        child2[self.fixed_indicies] = self.fixed_values
```

_uniform_cross_over: a private function that does the uniform cross-over. The uniform crossover uses a fixed mixing ratio between two parents. Unlike single- and two-point crossover, the uniform crossover enables the parent chromosomes to contribute the gene level rather than the segment level.

If the mixing ratio is 0.5, the offspring has approximately half of the genes from first parent and the other half from second parent, although cross over points can be randomly chosen as seen below:



Figure 2: Uniform Crossover

Inputs:

- pop: (ndarray) original population
- ind_prob: (float) the mixing ratio mentioned above

Outputs: Population after uniform cross over. (returns None but change the input pop)

_mutate: A private function that mutates individual's elements. The mutation is constrained by an input parameter called **scale**. And the formula for mutation is as follows: $pop[i][j] = \max\{0.0, pop[i][j] + (RandomNumber - 0.5) \cdot scale\}$ where pop[i][j] is the element that is been mutated

Inputs:

- pop: (ndarray) population given by 2D-array with shape ('pop_amount', 'num_feature')
- mut_prob : (attr form GA class) probability of an individual being selected to mutate.
- ind_prob : (float) probability of an element within an individual being selected to mutate.
- scale: (float) scaling constant of the random generated number for mutation.

Outputs: Population after mutating.

for j in feature_index:

_uniform_mutation: A private function that performs the uniform mutation which means the mutated value is the current value plus a scaled uniform [-0.5,0.5] random value. Inputs and Outputs are the same with **_mutate** but using a different mutation method.

```
def _uniform_mutation(self, pop, ind_prob, scale=2.0):
        """Mutates individual's elements. The individual has a probability of
        beeing selected and every element in this individual has a probability
        mutated. The mutated value is the current value plus a scaled uniform
        Parameters
        _____
        pop : ndarray
                population given by 2D-array with shape ('pop_amount', 'num_fe
    ind_prob : float
            probability of feature mutation
    scale : float
            scaling constant of the random generated number for mutation
    11 11 11
        pop_len = len(pop)
        mutate_index = np.random.choice(pop_len, int(self.mut_prob * pop_len), r
        for i in mutate_index:
                prob = np.random.random(self.num_feature)
                inc = (np.random.random(self.num_feature) - 0.5)*scale
                pop[i] += (prob > (1.0-ind_prob)).astype(int)*inc
                pop[i] = np.maximum(1e-5, pop[i])
                if self.fixed_values is not None:
                        pop[i][self.fixed_indicies] = self.fixed_values
```

_show_evolution: print statistics of the evolution of the population including min, max, average, std and the best individual of a population

```
def _show_evolution(self, fits, pop):
    """Print statistics of the evolution of the population."""
    length = len(pop)
    mean = fits.mean()
    std = fits.std()
    min_val = fits.min()
    max_val = fits.max()
    print (" Min {} \n Max {} \n Avg {}".format(min_val, max_val, mean))
    print (" Std {} \n Population Size {}".format(std, length))
    print (" Best Individual: ", pop[np.argmax(fits)])
```

_survive: the 80 percent of the individuals with best fitness survives to the next generation. **Inputs**:

- pop_tmp: (ndarray) population before survive process.
- fitness_tmp: (ndarray) utility for the population before survive process.

Outputs:

- **pop**: (ndarray) population after survive process.
- fitness: (ndarray) utility for the population after survive process.

```
def _survive(self, pop_tmp, fitness_tmp):
        """The 80 percent of the individuals with best fitness survives to
        the next generation.
        Parameters
        _____
        pop_tmp : ndarray
                population
        fitness_tmp : ndarray
                fitness values of `pop_temp`
        Returns
        _____
        ndarray
                individuals that survived
        .....
        index_fits = np.argsort(fitness_tmp)[::-1]
        fitness = fitness_tmp[index_fits]
        pop = pop_tmp[index_fits]
        num_survive = int(0.8*self.pop_amount)
        survive_pop = np.copy(pop[:num_survive])
        survive_fitness = np.copy(fitness[:num_survive])
        return np.copy(survive_pop), np.copy(survive_fitness)
```

run: main function of the GA class. Returns the (final population, the fitness for the final population). The whole algo follows these steps:

- 1. Select the individuals to perform cross-over and mutation.
- 2. Cross over among the selected candidate.
- 3. Mutate result as offspring.
- 4. Combine the result of offspring and parent together. And selected the top 80 percent of original population amount.

5. Random Generate 20 percent of original population amount new individuals and combine the above new population.

Within the process, the base model is doing uniform cross over with rate 0.5 and uniform mutation with rate 0.25 but the parameters can be changed and it can be changed to random cross-over or mutation.

Outputs:

- pop: (ndarray) final population
- fitness: (ndarray) utility for the final population.

```
def run(self):
       11 11 11
        Returns
        _____
        tuple
               final population and the fitness for the final population
        Note
        Uses the :mod: `~multiprocessing` package.
        11 11 11
       print("-----")
       pop = self._generate_population(self.pop_amount)
       pool = multiprocessing.Pool(processes=multiprocessing.cpu_count())
       fitness = pool.map(self._evaluate, pop) # how do we know pop[i] belongs
       fitness = np.array([val[0] for val in fitness])
       u_hist = np.zeros(self.num_gen) # not been used ...
       for g in range(0, self.num_gen):
               print ("-- Generation {} --".format(g+1))
               pop_select = self._select(np.copy(pop), rate=1)
               self._uniform_cross_over(pop_select, 0.50)
               self._uniform_mutation(pop_select, 0.25, np.exp(-float(g)/self.n
               #self._mutate(pop_select, 0.05)
               fitness_select = pool.map(self._evaluate, pop_select)
               fitness_select = np.array([val[0] for val in fitness_select])
               pop_tmp = np.append(pop, pop_select, axis=0)
               fitness_tmp = np.append(fitness, fitness_select, axis=0)
               pop_survive, fitness_survive = self._survive(pop_tmp, fitness_tm
```

pop_new = self._generate_population(self.pop_amount - len(pop_su

```
fitness_new = pool.map(self._evaluate, pop_new)
    fitness_new = np.array([val[0] for val in fitness_new])

pop = np.append(pop_survive, pop_new, axis=0)
    fitness = np.append(fitness_survive, fitness_new, axis=0)
    if self.print_progress:
        self._show_evolution(fitness, pop)
    u_hist[g] = fitness[0]

fitness = pool.map(self._evaluate, pop)
fitness = np.array([val[0] for val in fitness])
return pop, fitness
```

3 Gradient Search

3.1 Theory

The GS uses the gradient descent algorithm and the numerical gradient to find the optimal mitigation points. Moveover, it uses the Adaptive Moment Estimation (Adam) learning rate together with an accelerator scaler to update the points. Adam is a method that computes adaptive learning rates for each parameter.

In addition to storing an exponentially decaying average of past squared gradients, Adam also keeps an exponentially decaying average of past gradients. The accelerator is used to amplify low gradient values of mitigation values in nodes in the end of the tree, and thus reduce computation time. The **run** method takes **initial_point_list** and **topk** as arguments, runs the gradient descent optimization of the topk first elements of the initial_point_list, and picks the resulting point with the highest utility.

3.2 GS Class

Gradient search optimization algorithm for the EZ-Climate model

3.2.1 Inputs and Outputs

Inputs:

- utility: ('Utility' object) object of utility class
- learning_rate : (float) starting learning rate of gradient descent
- var_nums: (int) number of elements in array to optimize
- accuracy: (float) stop value for the gradient descent

- fixed_values: (ndarray, optional) nodes to keep fixed
- fixed_indicies : (ndarray, optional) indicies of nodes to keep fixed
- print_progress: (bool, optional) if the progress of the evolution should be printed
- scale_alpha: (ndarray, optional) array to scale the learning rate

Output:

The main output is from the **run** function same as the GA class. The function returns a tuple: (best mitigation point, the utility of the best mitigation point)

3.2.2 Attributes

- utility: ('Utility' object) object of utility class
- learning_rate : (float) starting learning rate of gradient descent
- var_nums: (int) number of elements in array to optimize. In the base case, it is 63 i.e. the number of nodes/decision points that we have in the binomial tree.
- accuracy: (float) stop value for the gradient descent
- fixed_values : (ndarray, optional) nodes to keep fixed
- fixed_indicies : (ndarray, optional) indicies of nodes to keep fixed
- print_progress: (bool, optional) if the progress of the evolution should be printed
- scale_alpha: (ndarray, optional) array to scale the learning rate

The attributes are the same as the inputs. All of this paramters is used to do the gradient search.

3.2.3 Methods

_partial_grad: A private function to calculate the gradient at a certain node. Gradient here is:

$$gradient = \frac{f(x+\Delta) - f(x-\Delta)}{2\Delta}$$
 (2)

where f(x) is the general fitness function for the GA Class. For the base case, it is the utility function.

Input:

• i: the index of the node in the utility array.

Output:

• grad: the gradient of the ith node

• i: the index of the node in the utility array.

```
def _partial_grad(self, i):
    """Calculate the ith element of the gradient vector."""
    m_copy = self.m.copy()
    m_copy[i] = m_copy[i] - self.delta if (m_copy[i] - self.delta)>=0 else 0
    minus_utility = self.u.utility(m_copy)
    m_copy[i] += 2*self.delta
    plus_utility = self.u.utility(m_copy)
    grad = (plus_utility-minus_utility) / (2*self.delta) # the math is trivereturn grad, i
```

numerical_gradient: calculate utility gradient for each node. Returns an array containing partial gradient on each node. **Inputs**:

- m: (ndarray) mitigation level on each node
- delta: (float) Δ in equation (2)

Outputs:

• grad : (ndarray) gradient vector for function U(m) def numerical_gradient(self, m, delta=1e-08, fixed_indicies=None): """Calculate utility gradient numerically. **Parameters** m : ndarray or list array of mitigation delta: float, optional change in mitigation fixed_indicies : ndarray or list, optional indicies of gradient that should not be calculated Returns _____ ndarrayqradientself.delta = delta self.m = mif fixed indicies is None:

fixed_indicies = []

if not isinstance(m, np.ndarray):
 self.m = np.array(m)

grad = np.zeros(len(m))

_accelerate_scale: An empirical accelerate function which does the following modification:

- 1. if the search direction remains the same, accelerate the search by 1.1 times the original search speed A.K.A. the learning rate. (equation (4) below)
- 2. otherwise, reset the search speed.

The accelerate ratio 1.1 is purely empirical and can be modified in the latter research. **Inputs**:

- accelerator: (float) accelerator ratio now.
- prev_grad: (ndarray) gradient on the last step
- grad: (ndarray) gradient vector now.

Outputs:

• accelerator: (float) accelerator now.

```
def _accelerate_scale(self, accelerator, prev_grad, grad):
    sign_vector = np.sign(prev_grad * grad)
    scale_vector = np.ones(self.var_nums) * ( 1 + 0.10)
    accelerator[sign_vector <= 0] = 1
    accelerator *= scale_vector
    return accelerator</pre>
```

gradient_descent: main body of the gradient search algorithm (Adam). In addition to storing an exponentially decaying average of past squared gradients v_t like Adadelta and RMSprop, Adam also keeps an exponentially decaying average of past gradients m_t , similar to momentum:

$$m_t = \beta_1 m_{t-1} + (1 - \beta_1) g_t$$

$$v_t = \beta_2 v_{t-1} + (1 - \beta_2) g_t^2$$

 m_t and v_t are estimates of the first moment (the mean) and the second moment (the uncentered variance) of the gradients respectively, hence the name of the method. As m_t and v_t are initialized as vectors of 0's, the authors of Adam observe that they are biased towards zero, especially during the initial time steps, and especially when the decay rates are small (i.e. β_1 and β_2 are close to 1, can be modified for latter research).

We counteract these biases by computing bias-corrected first and second moment estimates:

$$\hat{m}_t = \frac{m_t}{1 - \beta_1^t}$$

$$\hat{v}_t = \frac{v_t}{1 - \beta_2^t}$$

We then use these to update the parameters just as we have seen in Adadelta and RMSprop, which yields the Adam update rule:

$$\theta_{t+1} = \theta_t - \frac{\eta}{\sqrt{\hat{v}_t} + \epsilon} \hat{m}_t \tag{3}$$

In this case, we also add a acceleration coefficient which is define by above function to accelerate the searching process:

$$\theta_{t+1} = \theta_t - \frac{\eta}{\sqrt{\hat{v_t}} + \epsilon} \hat{m_t} \times \text{accelerator}$$
 (4)

Finally, we get the item in the search results with the highest utility.

gradient_descent: the function that search the best mitigation based on GS algorithm.

Inputs:

- initial_point: (ndarray) the start point of GS algorithm. In our case, it is the mitigation level on each node (63 nodes) given by GA algorithm
- return_last: (boolean) if True the function returns the last point, else the point with highest utility

Outputs:

- best mitigation level on each node
- consequently utility on period 0

def gradient_descent(self, initial_point, return_last=False):

"""Gradient descent algorithm. The `initial_point` is updated using the Adam algorithm. Adam uses the history of the gradient to compute indivistep sizes for each element in the mitigation vector. The vector of st sizes are calculated using estimates of the first and second moments of the gradient.

```
Parameters
```

initial_point : ndarray

initial guess of the mitigation

return_last : bool, optional

if True the function returns the last point, else the point with highest utility

```
Returns
_____
tuple
        (best point, best utility)
HHHH
num_decision_nodes = initial_point.shape[0]
x_hist = np.zeros((self.iterations+1, num_decision_nodes))
u_hist = np.zeros(self.iterations+1)
u_hist[0] = self.u.utility(initial_point)
x_hist[0] = initial_point
beta1, beta2 = 0.90, 0.90
eta = 0.0015 # learning rate
eps = 1e-3
m_t, v_t = 0, 0
prev_grad = 0.0
accelerator = np.ones(self.var_nums)
# formula at http://sebastianruder.com/optimizing-gradient-descent/ind
for i in range(self.iterations):
        grad = self.numerical_gradient(x_hist[i], fixed_indicies=self.fi
        m_t = beta1*m_t + (1-beta1)*grad
        v_t = beta2*v_t + (1-beta2)*np.power(grad, 2)
        m_hat = m_t / (1-beta1**(i+1))
        v_{hat} = v_t / (1-beta2**(i+1))
        if i != 0:
                accelerator = self._accelerate_scale(accelerator, prev_g
        new_x = x_hist[i] + ((eta*m_hat)/(np.square(v_hat)+eps)) * accel
        new_x[new_x < 0] = 0.0
        if self.fixed_values is not None:
                new_x[self.fixed_indicies] = self.fixed_values
        x_{hist}[i+1] = new_x
        u_hist[i+1] = self.u.utility(new_x)[0]
        prev_grad = grad.copy()
        if self.print_progress:
                print("-- Iteration {} -- \n Current Utility: {}".format
                print(new_x)
if return_last:
        return x_hist[i+1], u_hist[i+1]
```

```
best_index = np.argmax(u_hist)
return x_hist[best_index], u_hist[best_index]
```

run: run the GS on the init point (provided by GA) and get the optimized result. Returns the best mitigation level on each point and the utility on period 0.

```
def run(self, initial_point_list, topk=4):
        """Initiate the gradient search algorithm.
       Parameters
        initial\_point\_list : list
                list of initial points to select from
        topk: int, optional
               select and run gradient descent on the `topk` first points of
                `initial_point_list`
        Returns
        tuple
               best mitigation point and the utility of the best mitigation p
        Raises
        ValueError
               If `topk` is larger than the length of `initial_point_list`.
       Note
        Uses the :mod: `~multiprocessing` package.
        n n n
       print("-----")
       if topk > len(initial_point_list):
               raise ValueError("topk {} > number of initial points {}".format(
       candidate_points = initial_point_list[:topk]
       mitigations = []
       utilities = np.zeros(topk)
       for cp, count in zip(candidate_points, range(topk)):
               if not isinstance(cp, np.ndarray):
                       cp = np.array(cp)
               print("Starting process {} of Gradient Descent".format(count+1))
               m, u = self.gradient_descent(cp)
               mitigations.append(m)
```

```
utilities[count] = u
best_index = np.argmax(utilities)
return mitigations[best_index], utilities[best_index]
```

4 Coordinate Descent

Coordinate descent optimization algorithm for the EZ-Climate model.

4.1 Theory

Coordinate descent is based on the idea that the minimization of a multivariate function F(x) can be achieved by minimizing it along one direction at a time, i.e., solving univariate (or at least much simpler) optimization problems in a loop. In the simplest case of cyclic coordinate descent, one cyclically iterates through the directions, one at a time, minimizing the objective function with respect to each coordinate direction at a time. In the code, learning rate η is set to 0.0015 and $\beta 1 = 0.9$, $\beta 2 = 0.9$

4.2 Coordinate Descent

class CoordinateDescent(object):

utility: `Utility` object

var_nums : int

object of utility class

The function is runing **fmin** from scipy package for every single node at a time and cyclically iterates through the nodes.

```
"""Coordinate descent optimization algorithm for the EZ-Climate model.

Parameters
-----
utility: `Utility` object
object of utility class
var_nums: int
number of elements in array to optimize
accuracy: float
stop value for the utility increase
iterations: int
maximum number of iterations

Attributes
-------
```

number of elements in array to optimize

```
accuracy : float
        stop value for the utility increase
iterations: int
        maximum number of iterations
HHHH
def __init__(self, utility, var_nums, accuracy=1e-4, iterations=100):
       self.u = utility
       self.var_nums = var_nums
       self.accuracy = accuracy
       self.iterations = iterations
def _min_func(self, x, m, i):
       m_{copy} = m.copy()
       m_{copy}[i] = x
       return -self.u.utility(m_copy)[0]
def _minimize_node(self, node, m):
       from scipy.optimize import fmin
       return fmin(self._min_func, x0=m[node], args=(m, node), disp=False)
def run(self, m):
       """Run the coordinate descent iterations.
       Parameters
        -----
        m : initial point
       Returns
        _____
        tuple
               best mitigation point and the utility of the best mitigation p
       Note
        Uses the :mod: `~scipy` package.
       num_decision_nodes = m.shape[0]
       x_hist = []
       u_hist = []
       nodes = range(self.var_nums)
       x_hist.append(m.copy())
       u_hist.append(self.u.utility(m)[0])
       print("-----")
```