fitr

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Chapter 1

Overview & Foundations

Chapter 2

Tutorials

Getting Started

Installation

```
pip install git+https://github.com/abrahamnunes/fitr.git
```

Simulating and Fitting a Two-Armed Bandit

```
import numpy as np
import matplotlib.pyplot as plt
from fitr import generate behavioural data
from fitr.environments import TwoArmedBandit
from fitr.agents import RWSoftmaxAgent
from fitr.inference import mlepar
from fitr.utils import sigmoid
from fitr.utils import relu
from fitr.criticism.plotting import actual_estimate
N = 50 # number of subjects
T = 200 \# number of trials
# Generate synthetic data
data = generate_behavioural_data(TwoArmedBandit, RWSoftmaxAgent, N, T)
# Create log-likelihood function
def log_prob(w, D):
    lr = sigmoid(w[0], a_min=-6, a_max=6)
    ist = relu(w[1], a_max=10)
    agent = RWSoftmaxAgent(TwoArmedBandit(), lr, ist)
    L = 0
    for t in range(D.shape[0]):
        x=D[t,:3]; u=D[t,3:5]; r=D[t,5]; x_=D[t,6:]
```

Simulating and Fitting Data from a Random Contextual Bandit Task

```
import numpy as np
import matplotlib.pyplot as plt
from fitr import generate_behavioural_data
from fitr.agents import RWSoftmaxAgent
from fitr.environments import RandomContextualBandit
from fitr.criticism.plotting import actual_estimate
from fitr.inference import mlepar
from fitr.utils import sigmoid, relu
class MyBanditTask(RandomContextualBandit):
    def ___init___(self):
        super(). init (nactions=4,
                         noutcomes=3,
                         nstates=4,
                         min_actions_per_context=None,
                         alpha=0.1,
                         alpha_start=1.,
                         shift_flip='shift',
                         reward_lb=-1,
                         reward_ub=1,
                         reward_drift='on',
                         drift_mu=np.zeros(3),
                         drift sd=1.
data = generate behavioural data(MyBanditTask, RWSoftmaxAgent, 20, 200)
def log prob(w, D):
    agent = RWSoftmaxAgent(task=MyBanditTask(),
                           learning_rate=w[0],
                           inverse_softmax_temp=w[1])
    L=0
    for t in range(D.shape[0]):
        x=D[t,:7]; u=D[t,7:11]; r=D[t,11]; x_=D[t,12:]
```

Part I

API

Chapter 3

Environments

fitr.environments

Functions to synthesize data from behavioural tasks.

Graph

fitr.environments.graph.Graph()

Base object that defines a reinforcement learning task.

Definitions

- $\mathbf{x} \in \mathcal{X}$ be a one-hot state vector, where $|\mathcal{X}| = n_x$
- $\mathbf{u} \in \mathcal{U}$ be a one-hot action vector, where $|\mathcal{U}| = n_u$
- $T = p(\mathbf{x}_{t+1}|\mathbf{x}_t, \mathbf{u}_t)$ be a transition tensor
- $p(\mathbf{x})$ be a distribution over starting states
- $\mathcal{J}: \mathcal{X} \to \mathcal{R}$, where $\mathcal{R} \subseteq \mathbb{R}$ be a reward function

Arguments:

- T: Transition tensor
- R: Vector of rewards for each state such that scalar reward $r_t = \mathbf{r}^o p \mathbf{x}$
- end_states: A vector $\{0,1\}^{n_x}$ identifying which states terminate a trial (aka episode)
- **p_start**: Initial state distribution
- label: A string identifying a name for the task
- state_labels: A list or array of strings labeling the different states (for plotting purposes)
- action_labels: A list or array of strings labeling the different actions (for plotting purposes)
- rng: np.random.RandomState object
- **f_reward**: A function whose first argument is a vector of rewards for each state, and whose second argument is a state vector, and whose output is a scalar reward
- cmap: Matplotlib colormap for plotting.

Notes

There are two critical methods for the Graph class: observation() and step. All instances of a Graph must be able to call these functions. Let's say you have some bandit task MyBanditTask that inherits from Graph. To run such a task would look something like this:

```
env = MyBanditTask()  # Instantiate your environment object
agent = MyAgent()  # Some agent object (arbitrary, really)
for t in range(ntrials):
    x = env.observation()  # Samples initial state
    u = agent.action(x)  # Choose some action
    x_, r, done = agent.step(u) # Transition based on action
```

What differentiates tasks are the transition tensor T, starting state distribution $p(\mathbf{x})$ and reward function \mathcal{J} (which here would include the reward vector \mathbf{r}).

Graph.adjacency_matrix_decomposition

```
fitr.environments.graph.adjacency_matrix_decomposition(self)
```

Singular value decomposition of the graph adjacency matrix

Graph.get_graph_depth

```
fitr.environments.graph.get_graph_depth(self)
```

Returns the depth of the task graph.

Calculated as the depth from START (pre-initial state) to END (which absorbs trial from all terminal states), minus 2 to account for the START->node & node->END transitions.

Returns:

An int identifying the depth of the current graph for a single trial of the task

Graph.laplacian_matrix_decomposition

```
fitr.environments.graph.laplacian_matrix_decomposition(self)
```

Singular value decomposition of the graph Laplacian

Graph.make_action_labels

```
fitr.environments.graph.make_action_labels(self)
```

Creates labels for the actions (for plotting) if none provided

Graph.make_digraph

fitr.environments.graph.make_digraph(self)

Creates a networkx DiGraph object from the transition tensor for the purpose of plotting and some other analyses.

Graph.make_state_labels

```
fitr.environments.graph.make_state_labels(self)
```

Creates labels for the states (for plotting) if none provided

Graph.make_undirected_graph

fitr.environments.graph.make_undirected_graph(self)

Converts the DiGraph to undirected and computes some stats

Graph.observation

fitr.environments.graph.observation(self)

Samples an initial state from the start-state distribution $p(\mathbf{x})$

$$\mathbf{x}_0 \sim p(\mathbf{x})$$

Returns:

A one-hot vector ndarray ((nstates,)) indicating the starting state.

Examples:

x = env.observation()

Graph.plot action outcome probabilities

fitr.environments.graph.plot_action_outcome_probabilities(self, figsize=None, outfil

Plots the probabilities of different outcomes given actions.

Each plot is a heatmap for a starting state showing the transition probabilities for each action-outcome pair within that state.

Graph.plot_graph

fitr.environments.graph.plot_graph(self, figsize=None, node_size=2000, arrowsize=20,
Plots the directed graph of the task

Graph.plot_spectral_properties

fitr.environments.graph.plot_spectral_properties(self, figsize=None, outfile=None, out

Graph.random_action

fitr.environments.graph.random_action(self)

Samples a random one-hot action vector uniformly over the action space.

Useful for testing that your environment works, without having to create an agent.

$$\mathbf{u} \sim \text{Multinomial}\left(1, \mathbf{p} = \{p_i = \frac{1}{|\mathcal{U}|}\}_{i=1}^{|\mathcal{U}|}\right)$$

Returns:

A one-hot action vector of type ndarray ((nactions,))

Examples:

u = env.random_action()

Graph.set_seed

```
fitr.environments.graph.set_seed(self, seed=None)
```

Allows user to specify a seed for the pseudorandom number generator.

Arguments:

• **seed**: int. Seed value. Default is None, which results in a default random state object. If user enters a non-integer value, the default random state object will still be used and no error will be thrown!

Graph.step

```
fitr.environments.graph.step(self, action)
```

Executes a state transition in the environment.

Arguments:

action: A one-hot vector of type ndarray ((naction,)) indicating the action selected at the current state.

Returns:

A 3-tuple representing the next state (ndarray ((noutcomes,))), scalar reward, and whether the current step terminates a trial (bool).

Raises:

RuntimeError if env.observation() not called after a previous env.step(...) call yielded a terminal state.

TwoArmedBandit

```
fitr.environments.twoarmedbandit.TwoArmedBandit()
```

A simple 2-armed bandit task

TwoArmedBandit.adjacency_matrix_decomposition

```
fitr.environments.graph.adjacency_matrix_decomposition(self)
```

Singular value decomposition of the graph adjacency matrix

TwoArmedBandit.get_graph_depth

fitr.environments.graph.get_graph_depth(self)

Returns the depth of the task graph.

Calculated as the depth from START (pre-initial state) to END (which absorbs trial from all terminal states), minus 2 to account for the START->node & node->END transitions.

Returns:

An int identifying the depth of the current graph for a single trial of the task

TwoArmedBandit.laplacian_matrix_decomposition

fitr.environments.graph.laplacian_matrix_decomposition(self)

Singular value decomposition of the graph Laplacian

TwoArmedBandit.make_action_labels

fitr.environments.graph.make_action_labels(self)

Creates labels for the actions (for plotting) if none provided

TwoArmedBandit.make_digraph

fitr.environments.graph.make_digraph(self)

Creates a networkx DiGraph object from the transition tensor for the purpose of plotting and some other analyses.

TwoArmedBandit.make state labels

fitr.environments.graph.make_state_labels(self)

Creates labels for the states (for plotting) if none provided

TwoArmedBandit.make_undirected_graph

fitr.environments.graph.make_undirected_graph(self)

Converts the DiGraph to undirected and computes some stats

TwoArmedBandit.observation

fitr.environments.graph.observation(self)

Samples an initial state from the start-state distribution $p(\mathbf{x})$

 $\mathbf{x}_0 \sim p(\mathbf{x})$

Returns:

A one-hot vector ndarray ((nstates,)) indicating the starting state.

Examples:

x = env.observation()

TwoArmedBandit.plot action outcome probabilities

fitr.environments.graph.plot_action_outcome_probabilities(self, figsize=None, outfil

Plots the probabilities of different outcomes given actions.

Each plot is a heatmap for a starting state showing the transition probabilities for each action-outcome pair within that state.

TwoArmedBandit.plot_graph

fitr.environments.graph.plot_graph(self, figsize=None, node_size=2000, arrowsize=20, Plots the directed graph of the task

TwoArmedBandit.plot_spectral_properties

fitr.environments.graph.plot_spectral_properties(self, figsize=None, outfile=None, out

TwoArmedBandit.random_action

fitr.environments.graph.random_action(self)

Samples a random one-hot action vector uniformly over the action space.

Useful for testing that your environment works, without having to create an agent.

$$\mathbf{u} \sim \text{Multinomial}\left(1, \mathbf{p} = \left\{p_i = \frac{1}{|\mathcal{U}|}\right\}_{i=1}^{|\mathcal{U}|}\right)$$

Returns:

A one-hot action vector of type ndarray ((nactions,))

Examples:

u = env.random_action()

TwoArmedBandit.set_seed

fitr.environments.graph.set_seed(self, seed=None)

Allows user to specify a seed for the pseudorandom number generator.

Arguments:

• seed: int. Seed value. Default is None, which results in a default random state object. If user enters a non-integer value, the default random state object will still be used and no error will be thrown!

TwoArmedBandit.step

fitr.environments.graph.step(self, action)

Executes a state transition in the environment.

Arguments:

action: A one-hot vector of type ndarray ((naction,)) indicating the action selected at the current state.

Returns:

A 3-tuple representing the next state (ndarray ((noutcomes,))), scalar reward, and whether the current step terminates a trial (bool).

Raises:

RuntimeError if env.observation() not called after a previous env.step(...) call yielded a terminal state.

OrthogonalGoNoGo



OrthogonalGoNoGo.adjacency_matrix_decomposition

fitr.environments.graph.adjacency_matrix_decomposition(self)

Singular value decomposition of the graph adjacency matrix

OrthogonalGoNoGo.get_graph_depth

fitr.environments.graph.get_graph_depth(self)

Returns the depth of the task graph.

Calculated as the depth from START (pre-initial state) to END (which absorbs trial from all terminal states), minus 2 to account for the START->node & node->END transitions.

Returns:

An int identifying the depth of the current graph for a single trial of the task

OrthogonalGoNoGo.laplacian_matrix_decomposition

fitr.environments.graph.laplacian_matrix_decomposition(self)

Singular value decomposition of the graph Laplacian

$Orthogonal GoNoGo.make_action_labels$

fitr.environments.graph.make_action_labels(self)

Creates labels for the actions (for plotting) if none provided

OrthogonalGoNoGo.make_digraph

fitr.environments.graph.make_digraph(self)

Creates a networkx DiGraph object from the transition tensor for the purpose of plotting and some other analyses.

OrthogonalGoNoGo.make state labels

fitr.environments.graph.make_state_labels(self)

Creates labels for the states (for plotting) if none provided

OrthogonalGoNoGo.make_undirected_graph

fitr.environments.graph.make_undirected_graph(self)

Converts the DiGraph to undirected and computes some stats

OrthogonalGoNoGo.observation

fitr.environments.graph.observation(self)

Samples an initial state from the start-state distribution $p(\mathbf{x})$

$$\mathbf{x}_0 \sim p(\mathbf{x})$$

Returns:

A one-hot vector ndarray ((nstates,)) indicating the starting state.

Examples:

```
x = env.observation()
```

$Orthogonal GoNoGo.plot_action_outcome_probabilities$

fitr.environments.graph.plot_action_outcome_probabilities(self, figsize=None, outfil

Plots the probabilities of different outcomes given actions.

Each plot is a heatmap for a starting state showing the transition probabilities for each action-outcome pair within that state.

OrthogonalGoNoGo.plot_graph

fitr.environments.graph.plot_graph(self, figsize=None, node_size=2000, arrowsize=20,
Plots the directed graph of the task

OrthogonalGoNoGo.plot_spectral_properties

fitr.environments.graph.plot_spectral_properties(self, figsize=None, outfile=None, out

$Orthogonal GoNoGo.random_action$

fitr.environments.graph.random_action(self)

Samples a random one-hot action vector uniformly over the action space.

Useful for testing that your environment works, without having to create an agent.

$$\mathbf{u} \sim \text{Multinomial}\left(1, \mathbf{p} = \left\{p_i = \frac{1}{|\mathcal{U}|}\right\}_{i=1}^{|\mathcal{U}|}\right)$$

Returns:

A one-hot action vector of type ndarray ((nactions,))

Examples:

u = env.random_action()

OrthogonalGoNoGo.set_seed

fitr.environments.graph.set_seed(self, seed=None)

Allows user to specify a seed for the pseudorandom number generator.

Arguments:

• seed: int. Seed value. Default is None, which results in a default random state object. If user enters a non-integer value, the default random state object will still be used and no error will be thrown!

OrthogonalGoNoGo.step

fitr.environments.graph.step(self, action)

Executes a state transition in the environment.

Arguments:

action: A one-hot vector of type ndarray ((naction,)) indicating the action selected at the current state.

Returns:

A 3-tuple representing the next state (ndarray ((noutcomes,))), scalar reward, and whether the current step terminates a trial (bool).

Raises:

RuntimeError if env.observation() not called after a previous env.step(...) call yielded a terminal state.

DawTwoStep

fitr.environments.dawtwostep.DawTwoStep()

An implementation of the Two-Step Task from Daw et al. (2011).

Arguments:

- mu: float identifying the drift of the reward-determining Gaussian random walks
- sd: float identifying the standard deviation of the reward-determining Gaussian random walks

DawTwoStep.adjacency_matrix_decomposition

```
fitr.environments.graph.adjacency_matrix_decomposition(self)
```

Singular value decomposition of the graph adjacency matrix

$DawTwoStep.f_reward$

```
fitr.environments.dawtwostep.f_reward(self, R, x)
```

DawTwoStep.get_graph_depth

```
fitr.environments.graph.get_graph_depth(self)
```

Returns the depth of the task graph.

Calculated as the depth from START (pre-initial state) to END (which absorbs trial from all terminal states), minus 2 to account for the START->node & node->END transitions.

Returns:

An int identifying the depth of the current graph for a single trial of the task

DawTwoStep.laplacian_matrix_decomposition

```
fitr.environments.graph.laplacian_matrix_decomposition(self)
```

Singular value decomposition of the graph Laplacian

$DawTwoStep.make_action_labels$

```
fitr.environments.graph.make_action_labels(self)
```

Creates labels for the actions (for plotting) if none provided

DawTwoStep.make_digraph

```
fitr.environments.graph.make_digraph(self)
```

Creates a networkx DiGraph object from the transition tensor for the purpose of plotting and some other analyses.

DawTwoStep.make_state_labels

```
fitr.environments.graph.make_state_labels(self)
```

Creates labels for the states (for plotting) if none provided

DawTwoStep.make_undirected_graph

fitr.environments.graph.make_undirected_graph(self)

Converts the DiGraph to undirected and computes some stats

DawTwoStep.observation

fitr.environments.graph.observation(self)

Samples an initial state from the start-state distribution $p(\mathbf{x})$

$$\mathbf{x}_0 \sim p(\mathbf{x})$$

Returns:

A one-hot vector ndarray ((nstates,)) indicating the starting state.

Examples:

x = env.observation()

DawTwoStep.plot_action_outcome_probabilities

fitr.environments.graph.plot_action_outcome_probabilities(self, figsize=None, outfil

Plots the probabilities of different outcomes given actions.

Each plot is a heatmap for a starting state showing the transition probabilities for each action-outcome pair within that state.

DawTwoStep.plot_graph

fitr.environments.graph.plot_graph(self, figsize=None, node_size=2000, arrowsize=20,
Plots the directed graph of the task

DawTwoStep.plot_reward_paths

fitr.environments.dawtwostep.plot_reward_paths(self, outfile=None, outfiletype='pdf'

DawTwoStep.plot_spectral_properties

fitr.environments.graph.plot_spectral_properties(self, figsize=None, outfile=None, out

DawTwoStep.random_action

fitr.environments.graph.random_action(self)

Samples a random one-hot action vector uniformly over the action space.

Useful for testing that your environment works, without having to create an agent.

$$\mathbf{u} \sim \text{Multinomial}\left(1, \mathbf{p} = \left\{p_i = \frac{1}{|\mathcal{U}|}\right\}_{i=1}^{|\mathcal{U}|}\right)$$

Returns:

A one-hot action vector of type ndarray ((nactions,))

Examples:

u = env.random_action()

DawTwoStep.set_seed

fitr.environments.graph.set seed(self, seed=None)

Allows user to specify a seed for the pseudorandom number generator.

Arguments:

• seed: int. Seed value. Default is None, which results in a default random state object. If user enters a non-integer value, the default random state object will still be used and no error will be thrown!

DawTwoStep.step

fitr.environments.graph.step(self, action)

Executes a state transition in the environment.

Arguments:

action: A one-hot vector of type ndarray ((naction,)) indicating the action selected at the current state.

Returns:

A 3-tuple representing the next state (ndarray ((noutcomes,))), scalar reward, and whether the current step terminates a trial (bool).

Raises:

RuntimeError if env.observation() not called after a previous env.step(...) call yielded a terminal state.

KoolTwoStep

fitr.environments.kooltwostep.KoolTwoStep() From Kool & Gershman 2016. KoolTwoStep.adjacency_matrix_decomposition fitr.environments.graph.adjacency_matrix_decomposition(self) Singular value decomposition of the graph adjacency matrix KoolTwoStep.f reward fitr.environments.kooltwostep.f_reward(self, R, x) KoolTwoStep.get_graph_depth fitr.environments.graph.get_graph_depth(self) Returns the depth of the task graph. Calculated as the depth from START (pre-initial state) to END (which absorbs trial from all terminal states), minus 2 to account for the START->node & node->END transitions. Returns: An int identifying the depth of the current graph for a single trial of the task KoolTwoStep.laplacian_matrix_decomposition fitr.environments.graph.laplacian_matrix_decomposition(self) Singular value decomposition of the graph Laplacian KoolTwoStep.make_action_labels fitr.environments.graph.make_action_labels(self)

Creates labels for the actions (for plotting) if none provided

KoolTwoStep.make_digraph

fitr.environments.graph.make_digraph(self)

Creates a networkx DiGraph object from the transition tensor for the purpose of plotting and some other analyses.

KoolTwoStep.make_state_labels

fitr.environments.graph.make_state_labels(self)

Creates labels for the states (for plotting) if none provided

KoolTwoStep.make_undirected_graph

fitr.environments.graph.make_undirected_graph(self)

Converts the DiGraph to undirected and computes some stats

KoolTwoStep.observation

fitr.environments.graph.observation(self)

Samples an initial state from the start-state distribution $p(\mathbf{x})$

$$\mathbf{x}_0 \sim p(\mathbf{x})$$

Returns:

A one-hot vector ndarray ((nstates,)) indicating the starting state.

Examples:

```
x = env.observation()
```

KoolTwoStep.plot_action_outcome_probabilities

fitr.environments.graph.plot_action_outcome_probabilities(self, figsize=None, outfil

Plots the probabilities of different outcomes given actions.

Each plot is a heatmap for a starting state showing the transition probabilities for each action-outcome pair within that state.

KoolTwoStep.plot_graph

fitr.environments.graph.plot_graph(self, figsize=None, node_size=2000, arrowsize=20,
Plots the directed graph of the task

KoolTwoStep.plot_spectral_properties

fitr.environments.graph.plot_spectral_properties(self, figsize=None, outfile=None, out

KoolTwoStep.random_action

fitr.environments.graph.random_action(self)

Samples a random one-hot action vector uniformly over the action space.

Useful for testing that your environment works, without having to create an agent.

$$\mathbf{u} \sim \text{Multinomial}\left(1, \mathbf{p} = \left\{p_i = \frac{1}{|\mathcal{U}|}\right\}_{i=1}^{|\mathcal{U}|}\right)$$

Returns:

A one-hot action vector of type ndarray ((nactions,))

Examples:

u = env.random_action()

KoolTwoStep.set_seed

fitr.environments.graph.set_seed(self, seed=None)

Allows user to specify a seed for the pseudorandom number generator.

Arguments:

• seed: int. Seed value. Default is None, which results in a default random state object. If user enters a non-integer value, the default random state object will still be used and no error will be thrown!

KoolTwoStep.step

fitr.environments.graph.step(self, action)

Executes a state transition in the environment.

Arguments:

action: A one-hot vector of type ndarray ((naction,)) indicating the action selected at the current state.

Returns:

A 3-tuple representing the next state (ndarray ((noutcomes,))), scalar reward, and whether the current step terminates a trial (bool).

Raises:

RuntimeError if env.observation() not called after a previous env.step(...) call yielded a terminal state.

MouthTask

fitr.environments.mouthtask.MouthTask()

The Pizzagalli reward sensitivity signal-detection task

MouthTask.adjacency matrix decomposition

fitr.environments.graph.adjacency_matrix_decomposition(self)

Singular value decomposition of the graph adjacency matrix

MouthTask.get_graph_depth

fitr.environments.graph.get_graph_depth(self)

Returns the depth of the task graph.

Calculated as the depth from START (pre-initial state) to END (which absorbs trial from all terminal states), minus 2 to account for the START->node & node->END transitions.

Returns:

An int identifying the depth of the current graph for a single trial of the task

MouthTask.laplacian_matrix_decomposition

fitr.environments.graph.laplacian_matrix_decomposition(self)

Singular value decomposition of the graph Laplacian

MouthTask.make_action_labels

fitr.environments.graph.make_action_labels(self)

Creates labels for the actions (for plotting) if none provided

MouthTask.make_digraph

fitr.environments.graph.make_digraph(self)

Creates a networkx DiGraph object from the transition tensor for the purpose of plotting and some other analyses.

MouthTask.make_state_labels

fitr.environments.graph.make_state_labels(self)

Creates labels for the states (for plotting) if none provided

MouthTask.make_undirected_graph

fitr.environments.graph.make_undirected_graph(self)

Converts the DiGraph to undirected and computes some stats

MouthTask.observation

fitr.environments.graph.observation(self)

Samples an initial state from the start-state distribution $p(\mathbf{x})$

 $\mathbf{x}_0 \sim p(\mathbf{x})$

Returns:

A one-hot vector ndarray ((nstates,)) indicating the starting state.

Examples:

```
x = env.observation()
```

$MouthTask.plot_action_outcome_probabilities$

fitr.environments.graph.plot_action_outcome_probabilities(self, figsize=None, outfil

Plots the probabilities of different outcomes given actions.

Each plot is a heatmap for a starting state showing the transition probabilities for each action-outcome pair within that state.

MouthTask.plot_graph

```
fitr.environments.graph.plot_graph(self, figsize=None, node_size=2000, arrowsize=20, Plots the directed graph of the task
```

MouthTask.plot_spectral_properties

```
fitr.environments.graph.plot_spectral_properties(self, figsize=None, outfile=None, out
```

MouthTask.random_action

```
fitr.environments.graph.random_action(self)
```

Samples a random one-hot action vector uniformly over the action space.

Useful for testing that your environment works, without having to create an agent.

$$\mathbf{u} \sim \text{Multinomial}\left(1, \mathbf{p} = \left\{p_i = \frac{1}{|\mathcal{U}|}\right\}_{i=1}^{|\mathcal{U}|}\right)$$

Returns:

A one-hot action vector of type ndarray ((nactions,))

Examples:

```
u = env.random_action()
```

MouthTask.set seed

```
fitr.environments.graph.set_seed(self, seed=None)
```

Allows user to specify a seed for the pseudorandom number generator.

Arguments:

• seed: int. Seed value. Default is None, which results in a default random state object. If user enters a non-integer value, the default random state object will still be used and no error will be thrown!

MouthTask.step

```
fitr.environments.graph.step(self, action)
```

Executes a state transition in the environment.

Arguments:

action: A one-hot vector of type ndarray ((naction,)) indicating the action selected at the current state.

Returns:

A 3-tuple representing the next state (ndarray ((noutcomes,))), scalar reward, and whether the current step terminates a trial (bool).

Raises:

RuntimeError if env.observation() not called after a previous env.step(...) call yielded a terminal state.

IGT

```
fitr.environments.igt.IGT()
Iowa Gambling Task
```

IGT.adjacency_matrix_decomposition

```
fitr.environments.graph.adjacency_matrix_decomposition(self)
```

Singular value decomposition of the graph adjacency matrix

IGT.get_graph_depth

fitr.environments.graph.get_graph_depth(self)

Returns the depth of the task graph.

Calculated as the depth from START (pre-initial state) to END (which absorbs trial from all terminal states), minus 2 to account for the START->node & node->END transitions.

Returns:

An int identifying the depth of the current graph for a single trial of the task

IGT.laplacian_matrix_decomposition

fitr.environments.graph.laplacian_matrix_decomposition(self)

Singular value decomposition of the graph Laplacian

IGT.make_action_labels

fitr.environments.graph.make_action_labels(self)

Creates labels for the actions (for plotting) if none provided

IGT.make_digraph

fitr.environments.graph.make_digraph(self)

Creates a networkx DiGraph object from the transition tensor for the purpose of plotting and some other analyses.

IGT.make state labels

fitr.environments.graph.make_state_labels(self)

Creates labels for the states (for plotting) if none provided

IGT.make_undirected_graph

fitr.environments.graph.make_undirected_graph(self)

Converts the DiGraph to undirected and computes some stats

IGT.observation

fitr.environments.graph.observation(self)

Samples an initial state from the start-state distribution $p(\mathbf{x})$

 $\mathbf{x}_0 \sim p(\mathbf{x})$

Returns:

A one-hot vector ndarray ((nstates,)) indicating the starting state.

Examples:

x = env.observation()

IGT.plot action outcome probabilities

fitr.environments.graph.plot_action_outcome_probabilities(self, figsize=None, outfil

Plots the probabilities of different outcomes given actions.

Each plot is a heatmap for a starting state showing the transition probabilities for each action-outcome pair within that state.

IGT.plot_graph

fitr.environments.graph.plot_graph(self, figsize=None, node_size=2000, arrowsize=20, Plots the directed graph of the task

IGT.plot_spectral_properties

fitr.environments.graph.plot_spectral_properties(self, figsize=None, outfile=None, o

Creates a set of subplots depicting the graph Laplacian and its spectral decomposition.

IGT.random action

fitr.environments.graph.random_action(self)

Samples a random one-hot action vector uniformly over the action space.

Useful for testing that your environment works, without having to create an agent.

$$\mathbf{u} \sim \text{Multinomial}\left(1, \mathbf{p} = \left\{p_i = \frac{1}{|\mathcal{U}|}\right\}_{i=1}^{|\mathcal{U}|}\right)$$

Returns:

A one-hot action vector of type ndarray ((nactions,))

Examples:

u = env.random_action()

IGT.set_seed

fitr.environments.graph.set_seed(self, seed=None)

Allows user to specify a seed for the pseudorandom number generator.

Arguments:

• seed: int. Seed value. Default is None, which results in a default random state object. If user enters a non-integer value, the default random state object will still be used and no error will be thrown!

IGT.step

fitr.environments.graph.step(self, action)

Executes a state transition in the environment.

Arguments:

action: A one-hot vector of type ndarray ((naction,)) indicating the action selected at the current state.

Returns:

A 3-tuple representing the next state (ndarray ((noutcomes,))), scalar reward, and whether the current step terminates a trial (bool).

Raises:

RuntimeError if env.observation() not called after a previous env.step(...) call yielded a terminal state.

RandomContextualBandit

fitr.environments.randombandit.RandomContextualBandit()

Generates a random bandit task

Arguments:

- nactions: Number of actions
- **noutcomes**: Number of outcomes
- **nstates**: Number of contexts
- min_actions_per_context: Different contexts may have more or fewer actions than others (never more than nactions). This variable describes the minimum number of actions allowed in a context.
- alpha:
- alpha_start:
- shift_flip:
- reward_lb: Lower bound for drifting rewards
- reward_ub: Upper bound for drifting rewards
- reward_drift: Values (on or off) determining whether rewards are allowed to drift
- drift mu: Mean of the Gaussian random walk determining reward
- **drift_sd**: Standard deviation of Gaussian random walk determining reward

$Random Contextual Bandit.adjacency_matrix_decomposition$

fitr.environments.graph.adjacency_matrix_decomposition(self)

Singular value decomposition of the graph adjacency matrix

$Random Contextual Bandit. f_reward$

fitr.environments.randombandit.f_reward(self, R, x)

RandomContextualBandit.get_graph_depth

fitr.environments.graph.get_graph_depth(self)

Returns the depth of the task graph.

Calculated as the depth from START (pre-initial state) to END (which absorbs trial from all terminal states), minus 2 to account for the START->node & node->END transitions.

Returns:

An int identifying the depth of the current graph for a single trial of the task

$Random Contextual Bandit. laplacian_matrix_decomposition$

fitr.environments.graph.laplacian_matrix_decomposition(self)
Singular value decomposition of the graph Laplacian

$Random Contextual Band it. make_action_labels$

fitr.environments.graph.make_action_labels(self)

Creates labels for the actions (for plotting) if none provided

$Random Contextual Bandit.make_digraph$

fitr.environments.graph.make_digraph(self)

Creates a networkx DiGraph object from the transition tensor for the purpose of plotting and some other analyses.

$RandomContextualBandit.make_state_labels$

fitr.environments.graph.make_state_labels(self)

Creates labels for the states (for plotting) if none provided

RandomContextualBandit.make_undirected_graph

fitr.environments.graph.make_undirected_graph(self)

Converts the DiGraph to undirected and computes some stats

RandomContextualBandit.observation

fitr.environments.graph.observation(self)

Samples an initial state from the start-state distribution $p(\mathbf{x})$

 $\mathbf{x}_0 \sim p(\mathbf{x})$

Returns:

A one-hot vector ndarray ((nstates,)) indicating the starting state.

Examples:

```
x = env.observation()
```

$Random Contextual Bandit.plot_action_outcome_probabilities$

fitr.environments.graph.plot_action_outcome_probabilities(self, figsize=None, outfil

Plots the probabilities of different outcomes given actions.

Each plot is a heatmap for a starting state showing the transition probabilities for each action-outcome pair within that state.

RandomContextualBandit.plot_graph

```
fitr.environments.graph.plot_graph(self, figsize=None, node_size=2000, arrowsize=20,
Plots the directed graph of the task
```

$Random Contextual Band it.plot_spectral_properties$

```
fitr.environments.graph.plot_spectral_properties(self, figsize=None, outfile=None, out
```

$Random Contextual Bandit.random_action$

```
fitr.environments.graph.random_action(self)
```

Samples a random one-hot action vector uniformly over the action space.

Useful for testing that your environment works, without having to create an agent.

$$\mathbf{u} \sim \text{Multinomial}\left(1, \mathbf{p} = \left\{p_i = \frac{1}{|\mathcal{U}|}\right\}_{i=1}^{|\mathcal{U}|}\right)$$

Returns:

A one-hot action vector of type ndarray ((nactions,))

Examples:

```
u = env.random_action()
```

$RandomContextualBandit.set_seed$

fitr.environments.graph.set_seed(self, seed=None)

Allows user to specify a seed for the pseudorandom number generator.

Arguments:

• seed: int. Seed value. Default is None, which results in a default random state object. If user enters a non-integer value, the default random state object will still be used and no error will be thrown!

RandomContextualBandit.step

fitr.environments.graph.step(self, action)

Executes a state transition in the environment.

Arguments:

action: A one-hot vector of type ndarray ((naction,)) indicating the action selected at the current state.

Returns:

A 3-tuple representing the next state (ndarray ((noutcomes,))), scalar reward, and whether the current step terminates a trial (bool).

Raises:

RuntimeError if env.observation() not called after a previous env.step(...) call yielded a terminal state.

Chapter 4

Agents

fitr.agents

A modular way to build and test reinforcement learning agents.

There are three main submodules:

- fitr.agents.policies: which describe a class of functions essentially representing $f: \mathcal{X} \to \mathcal{U}$
- fitr.agents.value_functions: which describe a class of functions essentially representing $\mathcal{V}:\mathcal{X}\to\mathbb{R}$ and/or $\mathcal{Q}:\mathcal{Q}\times\mathcal{U}\to\mathbb{R}$
- fitr.agents.agents: classes of agents that are combinations of policies and value functions, along with some convenience functions for generating data from fitr.environments.Graph environments.

SoftmaxPolicy

fitr.agents.policies.SoftmaxPolicy()

Action selection by sampling from a multinomial whose parameters are given by a softmax.

Action sampling is

$$\mathbf{u} \sim \text{Multinomial}(1, \mathbf{p} = \varsigma(\mathbf{v})).$$

Parameters of that distribution are

$$p(\mathbf{u}|\mathbf{v}) = \varsigma(\mathbf{v}) = \frac{e^{\beta \mathbf{v}}}{\sum_{i}^{|\mathbf{v}|} e^{\beta v_{i}}}.$$

- inverse_softmax_temp: Inverse softmax temperature β
- rng: np.random.RandomState object

SoftmaxPolicy.action_prob

```
fitr.agents.policies.action_prob(self, x)
```

Computes the softmax

SoftmaxPolicy.log_prob

```
fitr.agents.policies.log_prob(self, x)
```

Computes the log-probability of an action \mathbf{u} , in addition to computing derivatives up to second order

$$\log p(\mathbf{u}|\mathbf{v}) = \beta \mathbf{v} - \log \sum_{v_i} e^{\beta \mathbf{v}_i}$$

Arguments:

• x: State vector of type ndarray ((nstates,))

Returns:

Scalar log-probability

SoftmaxPolicy.sample

```
fitr.agents.policies.sample(self, x)
```

Samples from the action distribution

StickySoftmaxPolicy

```
fitr.agents.policies.StickySoftmaxPolicy()
```

Action selection by sampling from a multinomial whose parameters are given by a softmax, but with accounting for the tendency to perseverate (i.e. choosing the previously used action without considering its value).

Let $\mathbf{u}_{t-1} = (u_{t-1}^{(i)})_{i=1}^{|\mathcal{U}|}$ be a one hot vector representing the action taken at the last step, and β^{ρ} be an inverse softmax temperature for the influence of this last action.

Action sampling is thus:

$$\mathbf{u} \sim \text{Multinomial}(1, \mathbf{p} = \varsigma(\mathbf{v}, \mathbf{u}_{t-1})).$$

Parameters of that distribution are

$$p(\mathbf{u}|\mathbf{v},\mathbf{u}_{t-1}) = \varsigma(\mathbf{v},\mathbf{u}_{t-1}) = \frac{e^{\beta \mathbf{v} + \beta^{\rho} \mathbf{u}_{t-1}}}{\sum_{i}^{|\mathbf{v}|} e^{\beta v_{i} + \beta^{\rho} u_{t-1}^{(i)}}}.$$

Arguments:

- inverse_softmax_temp: Inverse softmax temperature β
- **perseveration**: Inverse softmax temperature β^{ρ} capturing the tendency to repeat the last action taken.
- rng: np.random.RandomState object

StickySoftmaxPolicy.action_prob

fitr.agents.policies.action_prob(self, x)

Computes the softmax

Arguments:

• x: ndarray ((nactions,)) action value vector

Returns:

ndarray ((nactions,)) vector of action probabilities

StickySoftmaxPolicy.log_prob

fitr.agents.policies.log_prob(self, x)

Computes the log-probability of an action u

$$\log p(\mathbf{u}|\mathbf{v}, \mathbf{u}_{t-1}) = (\beta \mathbf{v} + \beta^{\rho} \mathbf{u}_{t-1}) - \log \sum_{v_i} e^{\beta \mathbf{v}_i + \beta^{\rho} u_{t-1}^{(i)}}$$

Arguments:

• x: State vector of type ndarray ((nactions,))

Returns:

Scalar log-probability

StickySoftmaxPolicy.sample

fitr.agents.policies.sample(self, x)

Samples from the action distribution

• x: ndarray ((nactions,)) action value vector

Returns:

```
ndarray((nactions,)) one-hot action vector
```

EpsilonGreedyPolicy

```
fitr.agents.policies.EpsilonGreedyPolicy()
```

A policy that takes the maximally valued action with probability $1 - \epsilon$, otherwise chooses randomly self.

Arguments:

- epsilon: Probability of not taking the action with highest value
- rng: numpy.random.RandomState object

EpsilonGreedyPolicy.action_prob

```
fitr.agents.policies.action_prob(self, x)
```

Creates vector of action probabilities for e-greedy policy

Arguments:

• x: ndarray((nstates,)) one-hot state vector

Returns:

```
ndarray ((nstates,)) vector of action probabilities
```

EpsilonGreedyPolicy.sample

```
fitr.agents.policies.sample(self, x)
```

Samples from the action distribution

Arguments:

• x: ndarray ((nstates,)) one-hot state vector

Returns:

```
ndarray ((nstates,)) one-hot action vector
```

ValueFunction

fitr.agents.value_functions.ValueFunction()

A general value function object.

A value function here is task specific and consists of several attributes:

- nstates: The number of states in the task, $|\mathcal{X}|$
- nactions: Number of actions in the task, $|\mathcal{U}|$
- V: State value function $\mathbf{v} = \mathcal{V}(\mathbf{x})$
- Q: State-action value function $\mathbf{Q} = \mathcal{Q}(\mathbf{x}, \mathbf{u})$
- rpe: Reward prediction error history
- etrace: An eligibility trace (optional)
- dV: A dictionary storing gradients with respect to parameters (named keys)
- dQ: A dictionary storing gradients with respect to parameters (named keys)

Note that in general we rely on matrix-vector notation for value functions, rather than function notation. Vectors in the mathematical typesetting are by default column vectors.

Arguments:

• env: A fitr.environments.Graph

ValueFunction.Qmax

fitr.agents.value_functions.Qmax(self, x)

Return maximal action value for given state

$$\max_{u_i} \mathcal{Q}(\mathbf{x}, u_i) = \max_{\mathbf{u}'} \mathbf{u}'^{\top} \mathbf{Q} \mathbf{x}$$

Arguments:

• x: ndarray ((nstates,)) one-hot state vector

Returns:

Scalar value of the maximal action value at the given state

ValueFunction.Qmean

fitr.agents.value_functions.Qmean(self, x)

Return mean action value for given state

$$Mean(\mathcal{Q}(\mathbf{x},:)) = \frac{1}{|\mathcal{U}|} \mathbf{1}^{\top} \mathbf{Q} \mathbf{x}$$

• x: ndarray((nstates,)) one-hot state vector

Returns:

Scalar value of the maximal action value at the given state

ValueFunction.Qx

fitr.agents.value_functions.Qx(self, x)

Compute action values for a given state

$$Q(\mathbf{x},:) = \mathbf{Q}\mathbf{x}$$

Arguments:

• x: ndarray((nstates,)) one-hot state vector

Returns:

ndarray ((nactions,)) vector of values for actions in the given state

ValueFunction.Vx

fitr.agents.value_functions.Vx(self, x)

Compute value of state x

$$\mathcal{V}(\mathbf{x}) = \mathbf{v}^{\top}\mathbf{x}$$

Arguments:

• x: ndarray ((nstates,)) one-hot state vector

Returns:

Scalar value of state x

ValueFunction.grad_Qx

fitr.agents.value_functions.grad_Qx(self, x)

Compute gradient of action values for a given state

$$Q(\mathbf{x},:) = \mathbf{Q}\mathbf{x},$$

where the gradient is defined as

$$\frac{\partial}{\partial \mathbf{Q}} \mathcal{Q}(\mathbf{x},:) = \mathbf{1} \mathbf{x}^{\top},$$

Arguments:

• x: ndarray ((nstates,)) one-hot state vector

Returns:

ndarray ((nactions,)) vector of values for actions in the given state

ValueFunction.grad_Vx

fitr.agents.value_functions.grad_Vx(self, x)

Compute the gradient of state value function with respect to parameters ${\bf v}$

$$\mathcal{V}(\mathbf{x}) = \mathbf{v}^{\top} \mathbf{x},$$

where the gradient is defined as

$$\nabla_{\mathbf{v}} \mathcal{V}(\mathbf{x}) = \mathbf{x}$$

Arguments:

• x: ndarray((nstates,)) one-hot state vector

Returns:

Scalar value of state x

ValueFunction.grad_uQx

fitr.agents.value_functions.grad_uQx(self, u, x)

Compute derivative of value of taking action \mathbf{u} in state \mathbf{x} with respect to value function parameters \mathbf{Q}

$$Q(\mathbf{x}, \mathbf{u}) = \mathbf{u}^{\top} \mathbf{Q} \mathbf{x},$$

where the derivative is defined as

$$\frac{\partial}{\partial \mathbf{Q}} \mathcal{Q}(\mathbf{x}, \mathbf{u}) = \mathbf{u} \mathbf{x}^{\top},$$

- **u**: ndarray ((nactions,)) one-hot action vector
- x: ndarray ((nstates,)) one-hot state vector

Returns:

Scalar value of action u in state x

ValueFunction.uQx

```
fitr.agents.value_functions.uQx(self, u, x)
```

Compute value of taking action \mathbf{u} in state \mathbf{x}

$$Q(\mathbf{x}, \mathbf{u}) = \mathbf{u}^{\top} \mathbf{Q} \mathbf{x}$$

Arguments:

- **u**: ndarray((nactions,)) one-hot action vector
- x: ndarray((nstates,)) one-hot state vector

Returns:

Scalar value of action u in state x

ValueFunction.update

```
fitr.agents.value_functions.update(self, x, u, r, x_, u_)
```

Updates the value function

In the context of the base ValueFunction class, this is merely a placeholder. The specific update rule will depend on the specific value function desired.

Arguments:

- x: ndarray ((nstates,)) one-hot state vector
- **u**: ndarray ((nactions,)) one-hot action vector
- r: Scalar reward
- x_: ndarray((nstates,)) one-hot next-state vector
- u_: ndarray((nactions,)) one-hot next-action vector

DummyLearner

```
fitr.agents.value_functions.DummyLearner()
```

A critic/value function for the random learner

This class actually contributes nothing except identifying that a value function has been chosen for an Agent object

Arguments:

• env: A fitr.environments.Graph

DummyLearner.Qmax

fitr.agents.value_functions.Qmax(self, x)

Return maximal action value for given state

$$\max_{u_i} \mathcal{Q}(\mathbf{x}, u_i) = \max_{\mathbf{u}'} \mathbf{u}'^{\top} \mathbf{Q} \mathbf{x}$$

Arguments:

• x: ndarray ((nstates,)) one-hot state vector

Returns:

Scalar value of the maximal action value at the given state

DummyLearner.Qmean

fitr.agents.value_functions.Qmean(self, x)

Return mean action value for given state

$$Meanig(\mathcal{Q}(\mathbf{x},:)ig) = rac{1}{|\mathcal{U}|}\mathbf{1}^{ op}\mathbf{Q}\mathbf{x}$$

Arguments:

• x: ndarray ((nstates,)) one-hot state vector

Returns:

Scalar value of the maximal action value at the given state

DummyLearner.Qx

```
fitr.agents.value_functions.Qx(self, x)
```

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Compute action values for a given state

$$\mathcal{Q}(\mathbf{x},:) = \mathbf{Q}\mathbf{x}$$

Arguments:

• x: ndarray((nstates,)) one-hot state vector

Returns:

ndarray ((nactions,)) vector of values for actions in the given state

DummyLearner.Vx

fitr.agents.value_functions.Vx(self, x)

Compute value of state x

$$V(\mathbf{x}) = \mathbf{v}^{\top} \mathbf{x}$$

Arguments:

• x: ndarray((nstates,)) one-hot state vector

Returns:

Scalar value of state x

DummyLearner.grad_Qx

fitr.agents.value_functions.grad_Qx(self, x)

Compute gradient of action values for a given state

$$Q(\mathbf{x},:) = \mathbf{Q}\mathbf{x},$$

where the gradient is defined as

$$\frac{\partial}{\partial \mathbf{Q}}\mathcal{Q}(\mathbf{x},:) = \mathbf{1}\mathbf{x}^\top,$$

Arguments:

• x: ndarray((nstates,)) one-hot state vector

Returns:

ndarray ((nactions,)) vector of values for actions in the given state

DummyLearner.grad_Vx

fitr.agents.value_functions.grad_Vx(self, x)

Compute the gradient of state value function with respect to parameters v

$$V(\mathbf{x}) = \mathbf{v}^{\top} \mathbf{x},$$

where the gradient is defined as

$$\nabla_{\mathbf{v}} \mathcal{V}(\mathbf{x}) = \mathbf{x}$$

Arguments:

• x: ndarray ((nstates,)) one-hot state vector

Returns:

Scalar value of state x

DummyLearner.grad_uQx

fitr.agents.value_functions.grad_uQx(self, u, x)

Compute derivative of value of taking action \mathbf{u} in state \mathbf{x} with respect to value function parameters \mathbf{Q}

$$\mathcal{Q}(\mathbf{x}, \mathbf{u}) = \mathbf{u}^{\top} \mathbf{Q} \mathbf{x},$$

where the derivative is defined as

$$\frac{\partial}{\partial \mathbf{Q}}\mathcal{Q}(\mathbf{x},\mathbf{u}) = \mathbf{u}\mathbf{x}^\top,$$

Arguments:

- **u**: ndarray((nactions,)) one-hot action vector
- x: ndarray ((nstates,)) one-hot state vector

Returns:

Scalar value of action u in state x

DummyLearner.uQx

fitr.agents.value_functions.uQx(self, u, x)

Compute value of taking action **u** in state **x**

$$Q(\mathbf{x}, \mathbf{u}) = \mathbf{u}^{\top} \mathbf{Q} \mathbf{x}$$

Arguments:

- **u**: ndarray((nactions,)) one-hot action vector
- x: ndarray ((nstates,)) one-hot state vector

Returns:

Scalar value of action u in state x

DummyLearner.update

fitr.agents.value_functions.update(self, x, u, r, x_, u_)

Updates the value function

In the context of the base ValueFunction class, this is merely a placeholder. The specific update rule will depend on the specific value function desired.

Arguments:

- x: ndarray ((nstates,)) one-hot state vector
- u: ndarray ((nactions,)) one-hot action vector
- r: Scalar reward
- x_: ndarray((nstates,)) one-hot next-state vector
- u_: ndarray((nactions,)) one-hot next-action vector

InstrumentalRescorlaWagnerLearner

fitr.agents.value_functions.InstrumentalRescorlaWagnerLearner()

Learns an instrumental control policy through one-step error-driven updates of the state-action value function

The instrumental Rescorla-Wagner rule is as follows:

$$\mathbf{Q} \leftarrow \mathbf{Q} + \alpha (r - \mathbf{u}^{\top} \mathbf{Q} \mathbf{x}) \mathbf{u} \mathbf{x}^{\top},$$

where $0 < \alpha < 1$ is the learning rate, and where the reward prediction error (RPE) is $\delta = (r - \mathbf{u}^{\top} \mathbf{Q} \mathbf{x})$.

\$\$

- env: A fitr.environments.Graph
- learning_rate: Learning rate α

InstrumentalRescorlaWagnerLearner.Qmax

fitr.agents.value_functions.Qmax(self, x)

Return maximal action value for given state

$$\max_{u_i} \mathcal{Q}(\mathbf{x}, u_i) = \max_{\mathbf{u}'} \mathbf{u}'^{\top} \mathbf{Q} \mathbf{x}$$

Arguments:

• x: ndarray((nstates,)) one-hot state vector

Returns:

Scalar value of the maximal action value at the given state

InstrumentalRescorlaWagnerLearner.Qmean

fitr.agents.value_functions.Qmean(self, x)

Return mean action value for given state

$$Meanig(\mathcal{Q}(\mathbf{x},:)ig) = rac{1}{|\mathcal{U}|}\mathbf{1}^{ op}\mathbf{Q}\mathbf{x}$$

Arguments:

• x: ndarray ((nstates,)) one-hot state vector

Returns:

Scalar value of the maximal action value at the given state

In strumental Rescorla Wagner Learner. Qx

fitr.agents.value_functions.Qx(self, x)

Compute action values for a given state

$$Q(\mathbf{x},:) = \mathbf{Q}\mathbf{x}$$

• x: ndarray((nstates,)) one-hot state vector

Returns:

ndarray ((nactions,)) vector of values for actions in the given state

In strumental Rescorla Wagner Learner. Vx

fitr.agents.value_functions.Vx(self, x)

Compute value of state \mathbf{x}

$$\mathcal{V}(\mathbf{x}) = \mathbf{v}^{\top} \mathbf{x}$$

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Arguments:

 \bullet x: ndarray ((nstates,)) $one\text{-}hot\ state\ vector$

Returns:

Scalar value of state x

InstrumentalRescorlaWagnerLearner.grad_Qx

fitr.agents.value_functions.grad_Qx(self, x)

Compute gradient of action values for a given state

$$Q(\mathbf{x},:) = \mathbf{Q}\mathbf{x},$$

where the gradient is defined as

$$\frac{\partial}{\partial \mathbf{Q}} \mathcal{Q}(\mathbf{x},:) = \mathbf{1} \mathbf{x}^{\top},$$

Arguments:

• x: ndarray ((nstates,)) one-hot state vector

Returns:

ndarray ((nactions,)) vector of values for actions in the given state

$Instrumental Rescorla Wagner Learner. grad_Vx$

fitr.agents.value_functions.grad_Vx(self, x)

Compute the gradient of state value function with respect to parameters v

$$\mathcal{V}(\mathbf{x}) = \mathbf{v}^{\top} \mathbf{x},$$

where the gradient is defined as

$$\nabla_{\mathbf{v}} \mathcal{V}(\mathbf{x}) = \mathbf{x}$$

Arguments:

• x: ndarray ((nstates,)) one-hot state vector

Returns:

Scalar value of state x

InstrumentalRescorlaWagnerLearner.grad_uQx

fitr.agents.value_functions.grad_uQx(self, u, x)

Compute derivative of value of taking action \mathbf{u} in state \mathbf{x} with respect to value function parameters \mathbf{Q}

$$\mathcal{Q}(\mathbf{x}, \mathbf{u}) = \mathbf{u}^{\top} \mathbf{Q} \mathbf{x},$$

where the derivative is defined as

$$\frac{\partial}{\partial \mathbf{Q}}\mathcal{Q}(\mathbf{x},\mathbf{u}) = \mathbf{u}\mathbf{x}^\top,$$

Arguments:

- **u**: ndarray((nactions,)) one-hot action vector
- x: ndarray ((nstates,)) one-hot state vector

Returns:

Scalar value of action u in state x

InstrumentalRescorlaWagnerLearner.uQx

fitr.agents.value_functions.uQx(self, u, x)

Compute value of taking action \mathbf{u} in state \mathbf{x}

$$\mathcal{Q}(\mathbf{x}, \mathbf{u}) = \mathbf{u}^{\top} \mathbf{Q} \mathbf{x}$$

Arguments:

- u: ndarray((nactions,)) one-hot action vector
- x: ndarray ((nstates,)) one-hot state vector

Returns:

Scalar value of action **u** in state **x**

InstrumentalRescorlaWagnerLearner.update

Computes the value function update of the instrumental Rescorla-Wagner learning rule and computes derivative with respect to the learning rate.

This derivative is defined as

$$\frac{\partial}{\partial \alpha} \mathcal{Q}(\mathbf{x}, \mathbf{u}; \alpha) = \delta \mathbf{u} \mathbf{x}^{\top} + \frac{\partial}{\partial \alpha} \mathcal{Q}(\mathbf{x}, \mathbf{u}; \alpha) (1 - \alpha \mathbf{u} \mathbf{x}^{\top})$$

and the second order derivative with respect to learning rate is

$$\frac{\partial}{\partial \alpha} \mathcal{Q}(\mathbf{x}, \mathbf{u}; \alpha) = -2\mathbf{u}\mathbf{x}^{\top} \partial_{\alpha} \mathcal{Q}(\mathbf{x}, \mathbf{u}; \alpha) + \partial_{\alpha}^{2} \mathcal{Q}(\mathbf{x}, \mathbf{u}; \alpha)(1 - \alpha \mathbf{u}\mathbf{x}^{\top})$$

Arguments:

- x: ndarray ((nstates,)). State vector
- u: ndarray((nactions,)). Action vector
- r: float. Reward received
- x_: ndarray((nstates,)). For compatibility
- u_: ndarray((nactions,)). For compatibility

QLearner

fitr.agents.value_functions.QLearner()

Learns an instrumental control policy through Q-learning

The Q-learning rule is as follows:

$$\mathbf{Q} \leftarrow \mathbf{Q} + \alpha (r + \gamma \max_{\mathbf{u}'} \mathbf{u}'^{\top} \mathbf{Q} \mathbf{x}' - \mathbf{u}^{\top} \mathbf{Q} \mathbf{x}) \mathbf{z},$$

where $0 < \alpha < 1$ is the learning rate, $0 \le \gamma \le 1$ is a discount factor, and where the reward prediction error (RPE) is $\delta = (r + \gamma \max_{\mathbf{u}'} \mathbf{u}'^{\top} \mathbf{Q} \mathbf{x}' - \mathbf{u}^{\top} \mathbf{Q} \mathbf{x})$. We have also included an eligibility trace \mathbf{z} defined as

$$\mathbf{z} = \mathbf{u} \mathbf{x}^{\top} + \gamma \lambda \mathbf{z}$$

Arguments:

• env: A fitr.environments.Graph

learning_rate: Learning rate α
 discount_factor: Discount factor γ
 trace_decay: Eligibility trace decay λ

QLearner.Qmax

fitr.agents.value_functions.Qmax(self, x)

Return maximal action value for given state

$$\max_{u_i} \mathcal{Q}(\mathbf{x}, u_i) = \max_{\mathbf{u}'} \mathbf{u}'^{\top} \mathbf{Q} \mathbf{x}$$

Arguments:

• x: ndarray ((nstates,)) one-hot state vector

Returns:

Scalar value of the maximal action value at the given state

QLearner.Qmean

fitr.agents.value_functions.Qmean(self, x)

Return mean action value for given state

$$Mean(\mathcal{Q}(\mathbf{x},:)) = \frac{1}{|\mathcal{U}|} \mathbf{1}^{\top} \mathbf{Q} \mathbf{x}$$

Arguments:

• x: ndarray((nstates,)) one-hot state vector

Returns:

Scalar value of the maximal action value at the given state

QLearner.Qx

fitr.agents.value_functions.Qx(self, x)

Compute action values for a given state

$$\mathcal{Q}(\mathbf{x},:) = \mathbf{Q}\mathbf{x}$$

Arguments:

• x: ndarray((nstates,)) one-hot state vector

Returns:

ndarray ((nactions,)) vector of values for actions in the given state

QLearner.Vx

fitr.agents.value_functions.Vx(self, x)

Compute value of state \mathbf{x}

$$V(\mathbf{x}) = \mathbf{v}^{\top} \mathbf{x}$$

Arguments:

• x: ndarray((nstates,)) one-hot state vector

Returns:

Scalar value of state x

QLearner.grad_Qx

fitr.agents.value_functions.grad_Qx(self, x)

Compute gradient of action values for a given state

$$Q(\mathbf{x},:) = \mathbf{Q}\mathbf{x},$$

where the gradient is defined as

$$\frac{\partial}{\partial \mathbf{Q}}\mathcal{Q}(\mathbf{x},:) = \mathbf{1}\mathbf{x}^\top,$$

Arguments:

• x: ndarray ((nstates,)) one-hot state vector

Returns:

ndarray ((nactions,)) vector of values for actions in the given state

QLearner.grad_Vx

fitr.agents.value_functions.grad_Vx(self, x)

Compute the gradient of state value function with respect to parameters \mathbf{v}

$$V(\mathbf{x}) = \mathbf{v}^{\mathsf{T}} \mathbf{x},$$

where the gradient is defined as

$$\nabla_{\mathbf{v}} \mathcal{V}(\mathbf{x}) = \mathbf{x}$$

Arguments:

• x: ndarray ((nstates,)) one-hot state vector

Returns:

Scalar value of state x

QLearner.grad_uQx

fitr.agents.value_functions.grad_uQx(self, u, x)

Compute derivative of value of taking action \mathbf{u} in state \mathbf{x} with respect to value function parameters \mathbf{Q}

$$Q(\mathbf{x}, \mathbf{u}) = \mathbf{u}^{\top} \mathbf{Q} \mathbf{x},$$

where the derivative is defined as

$$\frac{\partial}{\partial \mathbf{Q}} \mathcal{Q}(\mathbf{x}, \mathbf{u}) = \mathbf{u} \mathbf{x}^{\top},$$

Arguments:

• **u**: ndarray((nactions,)) one-hot action vector

• x: ndarray ((nstates,)) one-hot state vector

Returns:

Scalar value of action u in state x

QLearner.uQx

fitr.agents.value_functions.uQx(self, u, x)

Compute value of taking action \mathbf{u} in state \mathbf{x}

$$\mathcal{Q}(\mathbf{x},\mathbf{u}) = \mathbf{u}^{\top}\mathbf{Q}\mathbf{x}$$

Arguments:

- **u**: ndarray ((nactions,)) one-hot action vector
- x: ndarray ((nstates,)) one-hot state vector

Returns:

Scalar value of action **u** in state **x**

QLearner.update

fitr.agents.value_functions.update(self, x, u, r, x_, u_)

Computes value function updates and their derivatives for the Q-learning model

SARSALearner

fitr.agents.value_functions.SARSALearner()

Learns an instrumental control policy through the SARSA learning rule

The SARSA learning rule is as follows:

$$\mathbf{Q} \leftarrow \mathbf{Q} + \alpha (r + \gamma \mathbf{u}'^{\top} \mathbf{Q} \mathbf{x}' - \mathbf{u}^{\top} \mathbf{Q} \mathbf{x}) \mathbf{z},$$

where $0 < \alpha < 1$ is the learning rate, $0 \le \gamma \le 1$ is a discount factor, and where the reward prediction error (RPE) is $\delta = (r + \gamma \mathbf{u}'^{\top} \mathbf{Q} \mathbf{x}' - \mathbf{u}^{\top} \mathbf{Q} \mathbf{x})$. We have also included an eligibility trace \mathbf{z} defined as

$$\mathbf{z} = \mathbf{u} \mathbf{x}^\top + \gamma \lambda \mathbf{z}$$

• env: A fitr.environments.Graph

learning_rate: Learning rate α
 discount_factor: Discount factor γ
 trace_decay: Eligibility trace decay λ

SARSALearner.Qmax

fitr.agents.value_functions.Qmax(self, x)

Return maximal action value for given state

$$\max_{u_i} \mathcal{Q}(\mathbf{x}, u_i) = \max_{\mathbf{u}'} \mathbf{u}'^{\top} \mathbf{Q} \mathbf{x}$$

Arguments:

• x: ndarray ((nstates,)) one-hot state vector

Returns:

Scalar value of the maximal action value at the given state

SARSALearner.Qmean

fitr.agents.value_functions.Qmean(self, x)

Return mean action value for given state

$$Mean(\mathcal{Q}(\mathbf{x},:)) = \frac{1}{|\mathcal{U}|} \mathbf{1}^{\top} \mathbf{Q} \mathbf{x}$$

Arguments:

• x: ndarray ((nstates,)) one-hot state vector

Returns:

Scalar value of the maximal action value at the given state

SARSALearner.Qx

fitr.agents.value_functions.Qx(self, x)

Compute action values for a given state

$$\mathcal{Q}(\mathbf{x},:) = \mathbf{Q}\mathbf{x}$$

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Arguments:

• x: ndarray ((nstates,)) one-hot state vector

Returns:

ndarray ((nactions,)) vector of values for actions in the given state

SARSALearner.Vx

fitr.agents.value_functions.Vx(self, x)

Compute value of state x

$$\mathcal{V}(\mathbf{x}) = \mathbf{v}^{\top} \mathbf{x}$$

Arguments:

• x: ndarray((nstates,)) one-hot state vector

Returns:

Scalar value of state x

SARSALearner.grad_Qx

fitr.agents.value_functions.grad_Qx(self, x)

Compute gradient of action values for a given state

$$Q(\mathbf{x},:) = \mathbf{Q}\mathbf{x},$$

where the gradient is defined as

$$\frac{\partial}{\partial \mathbf{Q}} \mathcal{Q}(\mathbf{x},:) = \mathbf{1} \mathbf{x}^\top,$$

Arguments:

• x: ndarray((nstates,)) one-hot state vector

Returns:

ndarray ((nactions,)) vector of values for actions in the given state

SARSALearner.grad_Vx

fitr.agents.value_functions.grad_Vx(self, x)

Compute the gradient of state value function with respect to parameters \mathbf{v}

$$V(\mathbf{x}) = \mathbf{v}^{\top} \mathbf{x},$$

where the gradient is defined as

$$\nabla_{\mathbf{v}} \mathcal{V}(\mathbf{x}) = \mathbf{x}$$

Arguments:

• x: ndarray ((nstates,)) one-hot state vector

Returns:

Scalar value of state x

SARSALearner.grad_uQx

fitr.agents.value_functions.grad_uQx(self, u, x)

Compute derivative of value of taking action \mathbf{u} in state \mathbf{x} with respect to value function parameters \mathbf{Q}

$$\mathcal{Q}(\mathbf{x}, \mathbf{u}) = \mathbf{u}^{\top} \mathbf{Q} \mathbf{x},$$

where the derivative is defined as

$$\frac{\partial}{\partial \mathbf{Q}}\mathcal{Q}(\mathbf{x},\mathbf{u}) = \mathbf{u}\mathbf{x}^\top,$$

Arguments:

- **u**: ndarray((nactions,)) one-hot action vector
- x: ndarray ((nstates,)) one-hot state vector

Returns:

Scalar value of action u in state x

SARSALearner.uQx

fitr.agents.value_functions.uQx(self, u, x)

Compute value of taking action ${\bf u}$ in state ${\bf x}$

$$\mathcal{Q}(\mathbf{x},\mathbf{u}) = \mathbf{u}^{\top}\mathbf{Q}\mathbf{x}$$

Arguments:

- **u**: ndarray ((nactions,)) one-hot action vector
- x: ndarray((nstates,)) one-hot state vector

Returns:

Scalar value of action u in state x

SARSALearner.update

```
fitr.agents.value_functions.update(self, x, u, r, x_, u_)
```

Computes value function updates and their derivatives for the SARSA model

Agent

fitr.agents.agents.Agent()

Base class for synthetic RL agents.

Arguments:

meta: List of metadata of arbitrary type. e.g. labels, covariates, etc. params: List of parameters for the agent. Should be filled for specific agent.

Agent.action

Selects an action given the current state of environment.

The implementation will vary depending on the type of agent and environment.

Arguments:

• state: ndarray((nstates,)) one-hot state vector

Agent.learning

```
fitr.agents.agents.learning(self, state, action, reward, next_state, next_action)
```

Updates the model's parameters and computes gradients

The implementation will vary depending on the type of agent and environment.

Arguments:

- state: ndarray ((nstates,)) one-hot state vector
- action: ndarray((nactions,)) one-hot action vector
- reward: scalar reward
- next_state: ndarray((nstates,)) one-hot next-state vector
- next_action: ndarray((nactions,)) one-hot action vector

Agent.reset_trace

```
fitr.agents.agents.reset_trace(self, state_only=False)
```

For agents with eligibility traces, this resets the eligibility trace (for episodic tasks)

Arguments:

• **state_only**: bool. If the eligibility trace is only an nstate dimensional vector (i.e. for a Pavlovian conditioning model) then set to True. For instumental models, the eligibility trace should be an nactions by nstates matrix, so keep this to False in that case.

BanditAgent

```
fitr.agents.agents.BanditAgent()
```

A base class for agents in bandit tasks (i.e. with one step).

Arguments:

• task: fitr.environments.Graph

BanditAgent.action

```
fitr.agents.agents.action(self, state)
```

Selects an action given the current state of environment.

The implementation will vary depending on the type of agent and environment.

Arguments:

• state: ndarray((nstates,)) one-hot state vector

BanditAgent.generate_data

```
fitr.agents.agents.generate_data(self, ntrials)
```

For the parent agent, this function generates data from a bandit task

Arguments:

• **ntrials**: int number of trials

Returns:

fitr.data.BehaviouralData

BanditAgent.learning

```
fitr.agents.agents.learning(self, state, action, reward, next_state, next_action)
```

Updates the model's parameters and computes gradients

The implementation will vary depending on the type of agent and environment.

Arguments:

- state: ndarray ((nstates,)) one-hot state vector
- action: ndarray((nactions,)) one-hot action vector
- reward: scalar reward
- next_state: ndarray((nstates,)) one-hot next-state vector
- next_action: ndarray((nactions,)) one-hot action vector

BanditAgent.log prob

```
fitr.agents.agents.log_prob(self, state)
```

Computes the log-likelihood over actions for a given state under the present agent parameters.

Presently this only works for the state-action value function. In all other cases, you should define your own log-likelihood function. However, this can be used as a template.

Arguments:

• state: ndarray((nstates,)) one-hot state vector

Returns:

```
ndarray ((nactions,)) log-likelihood vector
```

BanditAgent.reset_trace

```
fitr.agents.agents.reset_trace(self, state_only=False)
```

For agents with eligibility traces, this resets the eligibility trace (for episodic tasks)

Arguments:

• **state_only**: bool. If the eligibility trace is only an nstate dimensional vector (i.e. for a Pavlovian conditioning model) then set to True. For instumental models, the eligibility trace should be an nactions by nstates matrix, so keep this to False in that case.

MDPAgent

```
fitr.agents.agents.MDPAgent()
```

A base class for agents that operate on MDPs.

This mainly has implications for generating data.

Arguments:

• task: fitr.environments.Graph

MDPAgent.action

```
fitr.agents.agents.action(self, state)
```

Selects an action given the current state of environment.

The implementation will vary depending on the type of agent and environment.

Arguments:

• state: ndarray((nstates,)) one-hot state vector

MDPAgent.generate_data

```
fitr.agents.agents.generate_data(self, ntrials, state_only=False)
```

For the parent agent, this function generates data from a Markov Decision Process (MDP) task

- **ntrials**: int number of trials
- **state_only**: bool. If the eligibility trace is only an nstate dimensional vector (i.e. for a Pavlovian conditioning model) then set to True. For instumental models, the eligibility trace should be an nactions by nstates matrix, so keep this to False in that case.

Returns:

```
fitr.data.BehaviouralData
```

MDPAgent.learning

```
fitr.agents.agents.learning(self, state, action, reward, next_state, next_action)
```

Updates the model's parameters and computes gradients

The implementation will vary depending on the type of agent and environment.

Arguments:

- state: ndarray((nstates,)) one-hot state vector
- action: ndarray((nactions,)) one-hot action vector
- reward: scalar reward
- next_state: ndarray((nstates,)) one-hot next-state vector
- next_action: ndarray((nactions,)) one-hot action vector

MDPAgent.reset_trace

```
fitr.agents.agents.reset_trace(self, state_only=False)
```

For agents with eligibility traces, this resets the eligibility trace (for episodic tasks)

Arguments:

• **state_only**: bool. If the eligibility trace is only an nstate dimensional vector (i.e. for a Pavlovian conditioning model) then set to True. For instumental models, the eligibility trace should be an nactions by nstates matrix, so keep this to False in that case.

RandomBanditAgent

```
fitr.agents.agents.RandomBanditAgent()
```

An agent that simply selects random actions at each trial

RandomBanditAgent.action

```
fitr.agents.agents.action(self, state)
```

Selects an action given the current state of environment.

The implementation will vary depending on the type of agent and environment.

Arguments:

```
• state: ndarray((nstates,)) one-hot state vector
```

RandomBanditAgent.generate_data

```
fitr.agents.agents.generate_data(self, ntrials)
```

For the parent agent, this function generates data from a bandit task

Arguments:

• **ntrials**: int number of trials

Returns:

```
fitr.data.BehaviouralData
```

RandomBanditAgent.learning

```
fitr.agents.learning(self, state, action, reward, next_state, next_action)
```

Updates the model's parameters and computes gradients

The implementation will vary depending on the type of agent and environment.

Arguments:

- state: ndarray((nstates,)) one-hot state vector
- action: ndarray ((nactions,)) one-hot action vector
- reward: scalar reward
- next_state: ndarray((nstates,)) one-hot next-state vector
- next_action: ndarray((nactions,)) one-hot action vector

RandomBanditAgent.log_prob

```
fitr.agents.agents.log_prob(self, state)
```

Computes the log-likelihood over actions for a given state under the present agent parameters.

Presently this only works for the state-action value function. In all other cases, you should define your own log-likelihood function. However, this can be used as a template.

Arguments:

```
• state: ndarray ((nstates,)) one-hot state vector
```

Returns:

```
ndarray ((nactions,)) log-likelihood vector
```

RandomBanditAgent.reset trace

```
fitr.agents.agents.reset_trace(self, state_only=False)
```

For agents with eligibility traces, this resets the eligibility trace (for episodic tasks)

Arguments:

• **state_only**: bool. If the eligibility trace is only an nstate dimensional vector (i.e. for a Pavlovian conditioning model) then set to True. For instumental models, the eligibility trace should be an nactions by nstates matrix, so keep this to False in that case.

RandomMDPAgent

```
fitr.agents.agents.RandomMDPAgent()
```

An agent that simply selects random actions at each trial

Notes

This has been specified as an OnPolicyAgent arbitrarily.

RandomMDPAgent.action

```
fitr.agents.agents.action(self, state)
```

Selects an action given the current state of environment.

The implementation will vary depending on the type of agent and environment.

Arguments:

• state: ndarray((nstates,)) one-hot state vector

RandomMDPAgent.generate_data

```
fitr.agents.agents.generate_data(self, ntrials, state_only=False)
```

For the parent agent, this function generates data from a Markov Decision Process (MDP) task

Arguments:

• **ntrials**: int number of trials

• **state_only**: bool. If the eligibility trace is only an nstate dimensional vector (i.e. for a Pavlovian conditioning model) then set to True. For instumental models, the eligibility trace should be an nactions by nstates matrix, so keep this to False in that case.

Returns:

```
fitr.data.BehaviouralData
```

RandomMDPAgent.learning

```
fitr.agents.agents.learning(self, state, action, reward, next_state, next_action)
```

Updates the model's parameters and computes gradients

The implementation will vary depending on the type of agent and environment.

Arguments:

- state: ndarray((nstates,)) one-hot state vector
- action: ndarray((nactions,)) one-hot action vector
- reward: scalar reward
- next_state: ndarray((nstates,)) one-hot next-state vector
- next_action: ndarray((nactions,)) one-hot action vector

RandomMDPAgent.reset_trace

```
fitr.agents.agents.reset_trace(self, state_only=False)
```

For agents with eligibility traces, this resets the eligibility trace (for episodic tasks)

Arguments:

• **state_only**: bool. If the eligibility trace is only an nstate dimensional vector (i.e. for a Pavlovian conditioning model) then set to True. For instumental models, the eligibility trace should be an nactions by nstates matrix, so keep this to False in that case.

SARSASoftmaxAgent

```
fitr.agents.agents.SARSASoftmaxAgent()
```

An agent that uses the SARSA learning rule and a softmax policy

The softmax policy selects actions from a multinomial

$$\mathbf{u} \sim \text{Multinomial}(1, \mathbf{p} = \varsigma(\mathbf{v})),$$

whose parameters are

$$p(\mathbf{u}|\mathbf{v}) = \varsigma(\mathbf{v}) = \frac{e^{\beta \mathbf{v}}}{\sum_{i}^{|\mathbf{v}|} e^{\beta v_{i}}}.$$

The value function is SARSA:

$$\mathbf{Q} \leftarrow \mathbf{Q} + \alpha (r + \gamma \mathbf{u}'^{\top} \mathbf{Q} \mathbf{x}' - \mathbf{u}^{\top} \mathbf{Q} \mathbf{x}) \mathbf{z},$$

where $0 < \alpha < 1$ is the learning rate, $0 \le \gamma \le 1$ is a discount factor, and where the reward prediction error (RPE) is $\delta = (r + \gamma \mathbf{u}'^{\top} \mathbf{Q} \mathbf{x}' - \mathbf{u}^{\top} \mathbf{Q} \mathbf{x})$. We have also included an eligibility trace \mathbf{z} defined as

$$\mathbf{z} = \mathbf{u} \mathbf{x}^{\top} + \gamma \lambda \mathbf{z}$$

Arguments:

• task: fitr.environments.Graph

learning_rate: Learning rate α
 discount_factor: Discount factor γ
 trace_decay: Eligibility trace decay λ

• inverse_softmax_temp: Inverse softmax temperature β

• rng: np.random.RandomState

SARSASoftmaxAgent.action

fitr.agents.agents.action(self, state)

Selects an action given the current state of environment.

The implementation will vary depending on the type of agent and environment.

Arguments:

• state: ndarray ((nstates,)) one-hot state vector

SARSASoftmaxAgent.generate_data

fitr.agents.agents.generate_data(self, ntrials, state_only=False)

For the parent agent, this function generates data from a Markov Decision Process (MDP) task

- ntrials: int number of trials
- **state_only**: bool. If the eligibility trace is only an nstate dimensional vector (i.e. for a Pavlovian conditioning model) then set to True. For instumental models, the eligibility trace should be an nactions by nstates matrix, so keep this to False in that case.

Returns:

fitr.data.BehaviouralData

SARSASoftmaxAgent.learning

fitr.agents.agents.learning(self, state, action, reward, next_state, next_action)

Updates the model's parameters and computes gradients

The implementation will vary depending on the type of agent and environment.

Arguments:

• state: ndarray((nstates,)) one-hot state vector

• action: ndarray((nactions,)) one-hot action vector

• reward: scalar reward

• next_state: ndarray((nstates,)) one-hot next-state vector

• next_action: ndarray((nactions,)) one-hot action vector

SARSASoftmaxAgent.log_prob

fitr.agents.agents.log_prob(self, state, action)

Computes the log-probability of the given action and state under the model, while also computing first and second order derivatives.

This model has four free parameters:

- Learning rate α
- Inverse softmax temperature β
- Discount factor γ
- Trace decay λ

First-order partial derivatives

We can break down the computation using the chain rule to reuse previously computed derivatives:

$$\frac{\partial \mathcal{L}}{\partial \alpha} = \frac{\partial \mathcal{L}}{\partial \boldsymbol{\pi}} \frac{\partial \boldsymbol{\pi}}{\partial \mathbf{q}} \frac{\partial \mathbf{q}}{\partial \mathbf{Q}} \frac{\partial \mathbf{Q}}{\partial \alpha}$$

$$\frac{\partial \mathcal{L}}{\partial \beta} = \frac{\partial \mathcal{L}}{\partial \boldsymbol{\pi}} \frac{\partial \boldsymbol{\pi}}{\partial \beta}$$

$$\frac{\partial \mathcal{L}}{\partial \gamma} = \frac{\partial \mathcal{L}}{\partial \boldsymbol{\pi}} \frac{\partial \boldsymbol{\pi}}{\partial \mathbf{q}} \frac{\partial \mathbf{q}}{\partial \mathbf{Q}} \frac{\partial \mathbf{Q}}{\partial \gamma}$$

$$\frac{\partial \mathcal{L}}{\partial \lambda} = \frac{\partial \mathcal{L}}{\partial \boldsymbol{\pi}} \frac{\partial \boldsymbol{\pi}}{\partial \mathbf{q}} \frac{\partial \mathbf{q}}{\partial \mathbf{Q}} \frac{\partial \mathbf{Q}}{\partial \lambda}$$

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Action Probabilities

$$\partial_{\alpha}\varsigma = \frac{\partial\varsigma}{\partial\boldsymbol{\pi}} \frac{\partial\boldsymbol{\pi}}{\partial\mathbf{q}} \frac{\partial\mathbf{q}}{\partial\mathbf{Q}} (\partial_{\alpha}\mathbf{Q}) = \beta(\partial_{\boldsymbol{\pi}}\varsigma)_{i} (\partial_{\alpha}Q)_{j}^{i} x^{j}$$

Value Function

$$\partial_{\alpha}Q_{ij} = \partial_{\alpha}Q_{ij} + (\delta + \alpha\partial_{\alpha}\delta)z_{ij}$$

$$\partial_{\gamma}Q_{ij} = \partial_{\gamma}Q_{ij} + \alpha((\partial_{\gamma}\delta)z_{ij} + \delta(\partial_{\gamma}z_{ij}))$$

$$\partial_{\lambda}Q_{ij} = \partial_{\lambda}Q_{ij} + \alpha((\partial_{\lambda}\delta)z_{ij} + \delta(\partial_{\lambda}z_{ij}))$$

Reward Prediction Error

$$\partial_{\alpha}\delta = (\partial_{\mathbf{Q}}\delta)_{ij}(\partial_{\alpha}Q)^{ij}$$

$$\partial_{\gamma}\delta = (\partial_{\mathbf{Q}}\delta)_{ij}(\partial_{\gamma}Q)^{ij} + \tilde{u}_{i}Q_{j}^{i}\tilde{x}^{j}$$

$$\partial_{\lambda}\delta = (\partial_{\mathbf{Q}}\delta)_{ij}(\partial_{\lambda}Q)^{ij}$$

Trace Decay

$$\partial_{\gamma} z_{ij} = \lambda (z_{ij} + \gamma (\partial_{\gamma} z_{ij}))$$

$$\partial_{\lambda} z_{ij} = \gamma (z_{ij} + \lambda (\partial_{\lambda} z_{ij}))$$

Simplified Components of the Gradient Vector

$$\begin{split} \frac{\partial \mathcal{L}}{\partial \alpha} &= \beta \big[\mathbf{u} - \varsigma(\boldsymbol{\pi}) \big]_i \big(\partial_{\alpha} Q \big)_j^i x^j = \beta \big[u_i (\partial_{\alpha} Q)_j^i x^j - p(u_i) (\partial_{\alpha} Q)_j^i x^j \big] \\ \frac{\partial \mathcal{L}}{\partial \beta} &= \big[\mathbf{u} - \varsigma(\boldsymbol{\pi}) \big]_i Q_j^i x^j = u_i Q_j^i x^j - p(u_i) Q_j^i x^j \\ \frac{\partial \mathcal{L}}{\partial \gamma} &= \beta \big[\mathbf{u} - \varsigma(\boldsymbol{\pi}) \big]_i \big(\partial_{\gamma} Q \big)_j^i x^j \\ \frac{\partial \mathcal{L}}{\partial \lambda} &= \beta \big[\mathbf{u} - \varsigma(\boldsymbol{\pi}) \big]_i \big(\partial_{\lambda} Q \big)_j^i x^j \end{split}$$

Second-Order Partial Derivatives

The Hessian matrix for this model is

$$\mathbf{H} = \begin{bmatrix} \frac{\partial^2 \mathcal{L}}{\partial \alpha^2} & \frac{\partial^2 \mathcal{L}}{\partial \alpha \partial \beta} & \frac{\partial^2 \mathcal{L}}{\partial \alpha \partial \gamma} & \frac{\partial^2 \mathcal{L}}{\partial \alpha \partial \lambda} \\ \frac{\partial^2 \mathcal{L}}{\partial \beta \partial \alpha} & \frac{\partial^2 \mathcal{L}}{\partial \beta^2} & \frac{\partial^2 \mathcal{L}}{\partial \beta \partial \gamma} & \frac{\partial^2 \mathcal{L}}{\partial \beta \partial \lambda} \\ \frac{\partial^2 \mathcal{L}}{\partial \gamma \partial \alpha} & \frac{\partial^2 \mathcal{L}}{\partial \gamma \partial \beta} & \frac{\partial^2 \mathcal{L}}{\partial \gamma^2} & \frac{\partial^2 \mathcal{L}}{\partial \gamma \partial \lambda} \\ \frac{\partial^2 \mathcal{L}}{\partial \lambda \partial \alpha} & \frac{\partial^2 \mathcal{L}}{\partial \lambda \partial \beta} & \frac{\partial^2 \mathcal{L}}{\partial \lambda \partial \gamma} & \frac{\partial^2 \mathcal{L}}{\partial \lambda^2} \end{bmatrix},$$

where the second-order partial derivatives are such that \mathbf{H} is symmetrical. We must therefore compute 10 second order partial derivatives, shown below:

$$\frac{\partial^{2} \mathcal{L}}{\partial \alpha^{2}} = \beta \left[(\mathbf{u} - \varsigma(\boldsymbol{\pi}))_{i} (\partial_{\alpha}^{2} Q)^{i} - (\partial_{\alpha} \varsigma)_{j} (\partial_{\alpha} Q)_{k}^{j} x^{k} \right]_{l} x^{l}$$

$$\frac{\partial^{2} \mathcal{L}}{\partial \beta^{2}} = \left(q_{i} \varsigma(\boldsymbol{\pi})^{i} \right)^{2} - \mathbf{q} \odot \mathbf{q} \odot \varsigma(\boldsymbol{\pi})$$

$$\frac{\partial^{2} \mathcal{L}}{\partial \gamma^{2}} = \beta \left[(\mathbf{u} - \varsigma(\boldsymbol{\pi}))_{i} (\partial_{\gamma}^{2} Q)^{i} - (\partial_{\gamma} \varsigma)_{j} (\partial_{\gamma} Q)_{k}^{j} x^{k} \right]_{l} x^{l}$$

$$\frac{\partial^{2} \mathcal{L}}{\partial \lambda^{2}} = \beta \left[(\mathbf{u} - \varsigma(\boldsymbol{\pi}))_{i} (\partial_{\lambda}^{2} Q)^{i} - (\partial_{\lambda} \varsigma)_{j} (\partial_{\lambda} Q)_{k}^{j} x^{k} \right]_{l} x^{l}$$

The off diagonal elements of the Hessian are as follows:

$$\frac{\partial^{2} \mathcal{L}}{\partial \alpha \partial \beta} = \left(\mathbf{u} - \varsigma(\boldsymbol{\pi}) - \beta(\partial_{\beta}\varsigma)\right)_{i} (\partial_{\alpha} Q)_{j}^{i} x^{j}$$

$$\frac{\partial^{2} \mathcal{L}}{\partial \beta \partial \gamma} = \left(\mathbf{u} - \varsigma(\boldsymbol{\pi}) - \beta(\partial_{\beta}\varsigma)\right)_{i} (\partial_{\gamma} Q)_{j}^{i} x^{j}$$

$$\frac{\partial^{2} \mathcal{L}}{\partial \beta \partial \lambda} = \left(\mathbf{u} - \varsigma(\boldsymbol{\pi}) - \beta(\partial_{\beta}\varsigma)\right)_{i} (\partial_{\lambda} Q)_{j}^{i} x^{j}$$

$$\frac{\partial^{2} \mathcal{L}}{\partial \alpha \partial \gamma} = \beta\left((\mathbf{u} - \varsigma(\boldsymbol{\pi}))_{i} (\partial_{\alpha} \partial_{\gamma} Q)^{i} - (\partial_{\gamma}\varsigma)_{j} (\partial_{\alpha} Q)^{j}\right)_{k} x^{k}$$

$$\frac{\partial^{2} \mathcal{L}}{\partial \alpha \partial \lambda} = \beta\left((\mathbf{u} - \varsigma(\boldsymbol{\pi}))_{i} (\partial_{\alpha} \partial_{\lambda} Q)^{i} - (\partial_{\lambda}\varsigma)_{j} (\partial_{\alpha} Q)^{j}\right)_{k} x^{k}$$

$$\frac{\partial^{2} \mathcal{L}}{\partial \gamma \partial \lambda} = \beta\left((\mathbf{u} - \varsigma(\boldsymbol{\pi}))_{i} (\partial_{\lambda} \partial_{\gamma} Q)^{i} - (\partial_{\lambda}\varsigma)_{j} (\partial_{\gamma} Q)^{j}\right)_{k} x^{k}$$

Reward Prediction Error

$$\partial_{\alpha}^{2} \delta = (\partial_{\mathbf{Q}} \delta)_{ij} (\partial_{\alpha}^{2} Q)^{ij}$$

$$\partial_{\gamma}^{2} \delta = (\partial_{\mathbf{Q}} \delta)_{ij} (\partial_{\gamma}^{2} Q)^{ij} + 2 \tilde{u}_{i} (\partial_{\gamma} Q)_{j}^{i} \tilde{x}^{j}$$

$$\partial_{\lambda}^{2} \delta = (\partial_{\mathbf{Q}} \delta)_{ij} (\partial_{\lambda}^{2} Q)^{ij}$$

$$\partial_{\alpha} \partial_{\gamma} \delta = (\partial_{\mathbf{Q}} \delta)_{ij} (\partial_{\gamma} \partial_{\alpha} Q)^{ij} + \tilde{u}_{i} (\partial_{\alpha} Q)_{j}^{i} \tilde{x}^{j}$$

$$\partial_{\alpha} \partial_{\lambda} \delta = (\partial_{\mathbf{Q}} \delta)_{ij} (\partial_{\gamma} \partial_{\lambda} Q)^{ij}$$

$$\partial_{\gamma} \partial_{\lambda} \delta = (\partial_{\mathbf{Q}} \delta)_{ij} (\partial_{\gamma} \partial_{\lambda} Q)^{ij} + \tilde{u}_{i} (\partial_{\lambda} Q)_{j}^{i} \tilde{x}^{j}$$

Value Function

$$\begin{split} \partial_{\alpha}^{2}Q_{ij} &= \partial_{\alpha}^{2}Q_{ij} + 2(\partial_{\alpha}\delta)z_{ij} + \alpha(\partial_{\alpha}^{2}\delta)z_{ij} \\ \partial_{\gamma}^{2}Q_{ij} &= \partial_{\gamma}^{2}Q_{ij} + \alpha\Big(\big(\partial_{\gamma}^{2}\delta\big)z_{ij} + \big(\partial_{\gamma}\delta\big)\big(\partial_{\gamma}z_{ij}\big) + \big(\partial_{\gamma}\delta\big)\big(\partial_{\gamma}^{2}z_{ij}\big)\Big) \\ \partial_{\lambda}^{2}Q_{ij} &= \partial_{\lambda}^{2}Q_{ij} + \alpha\Big(\big(\partial_{\lambda}^{2}\delta\big)z_{ij} + \big(\partial_{\lambda}\delta\big)\big(\partial_{\lambda}z_{ij}\big) + \big(\partial_{\lambda}\delta\big)\big(\partial_{\gamma}^{2}z_{ij}\big)\Big) \\ \partial_{\alpha}\partial_{\gamma}Q_{ij} &= \partial_{\alpha}\partial_{\gamma}Q_{ij} + \big(\partial_{\gamma}\delta\big)z_{ij} + \delta\big(\partial_{\gamma}z_{ij}\big) + \alpha\big(\partial_{\alpha}\delta\big)\big(\partial_{\gamma}z_{ij}\big) + \alpha\big(\partial_{\alpha}\partial_{\gamma}\delta\big)z_{ij} \\ \partial_{\alpha}\partial_{\lambda}Q_{ij} &= \partial_{\alpha}\partial_{\lambda}Q_{ij} + \big(\partial_{\lambda}\delta\big)z_{ij} + \delta\big(\partial_{\lambda}z_{ij}\big) + \alpha\big(\partial_{\alpha}\delta\big)\big(\partial_{\lambda}z_{ij}\big) + \alpha\big(\partial_{\alpha}\partial_{\lambda}\delta\big)z_{ij} \\ \partial_{\gamma}\partial_{\lambda}Q_{ij} &= \partial_{\gamma}\partial_{\lambda}Q_{ij} + \alpha\Big[\big(\partial_{\lambda}\partial_{\gamma}\delta\big)z_{ij} + \big(\partial_{\gamma}\delta\big)\big(\partial_{\lambda}z_{ij}\big) + \big(\partial_{\lambda}\delta\big)\big(\partial_{\gamma}z_{ij}\big) + \delta\big(\partial_{\lambda}\partial_{\gamma}z_{ij}\big)\Big] \end{split}$$

Trace Decay

$$\begin{split} \partial_{\gamma}^{2}z &= \lambda \Big(2(\partial_{\gamma}z) + \gamma(\partial_{\gamma}^{2}z) \Big) \\ \\ \partial_{\lambda}^{2}z &= \gamma \Big(2(\partial_{\lambda}z) + \lambda(\partial_{\lambda}^{2}z) \Big) \\ \\ \partial_{\gamma}\partial_{\lambda}z &= z + \gamma(\partial_{\gamma}z) + \lambda(\partial_{\lambda}z) + \lambda\gamma(\partial_{\gamma}\partial_{\lambda}z) \end{split}$$

- action: ndarray (nactions). One-hot action vector
- state: ndarray (nstates). One-hot state vector

SARSASoftmaxAgent.reset_trace

fitr.agents.agents.reset_trace(self, state_only=False)

For agents with eligibility traces, this resets the eligibility trace (for episodic tasks)

Arguments:

• state_only: bool. If the eligibility trace is only an nstate dimensional vector (i.e. for a Pavlovian conditioning model) then set to True. For instumental models, the eligibility trace should be an nactions by nstates matrix, so keep this to False in that case.

SARSAStickySoftmaxAgent

fitr.agents.agents.SARSAStickySoftmaxAgent()

An agent that uses the SARSA learning rule and a sticky softmax policy

The sticky softmax policy selects actions from a multinomial

$$\mathbf{u} \sim \text{Multinomial}(1, \mathbf{p} = \varsigma(\mathbf{v})),$$

whose parameters are

$$p(\mathbf{u}|\mathbf{v},\mathbf{u}_{t-1}) = \varsigma(\mathbf{v},\mathbf{u}_{t-1}) = \frac{e^{\beta \mathbf{v} + \beta^{\rho} \mathbf{u}_{t-1}}}{\sum_{i}^{|\mathbf{v}|} e^{\beta v_{i} + \beta^{\rho} u_{t-1}^{(i)}}}.$$

The value function is SARSA:

$$\mathbf{Q} \leftarrow \mathbf{Q} + \alpha (r + \gamma \mathbf{u}'^{\mathsf{T}} \mathbf{Q} \mathbf{x}' - \mathbf{u}^{\mathsf{T}} \mathbf{Q} \mathbf{x}) \mathbf{z},$$

where $0 < \alpha < 1$ is the learning rate, $0 \le \gamma \le 1$ is a discount factor, and where the reward prediction error (RPE) is $\delta = (r + \gamma \mathbf{u}'^{\top} \mathbf{Q} \mathbf{x}' - \mathbf{u}^{\top} \mathbf{Q} \mathbf{x})$. We have also included an eligibility trace \mathbf{z} defined as

$$\mathbf{z} = \mathbf{u}\mathbf{x}^\top + \gamma \lambda \mathbf{z}$$

- task: fitr.environments.Graph
- learning_rate: Learning rate α
- **discount_factor**: Discount factor γ
- **trace_decay**: Eligibility trace decay λ
- inverse_softmax_temp: Inverse softmax temperature β
- **perseveration**: Perseveration parameter β^{ρ}
- rng: np.random.RandomState

SARSAStickySoftmaxAgent.action

```
fitr.agents.agents.action(self, state)
```

Selects an action given the current state of environment.

The implementation will vary depending on the type of agent and environment.

Arguments:

• state: ndarray((nstates,)) one-hot state vector

SARSAStickySoftmaxAgent.generate_data

```
fitr.agents.agents.generate_data(self, ntrials, state_only=False)
```

For the parent agent, this function generates data from a Markov Decision Process (MDP) task

Arguments:

- **ntrials**: int number of trials
- **state_only**: bool. If the eligibility trace is only an nstate dimensional vector (i.e. for a Pavlovian conditioning model) then set to True. For instumental models, the eligibility trace should be an nactions by nstates matrix, so keep this to False in that case.

Returns:

```
fitr.data.BehaviouralData
```

SARSAStickySoftmaxAgent.learning

```
fitr.agents.agents.learning(self, state, action, reward, next_state, next_action)
```

Updates the model's parameters and computes gradients

The implementation will vary depending on the type of agent and environment.

Arguments:

- state: ndarray((nstates,)) one-hot state vector
- action: ndarray((nactions,)) one-hot action vector
- reward: scalar reward
- next_state: ndarray((nstates,)) one-hot next-state vector
- next_action: ndarray((nactions,)) one-hot action vector

SARSAStickySoftmaxAgent.reset_trace

```
fitr.agents.agents.reset_trace(self, state_only=False)
```

For agents with eligibility traces, this resets the eligibility trace (for episodic tasks)

Arguments:

• **state_only**: bool. If the eligibility trace is only an nstate dimensional vector (i.e. for a Pavlovian conditioning model) then set to True. For instumental models, the eligibility trace should be an nactions by nstates matrix, so keep this to False in that case.

QLearningSoftmaxAgent

fitr.agents.agents.QLearningSoftmaxAgent()

An agent that uses the Q-learning rule and a softmax policy

The softmax policy selects actions from a multinomial

$$\mathbf{u} \sim \text{Multinomial}(1, \mathbf{p} = \varsigma(\mathbf{v})),$$

whose parameters are

$$p(\mathbf{u}|\mathbf{v}) = \varsigma(\mathbf{v}) = \frac{e^{\beta \mathbf{v}}}{\sum_{i}^{|\mathbf{v}|} e^{\beta v_{i}}}.$$

The value function is Q-learning:

$$\mathbf{Q} \leftarrow \mathbf{Q} + \alpha (r + \gamma \max_{\mathbf{u}'} \mathbf{u}'^{\top} \mathbf{Q} \mathbf{x}' - \mathbf{u}^{\top} \mathbf{Q} \mathbf{x}) \mathbf{z},$$

where $0 < \alpha < 1$ is the learning rate, $0 \le \gamma \le 1$ is a discount factor, and where the reward prediction error (RPE) is $\delta = (r + \gamma \max_{\mathbf{u}'} \mathbf{u}'^{\top} \mathbf{Q} \mathbf{x}' - \mathbf{u}^{\top} \mathbf{Q} \mathbf{x})$. The eligibility trace \mathbf{z} is defined as

$$\mathbf{z} = \mathbf{u} \mathbf{x}^{\top} + \gamma \lambda \mathbf{z}$$

- task: fitr.environments.Graph
- learning_rate: Learning rate α
- **discount factor**: Discount factor γ
- **trace_decay**: Eligibility trace decay λ
- inverse_softmax_temp: Inverse softmax temperature β
- rng: np.random.RandomState

QLearningSoftmaxAgent.action

```
fitr.agents.agents.action(self, state)
```

Selects an action given the current state of environment.

The implementation will vary depending on the type of agent and environment.

Arguments:

• **state**: ndarray((nstates,)) **one-hot state vector**

QLearningSoftmaxAgent.generate_data

```
fitr.agents.agents.generate_data(self, ntrials, state_only=False)
```

For the parent agent, this function generates data from a Markov Decision Process (MDP) task

Arguments:

- **ntrials**: int number of trials
- **state_only**: bool. If the eligibility trace is only an nstate dimensional vector (i.e. for a Pavlovian conditioning model) then set to True. For instumental models, the eligibility trace should be an nactions by nstates matrix, so keep this to False in that case.

Returns:

```
fitr.data.BehaviouralData
```

QLearningSoftmaxAgent.learning

```
fitr.agents.agents.learning(self, state, action, reward, next_state, next_action)
```

Updates the model's parameters and computes gradients

The implementation will vary depending on the type of agent and environment.

Arguments:

- state: ndarray((nstates,)) one-hot state vector
- action: ndarray((nactions,)) one-hot action vector
- reward: scalar reward
- next_state: ndarray((nstates,)) one-hot next-state vector
- next_action: ndarray((nactions,)) one-hot action vector

QLearningSoftmaxAgent.reset_trace

```
fitr.agents.agents.reset_trace(self, state_only=False)
```

For agents with eligibility traces, this resets the eligibility trace (for episodic tasks)

Arguments:

• **state_only**: bool. If the eligibility trace is only an nstate dimensional vector (i.e. for a Pavlovian conditioning model) then set to True. For instumental models, the eligibility trace should be an nactions by nstates matrix, so keep this to False in that case.

RWSoftmaxAgent

fitr.agents.agents.RWSoftmaxAgent()

An instrumental Rescorla-Wagner agent with a softmax policy

The softmax policy selects actions from a multinomial

$$\mathbf{u} \sim \text{Multinomial}(1, \mathbf{p} = \varsigma(\mathbf{v})),$$

whose parameters are

$$p(\mathbf{u}|\mathbf{v}) = \varsigma(\mathbf{v}) = \frac{e^{\beta \mathbf{v}}}{\sum_{i}^{|\mathbf{v}|} e^{\beta v_{i}}}.$$

The value function is the Rescorla-Wagner learning rule:

$$\mathbf{Q} \leftarrow \mathbf{Q} + \alpha (r - \mathbf{u}^{\top} \mathbf{Q} \mathbf{x}) \mathbf{u} \mathbf{x}^{\top},$$

where $0 < \alpha < 1$ is the learning rate, $0 \le \gamma \le 1$ is a discount factor, and where the reward prediction error (RPE) is $\delta = (r - \mathbf{u}^{\top} \mathbf{Q} \mathbf{x})$.

Arguments:

- task: fitr.environments.Graph
- learning_rate: Learning rate α
- inverse_softmax_temp: Inverse softmax temperature β
- rng: np.random.RandomState

RWSoftmaxAgent.action

fitr.agents.agents.action(self, state)

Selects an action given the current state of environment.

The implementation will vary depending on the type of agent and environment.

Arguments:

• state: ndarray((nstates,)) one-hot state vector

RWSoftmaxAgent.generate_data

```
fitr.agents.agents.generate_data(self, ntrials)
```

For the parent agent, this function generates data from a bandit task

Arguments:

• **ntrials**: int number of trials

Returns:

fitr.data.BehaviouralData

RWSoftmaxAgent.learning

```
fitr.agents.agents.learning(self, state, action, reward, next_state, next_action)
```

Updates the model's parameters and computes gradients

The implementation will vary depending on the type of agent and environment.

Arguments:

- state: ndarray ((nstates,)) one-hot state vector
- action: ndarray((nactions,)) one-hot action vector
- reward: scalar reward
- next_state: ndarray((nstates,)) one-hot next-state vector
- next_action: ndarray((nactions,)) one-hot action vector

RWSoftmaxAgent.log prob

```
fitr.agents.agents.log_prob(self, state, action)
```

Computes the log-probability of an action taken by the agent in a given state, as well as updates all partial derivatives with respect to the parameters.

This function overrides the log_prob method of the parent class.

Let

- $n_u \in \mathbb{N}_+$ be the dimensionality of the action space
- $n_x \in \mathbb{N}_+$ be the dimensionality of the state space
- $\mathbf{u} = (u_0, u_1, u_{n_u})^{\top}$ be a one-hot action vector
- $\mathbf{x} = (x_0, x_1, x_{n_x})^{\top}$ be a one-hot action vector
- $\mathbf{Q} \in \mathbb{R}^{n_u \times n_x}$ be the state-action value function parameters
- $\beta \in \mathbb{R}$ be the inverse softmax temperature
- $\alpha \in [0, 1]$ be the learning rate

• $\varsigma(\pi) = p(\mathbf{u}|\mathbf{Q}, \beta)$ be a softmax function with logits $\pi_i = \beta Q_{ij}x^j$ (shown in Einstein summation convention).

- $\mathcal{L} = \log p(\mathbf{u}|\mathbf{Q}, \beta)$ be the log-likelihood function for trial t
- $q_i = Q_{ij}x^j$ be the value of the state x^j
- $v^i = e^{\beta q_i}$ be the softmax potential
- $\eta(\pi)$ be the softmax partition function.

Then we have the partial derivative of \mathcal{L} at trial t with respect to α

$$\partial_{\alpha} \mathcal{L} = \beta \left[\left(\mathbf{u} - \varsigma(\pi) \right)_{i} (\partial_{\alpha} Q)_{j}^{i} x^{j} \right],$$

and with respect to β

$$\partial_{\beta} \mathcal{L} = u_i \Big(\mathbf{I}_{n_u \times n_u} - \varsigma(\boldsymbol{\pi}) \Big)_j^i Q_{jk} x^k.$$

We also compute the Hessian H, defined as

$$\mathbf{H} = \left[\begin{array}{cc} \partial_{\alpha}^{2} \mathcal{L} & \partial_{\alpha} \partial_{\beta} \mathcal{L} \\ \partial_{\beta} \partial_{\alpha} \mathcal{L} & \partial_{\beta}^{2} \mathcal{L} \end{array} \right].$$

The components of **H** are

$$\partial_{\alpha}^{2} \mathcal{L} = \beta \Big((\mathbf{u} - \varsigma(\boldsymbol{\pi}))_{i} (\partial_{\alpha}^{2} \mathbf{Q})^{i} - \partial_{\alpha} \varsigma(\boldsymbol{\pi})_{i} (\partial_{\alpha} \mathbf{Q})^{i} \Big)_{j} x^{j},$$

$$\partial_{\beta}^{2} \mathcal{L} = u_{i}(),$$

$$\partial_{\alpha}\partial_{\beta}\mathcal{L} = \left[(u - \varsigma(\boldsymbol{\pi})) - \beta\partial_{\beta}\varsigma(\boldsymbol{\pi}) \right]_{i} (\partial_{\alpha}Q)_{k}^{i}x^{k}.$$

and where $\partial_{\beta}\partial_{\alpha}\mathcal{L} = \partial_{\alpha}\partial_{\beta}\mathcal{L}$ since the second derivatives of \mathcal{L} are continuous in the neighbourhood of the parameters.

Arguments:

- action: ndarray (nactions). One-hot action vector
- state: ndarray (nstates). One-hot state vector

RWSoftmaxAgent.reset_trace

```
fitr.agents.agents.reset_trace(self, state_only=False)
```

For agents with eligibility traces, this resets the eligibility trace (for episodic tasks)

• **state_only**: bool. If the eligibility trace is only an nstate dimensional vector (i.e. for a Pavlovian conditioning model) then set to True. For instumental models, the eligibility trace should be an nactions by nstates matrix, so keep this to False in that case.

RWStickySoftmaxAgent

fitr.agents.agents.RWStickySoftmaxAgent()

An instrumental Rescorla-Wagner agent with a 'sticky' softmax policy

The softmax policy selects actions from a multinomial

$$\mathbf{u} \sim \text{Multinomial}(1, \mathbf{p} = \varsigma(\mathbf{v}, \mathbf{u}_{t-1})).$$

whose parameters are

$$p(\mathbf{u}|\mathbf{v},\mathbf{u}_{t-1}) = \varsigma(\mathbf{v},\mathbf{u}_{t-1}) = \frac{e^{\beta \mathbf{v} + \beta^{\rho} \mathbf{u}_{t-1}}}{\sum_{i}^{|\mathbf{v}|} e^{\beta v_{i} + \beta^{\rho} u_{t-1}^{(i)}}}.$$

The value function is the Rescorla-Wagner learning rule:

$$\mathbf{Q} \leftarrow \mathbf{Q} + \alpha (r - \mathbf{u}^{\top} \mathbf{Q} \mathbf{x}) \mathbf{u} \mathbf{x}^{\top},$$

where $0 < \alpha < 1$ is the learning rate, $0 \le \gamma \le 1$ is a discount factor, and where the reward prediction error (RPE) is $\delta = (r - \mathbf{u}^{\mathsf{T}} \mathbf{Q} \mathbf{x})$.

Arguments:

- task: fitr.environments.Graph
- learning_rate: Learning rate α
- inverse softmax temp: Inverse softmax temperature β
- **perseveration**: Perseveration parameter $\beta^h o$
- rng: np.random.RandomState

RWStickySoftmaxAgent.action

fitr.agents.agents.action(self, state)

Selects an action given the current state of environment.

The implementation will vary depending on the type of agent and environment.

Arguments:

• state: ndarray((nstates,)) one-hot state vector

RWStickySoftmaxAgent.generate_data

```
fitr.agents.agents.generate_data(self, ntrials)
```

For the parent agent, this function generates data from a bandit task

Arguments:

• **ntrials**: int number of trials

Returns:

```
fitr.data.BehaviouralData
```

RWStickySoftmaxAgent.learning

```
fitr.agents.agents.learning(self, state, action, reward, next_state, next_action)
```

Updates the model's parameters and computes gradients

The implementation will vary depending on the type of agent and environment.

Arguments:

- state: ndarray((nstates,)) one-hot state vector
- action: ndarray ((nactions,)) one-hot action vector
- reward: scalar reward
- next_state: ndarray((nstates,)) one-hot next-state vector
- next_action: ndarray ((nactions,)) one-hot action vector

RWStickySoftmaxAgent.log_prob

```
fitr.agents.agents.log_prob(self, state, action)
```

Computes the log-probability of an action taken by the agent in a given state, as well as updates all partial derivatives with respect to the parameters.

This function overrides the log_prob method of the parent class.

Let

- $n_u \in \mathbb{N}_+$ be the dimensionality of the action space
- $n_x \in \mathbb{N}_+$ be the dimensionality of the state space
- $\mathbf{u} = (u_0, u_1, u_{n_n})^{\top}$ be a one-hot action vector
- \tilde{u} be a one-hot vector representing the last trial's action, where at trial 0, $\tilde{u} = 0$.
- $\mathbf{x} = (x_0, x_1, x_{n_x})^{\top}$ be a one-hot action vector
- $\mathbf{Q} \in \mathbb{R}^{n_u \times n_x}$ be the state-action value function parameters
- $\beta \in \mathbb{R}$ be the inverse softmax temperature scaling the action values
- $\rho \in \mathbb{R}$ be the inverse softmax temperature scaling the influence of the past trial's action
- $\alpha \in [0, 1]$ be the learning rate

• $\varsigma(\pi) = p(\mathbf{u}|\mathbf{Q}, \beta, \rho)$ be a softmax function with logits $\pi_i = \beta Q_{ij}x^j + \rho \tilde{u}_i$ (shown in Einstein summation convention).

- $\mathcal{L} = \log p(\mathbf{u}|\mathbf{Q}, \beta, \rho)$ be the log-likelihood function for trial t
- $q_i = Q_{ij}x^j$ be the value of the state x^j
- $v^i = e^{\beta q_i + \rho \tilde{u}_i}$ be the softmax potential
- $\eta(\pi)$ be the softmax partition function.

Then we have the partial derivative of \mathcal{L} at trial t with respect to α

$$\partial_{\alpha} \mathcal{L} = \beta \Big[(\mathbf{u} - \varsigma(\pi))_i (\partial_{\alpha} Q)_j^i x^j \Big],$$

and with respect to β

$$\partial_{\beta} \mathcal{L} = u_i \Big(\mathbf{I}_{n_u \times n_u} - \varsigma(\boldsymbol{\pi}) \Big)_{j}^{i} Q_{jk} x^k$$

and with respect to ρ

$$\partial_{\rho} \mathcal{L} = u_i \Big(\mathbf{I}_{n_u \times n_u} - \varsigma(\boldsymbol{\pi}) \Big)_j^i \tilde{u}^j.$$

We also compute the Hessian H, defined as

$$\mathbf{H} = \left[egin{array}{ccc} \partial_{lpha}^2 \mathcal{L} & \partial_{lpha} \partial_{eta} \mathcal{L} & \partial_{lpha} \partial_{
ho} \mathcal{L} \ \partial_{eta} \partial_{lpha} \mathcal{L} & \partial_{eta}^2 \mathcal{L} & \partial_{eta} \partial_{
ho} \mathcal{L} \ \partial_{
ho} \partial_{lpha} \mathcal{L} & \partial_{
ho} \partial_{eta} \mathcal{L} & \partial_{
ho}^2 \mathcal{L} \end{array}
ight].$$

The components of $\mathbf H$ are virtually identical to that of RWSoftmaxAgent, with the exception of the $\partial_\rho\partial_\alpha\mathcal L$ and $\partial_\beta\partial_\rho\mathcal L$

$$\partial_{\alpha}^{2} \mathcal{L} = \beta \Big((\mathbf{u} - \varsigma(\boldsymbol{\pi}))_{i} (\partial_{\alpha}^{2} \mathbf{Q})^{i} - \partial_{\alpha} \varsigma(\boldsymbol{\pi})_{i} (\partial_{\alpha} \mathbf{Q})^{i} \Big)_{j} x^{j},$$

$$\partial_{\beta}^{2} \mathcal{L} = u_{k} \left(\frac{(q_{i}q_{i}v^{i}v^{i}}{z^{2}} - \frac{q_{i}q_{i}v^{i}}{z} \right)^{k}$$

$$\partial_{\alpha} \partial_{\beta} \mathcal{L} = \left[(u - \varsigma(\boldsymbol{\pi})) - \beta \partial_{\beta} \varsigma(\boldsymbol{\pi}) \right]_{i} (\partial_{\alpha} Q)_{k}^{i} x^{k}$$

$$\partial_{\alpha} \partial_{\rho} \mathcal{L} = -\beta \Big(\partial_{\boldsymbol{\pi}} \varsigma(\boldsymbol{\pi})_{i} \tilde{u}^{i} \Big)_{i} (\partial_{\alpha} Q)_{k}^{j} x^{k}$$

and where \mathbf{H} is symmetric since the second derivatives of \mathcal{L} are continuous in the neighbourhood of the parameters.

- action: ndarray (nactions). One-hot action vector
- state: ndarray (nstates). One-hot state vector

Returns:

float

RWStickySoftmaxAgent.reset_trace

fitr.agents.agents.reset_trace(self, state_only=False)

For agents with eligibility traces, this resets the eligibility trace (for episodic tasks)

Arguments:

• **state_only**: bool. If the eligibility trace is only an nstate dimensional vector (i.e. for a Pavlovian conditioning model) then set to True. For instumental models, the eligibility trace should be an nactions by nstates matrix, so keep this to False in that case.

RWSoftmaxAgentRewardSensitivity

fitr.agents.agents.RWSoftmaxAgentRewardSensitivity()

An instrumental Rescorla-Wagner agent with a softmax policy, whose experienced reward is scaled by a factor ρ .

The softmax policy selects actions from a multinomial

$$\mathbf{u} \sim \text{Multinomial}(1, \mathbf{p} = \varsigma(\mathbf{v})),$$

whose parameters are

$$p(\mathbf{u}|\mathbf{v}) = \varsigma(\mathbf{v}) = \frac{e^{\beta \mathbf{v}}}{\sum_{i}^{|\mathbf{v}|} e^{\beta v_{i}}}.$$

The value function is the Rescorla-Wagner learning rule with scaled reward ρr :

$$\mathbf{Q} \leftarrow \mathbf{Q} + \alpha (\rho r - \mathbf{u}^{\top} \mathbf{Q} \mathbf{x}) \mathbf{u} \mathbf{x}^{\top},$$

where $0 < \alpha < 1$ is the learning rate, $0 \le \gamma \le 1$ is a discount factor, and where the reward prediction error (RPE) is $\delta = (\rho r - \mathbf{u}^{\top} \mathbf{Q} \mathbf{x})$.

- task: fitr.environments.Graph
- learning_rate: Learning rate α
- inverse softmax temp: Inverse softmax temperature β
- reward_sensitivity: Reward sensitivity parameter ρ
- rng: np.random.RandomState

RWS of tmax Agent Reward Sensitivity. action

```
fitr.agents.agents.action(self, state)
```

Selects an action given the current state of environment.

The implementation will vary depending on the type of agent and environment.

Arguments:

• state: ndarray((nstates,)) one-hot state vector

$RWS of tmax Agent Reward Sensitivity. generate_data$

```
fitr.agents.agents.generate_data(self, ntrials)
```

For the parent agent, this function generates data from a bandit task

Arguments:

• **ntrials**: int number of trials

Returns:

fitr.data.BehaviouralData

RWSoftmaxAgentRewardSensitivity.learning

```
fitr.agents.learning(self, state, action, reward, next_state, next_action)
```

Updates the model's parameters and computes gradients

The implementation will vary depending on the type of agent and environment.

Arguments:

- state: ndarray((nstates,)) one-hot state vector
- action: ndarray((nactions,)) one-hot action vector
- reward: scalar reward
- next state: ndarray((nstates,)) one-hot next-state vector
- next_action: ndarray((nactions,)) one-hot action vector

$RWS oftmax Agent Reward Sensitivity. log_prob$

```
fitr.agents.agents.log_prob(self, state)
```

Computes the log-likelihood over actions for a given state under the present agent parameters.

Presently this only works for the state-action value function. In all other cases, you should define your own log-likelihood function. However, this can be used as a template.

Arguments:

• **state**: ndarray((nstates,)) **one-hot state vector**

Returns:

ndarray((nactions,)) log-likelihood vector

 $RWS of tmax Agent Reward Sensitivity. reset_trace$

```
fitr.agents.agents.reset_trace(self, state_only=False)
```

For agents with eligibility traces, this resets the eligibility trace (for episodic tasks)

Arguments:

• **state_only**: bool. If the eligibility trace is only an nstate dimensional vector (i.e. for a Pavlovian conditioning model) then set to True. For instumental models, the eligibility trace should be an nactions by nstates matrix, so keep this to False in that case.

Chapter 5

Data

fitr.data

A module containing a generic class for behavioural data.

BehaviouralData

```
fitr.data.BehaviouralData()
```

A flexible and generic object to store and process behavioural data across tasks

Arguments:

- **ngroups**: Integer number of groups represented in the dataset. Only > 1 if data are merged
- **nsubjects**: Integer number of subjects in dataset
- **ntrials**: Integer number of trials done by each subject
- dict: Dictionary storage indexed by subject.
- params: ndarray((nsubjects, nparams + 1)) parameters for each (simulated) subject
- meta: Array of covariates of type ndarray ((nsubjects, nmetadata_features+1))
- tensor: Tensor representation of the behavioural data of type ndarray ((nsubjects, ntrials, nfeatures))

BehaviouralData.add_subject

```
fitr.data.add_subject(self, subject_index, parameters, subject_meta)
```

Appends a new subject to the dataset

- **subject_index**: Integer identification for subject
- parameters: list of parameters for the subject
- **subject_meta**: Some covariates for the subject (list)

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BehaviouralData.initialize data dictionary

fitr.data.initialize_data_dictionary(self)

BehaviouralData.make behavioural ngrams

```
fitr.data.make_behavioural_ngrams(self, n)
```

Creates N-grams of behavioural data

BehaviouralData.make_cooccurrence_matrix

```
fitr.data.make_cooccurrence_matrix(self, k, dtype=<class 'numpy.float32'>)
```

BehaviouralData.make_tensor_representations

```
fitr.data.make_tensor_representations(self)
```

Creates a tensor with all subjects' data

Notes

Assumes that all subjects did same number of trials.

BehaviouralData.numpy_tensor_to_bdf

```
fitr.data.numpy_tensor_to_bdf(self, X)
```

Creates BehaviouralData formatted set from a dataset stored in a numpy ndarray.

Arguments:

 \bullet X: ndarray ((nsubjects, ntrials, m)) with m being the size of flattened single-trial data

BehaviouralData.unpack_tensor

```
fitr.data.unpack_tensor(self, x_dim, u_dim, r_dim=1, terminal_dim=1, get='sarsat')
```

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Unpacks data stored in tensor format into separate arrays for states, actions, rewards, next states, and next actions.

Arguments:

 x_{dim} : Task state space dimensionality (int) u_{dim} : Task action space dimensionality (int) r_{dim} : Reward dimensionality (int, default=1) terminal_dim: Dimensionality of the terminal state indicator (int, default=1) get: String indicating the order that data are stored in the array. Can also be shortened such that fewer elements are returned. For example, the default is sarsat.

Returns:

List with data, where each element is in the order of the argument get

BehaviouralData.update

fitr.data.update(self, subject_index, behav_data)

Adds behavioural data to the dataset

Arguments:

- subject_index: Integer index for the subject
- behav_data: 1-dimensional ndarray of flattened data

merge_behavioural_data

fitr.data.merge_behavioural_data(datalist)

Combines BehaviouralData objects.

Arguments:

• datalist: List of BehaviouralData objects

Returns:

BehaviouralData with data from multiple groups merged.

Chapter 6

Inference

fitr.inference

Methods for inferring the parameters of generative models for reinforcement learning data.

OptimizationResult

fitr.inference.optimization_result.OptimizationResult()

Container for the results of an optimization run on a generative model of behavioural data

Arguments:

- subject_id: ndarray ((nsubjects,)) or None (default). Integer ids for subjects
- xmin: ndarray ((nsubjects, nparams)) or None (default). Parameters that minimize objective function
- fmin: ndarray ((nsubjects,)) or None (default). Value of objective function at minimum
- fevals: ndarray ((nsubjects,)) or None (default). Number of function evaluations required to minimize objective function
- niters: ndarray((nsubjects,)) or None (default). Number of iterations required to minimize objective function
- lme: ndarray ((nsubjects,)) or None (default). Log model evidence
- bic: ndarray((nsubjects,)) or None (default). Bayesian Information Criterion
- hess_inv: ndarray((nsubjects, nparams, nparams)) or None (default). Inverse Hessian at the optimum.
- err: ndarray ((nsubjects, nparams)) or None (default). Error of estimates at optimum.

OptimizationResult.transform_xmin

fitr.inference.optimization_result.transform_xmin(self, transforms, inplace=False)

Rescales the parameter estimates.

- transforms: list. Transformation functions where len(transforms) == self.xmin.shape[1]
- inplace: bool. Whether to change the values in self.xmin. Default is False, which returns an ndarray((nsubjects, nparams)) of the transformed parameters.

Returns:

ndarray((nsubjects, nparams)) of the transformed parameters if inplace=False

mlepar

fitr.inference.mle_parallel.mlepar(f, data, nparams, minstarts=2, maxstarts=10, maxs Computes maximum likelihood estimates using parallel CPU resources.

Wraps over the fitr.optimization.mle_parallel.mle function.

Arguments:

- **f**: Likelihood function
- data: A subscriptable object whose first dimension indexes subjects
- **optimizer**: Optimization function (currently only l_bfgs_b supported)
- nparams: int number of parameters to be estimated
- minstarts: int. Minimum number of restarts with new initial values
- maxstarts: int. Maximum number of restarts with new initial values
- maxstarts_without_improvement: int. Maximum number of restarts without improvement in objective function value
- init sd: Standard deviation for Gaussian initial values
- jac: bool. Set to True if f returns a Jacobian as the second element of the returned values
- hess: bool. Set to True if third output value of f is the Hessian matrix
- **method**: str. One of the scipy.optimize methods.

Returns:

fitr.inference.OptimizationResult

Todo:

• [] Raise errors when user selects inappropriate optimization function given values for jac and hess

l_bfgs_b

fitr.inference.mle_parallel.l_bfgs_b(f, i, data, nparams, jac, minstarts=2, maxstart

Minimizes the negative log-probability of data with respect to some parameters under function f using the L-BFGS-B algorithm.

This function is specified for use with parallel CPU resources.

Arguments:

• **f**: (Negative!) Log likelihood function

- i: int. Subject being optimized (slices first dimension of data)
- data: Object subscriptable along first dimension to indicate subject being optimized
- nparams: int. Number of parameters in the model
- jac: bool. Set to True if f returns a Jacobian as the second element of the returned values
- minstarts: int. Minimum number of restarts with new initial values
- maxstarts: int. Maximum number of restarts with new initial values
- maxstarts_without_improvement: int. Maximum number of restarts without improvement in objective function value
- init_sd: Standard deviation for Gaussian initial values

Returns:

- i: int. Subject being optimized (slices first dimension of data)
- xmin: ndarray ((nparams,)). Parameter values at optimum
- fmin: Scalar objective function value at optimum
- **fevals**: int. Number of function evaluations
- **niters**: int. Number of iterations
- lme_: Scalar log-model evidence at optimum
- bic_: Scalar Bayesian Information Criterion at optimum
- hess_inv: ndarray((nparams, nparams)). Inv at optimum

bms

fitr.inference.bms.bms(L, ftol=1e-12, nsamples=1000000, rng=<mtrand.RandomState objection as per Rigoux et al. (2014).

Arguments:

- L: ndarray((nsubjects, nmodels)). Log model evidence
- ftol: float. Threshold for convergence of prediction error
- **nsamples**: int>0. Number of samples to draw from Dirichlet distribution for computation of exceedence probabilities
- rng: np.random.RandomState
- verbose: bool (default=True). If False, no output provided.

Returns:

- pxp: ndarray (nmodels). Protected exceedance probabilities
- xp: ndarray (nmodels). Exceedance probabilities
- bor: ndarray (nmodels). Bayesian Omnibus Risk
- q_m: ndarray ((nsubjects, nmodels)). Posterior distribution over models for each subject
- alpha: ndarray (nmodels). Posterior estimates of Dirichlet parameters
- f0: float. Free energy of null model
- f1: float. Free energy of alternative model
- niter: int. Number of iterations of posterior optimization

Examples:

Assuming one is given a matrix of (\log -) model evidence values L of type ndarray((nsubjects, nmodels)),

from fitr.inference import spm_bms

pxp, xp, bor, q_m, alpha, f0, f1, niter = bms(L)
Todos:

• [] Add notes on derivation

Chapter 7

Criticism

fitr.criticism

Methods for criticism of model fits.

actual_estimate

fitr.criticism.plotting.actual_estimate(y_true, y_pred, xlabel='Actual', ylabel='Est

Plots parameter estimates against the ground truth values.

Arguments:

- ullet y_true: ndarray(nsamples). Vector of ground truth parameters
- y_pred: ndarray (nsamples). Vector of parameter estimates
- xlabel: str. Label for x-axis
- ylabel: str. Label for y-axis
- corr: bool. Whether to plot correlation coefficient.
- figsize: tuple. Figure size (inches).

Returns:

matplotlib.pyplot.Figure

Chapter 8

Statistics

fitr.metrics

Metrics and performance statistics.

bic

fitr.metrics.bic(log_prob, nparams, ntrials)

Bayesian Information Criterion (BIC)

Arguments:

• log_prob: Log probability

• **nparams**: Number of parameters in the model

• **ntrials**: Number of trials in the time series

Returns:

Scalar estimate of BIC.

linear_correlation

fitr.metrics.linear_correlation(X, Y)

Linear correlation coefficient.

Will compute the following formula

$$\rho = \frac{\mathbf{x}^{\top} \mathbf{y}}{\|\mathbf{x} Vert \cdot \|\mathbf{y} Vert}$$

where each vector \mathbf{x} and \mathbf{y} are rows of the matrices \mathbf{X} and \mathbf{Y} , respectively.

- X: ndarray ((nsamples, nfeatures)) of dimension 1 or 2. If X is a 1D array, it will be converted to 2D prior to computation
- Y: ndarray ((nsamples, nfeatures)) of dimension 1 or 2. If Y is a 1D array, it will be converted to 2D prior to computation

Returns:

• **rho**: ndarray ((nfeatures,)). Correlation coefficient(s)

TODO:

• [] Create error raised when X and Y are not same dimension

lme

fitr.metrics.lme(log_prob, nparams, hess_inv)

Laplace approximation to the log model evidence

Arguments:

- **log_prob**: Log probability
- nparams: Number of parameters in the model
- **hess_inv**: Hessian at the optimum (shape is $K \times K$)

Returns:

Scalar approximation of the log model evidence

log loss

fitr.metrics.log_loss(p, q)

Computes log loss.

$$\mathcal{L} = \mathbf{p}^{\top} \log \mathbf{q} + (1 - \mathbf{p})^{\top} \log(1 - \mathbf{q})$$

Arguments:

- p: Binary vector of true labels ndarray ((nsamples,))
- ullet q: Vector of estimates (between 0 and 1) of type ndarray ((nsamples,))

Returns:

Scalar log loss

Chapter 9

Utilities

fitr.utils

Functions used across fitr.

batch softmax

fitr.utils.batch_softmax(X, axis=1)

Computes the softmax function for a batch of samples

$$p(\mathbf{x}) = \frac{e^{\mathbf{x} - \max_i x_i}}{\mathbf{1}^\top e^{\mathbf{x} - \max_i x_i}}$$

Arguments:

• x: Softmax logits (ndarray ((nsamples, nfeatures)))

Returns:

Matrix of probabilities of size ndarray ((nsamples, nfeatures)) such that sum over nfeatures is 1.

batch_transform

fitr.utils.batch_transform(X, f_list)

Applies the fitr.utils.transform function over a batch of parameters

- X: ndarray((nsamples, nparams)). Raw parameters
- **f_list**: list where len(list) == nparams. Functions defining coordinate transformations on each element of x.

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Returns:

 $\verb|ndarray((nsamples, nparams))|. \\ \textit{Transformed parameters}|$

I

```
fitr.utils.I(x)
```

Identity transformation.

Mainly for convenience when using fitr.utils.transform with some vector element that should not be transformed, despite changing the coordinates of other variables.

Arguments:

• x: ndarray

Returns:

ndarray(shape=x.shape)

log_loss

fitr.utils.log_loss(p, q)

Computes log loss.

$$\mathcal{L} = -\frac{1}{n_s} (\mathbf{p}^{\top} \log \mathbf{q} + (1 - \mathbf{p})^{\top} \log(1 - \mathbf{q}))$$

Arguments:

- p: Binary vector of true labels ndarray ((nsamples,))
- q: Vector of estimates (between 0 and 1) of type ndarray ((nsamples,))

Returns:

Scalar log loss

logsumexp

fitr.utils.logsumexp(x)

Numerically stable logsumexp.

Computed as follows:

$$\max x + \log \sum_{x} e^{x - \max x}$$

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Arguments:

• x: 'ndarray(shape=(nactions,))"

Returns:

float

rank data

```
fitr.utils.rank_data(x)
```

Ranks a set of observations, assigning the average of ranks to ties.

Arguments:

• x: ndarray (nsamples). Vector of data to be compared

Returns:

• ranks: ndarray (nsamples). Ranks for each observation

rank_grouped_data

```
fitr.utils.rank_grouped_data(x, g)
```

Ranks observations taken across several groups

Arguments:

- x: ndarray (nsamples). Vector of data to be compared
- g: ndarray (nsamples). Group ID's

Returns:

- ranks: ndarray (nsamples). Ranks for each observation
- G: ndarray (nsamples, ngroups). Matrix indicating whether sample i is in group j
- R: ndarray ((nsamples, ngroups)). Matrix indicating the rank for sample i in group j
- lab: ndarray (ngroups). Group labels

reduce then tile

```
fitr.utils.reduce_then_tile(X, f, axis=1)
```

Computes some reduction function over an axis, then tiles that vector to create matrix of original size

- **X**: ndarray ((n, m)). Matrix.
- f: function that reduces data across some axis (e.g. np.sum(), np.max())

• axis: int which axis the data should be reduced over (only goes over 2 axes for now)

Returns:res

```
ndarray((n, m))
```

Examples:

Here is one way to compute a softmax function over the columns of X, for each row.

```
import numpy as np
X = np.random.normal(0, 1, size=(10, 3))**2
max_x = reduce_then_tile(X, np.max, axis=1)
exp_x = np.exp(X - max_x)
sum_exp_x = reduce_then_tile(exp_x, np.sum, axis=1)
y = exp_x/sum_exp_x
```

relu

```
fitr.utils.relu(x, a_max=None)
```

Rectified linearity

$$\mathbf{x}' = \max(x_i, 0)_{i=1}^{|\mathbf{x}|}$$

Arguments:

- x: Vector of inputs
- a_max: Upper bound at which to clip values of x

Returns:

Exponentiated values of x.

scale_data

```
fitr.utils.scale_data(X, axis=0, with_mean=True, with_var=True)
```

Rescales data by subtracting mean and dividing by variance

$$\mathbf{x}' = \frac{\mathbf{x} - \frac{1}{n} \mathbf{1}^{\mathsf{T}} \mathbf{x}}{Var(\mathbf{x})}$$

- X: ndarray ((nsamples, [nfeatures])). Data. May be 1D or 2D.
- with mean: bool. Whether to subtract the mean
- with_var: bool. Whether to normalize for variance

Returns:

ndarray (X. shape). Rescaled data.

sigmoid

fitr.utils.sigmoid(x, a_min=-10, a_max=10)

Sigmoid function

$$\sigma(x) = \frac{1}{1 + e^{-x}}$$

Arguments:

- x: Vector
- a_min: Lower bound at which to clip values of x
- a_max: Upper bound at which to clip values of x

Returns:

Vector between 0 and 1 of size x.shape

softmax

fitr.utils.softmax(x)

Computes the softmax function

$$p(\mathbf{x}) = \frac{e^{\mathbf{x} - \max_i x_i}}{\mathbf{1}^\top e^{\mathbf{x} - \max_i x_i}}$$

Arguments:

• x: Softmax logits (ndarray ((N,)))

Returns:

Vector of probabilities of size ndarray ((N,))

stable_exp

fitr.utils.stable_exp(x, a_min=-10, a_max=10)

Clipped exponential function

Avoids overflow by clipping input values.

- x: Vector of inputs
- a_min: Lower bound at which to clip values of x
- a_max: Upper bound at which to clip values of x

Returns:

Exponentiated values of x.

transform

```
fitr.utils.transform(x, f_list)
```

Transforms parameters from domain in x into some new domain defined by f_list

Arguments:

- x: ndarray ((nparams,)). Parameter vector in some domain.
- **f_list**: list where len(list) == nparams. Functions defining coordinate transformations on each element of x.

Returns:

• x_: ndarray ((nparams,)) . Parameter vector in new coordinates.

Examples:

Applying fitr transforms can be done as follows.

```
import numpy as np
from fitr.utils import transform, sigmoid, relu

x = np.random.normal(0, 5, size=3)
x_= transform(x, [sigmoid, relu, relu])
```

You can also apply other functions, so long as dimensions are equal for input and output.

```
import numpy as np
from fitr.utils import transform

x = np.random.normal(0, 10, size=3)
x_ = transform(x, [np.square, np.sqrt, np.exp])
```