https://neorl.readthedocs.io/en/latest/index.html

NEORL Workshop
(NeuroEvolution Optimization with Reinforcement Learning)

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American Nuclear Society
Oak Ridge/Knoxville Section

M&C 2021

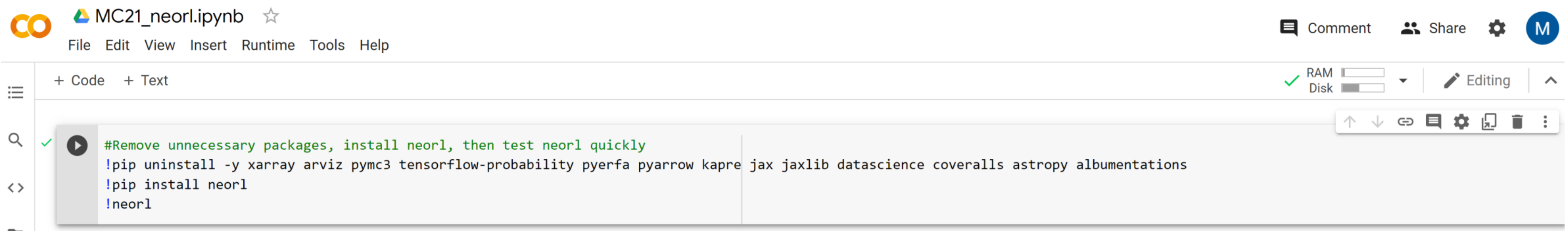
Oct 3rd, 2021

Massachusetts Institute of Technology

Lets Setup our Colab Early on

- Go to colab and start a new session.
  - https://colab.research.google.com/notebooks/intro.ipynb#recent=true
- Name the session the way you like (e.g. MC21_neorl.ipynb).
- Run the following commands:

```
#Remove unnecessary packages, install neorl, then test neorl quickly
!pip uninstall -y xarray arviz pymc3 tensorflow-probability pyerfa pyarrow kapre jax jaxlib datascience coveralls astropy albumentations
!pip install neorl
!neorl
```



Content

- **Background**
- NEORL Framework
- Problem 1: Ackley Mathematical Function
- Problem 2: Pressure Vessel Design
- Problem 3: Three-bar Truss (Homework)
- Summary

Optimization

Single-objective optimization

$$\min_{\vec{x}} \ f(\vec{x}),$$

subject to,

$$g_i(\vec{x}) \geq 0, \quad i = 1, 2, ..., m,$$

$$h_j(\vec{x}) = 0, \quad j = 1, 2, ..., p,$$

Multi-objective optimization

$$\min_{\vec{x}} \ F(\vec{x}) = (f_1(\vec{x}), f_2(\vec{x}), ..., f_k(\vec{x}))$$

subject to,

$$g_i(\vec{x}) \geq 0, \quad i = 1, 2, ..., m,$$

$$h_j(\vec{x}) = 0, \quad j = 1, 2, ..., p,$$

$$k \geq 2,$$

Optimization while in high school

4. An open-top box with a square bottom and rectangular sides is to have a volume of 256 cubic inches. Find the dimensions that require the *minimum* amount of material.

$$S = x^2 + 4xy$$

$$V = x^2 y = 256$$

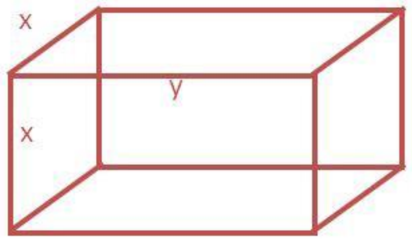
$$\rightarrow S = x^2 + 4x\left(\frac{256}{x^2}\right)$$

$$S = x^2 + \frac{1024}{x}$$

$$S' = 2x - \frac{1024}{x^2}$$

$$0 = 2x - \frac{1024}{x^2}$$

$$\boxed{x = 8 \quad \rightarrow y = 4}$$



$$S'' = 2 + \frac{2048}{x^3} > 0$$

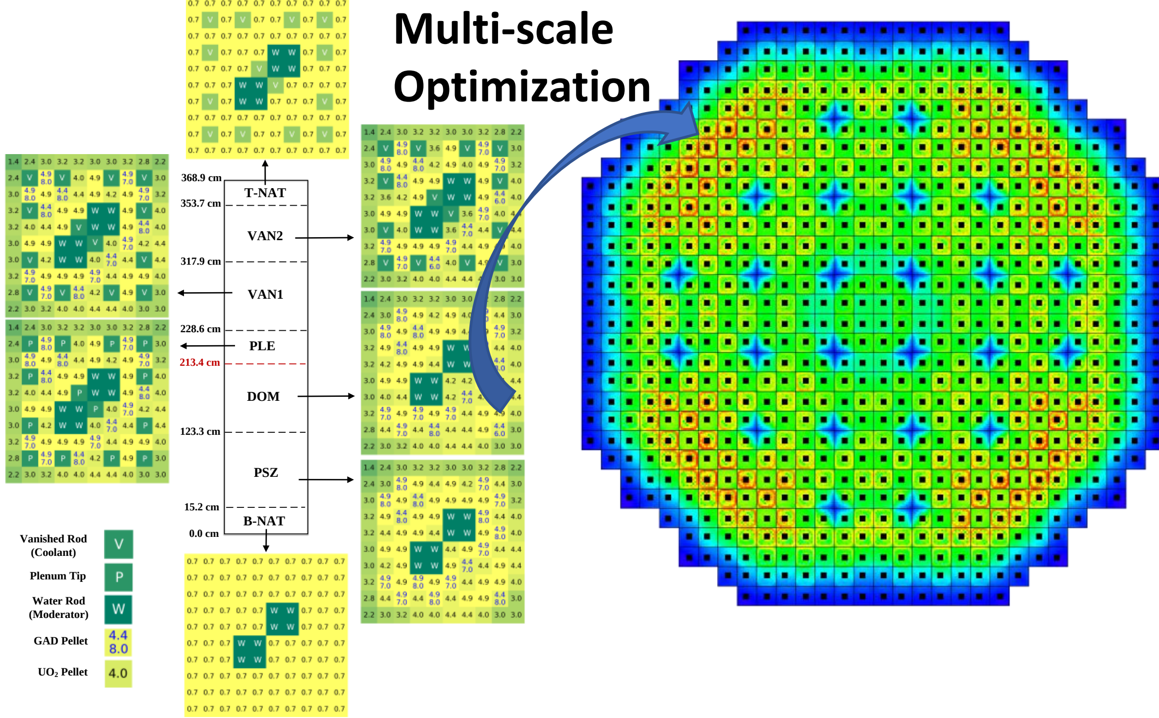
therefore a min

8 x 8 x 4

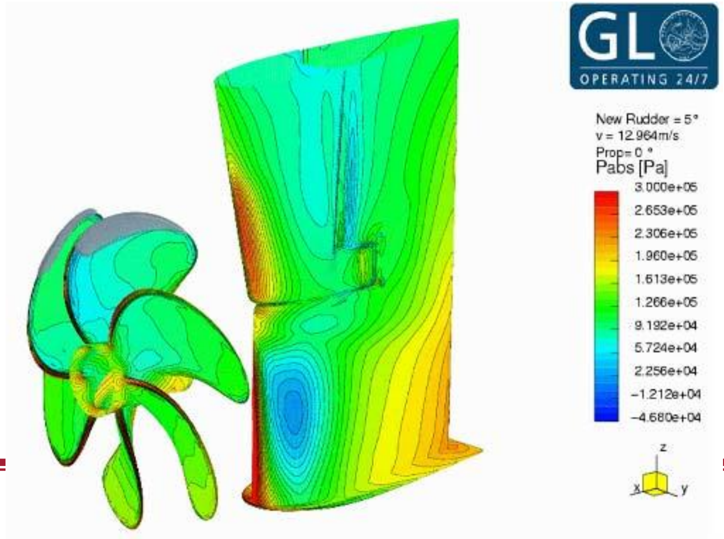
Large-scale optimization

- We don’t always have a closed-form objective function!
- We don’t always have access to derivatives!
- We don’t always have fast analytical computation!
- **Thus, we need smart optimizers!**

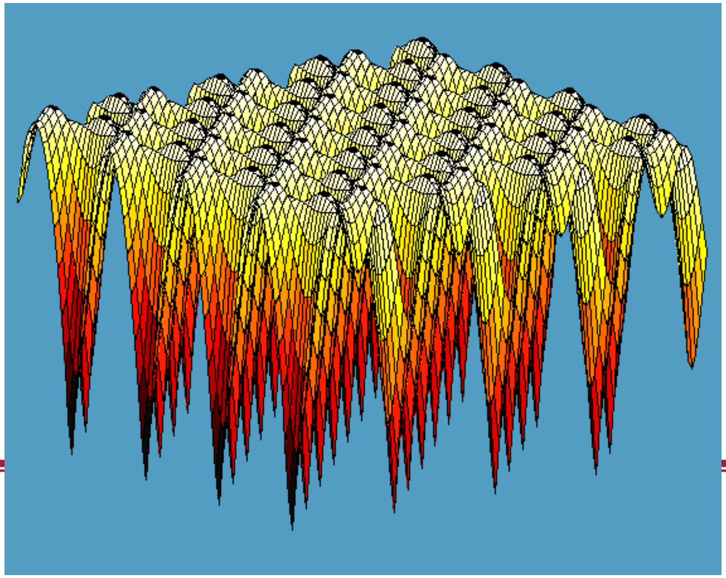
Multi-scale Optimization



Expensive Simulations



Multimodal Multi-local Optima



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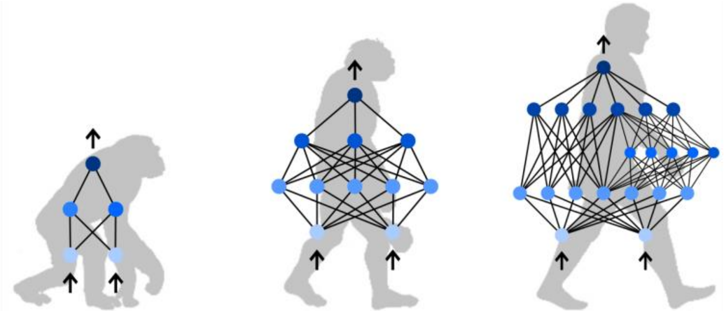
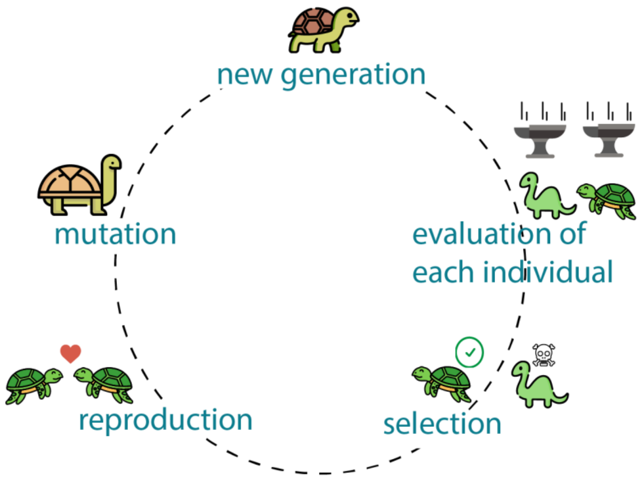
Optimization Categories

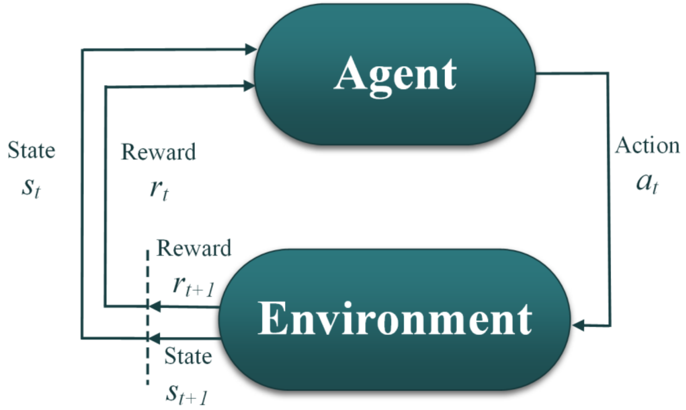


Hybrid Algorithms (Neuroevolution)



Evolutionary Algorithms (Metaheuristics)

Neural Networks (Reinforcement Learning)



For gradient-based algorithms, see:
https://nlopt.readthedocs.io/en/latest/
https://docs.scipy.org/doc/scipy/reference/optimize.html

NEORL in a Nutshell

https://neorl.readthedocs.io/en/latest/index.html

Basic Features

Features	NEORL
Reinforcement Learning (standalone)	✔
Evolutionary Computation (standalone)	✔
Hybrid Neuroevolution	✔
Supervised Learning	✔
Parallel processing	✔
Combinatorial/Discrete Optimization	✔
Continuous Optimization	✔
Mixed Discrete/Continuous Optimization	✔
Hyperparameter Tuning	✔
Ipython / Notebook friendly	✔
Detailed Documentation	✔
Advanced logging	✔
Optimization Benchmarks	✔

Implemented Algorithms

NEORL offers a wide range of algorithms, where some algorithms could be used with a specific parameter space.

Algorithm	Discrete Space	Continuous Space	Mixed Space	Multiprocessing
ACER	✔	✘	✘	✔
ACKTR	✔	✔	✔	✔
A2C	✔	✔	✔	✔
PPO	✔	✔	✔	✔
DQN	✔	✘	✘	✘
ES	✔	✔	✔	✔
PSO	✔	✔	✔	✔
DE	✔	✔	✔	✔
XNES	✘	✔	✘	✔
GWO	✔	✔	✔	✔
PESA	✔	✔	✔	✔
PESA2	✔	✔	✔	✔
RNEAT	✘	✔	✘	✔
FNEAT	✘	✔	✘	✔
SA	✔	✔	✔	✔
SSA	✔	✔	✔	✔
WOA	✔	✔	✔	✔
JAYA	✔	✔	✔	✔
MFO	✔	✔	✔	✔
HHO	✔	✔	✔	✔
BAT	✔	✔	✔	✔
PPO-ES	✔	✔	✔	✔
ACKTR-DE	✔	✔	✔	✔
ACO	✘	✔	✘	✔
NGA	✘	✔	✘	✘
NHHO	✔	✔	✔	✔
CS	✔	✔	✔	✔
TS	✔	✔	✘	✘

NEORL Team

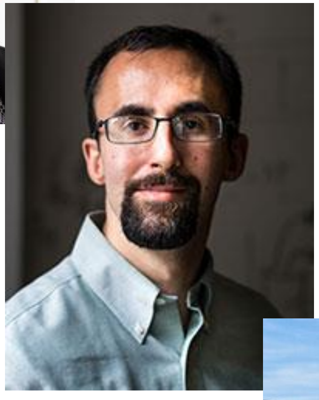
Katelin

Haijia

Devin

John

Paul



Koroush

Xubo

Majdi

NEORL Detailed Documentation

https://neorl.readthedocs.io/en/latest/index.html

Neuro**E**volution **O**ptimization with **R**einforcement **L**earning

NEORL

latest

Search docs

GENERAL GUIDE

- Quick Installation
- Detailed Installation
- Getting Started
- Reinforcement Learning
- Evolutionary Algorithms
- Hyperparameter Tuning

ALGORITHMS

- Advantage Actor Critic (A2C)
- Actor-Critic with Experience Replay (ACER)
- Actor Critic using Kronecker-Factored Trust Region (ACKTR)
- Deep Q Learning (DQN)

» Welcome to NEORL Website!

Edit on GitHub

Welcome to NEORL Website!

Latest News:

- September 10, 2021: First NEORL stable release 1.6 is out.

Primary contact to report bugs/issues: Majdi I. Radaideh (radaideh@mit.edu)

NEORL (**N**euro**E**volution **O**ptimisation with **R**einforcement **L**earning) is a set of implementations of hybrid algorithms combining neural networks and evolutionary computation based on a wide range of machine learning and evolutionary intelligence architectures. NEORL aims to solve large-scale optimisation problems relevant to operation & optimisation research, engineering, business, and other disciplines.

Github repository: https://github.com/mradaideh/neorl

Copyright

You can read the first successful application of NEORL for nuclear fuel optimisation in this News Article.

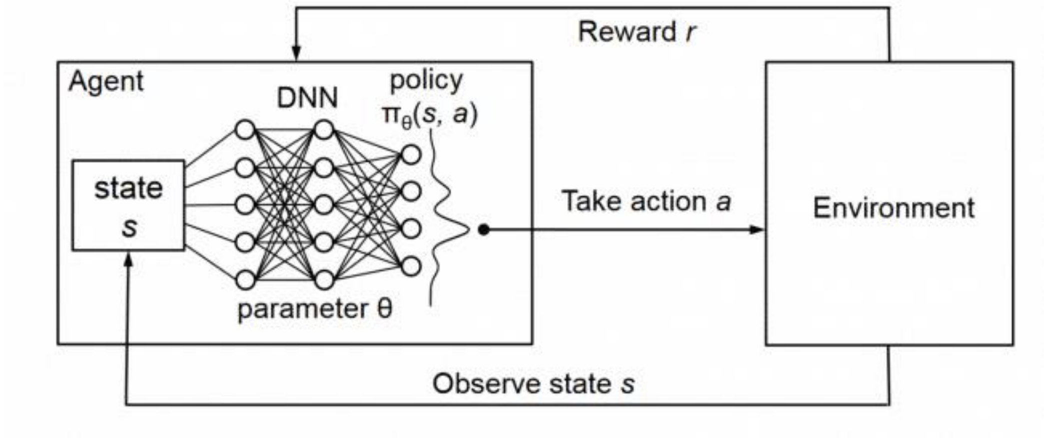
User Guide

General Guide

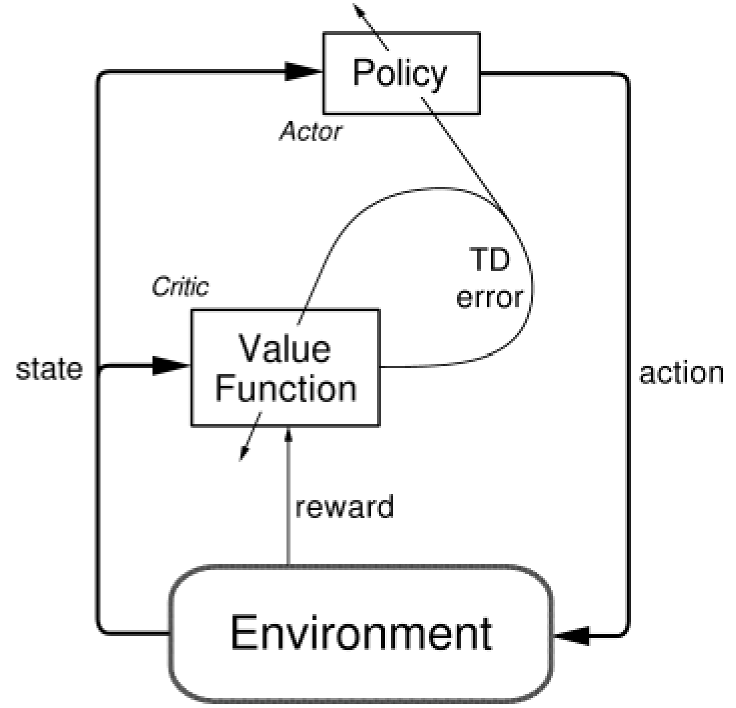
Neural-based Algorithms

- Reinforcement Learning: Combination of **state-reward-action** learning, guided by **deep neural networks**
  - PPO
  - ACKTR
  - A2C
  - DQN
  - ACER

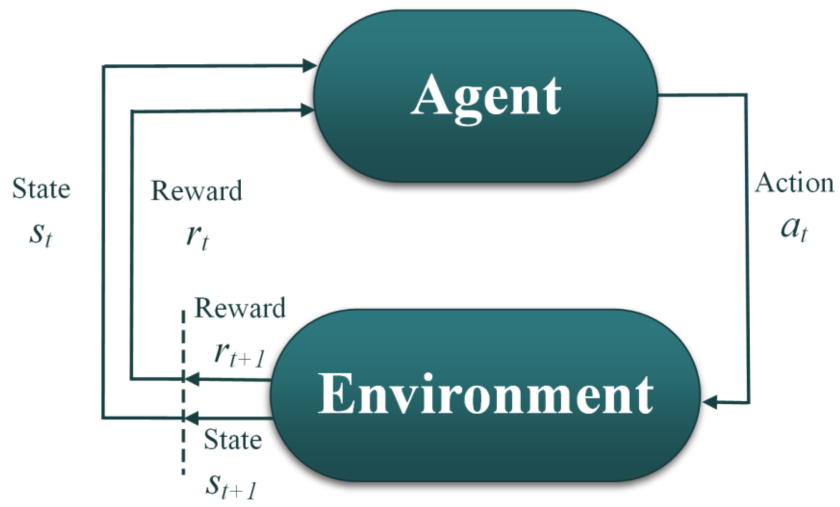
Deep Q Learning



Actor-Critic Policies



General RL

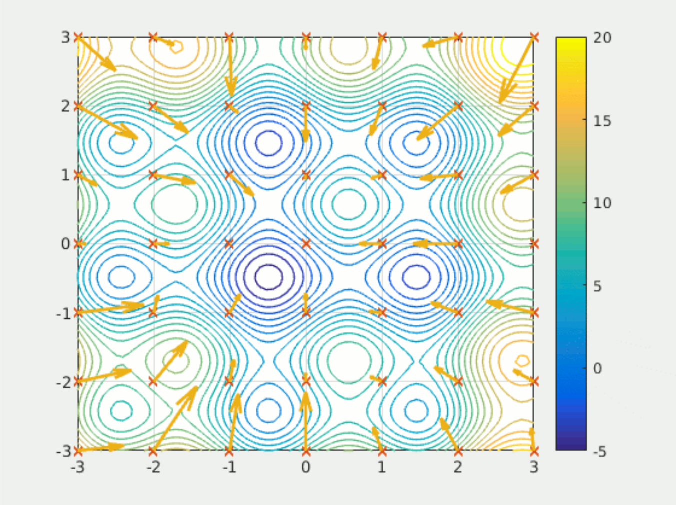


Evolutionary Algorithms

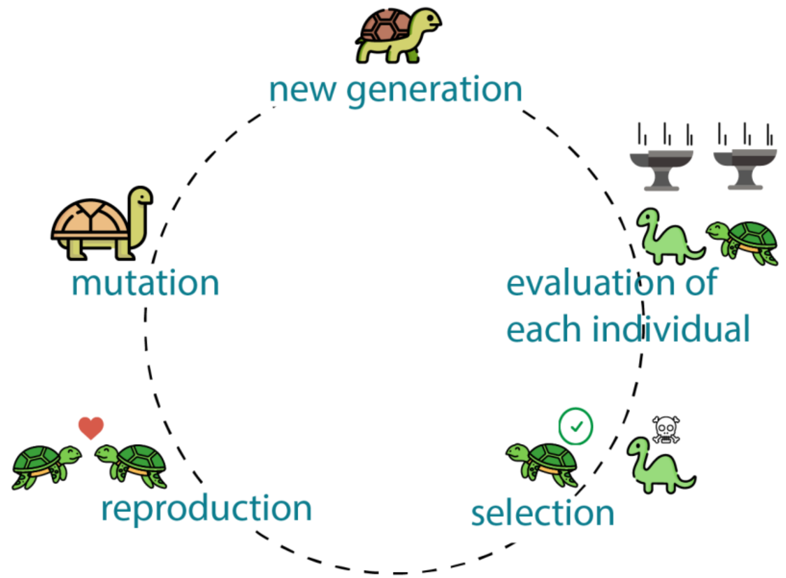
https://neorl.readthedocs.io/en/latest/index.html

- 1- Random population is generated,
- 2- Population is evaluated by a fitness function,
- 3- Best individuals are survived for next generation.
- 4- The population is updated using natural operations (crossover, mutation, hunting strategies) for next generation.
- Repeat 1-4

Particle Swarm Optimization



Genetic Algorithms

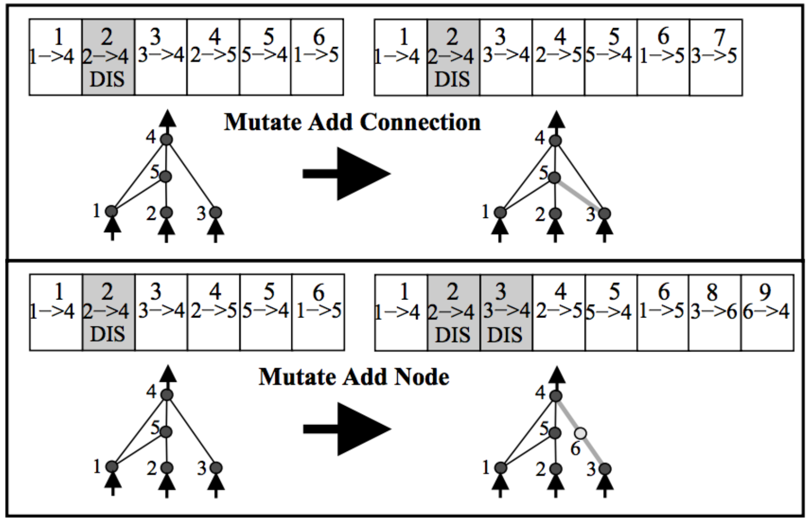


Grey wolf Optimization

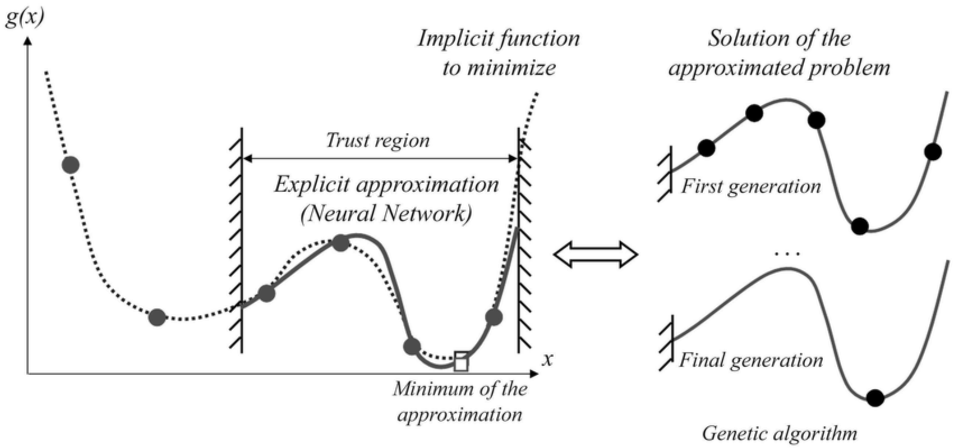
Hybrid/Neuroevolution Algorithms

- **Neuroevolution algorathims are advanced optimizers:**
- NEAT (RNEAT, FNEAT)
- PESA
- PESA2
- PPO-ES
- ACKTR-DE
- NHHO
- NGA

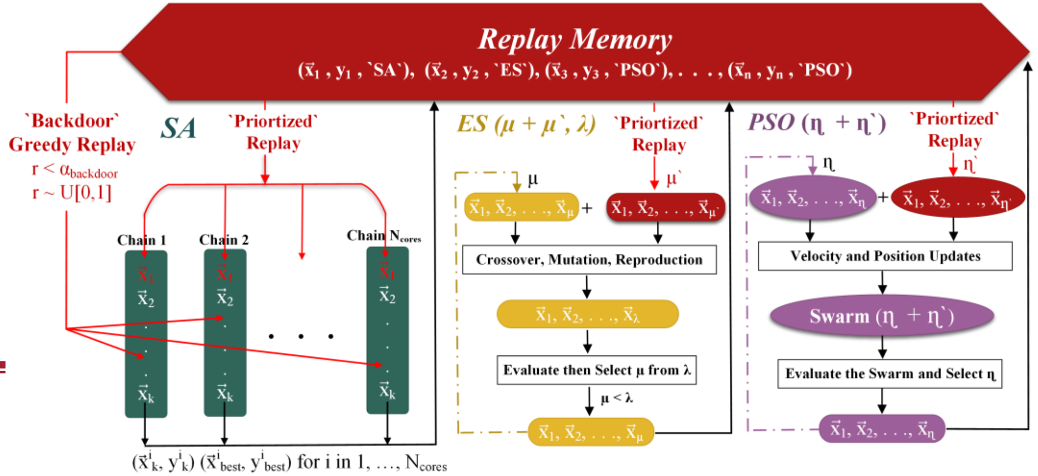
Neuroevolution of Augmenting Topologies (NEAT)



Surrogate-based Evolutionary Algorithms

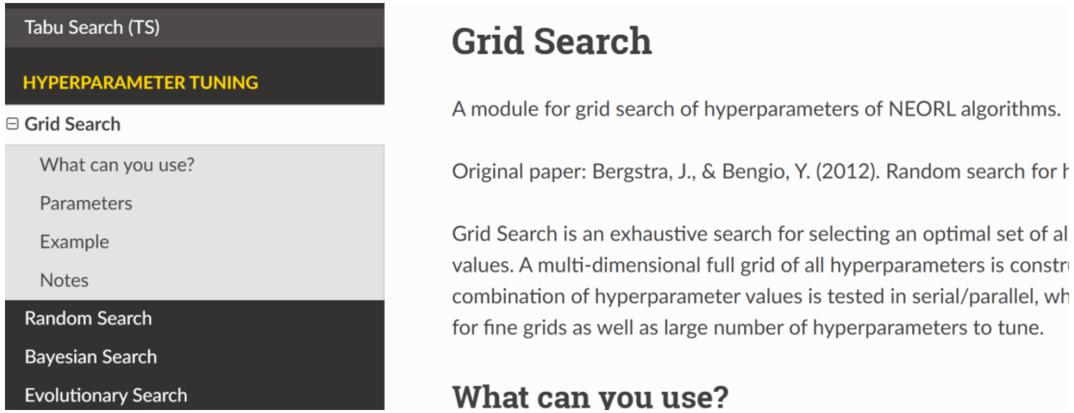


Prioritized replay Evolutionary and Swarm Algorithm (PESA)



Hyperparameter Tuning and Parallel Computing

- Tune the optimizer hyperparameters **for maximum performance**
- NEORL offers **four automatic tuners**!


Tabu Search (TS)
HYPERPARAMETER TUNING
⊟ Grid Search
What can you use?
Parameters
Example
Notes
Random Search
Bayesian Search
Evolutionary Search

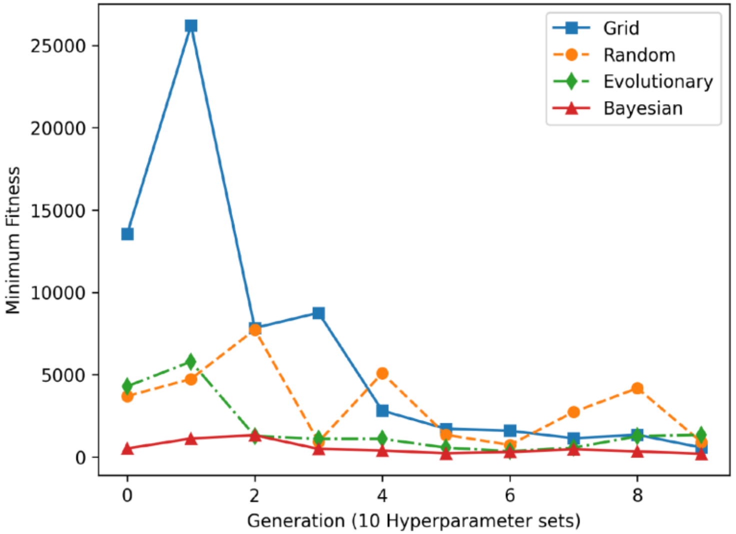
Grid Search

A module for grid search of hyperparameters of NEORL algorithms.

Original paper: Bergstra, J., & Bengio, Y. (2012). Random search for h

Grid Search is an exhaustive search for selecting an optimal set of al values. A multi-dimensional full grid of all hyperparameters is constru combination of hyperparameter values is tested in serial/parallel, wh for fine grids as well as large number of hyperparameters to tune.

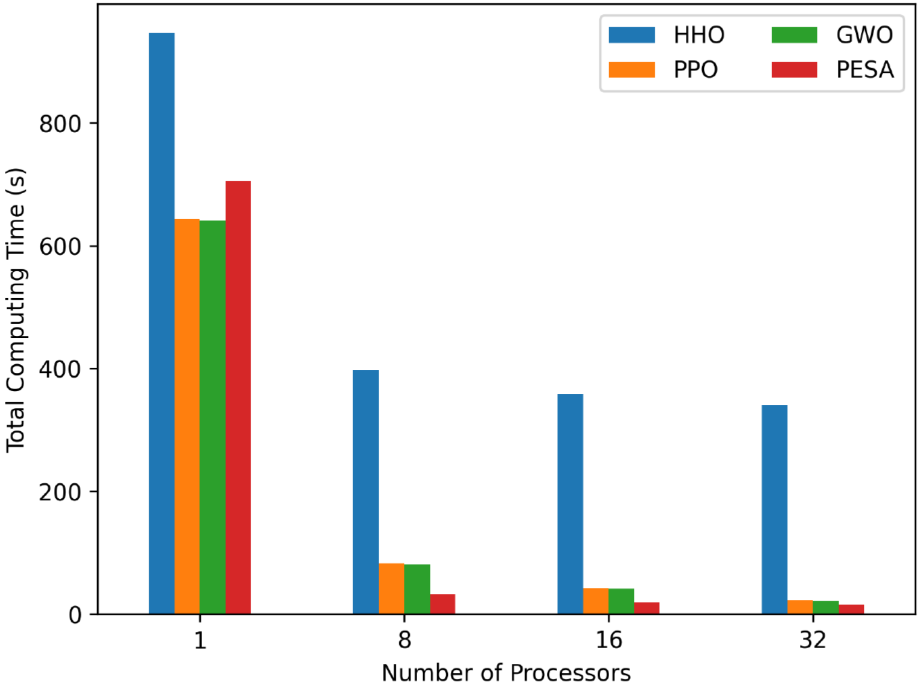
What can you use?



- **Automatic search** makes hyperparameter tuning a much **less burden** to **focus on the optimization** problem itself!

Parallelization in NEORL is straightforward, turn on "ncores" flag!

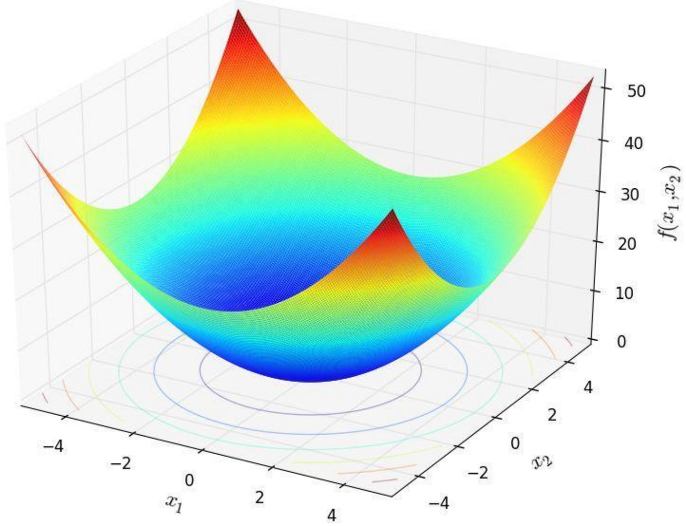
```
gwo=GWO(mode='min', bounds=BOUNDS,
fit=ACKLEY, nwolves=20, ncores=16, seed=1)
```



Toy Example (Sphere Function)

```
#1- Import an algorithm from NEORL
from neorl import DE

#2- Define the fitness function
def FIT(individual):
    #sphere function
    y=sum(x**2 for x in individual)
    return y

#3-Setup the parameter space (n=5)
nx=5
BOUNDS={}
for i in range(1,nx+1):
    BOUNDS['x'+str(i)]=['float', -5.12, 5.12]

#4- setup and run the optimizer
de=DE(mode='min', bounds=BOUNDS, fit=FIT, npop=60, F=0.5, CR=0.7, ncores=1, seed=1)
x_best, y_best, de_hist=de.evolute(ngen=100, verbose=1)

print(x_best, y_best)
```

2D Sphere (n=2)



$$f(x_1 \cdots x_n) = \sum_{i=1}^{n} x_i^2$$

$$-5.12 \leq x_i \leq 5.12$$

$$\text{minimum at } f(0, \cdots, 0) = 0$$

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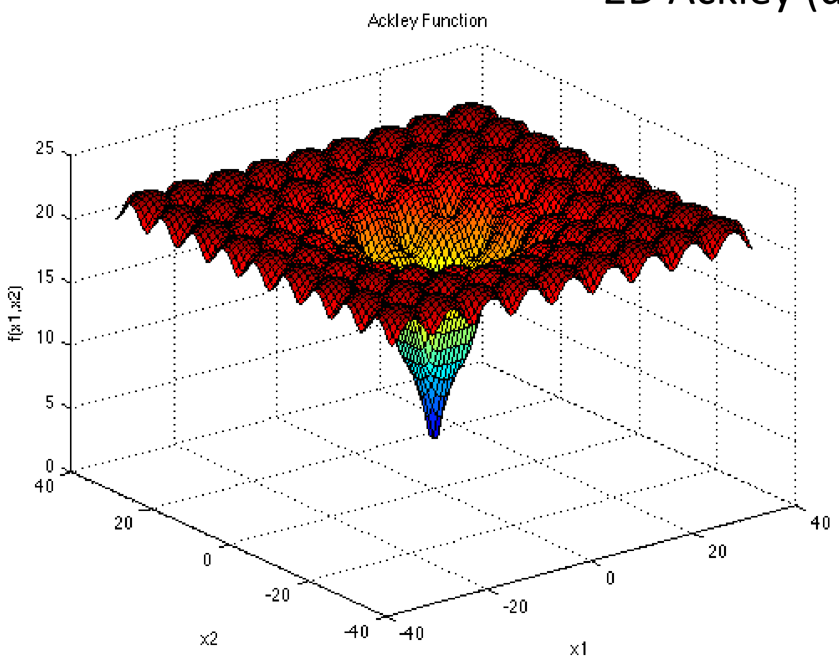
Problem Statement

2D Ackley (d=2)



- Find the optimal value of $\vec{x}$ *such that $f(\vec{x})$ is minimized, where d=10.*
- Solution through NEORL:
  - Set the objective function.
  - Set the parameter space.
  - Set the algorithm object.
  - Optimize!
  - Make a plot (optional)

$$f(\vec{x}) = 20 - 20exp\Big(-0.2\sqrt{\frac{1}{d}\sum_{i=1}^{d} x_i^2}\Big) - exp\Big(\frac{1}{d}\sum_{i=1}^{d} cos(2\pi x_i)\Big) + exp(1)$$

$x_i \in [-32, 32]$, for all $i = 1, \ldots, d$.

Sample Script

- DE group
  - Use hyperparameters **npop=80, F=0.3, CR=0.7**
  - Set **seed = 1**.
  - Use **ngen=120** in evolute function.
  - For plotting access the fitness via the key fitness in the returned dictionary.
    - **x_gwo, y_gwo, gwo_hist=gwo.evolute(ngen=120, verbose=1)**
    - Use **gwo_hist['fitness']** for plotting.
- GWO group
  - Use **nwolves=20**
  - Set **seed = 1**
  - Use **ngen=120** in evolute function
  - For plotting access the fitness directly from the variable fitness.
    - **x_de, y_de, de_hist=de.evolute(ngen=120, verbose=1)**
    - Use **de_hist** for plotting.

```python
#---------------------------------
# Import packages
#---------------------------------
import numpy as np
import matplotlib.pyplot as plt
from neorl import DE, GWO
from math import exp, sqrt, cos, pi
#---------------------------------
# Fitness function
#---------------------------------
def ACKLEY(individual):
    #Ackley objective function.
    d = len(individual)
    f=20 - 20 * exp(-0.2*sqrt(1.0/d * sum(x**2 for x in individual))) \
            + exp(1) - exp(1.0/d * sum(cos(2*pi*x) for x in individual))
    return f
#---------------------------------
# Parameter Space
#---------------------------------
#Setup the parameter space (d=8)
d=10
lb=-32
ub=32
BOUNDS={}
for i in range(1,d+1):
    BOUNDS['x'+str(i)]=['float', lb, ub]
#---------------------------------
# GWO
#---------------------------------
gwo=GWO(mode='min', bounds=BOUNDS, fit=ACKLEY, nwolves=20, seed=1)
x_gwo, y_gwo, gwo_hist=gwo.evolute(ngen=120, verbose=1)
#---------------------------------
# DE
#---------------------------------
de=DE(mode='min', bounds=BOUNDS, fit=ACKLEY, npop=80, F=0.3, CR=0.7, ncores=1,
seed=1)
x_de, y_de, de_hist=de.evolute(ngen=120, verbose=1)
#---------------------------------
# Plot
#---------------------------------
#Plot fitness for both methods
plt.figure()
plt.plot(gwo_hist['fitness'], label='GWO')
plt.plot(np.array(de_hist), label='DE')
plt.xlabel('Generation')
plt.ylabel('Fitness')
plt.legend()
plt.savefig('ackley_fitness.png',format='png', dpi=300, bbox_inches="tight")
plt.show()
```

Required arguments in NEORL algorithms:

mode, bounds, fit

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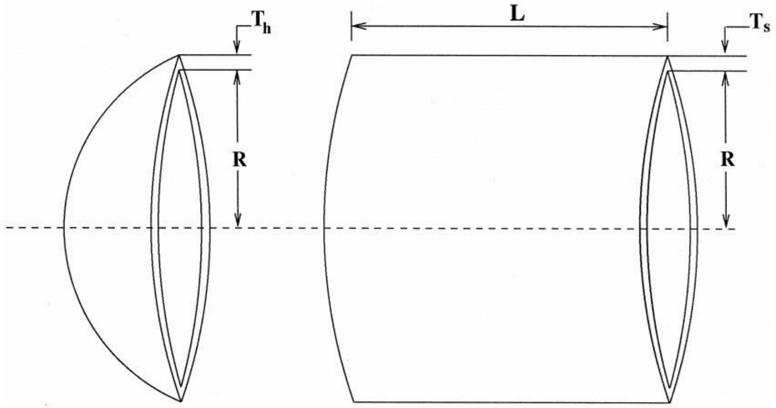
Problem Statement

- Find the optimal value of $\vec{x}$
  - $T_s = x_1$
  - $T_h = x_2$
  - $R = x_3$
  - $L = x_4$
  - such that *$f(\vec{x})$* is minimized (cost of pressure vessel is minimized)
- Solution through NEORL:
  - Set the objective function, including the constraints.
  - Set the parameter space.
  - Set the algorithm object.
  - Optimize!
  - Make a plot (optional).



$$\min_{\vec{x}} f(\vec{x}) = 0.6224x_1x_3x_4 + 1.7781x_2x_3^2 + 3.1661x_1^2x_4 + 19.84x_1^2x_3,$$

$$g_1 = -x_1 + 0.0193x_3 \leq 0,$$
$$g_2 = -x_2 + 0.00954x_3 \leq 0,$$
$$g_3 = -\pi x_3^2x_4 - \frac{4}{3}\pi x_3^3 + 1296000 \leq 0,$$
$$g_4 = x_4 - 240 \leq 0,$$

$0.0625 \leq x_1 \leq 6.1875$ (with step of 0.0625)

$$x_2 \in \{0.0625, 0.125, 0.1875, 0.25, 0.3125, 0.375, 0.4375, 0.5, 0.5625, 0.625\}$$

$$10 \leq x_3 \leq 200,$$

$$10 \leq x_4 \leq 200$$

Problem Setup

Required arguments in NEORL algorithms:

mode, bounds, fit

- HHO group
  - Use hyperparameters **nhawks=50, int_transform='minmax'**
  - Set **seed = 1**.
  - Use **ngen=200** in evolute function.
  - For plotting access the fitness via the key fitness in the returned dictionary.
    - **x_hho, y_hho, hho_hist=hho.evolute(ngen=200, verbose=False)**
    - Use **hho_hist['global_fitness']** for plotting.
- BAT group
  - Use **nbats=50, levy = True**
  - Set **seed = 1**
  - Use **ngen=200** in evolute function
  - For plotting access the fitness directly from the variable fitness.
    - **x_bat, y_bat, bat_hist=bat.evolute(ngen=200, verbose=1)**
    - Use **bat_hist['global_fitness']** for plotting.

```python
def Vessel(individual):
    """
    Pressure vesssel design
    x1: thickness (d1)  --> discrete value multiple of 0.0625 in
    x2: thickness of the heads (d2) ---> categorical value from a pre-defined grid
    x3: inner radius (r)  ---> cont. value between [10, 200]
    x4: length (L)  ---> cont. value between [10, 200]
    """
    x=individual.copy()
    x[0] *= 0.0625   #convert d1 to "in"
    y = 0.6224*x[0]*x[2]*x[3]+1.7781*x[1]*x[2]**2+3.1661*x[0]**2*x[3]+19.84*x[0]**2*x[2];
    g1 = -x[0]+0.0193*x[2];
    g2 = -x[1]+0.00954*x[2];
    g3 = -math.pi*x[2]**2*x[3]-(4/3)*math.pi*x[2]**3 + 1296000;
    g4 = x[3]-240;
    g=[g1,g2,g3,g4]
    phi=sum(max(item,0) for item in g)
    eps=1e-5 #tolerance to escape the constraint region
    penality=1e6 #large penality to add if constraints are violated
    if phi > eps:
        fitness=phi+penality
    else:
        fitness=y
    return fitness
```

Sample Script

```python
########################
# Import Packages
########################
from neorl import HHO, BAT
import math
import matplotlib.pyplot as plt
#################################
# Define Vessel Function
#Mixed discrete/continuous/grid
#################################
def Vessel(individual):
    """
    Pressure vesssel design
    x1: thickness (d1)  --> discrete value multiple of 0.0625 in
    x2: thickness of the heads (d2) ---> categorical value from a pre-defined grid
    x3: inner radius (r)  ---> cont. value between [10, 200]
    x4: length (L)  ---> cont. value between [10, 200]
    """
    x=individual.copy()
    x[0] *= 0.0625   #convert d1 to "in"
    y = 0.6224*x[0]*x[2]*x[3]+1.7781*x[1]*x[2]**2+3.1661*x[0]**2*x[3]+19.84*x[0]**2*x[2];
    g1 = -x[0]+0.0193*x[2];
    g2 = -x[1]+0.00954*x[2];
    g3 = -math.pi*x[2]**2*x[3]-(4/3)*math.pi*x[2]**3 + 1296000;
    g4 = x[3]-240;
    g=[g1,g2,g3,g4]
    phi=sum(max(item,0) for item in g)
    eps=1e-5 #tolerance to escape the constraint region
    penality=1e6 #large penality to add if constraints are violated
    if phi > eps:
        fitness=phi+penality
    else:
        fitness=y
    return fitness
########################
# Setup the Space
########################
bounds = {}
bounds['x1'] = ['int', 1, 99]
bounds['x2'] = ['grid', (0.0625, 0.125, 0.1875, 0.25, 0.3125, 0.375, 0.4375, 0.5, 0.5625, 0.625)]
bounds['x3'] = ['float', 10, 200]
bounds['x4'] = ['float', 10, 200]
```

```python
########################
# Setup and evolute HHO
########################
hho = HHO(mode='min', bounds=bounds, fit=Vessel, nhawks=50,
                  int_transform='minmax', ncores=1, seed=1)
x_hho, y_hho, hho_hist=hho.evolute(ngen=200, verbose=False)
########################
# Setup and evolute BAT
########################
bat=BAT(mode='min', bounds=bounds, fit=Vessel, nbats=50, levy = True, seed
= 1, ncores=1)
x_bat, y_bat, bat_hist=bat.evolute(ngen=200, verbose=1)
########################
# Plotting
########################
plt.figure()
plt.plot(hho_hist['global_fitness'], label='HHO')
plt.plot(bat_hist['global_fitness'], label='BAT')
plt.xlabel('Generation')
plt.ylabel('Fitness')
plt.ylim([0,10000]) #zoom in
plt.legend()
plt.savefig('ex8_pv_fitness.png',format='png', dpi=300,
bbox_inches="tight")
########################
# Comparison
########################
print('---Best HHO Results---')
print(x_hho)
print(y_hho)
print('---Best BAT Results---')
print(x_bat)
print(y_bat)
```

Content

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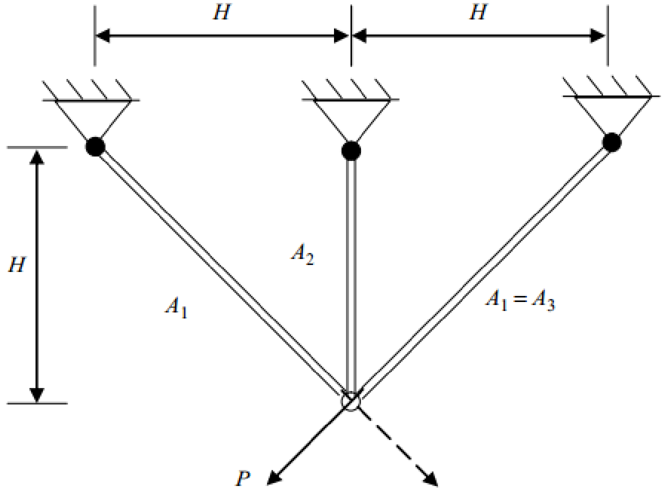
- **Problem 3: Three-bar Truss (Homework)**
- Summary

Three-bar Truss (Enjoy it!)

- Solve it with PSO and MFO in NEORL.
- Look for a minimum $f(\vec{x})$ of **263.9**




```python
#----------------------------------
# Fitness function
#----------------------------------
def TBT(individual):
    """Three-bar truss Design
    """
    x1 = individual[0]
    x2 = individual[1]
    y = (2*sqrt(2)*x1 + x2) * 100

    #Constraints
    if x1 <= 0:
            g = [1,1,1]
    else:
            g1 = (sqrt(2)*x1+x2)/(sqrt(2)*x1**2 + 2*x1*x2) * 2 - 2
            g2 = x2/(sqrt(2)*x1**2 + 2*x1*x2) * 2 - 2
            g3 = 1/(x1 + sqrt(2)*x2) * 2 - 2
            g = [g1,g2,g3]

    g_round=np.round(np.array(g),6)
    w1=100
    w2=100
    phi=sum(max(item,0) for item in g_round)
    viol=sum(float(num) > 0 for num in g_round)

    return y + w1*phi + w2*viol
```

$$\min_{\vec{x}} f(\vec{x}) = (2\sqrt{2}x_1 + x_2) \times H,$$

$$g_1 = \frac{\sqrt{2}x_1 + x_2}{\sqrt{2}x_1^2 + 2x_1x_2}P - \sigma \leq 0,$$
$$g_2 = \frac{x_2}{\sqrt{2}x_1^2 + 2x_1x_2}P - \sigma \leq 0,$$
$$g_3 = \frac{1}{x_1 + \sqrt{2}x_2}P - \sigma \leq 0,$$

where $0 \leq x_1 \leq 1, 0 \leq x_2 \leq 1, H = 100cm, P = 2KN/cm^2$, and $\sigma = 2KN/cm^2$

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Summary

Share your NEORL project with us!

- Bring your **objective function** and let NEORL **takes care of the rest**.
- NEORL has:
  - more than 25 algorithms,
  - neural, evolutionary, and neuroevolution categories,
  - Discrete, continuous, and mixed optimization spaces,
  - parallel computing,
  - hyperparameter tuning.
  - friendly interface,
  - detailed documentation,

RL-informed Differential Evolution (ACKTR-DE)
Ant Colony Optimization (ACO)
Neural Genetic Algorithms (NGA)
Neural Harris Hawks Optimization (NHHO)
Cuckoo Search (CS)
Tabu Search (TS)

HYPERPARAMETER TUNING

Grid Search
Random Search
Bayesian Search
Evolutionary Search

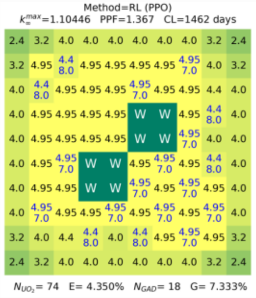
EXAMPLES

Example 1: Traveling Salesman Problem
Example 2: Ackley with EA
Example 3: Welded-beam design
Example 4: Benchmarks
Example 5: CEC'2017 Test Suite
Example 6: Three-bar Truss Design

Projects

This is a list of projects using NEORL. Please contact us if you want your project to appear on this page.

Physics-informed Reinforcement Learning Optimisation with NEORL



Optimization of nuclear fuel assemblies if performed effectively, will lead to fuel efficiency improvement, cost reduction, and safety assurance. However, assembly optimization involves solving high-dimensional and computationally expensive combinatorial problems. As such, fuel designers' expert judgement has commonly prevailed over the use of stochastic optimization (SO) algorithms such as genetic algorithms and simulated annealing. To improve the state-of-art, we explore a class of artificial intelligence (AI) algorithms, namely, reinforcement learning (RL) in this work. We propose a physics-informed AI optimization methodology by establishing a connection through reward shaping between RL and the tactics fuel designers follow in practice by moving fuel rods in the assembly to meet specific constraints and objectives. The methodology utilizes RL algorithms, deep Q learning and proximal policy optimization, and compares their performance to SO algorithms. The methodology is applied on two boiling water reactor assemblies of low-dimensional (combinations) and high-dimensional (combinations) natures. The results demonstrate that RL is more effective than SO in solving high dimensional problems, i.e., 10 × 10 assembly, through embedding expert knowledge in form of game rules and effectively exploring the search space. For a given computational resources and timeframe relevant to fuel designers, RL algorithms outperformed SO through finding more feasible patterns, 4–5 times more than SO, and through increasing search speed, as indicated by the RL outstanding computational efficiency. The results of this work clearly demonstrate RL effectiveness as another decision support tool for nuclear fuel assembly optimization.

Authors: Majdi I. Radaideh et al., 2021.
Reference: https://doi.org/10.1016/j.nucengdes.2020.110966

Questions?

- For detailed examples and info, check our website and Github:
- https://neorl.readthedocs.io/en/latest/index.html
- https://github.com/mradaideh/neorl

Thanks to our collaborators and sponsor:

You can download all workshop materials/scripts from this link:
https://github.com/mradaideh/neorl/tree/master/examples/MC-2021-workshop