# aqua-blue.aqua\_blue

# aqua-blue

Lightweight and basic reservoir computing library

```
gh-pages docs

pypi v0.2.17 python 3.9 | 3.10 | 3.11 | 3.12
```

# What is aqua-blue?

aqua-blue is a lightweight python library for reservoir computing (specifically echo state networks) depending only on numpy. aqua-blue 's namesake comes from:

- A blue ocean of data, aka a reservoir
- A very fancy cat named Blue

# Found a bug?

Please open an issue <u>here</u> if you found a bug! The easier it is to reproduce the bug, the faster we will find a solution to the problem. Please consider including the following info in your issue:

- Steps to reproduce
- Expected and actual behavior
- Version info, OS, etc.

# **Contributing**

Please see <u>CONTRIBUTING.md</u> for instructions on how to contribute to aquablue

# Installation

aqua-blue is on PyPI, and can therefore be installed with pip:

```
pip install aqua-blue
```

# Quickstart

```
import numpy as np
import aqua_blue
# generate arbitrary two-dimensional time series
```

```
\# y_1(t) = \cos(t), y_2(t) = \sin(t)
# resulting dependent variable has shape (number of timesteps, 2)
t = np.linspace(0, 4.0 * np.pi, 10 000)
y = np.vstack((2.0 * np.cos(t) + 1, 5.0 * np.sin(t) - 1)).T
# create time series object to feed into echo state network
time series = aqua blue.time series.TimeSeries(dependent variable=y, times=t)
# normalize
normalizer = aqua blue.utilities.Normalizer()
time series = normalizer.normalize(time series)
# make model and train
model = aqua blue.models.Model(
   reservoir=aqua blue.reservoirs.DynamicalReservoir(
       reservoir_dimensionality=100,
        input dimensionality=2
    ),
    readout=aqua blue.readouts.LinearReadout()
model.train(time series)
# predict and denormalize
prediction = model.predict(horizon=1 000)
prediction = normalizer.denormalize(prediction)
```

# License

agua-blue is released under the MIT License.



Blue, the cat behind aqua-blue.

# **Examples**

# **Basic Lotka-Volterra example**

Below is an example of using aqua-blue to predict the predator-prey <u>Lotka-Volterra equations</u>:

```
\dot{x} = \alpha x - \beta x y \dot{y} = -\gamma y + \delta x y
```

with parameters  $\alpha=0.1$ ,  $\beta=0.02$ ,  $\gamma=0.3$ , and  $\delta=0.01$ , and initial conditions  $(x_0,y_0)=(20,9)$ . We train a reservoir computer with a reservoir dimensionality of 1000 over  $0 \le t \le 10$ , with 1000 timesteps. Then, we predict the next 1000 timesteps.

Here, we use <code>scipy.integrate.solve\_ivp</code> to integrate the system of differential equations.

```
import numpy as np
from scipy.integrate import solve ivp
import matplotlib.pyplot as plt
import aqua blue
def lotka volterra(t, z, alpha, beta, delta, gamma):
   x, y = z
   dxdt = alpha * x - beta * x * y
   dydt = delta * x * y - gamma * y
   return [dxdt, dydt]
def solve lv(t start, t end, no, alpha=0.1, beta=0.02, gamma=0.3, delta=0.01, x0=20,
y0=9):
   t eval = np.linspace(t start, t end, no)
   solution = solve ivp(lotka volterra, [t start, t end], [x0, y0], t eval=t eval,
args=(alpha, beta, delta, gamma))
   x, y = solution.y
   lotka volterra array = np.vstack((x, y)).T
   return lotka volterra array
def main():
   y = solve lv(0, 10, 1000)
   t = np.linspace(0, 10, 1000)
    time series = aqua blue.time series.TimeSeries(dependent variable=y, times=t)
   normalizer = aqua blue.utilities.Normalizer()
    time series = normalizer.normalize(time series)
```

```
model = aqua blue.models.Model(
        reservoir=aqua blue.reservoirs.DynamicalReservoir(
            reservoir dimensionality=100,
            input dimensionality=2
       ),
        readout=aqua blue.readouts.LinearReadout()
   model.train(time series)
   prediction = model.predict(horizon=1 000)
    prediction = normalizer.denormalize(prediction)
    actual future = solve lv(prediction.times[0], prediction.times[-1], 1 000)
   plt.plot(prediction.times, actual future)
    plt.xlabel('t')
    plt.plot(prediction.times, prediction.dependent variable)
    plt.legend(['actual x', 'actual y', 'predicted x', 'predicted y'], shadow=True)
    plt.title('Lotka-Volterra System')
    plt.show()
if __name__ == "__main__":
   main()
```

# Using datetime objects

Below is an example of a simple sine-cosine task similar to above, using datetime objects as times.

```
import numpy as np
import matplotlib.pyplot as plt

import datetime
from zoneinfo import ZoneInfo

import aqua_blue

def main():

    start_date = datetime.datetime.now().astimezone(ZoneInfo("Indian/Maldives"))
```

```
# Generate 10,000 datetime objects, each 1 minute apart
    t = [start date + datetime.timedelta(minutes=i) for i in range(10000)]
   a = np.arange(len(t)) / 100
   y = np.vstack((np.cos(a)+1, np.sin(a)-1)).T
    time series = aqua blue.time series.TimeSeries(dependent variable=y, times=t)
    normalizer = aqua blue.utilities.Normalizer()
    time series = normalizer.normalize(time series)
   model = aqua blue.models.Model(
       reservoir=aqua blue.reservoirs.DynamicalReservoir(
           reservoir dimensionality=100,
           input dimensionality=2
       ),
       readout=aqua blue.readouts.LinearReadout()
   model.train(time series)
   horizon = 1 000
   prediction = model.predict(horizon=horizon)
   prediction = normalizer.denormalize(prediction)
   dt = np.diff(a)[0]
    actual future = np.vstack((
        (np.cos(a[-1] + dt * np.arange(horizon)) + 1, np.sin(a[-1] + dt *
np.arange(horizon)) - 1)
   )).T
   root_mean_square_error = np.sqrt(np.mean((actual future -
prediction.dependent variable) ** 2))
   print(root mean square error)
   plt.plot(prediction.times, actual future)
   plt.plot(prediction.times, prediction.dependent variable)
   plt.legend(['actual x', 'actual y', 'predicted x', 'predicted y'])
   plt.show()
if __name__ == "__main__":
   main()
```

# Load and output a JSON string

Below is an example of inputting a json string as the training data, and outputting a json string for the prediction. This is particularly useful for interfacing aqua-blue with already-existing systems.

```
import json
import aqua blue
def main():
    # some string that is valid json
   json str = """
"dependent variable": [
[2.0, -1.0],
[1.5403023058681398, -0.1585290151921035],
[0.5838531634528576, -0.09070257317431829],
[0.010007503399554585, -0.8588799919401328],
[0.34635637913638806, -1.7568024953079282],
[1.2836621854632262, -1.9589242746631386],
[1.9601702866503659, -1.2794154981989259],
[1.7539022543433047, -0.34301340128121094],
[0.8544999661913865, -0.010641753376618213],
[0.08886973811532306, -0.5878815147582435]
],
"times": [0, 1, 2, 3, 4, 5, 6, 7, 8, 9]
11 11 11
    # turn into a TimeSeries instance
    time series = aqua blue.time series.TimeSeries(**json.loads(json str))
    # normalize and feed into model
    normalizer = aqua_blue.utilities.Normalizer()
    normalized time series = normalizer.normalize(time series)
    model = aqua_blue.models.Model(
       reservoir=aqua blue.reservoirs.DynamicalReservoir(
            reservoir dimensionality=100,
            input dimensionality=2
        ),
        readout=aqua blue.readouts.LinearReadout()
```

```
model.train(normalized_time_series)

# predict 5 more steps
horizon = 5
prediction = model.predict(horizon=horizon)
prediction = normalizer.denormalize(prediction)

# concatenate prediction and original time series, and print out a new json concatenated = time_series >> prediction

# turn into a dictionary and json dump it
print(json.dumps(concatenated.to_dict()))

if __name__ == "__main__":
    main()
```

# **Explicit weights**

Below is an example of generating explicit matrices for  $w_{\rm in}$  and  $w_{\rm res}$ . Here, sparsity=0.99 and spectral\_radius=1.2 respectively zero-out 99% of  $w_{\rm res}$ 's elements and force  $w_{\rm res}$  to have a spectral radius of 1.2. We also showcase the >> operator, which concatenates instances of aqua blue.time series. TimeSeries.

```
import numpy as np
import matplotlib.pyplot as plt

import aqua_blue

def main():
    t = np.arange(5_000) / 100
    y = np.vstack((np.cos(t) ** 2, np.sin(t))).T

    time_series = aqua_blue.time_series.TimeSeries(dependent_variable=y, times=t)
    normalizer = aqua_blue.utilities.Normalizer()
    normalized_time_series = normalizer.normalize(time_series)
    generator = np.random.default_rng(seed=0)

    w_res = generator.uniform(
        low=-0.5,
        high=0.5,
```

```
size=(100, 100)
   )
   w in = generator.uniform(
       low=-0.5,
       high=0.5,
       size=(100, 2)
   model = aqua blue.models.Model(
       reservoir=aqua blue.reservoirs.DynamicalReservoir(
           reservoir dimensionality=100,
           input dimensionality=2,
           w res=w res,
            w in=w in,
            spectral radius=1.2,
            sparsity=0.99
       ),
       readout=aqua blue.readouts.LinearReadout()
   model.train(normalized time series)
   horizon = 1 000
   prediction = model.predict(horizon=horizon)
   prediction = normalizer.denormalize(prediction)
   actual future = aqua blue.time series.TimeSeries(
       dependent variable=np.vstack((np.cos(prediction.times) ** 2,
np.sin(prediction.times))).T,
       times=prediction.times
   )
   ground truth = time series >> actual future
   predicted = time series >> prediction
   plt.plot(ground_truth.times, ground_truth.dependent_variable)
   plt.plot(predicted.times, predicted.dependent variable)
   plt.axvline(time_series.times[-1], color="black", linestyle="--")
   plt.legend(['actual x', 'actual y', 'predicted x', 'predicted y', 'knowledge
horizon'])
   plt.title("Explicit Weight Matrix Example")
   plt.show()
```

```
if __name__ == "__main__":
    main()
```

# **Explicit activation function**

Below is an example of using a different activation function to map from the input state to the reservoir. Here, we use both hyperbolic tangent ( tanh ) and the <u>error function</u> ( erf ), and compare the results.

```
from typing import Dict, Callable
import numpy as np
import matplotlib.pyplot as plt
import scipy
import aqua blue
def main():
   fig, axs = plt.subplots(nrows=1, ncols=2, sharex=True, sharey=True)
   activation functions: Dict[str, Callable] = {"tanh": np.tanh, "erf":
scipy.special.erf}
   t = np.arange(10 000) / 100
   y = np.vstack((np.cos(t) ** 2, np.sin(t))).T
    for ax, activation function in zip(axs, activation functions):
       time series = aqua blue.time series.TimeSeries(dependent variable=y, times=t)
       normalizer = aqua blue.utilities.Normalizer()
       time series = normalizer.normalize(time series)
       model = aqua blue.models.Model(
           reservoir=aqua blue.reservoirs.DynamicalReservoir(
               reservoir_dimensionality=100,
               input dimensionality=2,
               activation function=activation functions[activation function]
            ),
            readout=aqua blue.readouts.LinearReadout()
       model.train(time_series)
       prediction = model.predict(horizon=1_000)
```

```
prediction = normalizer.denormalize(prediction)

actual_future = np.vstack((np.cos(prediction.times) ** 2,

np.sin(prediction.times))).T

ax.plot(prediction.times, actual_future)
ax.plot(prediction.times, prediction.dependent_variable)
ax.legend(['actual_x', 'actual_y', 'predicted_x', 'predicted_y'])
ax.set_title(activation_function)

plt.show()

if __name__ == "__main__":
    main()
```

# **HTTP Requests**

Below is an example of pulling csv file data from a resource URL using the <u>requests</u> library. Here, we retrieve a time series of temperature data from <u>NCEI NOAA</u> and use it for training and predicting temperatures.

```
import requests
import aqua blue
from io import BytesIO
import matplotlib.pyplot as plt
import numpy as np
import time
def main():
   req = requests.get("https://www.ncei.noaa.gov/data/global-summary-of-the-
day/access/2024/01001099999.csv")
    time col = "DATE"
   dependent var cols = ["TEMP"]
   with BytesIO() as file:
       txt = req.text
       file.write(txt.encode('utf-8'))
       file.seek(0)
       DATA = aqua blue.time series.TimeSeries.from csv(
           fp=file,
```

```
time col=time col,
        dependent var cols=dependent var cols,
        times dtype='datetime64[s]',
        max rows=87,
TRAIN DATA = aqua blue.time series.TimeSeries(
    times=DATA.times[:82],
    dependent variable=DATA.dependent variable[:82, :]
normalizer = aqua blue.utilities.Normalizer()
normalized time series = normalizer.normalize(TRAIN DATA)
seed = int(time.time())
generator = np.random.default rng(seed)
w res = generator.uniform(
   low=-0.5,
   high=0.5,
    size=(100, 100)
w in = generator.uniform(
   low=-0.5,
   high=0.5,
   size=(100, 1)
model = aqua blue.models.Model(
    reservoir=aqua blue.reservoirs.DynamicalReservoir(
        reservoir dimensionality=100,
        w_{in} = w_{in}
        w res = w res,
        input dimensionality=1,
    ),
    readout=aqua blue.readouts.LinearReadout(1e-1)
model.train(normalized time series)
horizon = 5
prediction = model.predict(horizon=horizon)
prediction = normalizer.denormalize(prediction)
```

```
concatenated = TRAIN_DATA >> prediction

plt.plot(concatenated.times, concatenated.dependent_variable, label='Predicted
Future')

plt.plot(DATA.times, DATA.dependent_variable, label='Actual Future')

plt.legend()

plt.show()

if __name__ == '__main__':
    main()
```

# Read from and write to CSV files

Below is an example of parsing data from a csv file (goldstocks.csv) and writing it to a TimeSeries object, which is used for training and predictions. The predictions are written to a new csv file (predicted-goldstocks.csv).

```
import aqua blue
from pathlib import Path
def main():
   goldstocks = aqua blue.time series.TimeSeries.from csv(
        fp=Path('examples/goldstocks.csv'),
       time col='DATE',
        times dtype='datetime64[s]',
       dependent_var_cols=['X', 'Y', 'Z', 'A', 'B'],
   )
   normalizer = aqua blue.utilities.Normalizer()
    normalized time series = normalizer.normalize(goldstocks)
   model = aqua blue.models.Model(
       reservoir=aqua blue.reservoirs.DynamicalReservoir(
           reservoir_dimensionality=100,
            input dimensionality=5
       ),
       readout=aqua blue.readouts.LinearReadout()
   )
   model.train(normalized time series)
   horizon = 100
```

```
prediction = model.predict(horizon=horizon)
prediction = normalizer.denormalize(prediction)

concatenated = goldstocks >> prediction

concatenated.save(
    fp=Path('examples/predicted_goldstocks.csv'),
    header='DATE,X,Y,Z,A,B',
    fmt=('%s', '%.2f', '%.2f', '%.2f', '%.2f', '%.2f')
)

if __name__ == '__main__':
    main()
```

# Logging

aqua-blue utilizes the native logging library to do some additional logging. An example of this is below:

```
import logging
import sys
import numpy as np
import aqua blue
def main():
   logging.basicConfig(stream=sys.stdout, level=logging.DEBUG)
   t = np.arange(5 000) / 100
   y = np.vstack((np.cos(t) ** 2, np.sin(t))).T
    time_series = aqua_blue.time_series.TimeSeries(dependent_variable=y, times=t)
   normalizer = aqua blue.utilities.Normalizer()
    normalized_time_series = normalizer.normalize(time_series)
   model = aqua blue.models.Model(
       reservoir=aqua_blue.reservoirs.DynamicalReservoir(
           reservoir_dimensionality=100,
           input dimensionality=2,
            sparsity=0.5,
            spectral radius=0.95
```

# which prints:

```
INFO:root:times dtype set to float64
INFO:root:times dtype set to float64
DEBUG:root:DynamicalReservoir.w_res sparsity set to 50.67%
DEBUG:root:DynamicalReservoir.w_res spectral radius set to 4.7707258199919655
INFO:root:LinearReadout layer trained. Inaccuracy = 5.025374978118052e-09 and pcc = 1.0
DEBUG:root:Model.timestep set to 0.01
DEBUG:root:Model.final_time set to 49.99
DEBUG:root:Model.tz set to None
DEBUG:root:Model.times_detype set to float64
```

For my favorite video about logging in Python, see a wonderful video below by mCoding:

# <u>aqua-blue.aqua\_blue</u>.datetimelikearray

Module providing a timezone-aware wrapper for NumPy arrays.

Timezone awareness is a deprecated NumPy feature due to the deprecation of pytz. This module provides a workaround by storing the timezone information separately in the array. The datetime objects are stored in UTC and converted to the specified timezone when accessed.

This implementation is designed specifically for one-dimensional arrays and is intended to satisfy the datetime processing requirements of the project, rather than general NumPy timezone integration.

```
DatetimeLike = ~DatetimeLike
```

Datetime like, representing either dates or numerical values

TimeDeltaLike = ~TimeDeltaLike

Corresponding object representing timesteps, which are either float if the two times are floats, or a timedelta

class DatetimeLikeArray(numpy.ndarray):

A subclass of NumPy ndarray that provides timezone awareness for datetime arrays.

The timezone information is stored separately since NumPy does not natively support timezone-aware datetime objects. All datetime values are stored in UTC and converted back to the specified timezone when accessed.

DatetimeLikeArray( input\_array: Sequence[~DatetimeLike], dtype, buffer=None, offset=0, strides=None, order=None)

Create a new instance of DatetimeLikeArray.

## Arguments:

- **input\_array** (**Sequence[DatetimeLike]**): List of datetime-like objects to be stored in the array.
- **dtype:** Data type for the NumPy array.
- **buffer:** Optional buffer for the array.
- **offset:** Offset for the array.
- **strides:** Strides for the array.
- **order:** Memory layout order.

#### Returns:

DatetimeLikeArray: A new instance of the class.

tz: Optional[datetime.tzinfo] = None

The timezone associated with the array. Defaults to None (assumed UTC).

tz\_offset: Optional[datetime.timedelta] = None

The timezone offset from UTC for the stored datetime values. Defaults to None.

def to list(self) -> List[~DatetimeLike]:

Convert the array back to a list of datetime-like objects with timezone information.

#### Returns:

List[DatetimeLike]: A list of datetime objects with their original timezone restored.

def to file(self, fp: Union[IO, str, pathlib.Path], tz: Optional[datetime.tzinfo] = None):

Save a DatetimeLikeArray instance to a text file.

#### Arguments:

- **fp** (**Union**[**IO**, **str**, **Path**]): File path or file-like object to write to.
- tz (datetime.tzinfo, optional): Timezone in which to write the data.

## @classmethod

def from\_array( cls, input\_array: numpy.ndarray[typing.Any, numpy.dtype[typing.Union[numpy.number, numpy.datetime64]]], tz: Optional[datetime.tzinfo] = None):

Convert a numpy array to a DatetimeLikeArray instance.

## **Arguments:**

- **input\_array** (**np.ndarray**): NumPy array containing datetime values.
- tz (datetime.tzinfo, optional): Timezone of the input datetime values.

#### Returns:

DatetimeLikeArray: A new instance with timezone awareness.

#### @classmethod

def from fp( cls, fp: Union[IO, str, pathlib.Path], dtype: Type, tz: Optional[datetime.tzinfo] = None):

Load a text file and convert it to a DatetimeLikeArray instance.

## **Arguments:**

- **fp** (**Union**[**IO**, **str**, **Path**]): File path or file-like object to read from.
- **dtype (Type):** Data type of the values in the file.
- tz (datetime.tzinfo, optional): Timezone to assign to the loaded data.

### Returns:

DatetimeLikeArray: A new instance with timezone awareness.

## @classmethod

def from\_iter( cls, gen: Generator[~DatetimeLike, NoneType, NoneType], dtype: Type, tz: Optional[datetime.tzinfo] = None):

Create a DatetimeLikeArray object from an Iterable with DatetimeLike yields

## Arguments:

- **gen (Generator[DatetimeLike, None, None]):** A generator that yields DatetimeLike values
- **dtype (Type):** Data type of the values in the file.
- tz (datetime.tzinfo, optional): Timezone to assign to the loaded data.

DatetimeLikeArray: A new instance with timezone awareness.

# <u>aqua-blue</u>.aqua\_blue.models

Module defining models, i.e., compositions of reservoir(s) and readout layers.

This module implements the Model class, which integrates a reservoir and a readout layer to process time series data. The model enables training using input time series data and forecasting future values based on learned patterns.

#### Classes:

 Model: Represents an Echo State Network (ESN)-based model that learns from input time series data and makes future predictions.

logger = <Logger aqua-blue.aqua\_blue.models (WARNING)>
@dataclass
class Model(typing.Generic[~DatetimeLike, ~TimeDeltaLike]):

A machine learning model that integrates a reservoir with a readout layer for time series forecasting.

This class implements an Echo State Network (ESN) approach, where the reservoir serves as a high-dimensional dynamic system, and the readout layer maps reservoir states to output values.

### Attributes:

- **reservoir (Reservoir):** The reservoir component, defining the input-to-reservoir mapping.
- readout (Readout): The readout layer, mapping reservoir states to output values.
- **final\_time (float):** The last timestamp seen during training. This is set automatically after training.
- **timestep (float):** The fixed time interval between consecutive steps in the input time series, set during training.
- **initial\_guess (np.ndarray):** The last observed state of the system during training, used as an initial condition for predictions.
- tz (Union[datetime.tzinfo, None]): The timezone associated with the time series. Set to None if the DatetimeLikeArray is incompatible.

Model( reservoir: aqua-blue.aqua\_blue.reservoirs.Reservoir, readout: aqua-blue.aqua\_blue.readouts.Readout)
reservoir: aqua-blue.aqua\_blue.reservoirs.Reservoir

The reservoir component that defines the input-to-reservoir mapping.

readout: aqua-blue.aqua blue.readouts.Readout

The readout component that defines the reservoir-to-output mapping.

final\_time: ~DatetimeLike

The final timestamp encountered in the training dataset (set during training).

timestep: ~TimeDeltaLike

The fixed time step interval of the training dataset (set during training).

initial guess: numpy.ndarray[typing.Any, numpy.dtype[numpy.floating]]

The last observed state of the system, used for future predictions (set during training).

tz: Optional[datetime.tzinfo]

The timezone associated with the independent variable. Set to None if unsupported.

def train( self, input\_time\_series: aqua-blue.aqua\_blue.time\_series.TimeSeries, warmup: int = 0):

Trains the model on the provided time series data.

This method fits the readout layer using reservoir states obtained from the input time series data. A warmup period can be specified to exclude initial steps from training.

## **Arguments:**

- **input\_time\_series (TimeSeries):** The time series instance used for training.
- warmup (int): The number of initial steps to ignore in training (default: 0).

#### Raises:

• **ValueError:** If warmup is greater than or equal to the number of timesteps in the input time series.

def predict(self, horizon: int) -> aqua-blue.aqua blue.time series.TimeSeries:

Generates future predictions for a specified time horizon.

This method uses the trained model to generate future values based on the learned dynamics of the input time series.

# Arguments:

• **horizon (int):** The number of steps to forecast into the future.

#### Returns:

TimeSeries: A TimeSeries instance containing the predicted values and corresponding timestamps.

# <u>aqua-blue</u>.aqua\_blue.readouts

Module defining readout layers.

This module provides the abstract Readout class and its concrete implementation, LinearReadout. Readout layers map the internal reservoir states of an Echo State Network (ESN) to output values.

#### Classes:

- Readout: Abstract base class defining the interface for readout layers.
- LinearReadout: A linear mapping readout layer that transforms reservoir states into output values using learned coefficients.

logger = <Logger aqua-blue.aqua\_blue.readouts (WARNING)>
@dataclass
class Readout(abc.ABC):

Abstract base class for readout layers in Echo State Networks (ESNs).

Readout layers transform the high-dimensional reservoir states into output predictions. The transformation is typically learned during training.

## Attributes:

• **coefficients (np.ndarray):** The learned weights for mapping reservoir states to output values. This is set after training.

coefficients: numpy.ndarray[typing.Any, numpy.dtype[numpy.floating]]

The learned weight matrix for the readout layer, initialized during training.

#### @abstractmethod

def train( self, independent\_variables: numpy.ndarray[typing.Any, numpy.dtype[numpy.floating]], dependent variables: numpy.ndarray[typing.Any, numpy.dtype[numpy.floating]]):

Trains the readout layer by learning the mapping from reservoir states to output values.

This method takes independent input variables (reservoir states) and corresponding dependent variables (target outputs) to compute the optimal readout weights.

#### **Arguments:**

- **independent\_variables (np.ndarray):** The reservoir state matrix used as input for training.
- **dependent\_variables (np.ndarray):** The expected output values corresponding to the input states.

#### @abstractmethod

def reservoir\_to\_output( self, reservoir\_state: numpy.ndarray[typing.Any, numpy.dtype[numpy.floating]]) -> numpy.ndarray[typing.Any, numpy.dtype[numpy.floating]]:

Maps a given reservoir state to an output value.

#### Arguments:

• reservoir\_state (np.ndarray): The current state of the reservoir.

#### Returns:

np.ndarray: The predicted output corresponding to the given reservoir state.

## @dataclass

class LinearReadout(Readout):

A linear readout layer that applies a learned linear transformation to reservoir states.

This readout layer learns a set of coefficients during training and applies a simple linear mapping to transform reservoir states into output predictions.

#### Attributes:

• **rcond (float):** A regularization parameter used in the pseudo-inverse calculation to prevent numerical instability in the least squares solution.

```
LinearReadout(rcond: float = 1e-10)
rcond: float = 1e-10
```

Regularization parameter for pseudo-inverse computation.

This controls the minimum singular value considered for the pseudo-inverse computation. A lower value ensures more stable training.

def train( self, independent\_variables: numpy.ndarray[typing.Any, numpy.dtype[numpy.floating]], dependent\_variables: numpy.ndarray[typing.Any, numpy.dtype[numpy.floating]]):

Trains the linear readout layer by solving the least-squares optimization problem.

The training process determines the optimal readout coefficients  $w^*$  by solving the optimization problem below:

$$W^* = \underset{\lambda \rightarrow 0^+}{\lim} \arg \overset{\min}{W} \| \mathit{XW} - \mathit{Y} \|_F^2 + \lambda \| \mathit{W} \|_F^2$$

where  $_X$  is the matrix of reservoir states (independent variables) and  $_Y$  is the matrix of target output values (dependent variables).

## **Arguments:**

- independent\_variables (np.ndarray): The reservoir state matrix used for training.
- **dependent\_variables (np.ndarray):** The target output values corresponding to the reservoir states.

def reservoir\_to\_output( self, reservoir\_state: numpy.ndarray[typing.Any, numpy.dtype[numpy.floating]]) -> numpy.ndarray[typing.Any, numpy.dtype[numpy.floating]]:

Computes the output from a given reservoir state using a learned linear mapping.

This method applies the learned weight matrix (self.coefficients) to map the reservoir state to an output value.

## **Arguments:**

• reservoir\_state (np.ndarray): The reservoir state to be mapped to an output value.

# Returns:

np.ndarray: The predicted output value.

#### Raises:

• **ValueError:** If the readout layer has not been trained (i.e., coefficients are not set).

#### **Inherited Members**

## Readout

coefficients

# <u>aqua-blue</u>.aqua\_blue.reservoirs

Module defining reservoirs.

This module contains the base Reservoir class and its concrete implementation, DynamicalReservoir. Reservoirs serve as dynamic memory structures in Echo

State Networks (ESNs) by transforming input signals into high-dimensional representations.

#### Classes:

- Reservoir: Abstract base class defining the structure of a reservoir.
- DynamicalReservoir: A specific implementation of a reservoir with tunable dynamics and activation functions.

ActivationFunction = typing.Callable[[numpy.ndarray[typing.Any, numpy.dtype[numpy.floating]]], numpy.ndarray[typing.Any, numpy.dtype[numpy.floating]]]

activation function, taking in a numpy array and returning a numpy array of the same shape

logger = <Logger aqua-blue.aqua\_blue.reservoirs (WARNING)>
@dataclass
class Reservoir(abc.ABC):

Abstract base class defining a reservoir in an Echo State Network (ESN).

Reservoirs are responsible for transforming input signals into high-dimensional representations, which are then used by the readout layer for predictions.

#### Attributes:

- **input\_dimensionality (int):** The number of input features.
- **reservoir\_dimensionality (int):** The number of reservoir neurons (i.e., the size of the reservoir).
- **res\_state (np.ndarray):** The current state of the reservoir, which is updated at each time step.

input dimensionality: int

Dimensionality of the input state.

reservoir dimensionality: int

Dimensionality of the reservoir state, equivalently the reservoir size.

res\_state: numpy.ndarray[typing.Any, numpy.dtype[numpy.floating]]

Reservoir state, necessary property when performing training loop.

# @abstractmethod

def update\_reservoir( self, input\_state: numpy.ndarray[typing.Any, numpy.dtype[numpy.floating]]) -> numpy.ndarray[typing.Any, numpy.dtype[numpy.floating]]:

Updates the reservoir state given an input state.

This method defines the transformation applied to an input vector when passed through the reservoir.

class DynamicalReservoir(Reservoir):

A dynamical reservoir with tunable properties.

This reservoir is defined by the equation:

$$y_t = (1 - \alpha)y_{t-1} + \alpha f(W_{\text{in}}x_t + W_{\text{res}}y_{t-1})$$

where  $x_t$  is the input at time step t,  $y_t$  is the reservoir state at time t,  $W_{in}$  is the input weight matrix,  $W_{res}$  is the reservoir weight matrix, t (leaking\_rate) controls how much of the previous state influences the next state, and t is a nonlinear activation function.

#### Attributes:

- **generator (Optional[np.random.Generator]):** Random number generator for weight initialization.
- w\_in (Optional[np.ndarray]): Input weight matrix of shape (reservoir\_dimensionality, input\_dimensionality) . Auto-generated if not provided.
- w\_res (Optional[np.ndarray]): Reservoir weight matrix of shape (reservoir\_dimensionality, reservoir\_dimensionality) . Auto-generated if not provided.
- activation\_function (ActivationFunction): Activation function applied to the reservoir state. Defaults to np.tanh.
- **leaking\_rate (float):** Leaking rate that controls the contribution of the previous state.

DynamicalReservoir(input\_dimensionality: int, reservoir\_dimensionality: int, generator:

Optional[numpy.random.\_generator.Generator] = None, w\_in: Optional[numpy.ndarray[Any, numpy.dtype[numpy.floating]]] = None, w\_res: Optional[numpy.ndarray[Any, numpy.dtype[numpy.floating]]] = None, activation\_function: Callable[[numpy.ndarray[Any, numpy.dtype[numpy.floating]]], numpy.ndarray[Any, numpy.dtype[numpy.floating]]] = <ufunc 'tanh'>, leaking\_rate: float = 1.0, sparsity:
Optional[float] = None, spectral\_radius: Optional[float] = 0.95)
generator: Optional[numpy.random.\_generator.Generator] = None

Random generator for initializing weights. Defaults to np.random.default\_rng(seed=0) if not specified.

w\_in: Optional[numpy.ndarray[Any, numpy.dtype[numpy.floating]]] = None

Input weight matrix. Must have shape (reservoir\_dimensionality, input\_dimensionality) . If not provided, it is auto-generated with values in [-0.5, 0.5].

w\_res: Optional[numpy.ndarray[Any, numpy.dtype[numpy.floating]]] = None

Reservoir weight matrix. Must have shape (reservoir\_dimensionality, reservoir\_dimensionality). If not provided, it is auto-generated and normalized to have a spectral radius of 0.95.

activation\_function: Callable[[numpy.ndarray[Any, numpy.dtype[numpy.floating]]], numpy.ndarray[Any, numpy.dtype[numpy.floating]]] = <ufunc 'tanh'>

Nonlinear activation function applied to the reservoir state. Defaults to np.tanh, but can be replaced with other functions like ReLU.

```
leaking rate: float = 1.0
```

Leaking rate ((\alpha)) that controls how much of the previous state contributes to the next. Defaults to 1.0, meaning the state is fully updated at each time step.

```
sparsity: Optional[float] = None
```

sparsity of the reservoir weight matrix. (0, 1]

```
spectral_radius: Optional[float] = 0.95
```

spectral radius of reservoir weight matrix. Recommended values - [0.9, 1.2]

def update\_reservoir( self, input\_state: numpy.ndarray[typing.Any, numpy.dtype[numpy.floating]]) -> numpy.ndarray[typing.Any, numpy.dtype[numpy.floating]]:

Updates the reservoir state given an input.

This method applies the state update equation:

$$y_t = (1 - \alpha)y_{t-1} + \alpha f(W_{\text{in}}x_t + W_{\text{res}}y_{t-1})$$

#### Arguments:

• input\_state (np.ndarray): The input state vector.

#### Returns:

np.ndarray: The updated reservoir state.

#### **Inherited Members**

# Reservoir

input\_dimensionality reservoir\_dimensionality res\_state

# <u>aqua-blue.aqua\_blue</u>.time\_series

Module defining the TimeSeries object

```
logger = <Logger aqua-blue.aqua_blue.time_series (WARNING)>
def parse_time(s: str):
class ShapeChangedWarning(builtins.Warning):
```

Warning for cases where <u>TimeSeries</u>.\_\_post\_init\_\_ alters the shape of the dependent variable.

```
class TimeSeriesTypedDict(typing.TypedDict):
```

TypedDict form of a TimeSeries object, useful for turning into json

```
dependent_variable: Sequence[Sequence[float]]
times: Sequence[Union[float, str]]
@dataclass
class TimeSeries(typing.Generic[~TimeDeltaLike]):
```

A class representing a time series, encapsulating dependent variables and corresponding timestamps.

```
TimeSeries( dependent_variable: numpy.ndarray[typing.Any, numpy.dtype[numpy.floating]], times: aqua-blue.aqua_blue.datetimelikearray.DatetimeLikeArray) dependent_variable: numpy.ndarray[typing.Any, numpy.dtype[numpy.floating]]
```

Array of dependent variables representing the time series values.

```
times: aqua-blue.aqua_blue.datetimelikearray.DatetimeLikeArray
```

Array of time values associated with the dependent variable.

```
def save( self, fp: Union[IO, str, pathlib.Path], header: str = ", delimiter=',', fmt: Union[str, Tuple[str]] = '%s'):

Saves the time series data to a file.
```

## Arguments:

- **fp (Union[IO, str, Path]):** File path or object where the TimeSeries instance will be saved.
- header (str, optional): An optional header. Defaults to an empty string.
- **delimiter (str, optional):** The delimiter used in the output file. Defaults to a comma.
- **fmt (Tuple(str), optional):** Format specifier used for saving the data to fp. Defaults to '%s' (String representation)

```
num dims: int
```

Returns the dimensionality of the dependent variable.

## Returns:

int: Number of dimensions of the time series.

#### @classmethod

def from\_csv( cls, fp: Union[IO, str, pathlib.Path], time\_col: str, times\_dtype: Type, dependent\_var\_cols: List[str], times\_conversion: Callable[[str], ~DatetimeLike] = <function parse\_time>, dep\_var\_conversion: Callable[[str], float] = <class 'float'>, max\_rows: Optional[int] = 0):

Loads time series data from a CSV file.

#### **Arguments:**

- fp (Union[IO, str, Path]): File path or object to read from.
- **time\_col (str):** Name of the times column.
- times\_dtype (dtype): Type of the times column
- **dependent\_var\_cols** (List[str]): Names of the dependent variable columns
- **times\_conversion (Callable[[str], DatetimeLike]):** Function determining how to parse elements of the times column. Defaults to parse time
- **dep\_var\_conversion (Callable[[str], float]):** Function determining how to parse elements of the dependent variable columns. Defaults to float
- max\_rows (float): Maximum number of rows that should be parsed. If set to zero, all rows are parsed. Defaults to 0

#### Returns:

TimeSeries: A TimeSeries instance populated by data from the csv file.

def to dict(self) -> aqua-blue.aqua blue.time series.TimeSeriesTypedDict:

convert to a typed dictionary

timestep: ~TimeDeltaLike

Returns the time step between consecutive observations.

#### Returns:

TimeDeltaLike: The timestep of the time series.

# <u>aqua-blue</u>.aqua\_blue.utilities

This module provides simple utilities for processing TimeSeries instances.

#### @dataclass

class Normalizer:

A utility class for normalizing and denormalizing TimeSeries instances.

This class computes and stores the mean and standard deviation of the dependent variable during normalization. These statistics are later used to restore the original scale of the data when denormalizing.

means: numpy.ndarray[typing.Any, numpy.dtype[numpy.floating]]

Mean values of the dependent variable, computed during normalization.

standard deviations: numpy.ndarray[typing.Any, numpy.dtype[numpy.floating]]

Standard deviation values of the dependent variable, computed during normalization.

def normalize( self, time\_series: aqua-blue.aqua\_blue.time\_series.TimeSeries) -> aqua-blue.aqua\_blue.time\_series.TimeSeries:

Normalize a TimeSeries instance by adjusting its values to have zero mean and unit variance.

## **Arguments:**

• **time\_series (TimeSeries):** The time series to be normalized.

#### Returns:

TimeSeries: A new TimeSeries instance with normalized values.

#### Raises:

• **ValueError:** If the normalizer has already been used, since it is intended for one-time use.

def denormalize( self, time\_series: aqua-blue.aqua\_blue.time\_series.TimeSeries) ->
aqua-blue.aqua blue.time series.TimeSeries:

Denormalize a previously normalized TimeSeries instance, restoring it to its original scale.

#### **Arguments:**

• time\_series (TimeSeries): Time series to denormalize

# Returns:

TimeSeries: The denormalized time series

## Raises:

• **ValueError:** If normalization has not been performed before calling this method.

def make\_sparse( weight\_matrix: numpy.ndarray[typing.Any, numpy.dtype[numpy.floating]], sparsity: float, generator: Optional[numpy.random.\_generator.Generator] = None) -> numpy.ndarray[typing.Any, numpy.dtype[numpy.floating]]:

Make a weight matrix sparse

#### Arguments:

- weight\_matrix (np.typing.NDArray[np.floating]): Weight matrix to be made sparse
- **sparsity (float):** Extent of how sparse to make the weight matrix. Ranges from 0 to 1.
- **generator (np.random.Generator):** NumPy Generator to create random numbers

def set\_spectral( weight\_matrix: numpy.ndarray[typing.Any, numpy.dtype[numpy.floating]], spectral\_radius: float) -> numpy.ndarray[typing.Any, numpy.dtype[numpy.floating]]:

Set the spectral radius of the weight matrix

## Arguments:

- weight\_matrix (np.typing.NDArray[np.floating]): Weight matrix whose spectral radius is to be set
- **spectral\_radius (float):** The largest absolute singular value of the weight matrix. Values less than 1.0 are recommended for tasks that require significant memory fading. Values between 1-1.5 are recommended for tasks that are memory dependent.