

# Time Series Classification in Python

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# Outline

- 1 Time series classification
  - Metric-based approaches
  - Feature-based approaches
- 2 Managing your project as a software
- 3 `pyts`: A Python Package for Time Series Classification

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# Machine learning - classification

- **Data:** a set of samples  $(x, y)$  where  $x$  is the **input** and  $y$  is the **label**.
- **Objective:** To predict the label  $y$  from with its corresponding input  $x$ .
- Find a **mapping**  $f$  with **parameters**  $\theta$  from  $x$  to  $y$ :  $\hat{y} = f(x; \theta)$
- **Optimize** the parameters  $\theta$  on a **training set** of samples.
- **Evaluate** the **performance** of the model on an **independent test set** of samples.

# Machine learning for time series

- Time series data is **unstructured** → not suited as raw input to standard machine learning classifiers (e.g., logistic regression).
- Two main approaches: **feature-based** and **metric-based** approaches.
- Feature-based methods:
  - ▶ **Independent process**: Running the feature extraction process before fitting the classifier on the extracted features.
  - ▶ **Incorporated process**: Including the feature extraction process in the classifier (e.g., neural networks with several layers).
- Metric-based methods: **Adapting** existing machine learning classifiers to time series data (e.g., with specific metrics for nearest-neighbor methods and specific kernels for kernel methods).

# Literature overview

- Not an exhaustive literature review.
- Highlight the **main algorithms** and the **variety of methods**.
- Time series are assumed to be **univariate** (a real number at each timestamp) and **not multivariate** (a real-valued vector at each timestamps, e.g. (latitude, longitude) pairs for GPS coordinates).

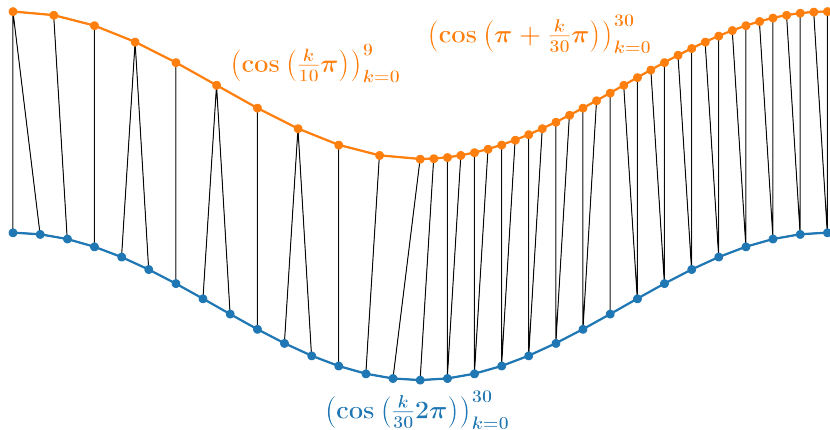
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# Limitations of the Euclidean distance

- Simple example from speech recognition:
  - ▶ Two audio recordings of the **same person** pronouncing the **same sentence** but at **different speech rates**.
  - ▶ Expectations: a relevant metric should return a **low value** (i.e., both time series are similar).
- Two time series  $X = (x_1, \dots, x_n) \in \mathbb{R}^n$  and  $Y = (y_1, \dots, y_m) \in \mathbb{R}^m$
- Limitations of the Euclidean distance for time series:  $\left( \sum_i (x_i - y_i)^2 \right)^{1/2}$ 
  - ▶ Independent comparison (squared difference) in each dimension
  - ▶ Not defined for two vectors of different sizes

# Global alignment



# Dynamic time warping

- **Local divergence:** function that measures closeness between two values, e.g.:

$$\forall x, y \in \mathbb{R}, f(x, y) = (x - y)^2$$

- **Cost matrix:** evaluation of the local divergence for every pair  $(x_i, y_j)$

$$\forall i, j \in \{1, \dots, n\} \times \{1, \dots, m\}, C_{ij} = f(x_i, y_j)$$

- **Warping path:** sequence  $p = (p_1, \dots, p_L)$  such that:
  - ▶ value condition:  $\forall l \in \{1, \dots, L\}, p_l = (i_l, j_l) \in \{1, \dots, n\} \times \{1, \dots, m\}$
  - ▶ boundary condition:  $p_1 = (1, 1)$  and  $p_L = (n, m)$
  - ▶ step condition:  $\forall l \in \{1, \dots, L - 1\}, p_{l+1} - p_l \in \{(0, 1), (1, 0), (1, 1)\}$

# Dynamic time warping

- **Cost associated with a warping path:**

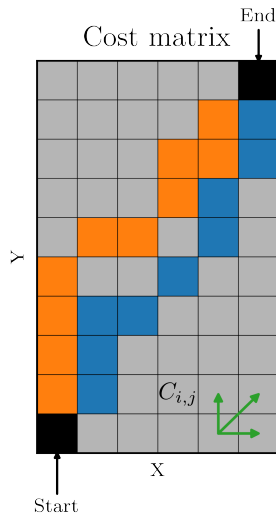
$$C_p(X, Y) = \sum_{l=1}^L C_{i_l, j_l}$$

- **Dynamic time warping [SC78]:** minimum cost among all the possible warping paths:

$$\text{DTW}(X, Y) = \min_{p \in \mathcal{P}} C_p(X, Y)$$

- Computed using **dynamic programming**:

$$\text{DTW}(X_{:i}, Y_{:j}) = C_{i,j} + \min \left\{ \begin{array}{l} \text{DTW}(X_{:i-1}, Y_{:j-1}) \\ \text{DTW}(X_{:i-1}, Y_{:j}) \\ \text{DTW}(X_{:i}, Y_{:j-1}) \end{array} \right\}$$



# Limitations of dynamic time warping

- **High complexity:**  $\mathcal{O}(nm)$  for two time series of sizes  $n$  and  $m$ .
- (Possibly too) large time warps.
- **Not a distance** (separation property and **triangle inequality** not satisfied)  $\longrightarrow$  no efficient nearest-neighbor search algorithm.

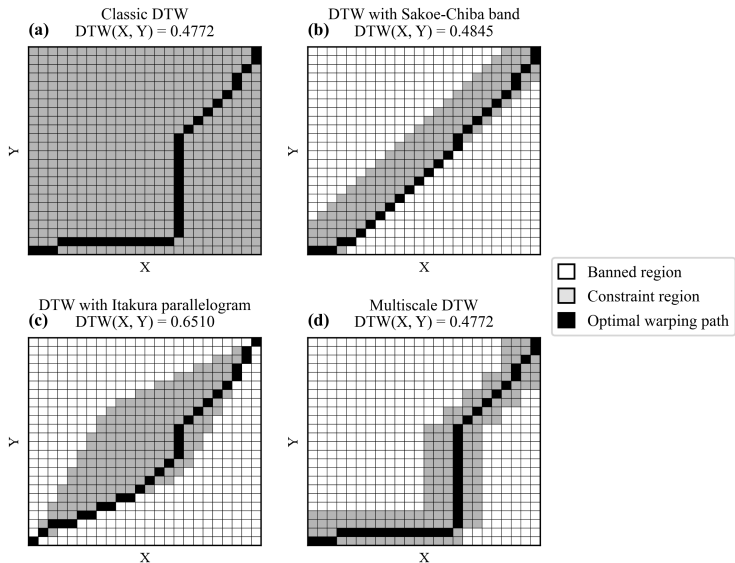
# Constraint regions

- **Idea:** Limit the possible values in a warping path.

Pros	Cons
Decrease maximum time warp	May not retrieve the optimal path
Decrease computational complexity	Hyperparameter

- A constraint region may depend on the values of both time series.
  - ▶ Series-independent constraint regions: Sakoe-Chiba band [SC78], Itakura parallelogram [Ita75].
  - ▶ Series-dependent constraint regions: Multiscale-DTW [MMK06], FastDTW [SC07].

# Dynamic time warping (with constraint regions)



# Global alignment kernel

- Dynamic time warping cannot be used to define a positive definite kernel since it does not satisfy the triangle inequality.
- **Global alignment kernel** [Cut11]:

$$k_{\text{GA}}^{\gamma}(x, y) = \sum_{p \in \mathcal{P}} \exp(-C_p(x, y)/\gamma)$$

- $k_{\text{GA}}^{\gamma}$  is a positive definite kernel under mild conditions.
- Soft dynamic time warping [CB17] (differentiable loss function):

$$\text{soft-dtw}_{\gamma} = -\gamma \log k_{\text{GA}}^{\gamma}$$

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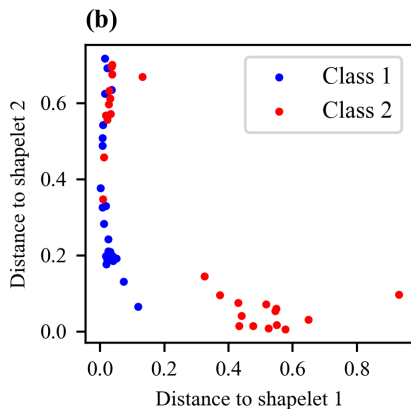
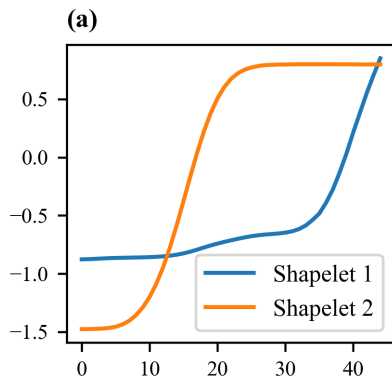
# Shapelet-based algorithms

- **Idea:** Some small sequences of consecutive values may be specific to certain classes.
- **Shapelet:** real-valued vector of size  $l \leq n$  ( $n$  being the size of the time series).
- **“Distance”** between a time series  $X = (x_1, \dots, x_n)$  and a shapelet  $S = (s_1, \dots, s_l)$ :

$$d(X, S) = \min_{j \in \{0, \dots, n-l\}} \sum_{i=1}^l (x_{i+j} - s_i)^2$$

- **Algorithms:** Shapelet transform [Lin+12], Learning shapelets [Gra+14].

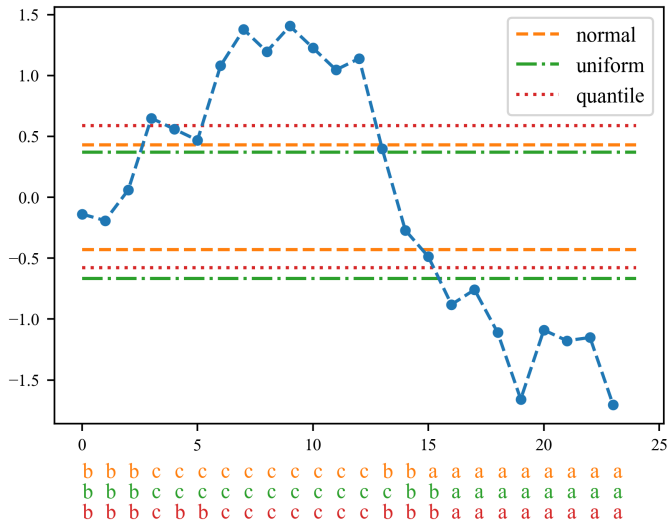
# Learning shapelets



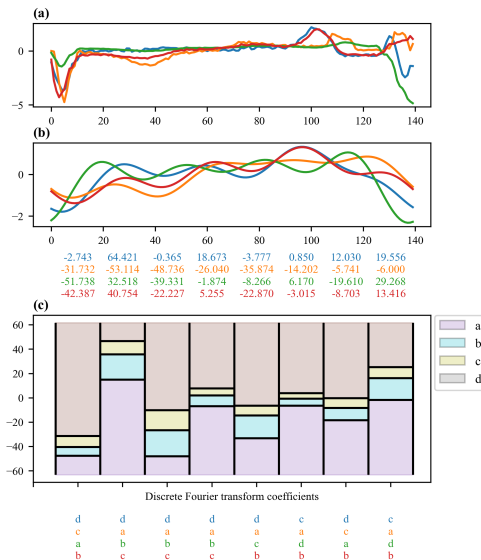
# Dictionary-based approaches

- **Idea:** transform a time series into a bag of words.
- **General algorithm:**
  - 1 Extract subsequences using a sliding window.
  - 2 Transform each subsequence into a word.
  - 3 Perform classification based on the word frequencies.
- **Algorithms:** Bag-of-Patterns [LKL12], SAXVSM [SM13], BOSS [Sch15], BOSSVS [Sch16], WEASEL [SL17]...
- **Two main methods** to transform a subsequence into a word:
  - ▶ discretization of (standardized) values: SAX [Lin+07]
  - ▶ discretization of Fourier coefficient: SFA [SH12]

# Symbolic Aggregate approXimation (SAX)



# Symbolic Fourier Approximation (SFA)



# Imaging time series

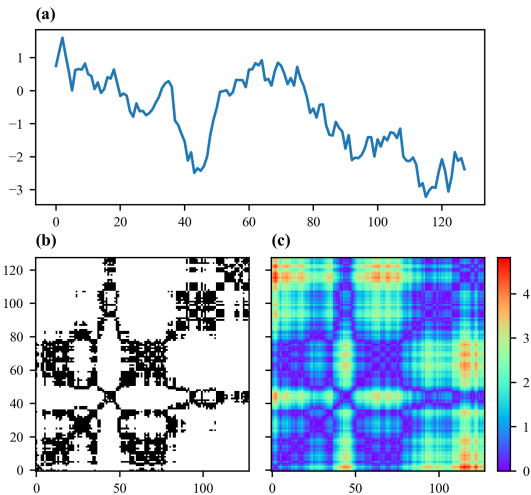
- Old concept (for visualizing dynamic systems).
- Motivated by **breakthroughs in computer vision** (convolutional neural networks).
- **Algorithms**: Recurrence plot [[EKR87](#)], Gramian angular field [[WO15](#)], Markov transition field [[WO15](#)].

# Imaging time series: recurrence plots

$$\vec{x}_i = (x_i, x_{i+\tau}, \dots, x_{i+(m-1)\tau})$$

$$R_{ij} = \mathbb{1} (\|\vec{x}_i - \vec{x}_j\|_2 < \varepsilon)$$

$$R_{ij} = \|\vec{x}_i - \vec{x}_j\|_2$$



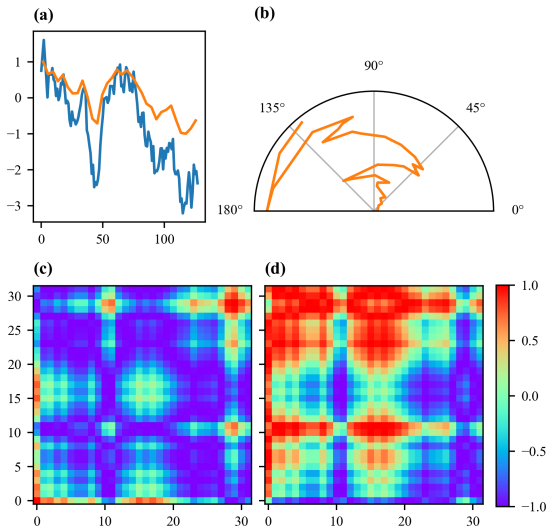
# Imaging time series: Gramian angular fields

$$\tilde{x}_i = -1 + 2 \frac{x_i - \min(x)}{\max(x) - \min(x)}$$

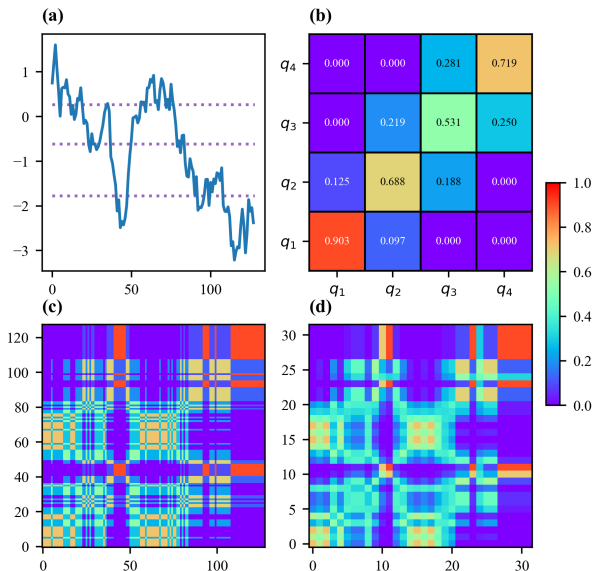
$$\phi_i = \arccos(\tilde{x}_i)$$

$$\text{GASF}_{i,j} = \cos(\phi_i + \phi_j)$$

$$\text{GADF}_{i,j} = \sin(\phi_i - \phi_j)$$



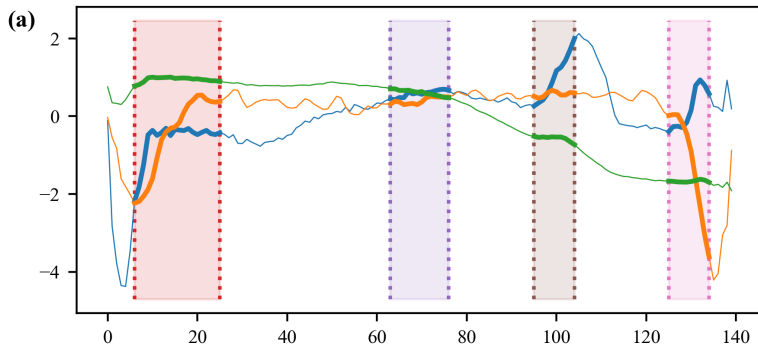
# Imaging time series: Markov transition fields



# Tree-based algorithms

- Motivated by the **success** of the **random forest** and **extremely randomized trees** algorithms.
- Two main approaches:
  - ▶ **Extract features** that are then used to **fit a standard tree-based algorithm**.
  - ▶ **Modify the tree building process** to make use of the different **metrics for time series** published in the literature.
- **Algorithms:** Time series forest [Den+13], time series bag-of-features [BRT13], Proximity forest [Luc+19].

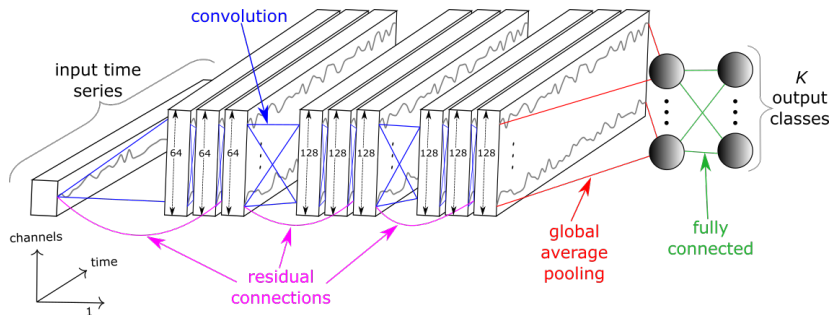
# Tree-based algorithms: Time series forest



(b)

	Interval 1			Interval 2			Interval 3			Interval 4		
	Mean	SD	Slope	Mean	SD	Slope	Mean	SD	Slope	Mean	SD	Slope
Time series 1	-0.61	0.504	0.052	0.58	0.086	0.02	1.004	0.572	0.197	0.189	0.504	0.156
Time series 2	-0.467	0.977	0.158	0.403	0.084	0.017	0.568	0.061	0.011	-1.204	1.305	-0.431
Time series 3	0.944	0.061	0.002	0.604	0.075	-0.018	-0.57	0.065	-0.017	-1.671	0.024	0.003

# Neural networks: InceptionTime [Ism+20]



# Random convolutional kernels

- Generating **random** convolutional kernels instead of learning them.
- **Different aggregated features** computed from each feature map from usual global average/max pooling:
  - ▶ proportion of positive values
  - ▶ longest period of consecutive positive values
- Ridge classifier fitted on these extracted features.
- **Algorithms:** ROCKET [DPW20], MiniROCKET [DSW21], MultiROCKET [Tan+21].

# Ensemble models

- Ensemble of **several models** (different algorithms, same algorithms with different hyperparameters).
- **State-of-the-art** in terms of **predictive performance** only, but **very high algorithmic complexity**.
- **Algorithms**: COTE [[Bag+15](#)], HIVE-COTE [[LTB18](#); [Bag+20](#); [Mid+21](#)], TS-CHIEF [[Shi+20](#)].

# Time Series Classification Archive

- **Website:** <http://timeseriesclassification.com>
- Over 100 univariate (and 30 multivariate) time series classification datasets.
- **Benchmark results** for many algorithms.

# Conclusion

- **Many papers** describing **new algorithms** dedicated to time series classification have been published in the literature, with a **wide variety** of approaches being investigated.
- **Concrete application:**
  - ▶ One wants to tackle a real-world use case which is formulated as a time series classification task.
  - ▶ What are their possibilities?

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# Barriers to work on a real-world application

- Investigate **several algorithms** to see what works best.
- Possible issues with source code:
  - ▶ **Not available.**
  - ▶ Written in **different programming languages** (Java, MATLAB, Python, R, etc.).
  - ▶ Provided commands only aiming at **reproducing the results on some given datasets.**
  - ▶ **Barely commented** and **not easily extendable.**
  - ▶ **Barely documented.**

# Replication crisis

- Little incentive to publish the source code associated to a paper (until recently).
- Source code rarely peer reviewed (until recently).
- **Yet, all the experiments, thus the results and conclusions, rely on the source code.**

# Source code - different levels of usability

- **Code availability:** Easily accessing the source code of a project.
- **Reproducibility:** Reproducing (almost) the same experiments and obtaining (almost) the same results (hardware, float precision, etc.).
- **Replicability:** Slightly modifying the experiments (different dataset, different use case) and obtaining “good” results.
- **Reusability:** Easily integrating the tools made available in one project in another project.

# Objective

- **Present the notions and tools that make producing reusable code easier.**
- **Advocate for managing your project as a software.**

# Version control

- **Problem:** Updating the source code of a software may quickly become a mess because of multiple versions of the same software at any given time:
  - ▶ Remote version
  - ▶ Local version for each developer
- **Version control:** Tracking and providing control over changes to source code.
- **Distributed version control:** The complete codebase, including its full history, is mirrored on every developer's computer, enabling automatic management branching and merging.
- **Tools:**



▶ Mercurial

# Hosting your source code

- GitHub



- GitLab



- Bitbucket



- SourceForge



# Hosting your (Python) package

- Some programming languages (e.g., Python, R, TeX) have an **official archive** to upload and download packages.

- PyPI: Python Package Index**

- ▶ Over 330 thousand projects
- ▶ Over 3 million releases
- ▶ Over 500k users

```
pip install pyts
```

```
conda install -c conda-forge pyts
```

- conda**: package, dependency and environment management:
  - ▶ **Limitation**: Only a few packages are available in the default channel; anyone can create their own channel to host their packages (but this has several disadvantages).
  - ▶ **conda-forge** is a community effort that provides conda packages for a wide range of software in a single channel.

# Semantic versioning

- Website: <https://semver.org>
- Summary:

*Given a **version number MAJOR.MINOR.PATCH**, increment the:*

- ▶ *MAJOR version when you make **incompatible API changes**,*
- ▶ *MINOR version when you add **functionality in a backwards compatible manner**, and*
- ▶ *PATCH version when you make **backwards compatible bug fixes**.*

*Additional labels for pre-release and build metadata are available as extensions to the MAJOR.MINOR.PATCH format.*

# Linting

- **Definition:** Process of checking the source code for programmatic and stylistic errors.
- Examples of stylistic errors:
  - ▶ Lines too long
  - ▶ Defining variables that are never used
  - ▶ Missing (or too many) whitespaces (or blank lines)

# Linting in Python

- Mainly defined by two **Python Enhancement Proposals** (PEP):
  - ▶ [PEP 8](#): Style Guide for Python Code
  - ▶ [PEP 257](#): Docstring Conventions
- Main Python package: [flake8](#)
  - ▶ `flake8` itself does not implement checks but builds a strong foundation for a plugin ecosystem.
  - ▶ Popular plugins:
    - ★ [pyflakes](#): checks Python code for errors.
    - ★ [pycodestyle](#): checks Python code against some PEP 8 style conventions.
    - ★ [mccabe](#): checks McCabe complexity using Ned's script.
    - ★ [pep8-naming](#): checks Python code against PEP 8 naming conventions.
    - ★ [flake8-docstrings](#): is an extension for [pydocstyle](#) to `flake8`.

# Code style (in Python)

- Even when abiding by PEP 8 style conventions, there are still **many ways to write the same piece of code**.



- **Black**: The uncompromising code formatter:
  - ▶ Blackened code looks the same regardless of the project you're reading.
  - ▶ Formatting becomes transparent after a while and you can focus on the content instead.
  - ▶ Black makes code review faster by producing the smallest diffs possible.

# Testing

- Would you state a new theorem without giving its proof?

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- Would you state a new theorem without giving its proof?
- Would you apply a theorem without checking if the hypotheses are satisfied?
- Would you trust anyone's code (including yours) without it being tested?

# Testing

**Objective:** Testing that your code **works** and **does what it is supposed to do**.

- **Unit testing:** Testing individual modules of an application in isolation to confirm that the code is doing things right.
- **Integration testing:** Checking if different submodules of your project are working fine when combined together.
- **Functional testing:** Testing a functionality in the project (may interact with dependencies) to confirm that the code is doing the right things.

# Testing in Python

- `unittest`: Python package from the standard library.
- `nose`: deprecated Python package.
- `pytest`: the most popular Python package (easier, more flexible).

# Code coverage

- **Definition:** a measure used to describe the degree to which the source code of a program is executed when a particular test suite is run.
- Common metric: percentage of lines that have been executed at least once. Available at any level:
  - ▶ in the whole module,
  - ▶ in any submodule,
  - ▶ in any file.
- Reliant on the report of the testing tool used to run the test suite.

# Code coverage in Python

- `coverage`: general tool (initially developed to be used with `unittest`).

- `pytest-cov`: plugin for `pytest`.

# Code coverage (online)

- Reporting the code coverage results online has several upsides:
  - ▶ **Information easily available to anyone** (no need to run a command)
  - ▶ **User-friendly report** (sunburst graph, code coverage at any level, etc.)
  - ▶ Can be included in the **continuous integration** pipeline (e.g., monitoring the change in code coverage in a pull request)
- Available tools:
  - ▶ [Codecov](#)
  - ▶ [Coveralls](#)



# Documentation

- A software (and more generally any source code) **without its corresponding documentation** is almost **useless**.
- **Key elements** of any documentation:
  - ▶ Installation instructions
  - ▶ User guide
  - ▶ API documentation
  - ▶ Examples
- Other useful elements: getting started, tutorials, changelog, glossary, developer guide, etc.

# Documentation in Python

- **Sphinx**: Python documentation generator

- ▶ Originally created for the Python documentation
- ▶ Expanded to other programming languages (C, PHP, Ruby, JavaScript, etc.)
- ▶ Many useful extensions, including:
  - ★ `sphinx.ext.autodoc`: Include documentation from docstrings
  - ★ `sphinx.ext.autodoc`: Generate autodoc summaries
  - ★ `sphinx.ext.viewcode`: Add links to highlighted source code
  - ★ `sphinx.ext.doctest`: Test snippets in the documentation
  - ★ `sphinx_gallery`: Build an HTML gallery of examples from any set of Python scripts

- **MkDocs**: project documentation with Markdown

# Documentation (online)

- A **website** dedicated to the documentation is much more user-friendly than a PDF file with hundreds or even thousands of pages.
- **ReadTheDocs**: Simplify software documentation by automating building, versioning, and hosting of your docs for you.
- **GitHub Pages**: Websites for you and your projects.
  - ▶ Hosted directly from your GitHub repository.
  - ▶ Just edit, push, and your changes are live.
- Automatically redirect to another website if you own a dedicated domain.

# Continuous integration

- **Rationale:** Making sure that any version of the remote source code always works.
- **Content:** linting, testing, code coverage, documentation, etc.
- **Workflow:** Before changing the remote source code:
  - 1 Run the continuous integration locally.
  - 2 Run the continuous integration remotely (several operating systems, several versions of dependencies, etc.).
  - 3 If successful, the changes can be merged.

# Continuous integration (online)

Many services available, all of them being free for open source projects (with reasonable restrictions), including:

- Azure Pipelines



- Travis CI



- CircleCI



- AppVeyor



- Jenkins



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# What is `pyts`?

- Python package dedicated to time series classification.
- **Objective:** Make working on time series classification easy:
  - ▶ Data loading utilities, preprocessing tools, implementations of many algorithms,
  - ▶ Under a unified application programming interface,
  - ▶ Compatible with `scikit-learn` tools such as cross-validation and pipelines.
- Published in the *Open Source Section of Journal of Machine Learning Research* in 2020 [FJ20].

# Concrete example



Let's see how the tools presented in the second section are applied in this package.

# Thanks

Thank you for your attention

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