Input Data and Distance Measures

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Anatomy of unsupervised algorithms

Internal choices / cost function:
- Usually, we cannot control these.
- Strongly affect the result, and define the range of possible outputs.

Algorithm output:
- Density distribution.
- Clusters.
- Embedding in low-D space.
- Outliers.

$$f(\overrightarrow{X}, \{a_1, a_2, ...\}) = \overrightarrow{y}$$

Input dataset:
- Raw data (spectra, images, light-curves).
- Extracted features.
- Measured relations between different objects (distances, correlations).

Hyperparameters:
- Tuning parameters of the algorithm.
- Can strongly affect the result.
- Traditionally, cannot be optimized for.

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Distance will be estimated using either!

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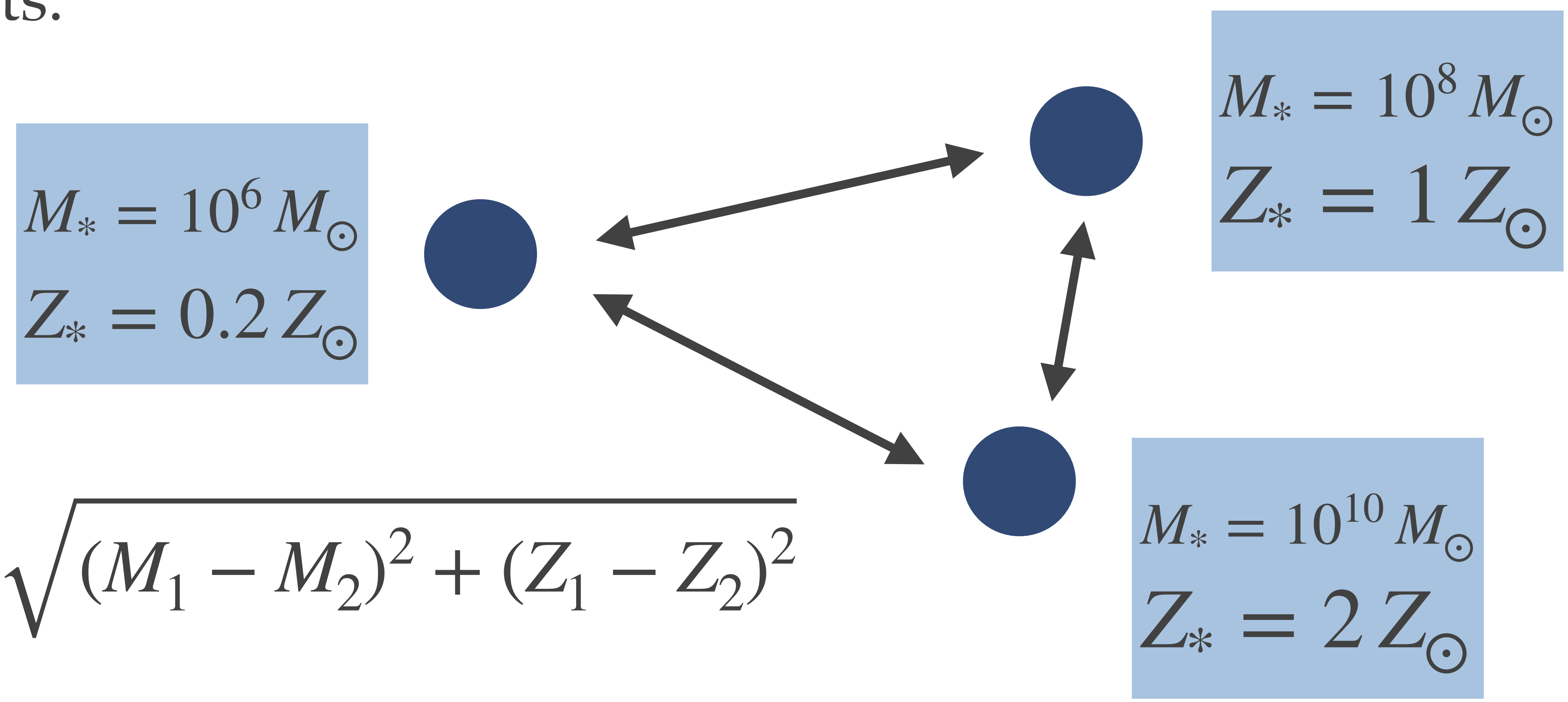
- **Interpretability:** it is easier to understand what is the meaning of the algorithm's output using derived features.
- **Potential for new discoveries:** by using derived features we are limiting ourselves to a fewer number of parameters which we are already familiar with, which reduces the discovery potential. We only derive features for what we already know, what about the things we don't know?

Derived features: aspects to consider

- **Feature scaling and normalization:** features derived from astronomical observations have physical units, and might have different dynamical scales. Features with larger variance will dominate the summed Euclidean distance between individual objects.



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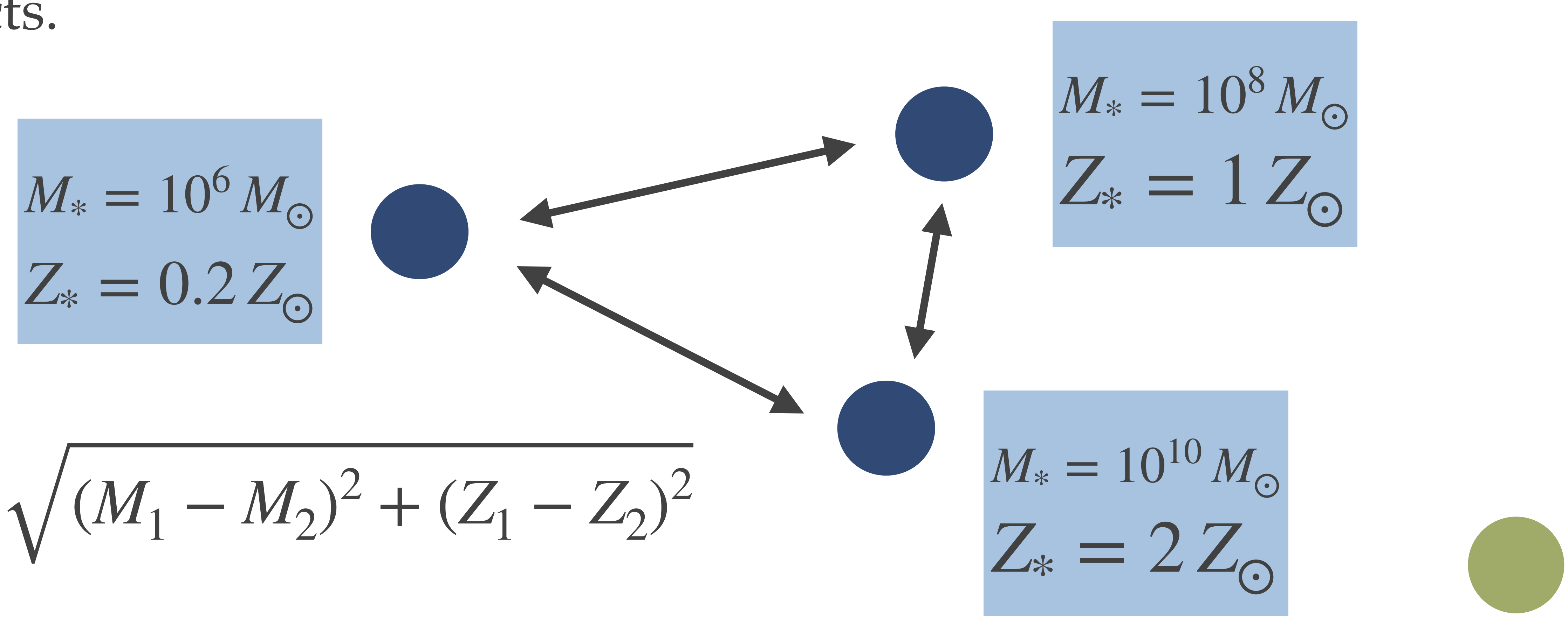

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- **What to do?** Apply rescaling and normalization to all the features. Use the logarithm of the feature as the new feature, and/or normalize using the mean and standard deviation of the distribution: $f_{norm} = (f - \mu_f)/\sigma_f$.

Derived features: aspects to consider

- **Outliers:** some algorithms are based on the variance within each feature and are highly-sensitive to the presence of outliers in the data.
- **What to do?** Use histograms to inspect each feature separately and identify and/or remove outliers. A common practice is also to clip the feature values to be between the 0.5th and 99.5th percentiles of the distribution.

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- **Correlated features:** a set of highly-correlated features in the dataset will result in a higher weight in the summed Euclidean distance, which may wash-out other structures in the dataset.
- **What to do?**
  - Use PCA to obtain features in an orthogonal space. Might not be very interpretable.
  - Instead of using the correlated features, use the deviation of one feature from the correlation with another. Might not scale well for multiple features with multiple correlations.

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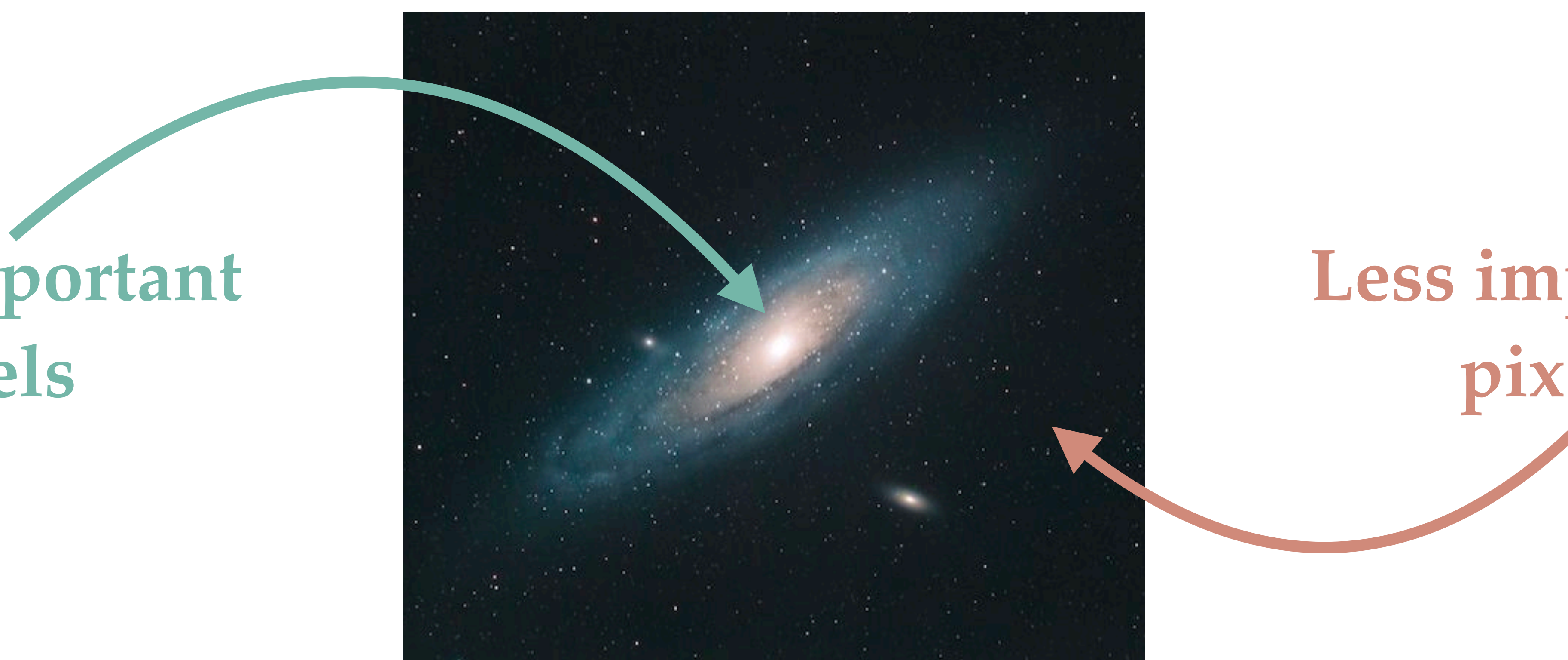

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  - Frequency domain for time series data.
  - Wavelet transform for imaging data.
  - Representation using "eigenvectors" of spectral information.

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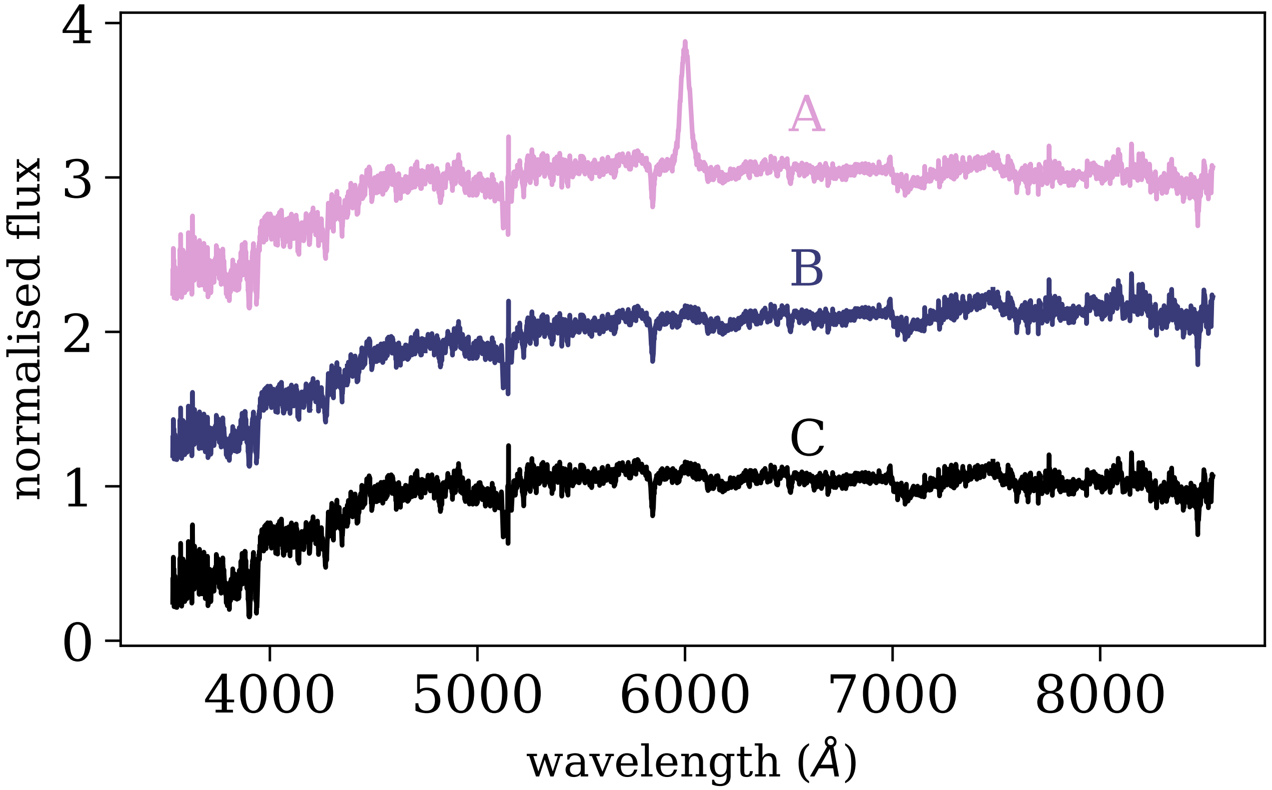
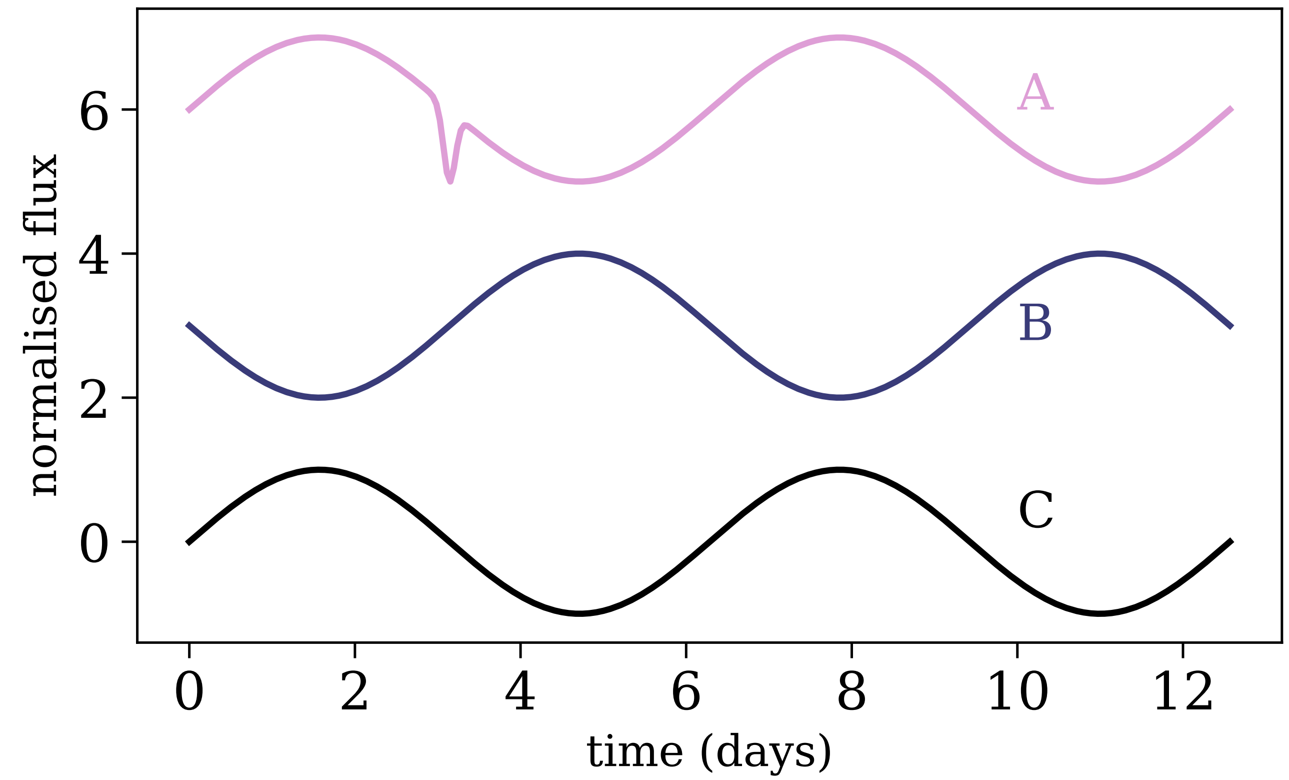
Example of spectra:



Example of time-series:



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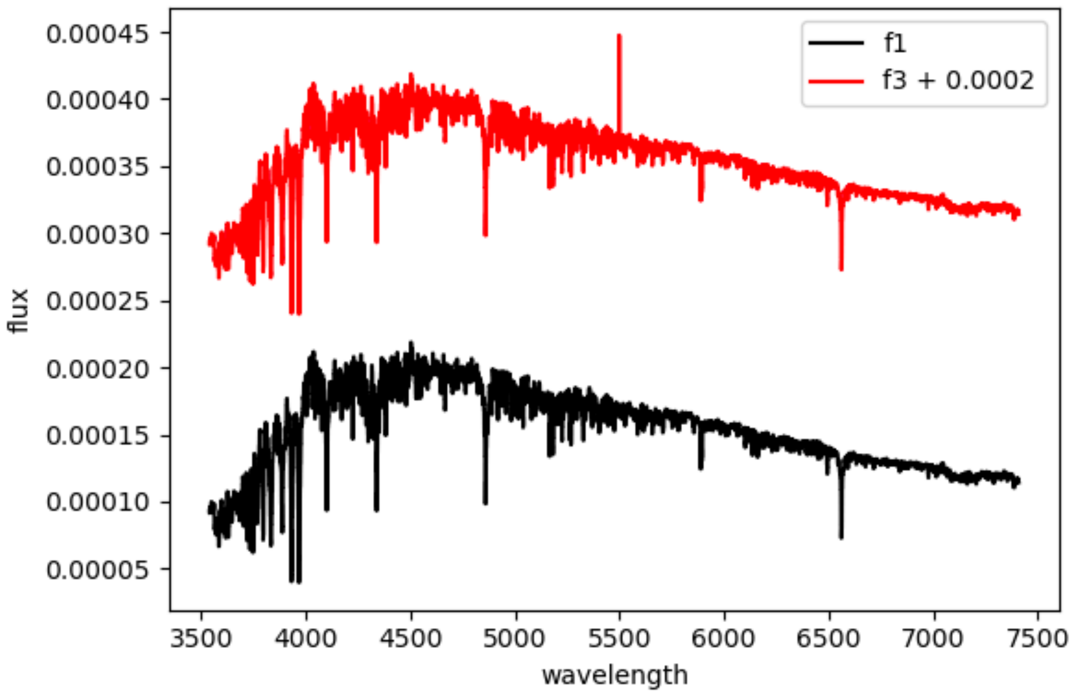

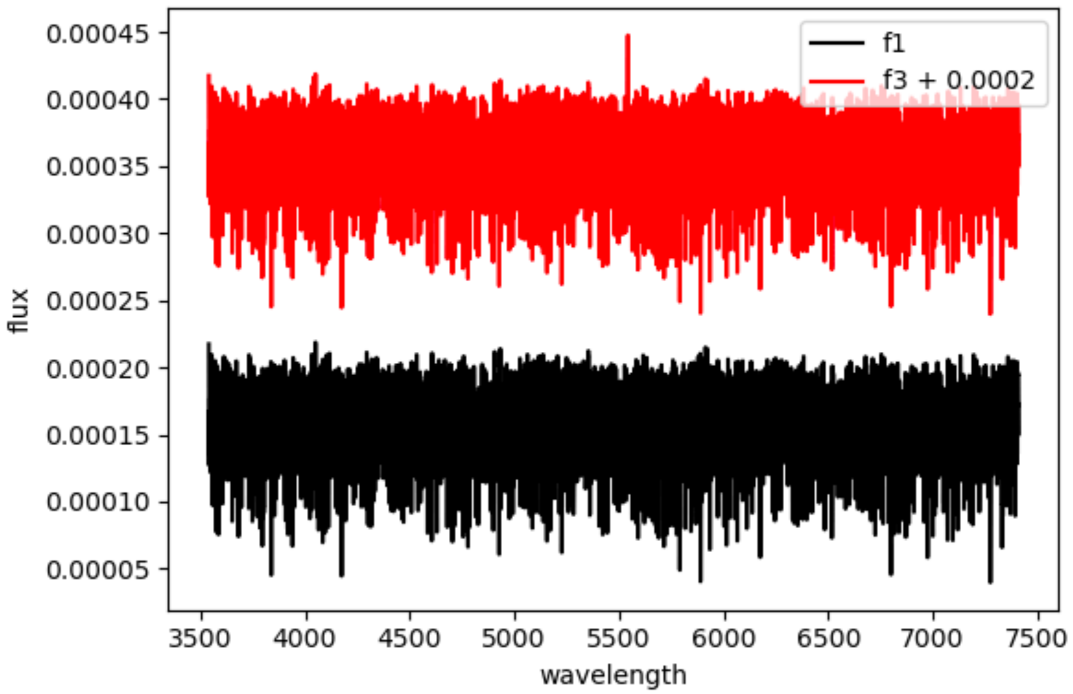

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- Other metrics:
  - Pearson/Spearman correlation coefficient.
  - KL-divergence.
  - Earth mover's distance or energy distance: the relative order of the features matters!!.
  - A list of popular metrics can be found here.