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Machine learning interpretability to explain supernovae progenitor's characteristics

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Scientific Rationale

- In the next few years, the **number of available supernovae observations will increase exponentially** thanks to the **Legacy Survey of Space and Time (LSST)** Survey

- **Inferring the supernovae's progenitor characteristics is** currently performed using several **computationally expensive** methods
  - An example is **Bayesian inference**, that is computationally challenging as a Monte Carlo search is involved to test the parameters
  - Supernovae classification (e.g., 87A, type 1, etc.) , on the other hand, is an easier task

Scientific Rationale

- Given the increasing number of observations, **finding the characteristics of all the supernovae' progenitors will be** practically **unfeasible** with current methods
- Moreover, **observational resources** are **scarce and shared** by many researchers
- Identifying the **key phases (in days) for the characterization tasks** can…
  - **… help researchers spare observational resources** that can be employed elsewhere
  - **… optimize the data collection process**

Technical Objectives

- In this work, **we aim at training a machine to infer the characteristics of the supernovae's progenitor**: **energy, mass, radius, and nickel content**
  - **World-first** approach, never done before

- **Machine Learning is well-suited** for the task:
  - **Noise and error-tolerance**
  - **Fast computation**
  - Easily trainable on new data
  - Can provide insights on the problem itself trough interpretability tools

- **This work is also meant as a test-bench for the new HPC capabilities** that are under deployment

Methodologies and Solutions

- Each **observation** includes **two timeseries** the **bolometric luminosity** and **photo-spheric velocity**. Moreover, **real-world observations are scarce, and fully-characterized ones are even less**

- **We employ** the **state-of-the-art** of trainable algorithms, the ***InceptionTime*** **model**, **for time-series data to infer** (through regression) the characteristics
  - **We train the model on generated** time-series **data from synthetic models**, that provide **bolometric luminosity** and **photo-spheric velocity**
- Then, **we "open" the black-box and gain insights** on the problem **via *Occlusion***, a machine-learning **model-interpretability tool**
  - **The consistency of explainer results with astrophysical models is a significant step towards developing an ML-based automatic characterization procedure**

Methodologies and Solutions

- **Synthetic models available**:
  - **Semi-analitical**: very **fast**, produces **rough approximations** that do not exactly match the real-world observations
  - **Hydrodynamical** simulations: **computationally expensive** and **slow**, accounts for many phenomena happening in the star
- **Dataset generated**:
  - **205k semi-analitical observations of 87A-like**
  - **59 hydrodynamical observations of 87A-like**

Accomplished Work, Results

- **Curriculum-learning** strategy**: models** are **trained starting with simpler examples and gradually increasing in complexity**, mimicking the human learning process
  - It helps models to generalize better and can lead to faster convergence during training, while also being data efficient

- **Three** learning **phases:**

1. **Training on** the **semi-analitical** data, **testing on** the **hydrodynamical** observations

2. **Training on** (a subset of) the **hydrodynamical** data**, validation and testing on** the **ones left** out the training set

3. **Training on** all the **hydrodynamical** data**, testing on the real-world observations**

Accomplished Work, Results

- **First vs second phase** result **comparison on hydrodynamical** data
  - **Major improvement in results (MAPE)**

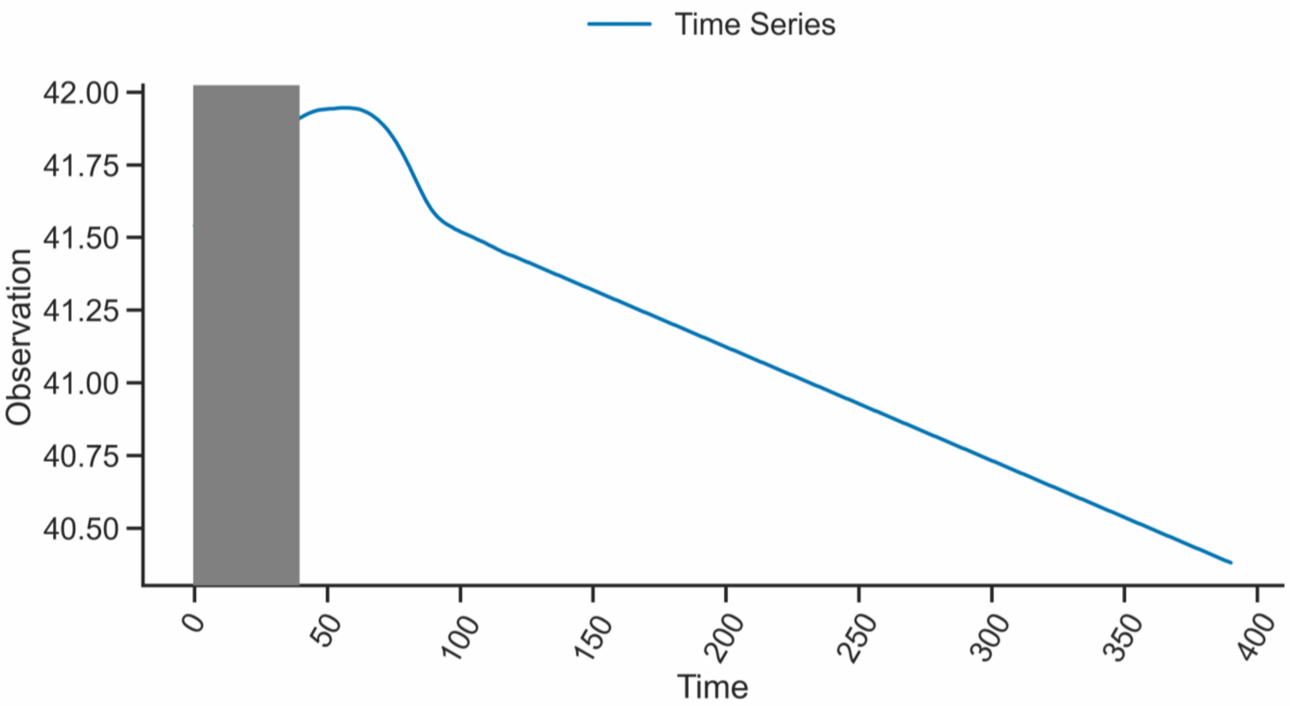
	Radius	Mass	Energy	Nickel
baseline	98%	48%	193%	186%
C. learning (old)	61%	20%	41%	39%
C. learning	**50%**	**20%**	**13%**	**18%**

- **[WIP] Real-world data performances**

	Radius	Mass	Energy	Nickel
C. learning	**108%**	**178%**	**112%**	**22%**

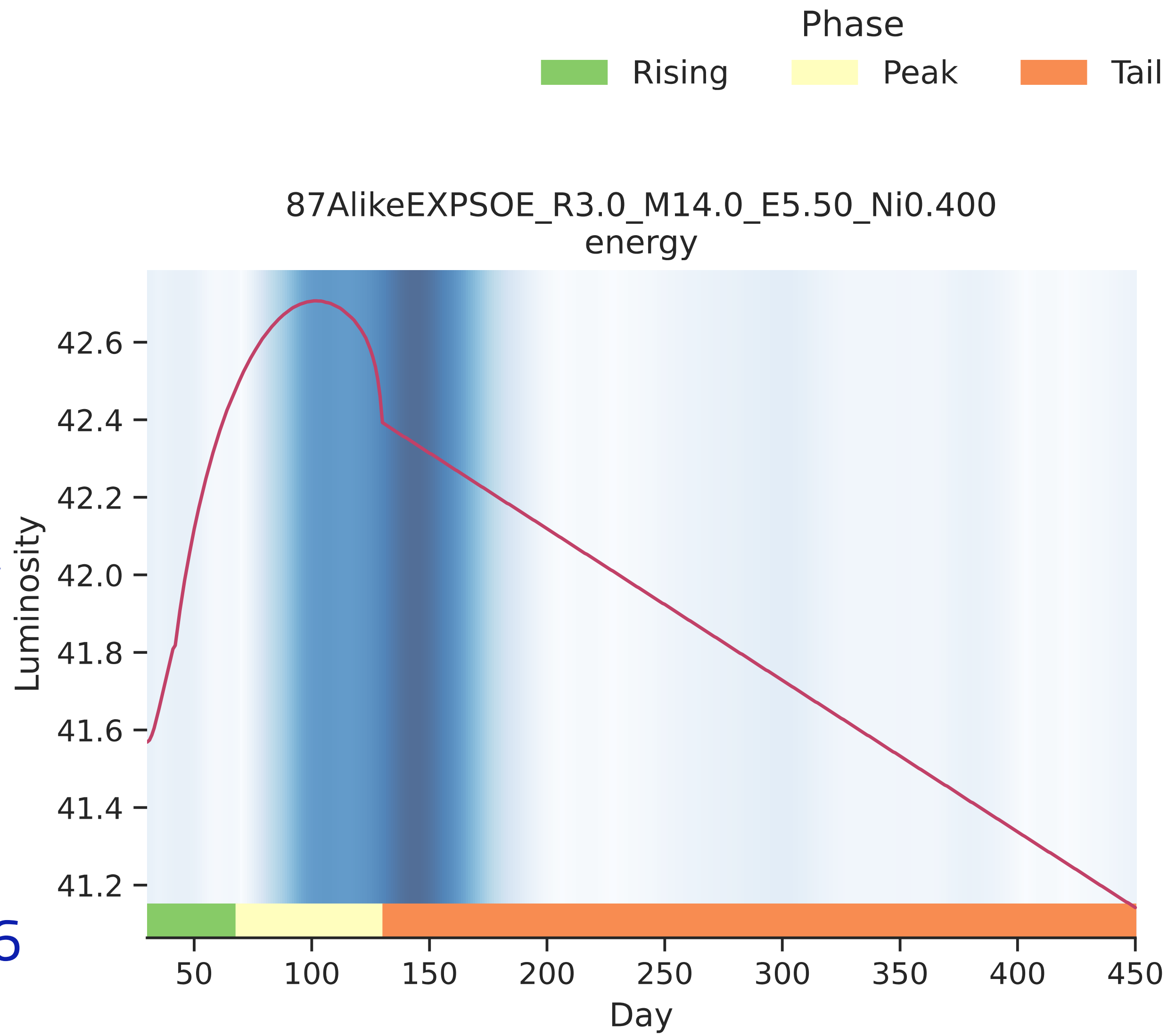
Accomplished Work, Results

- ***Occlusion*** is a **technique used** in machine learning interpretability **to understand** the **importance of different parts of the input** data…
- … **by** systematically **masking** or "**occluding**" **parts of the input and observing the effect on the model's output**
- **This** helps **in identifying the most influential parts and interpreting the model's behavior**



Accomplished Work, Results

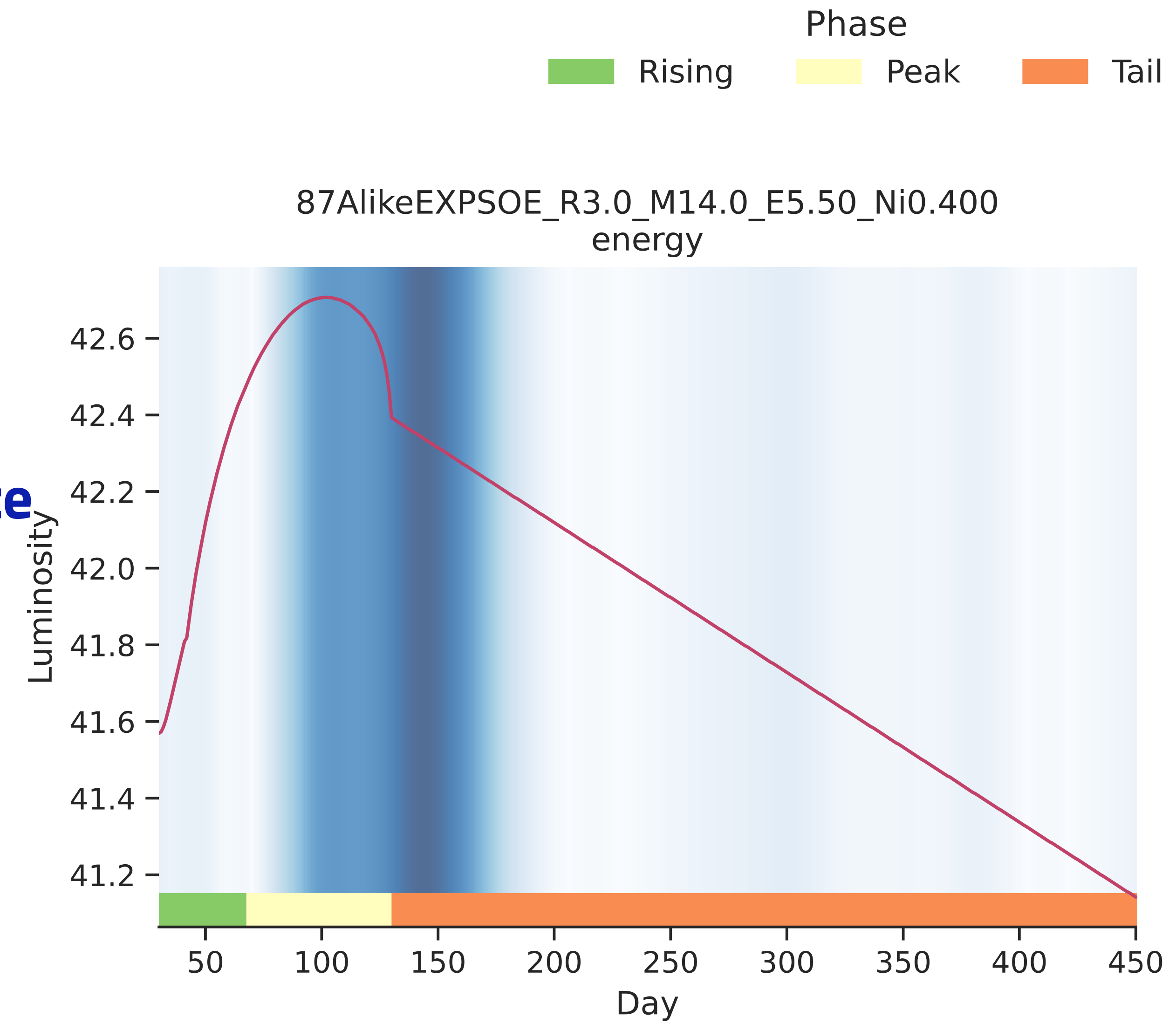
- **We divide** the **light curve** in **three phases**: **rise**, **peak** and **tail**
  - ***Rise*** phase…
  - **…** that **halts at a *peak* phase with maximum luminosity followed by** a **rapid decline**
  - **After this**, the ***tail* phase begins**, where **logarithm** of **luminosity becomes linear**, resulting from radioactive elements like Nickel-56 and Cobalt-56



Accomplished Work, Results

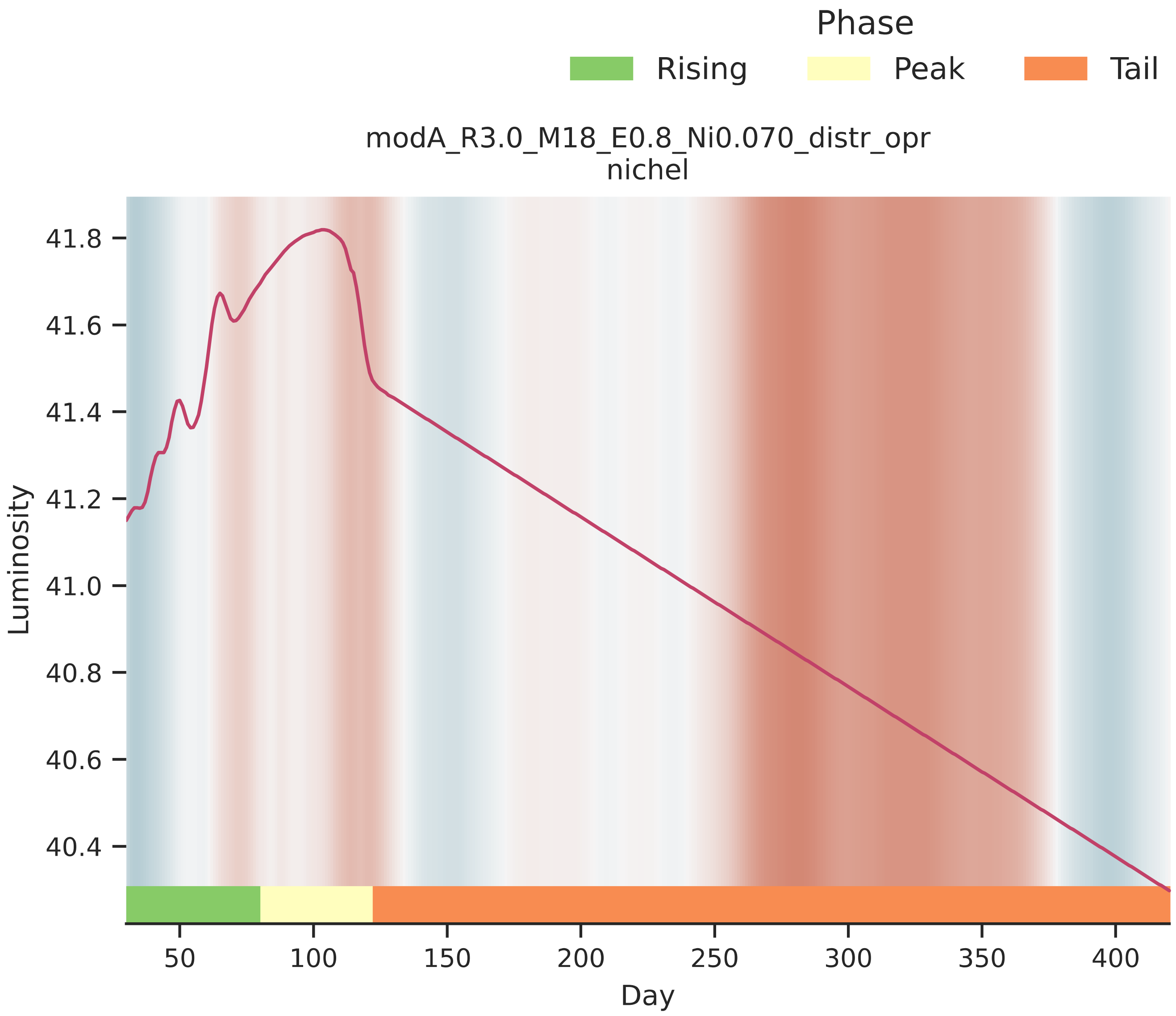
- We first test ***Occlusion*** **on** some **test-samples from** the **semi-analytical dataset**

- **The model learns to** effectively **utilize the rise, peak, and tail phases as expected, but also the knee** on the transition between the peak and the tail



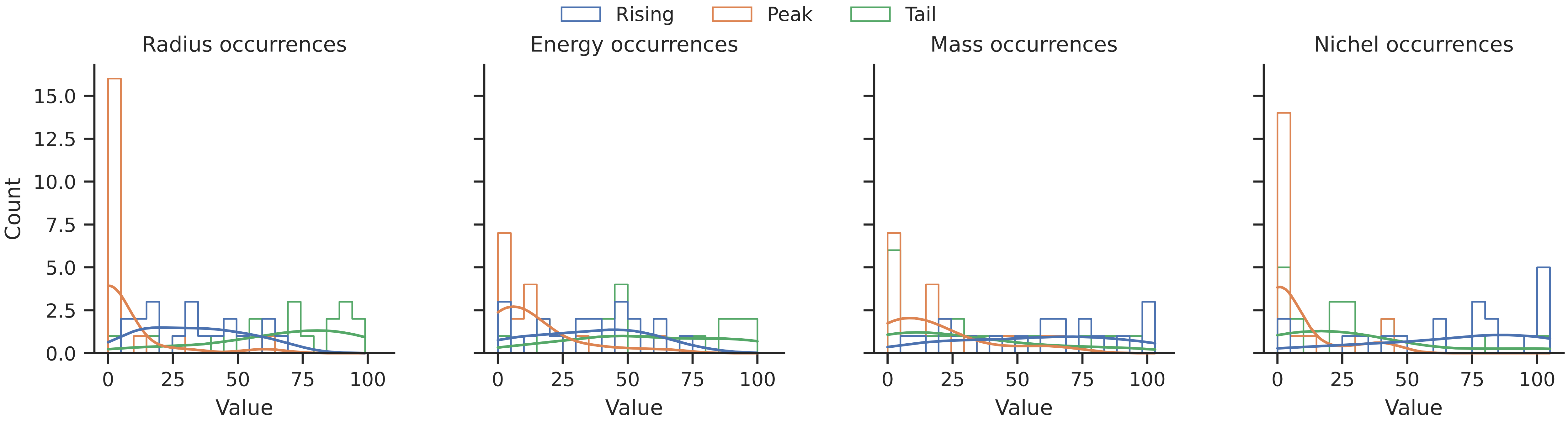
Accomplished Work, Results

- Then, **we test *Occlusion*** on the hydrodynamical observations
- The **results observed** in **the semi-analytical case are also validated with hydrodynamic data**
- The **color** here **represents** the fact that if the **corresponding point** is **missing**, the **value is underestimated (red) or overestimated (blue)**



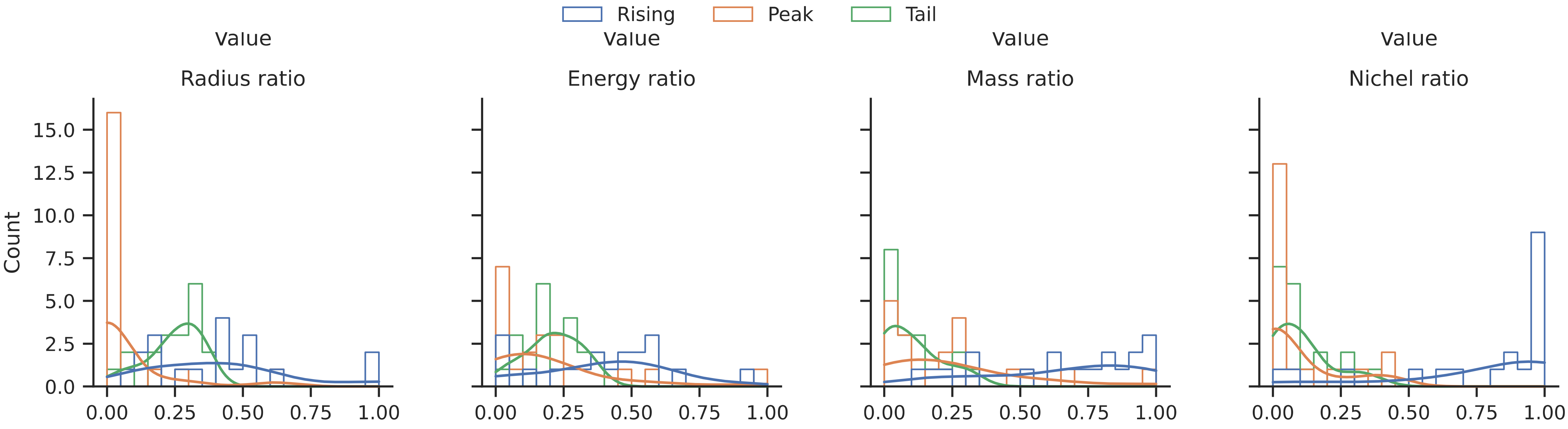
Accomplished Work, Results

- By **studying multiple simulations** and repeating the process **for all four supernova parameters**, **we** can **evaluate** the **importance distribution across the three** main light curve **phases**



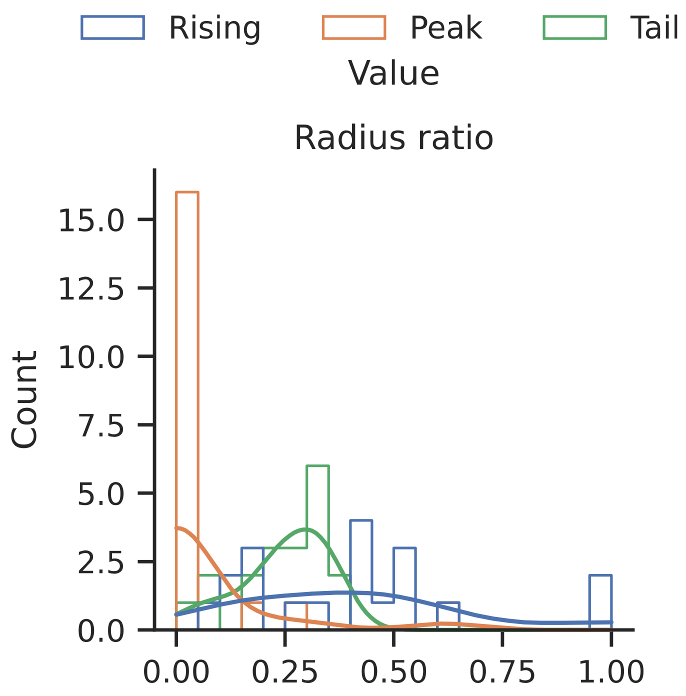
Accomplished Work, Results

- We also **evaluate ratios** rather than raw number of occurrences, **as different phases have varying** point counts based on their **temporal width**



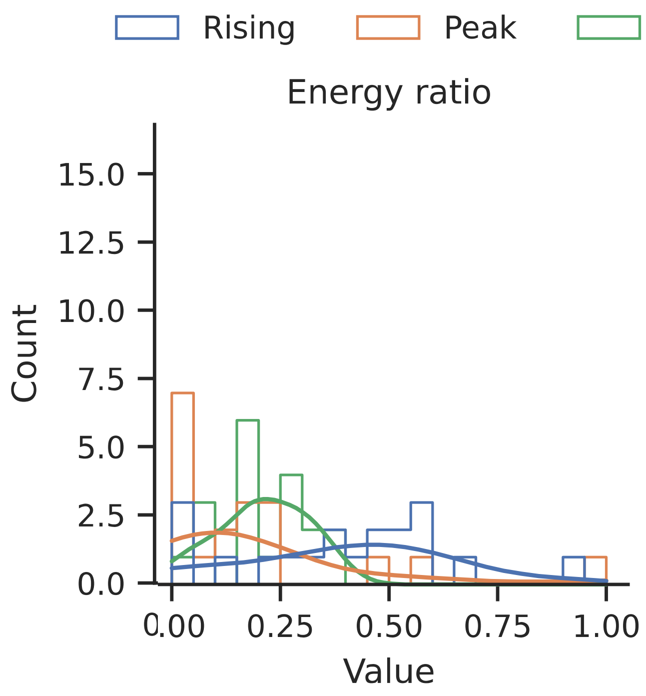
Accomplished Work, Results

- The **radius represents** the **initial radius of the star before** the **explosion**. **During the first phase**, **the supernova expands adiabatically**, and **the rise is linked to the increase in radius**
- The **ML model leverages this dependence dependence on the the rise phase**
- The initial radius also influences the end of the recombination phase during the peak
- The tail phase is weakly influenced by the radius, as the SN's photosphere ceases to exist, and the emission is related to the thermalization of Nickel distributed within the ejecta



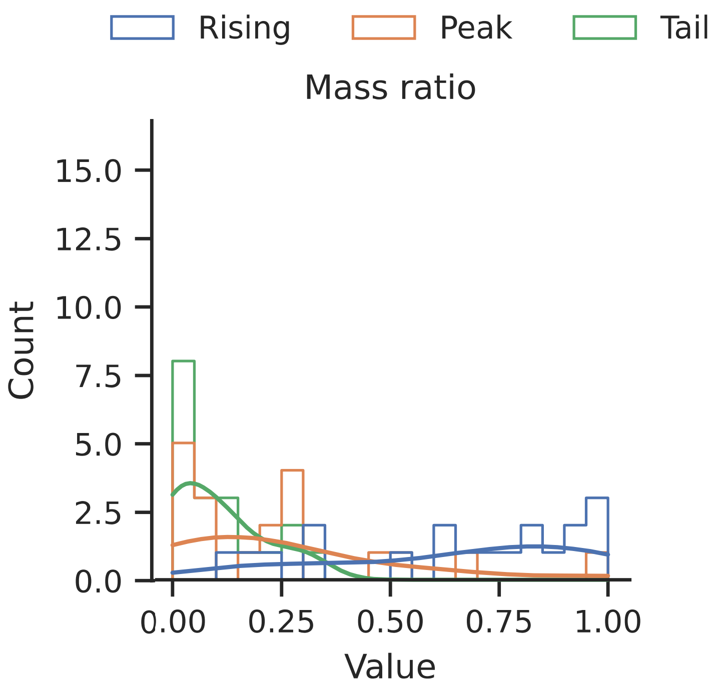
Accomplished Work, Results

- **Energy** strongly **influences** the **expansion speed** of the ejecta
- **Faster expansion leads** to a **quicker peak** evolution **and higher luminosity** during the rise phase
- This effect is evident from the strength distribution in the second column of the plot
- Energy is **most influenced by the rise phase and** bimodally during **the peak**



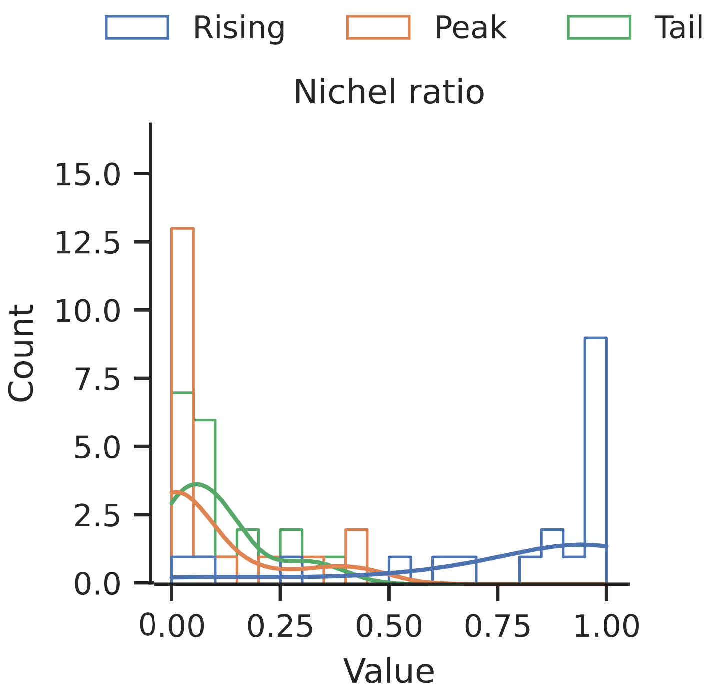
Accomplished Work, Results

- **Mass influences the expansion speed** of the ejecta in the **opposite** manner (see e.g., Pumo & Zampieri 2011) **than energy**
- **Tends to slow down** the **recombination process**, **extending** both the **rise and peak phases** in terms of time
- These effects are **also evident in the what the ML model learned**, where the importance of the peak phase varies significantly around 25%



Accomplished Work, Results

- The **tail phase** is **primarily influenced by** the behavior of **Nickel mass**, as suggested by theoretical models
- **Nickel can also significantly impact earlier phases**, especially in SNe 87A-like events (see e.g., Pumo & Cosentino 2024)
- This **connection between Nickel and the** other two **phases** is **evident from the ratio** parameter, calculated as the ratio of significant points above a certain threshold in a phase to all points in that phase



Next Steps and Expected Results

- **Improve and "explain" the predictions on real-world data**

- **Dataset improvement**
  - New and more accurate synthetic model to improve the training data
  - More hydrodynamical simulations
  - Train on real-world ones

- **Timeseries generation using ML**

Timescale, Milestones and KPIs

- **M7:**
  - **Model refinement**
  - **Code development and improvements**
  - **KPI: code / data**
- **M8**
  - **Grid search** of hyper-parameters
  - **KPI: numerical results, code / data**
- **M9**
  - Design and development of **timeseries key points extraction**
  - **Generalization to real-world examples**
  - **KPI: numerical results, code / data**
- **M10**
  - **KPI: paper preparation + results**

Timescale, Milestones and KPIs

- **M10**
  - **KPI: paper preparation + results**
- **M11**
  - **Grid search** of hyper-parameters
  - **KPI: numerical results, code / data**
- **M12**
  - Design and development of **timeseries key points extraction**
  - **Generalization to real-world examples**
  - **KPI: numerical results, code / data**
- **M10**
  - **KPI: paper preparation + results**

Thank you!

InceptionTime model

- Proposed for **Time Series Classification (TSC) tasks**
  - **Stacks multiple Inception-v4 layers** initialized with various weights
  - **Convolutional Neural Networks** (CNNs) are **at the core**
  - Combines **pooling, batch normalization** and
  - optionally includes **residual connections**