

Laboratory of Computational Physics 2022-2023
Astrophysics Project

The Formation of Binary Black Holes

Bhatti Roben

Bedin Veronica

Bonato Diego

Sapkas Michail

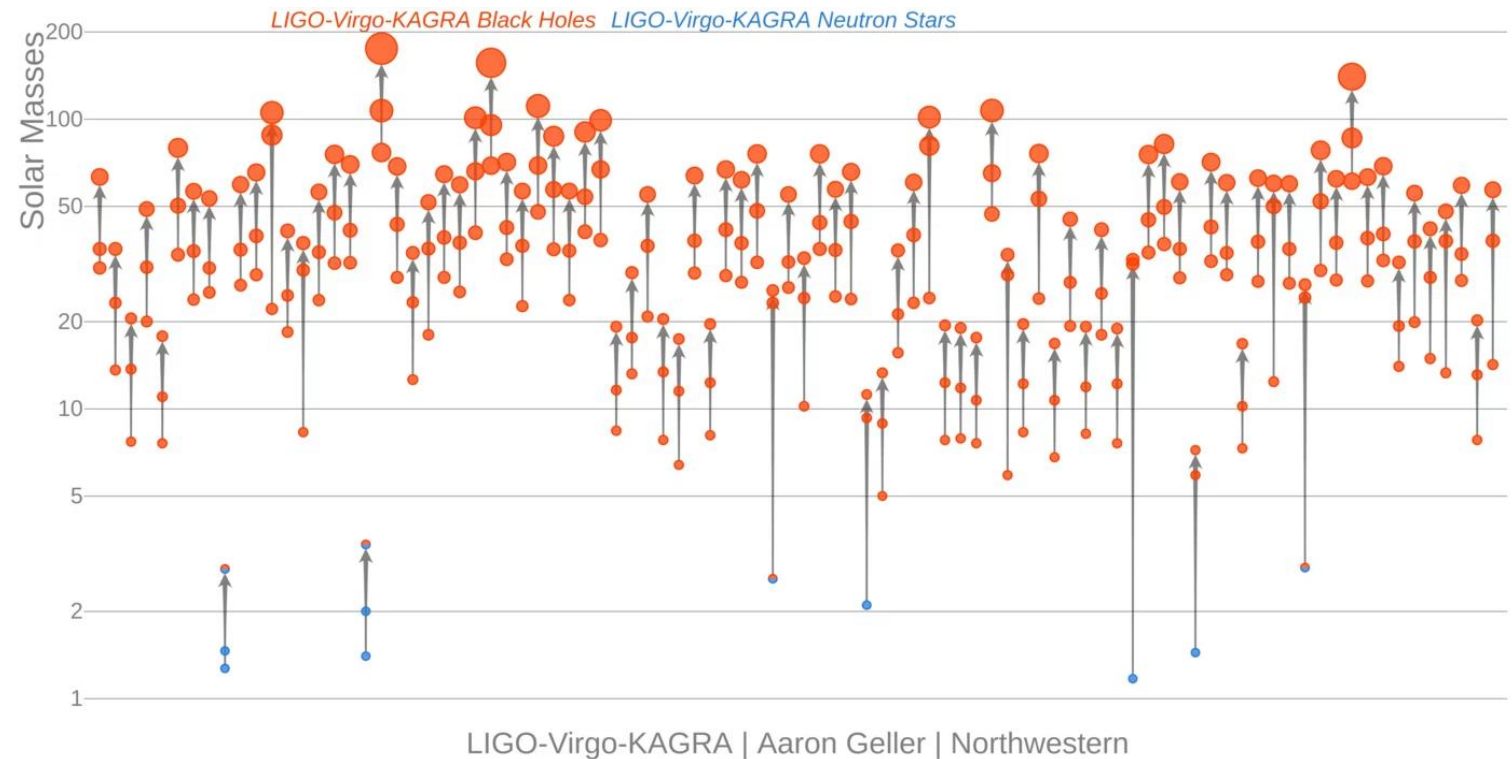
Binary black holes and gravitational waves



90 events of
gravitational waves



80 mergers of **binary
black holes**



Masses in the stellar graveyard

Goal of the project



Goal of the project:
finding **what features** have
the highest impact on the
evolution of a binary system
into a Binary Black Hole

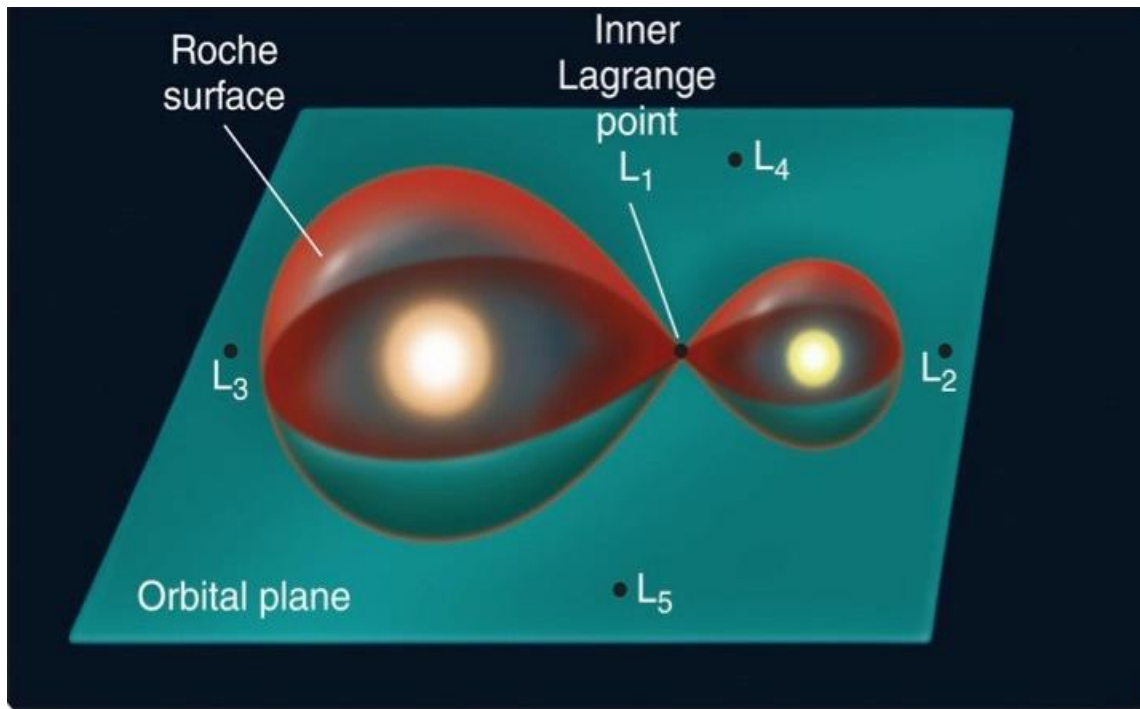


Credits: ESO/M. Kornmesser/S.E. de Mink

Mass transfer via Roche Lobe Overflow



Roche Lobe: region where
orbiting material
is gravitationally bound

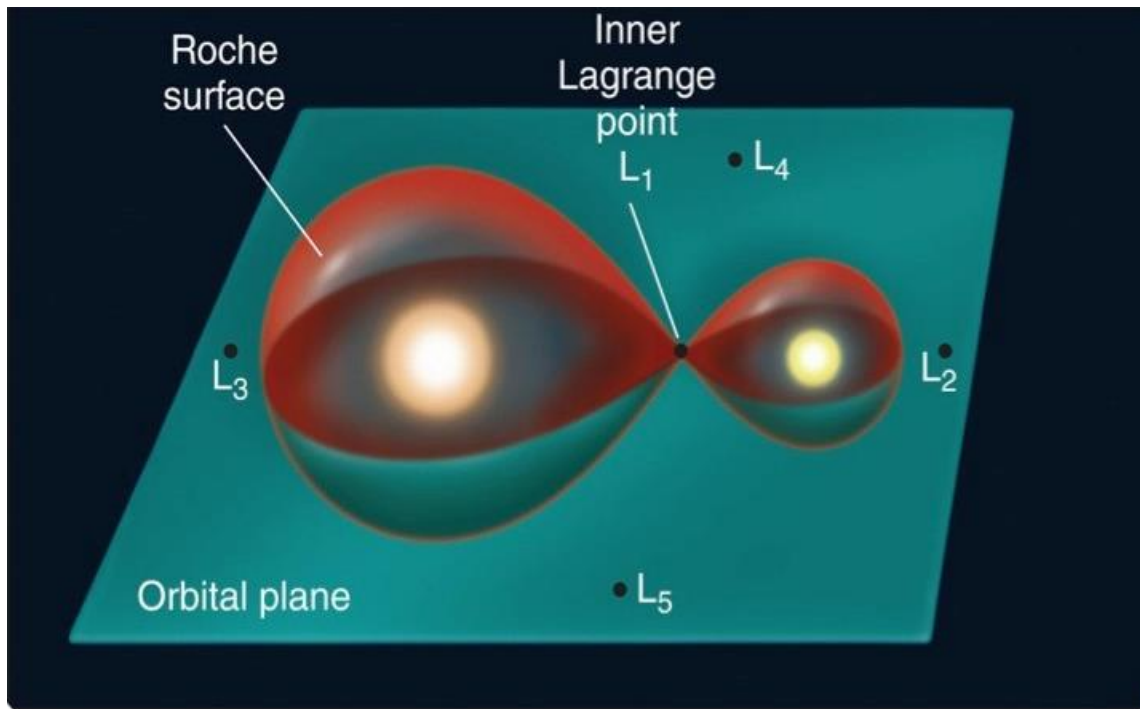


Credits: Cengage Learning (2016)

Mass transfer via Roche Lobe Overflow



Roche Lobe: region where orbiting material is gravitationally bound



Roche lobe
overflow

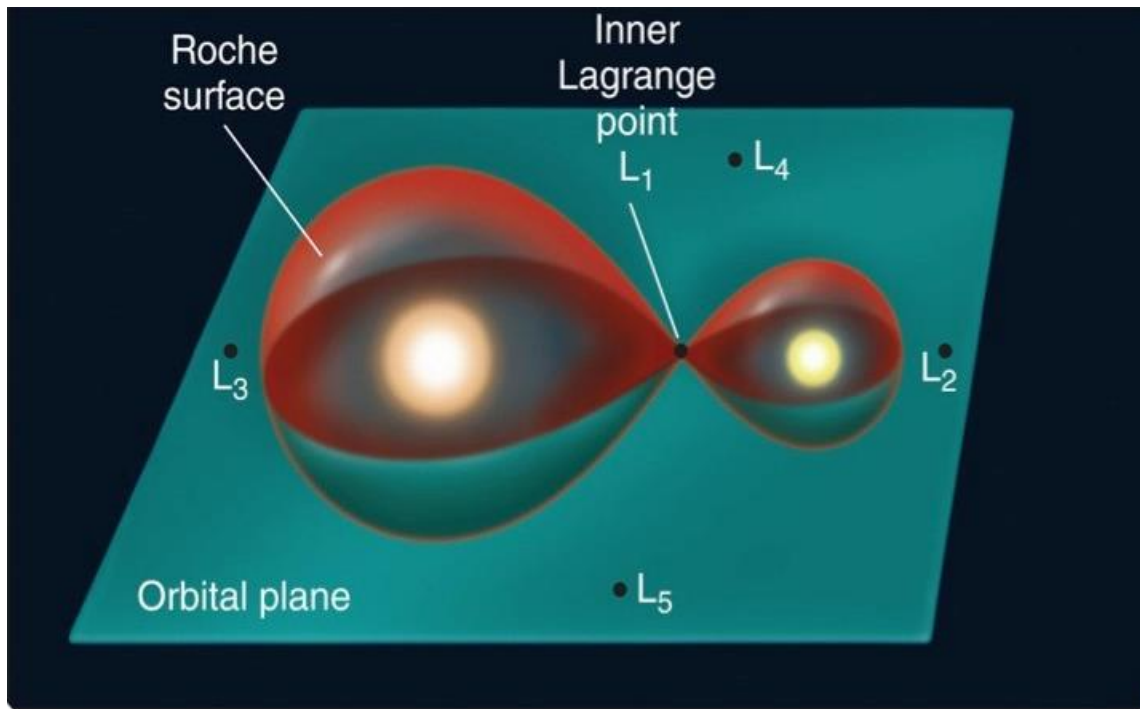


Credits: Cengage Learning (2016)

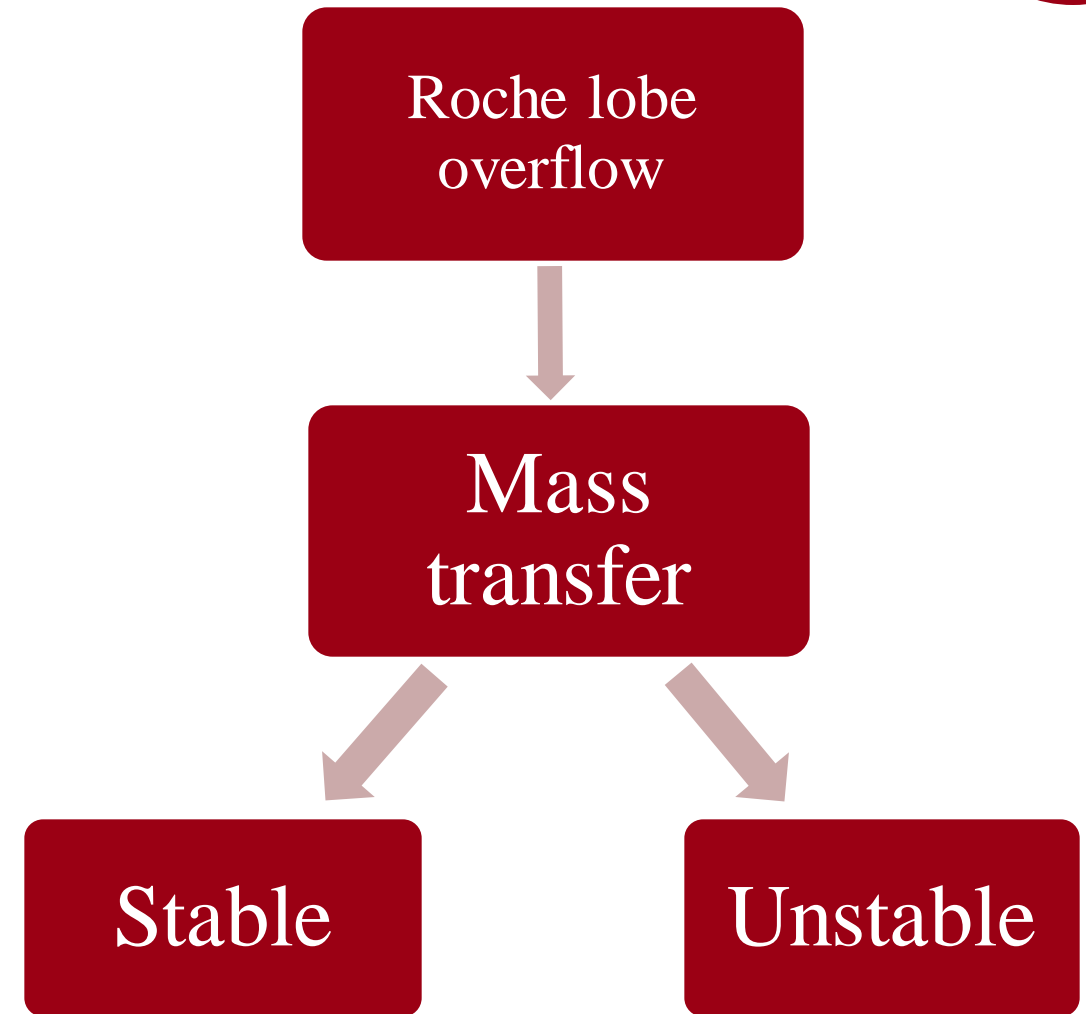
Mass transfer via Roche Lobe Overflow



Roche Lobe: region where orbiting material is gravitationally bound



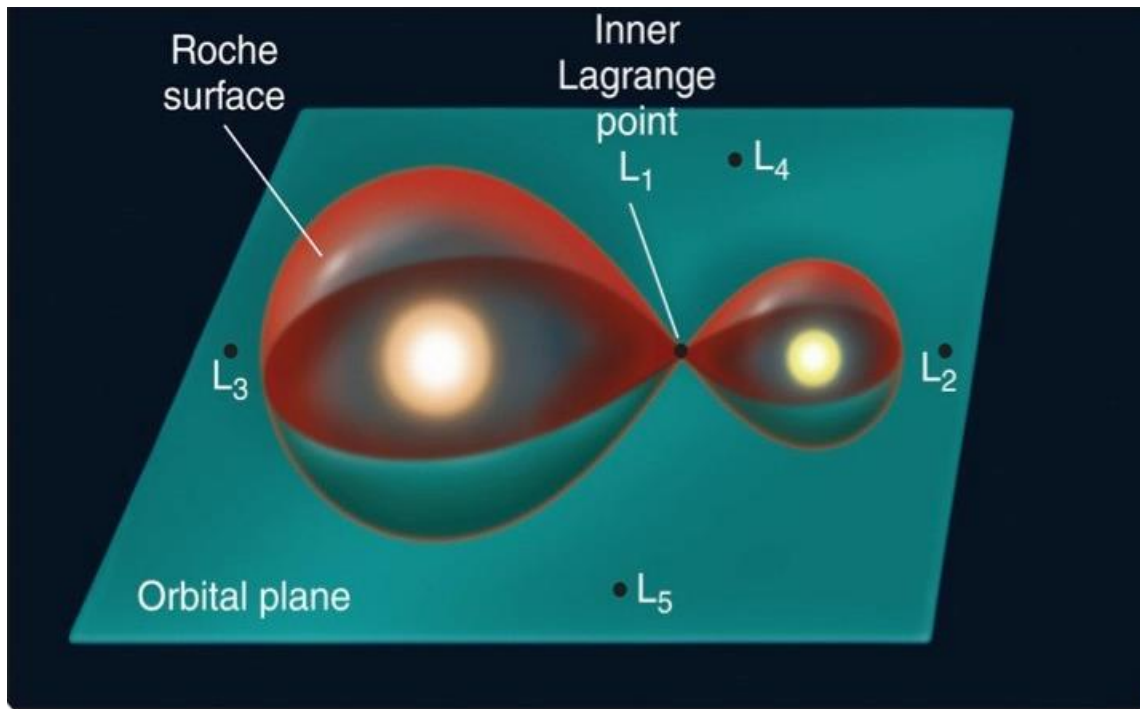
Credits: Cengage Learning (2016)



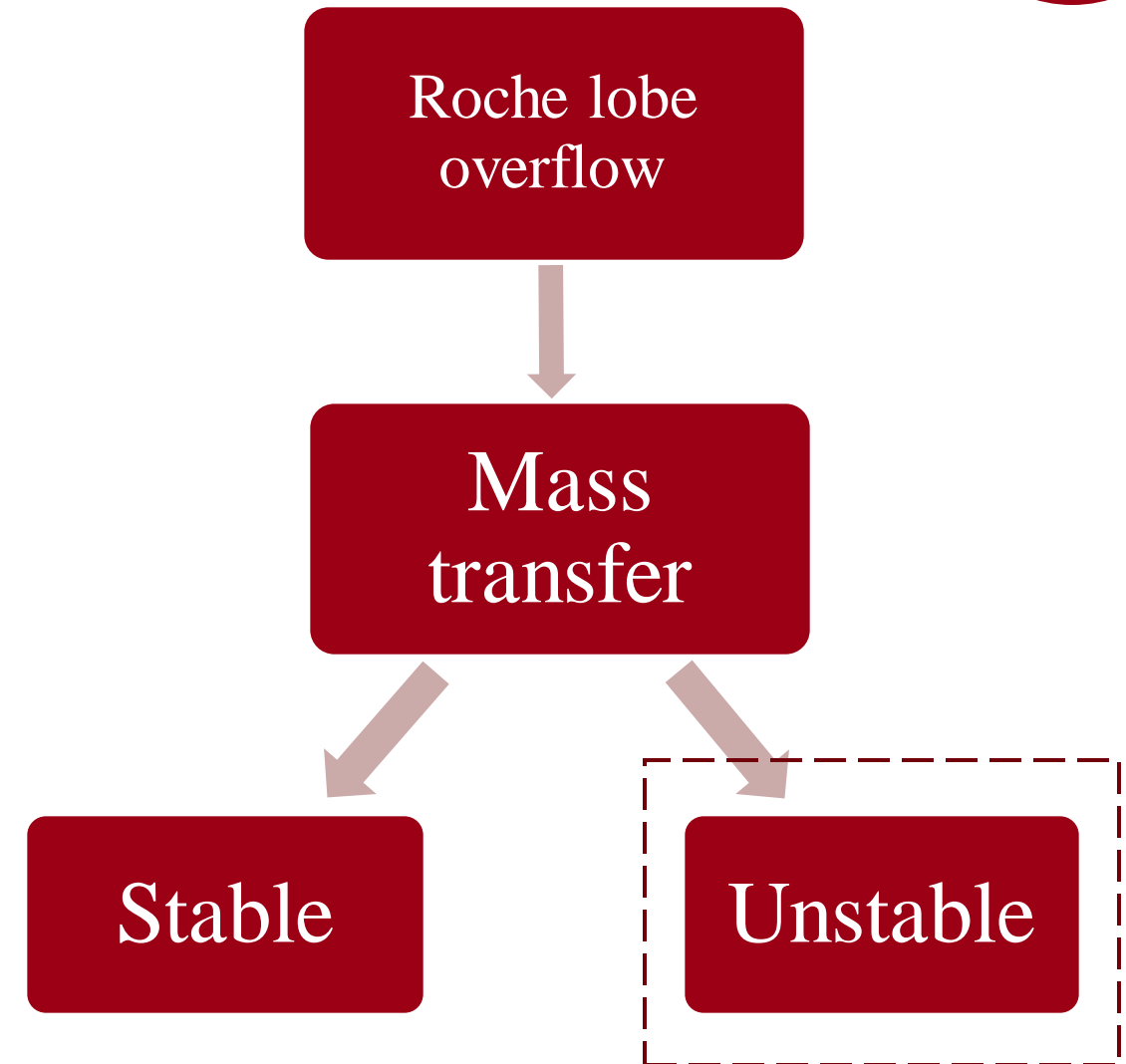
Mass transfer via Roche Lobe Overflow



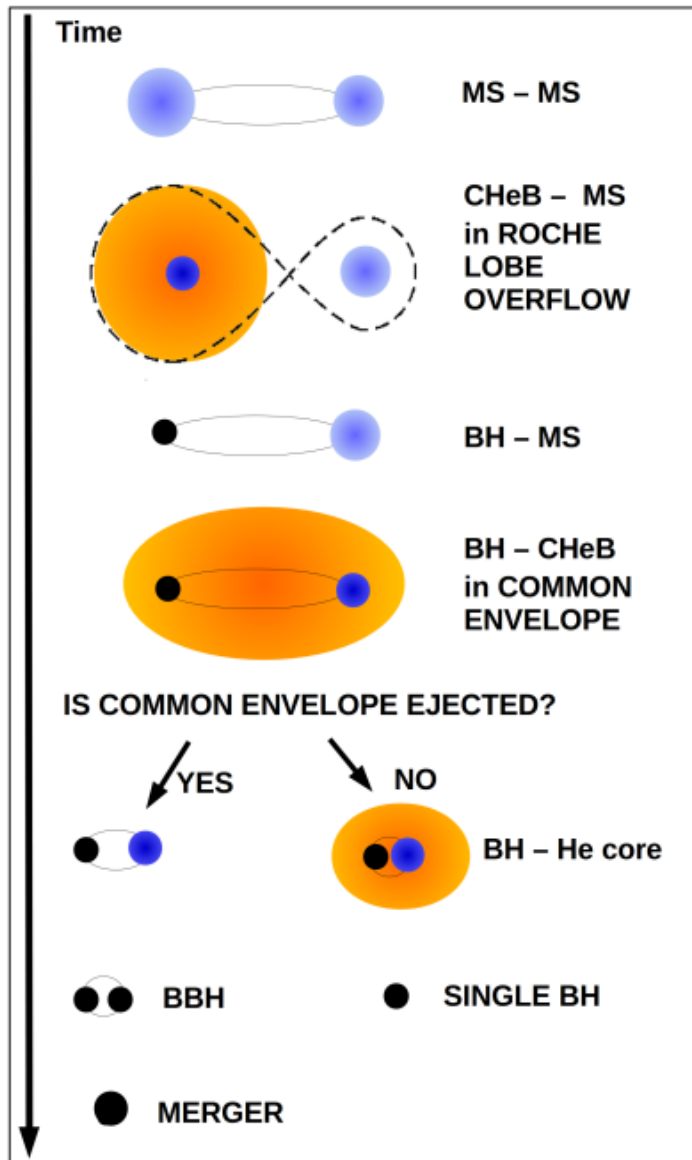
Roche Lobe: region where orbiting material is gravitationally bound



Credits: Cengage Learning (2016)



Unstable mass transfer



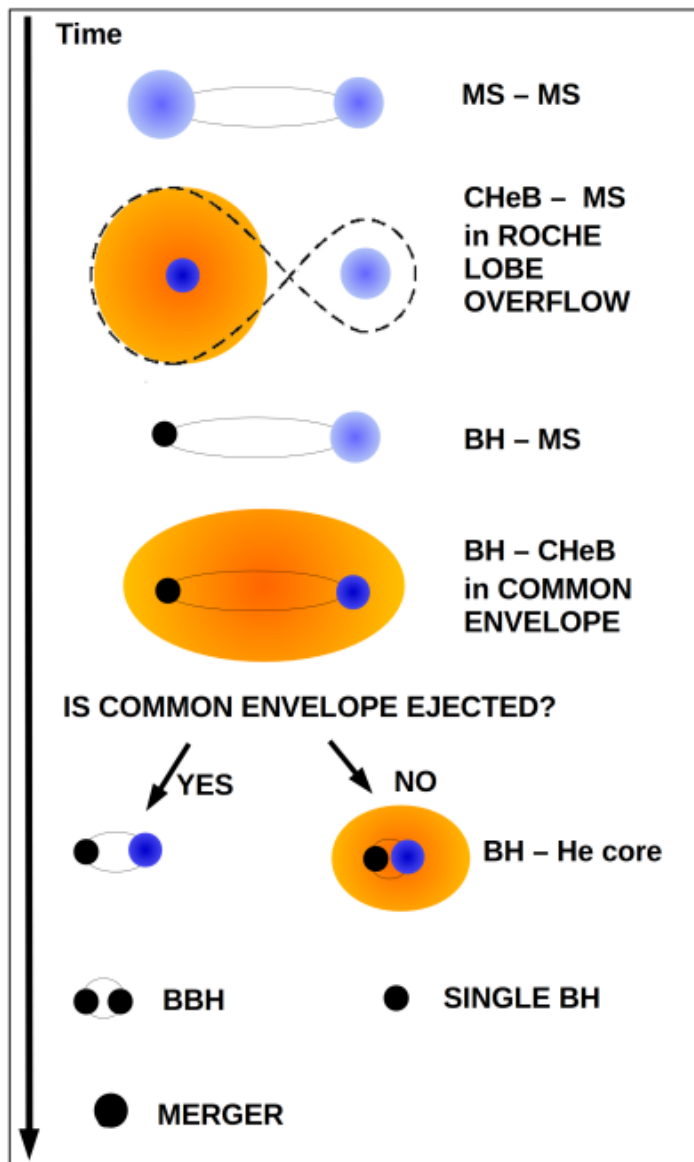
→ Binary system with stars in main sequence

→ Roche lobe overflow

→ Black hole - main sequence star

→ Common envelope phase

Unstable mass transfer



Binary system with stars in main sequence

Roche lobe overflow

Black hole - main sequence star

Common envelope phase

- Yes: Binary Black Hole and merger
- No: two components merge without gravitational waves event

The α formalism

The **α formalism** describes the **energy balance** during the common envelope phase.

$$\Delta E = \alpha(E_{b,f} - E_{b,i}) = \alpha \frac{G m_{c,1} m_{c,2}}{2} \left(\frac{1}{a_f} - \frac{1}{a_i} \right)$$

The α formalism

The **α formalism** describes the **energy balance** during the common envelope phase.

$$\Delta E = \alpha(E_{b,f} - E_{b,i}) = \alpha \frac{Gm_{c,1}m_{c,2}}{2} \left(\frac{1}{a_f} - \frac{1}{a_i} \right)$$

→ Encodes the **efficiency** of the conversion between **gravitational energy** and **internal energy** of the envelope.

Dataset



▪ **Dataset:** set of simulated binary black holes formations.

	Binary ID	ZAMS Mass 1 [Msun]	ZAMS Mass 2 [Msun]	Black Hole Mass 1 [Msun]	Black Hole Mass 2 [Msun]	Formation Delay Time [Myrs]	Semi Major Axis [Rsun]	Orbital Eccentricity	Formation by Common Envelope	Alpha	Metallicity	Q	Q_BH
1878045	1_1339891	27.795000	27.720300	4.737200	4.619000	11795.084000	11.461000	0.174990	True	3.000000	0.001600	1.002695	1.025590
1589326	1_1272522	26.738100	20.396400	5.877000	11.986900	915.528200	9.288200	0.114790	True	3.000000	0.000400	1.310923	0.490285
835409	1_1434130	25.979100	25.630200	5.908600	5.208300	8001.689900	17.491000	0.617170	True	1.000000	0.000400	1.013613	1.134458
1091111	4_1581057	21.064600	18.994800	3.024900	7.702200	185.318000	4.539100	0.347010	True	1.000000	0.001200	1.108967	0.392732
1325494	0_1915046	46.360100	35.359700	18.162200	24.748700	432.073700	15.031000	0.011652	True	3.000000	0.000200	1.311100	0.733865
332780	2_65743	67.952300	42.653100	25.226800	30.465300	183.218100	14.739000	0.008978	True	0.500000	0.001200	1.593139	0.828050
1339656	1_537277	43.895600	25.066100	16.281300	19.313400	145.338200	9.888200	0.014047	True	3.000000	0.000200	1.751194	0.843005
2022989	1_1307248	24.482000	17.403100	4.418400	9.325700	861.019600	7.704200	0.209460	True	5.000000	0.000200	1.406761	0.473787
952697	4_1973207	66.332400	48.536300	26.816900	33.535400	173.236400	15.426000	0.019395	True	1.000000	0.000400	1.366655	0.799659
1712477	4_1088638	36.890900	22.139700	13.769600	16.231300	8287.779300	24.353000	0.016666	True	3.000000	0.000400	1.666278	0.848336

Dataset



■ Features

	Binary ID	ZAMS Mass 1 [Msun]	ZAMS Mass 2 [Msun]	Black Hole Mass 1 [Msun]	Black Hole Mass 2 [Msun]	Formation Delay Time [Myrs]	Semi Major Axis [Rsun]	Orbital Eccentricity	Formation by Common Envelope	Alpha	Metallicity	Q	Q_BH
1878045	1_1339891	27.795000	27.720300	4.737200	4.619000	11795.084000	11.461000	0.174990	True	3.000000	0.001600	1.002695	1.025590
1589326	1_1272522	26.738100	20.396400	5.877000	11.986900	915.528200	9.288200	0.114790	True	3.000000	0.000400	1.310923	0.490285
835409	1_1434130	25.979100	25.630200	5.908600	5.208300	8001.689900	17.491000	0.617170	True	1.000000	0.000400	1.013613	1.134458
1091111	4_1581057	21.064600	18.994800	3.024900	7.702200	185.318000	4.539100	0.347010	True	1.000000	0.001200	1.108967	0.392732
1325494	0_1915046	46.360100	35.359700	18.162200	24.748700	432.073700	15.031000	0.011652	True	3.000000	0.000200	1.311100	0.733865
332780	2_65743	67.952300	42.653100	25.226800	30.465300	183.218100	14.739000	0.008978	True	0.500000	0.001200	1.593139	0.828050
1339656	1_537277	43.895600	25.066100	16.281300	19.313400	145.338200	9.888200	0.014047	True	3.000000	0.000200	1.751194	0.843005
2022989	1_1307248	24.482000	17.403100	4.418400	9.325700	861.019600	7.704200	0.209460	True	5.000000	0.000200	1.406761	0.473787
952697	4_1973207	66.332400	48.536300	26.816900	33.535400	173.236400	15.426000	0.019395	True	1.000000	0.000400	1.366655	0.799659
1712477	4_1088638	36.890900	22.139700	13.769600	16.231300	8287.779300	24.353000	0.016666	True	3.000000	0.000400	1.666278	0.848336

$$Q = \frac{ZAMS\ Mass\ 1}{ZAMS\ Mass\ 2} \quad BHQ = \frac{Black\ Hole\ Mass\ 1}{Black\ Hole\ Mass\ 2}$$

these features were added for **physical** and **computational** reasons

Dataset



■ **Label:** value we want to predict

	Binary ID	ZAMS Mass 1 [Msun]	ZAMS Mass 2 [Msun]	Black Hole Mass 1 [Msun]	Black Hole Mass 2 [Msun]	Formation Delay Time [Myrs]	Semi Major Axis [Rsun]	Orbital Eccentricity	Formation by Common Envelope	Alpha	Metallicity	Q	Q_BH
1878045	1_1339891	27.795000	27.720300	4.737200	4.619000	11795.084000	11.461000	0.174990	True	3.000000	0.001600	1.002695	1.025590
1589326	1_1272522	26.738100	20.396400	5.877000	11.986900	915.528200	9.288200	0.114790	True	3.000000	0.000400	1.310923	0.490285
835409	1_1434130	25.979100	25.630200	5.908600	5.208300	8001.689900	17.491000	0.617170	True	1.000000	0.000400	1.013613	1.134458
1091111	4_1581057	21.064600	18.994800	3.024900	7.702200	185.318000	4.539100	0.347010	True	1.000000	0.001200	1.108967	0.392732
1325494	0_1915046	46.360100	35.359700	18.162200	24.748700	432.073700	15.031000	0.011652	True	3.000000	0.000200	1.311100	0.733865
332780	2_65743	67.952300	42.653100	25.226800	30.465300	183.218100	14.739000	0.008978	True	0.500000	0.001200	1.593139	0.828050
1339656	1_537277	43.895600	25.066100	16.281300	19.313400	145.338200	9.888200	0.014047	True	3.000000	0.000200	1.751194	0.843005
2022989	1_1307248	24.482000	17.403100	4.418400	9.325700	861.019600	7.704200	0.209460	True	5.000000	0.000200	1.406761	0.473787
952697	4_1973207	66.332400	48.536300	26.816900	33.535400	173.236400	15.426000	0.019395	True	1.000000	0.000400	1.366655	0.799659
1712477	4_1088638	36.890900	22.139700	13.769600	16.231300	8287.779300	24.353000	0.016666	True	3.000000	0.000400	1.666278	0.848336



Imbalanced dataset:

- 86 % Common envelope
- 14 % Stable mass transfer

Solution: under-sampling to obtain 50/50 dataset

Dataset imbalance

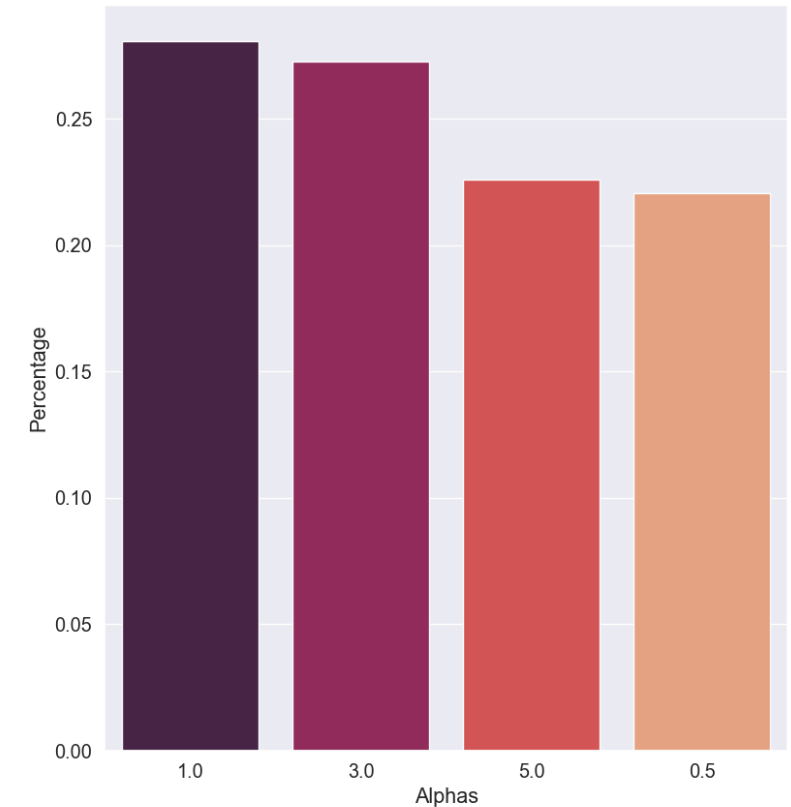
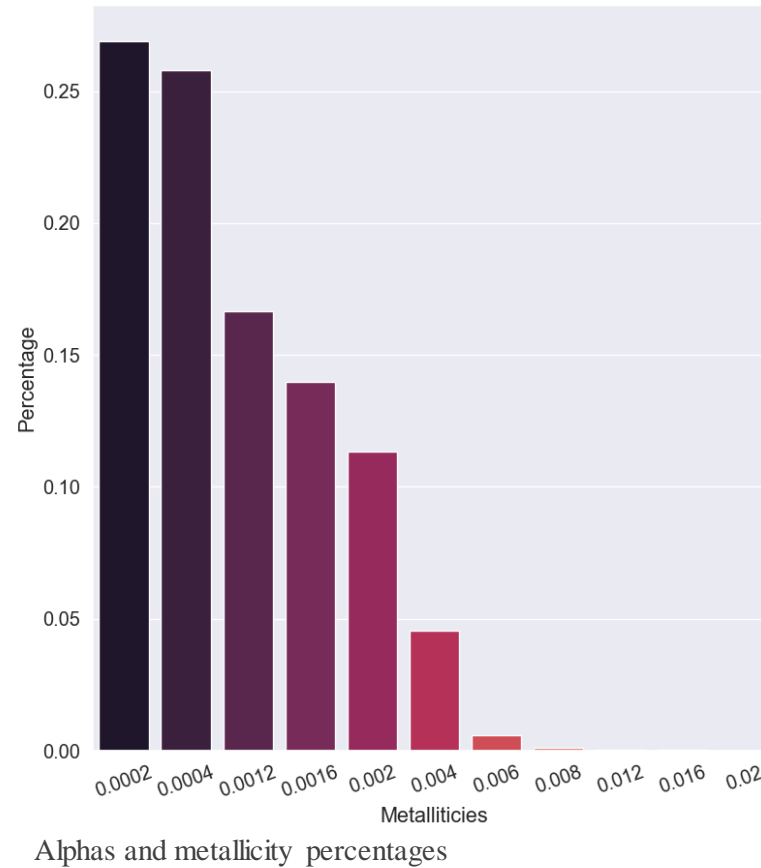


Imbalanced dataset:

- 86 % Common envelope
- 14 % Stable mass transfer

Solution: under-sampling to obtain 50/50 dataset

- **Alphas** well distributed
- Mainly low **metallicities** → merger is more likely



Removing the outliers



High stds and extreme outliers makes it difficult to cluster our data

	count	mean	std	min	1%	50%	99%	max
Orbital Eccentricity	692008.0	0.074763	0.139523	0.000015	0.007946	0.01602	0.686288	1.0
Semi Major Axis [Rsun]	692008.0	26.397353	607.786604	0.664170	3.389100	19.46700	53.129650	329100.0

Removing the outliers



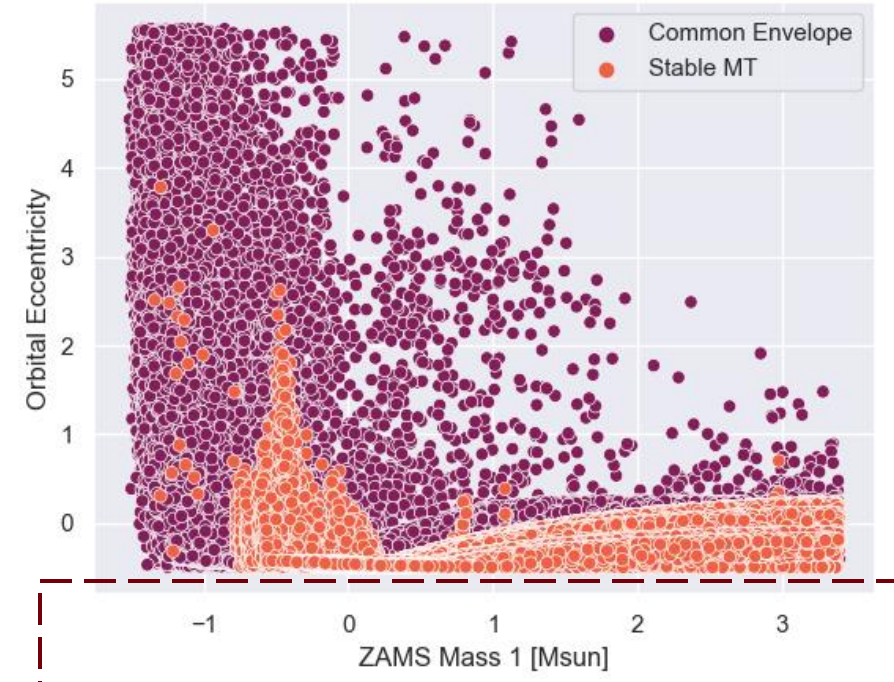
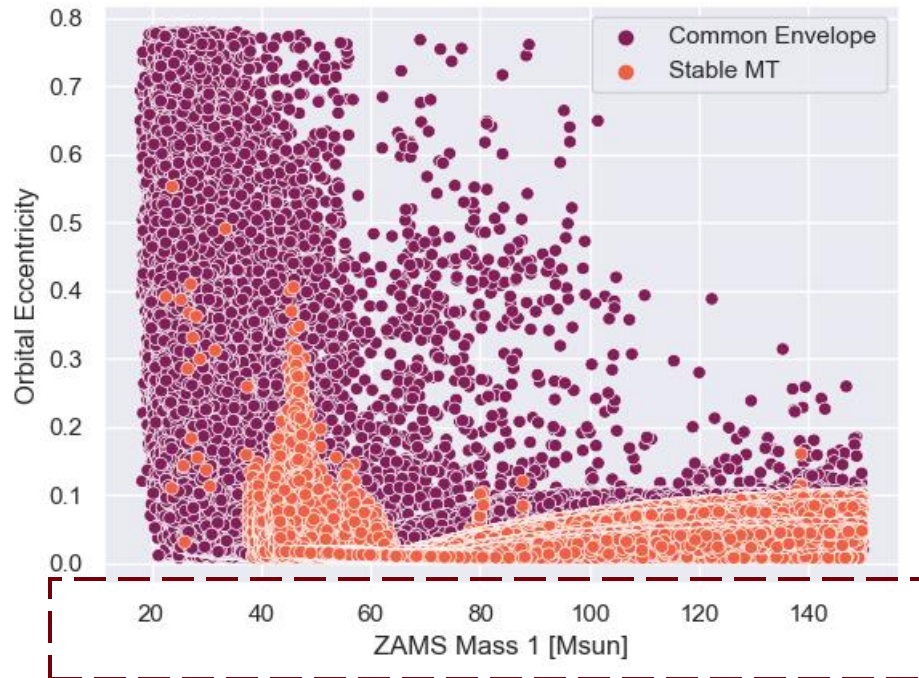
High stds and extreme outliers makes it difficult to cluster our data

	count	mean	std	min	1%	50%	99%	max
Orbital Eccentricity	692008.0	0.074763	0.139523	0.000015	0.007946	0.01602	0.686288	1.0
Semi Major Axis [Rsun]	692008.0	26.397353	607.786604	0.664170	3.389100	19.46700	53.129650	329100.0

Filtering the extreme 1%

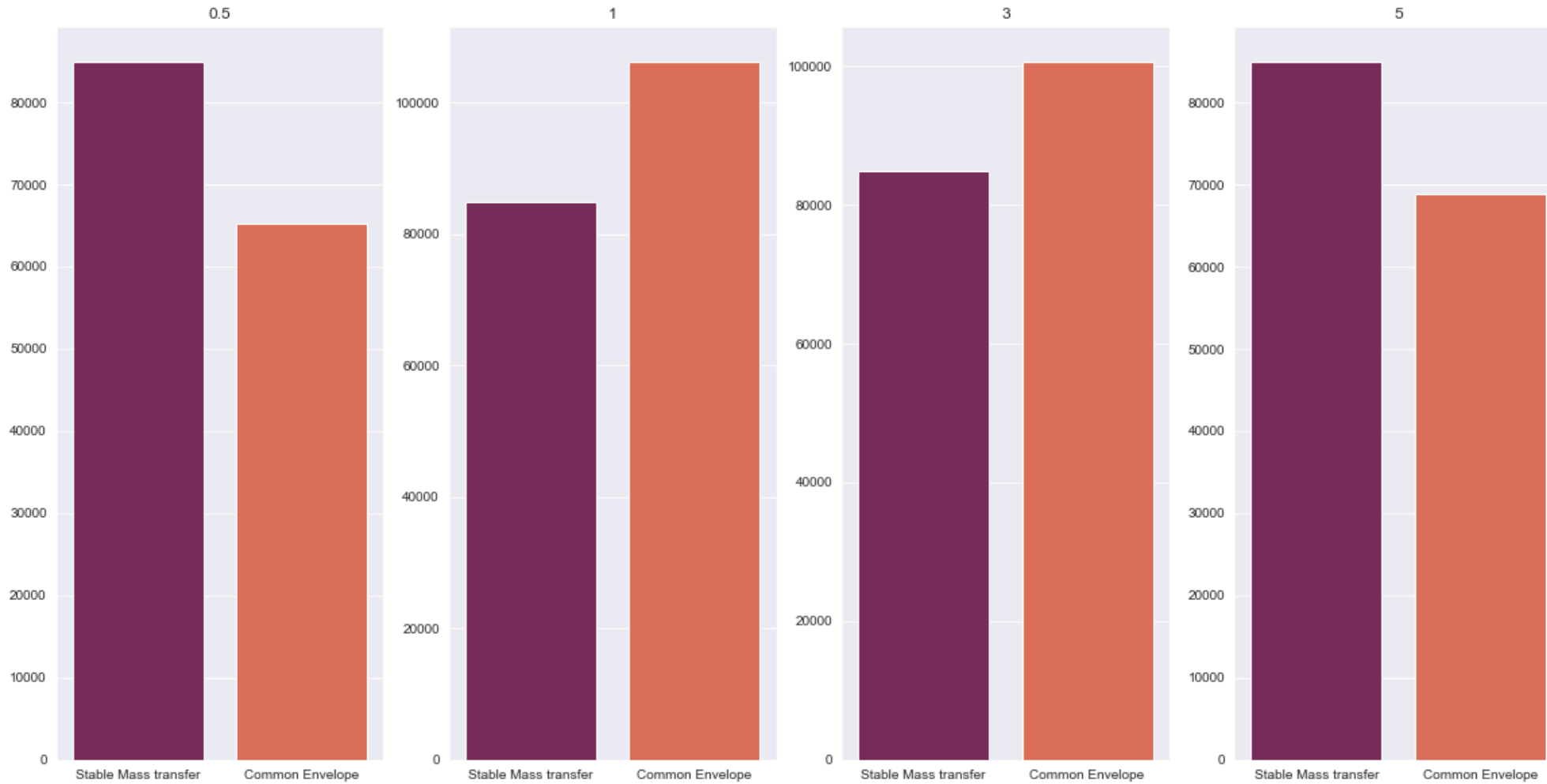
	count	mean	std	min	1%	50%	99%	max
Orbital Eccentricity	680471.0	0.071232	0.127306	0.00800	0.008286	0.016089	0.61662	0.77999
Semi Major Axis [Rsun]	680471.0	20.767367	12.262600	0.66417	3.412000	19.321000	52.60300	88.30800

Normalization



Normalization is important for
distance-based algorithms

Alpha



Alpha distribution for different labels

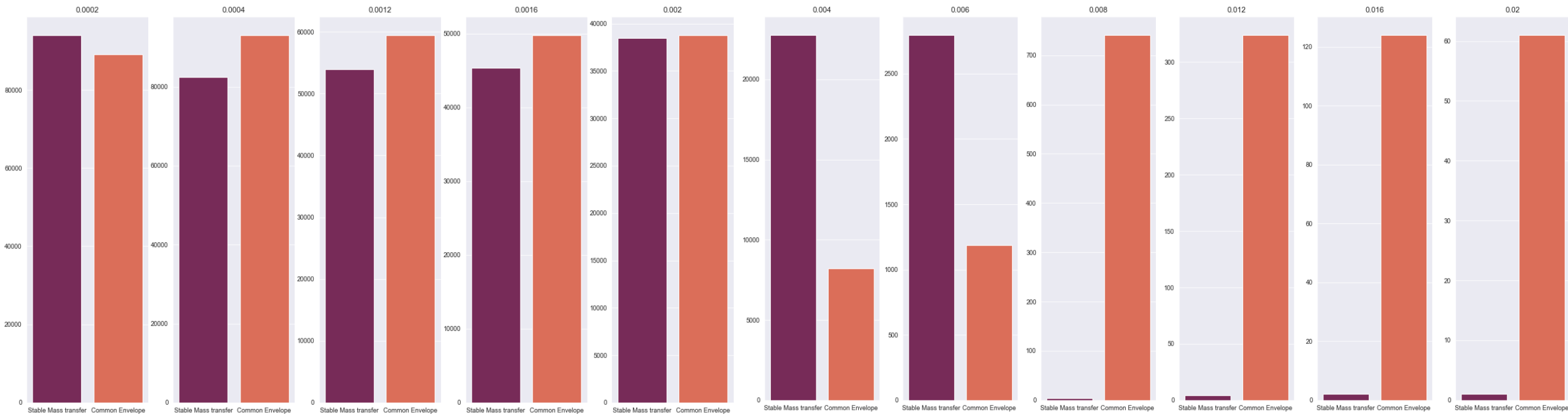
Alpha parameters are **well distributed** between the two evolution cases

Metallicities



The **metallicities** are **imbalanced**

For **higher** metallicities only Common envelope



Metallicity distribution for different labels

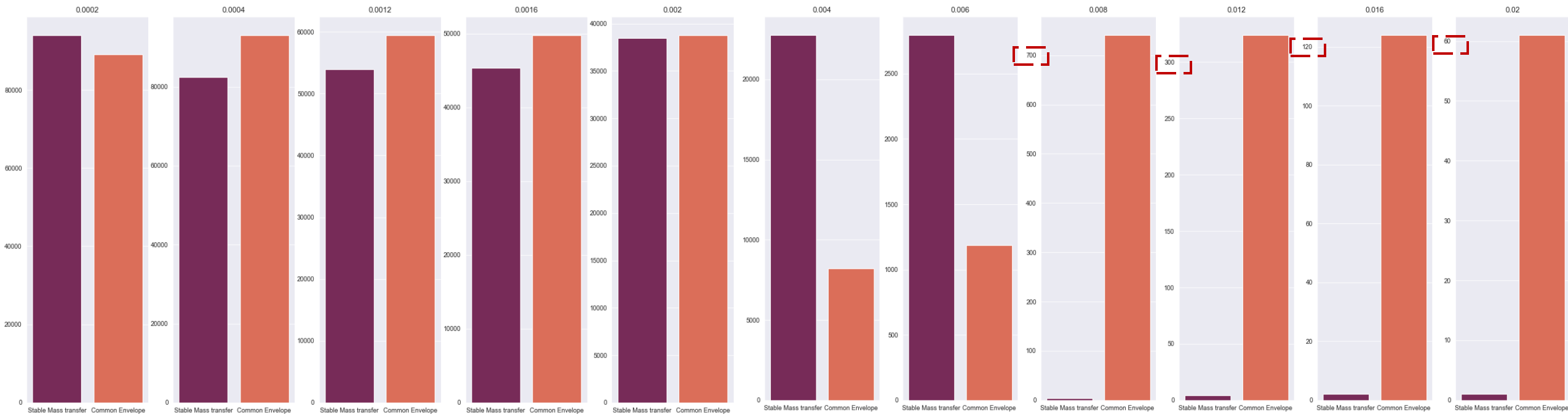
Metallicities



The **metallicities** are **imbalanced**

For **higher** metallicities only Common envelope

Small number of instances, **negligible**

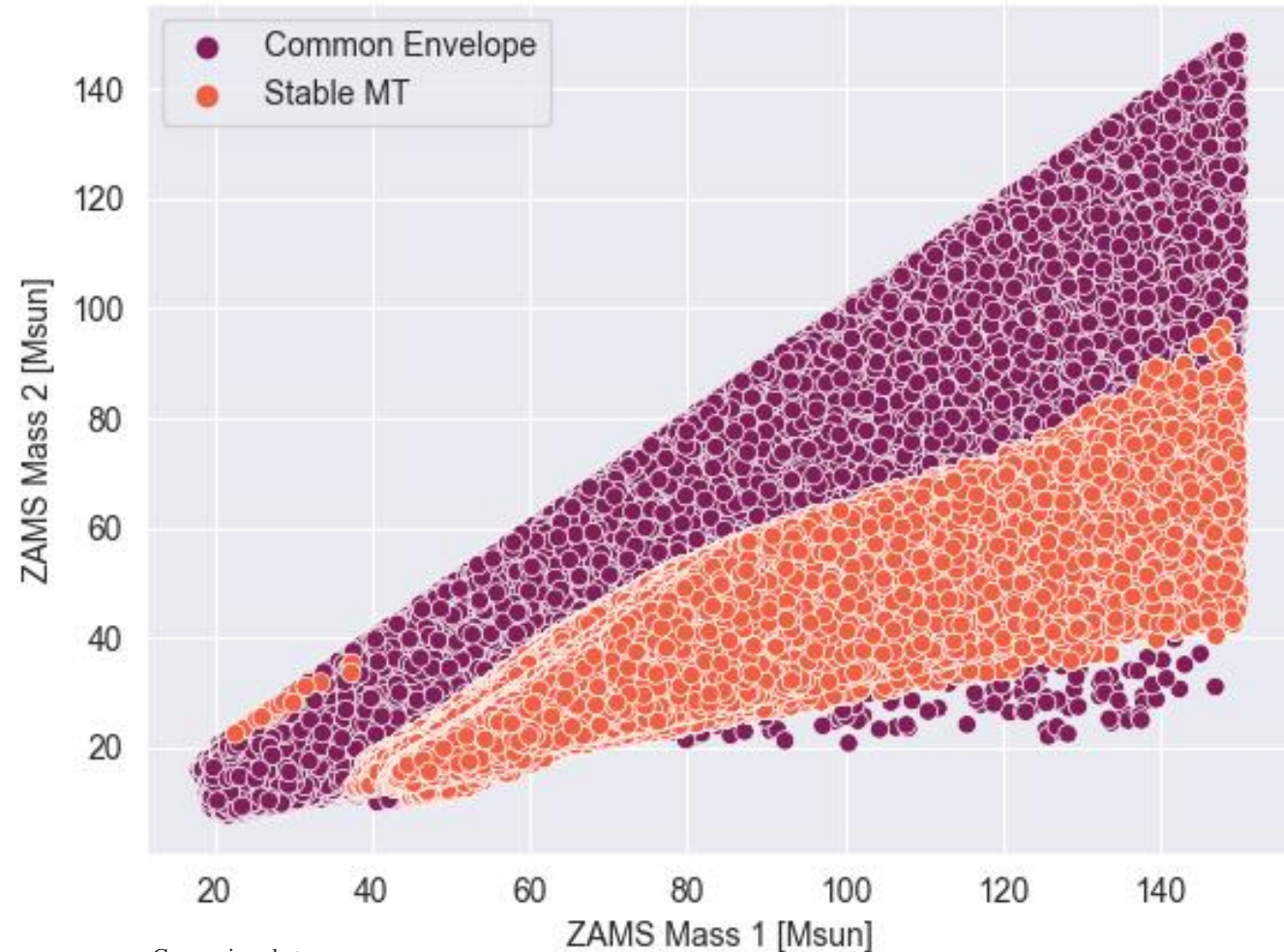


Metallicity distribution for different labels

Masses considerations



ZAMS Mass 1 > ZAMS Mass2
by **construction**



Comparison between masses

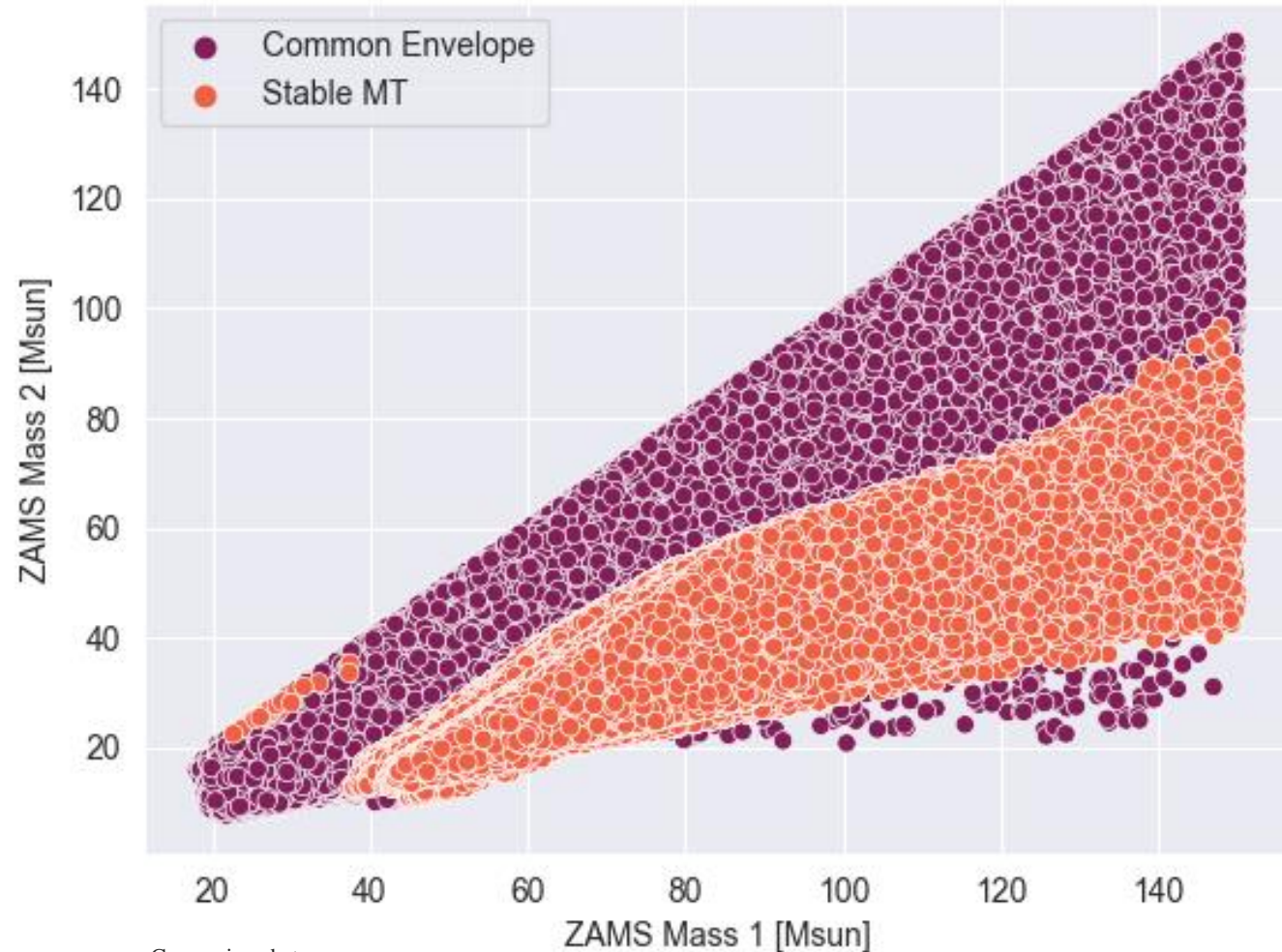
Masses considerations



ZAMS Mass 1 > ZAMS Mass2
by **construction**



Introduces a **bias**



Comparison between masses

Masses considerations



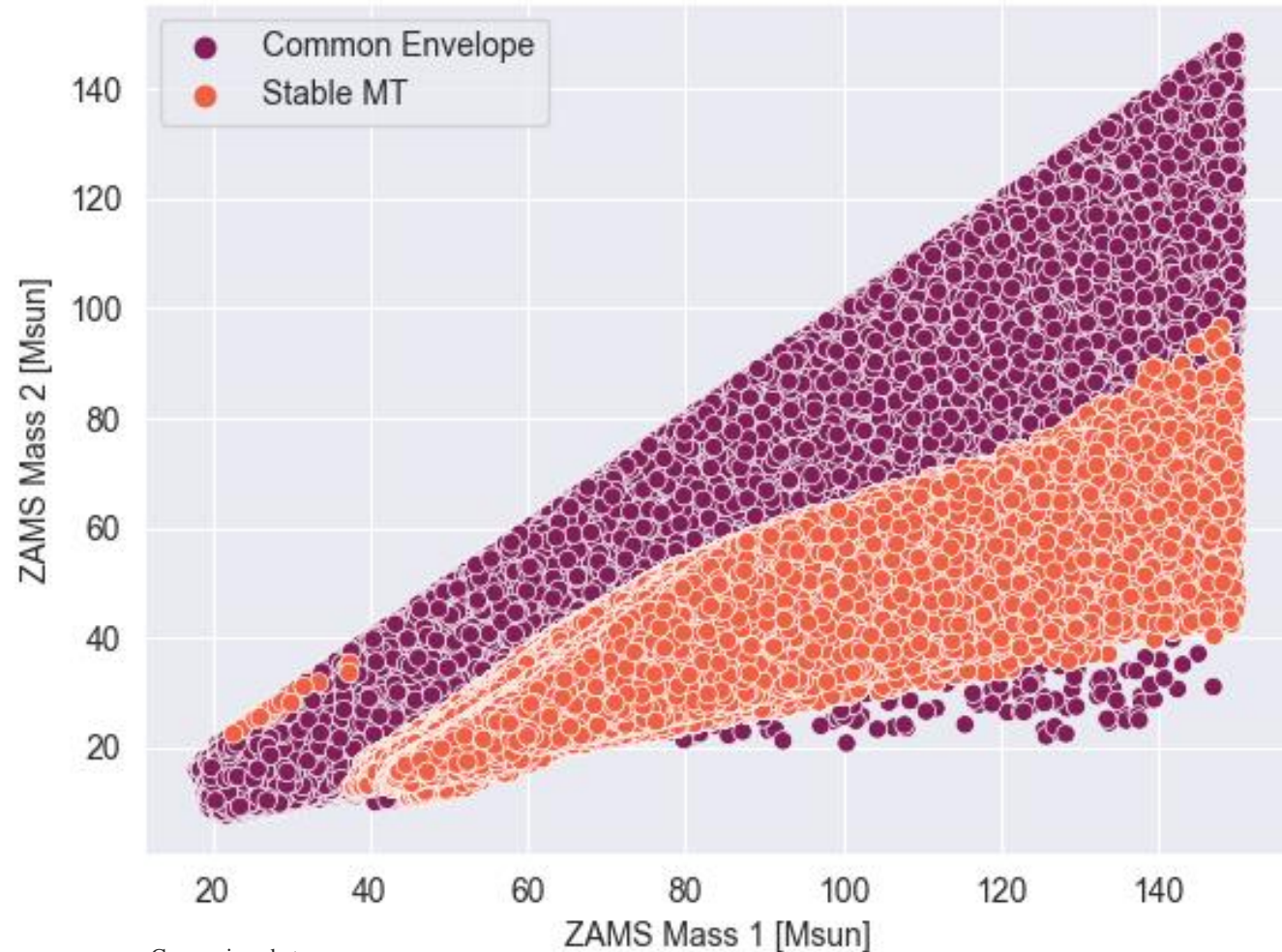
ZAMS Mass 1 > ZAMS Mass2
by **construction**



Introduces a **bias**



Problems with Machine
Learning algorithms



Comparison between masses

Masses considerations

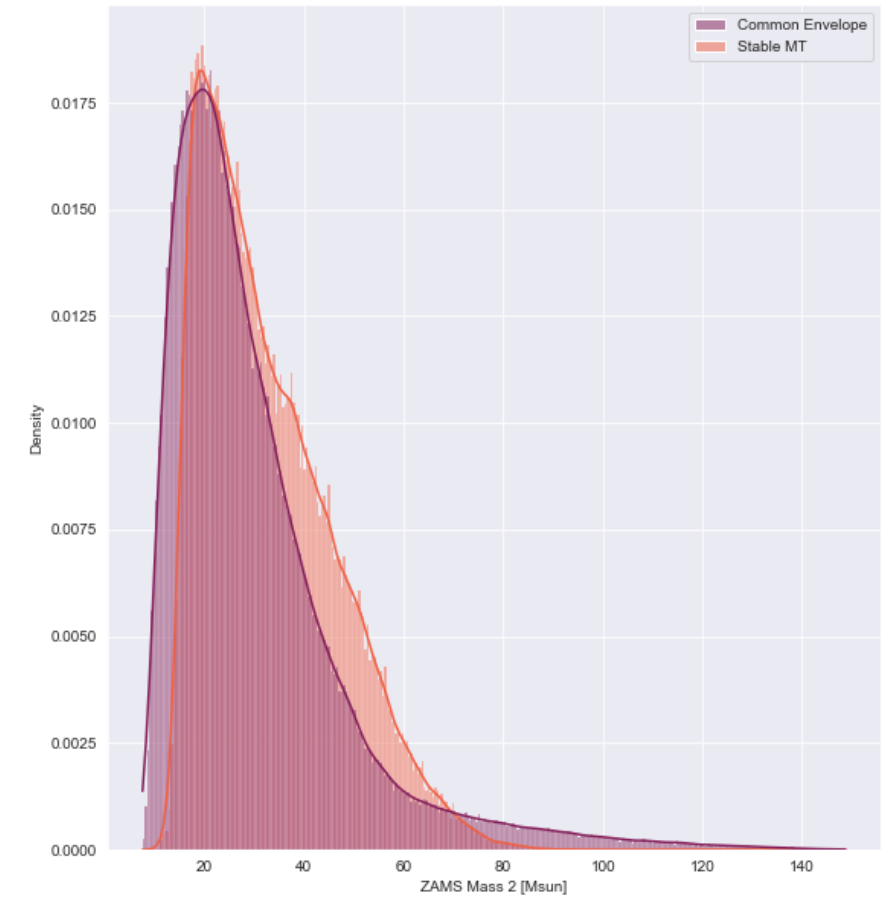
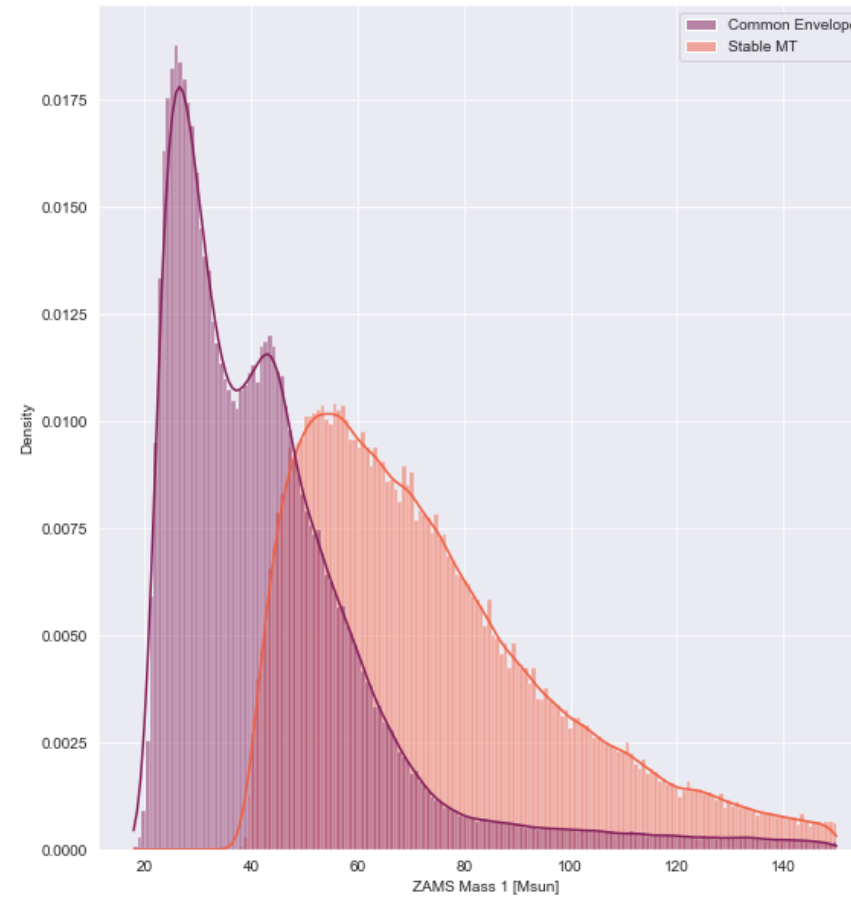


Primary mass

- Clear pattern
- CE – SMT boundary at around 40[Msun]

Secondary mass:

- Overlapping distributions



Probability density of events for Mass 1 and Mass 2

Masses considerations



Primary mass

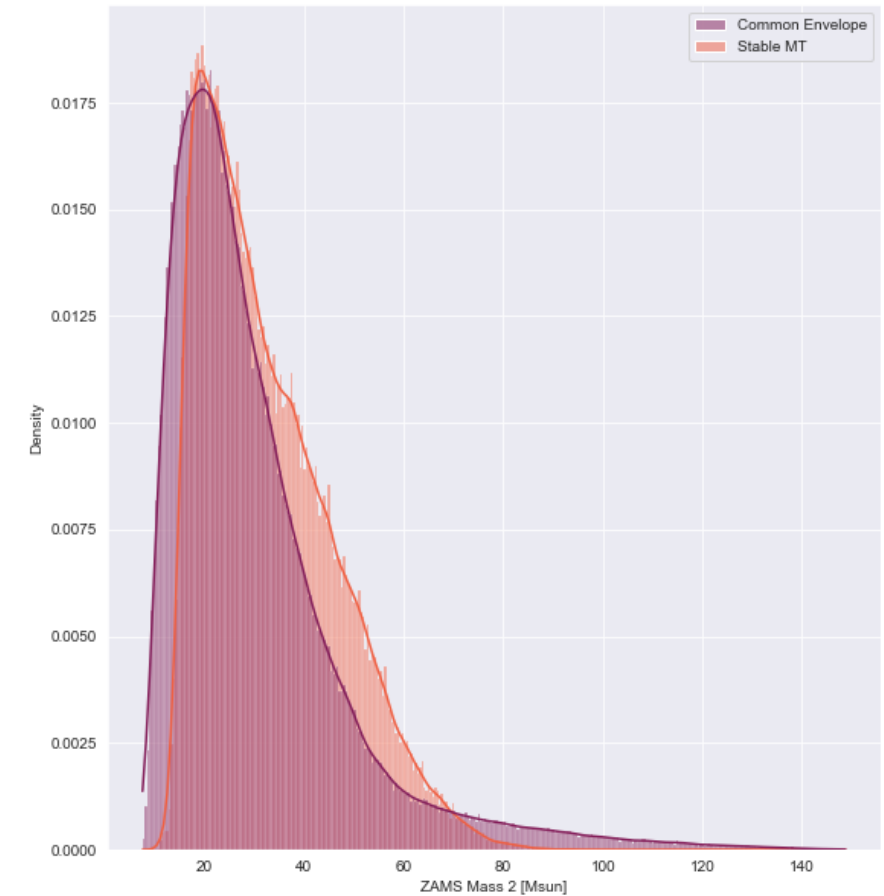
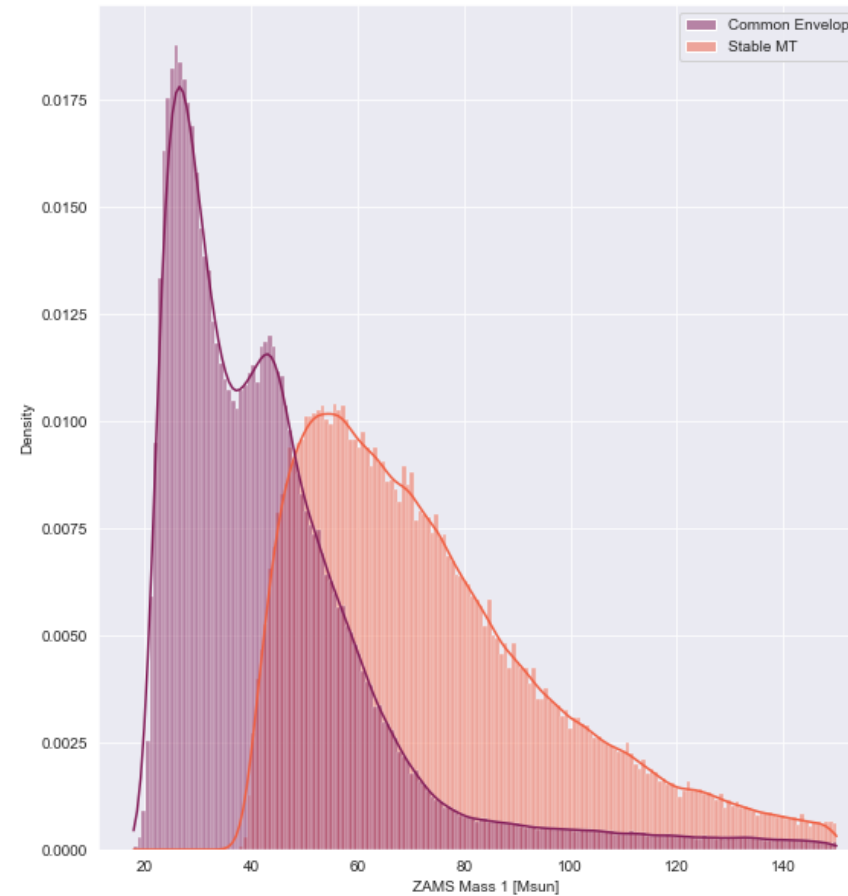
- Clear pattern
- CE – SMT boundary at around 40[Msun]

Secondary mass:

- Overlapping distributions



Problems with **machine learning** algorithms



Probability density of events for Mass 1 and Mass 2

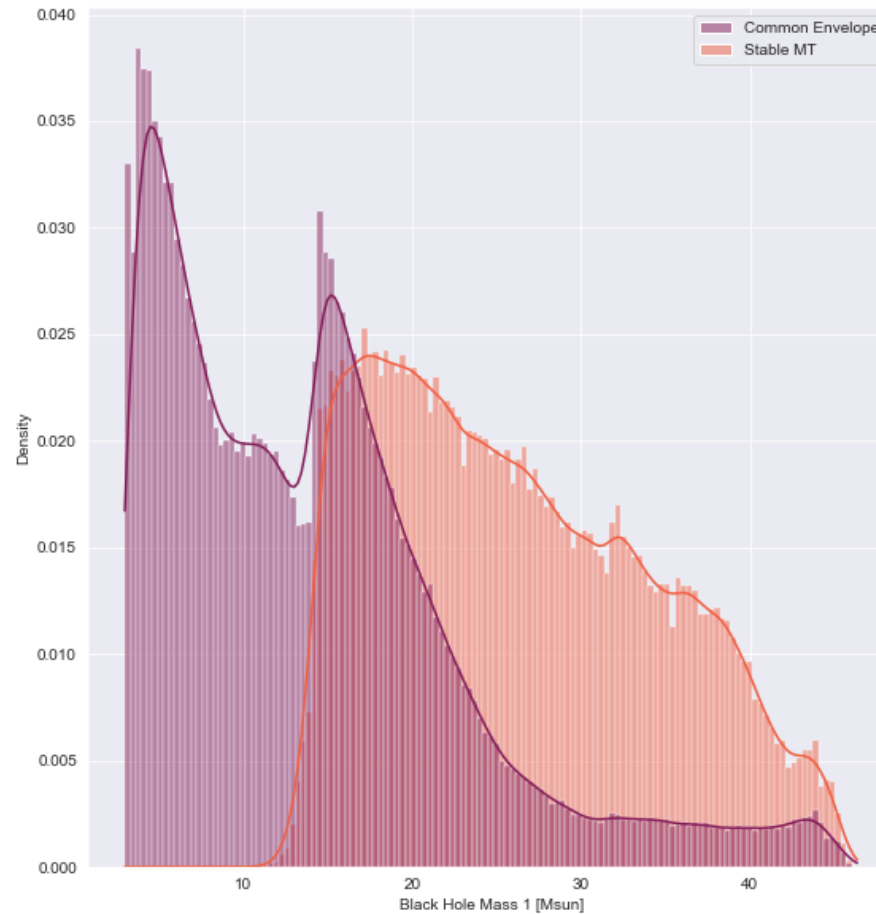
BBH masses considerations



Binary black holes
masses



Same pattern of
primary ZAMS mass



Probability density of events for BBH Mass 1 and BBH Mass 2

Q and BHQ

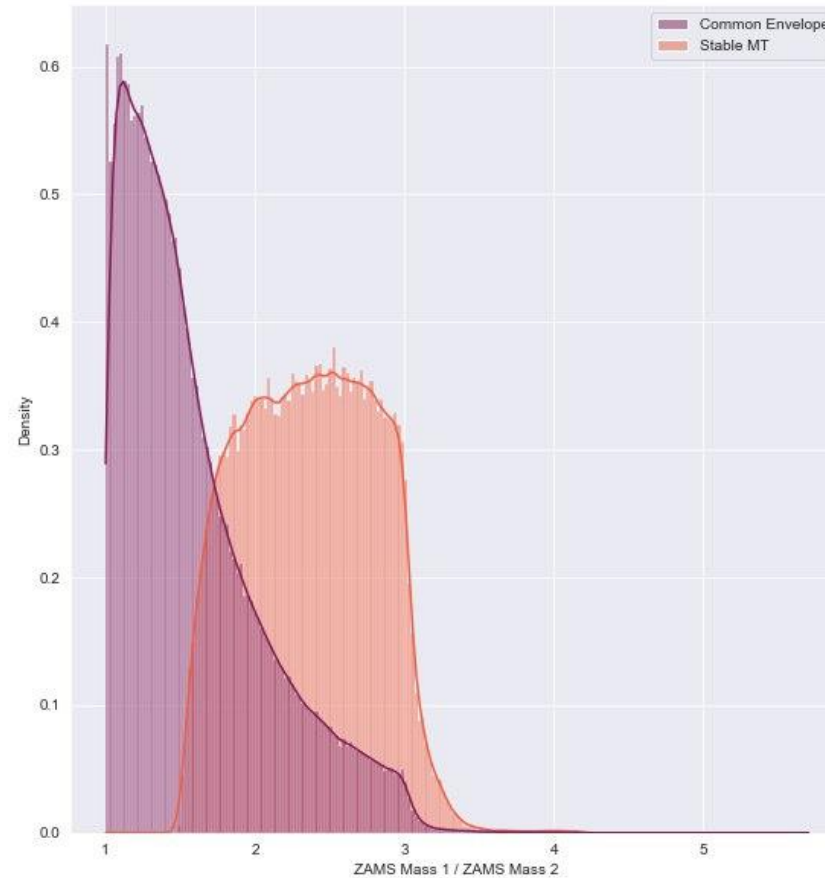


$$Q = \frac{ZAMS\ Mass\ 1}{ZAMS\ Mass\ 2}$$

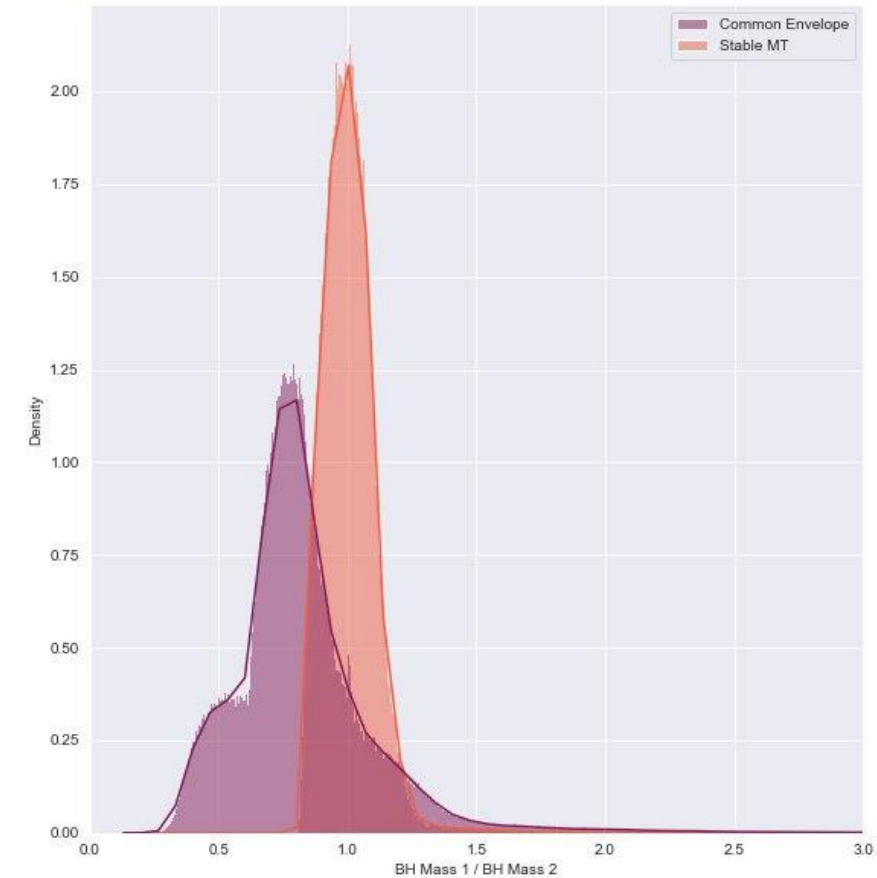
$$BHQ = \frac{Black\ Hole\ Mass\ 1}{Black\ Hole\ Mass\ 2}$$

these features were added for **physical** and **computational** reasons

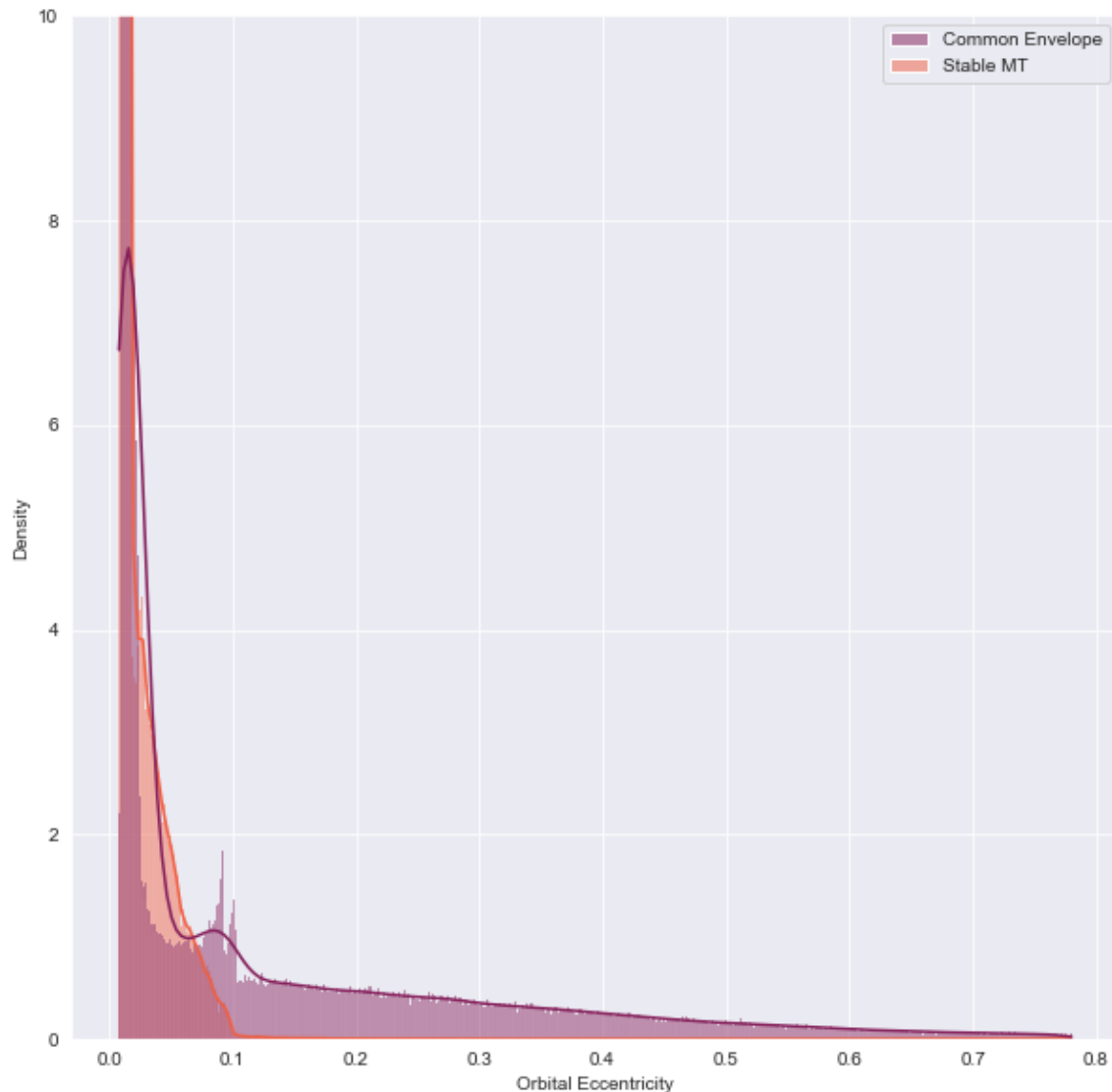
Q and BHQ show a good separation between the two classes and a small std



Probability density of events for BBH Mass 1 and BBH Mass 2



Orbital Eccentricity



Probability density of events for orbital eccentricity

Low eccentricity → • Common Envelope
• Stable MT

High eccentricity → Common Envelope

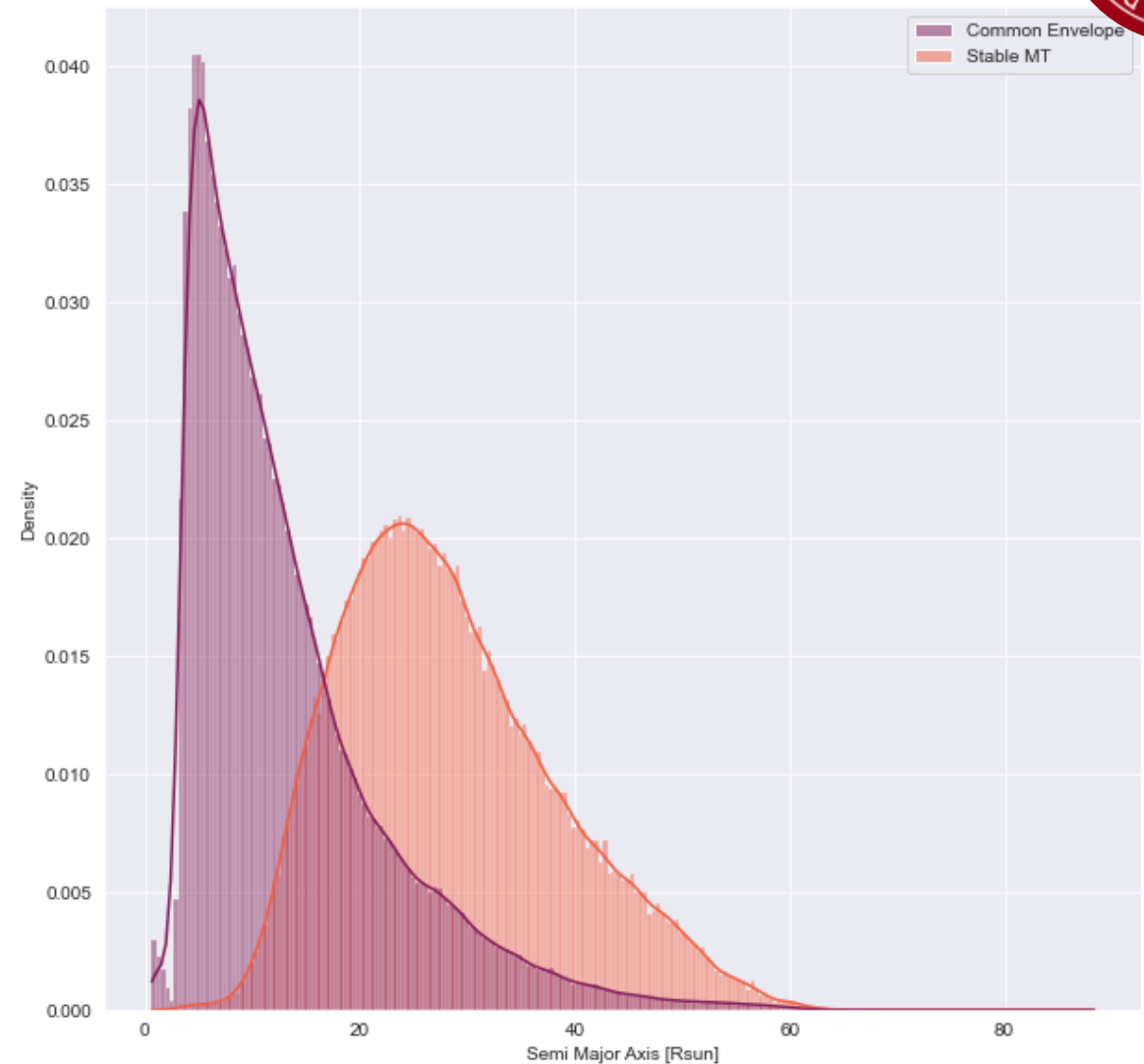
Semi Major Axis



Low orbital separation



Common envelope more likely



Probability density of events for Semi Major Axis

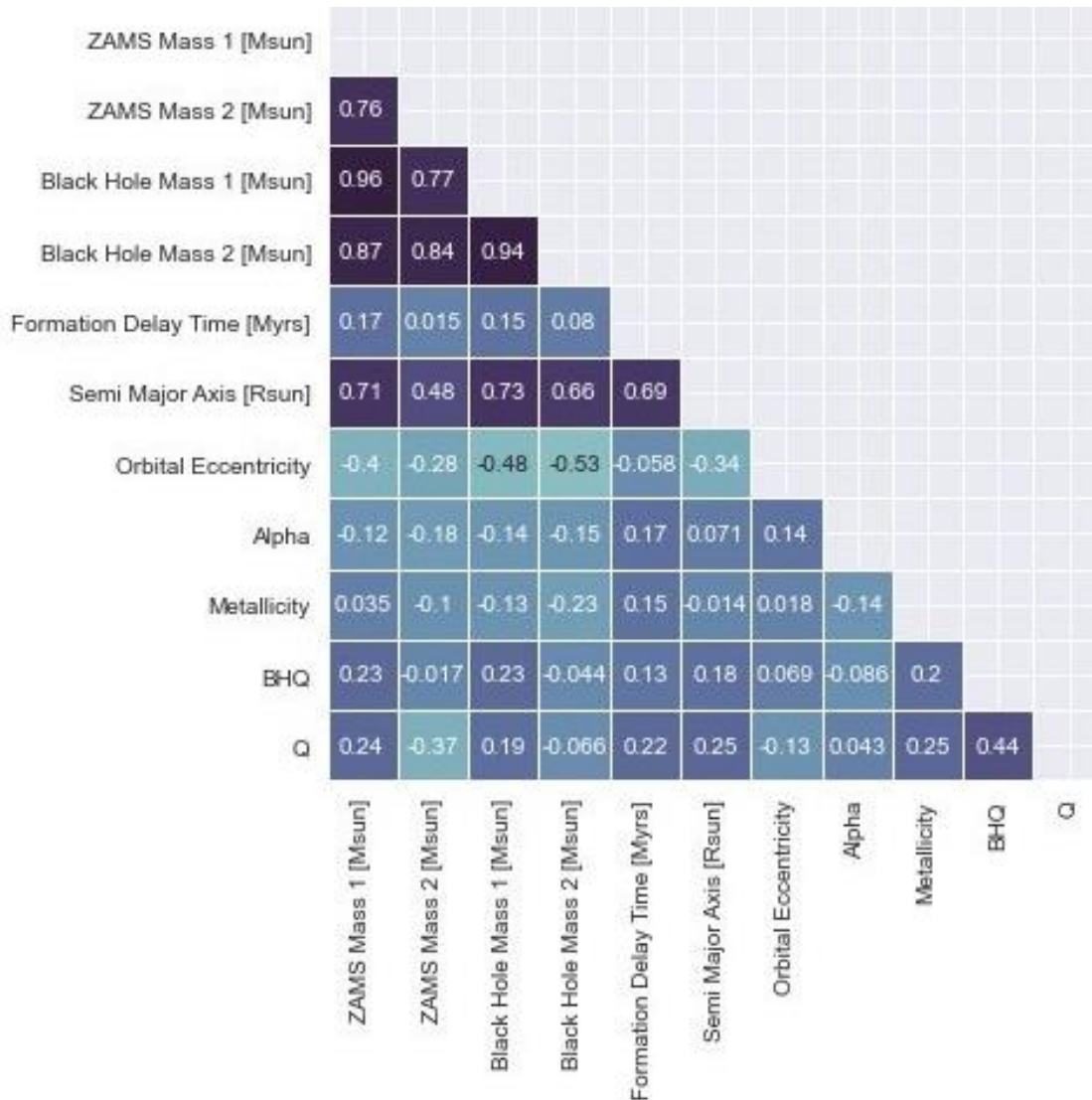
Dataset



▪Expectations: from dataset visualization

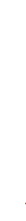
	Binary ID	ZAMS Mass 1 [Msun]	ZAMS Mass 2 [Msun]	Black Hole Mass 1 [Msun]	Black Hole Mass 2 [Msun]	Formation Delay Time [Myrs]	Semi Major Axis [Rsun]	Orbital Eccentricity	Formation by Common Envelope	Alpha	Metallicity	Q	Q_BH
1878045	1_1339891	27.795000	27.720300	4.737200	4.619000	11795.084000	11.461000	0.174990	True	3.000000	0.001600	1.002695	1.025590
1589326	1_1272522	26.738100	20.396400	5.877000	11.986900	915.528200	9.288200	0.114790	True	3.000000	0.000400	1.310923	0.490285
835409	1_1434130	25.979100	25.630200	5.908600	5.208300	8001.689900	17.491000	0.617170	True	1.000000	0.000400	1.013613	1.134458
1091111	4_1581057	21.064600	18.994800	3.024900	7.702200	185.318000	4.539100	0.347010	True	1.000000	0.001200	1.108967	0.392732
1325494	0_1915046	46.360100	35.359700	18.162200	24.748700	432.073700	15.031000	0.011652	True	3.000000	0.000200	1.311100	0.733865
332780	2_65743	67.952300	42.653100	25.226800	30.465300	183.218100	14.739000	0.008978	True	0.500000	0.001200	1.593139	0.828050
1339656	1_537277	43.895600	25.066100	16.281300	19.313400	145.338200	9.888200	0.014047	True	3.000000	0.000200	1.751194	0.843005
2022989	1_1307248	24.482000	17.403100	4.418400	9.325700	861.019600	7.704200	0.209460	True	5.000000	0.000200	1.406761	0.473787
952697	4_1973207	66.332400	48.536300	26.816900	33.535400	173.236400	15.426000	0.019395	True	1.000000	0.000400	1.366655	0.799659
1712477	4_1088638	36.890900	22.139700	13.769600	16.231300	8287.779300	24.353000	0.016666	True	3.000000	0.000400	1.666278	0.848336

Correlation matrix



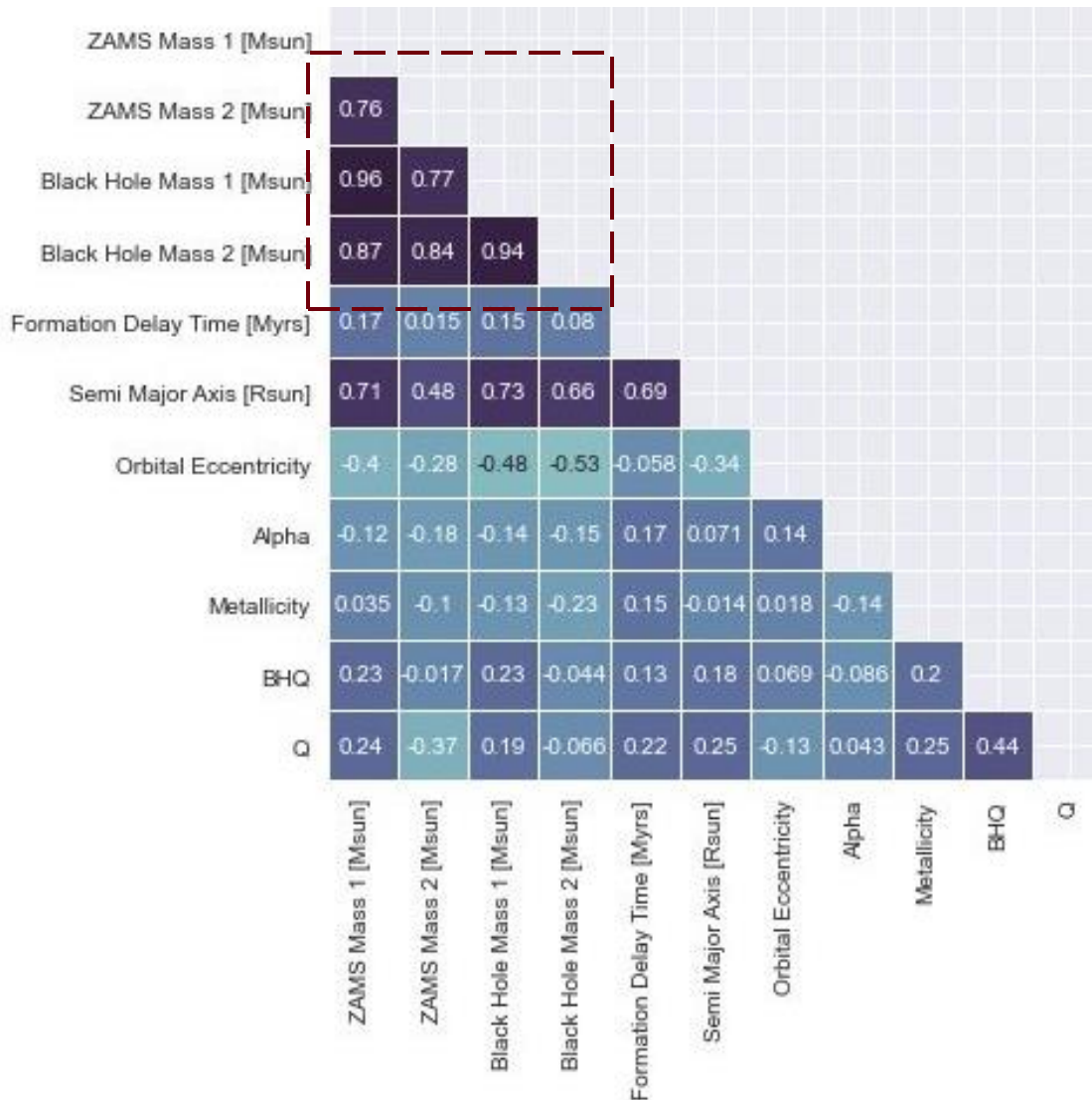
Feature correlation matrix

Masses are **highly correlated**



This could **negatively affect** prediction of the feature importances

Correlation matrix



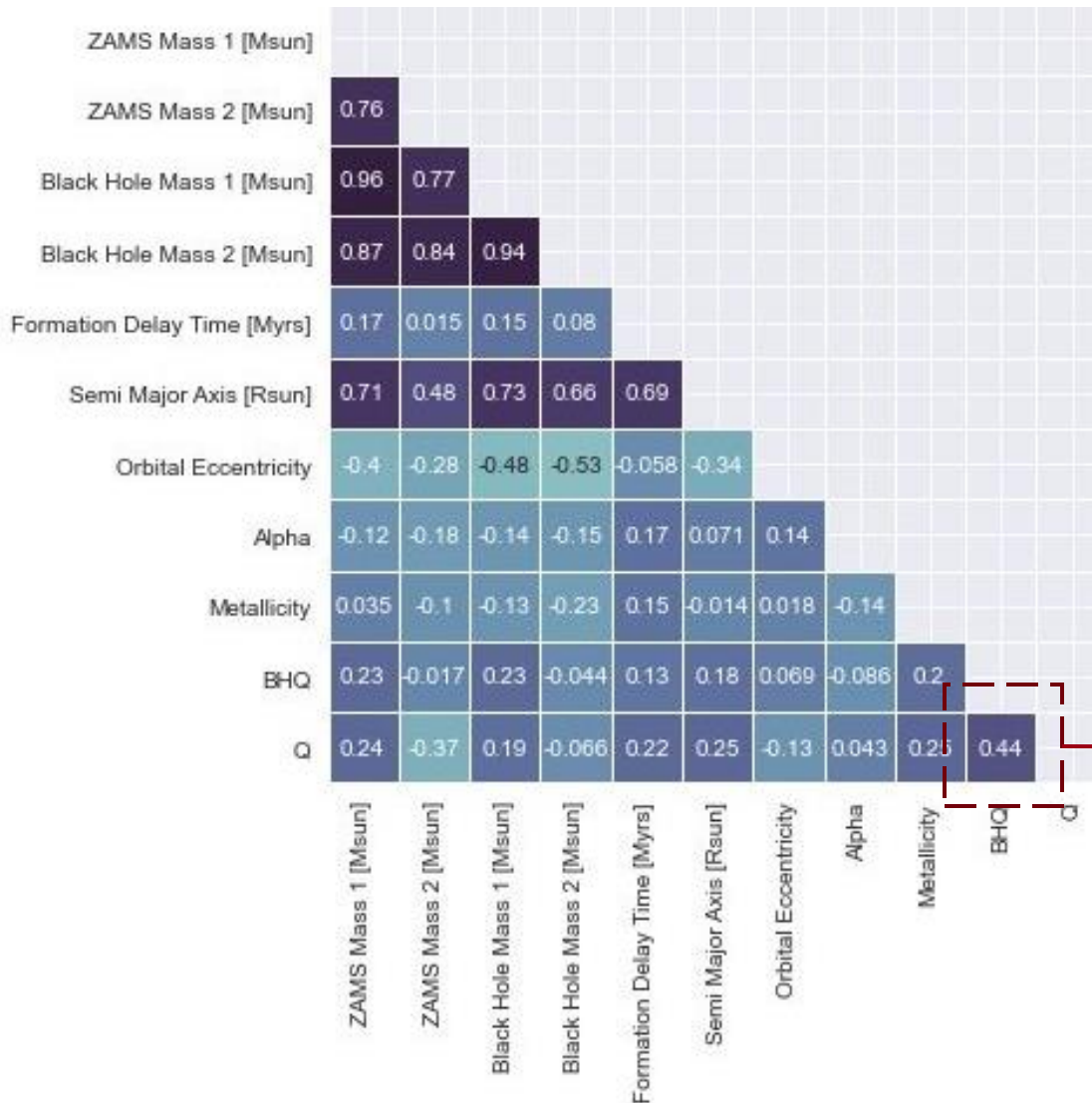
Feature correlation matrix

Masses are **highly correlated**



This could **negatively affect** prediction of the feature importances

Correlation matrix



Feature correlation matrix

Masses are **highly correlated**

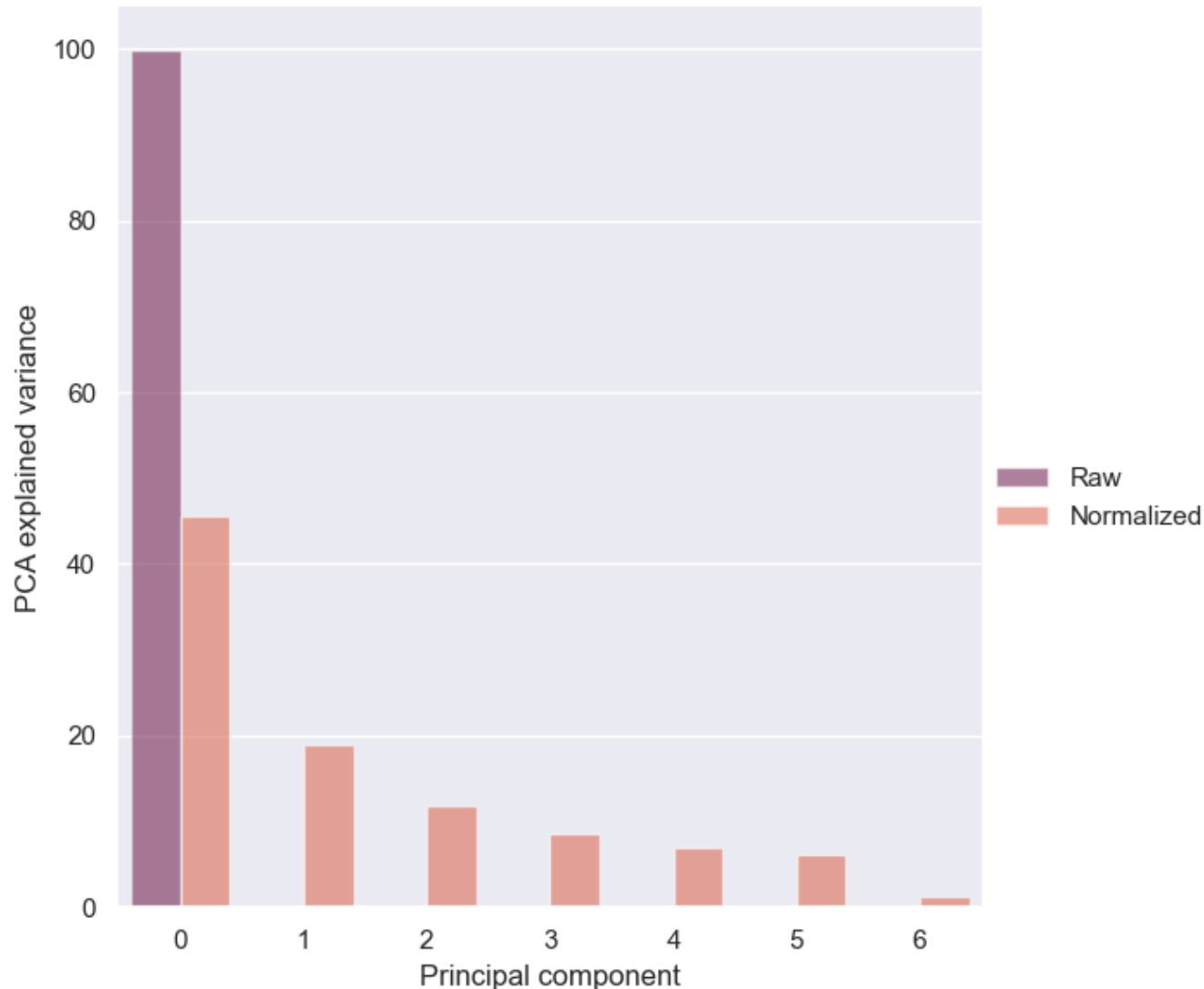
This could **negatively affect** prediction of the feature importances

$$Q = \frac{ZAMS\ Mass\ 1}{ZAMS\ Mass\ 2}$$

$$BHQ = \frac{Black\ Hole\ Mass\ 1}{Black\ Hole\ Mass\ 2}$$

these features were added for **physical** and **computational** reasons

Principal Component Analysis



**Without
normalization:**
1 PC ~ 99% variance

With normalization:
variance is distributed
across more PC

Feature importance



Model in-built method:

Weight for Linear
SVM

Medium
Difference in
Impurity for RFC

Model agnostic methods:

Permutation
importance

Feature-
dropping



Mean Decrease Impurity (MDI): total decrease in node impurity, weighted by the probability of reaching that node (approximated by the proportion of samples reaching that node), averaged over all trees of the ensemble

Disadvantage:

- Biased toward high cardinality and continuous features



Permutation feature importance doesn't suffer from this

Feature permutation: decrease in a model score when a single **feature is randomly shuffled**

Disadvantages:

- Misleading values on strongly correlated features
- Creates new instances that can be physically impossible



Feature-dropping could be a good fallback

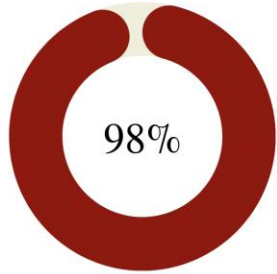
Feature-dropping: change in model score when a single **feature is removed**

Every time the model is retrained

Disadvantage:

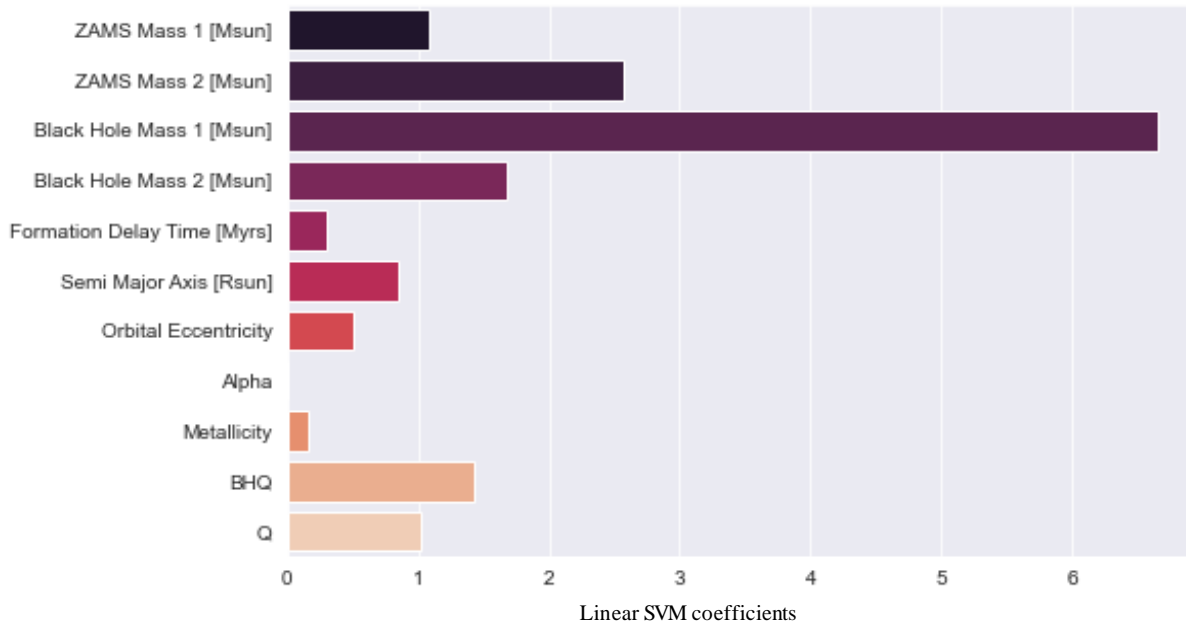
- Long calculation time
- Larger algorithm complexity

Linear SVM

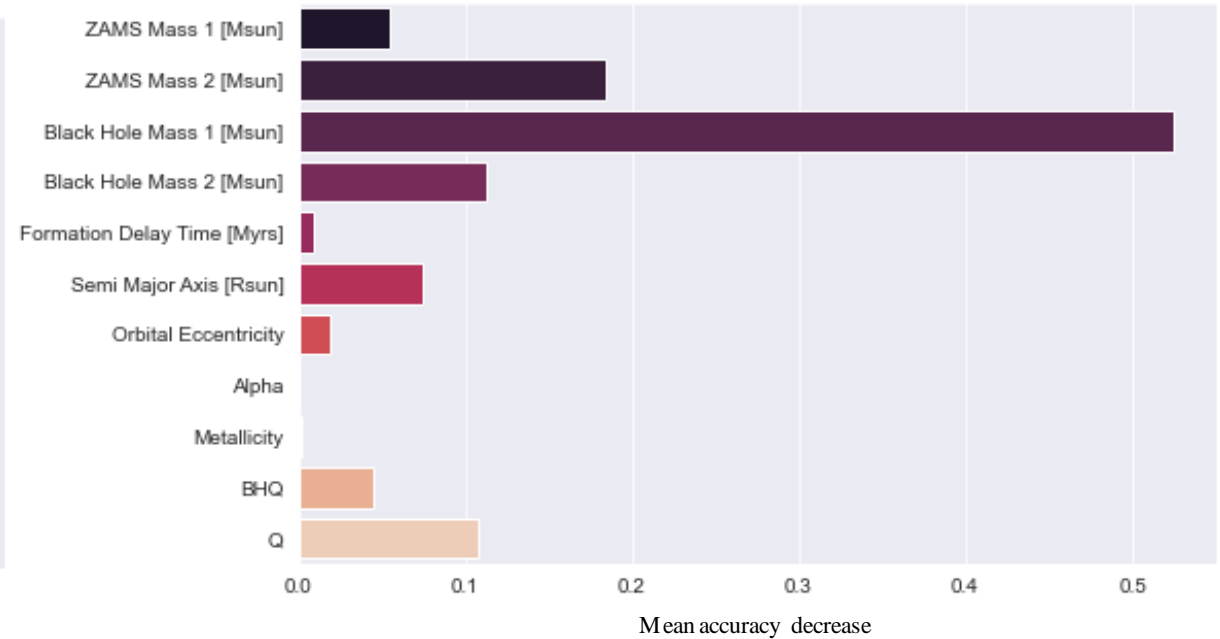
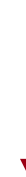


Accuracy

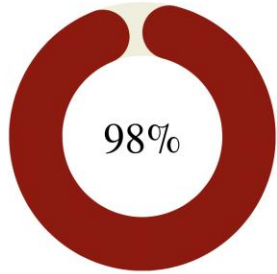
SVM coefficients



Feature permutation



Linear SVM

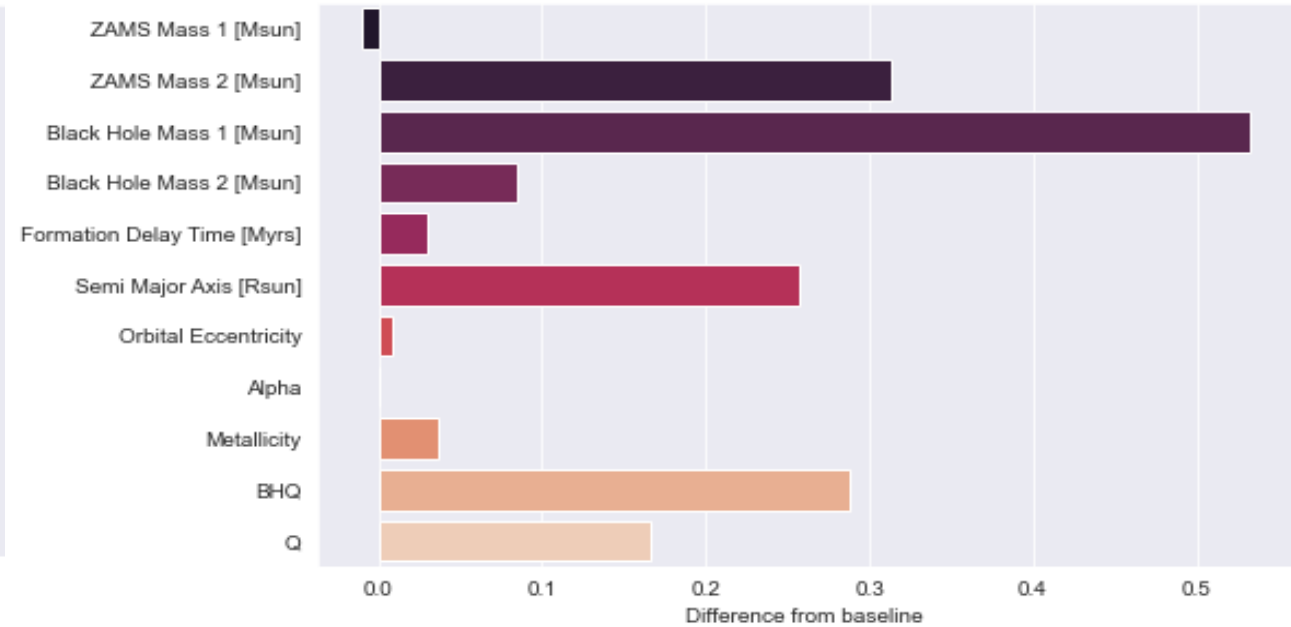
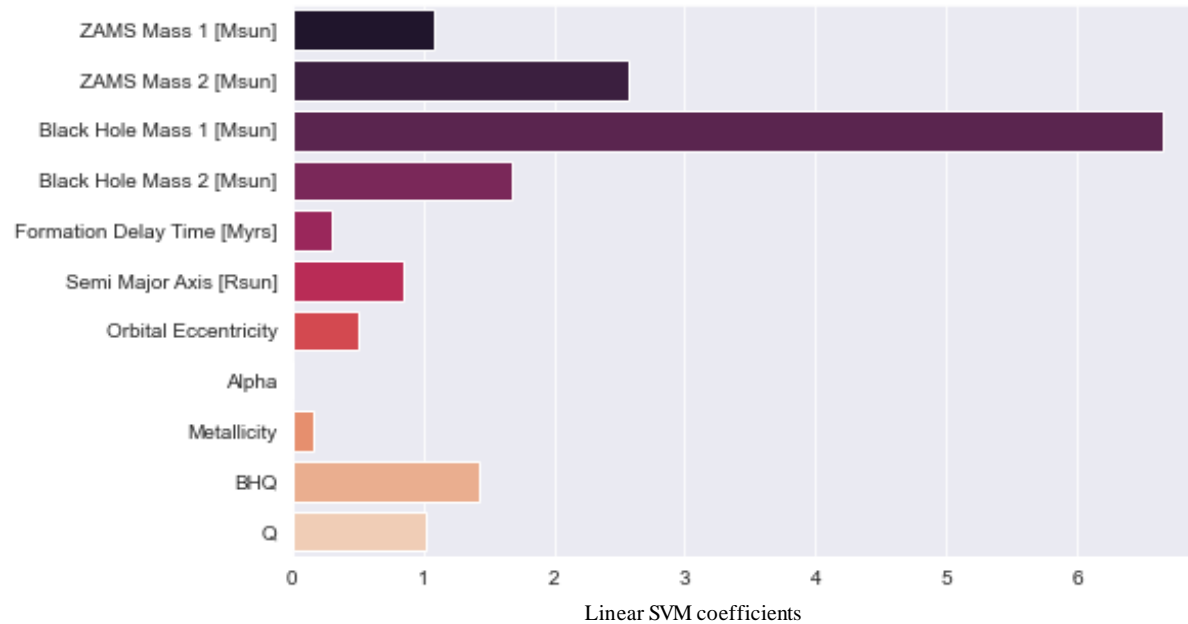


Accuracy

SVM coefficients



Feature-dropping

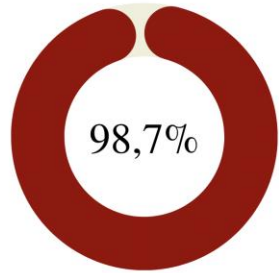


Linear SVM: ranking



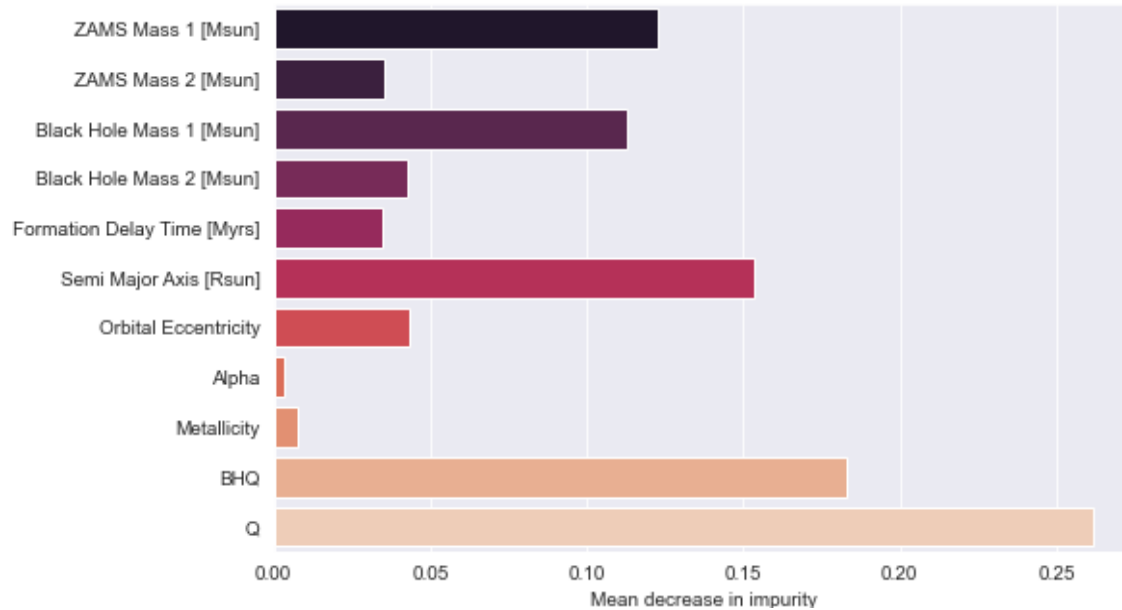
Ranking	Linear SVM	Feature permutation	Feature-dropping
1	BH Mass 1	BH Mass 1	BH Mass 1
2	ZAMS Mass 2	ZAMS Mass 2	ZAMS Mass 2
3	BH Mass 2	BH Mass 2	BHQ
10	Metallicity	Metallicity	Orbital eccentricity
11	Alpha	Alpha	Alpha

Random Forest

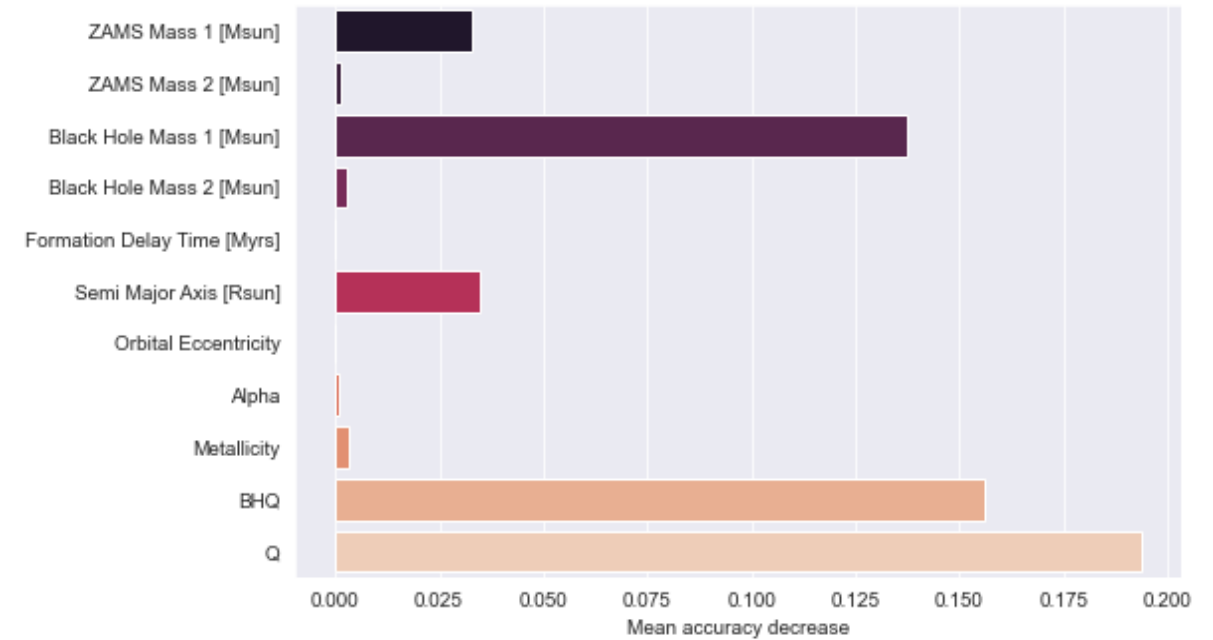


Accuracy

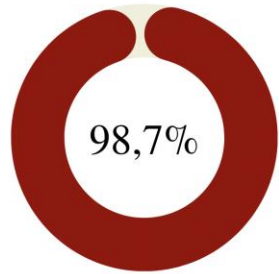
Mean Decrease in
Impurity



Feature permutation

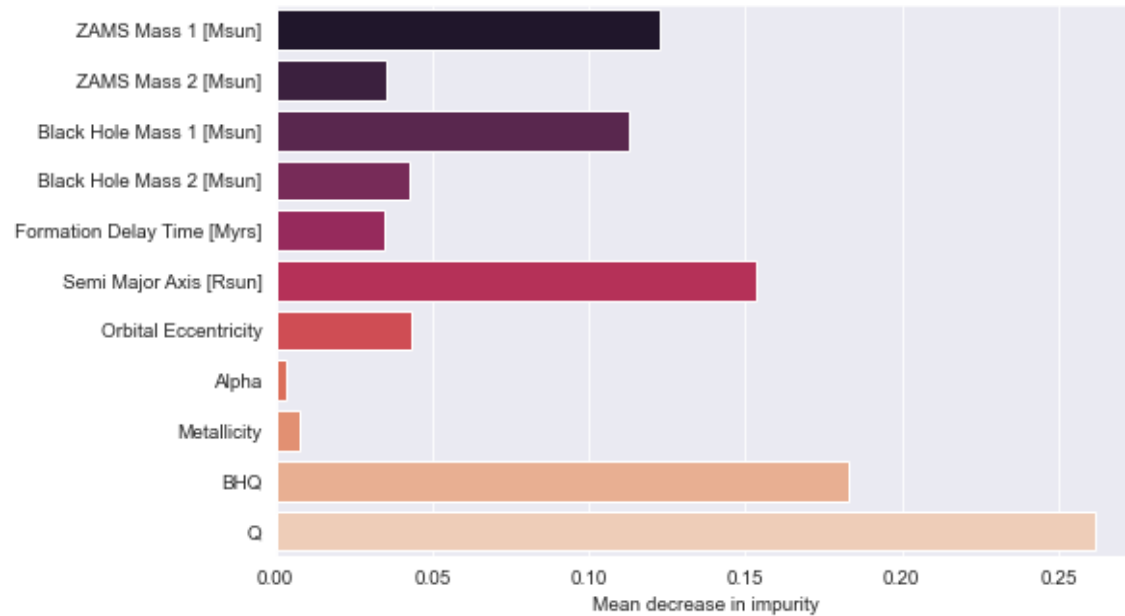


Random Forest

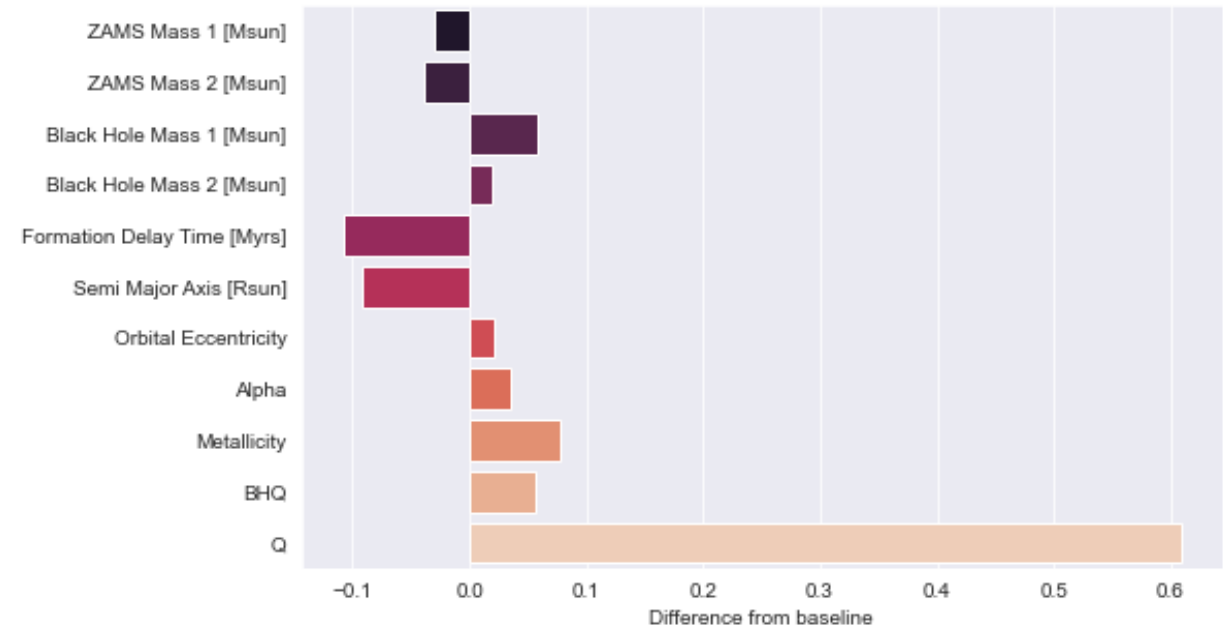


Accuracy

Mean Decrease in
Impurity



Feature-dropping

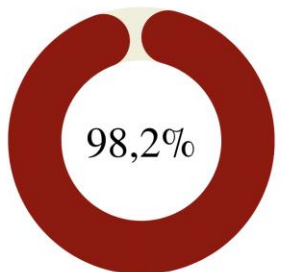
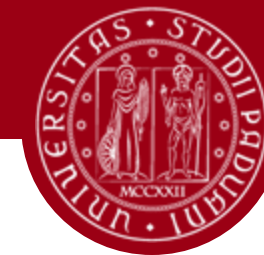


Random Forest: ranking



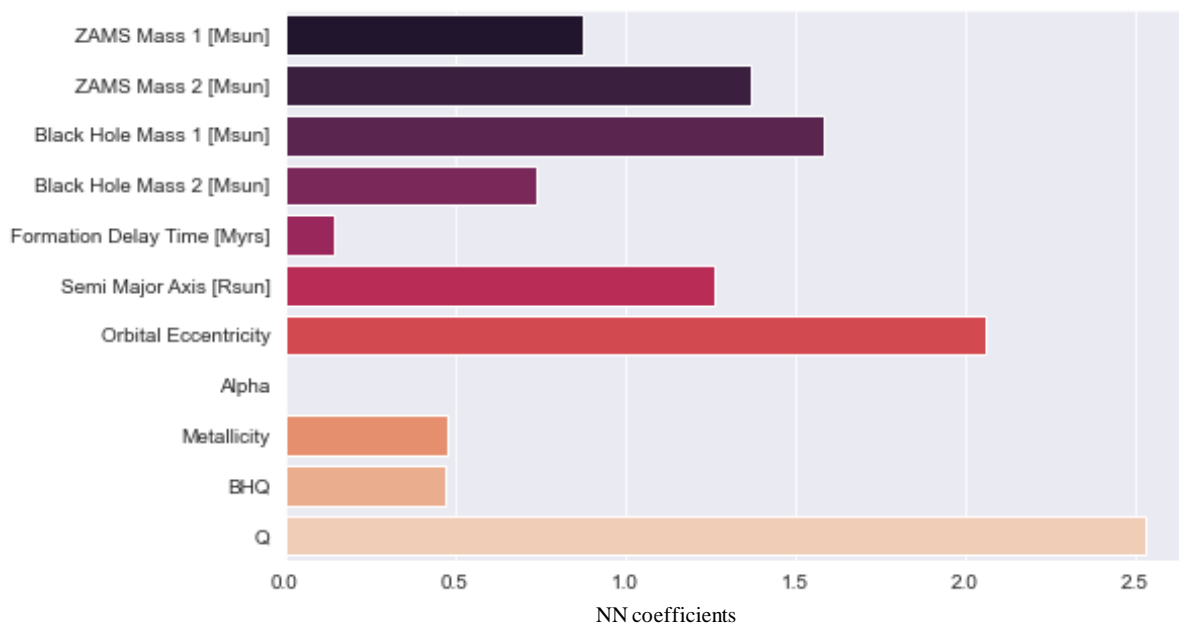
Ranking	MDI	Feature permutation	Feature-dropping
1	Q	Q	x
2	BHQ	BHQ	x
3	Semi-major axis	BH Mass 1	x
10	Metallicity	Formation delay time	x
11	Alpha	Orbital eccentricity	x

Neural Network

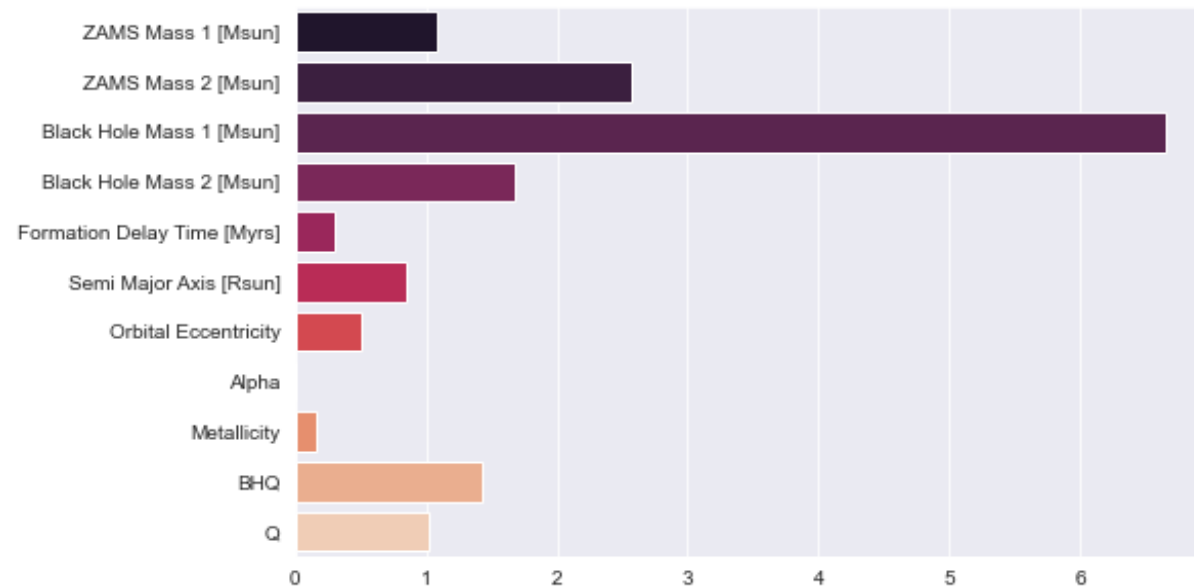


Accuracy

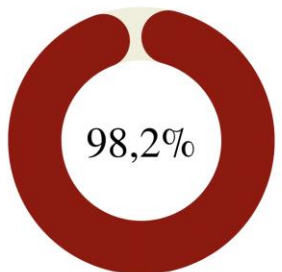
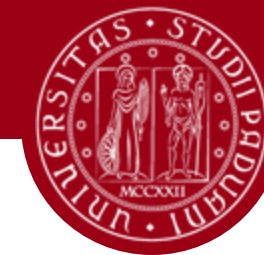
NN coefficients



Linear SVM coefficients

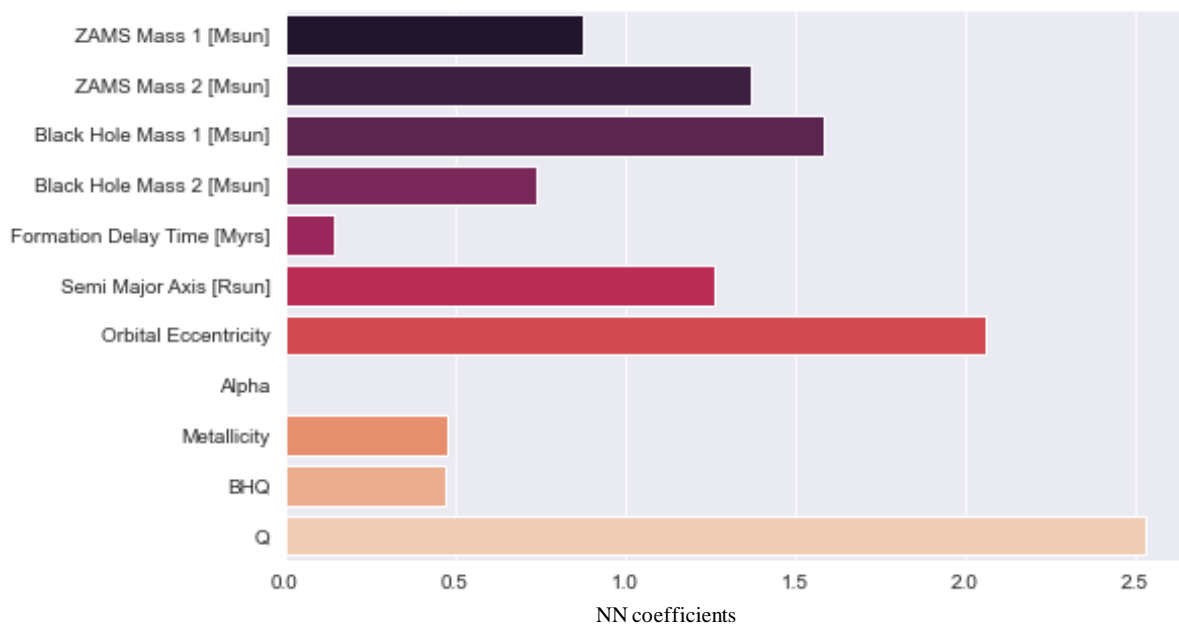


Neural Network

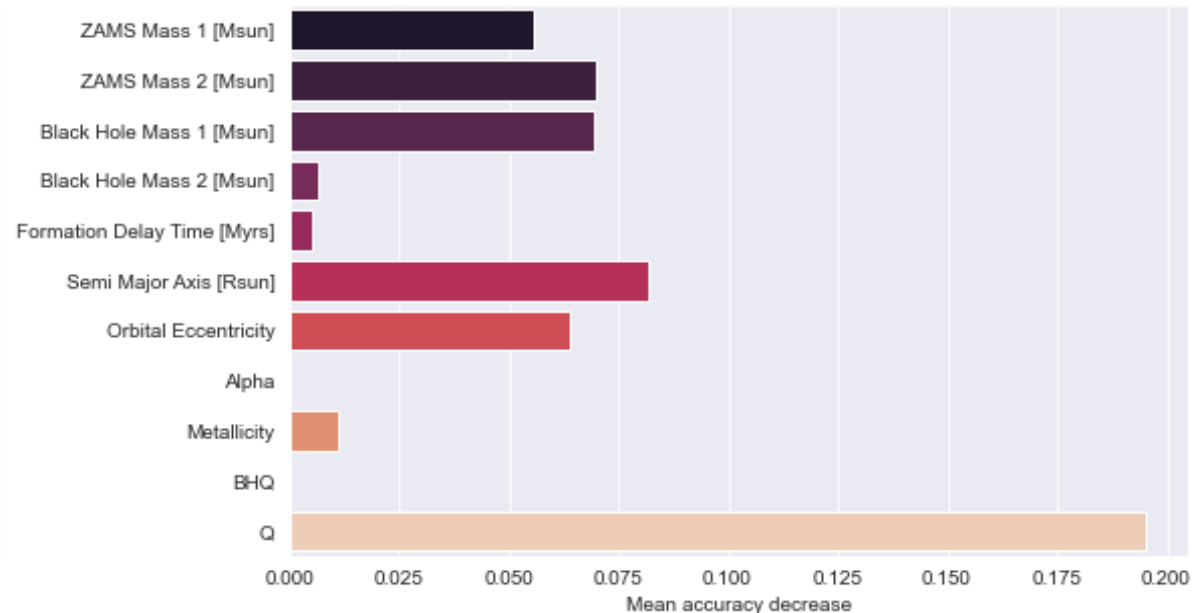


Accuracy

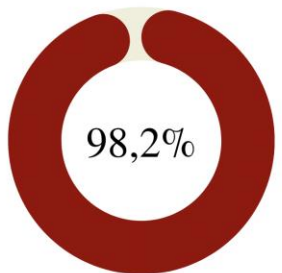
NN coefficients



Feature-permutation

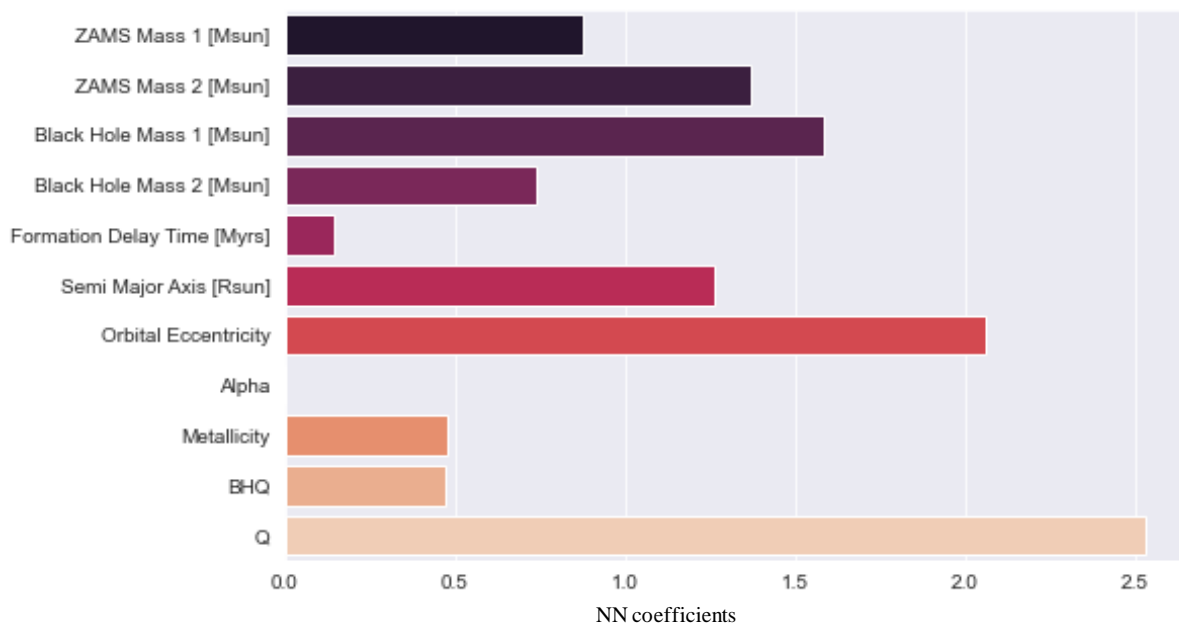


Neural Network

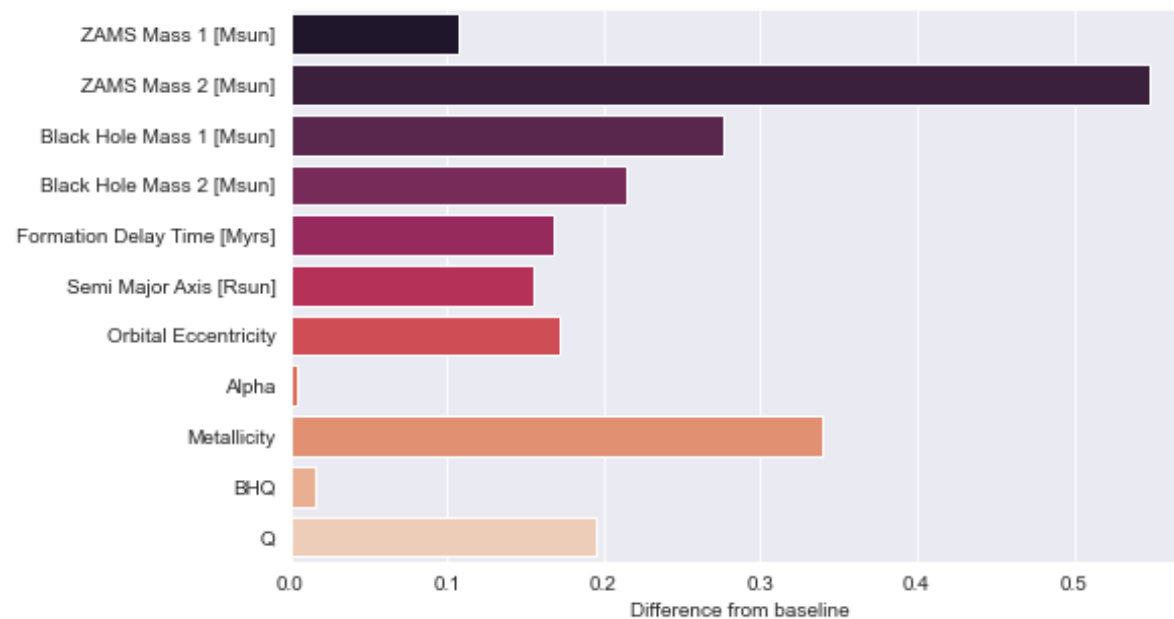


Accuracy

NN coefficients



Feature-dropping



Neural Network: ranking




Ranking	NN coefficients	Feature permutation	Feature-dropping
1	Q	Q	ZAMS Mass 2
2	Orbital eccentricity	Semi-major axis	Metallicity
3	BH Mass 1	ZAMS Mass 2	BH Mass 1
10	Formation delay time	BHQ	BHQ
11	Alpha	Alpha	Alpha

Conclusion



- **Goal:** Infer what are the most important features for determining the evolution of binary stars into binary black holes
- **Dataset preprocess:**
 - Balance the possible evolution paths
 - Removal of the outliers
 - Normalization
- **Data evaluation** → qualitative observation of 1:1 feature plots :
 - ZAMS Masses
 - BBH masses
 - Q and BHQ values
 - Orbital eccentricity
 - Semi-major axis



```
graph LR; A[ZAMS Masses] --- B[ ]; B[BBH masses] --- B; B[Q and BHQ values] --- B; B[Orbital eccentricity] --- B; B[Semi-major axis] --- B; B --> C[Expected important features];
```

- **Machine learning algorithm:**

- Built-in vs custom methods:

- MDI (built-in)
 - Feature permutation (custom)
 - Feature dropping (custom)

- Models:

- Linear SVM
 - Random Forest
 - Neural Network

- **Best model** → Random Forest, it resembles expectations

- **Most important features** → Masses (alone or ratios) and semi-major axis