

Laboratory of Computational Physics 2022-2023
Astrophysics Project

The Formation of Binary Black Holes

Bhatti Roben

Bedin Veronica

Bonato Diego

Sapkas Michail

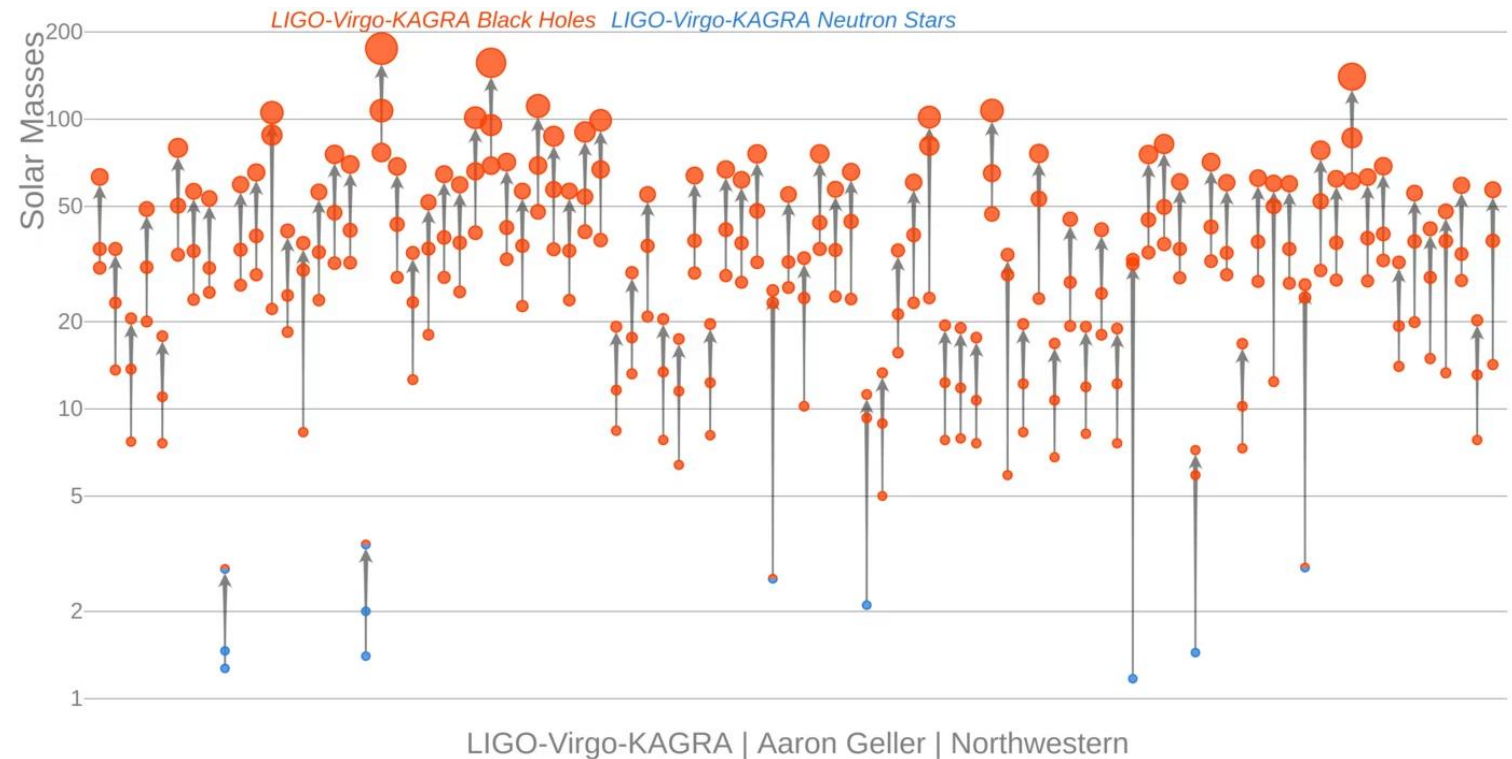
Binary black holes and gravitational waves



90 events of
gravitational waves

↓

80 mergers of **binary
black holes**



Masses in the stellar graveyard

Goal of the project

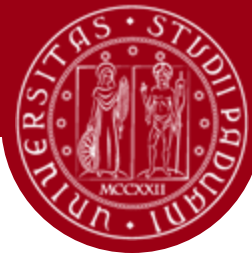


Goal of the project:
finding **what features** have
the highest impact on the
evolution of a binary system
into a Binary Black Hole

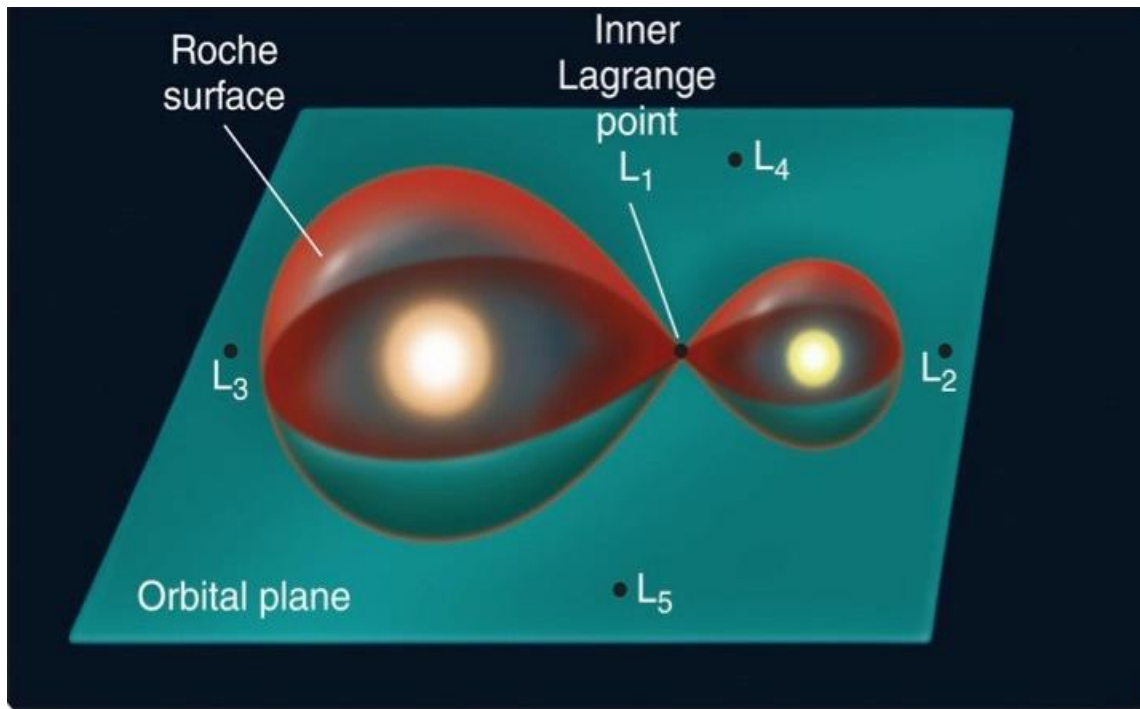


Credits: ESO/M. Kornmesser/S.E. de Mink

Mass transfer via Roche Lobe



Roche Lobe: region where
orbiting material
is gravitationally bound

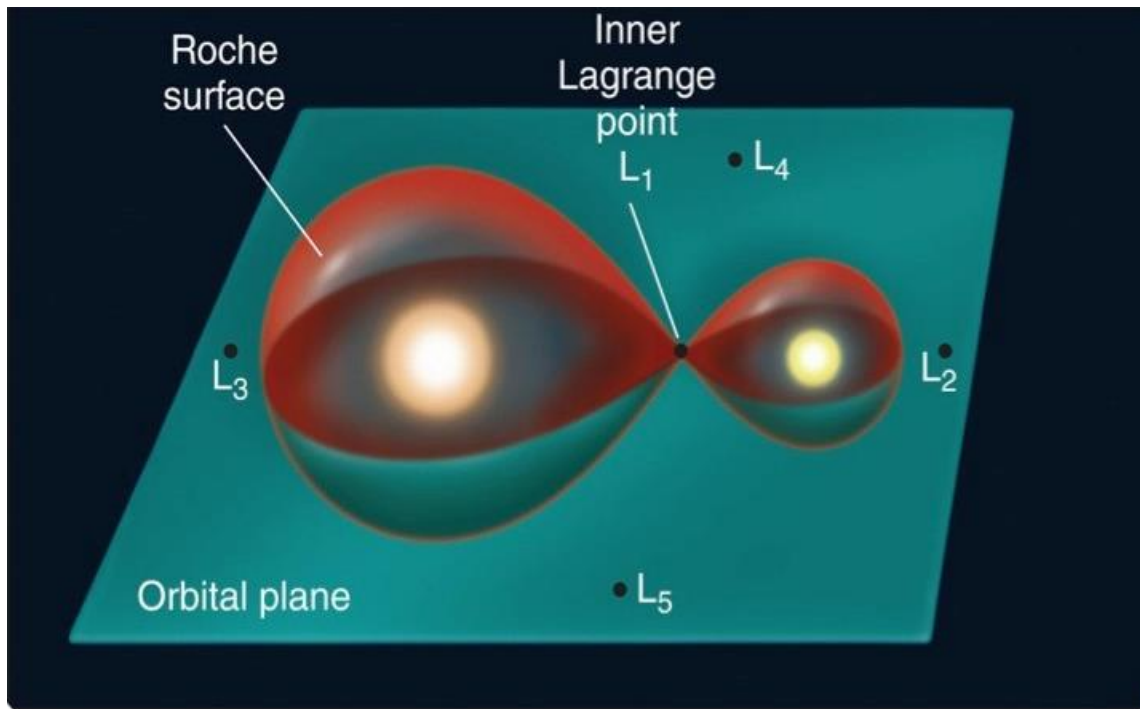


Credits: Cengage Learning (2016)

Mass transfer via Roche Lobe



Roche Lobe: region where
orbiting material
is gravitationally bound



Roche lobe
overflow

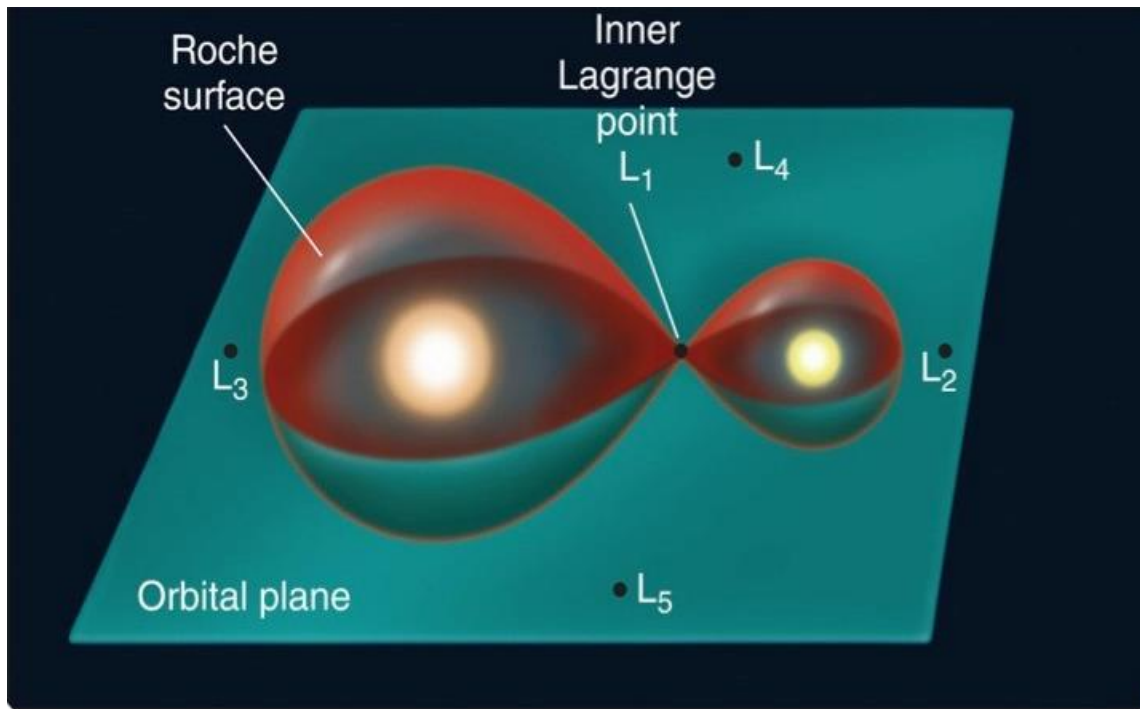


Credits: Cengage Learning (2016)

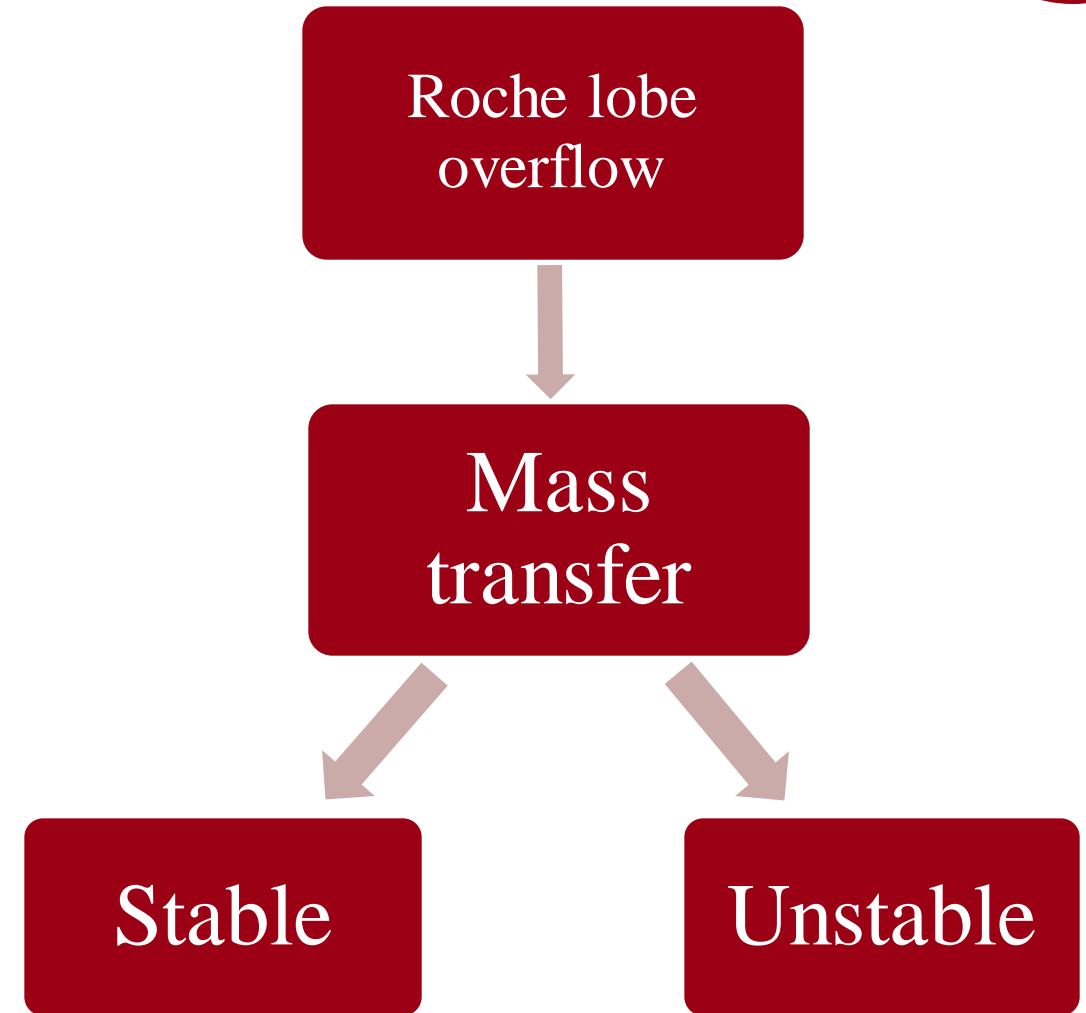
Mass transfer via Roche Lobe



Roche Lobe: region where orbiting material is gravitationally bound



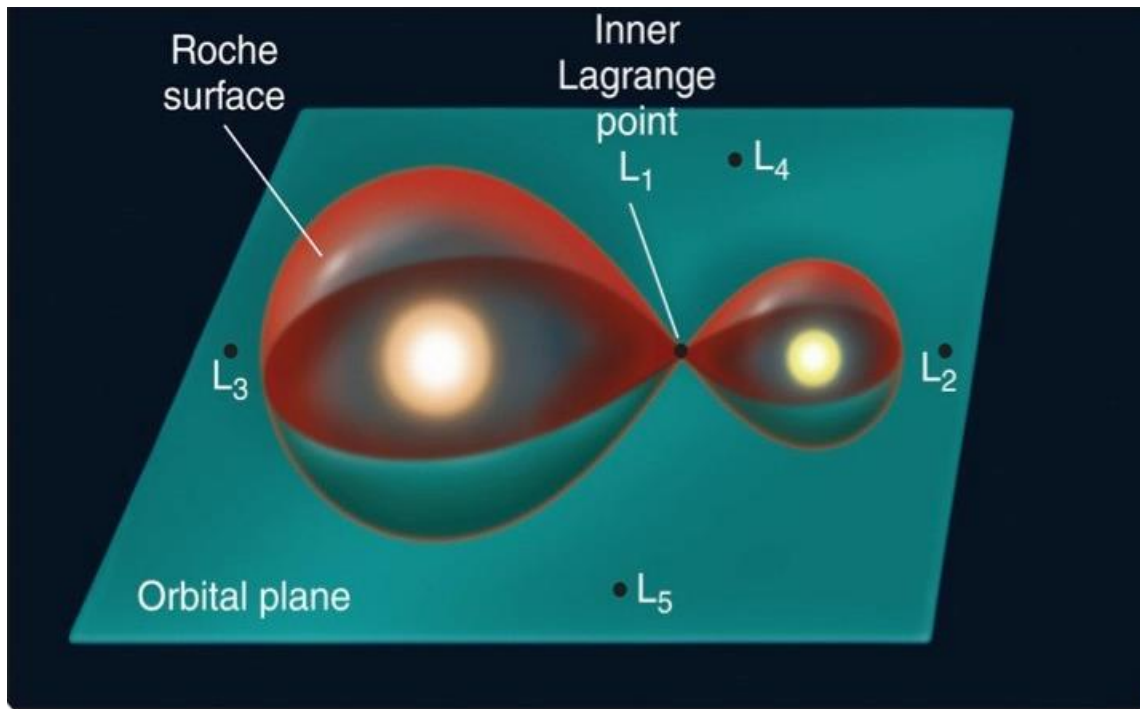
Credits: Cengage Learning (2016)



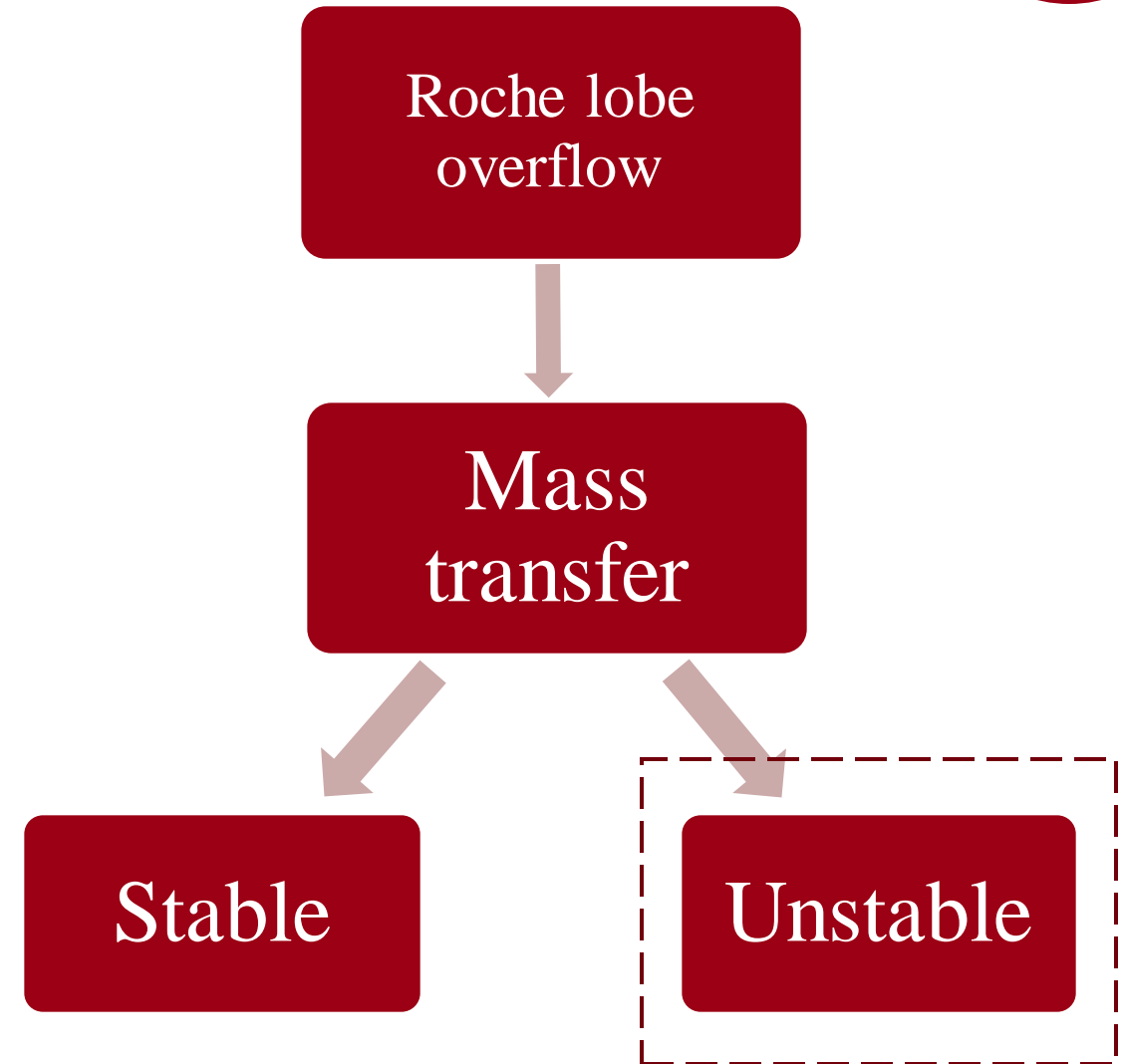
Mass transfer via Roche Lobe



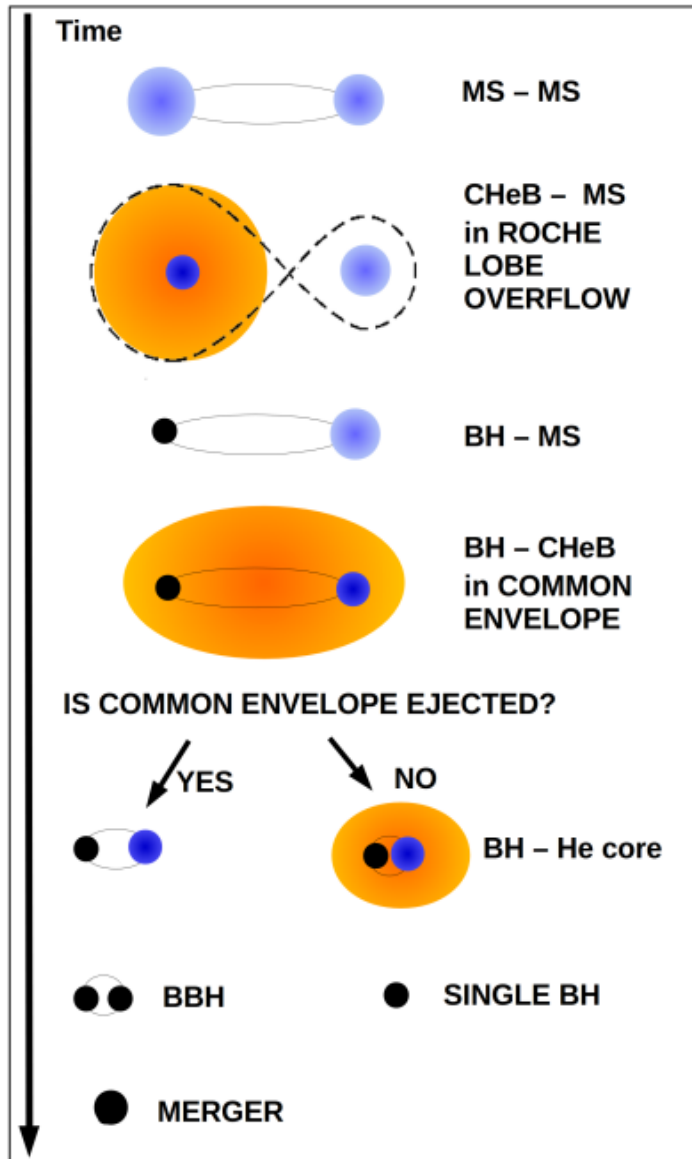
Roche Lobe: region where orbiting material is gravitationally bound



Credits: Cengage Learning (2016)



Unstable mass transfer



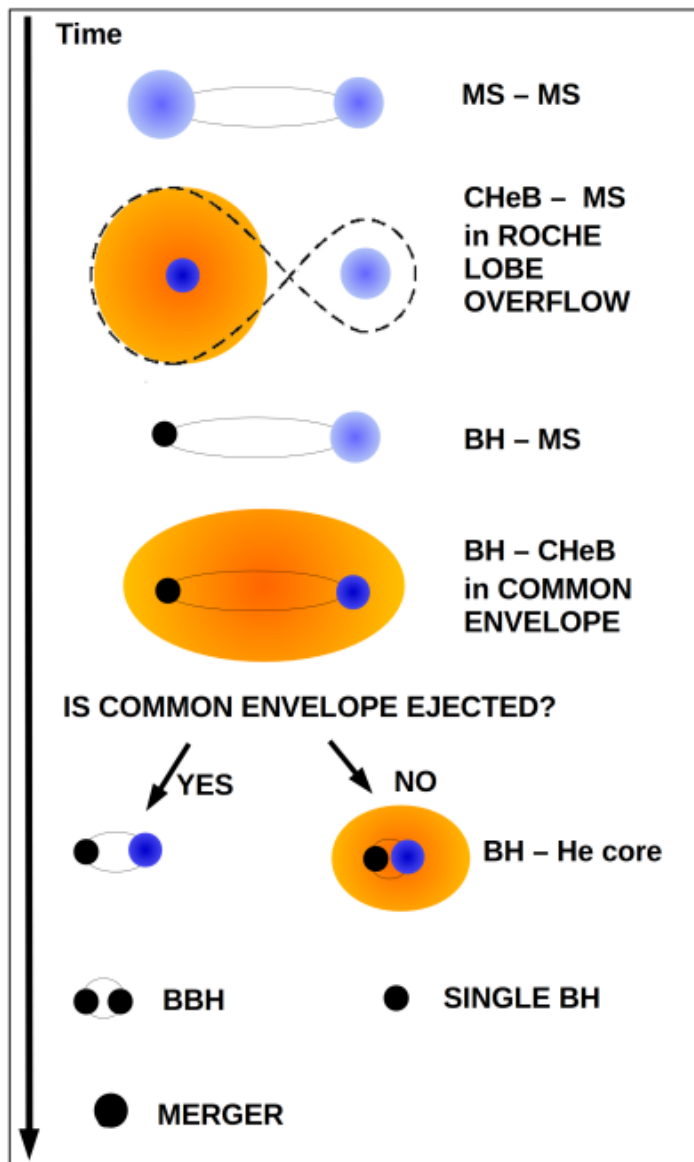
Binary system with stars in main sequence

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.

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

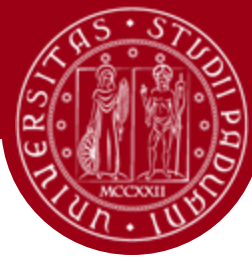
The α formalism

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



▪ **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

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

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

Dataset



■ 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

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

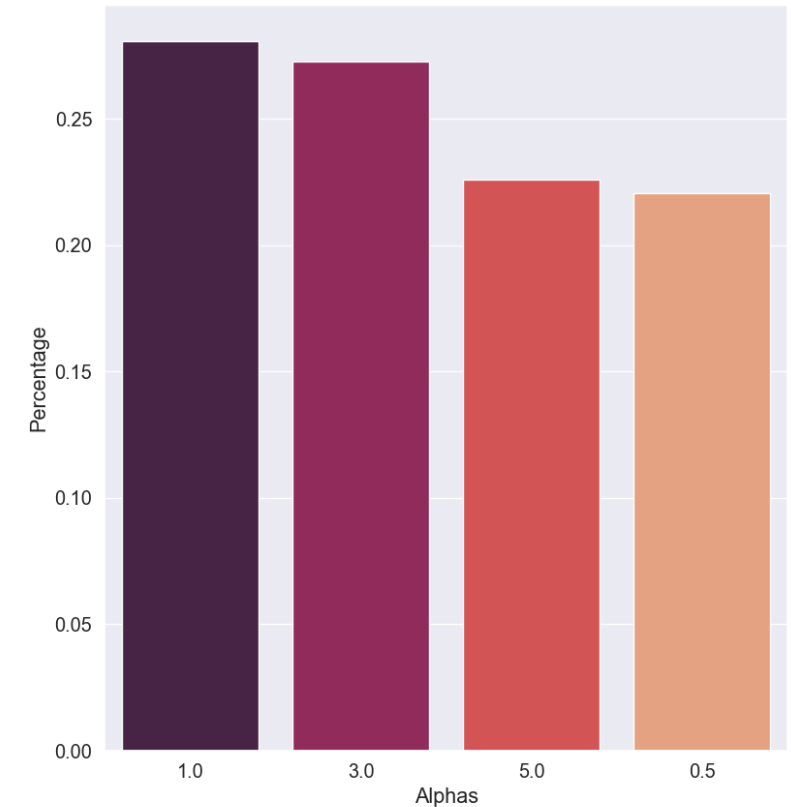
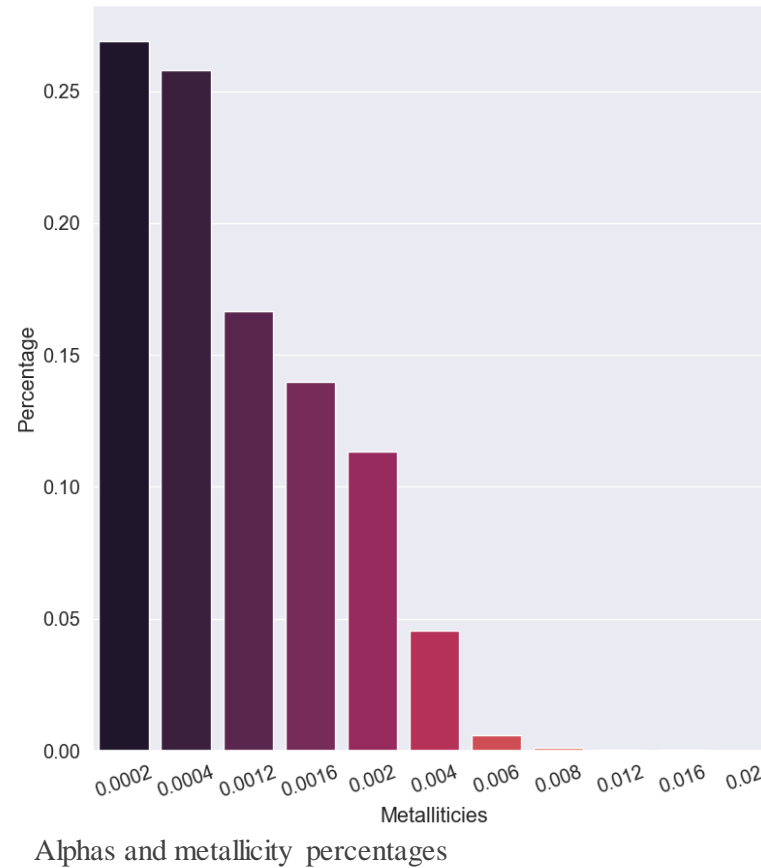


Imbalanced dataset:

- 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



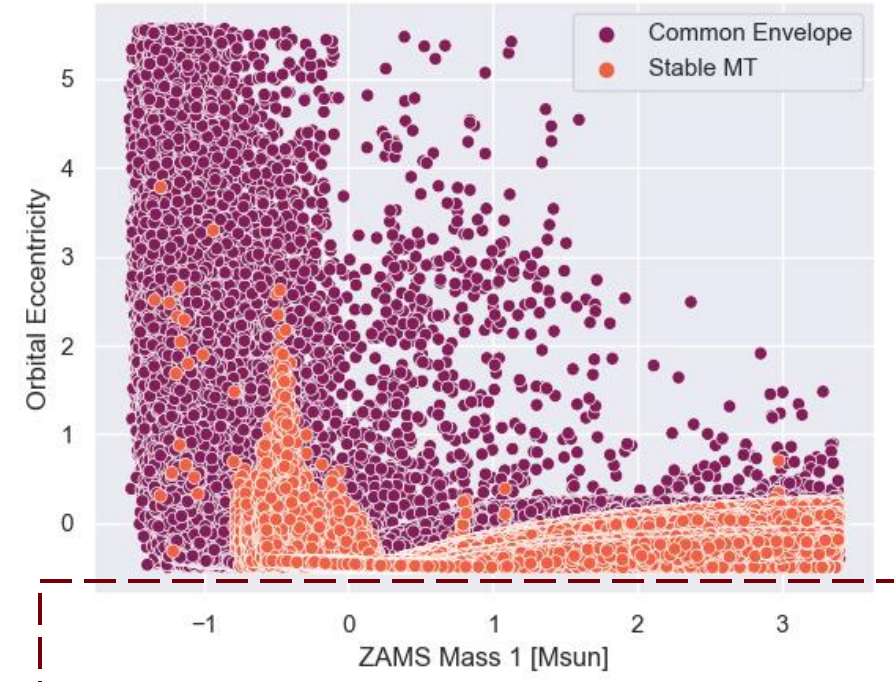
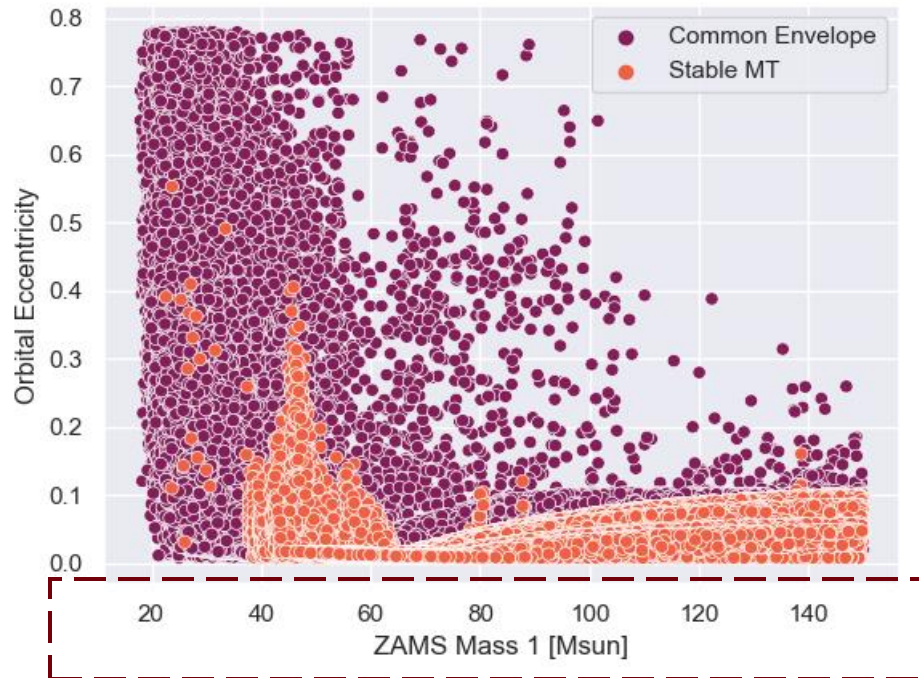
High stds and extreme outliers makes it difficult to cluster our data

	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%

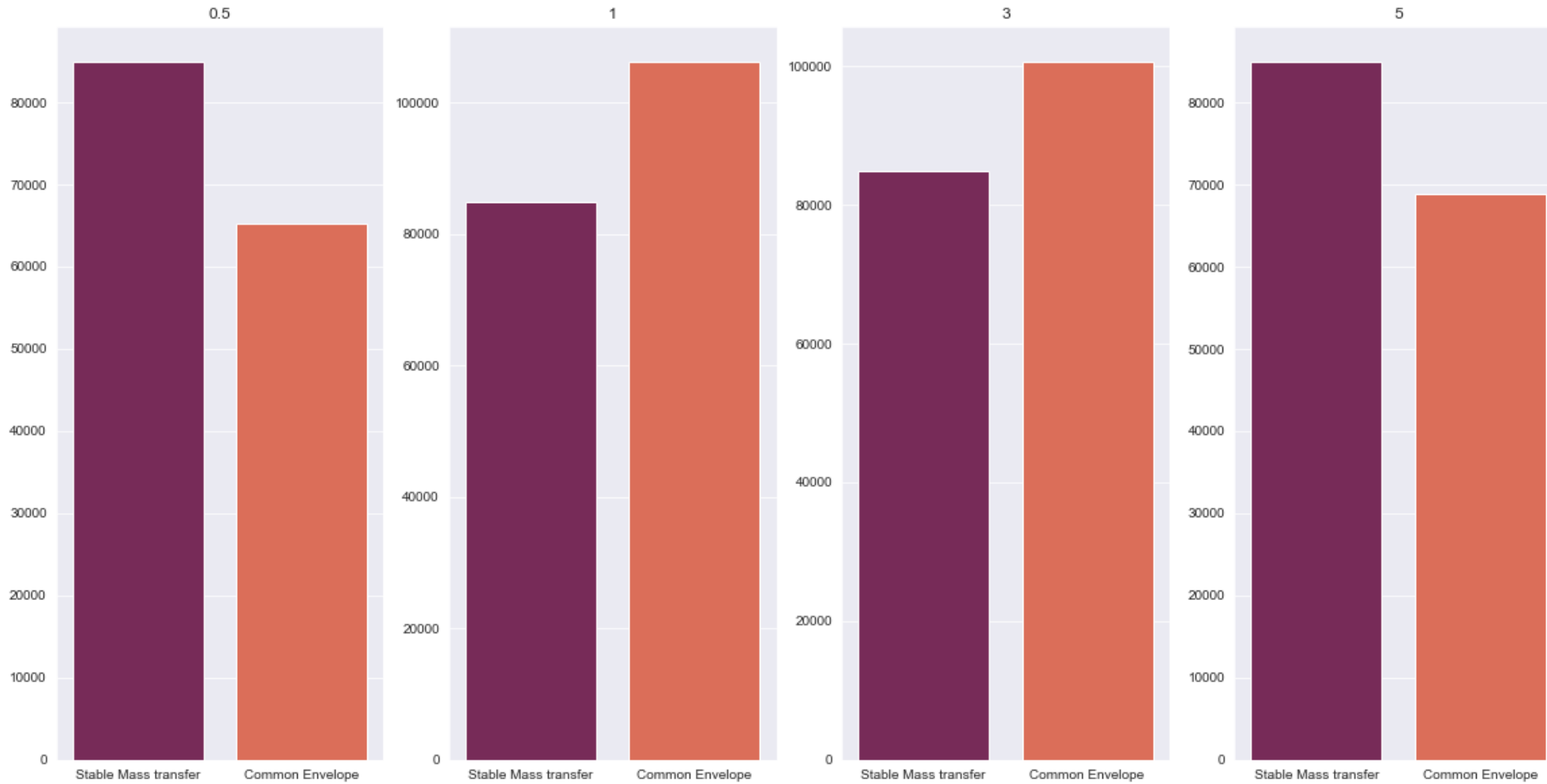
	count	mean	std	min	1%	50%	99%	max
Orbital Eccentricity	680471.0	0.071232	0.127306	0.00800	0.008286	0.016089	0.61662	0.77999
Semi Major Axis [Rsun]	680471.0	20.767367	12.262600	0.66417	3.412000	19.321000	52.60300	88.30800

Normalization



Normalization is important for
distance-based algorithms

Alpha



Alpha distribution for different labels

Alpha parameters are
well distributed
between the two
evolution cases

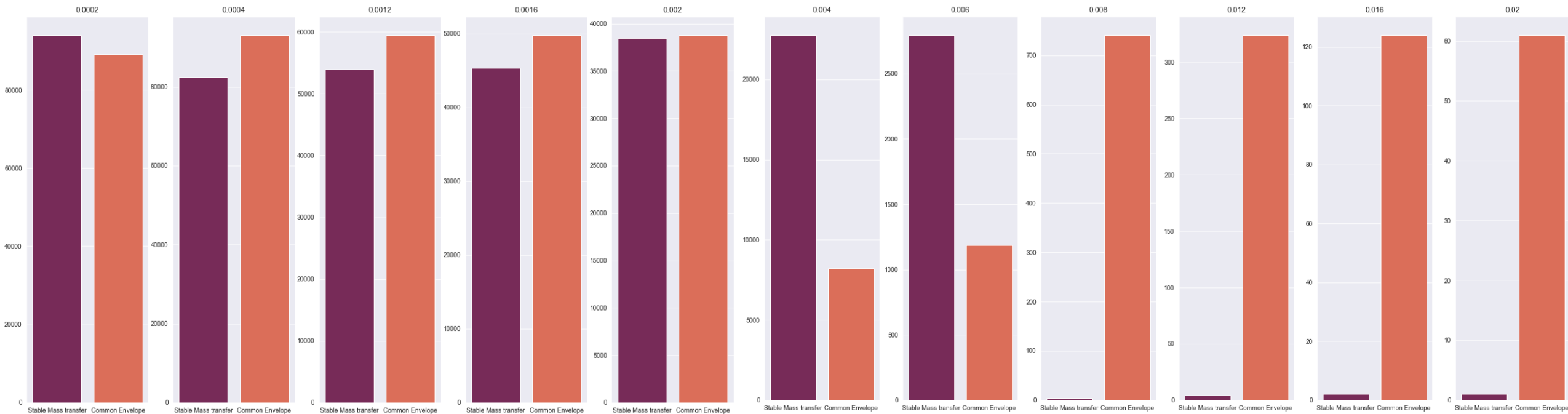
Metallicities



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



For **higher** metallicities only Common envelope



Metallicity distribution for different labels

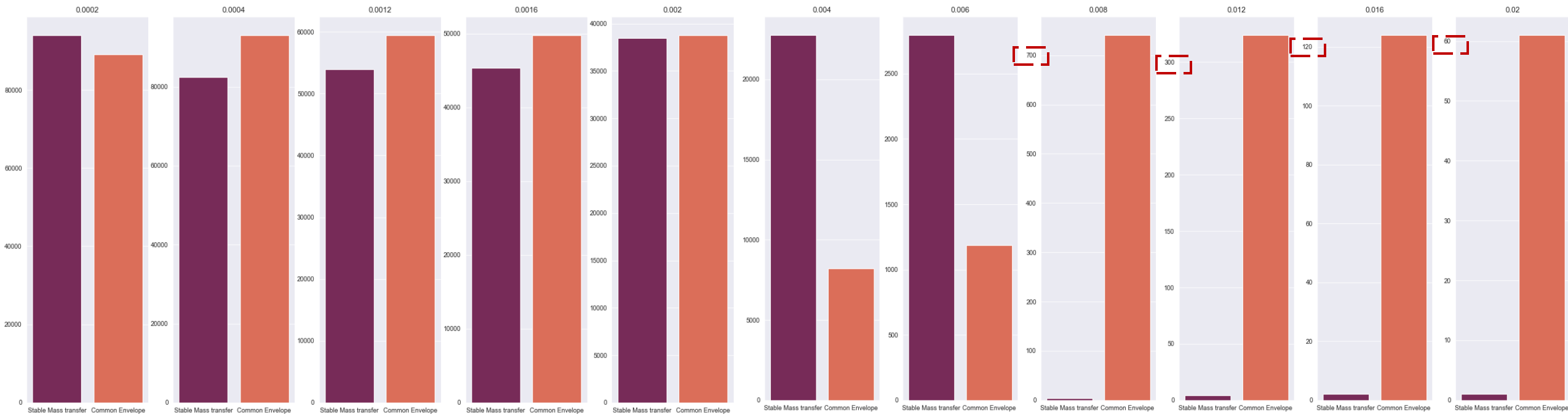
Metallicities



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

For **higher** metallicities only Common envelope

Small number of instances, **negligible**

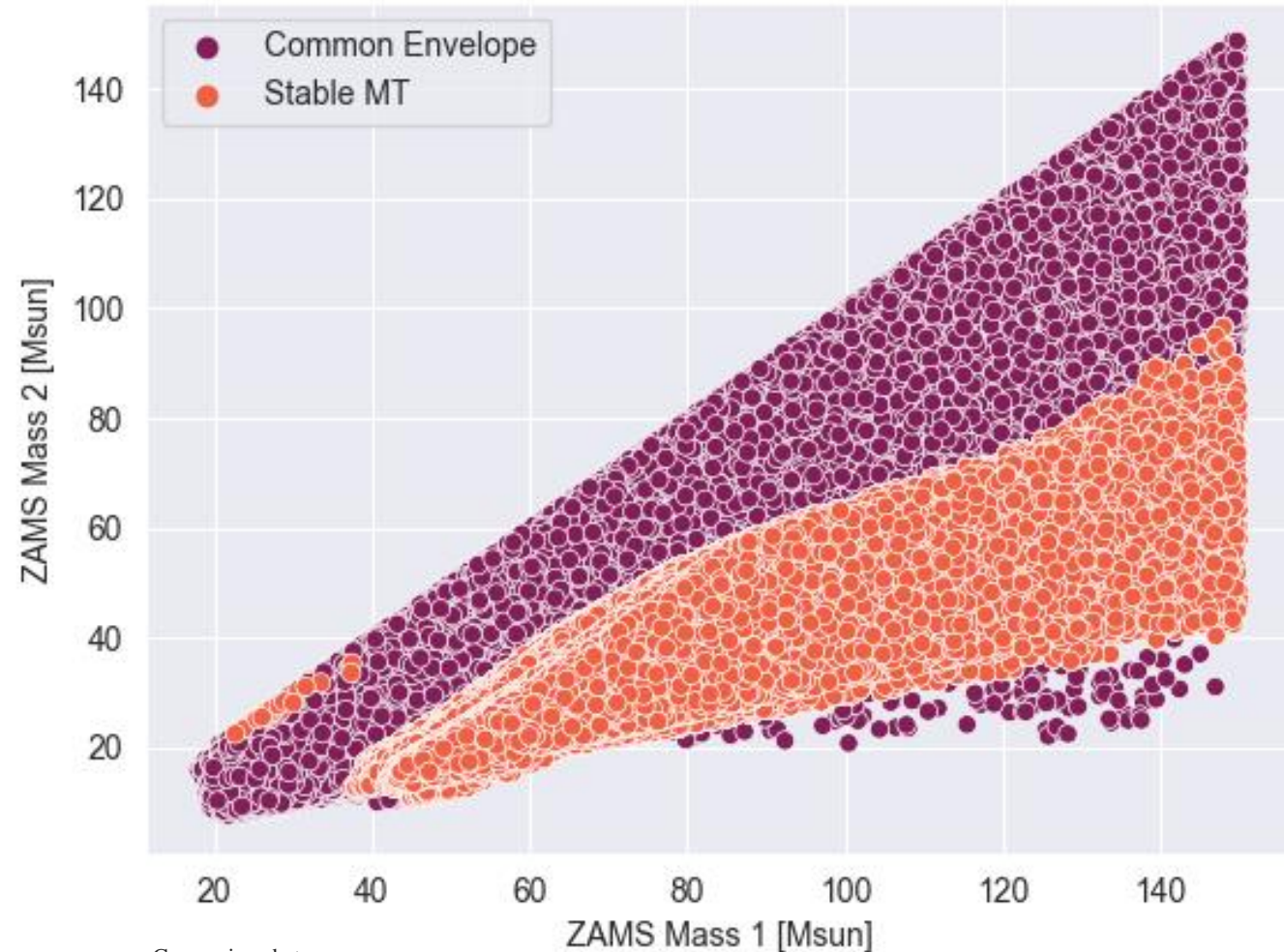


Metallicity distribution for different labels

Masses considerations



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



Comparison between masses

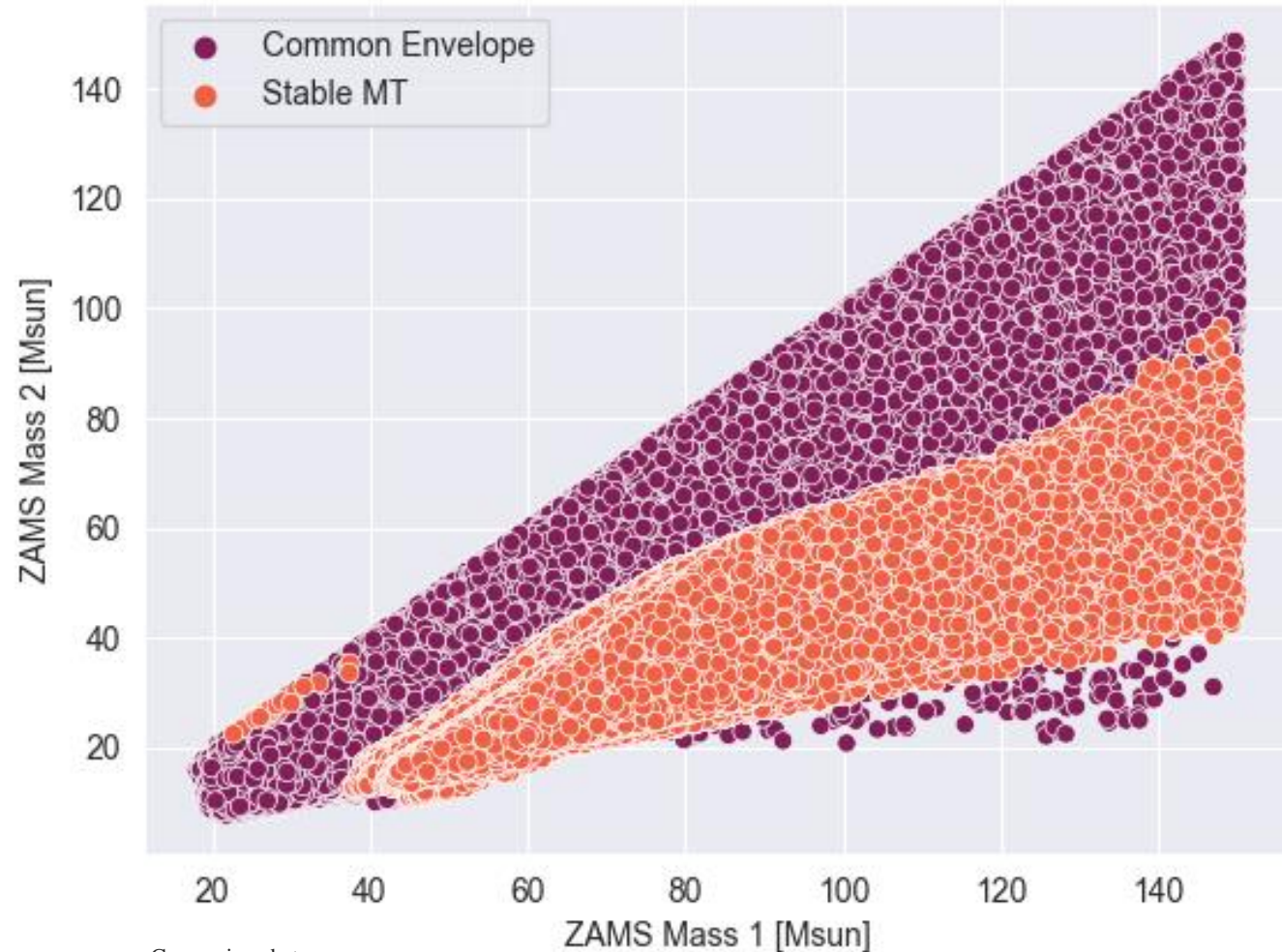
Masses considerations



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



Introduces a **bias**



Comparison between masses

Masses considerations



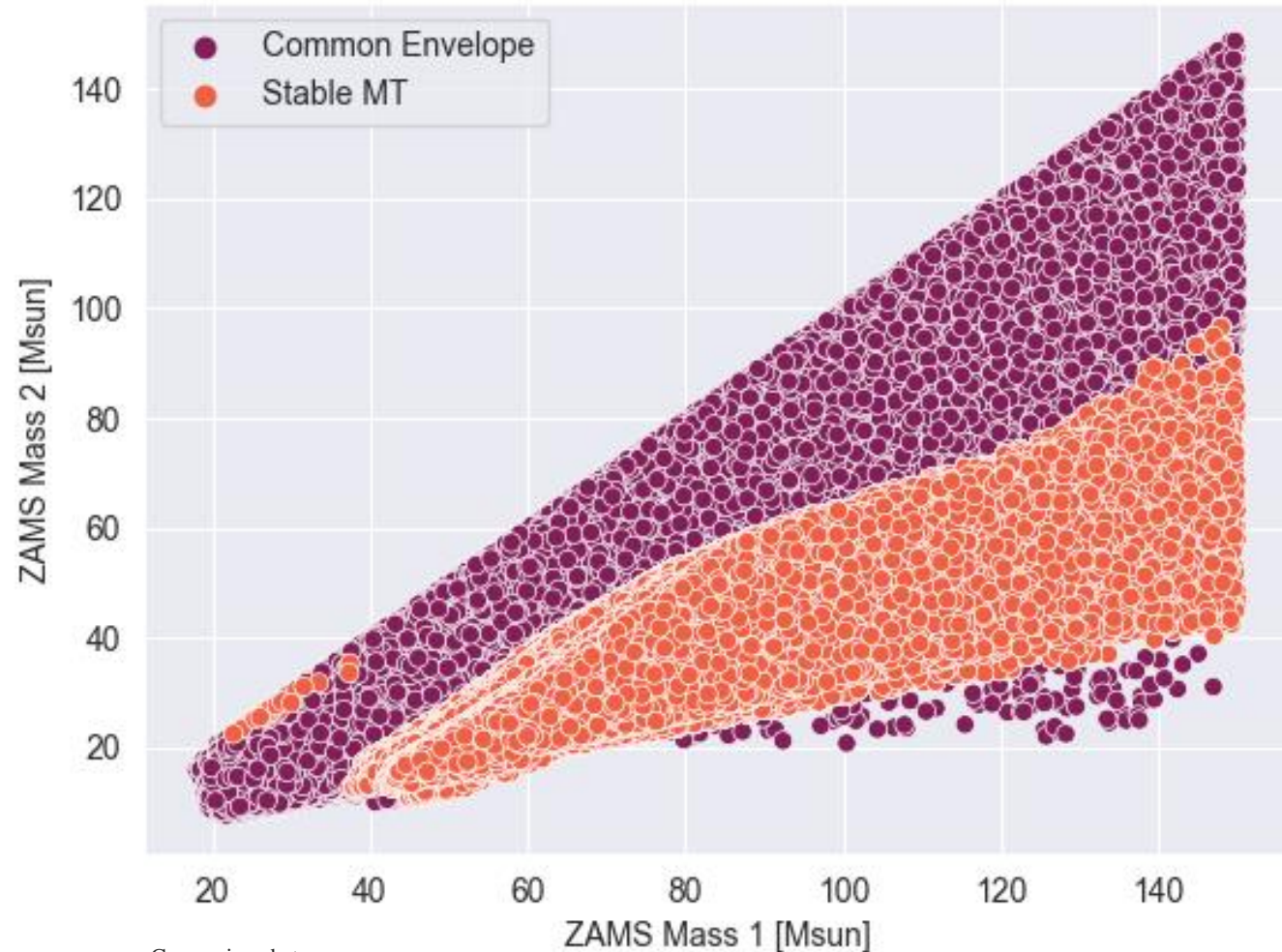
ZAMS Mass 1 > ZAMS Mass2
by **construction**



Introduces a **bias**



Problems with Machine
Learning algorithms



Comparison between masses

Masses considerations

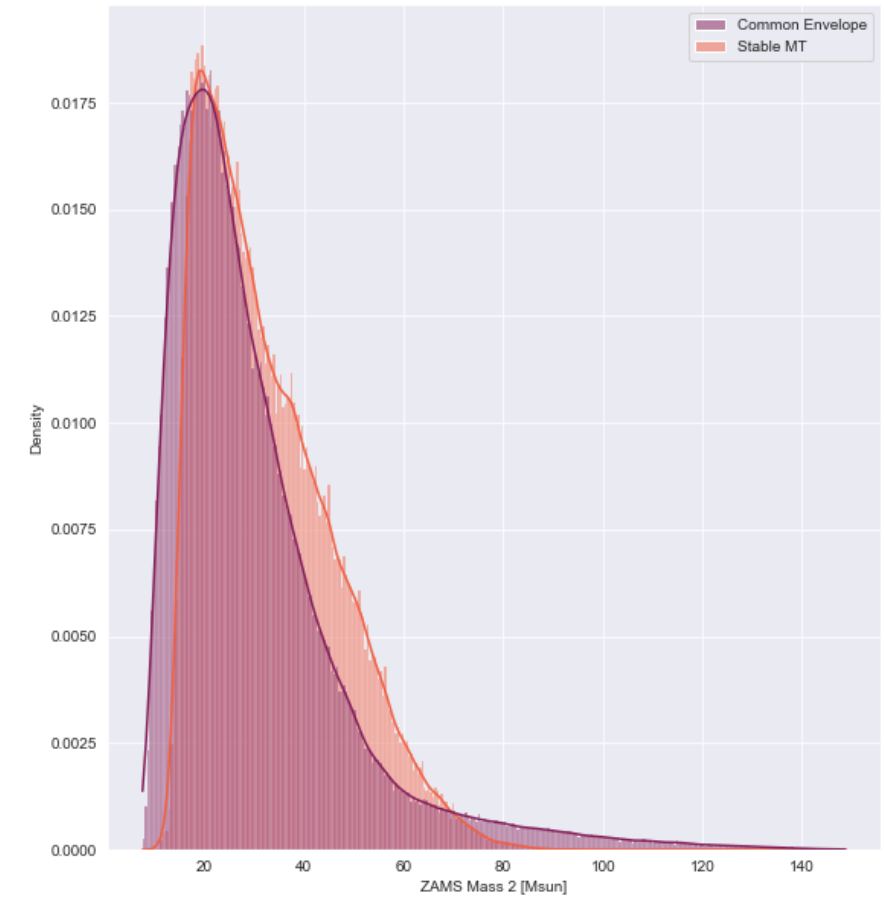
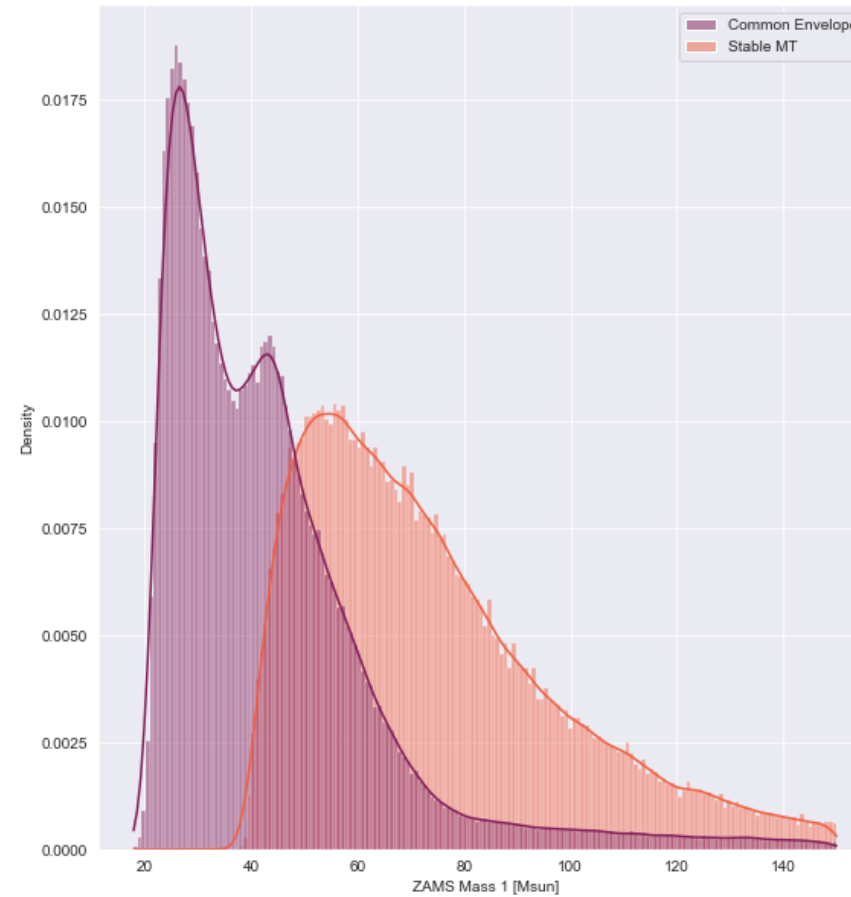


Primary mass

- 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

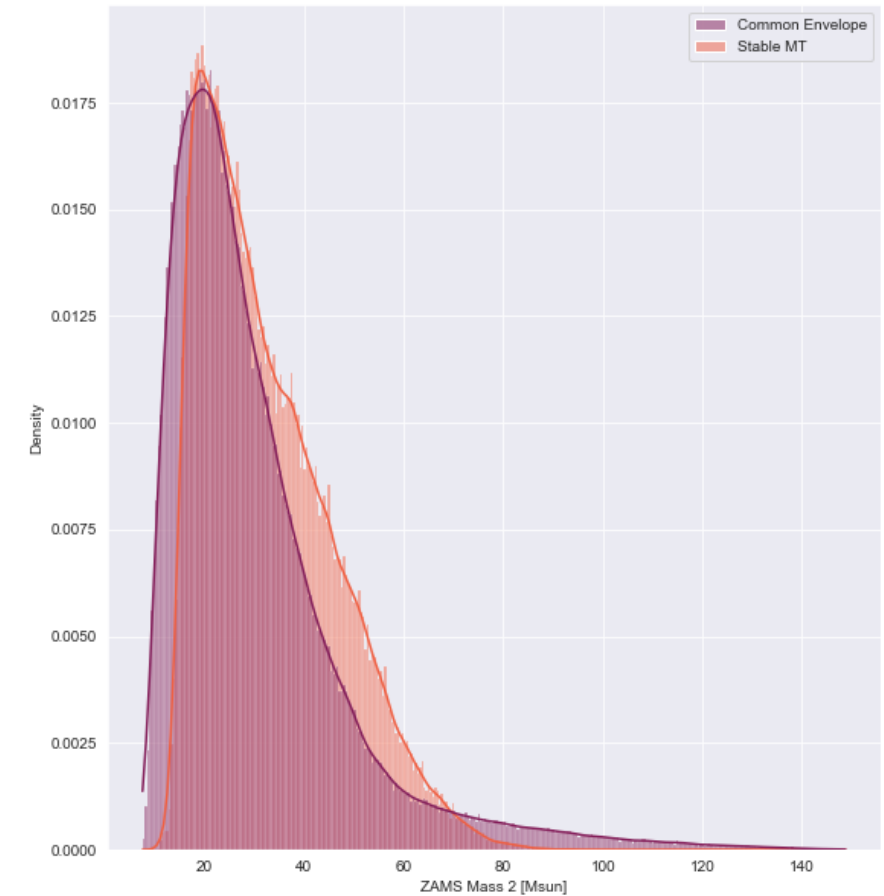
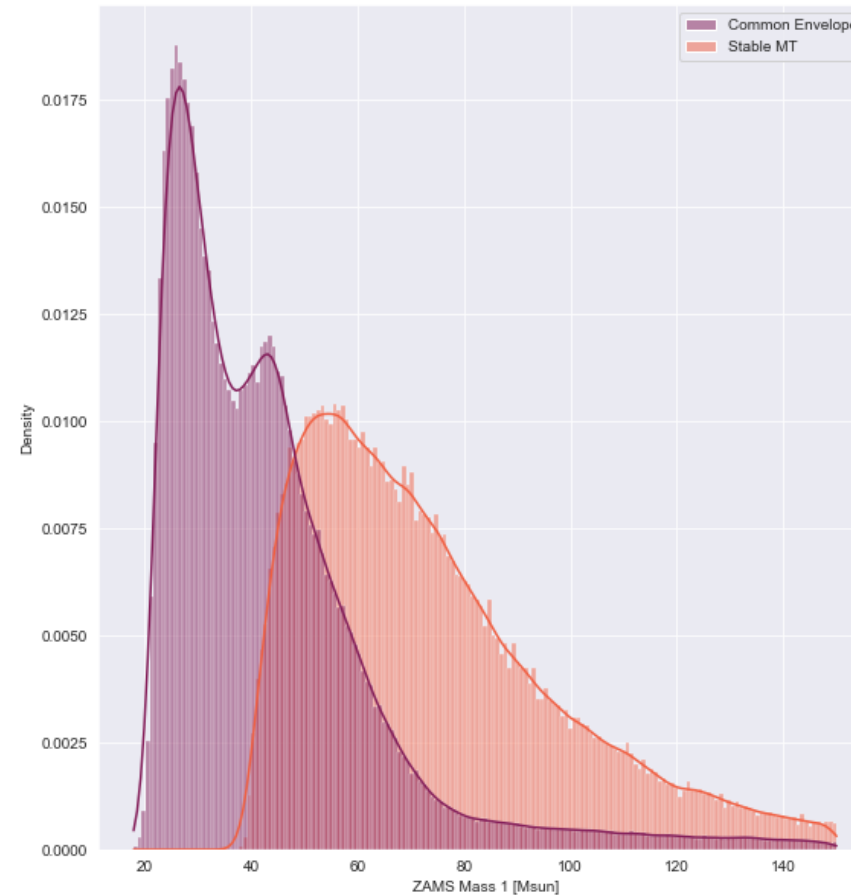
- Clear pattern
- CE – SMT boundary at around 40[Msun]

Secondary mass:

- Overlapping distributions



Problems with **machine learning** algorithms



Probability density of events for Mass 1 and Mass 2

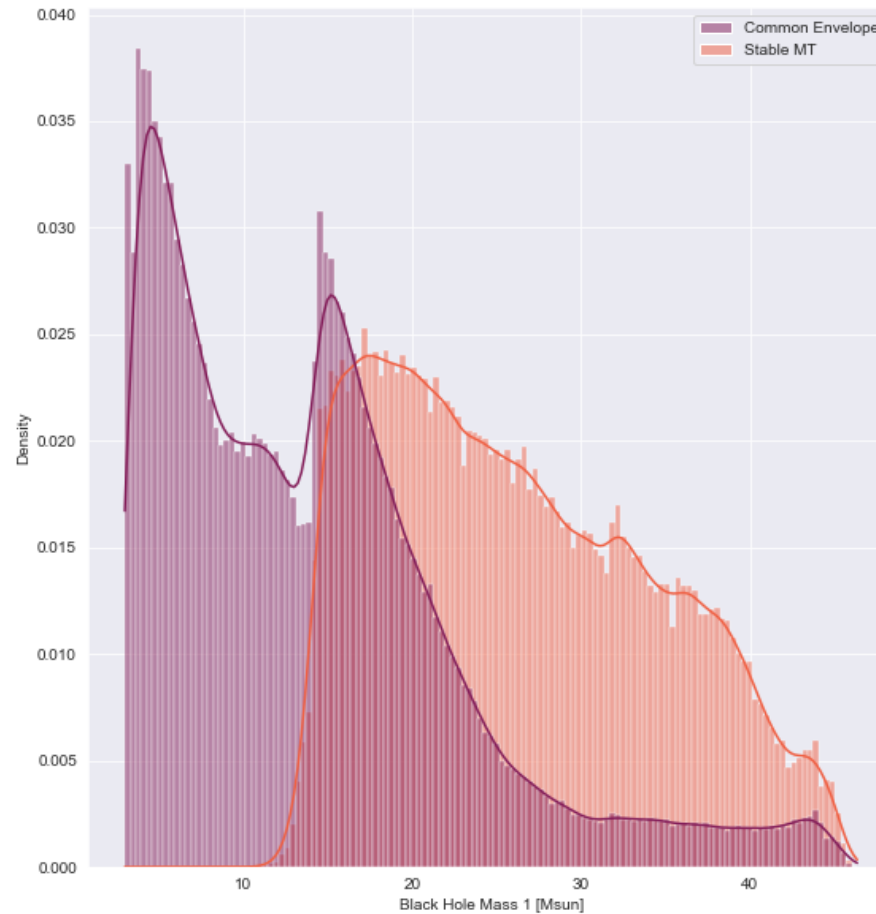
BBH masses considerations



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

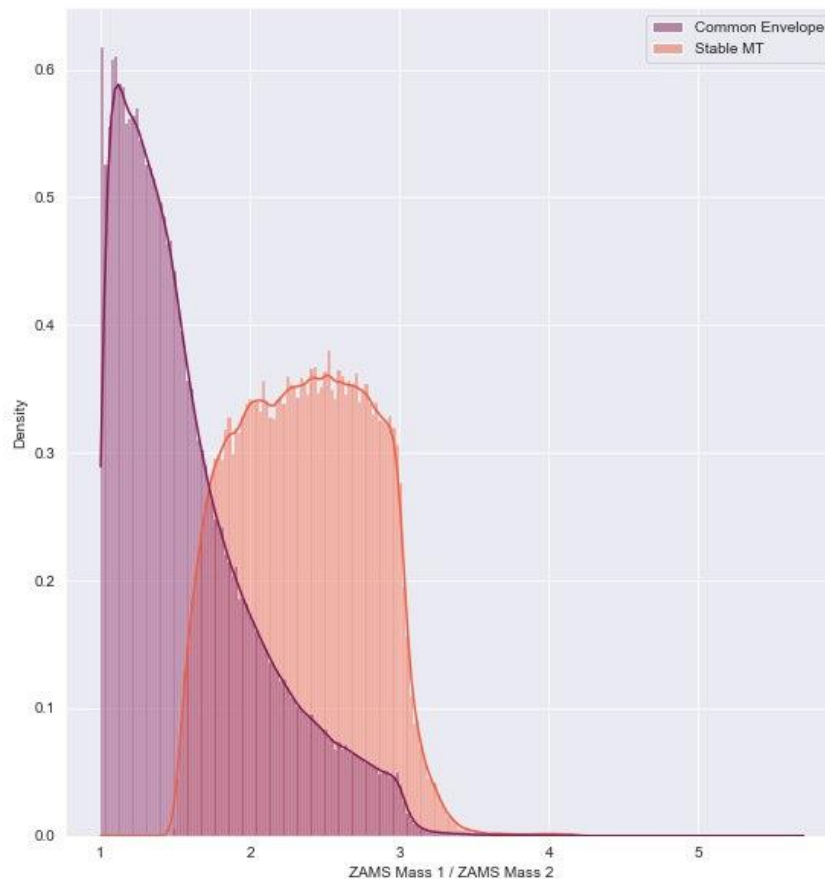


$$Q = \frac{ZAMS\ Mass\ 1}{ZAMS\ Mass\ 2}$$

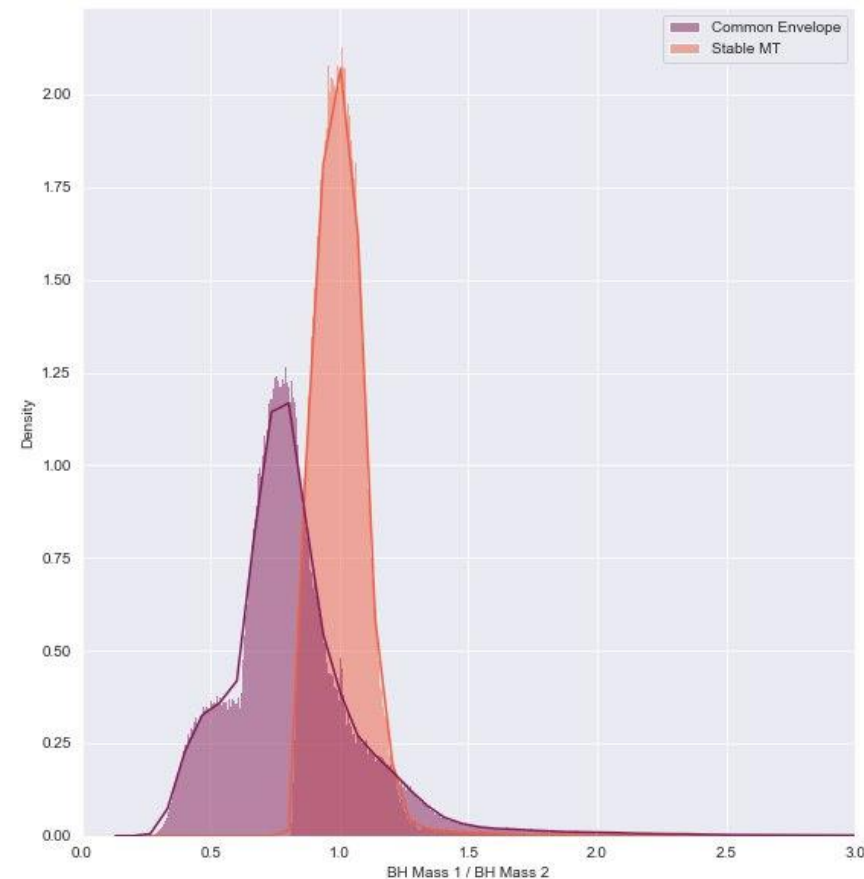
$$BHQ = \frac{Black\ Hole\ Mass\ 1}{Black\ Hole\ Mass\ 2}$$

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

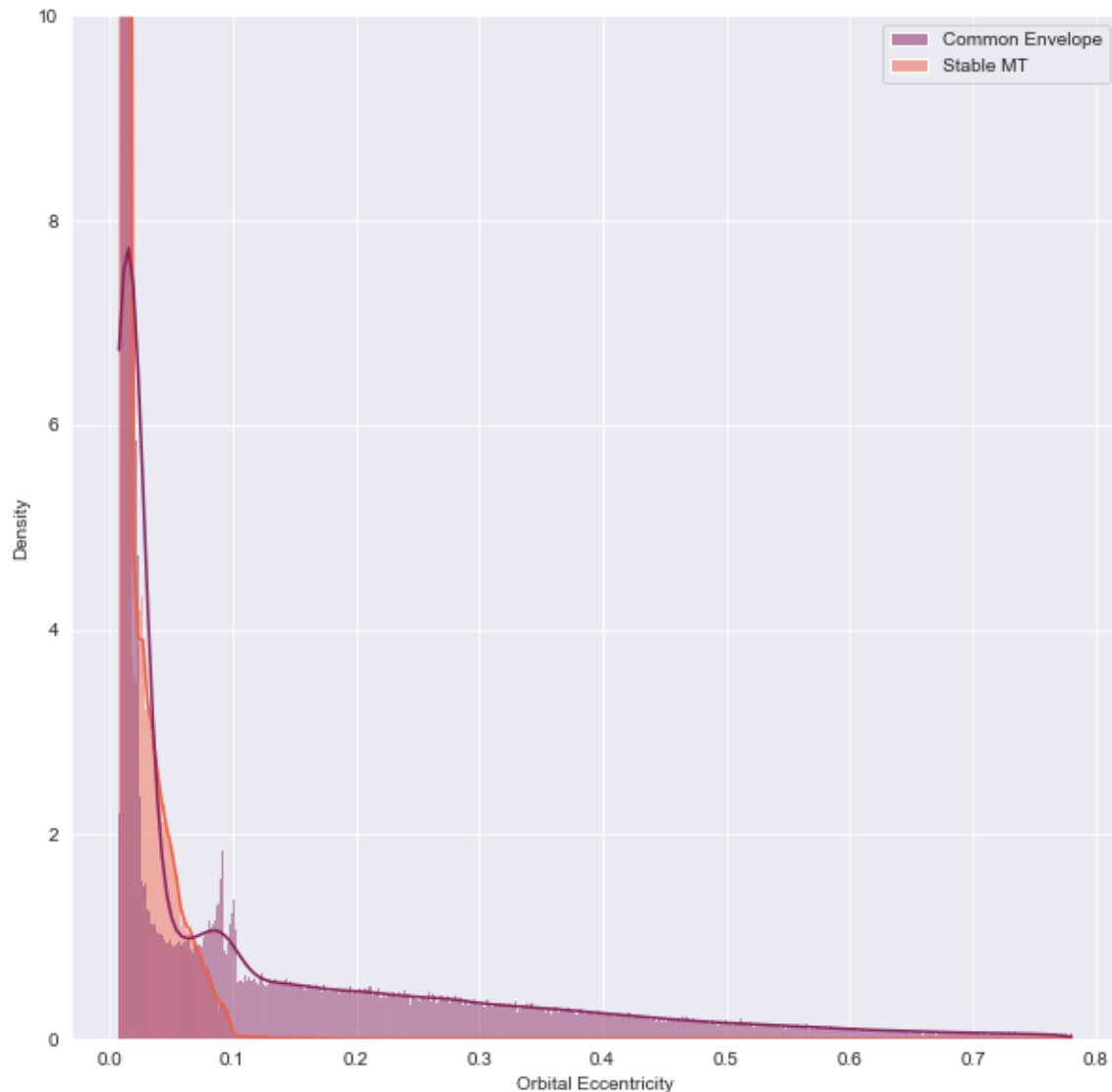
Q and BHQ show a good separation between the two classes and a small std



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

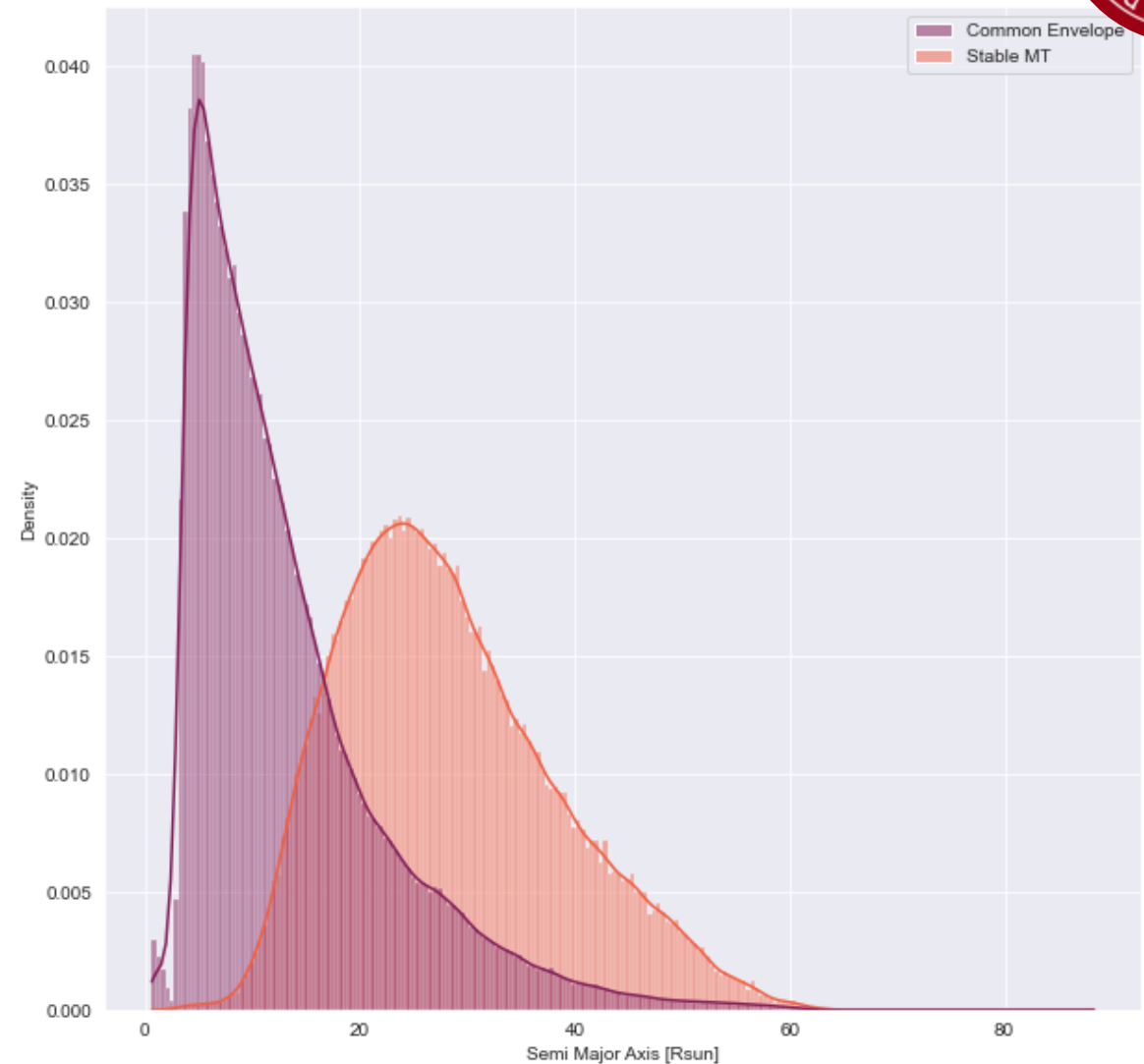
Semi Major Axis



Low orbital separation



Common envelope more likely



Probability density of events for Semi Major Axis

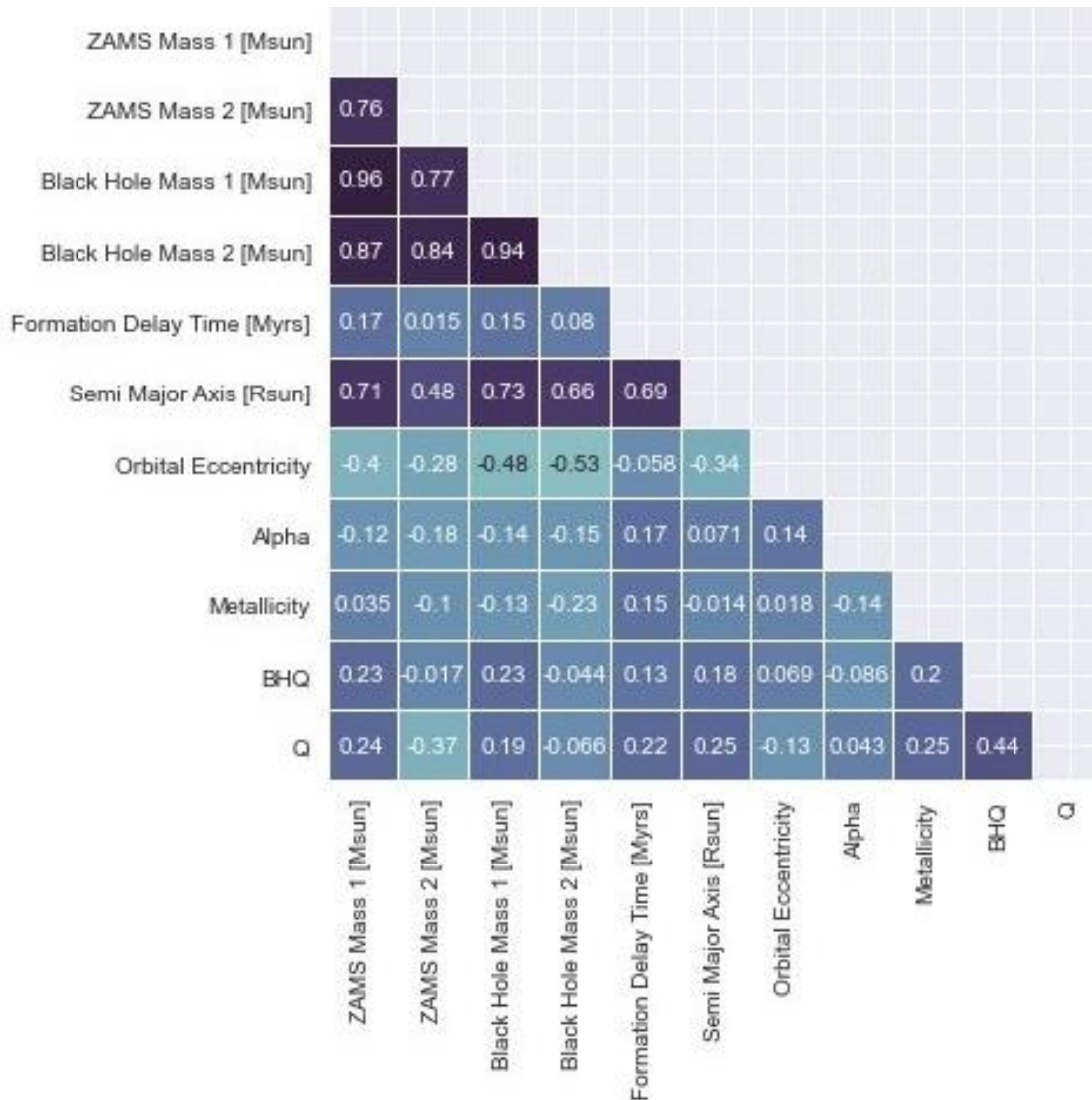
Dataset



▪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



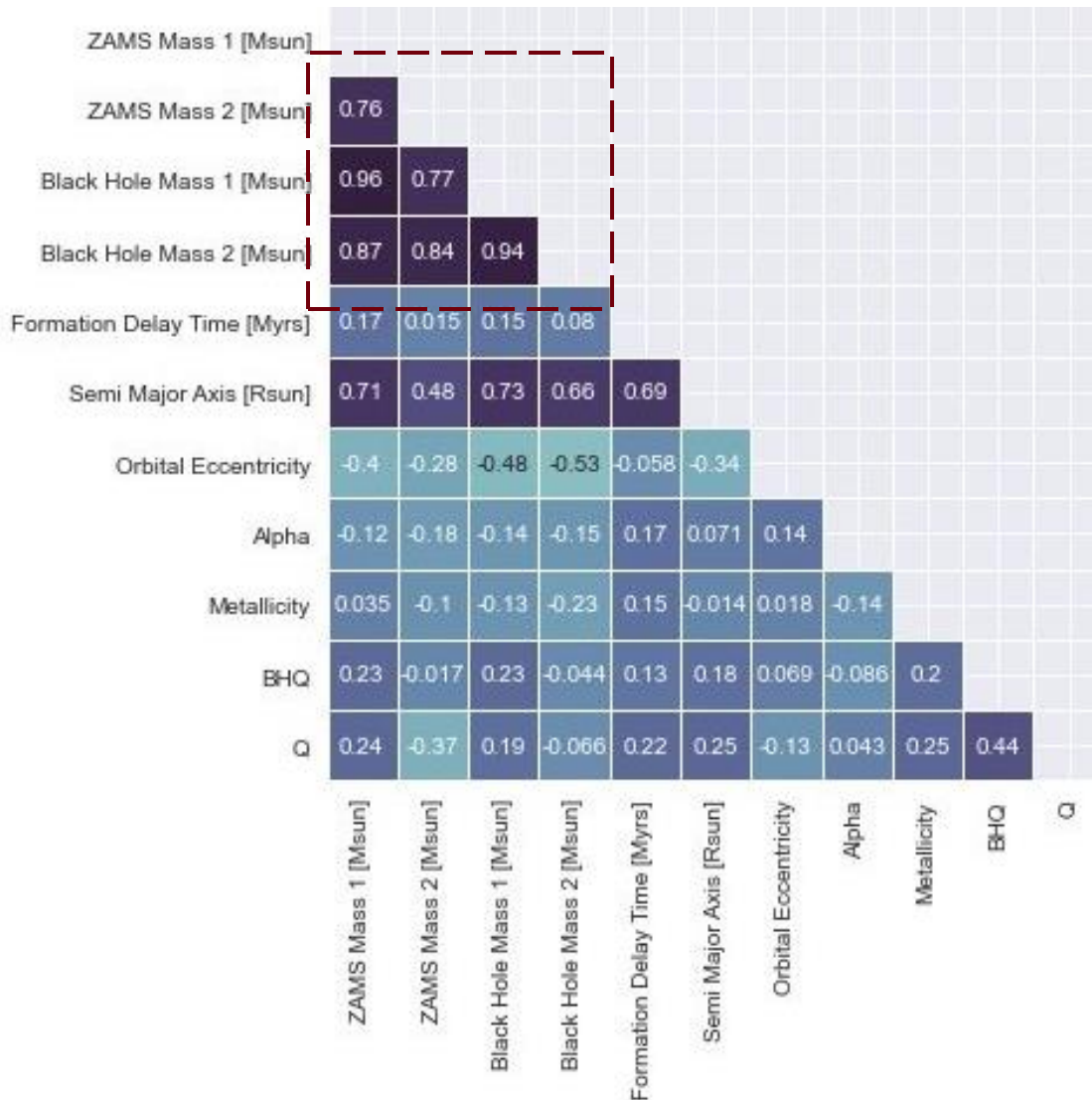
Feature correlation matrix

Masses are **highly correlated**



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

Correlation matrix



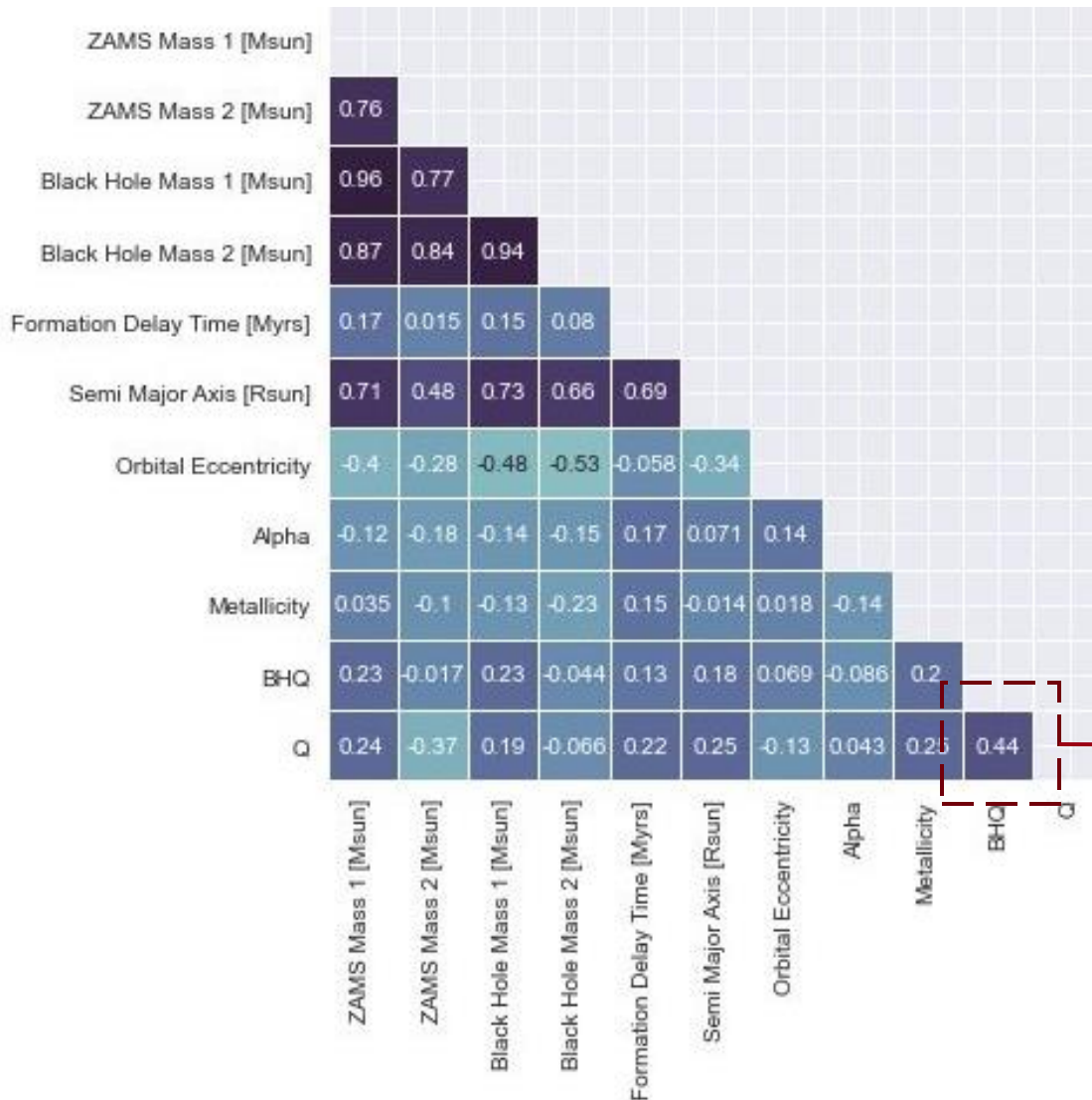
Feature correlation matrix

Masses are **highly correlated**



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

Correlation matrix



Feature correlation matrix

Masses are **highly correlated**

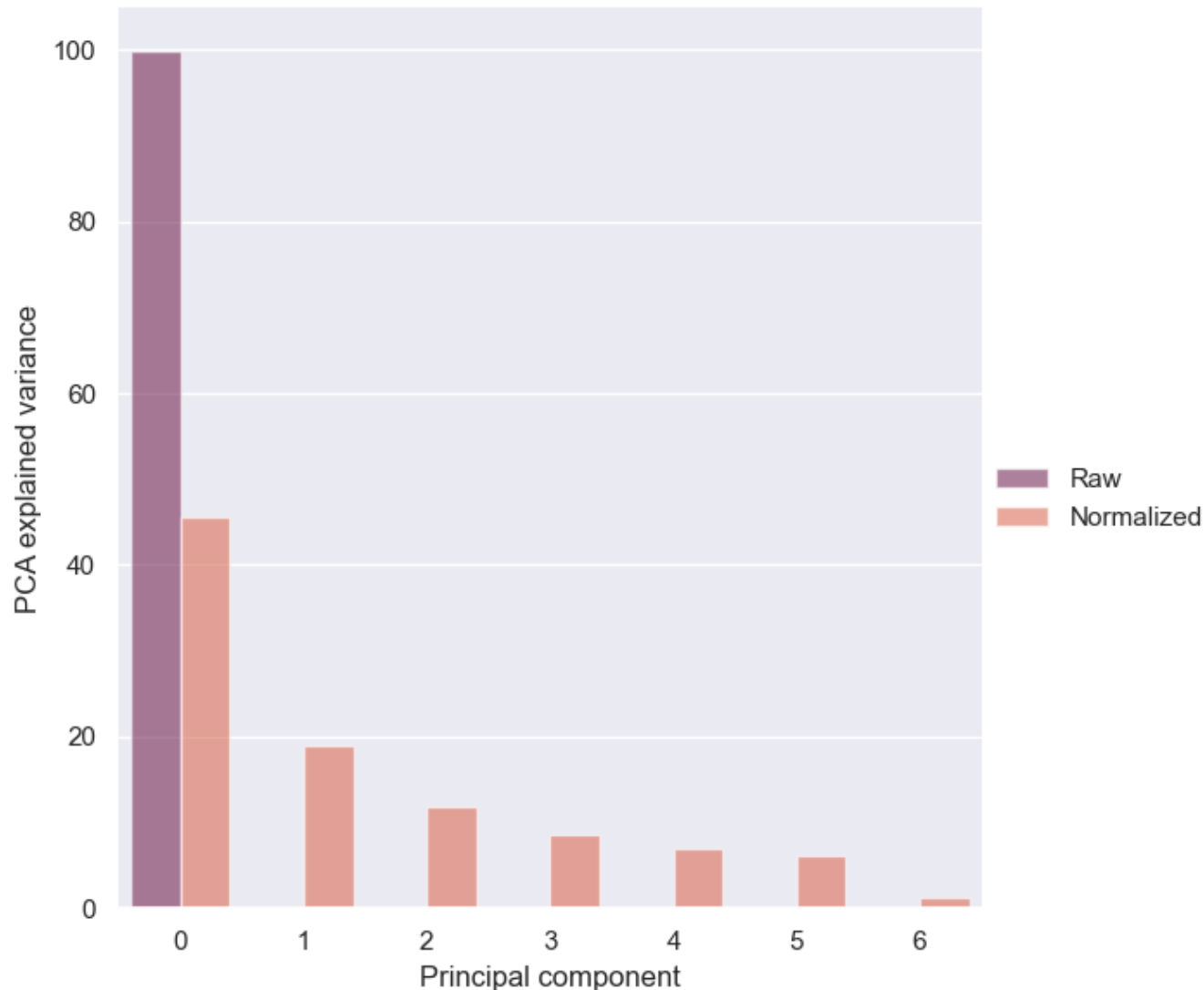
This could **negatively affect** prediction of the feature importances

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

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

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

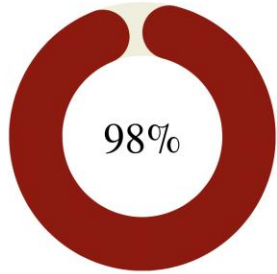
Feature-dropping: change in model score when a single **feature is removed**

Every time the model is retrained

Disadvantage:

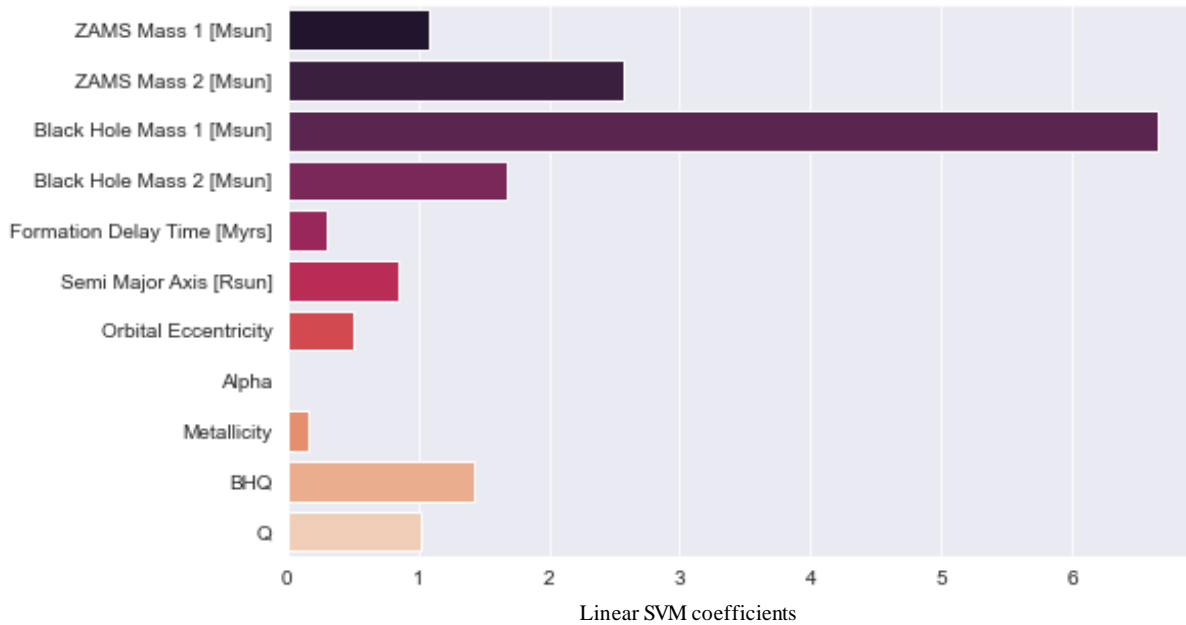
- Long calculation time
- Larger algorithm complexity

Linear SVM

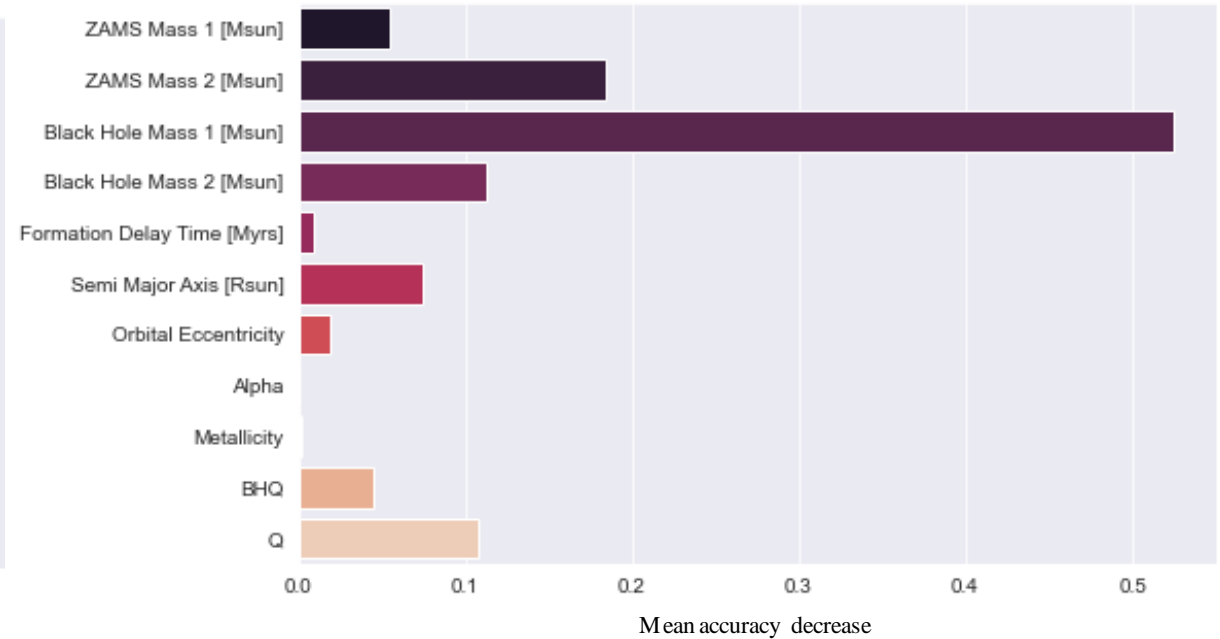
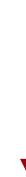


Accuracy

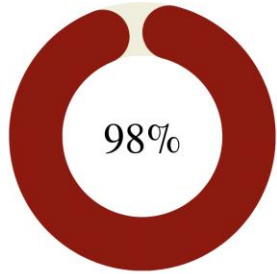
SVM coefficients



Feature permutation



Linear SVM

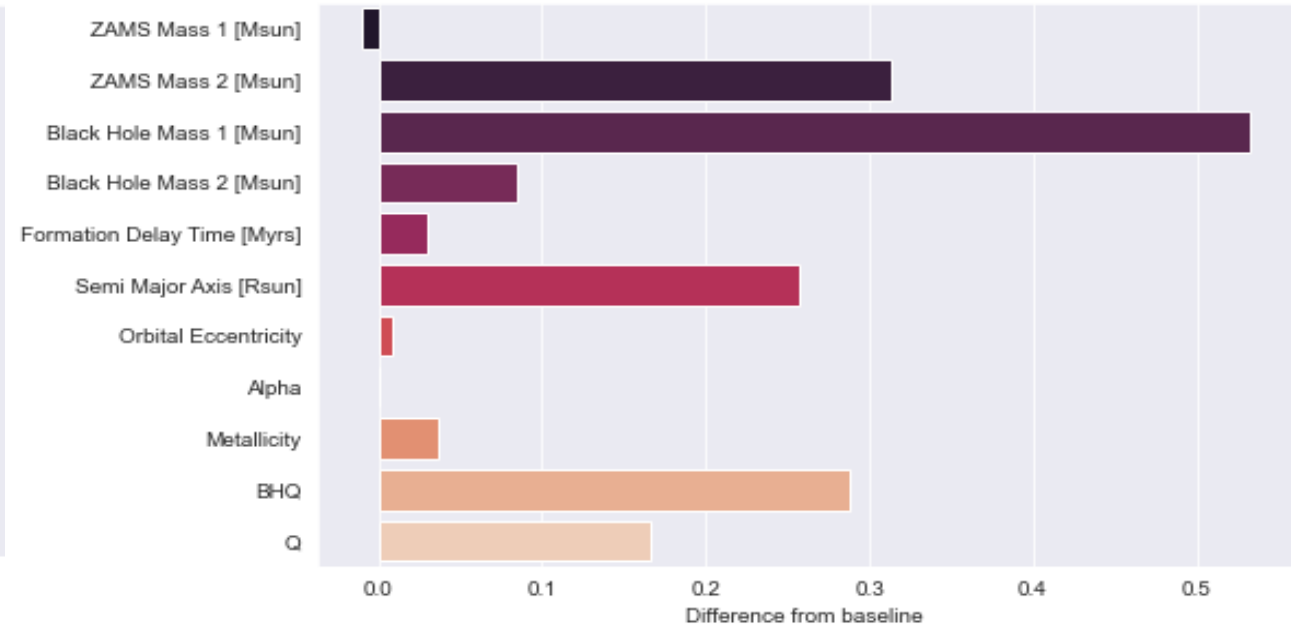
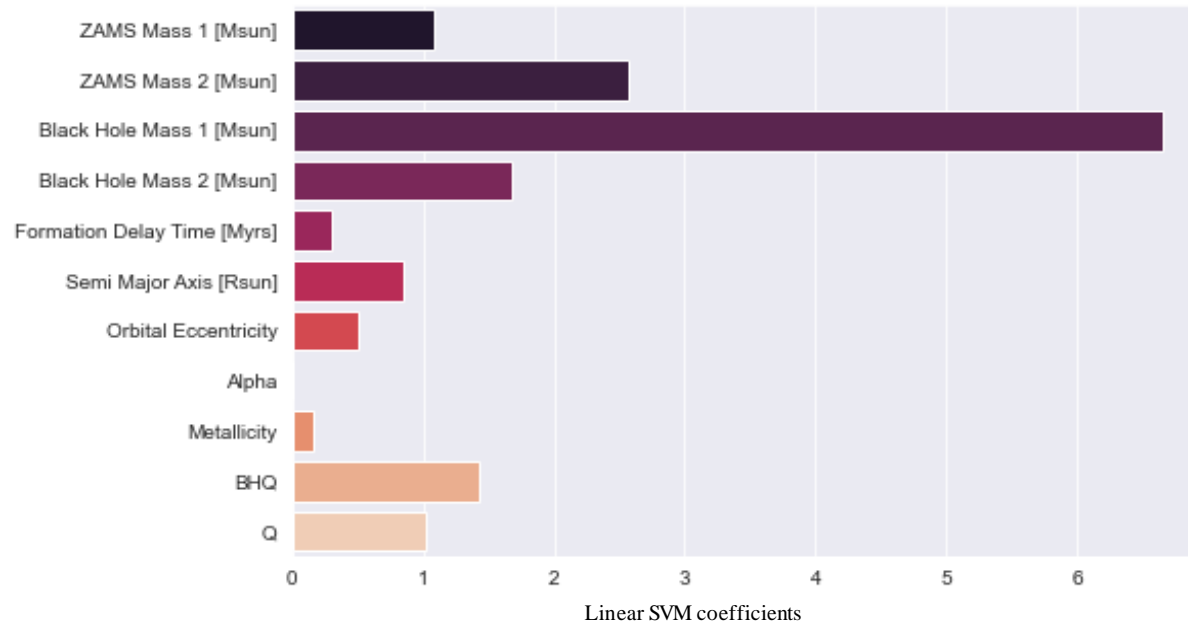


Accuracy

SVM coefficients



Feature-dropping

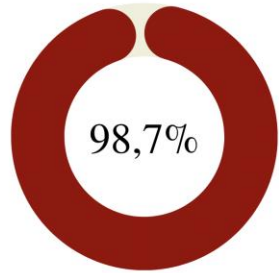


Linear SVM: ranking



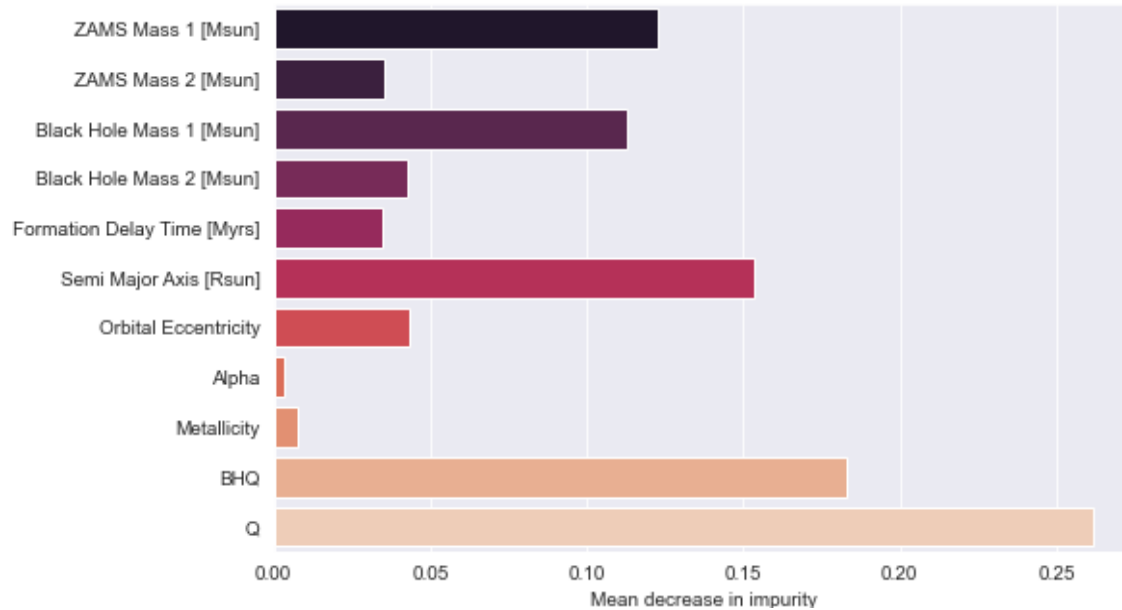
Ranking	Linear SVM	Feature permutation	Feature-dropping
1	BH Mass 1	BH Mass 1	BH Mass 1
2	ZAMS Mass 2	ZAMS Mass 2	ZAMS Mass 2
3	BH Mass 2	BH Mass 2	BHQ
10	Metallicity	Metallicity	Orbital eccentricity
11	Alpha	Alpha	Alpha

Random Forest

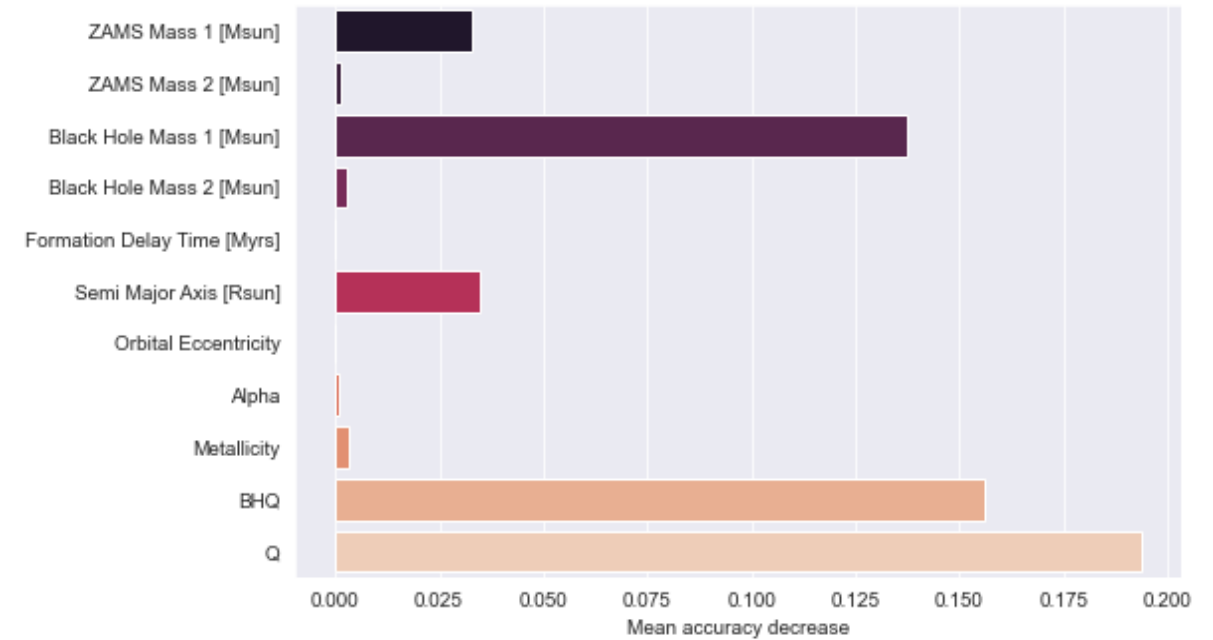


Accuracy

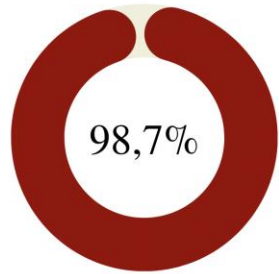
Mean Decrease in
Impurity



Feature permutation

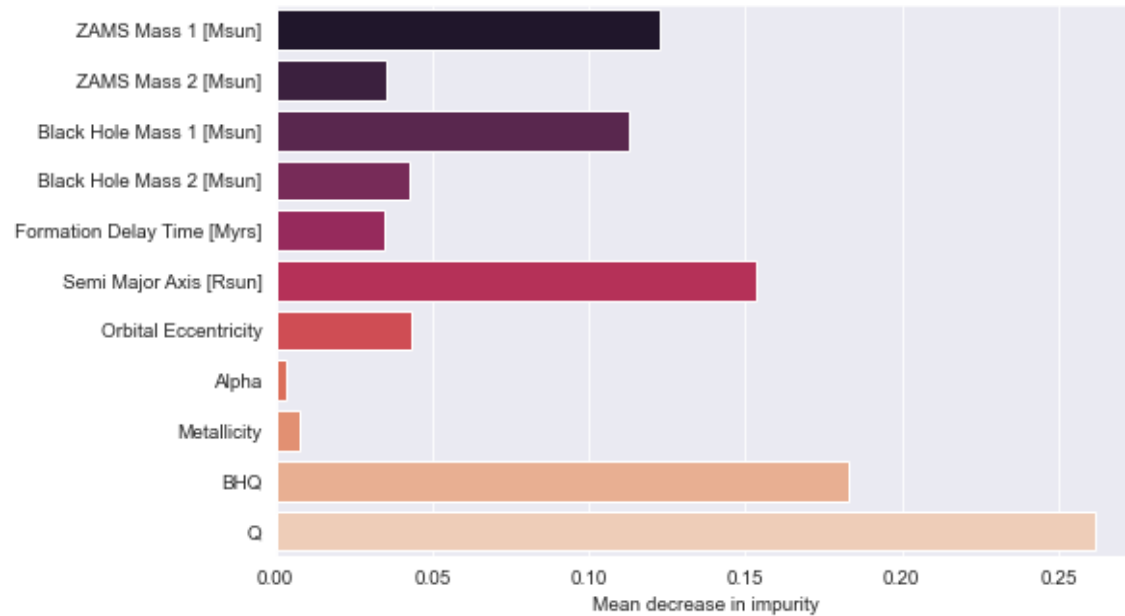


Random Forest

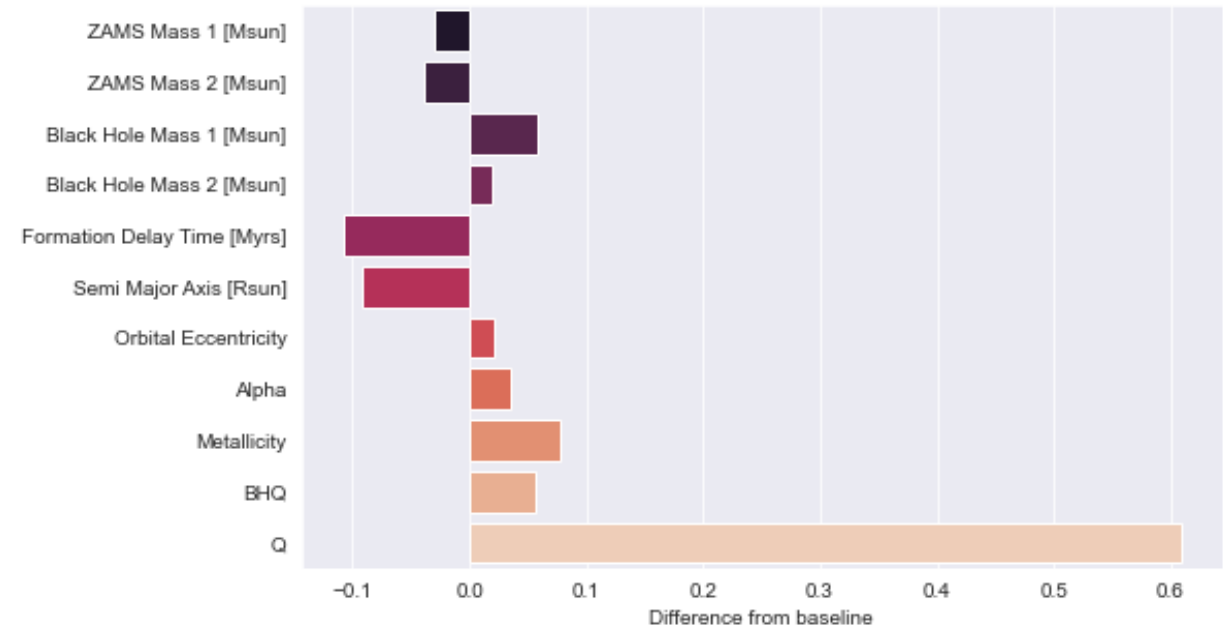


Accuracy

Mean Decrease in
Impurity



Feature-dropping

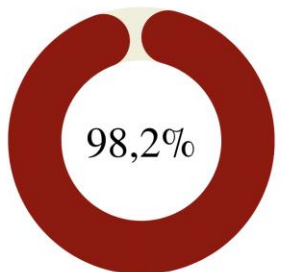
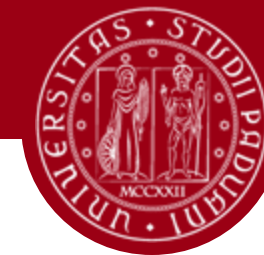


Random Forest: ranking



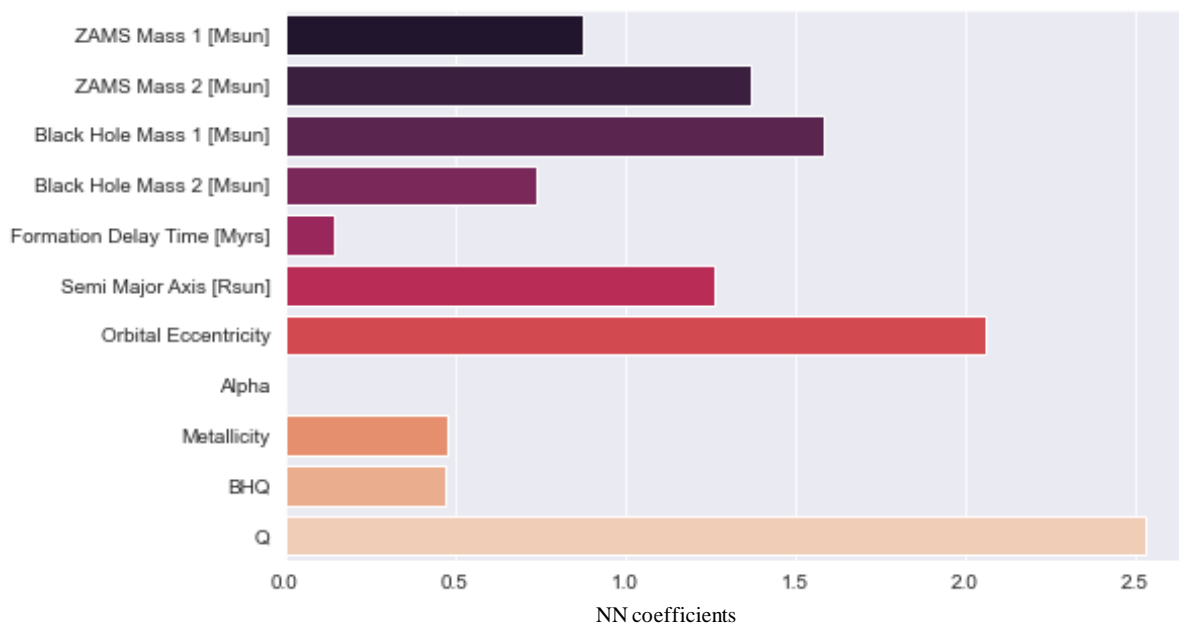
Ranking	MDI	Feature permutation	Feature-dropping
1	Q	Q	x
2	BHQ	BHQ	x
3	Semi-major axis	BH Mass 1	x
10	Metallicity	Formation delay time	x
11	Alpha	Orbital eccentricity	x

Neural Network

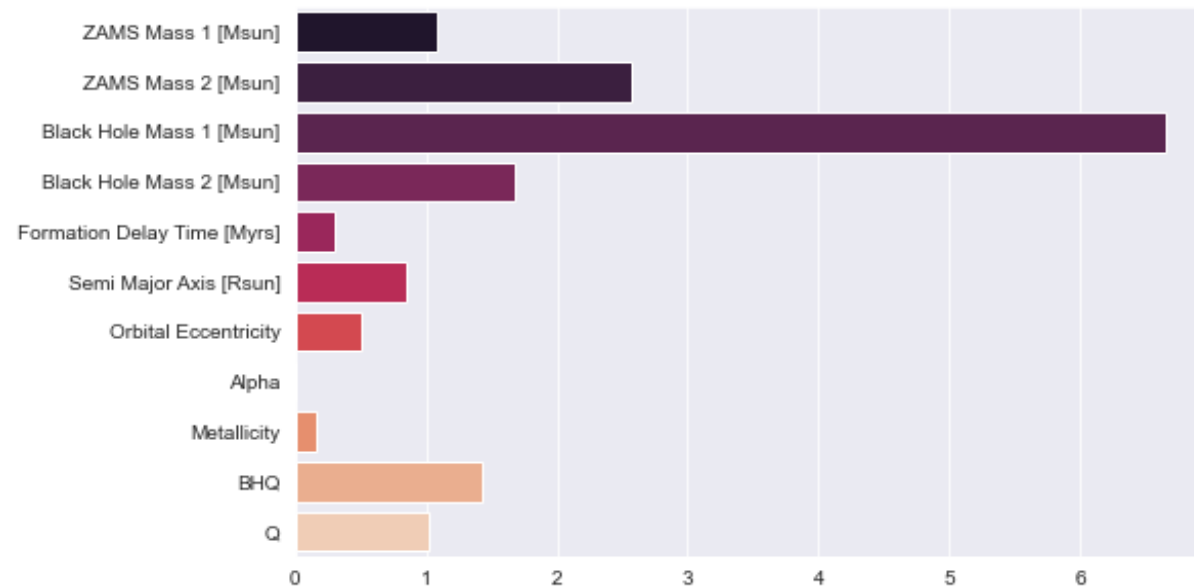


Accuracy

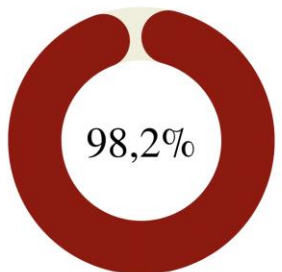
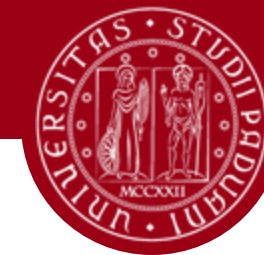
NN coefficients



Linear SVM coefficients

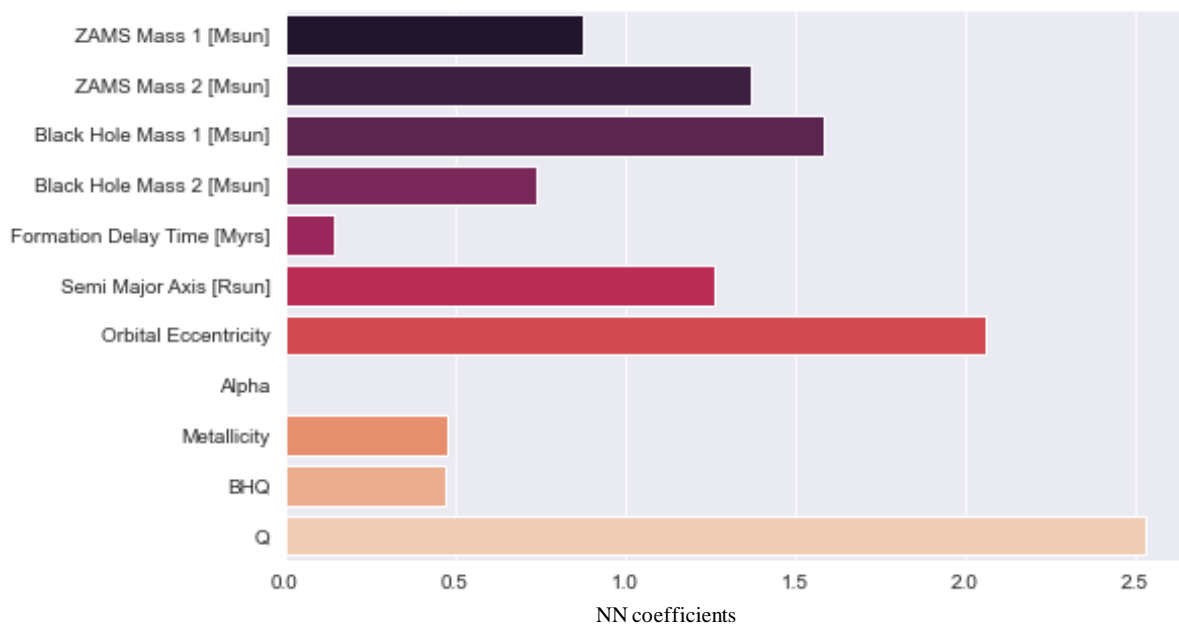


Neural Network

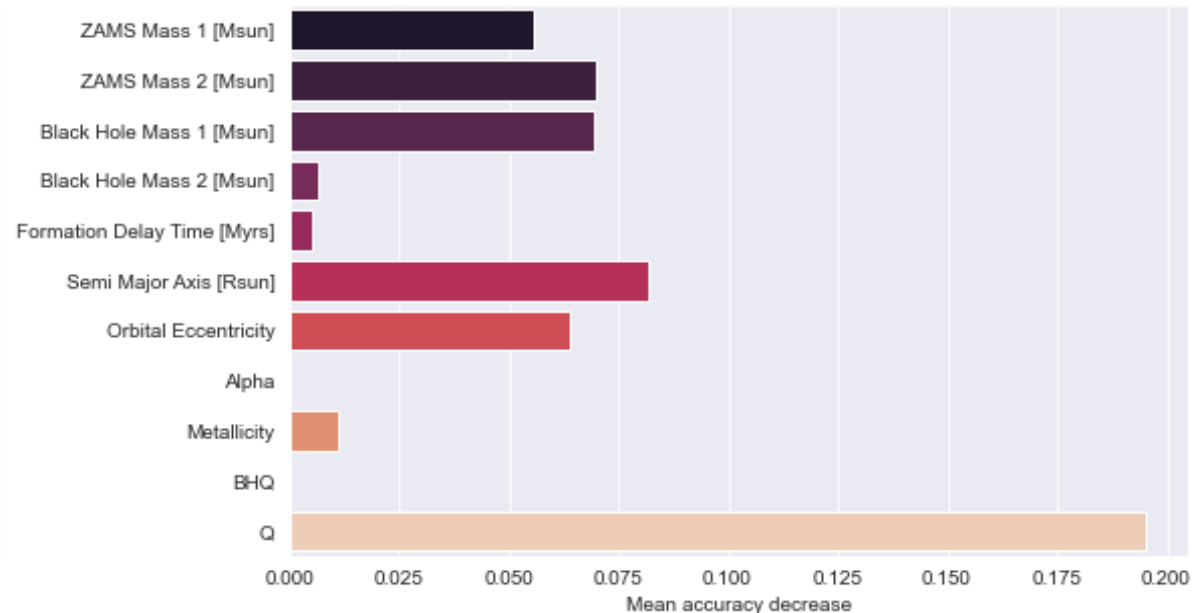


Accuracy

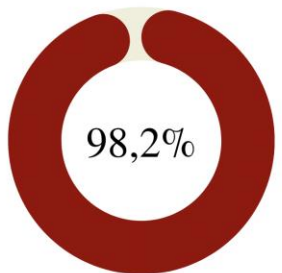
NN coefficients



Feature-permutation

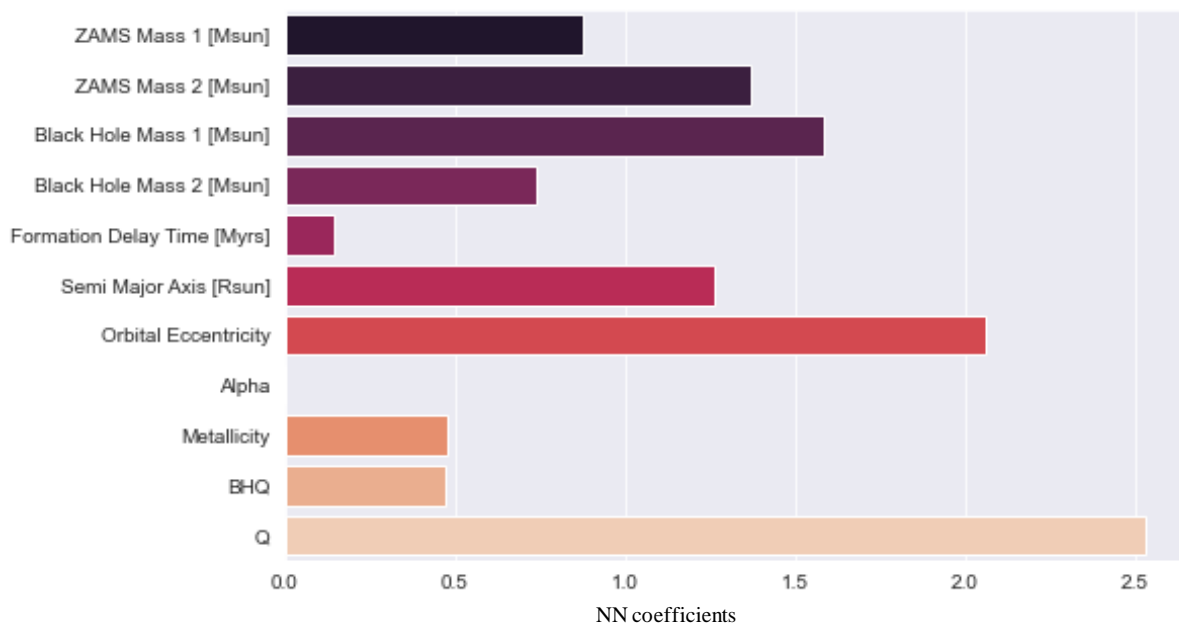


Neural Network

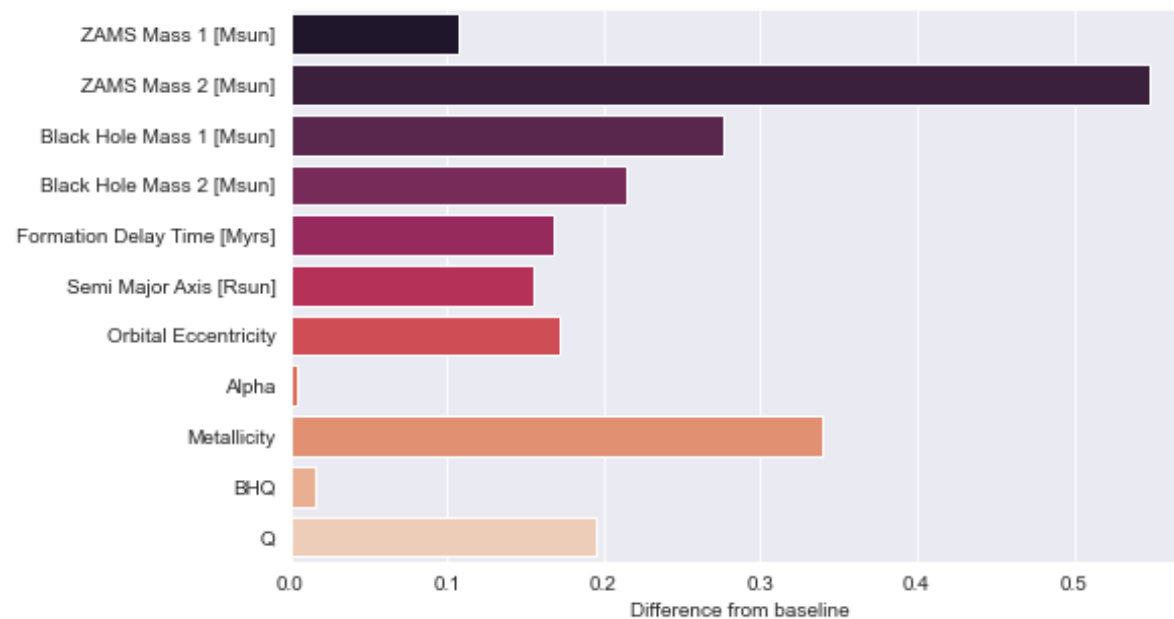


Accuracy

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 axisA diagram consisting of a large right-facing curly bracket on the left side of the list of features. A horizontal arrow points from the center of the bracket to the text '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



- **Most important features:**
 - Most important features --> masses (alone or ratios)
 - Least important features --> Metallicity (metal-poor stars) ; Alpha parameter
-

Conclusion



- Show all results in the same slide
- Do the models agree with each other?
- If yes, do they produce the expected results?
- If no, why do we think they fail?

-Other ways of dealing with unbalanced dataset

<https://machinelearningmastery.com/tactics-to-combat-imbalanced-classes-in-your-machine-learning-dataset/>

-why theory?

-<https://towardsdatascience.com/all-about-feature-scaling-bcc0ad75cb35>