UNIVERSIDADE D
COIMBRA

Nuclear matter properties: Supervised Machine Learning Approach

Valéria Carvalho

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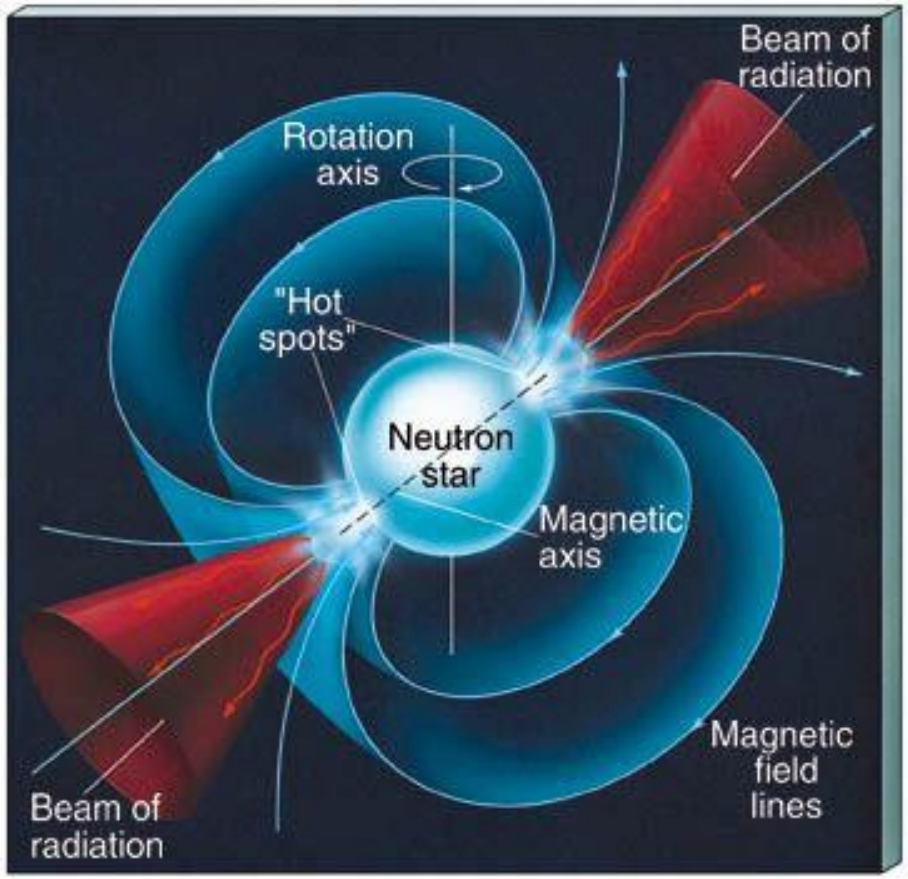
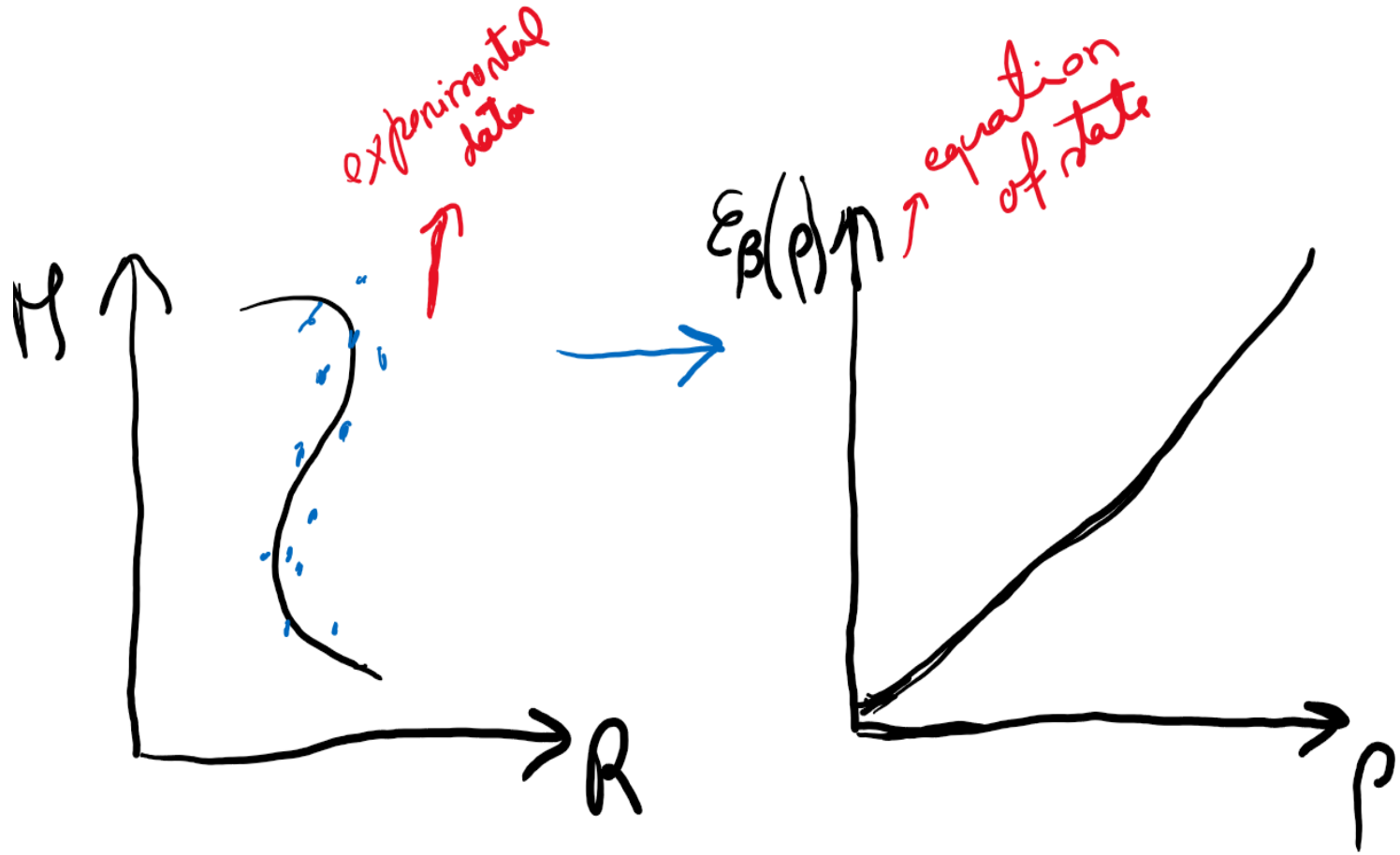
Statistical Data Analysis


Beam of radiation
Rotation axis
"Hot spots"
Neutron star
Magnetic axis
Magnetic field lines
Beam of radiation


experimental data
equation of state
M
R
ε(ρ)
ρ

How things work

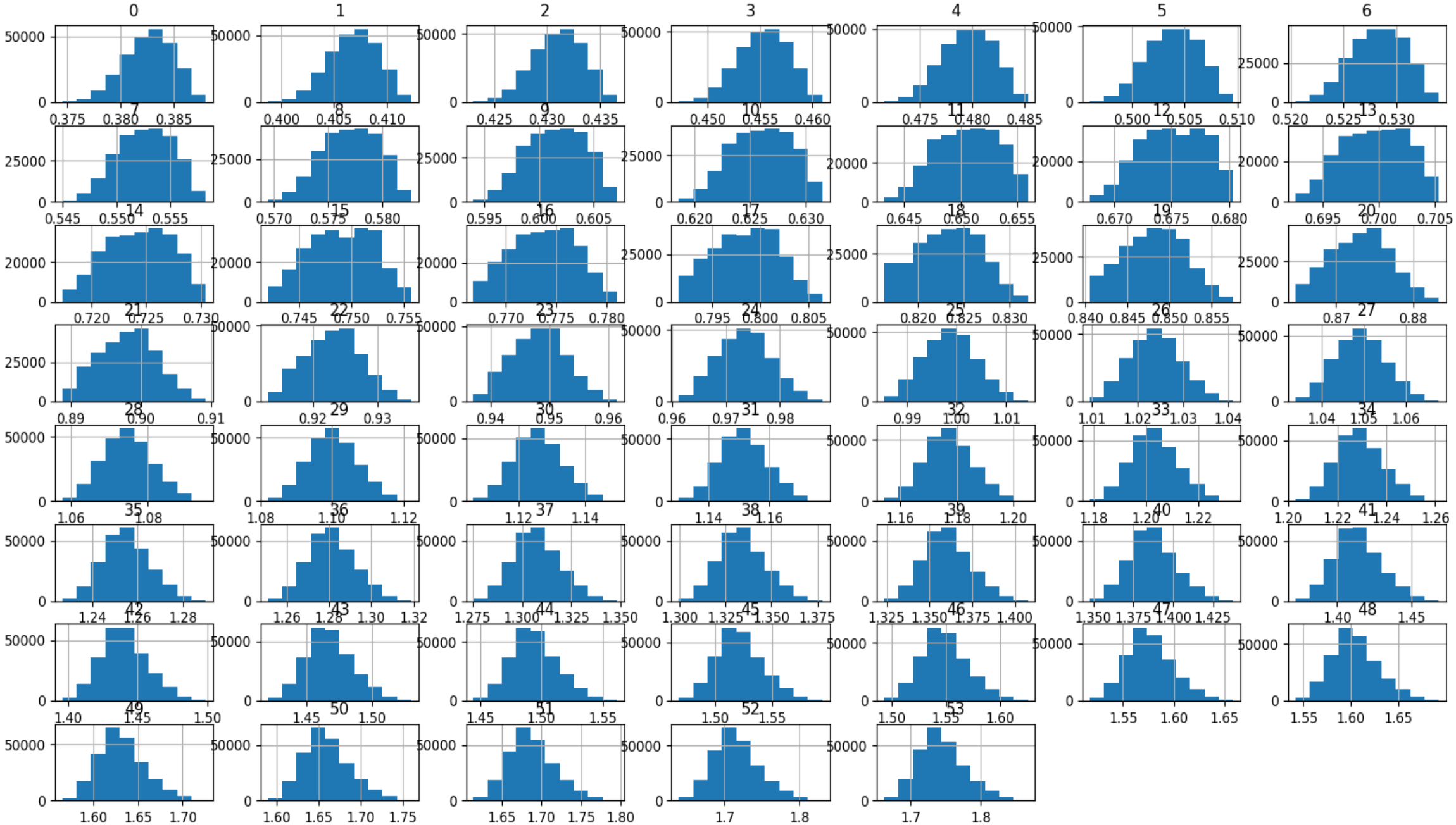
$$\varepsilon_{nuc}(\rho) = E_0 + \frac{1}{2}K_0(\frac{\rho-\rho_0}{3\rho_0})^2 + \frac{1}{6}J_0(\frac{\rho-\rho_0}{3\rho_0})^3 + \frac{1}{24}Z_0(\frac{\rho-\rho_0}{3\rho_0})^4 +$$

$$\left(E_{sym} + Lsym(\frac{\rho-\rho_0}{3\rho_0}) + \frac{1}{2}K_{sym}(\frac{\rho-\rho_0}{3\rho_0})^2 + \frac{1}{6}Q_{sym}(\frac{\rho-\rho_0}{3\rho_0})^3 + \frac{1}{24}Z_{sym}(\frac{\rho-\rho_0}{3\rho_0})^4\right)\left(\frac{(\rho_n-\rho_p)}{(\rho_n+\rho_p)}\right)$$

$$\varepsilon_\beta(\rho;\mathbf{w}) = \rho\left(\mathcal{E}_{nuc}(\rho,\delta;\mathbf{w}) + \bar{m}_N\right) + \varepsilon_{lep}(\rho,\delta;\mathbf{w}),$$

$$\mathbf{x}_i = [\mathcal{E}_\beta(\rho_1), \mathcal{E}_\beta(\rho_2), \mathcal{E}_\beta(\rho_3), \cdots, \mathcal{E}_\beta(\rho_N)]^T \quad [N \times 1]$$

w= $\mathbf{y}_i = [\rho_0, E_0, K_0, J_0, Z_0, E_{\rm sym}, L_{\rm sym}, K_{\rm sym}, Q_{\rm sym}, Z_{\rm sym}]^T \quad [10 \times 1]$


0
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
21
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42
43
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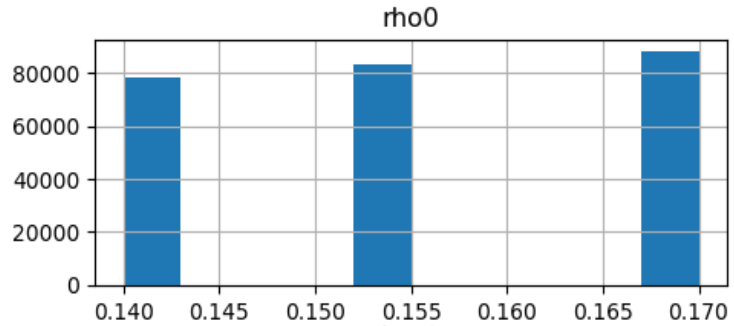
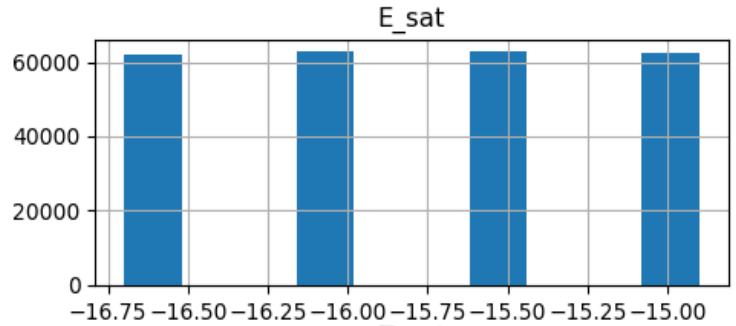
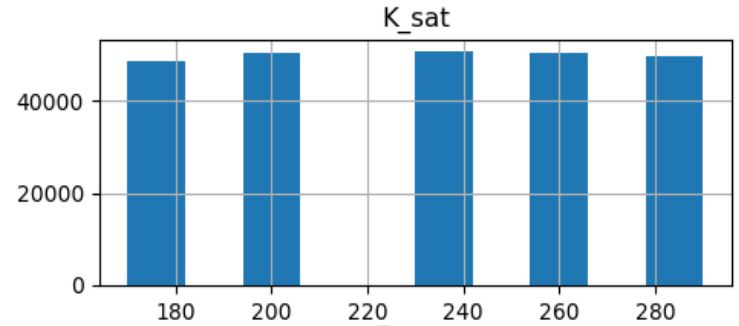
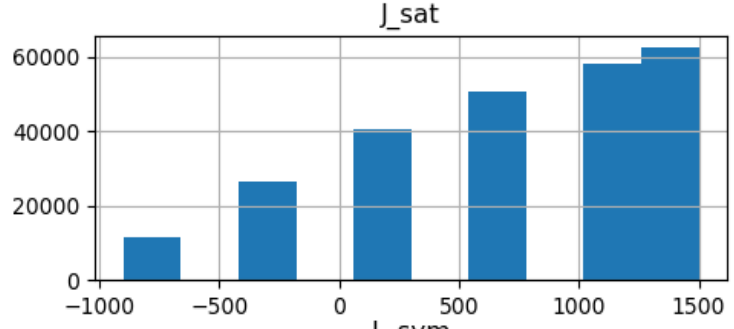
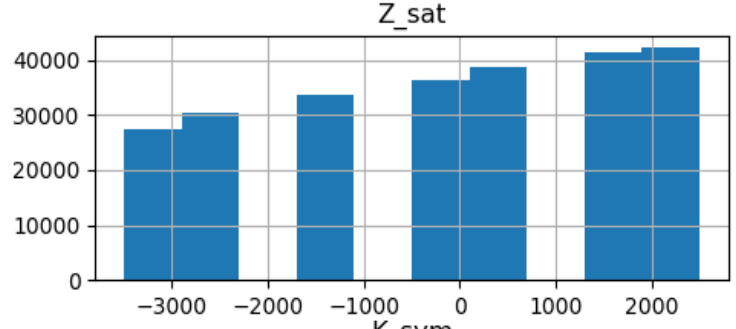
48
49
50
51
52
53

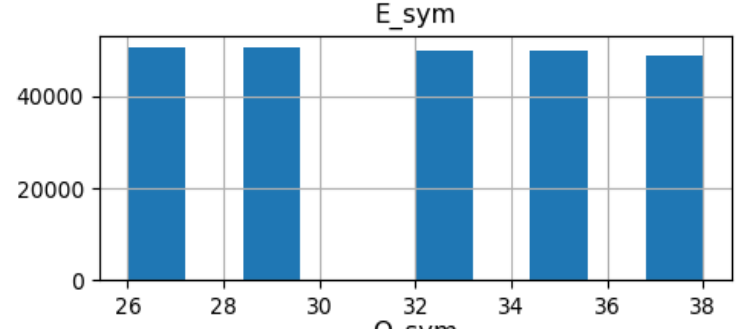

rho0
0
20000
40000
60000
80000
0.140
0.145
0.150
0.155
0.160
0.165
0.170

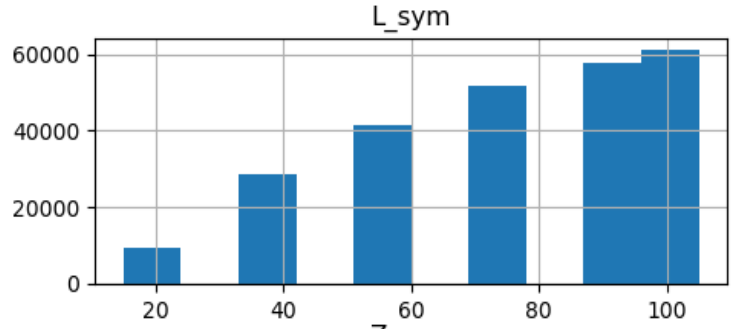

E_sat
0
20000
40000
60000
−16.75
−16.50
−16.25
−16.00
−15.75
−15.50
−15.25
−15.00

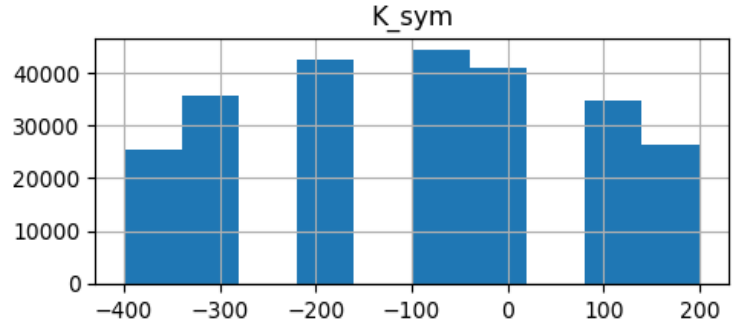

K_sat
0
20000
40000
180
200
220
240
260
280

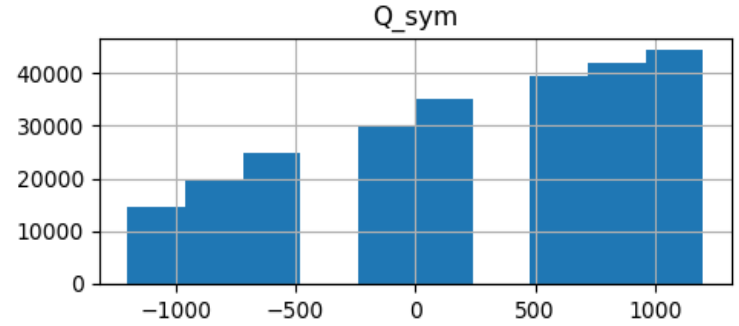

J_sat
0
20000
40000
60000
−1000
−500
0
500
1000
1500

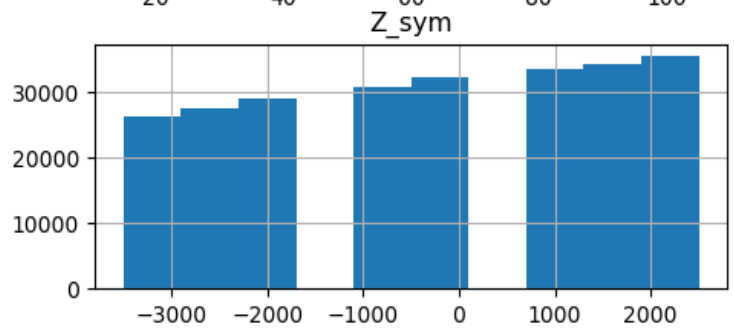

Z_sat
0
10000
20000
30000
40000
−3000
−2000
−1000
0
1000
2000

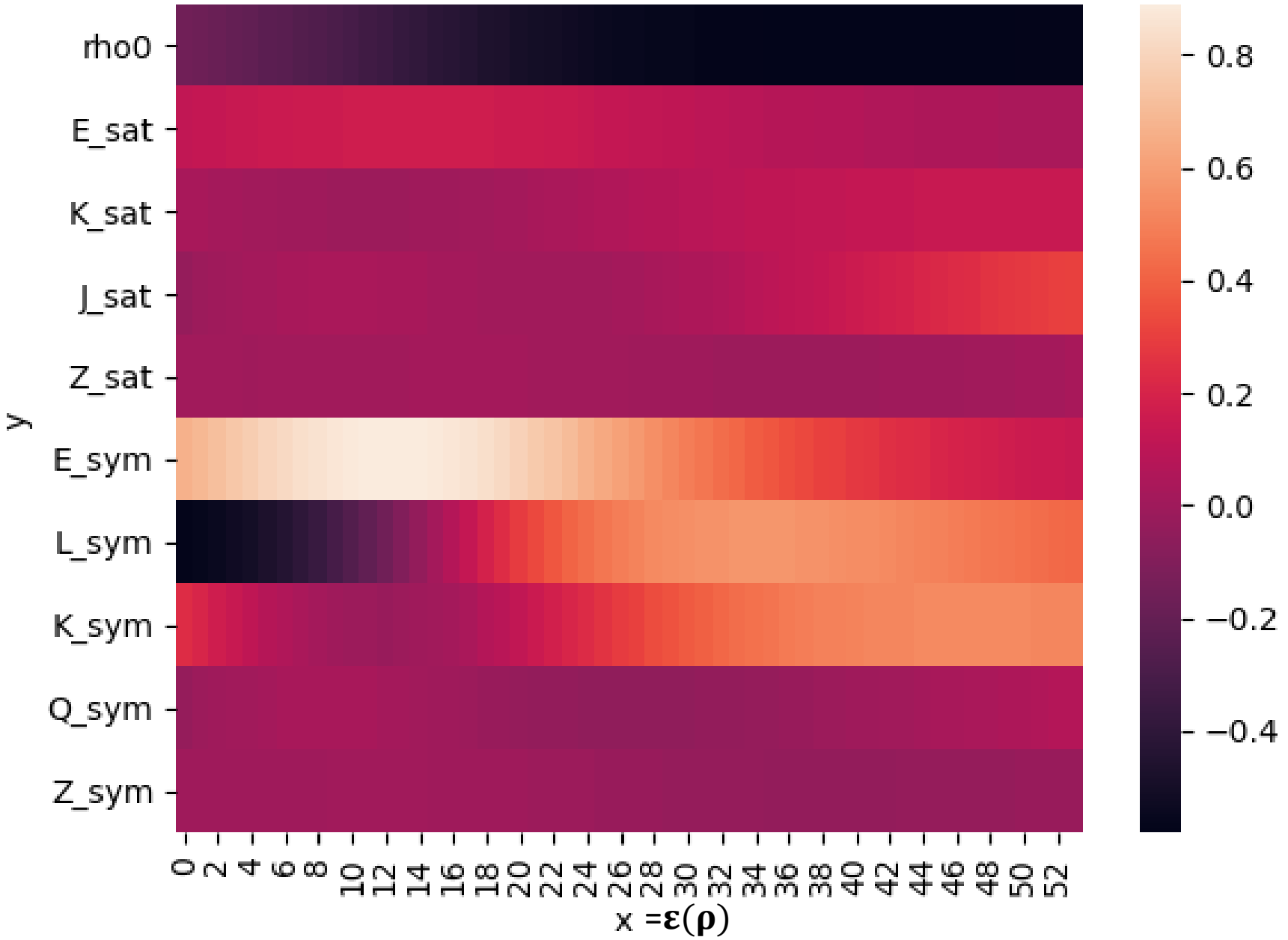

E_sym
0
20000
40000
26
28
30
32
34
36
38


L_sym
0
20000
40000
60000
20
40
60
80
100


K_sym
0
10000
20000
30000
40000
−400
−300
−200
−100
0
100
200


Q_sym
0
10000
20000
30000
40000
−1000
−500
0
500
1000


Z_sym
0
10000
20000
30000
−3000
−2000
−1000
0
1000
2000


Heatmap of all features without correlation values
rho0
E_sat
K_sat
J_sat
Z_sat
E_sym
L_sym
K_sym
Q_sym
Z_sym
y
0 2 4 6 8 10 12 14 16 18 20 22 24 26 28 30 32 34 36 38 40 42 44 46 48 50 52
x =ε(ρ)
0.8
0.6
0.4
0.2
0.0
−0.2
−0.4

Normalization of the data

Index	model	RMSE	MAE	loss	epoch
0	y_norm_stand.|x_standardized	608.2345998287	268.1045037466	[0.22293197 0.22293197]	1233
1	y_normalized|x_normalized	1253.1543181558	637.8255659247	[0.14080147 0.14080147]	2403
2	y_standardized|x_standardized	608.2345994032	268.1045038949	[0.22293197 0.22293197]	1233
3	y_normalized|x_standardized	666.6807056856	302.9693430133	[0.03010081 0.03010081]	683
4	unscaled	933.7910585497	480.3372874785	[871965.5 871965.5]	1770

Grid search :

→ Batch grid -> 100;
→Epochs -> 100-300;

For 0.2GB of data:

- 4 hidden layers ;
- 3 different values for neurons=[80,100,140];
- 3 active functions: ['tanh', 'relu', 'sigmoid’];
- 7380 combinations.

For the 16.5 GB of data:

- The best 40 combinations.

Best seven values for big data

HL	Active_function	Nodes	val_MSE	val_MAE	Loss_MSE
4	('tanh', 'tanh', 'sigmoid', 'sigmoid')	(140, 140, 140, 100)	0.121150516	0.2010177672	0.1374571621
4	('tanh', 'tanh', 'sigmoid', 'sigmoid')	(100, 140, 140, 140)	0.128176555	0.2095577121	0.1375417858
4	('tanh', 'tanh', 'sigmoid', 'sigmoid')	(100, 100, 140, 140)	0.1281408817	0.2115080357	0.1427749395
4	('tanh', 'tanh', 'tanh', 'sigmoid')	(100, 80, 140, 80)	0.1311056316	0.2115254998	0.1410267502
4	('tanh', 'tanh', 'sigmoid', 'tanh')	(140, 100, 100, 100)	0.1311052293	0.2145950049	0.145413354
4	('tanh', 'tanh', 'sigmoid', 'sigmoid')	(100, 100, 140, 80)	0.1368201971	0.216223225	0.1495948136
4	('tanh', 'tanh', 'sigmoid', 'tanh')	(100, 140, 80, 140)	0.1300683618	0.2164411396	0.1430959851

The best result was:

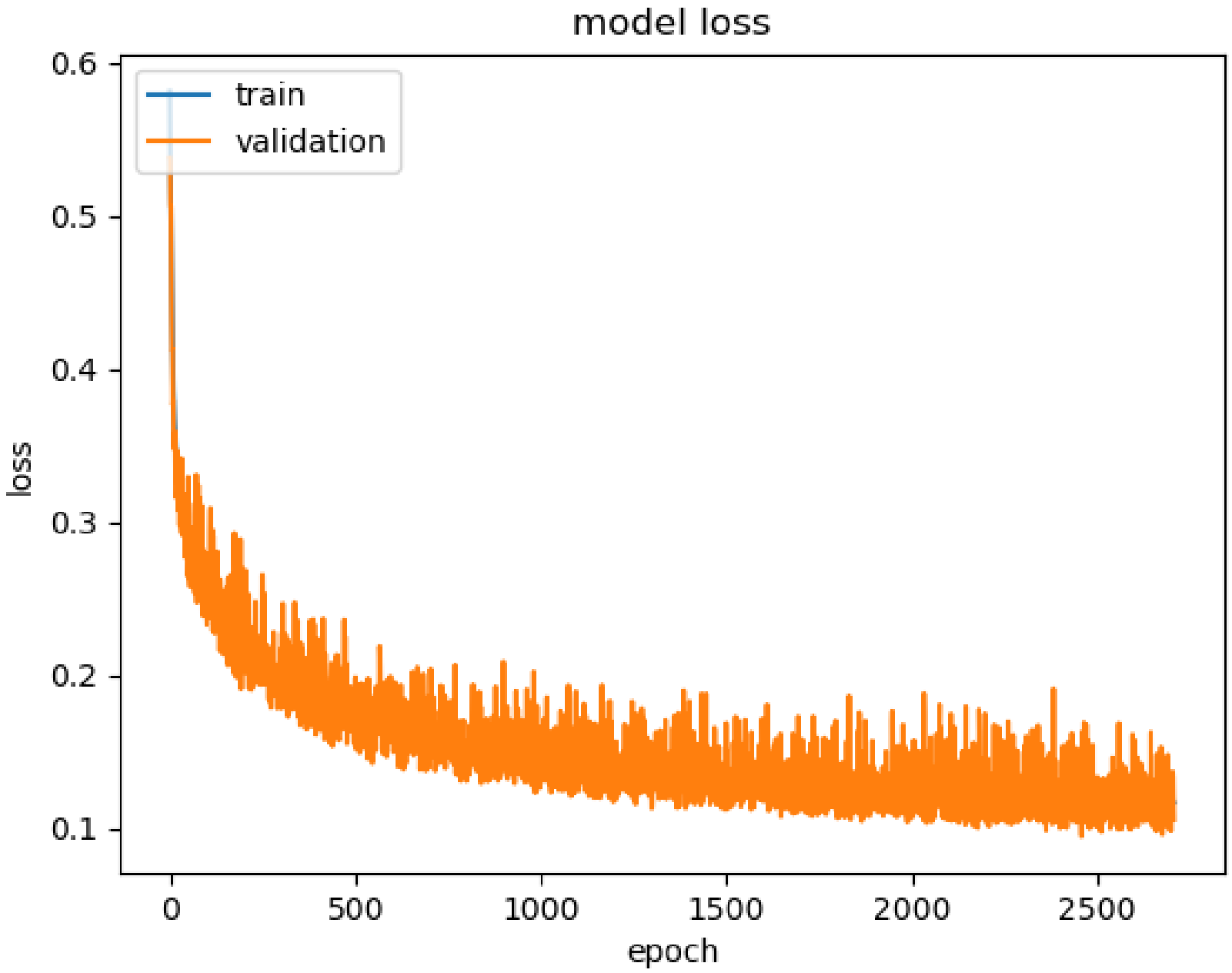
```
model.add(Dense(140, input_dim=xi.shape[1],acti.= 'tanh’))
model.add(Dense(140, activation= 'tanh'))
model.add(Dense(140, activation= 'sigmoid’))
model.add(Dense(100, activation= 'sigmoid'))
model.add(Dense(yi.shape[1], activation='linear'))
```

Best result:

Loss for the test set ->
0.10565873235464096

RMSE ->
488.7912724466753

MAE ->
206.65862626838552

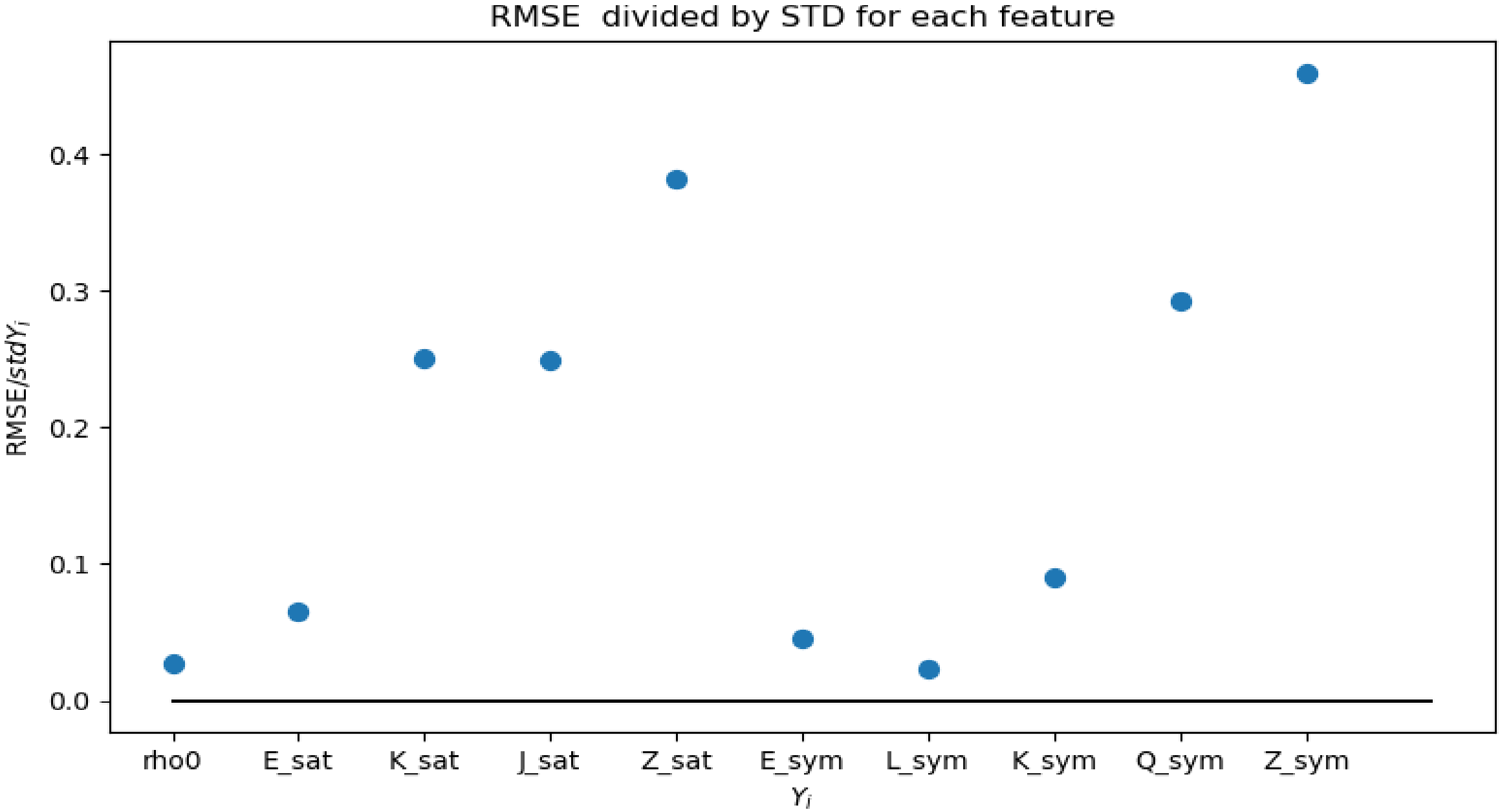


Best result – RMSE for each Y

- 0.00033452706578327 31 -> rho0
- 0.04336347443759167 -> E_sat
- 10.600287267671552 -> K_sat
- 177.2540943515378 -> J_sat
- 751.4311745041396 -> Z_sat
- 0.189389271800814 2 -> E_sym
- 0.588633086364825m -> L_sym
- 16.33575380026284 -> K_sym
- 213.23232978902993 -> Q_sym
- 896.910902604915 -> Z_sym

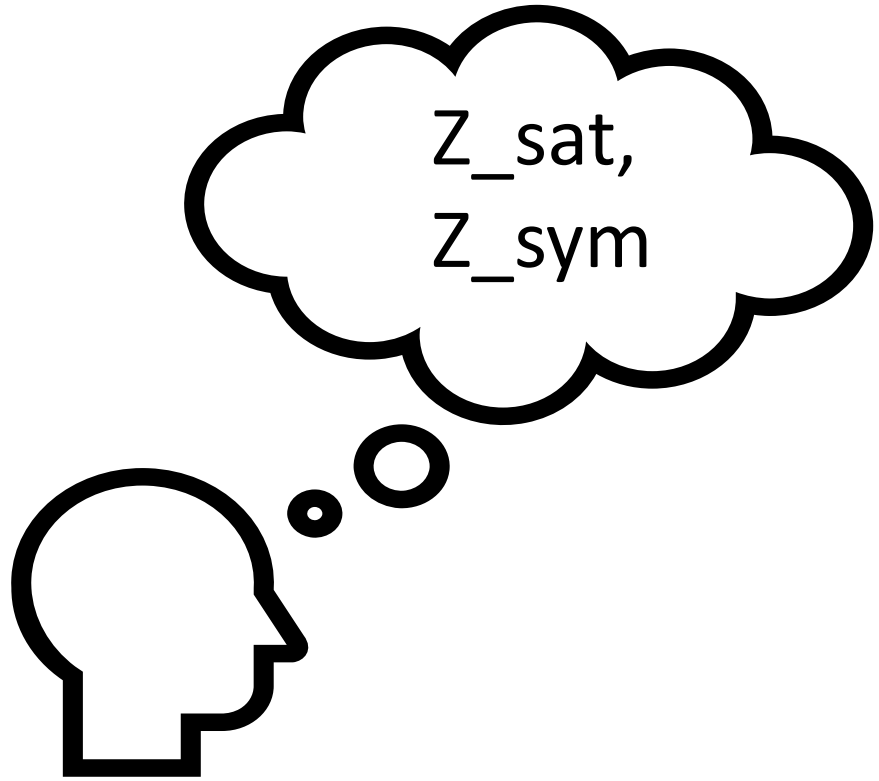
Best result – RMSE for each Y

- 0.0003345270657832731 -> rho0
- 0.0433634744375916 7 -> E_sat
- 10.600287267671552 -> K_sat
- 177.2540943515378 -> J_sat
- 751.4311745041396 -> Z_sat
- 0.189389271800814 2 -> E_sym
- 0.588633086364825m -> L_sym
- 16.33575380026284 -> K_sym
- 213.23232978902993 -> Q_sym
- 896.910902604915 -> Z_sym


RMSE divided by STD for each feature
RMSE/stdY_i
0.0
0.1
0.2
0.3
0.4
rho0
E_sat
K_sat
J_sat
Z_sat
E_sym
L_sym
K_sym
Q_sym
Z_sym
Y_i

Conclusion

- I reached my goal but:



- Cross validation;
- Improving the code to train the complete data set;
- Neural network is a stochastic method;
- Bigger grid search.

THANK YOU!

Backup Slides

How things work

$$\mathcal{E}_{nuc}(\rho,\delta) = \mathcal{E}_{SNM}(\rho) + S(\rho)\,\delta^2, \qquad S(\rho) = \frac{1}{2}\left.\frac{\partial^2 \mathcal{E}_{nuc}}{\partial \delta^2}\right|_{\delta=0}.$$

$$P_{is}^k = (3n_0)^k \left.\frac{\partial^k \mathcal{E}_{SNM}/A}{\partial n^k}\right|_{\{\delta=0, n=n_0\}} \quad \text{and} \quad P_{iv}^k = (3n_0)^k \left.\frac{\partial^k S(\rho)}{\partial n^k}\right|_{\{\delta=0, n=n_0\}}.$$

$$\mathcal{E}_{SNM}(\rho) = E_0 + \frac{1}{2}K_0 x^2 + \frac{1}{6}J_0 x^3 + \frac{1}{24}Z_0 x^4$$

$$S(\rho) = E_{\rm sym} + L_{\rm sym} x + \frac{1}{2}K_{\rm sym} x^2 + \frac{1}{6}Q_{\rm sym} x^3 + \frac{1}{24}Z_{\rm sym} x^4$$

$$\{P_{is}^0 = E_0, P_{is}^2 = K_0, P_{is}^3 = J_0, P_{is}^4 = Z_0\}$$

$$\{P_{iv}^0 = E_{\rm sym}, P_{iv}^1 = L_{\rm sym}, P_{iv}^2 = K_{\rm sym}, P_{iv}^3 = Q_{\rm sym}, P_{iv}^4 = Z_{\rm sym}\}$$

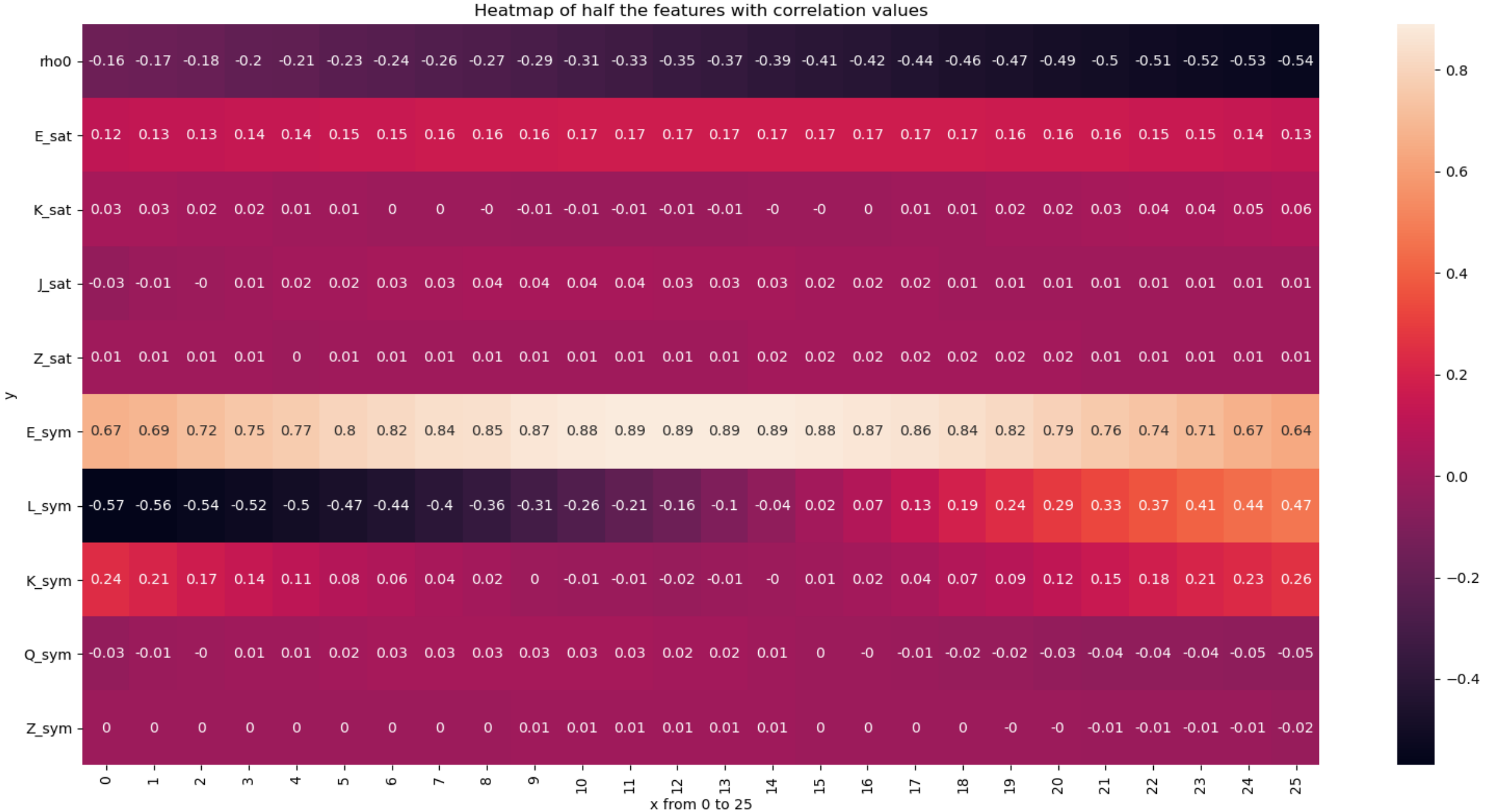
$$\varepsilon_{lep}(\rho, \delta; \mathbf{w}) = \varepsilon_e(\rho, \delta; \mathbf{w}) + \varepsilon_\mu(\rho, \delta; \mathbf{w})$$

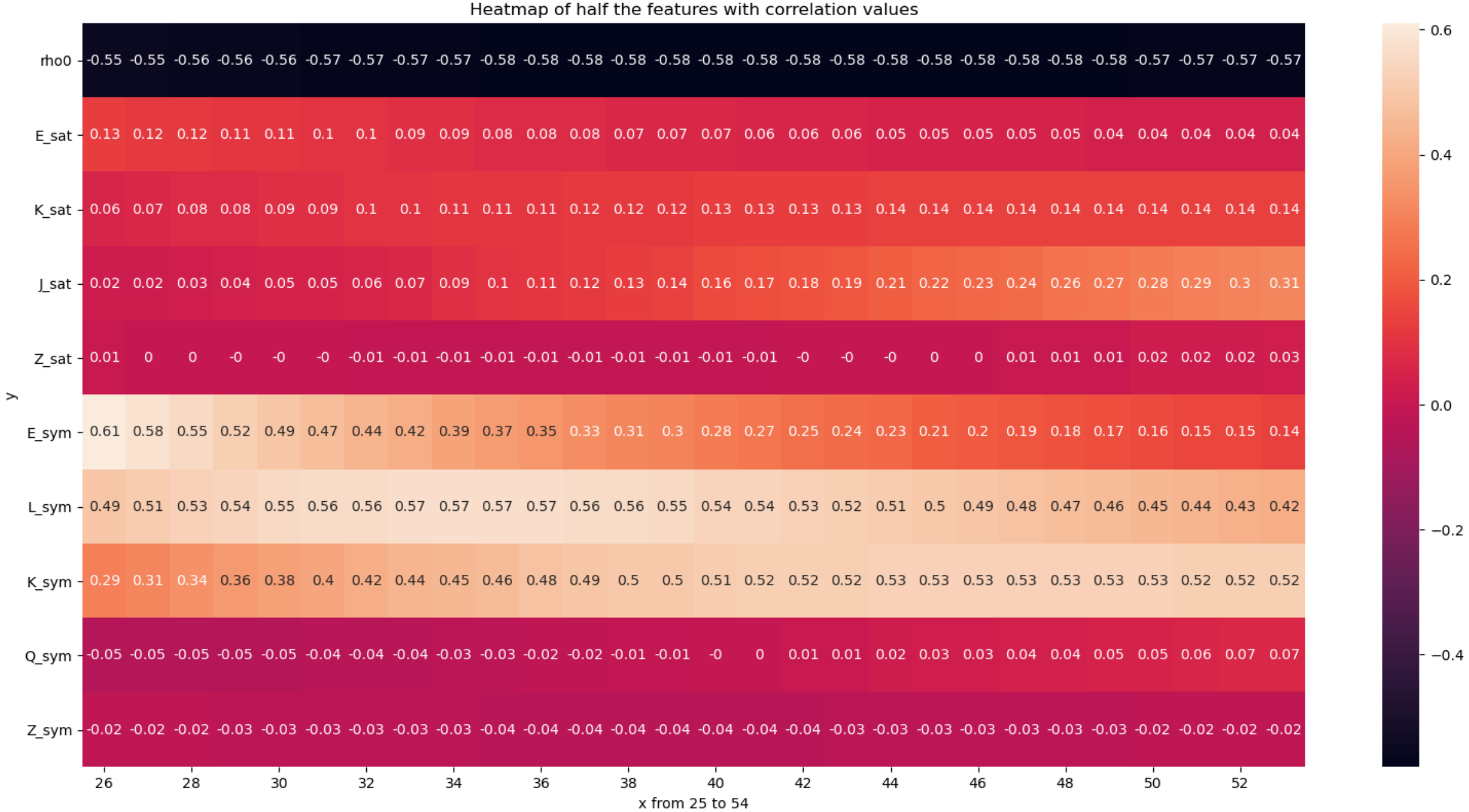
$$\bar{m}_N = (m_n + m_p)/2$$

$$\varepsilon_\beta(\rho; \mathbf{w}) = \rho\left(\mathcal{E}_{nuc}(\rho, \delta; \mathbf{w}) + \bar{m}_N\right) + \varepsilon_{lep}(\rho, \delta; \mathbf{w}),$$

index	rho0	E_sat	K_sat	J_sat	Z_sat	E_sym	L_sym	K_sym	Q_sym	Z_sym
count	250000	250000	250000	250000	250000	250000	250000	250000	250000	250000
mean	0.155582…	-15.7990…	230.28416	643.32288	-213.432	31.945388	72.827376	-100.2744	252.7351…	-304.516…
std	0.012228…	0.669884…	42.19845…	711.5798…	1964.828…	4.234462…	26.23837…	182.2650…	729.1679…	1948.430…
min	0.14	-16.7	170	-900	-3500	26	15	-400	-1200	-3500
25%	0.14	-16.1	200	60	-1500	29	51	-200	-171.429	-1785.714
50%	0.155	-15.5	230	540	-500	32	69	-100	514.286	-71.429
75%	0.17	-15.5	260	1500	1500	35	87	0	857.143	1642.857
max	0.17	-14.9	290	1500	2500	38	105	200	1200	2500

index	0	1	2	3	4	33	51	52	53
count	250000	250000	250000	250000	250000	250000	250000	250000	250000
mean	0.382661…	0.406853…	0.431075…	0.455327…	0.479610…	1.203134…	1.688050…	1.716311…	1.744736…
std	0.002258…	0.002297…	0.002334…	0.002370…	0.002406…	0.008924…	0.029039…	0.030853…	0.032764…
min	0.374544…	0.398720…	0.422958…	0.447254…	0.471603…	1.178598…	1.613980…	1.638176…	1.662375…
25%	0.381112…	0.405266…	0.429448…	0.453661…	0.477901…	1.196877…	1.667760…	1.694684…	1.721744…
50%	0.382797…	0.406980…	0.431190…	0.455435…	0.479711…	1.202701…	1.685023…	1.713009…	1.741134…
75%	0.384336…	0.408559…	0.432815…	0.457104…	0.481431…	1.209007…	1.705729…	1.734989…	1.764450…
max	0.388019…	0.412326…	0.436638…	0.460967…	0.485302…	1.233160…	1.795425…	1.831210…	1.867569…


Heatmap of half the features with correlation values
rho0 -0.16 -0.17 -0.18 -0.2 -0.21 -0.23 -0.24 -0.26 -0.27 -0.29 -0.31 -0.33 -0.35 -0.37 -0.39 -0.41 -0.42 -0.44 -0.46 -0.47 -0.49 -0.5 -0.51 -0.52 -0.53 -0.54
E_sat 0.12 0.13 0.13 0.14 0.14 0.15 0.15 0.16 0.16 0.16 0.17 0.17 0.17 0.17 0.17 0.17 0.17 0.17 0.17 0.16 0.16 0.16 0.15 0.15 0.14 0.13
K_sat 0.03 0.03 0.02 0.02 0.01 0.01 0 0 -0 -0.01 -0.01 -0.01 -0.01 -0.01 -0 -0 0 0.01 0.01 0.02 0.02 0.03 0.04 0.04 0.05 0.06
J_sat -0.03 -0.01 -0 0.01 0.02 0.02 0.03 0.03 0.04 0.04 0.04 0.04 0.03 0.03 0.03 0.02 0.02 0.02 0.01 0.01 0.01 0.01 0.01 0.01 0.01 0.01
Z_sat 0.01 0.01 0.01 0.01 0 0.01 0.01 0.01 0.01 0.01 0.01 0.01 0.01 0.01 0.02 0.02 0.02 0.02 0.02 0.02 0.02 0.01 0.01 0.01 0.01 0.01
E_sym 0.67 0.69 0.72 0.75 0.77 0.8 0.82 0.84 0.85 0.87 0.88 0.89 0.89 0.89 0.89 0.88 0.87 0.86 0.84 0.82 0.79 0.76 0.74 0.71 0.67 0.64
L_sym -0.57 -0.56 -0.54 -0.52 -0.5 -0.47 -0.44 -0.4 -0.36 -0.31 -0.26 -0.21 -0.16 -0.1 -0.04 0.02 0.07 0.13 0.19 0.24 0.29 0.33 0.37 0.41 0.44 0.47
K_sym 0.24 0.21 0.17 0.14 0.11 0.08 0.06 0.04 0.02 0 -0.01 -0.01 -0.02 -0.01 -0 0.01 0.02 0.04 0.07 0.09 0.12 0.15 0.18 0.21 0.23 0.26
Q_sym -0.03 -0.01 -0 0.01 0.01 0.02 0.03 0.03 0.03 0.03 0.03 0.03 0.02 0.02 0.01 0 -0 -0.01 -0.02 -0.02 -0.03 -0.04 -0.04 -0.04 -0.05 -0.05
Z_sym 0 0 0 0 0 0 0 0 0 0.01 0.01 0.01 0.01 0.01 0.01 0 0 0 0 -0 -0 -0.01 -0.01 -0.01 -0.01 -0.02
y
0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25
x from 0 to 25
0.8
0.6
0.4
0.2
0.0
−0.2
−0.4


Heatmap of half the features with correlation values
rho0 -0.55 -0.55 -0.56 -0.56 -0.56 -0.57 -0.57 -0.57 -0.57 -0.58 -0.58 -0.58 -0.58 -0.58 -0.58 -0.58 -0.58 -0.58 -0.58 -0.58 -0.58 -0.58 -0.58 -0.58 -0.57 -0.57 -0.57 -0.57
E_sat 0.13 0.12 0.12 0.11 0.11 0.1 0.1 0.09 0.09 0.08 0.08 0.08 0.07 0.07 0.07 0.06 0.06 0.06 0.05 0.05 0.05 0.05 0.05 0.04 0.04 0.04 0.04 0.04
K_sat 0.06 0.07 0.08 0.08 0.09 0.09 0.1 0.1 0.11 0.11 0.11 0.12 0.12 0.12 0.13 0.13 0.13 0.13 0.14 0.14 0.14 0.14 0.14 0.14 0.14 0.14 0.14 0.14
J_sat 0.02 0.02 0.03 0.04 0.05 0.05 0.06 0.07 0.09 0.1 0.11 0.12 0.13 0.14 0.16 0.17 0.18 0.19 0.21 0.22 0.23 0.24 0.26 0.27 0.28 0.29 0.3 0.31
Z_sat 0.01 0 0 -0 -0 -0 -0.01 -0.01 -0.01 -0.01 -0.01 -0.01 -0.01 -0.01 -0.01 -0.01 -0 -0 -0 0 0 0.01 0.01 0.01 0.02 0.02 0.02 0.03
E_sym 0.61 0.58 0.55 0.52 0.49 0.47 0.44 0.42 0.39 0.37 0.35 0.33 0.31 0.3 0.28 0.27 0.25 0.24 0.23 0.21 0.2 0.19 0.18 0.17 0.16 0.15 0.15 0.14
L_sym 0.49 0.51 0.53 0.54 0.55 0.56 0.56 0.57 0.57 0.57 0.57 0.56 0.56 0.55 0.54 0.54 0.53 0.52 0.51 0.5 0.49 0.48 0.47 0.46 0.45 0.44 0.43 0.42
K_sym 0.29 0.31 0.34 0.36 0.38 0.4 0.42 0.44 0.45 0.46 0.48 0.49 0.5 0.5 0.51 0.52 0.52 0.52 0.53 0.53 0.53 0.53 0.53 0.53 0.53 0.52 0.52 0.52
Q_sym -0.05 -0.05 -0.05 -0.05 -0.05 -0.04 -0.04 -0.04 -0.03 -0.03 -0.02 -0.02 -0.01 -0.01 -0 0 0.01 0.01 0.02 0.03 0.03 0.04 0.04 0.05 0.05 0.06 0.07 0.07
Z_sym -0.02 -0.02 -0.02 -0.03 -0.03 -0.03 -0.03 -0.03 -0.03 -0.04 -0.04 -0.04 -0.04 -0.04 -0.04 -0.04 -0.04 -0.03 -0.03 -0.03 -0.03 -0.03 -0.03 -0.03 -0.02 -0.02 -0.02 -0.02
y
26 28 30 32 34 36 38 40 42 44 46 48 50 52
x from 25 to 54
0.6 0.4 0.2 0.0 −0.2 −0.4