

Article

Using Machine Learning Techniques for Asserting Cellular Damage Induced by High-LET Particle Radiation

Supplementary Material

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1 **Keywords:** Machine Learning; Ionizing Radiation; Cell Survival; DNA Damage, Computational
2 modelling

3 S1. Code

4 The Python code of this study can be found [GitHub](#) as a jupyter notebook.

5 Python packages that were used:

- 6 • python==3.6.12
- 7 • matplotlib==3.2.2
- 8 • seaborn==0.11.0
- 9 • pandas==0.25.3
- 10 • hyperopt==0.2.5
- 11 • scipy==1.5.2
- 12 • statsmodels==2.12.0
- 13 • xlrd==1.2.0
- 14 • numpy==1.17.4
- 15 • joblib==0.17.0
- 16 • category_encoders==2.2.2
- 17 • scikit_learn==0.23.2

18 S2. Tables & Figures

19 Here, in Figures [S1](#), [S2](#) we present the partial dependence of the β parameter. Given the poor
20 performance of the model in predicting the β parameter, the interpretation plots of the parameters was
21 omitted and included in the supplementary material.

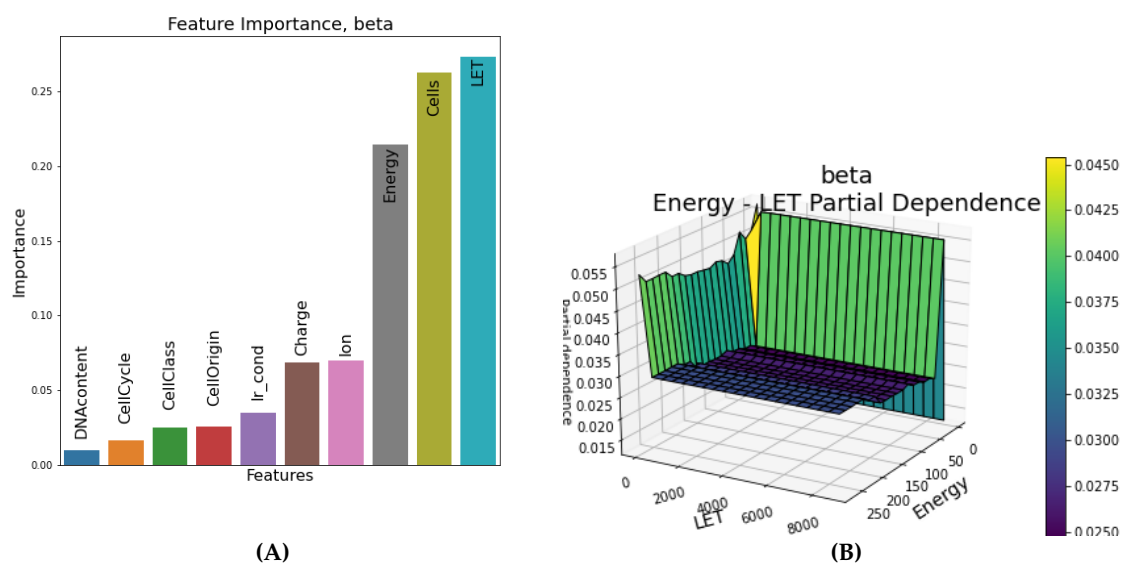


Figure S2. (A) Feature importance for the β parameter, (B) LET - Energy two-way partial dependence for the β parameter

22 Below in Table S1 are presented the hyper-parameters for each model that was trained.

Hyper Parameter	α parameter	β parameter	All clusters (hypoxic cells)	All clusters (oxic cells)
bootstrap	true	true	true	true
criterion	mse	mae	mae	mae
max_depth	None	None	None	None
max_features	log2	log2	auto	auto
max_samples	0.9	0.9	0.9	0.9
min_samples_leaf	1	4	1	1
min_samples_split	2	2	2	2
n_estimators	50	10	15	13
oob_score	true	true	true	true

Table S1. Optimized Parameters, as were calculated by the hyperopt algorithm

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