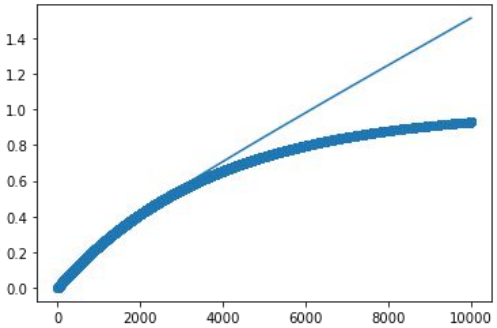
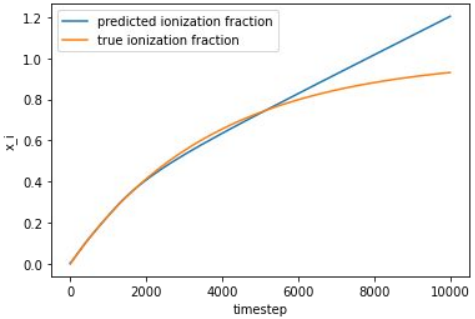
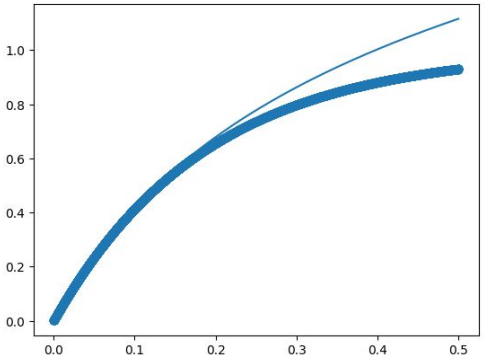
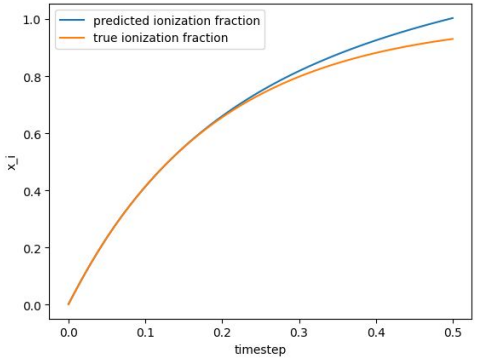
ML4Science

Week 4

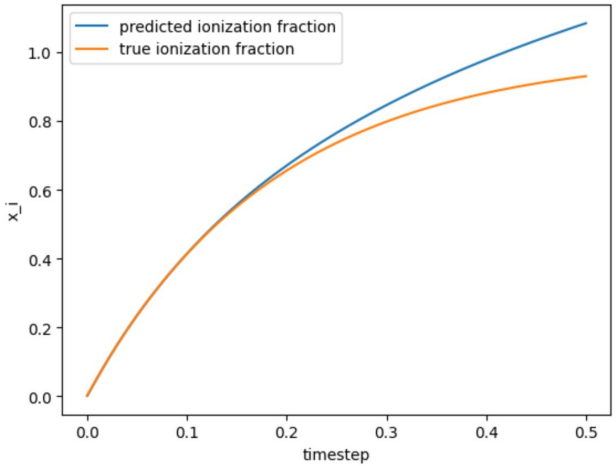
What we did

- experimented with time scaling
- approximated function with deviated physics parameters
- implemented (Γ, n) parameter handling
- implemented cross-validation for hyperparameter tuning

Time Scaling (scaling factor of 1e-6)

	Simple model		Model with physics loss	
No scaling		R2-Score: -0.0216		R2-Score: 0.8409
With scaling		R2-Score: 0.8890		R2-Score: 0.9852

Deviated physics parameters



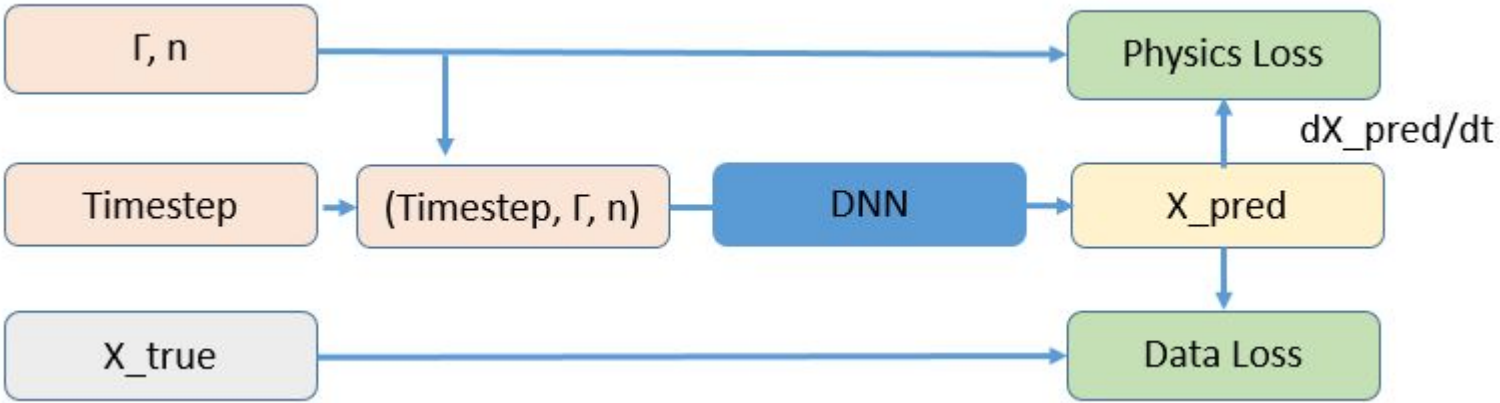
- R2-Score: 0.9290
- Physics loss coefficient: 1000
- Scaling: 1e-6

(|nH[i] - nH[0]|, |gamma[i] - gamma[0]|): R2-Score

(8.829006709039466e-09, 2.388218114161164e-14) : 0.9556017518043518
(1.4993662971480848e-08, 2.2878043172973725e-14) : 0.9555726647377014
(2.015543801326738e-08, 2.1991478230090445e-14) : 0.9554858207702637
(1.3953909615581705e-08, 2.5642846736391315e-14) : 0.9554798007011414
(1.278455418001184e-08, 2.632311102022812e-14) : 0.955375075340271
(1.1482866414972331e-08, 2.0827649563095413e-14) : 0.9552826285362244
(6.396633391851045e-09, 2.01977954456038e-14) : 0.9551296830177307
(1.2989952340825574e-08, 2.761311630717725e-14) : 0.9550908207893372
(5.688696782222474e-08, 2.851340002274781e-14) : 0.9548271894454956
(1.494877105893237e-08, 1.9150922841484917e-14) : 0.9548071622848511
(8.183570823172837e-08, 2.945351526986744e-14) : 0.9544958472251892
(1.1392263915930119e-08, 1.8054106613631158e-14) : 0.9543760418891907
(1.4620253678708627e-08, 1.7130120503178276e-14) : 0.9539368748664856
(1.20338830598972e-08, 3.134219916811571e-14) : 0.9536619782447815
(1.4567341835511319e-08, 3.2093942501190725e-14) : 0.9532691240310669
(1.2073837678420326e-08, 1.535897232472388e-14) : 0.9528956413269043
(1.505322610103436e-08, 1.4945384581438753e-14) : 0.9526137709617615
(7.221728651405888e-09, 3.392513692151445e-14) : 0.9521710276603699
…

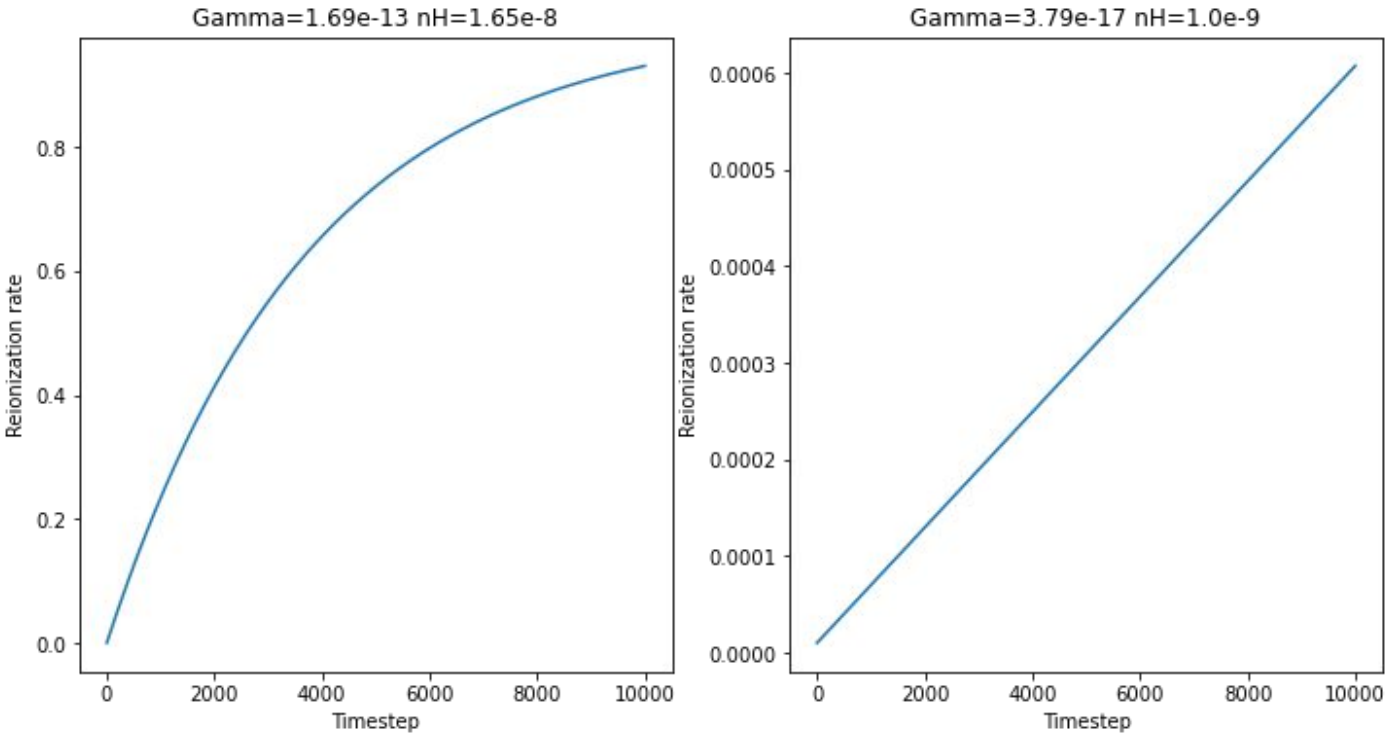
Physics Parameters Handling

Goal is to train a single model for all possible combinations of physics parameters



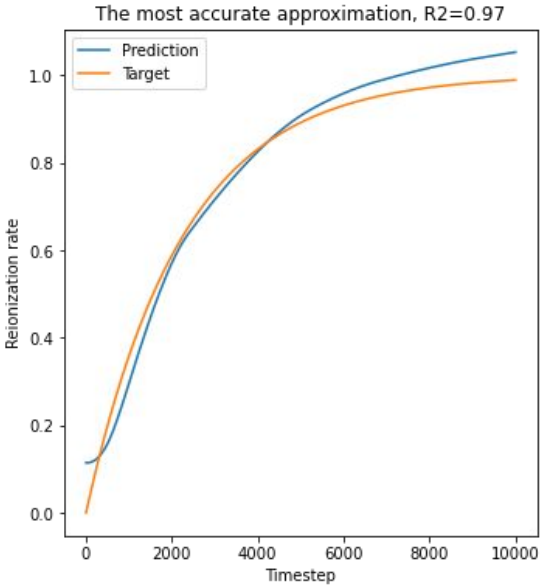
Our suggestion on handling Γ, n

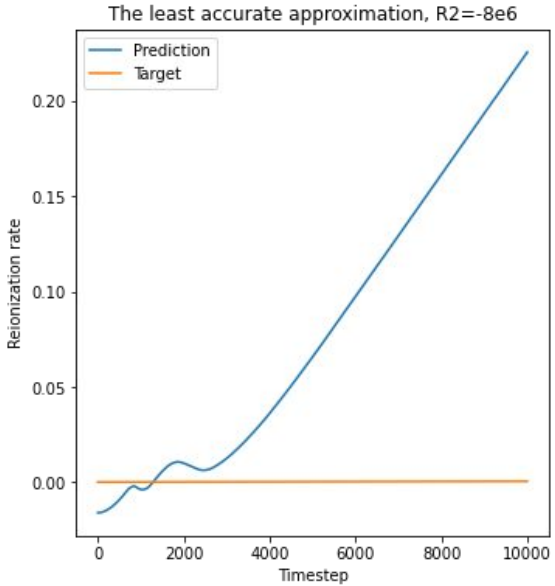
Parameter Handling: Influence of gamma and n on the target function



Left example is a common behavior of target function, right example is a rare case (10% of all simulations)

Result





- feature tensor of format (timestep, n, gamma)
- tested on 10% of all simulations

The model performs better in case of expected behaviour of reionization rate, but fails in case of rare behaviour of target function and produces artifacts(negative values, extremums)

Plan for the coming week

- refactor code
- put together a set of most meaningful setups
- balancing the fraction of “bad” and “good” simulations: sampling more simulations which are challenging for the model on the training stage
- start writing report