

# MACHINE LEARNING-BASED MODELING OF MUON BEAM IONIZATION COOLING

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## Abstract

Surrogate modeling can lead to significant improvements of beam dynamics simulations in terms of computational time and resources. Application of supervised machine learning, using collected simulation data allows to build surrogate models which can estimate beam parameters evolution based on the provided cooling channel design. The created models help to understand the correlations between different lattice components and the importance of specific beam properties for the cooling performance. We present the application of surrogate modeling to enhance final muon cooling design studies, demonstrating the potential of such approach to be integrated into the design and optimization of other components of future colliders.

## INTRODUCTION

In light of rising activities on the muon collider studies [1], the applied simulation tools, optimization of design parameters and overall software and data handling infrastructure gain more importance. Currently, one of the more active areas of the design study is the final cooling system. The reduction of the muon beam emittance is based on the concept of ionization cooling [2], where careful choice of the lattice and beam parameters is required. First results obtained from a prototype of an automatic optimization framework for the final cooling are presented in [3]. With the growing number of parameters and objectives to be considered in the design, the choice of initial simulation settings will become more challenging. Moreover, the required time and computational resources might become a bottleneck in optimization studies based on complex simulations. Applying supervised learning-based surrogate models promises a solution of both challenges. The results presented in this work first, demonstrate how optimization can be speeded up significantly by replacing tracking simulation with Machine Learning (ML) model prediction. Second, the application of inverted surrogate models is presented, allowing to obtain initial guess for optimization parameters, reducing the number of steps needed to reach an optimal solution.

## Supervised Learning

Supervised learning methods allow to make predictions on unseen data, after learning a mapping function between input variables and output targets in the provided training samples. In this context, *supervision* is provided in the form of sets of data inputs with corresponding true output targets. While *learning* means adjusting parameters of the mapping function aiming to minimize the difference

between prediction made by the model and true target values of the provided input-output pairs. The complexity of the mapping function depends on characteristics of the data and selected method, such that mapping between linearly related input and output variables can be built e.g. using linear regression models while for complex non-linear problems neural networks with various possible architectures are applied. Decision Trees, where each final node corresponds to a prediction of a single output target, are also widely used in supervised learning. Since decision trees are graphs, their predictions are easier to interpret than others such as deep neural networks. Combining several decision trees and making predictions by averaging the individual output helps to overcome the problem of over-fitting on training data and allows to make more reliable prediction on unseen data.

In this work, we apply the Random Forest algorithm [4], an ensemble method, where each tree in the ensemble is trained on different parts of the training data set. This is done in order to reduce the variance, usually causing a small increase of bias which is then mitigated by averaging the final prediction, allowing Random Forest to outperform a single decision tree.

## MODELING BEAM DYNAMICS USING SUPERVISED LEARNING

Machine Learning concepts became a popular tool in various accelerator physics areas, ranging from operation and automatic control of machine parameters [5, 6] to beam instrumentation analysis to improve the quality of measurements data detecting anomalous signals [7]. While the advantages of unsupervised learning have been mostly demonstrated in online applications, supervised learning and in particular data-driven surrogate modeling is used also outside of operation, e.g. to model virtual diagnostics tools [8].

Also, solving optimization problems with the help of surrogate models brings the advantage of speeding up the optimization process by replacing measurements or slow-executable simulations with beam dynamics models. Such models can be built from measurements or simulations data to be used as training sets for supervised learning algorithms. The application of surrogate models for the optimization of existing accelerators and experiments planning has been demonstrated [9], however this approach did not find a wide application in the design of future facilities. Here we present the first results of improving the optimization of one of the most crucial components of the muon collider, the final cooling system with the help of supervised learning.

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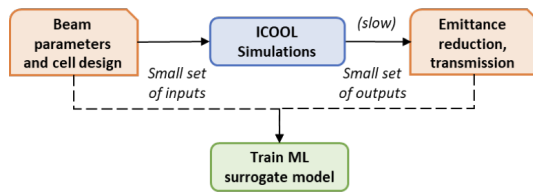


Figure 1: How to make use of simulation data created during optimization for further design enhancement.

## Data Preparation

As training data for the surrogate model of final cooling, we use the simulations configuration and tracking results from ICOOL, as shown in Fig. 1. Data can be generated passively, without performing dedicated simulations, but making use of a well structured data handling, combining first optimization steps and data preparation for more advanced computationally efficient optimization. Another advantage compared to generating the training data from simple parameter scans, is the distribution of parameter values. When collecting data from optimization steps, the values will be centered around potential optima, providing trained models with additional information about the physics underlying in the data. A detailed description of ICOOL simulations and optimization set up for final cooling studies is presented in [3]. To build the first prototype and verify the concept of applying surrogate models to the design of final cooling channel, we consider transverse beam dynamics only, without including longitudinal emittance growth and re-acceleration of the muon beam cooled in the absorbers. In the following, we present different options, how surrogate model can be used in the final cooling optimization.

## PREDICTION OF COOLING PERFORMANCE

In the simplified case considering the transverse dynamics only, the optimization is performed towards the reduction of the transverse emittance, while keeping the transmission rate high, passing the beam through two consecutive cooling cells with liquid hydrogen absorber placed in a solenoid field up to 30 T. As optimization variables, we use the radii of the coils which built the solenoid field inside the cooling cell to control the optics parameters  $\beta$ -function and  $\alpha$  at the location of absorber. Absorber densities,  $\beta$ -function and kinetic energy of the incoming beam are also included as free variables. These parameters build the input of surrogate model, while the resulting emittance reduction, the change of the longitudinal momentum and transmission rate are the corresponding output targets to be predicted by the surrogate model. The ML-based objective function evaluation during optimization is then performed in two steps. First we evaluate the optics matching by predicting  $\alpha$  and  $\beta$  in the absorber regions from the solenoid field configuration, 6 input variables in total, corresponding to the radii of matching coils and main 30 T solenoid coils. As a second step, the model predicts transmission, emittance and momentum reduction (3 output targets) from the initial beam energy

and  $\beta$ -function at the start of the cell, absorber densities and average  $\alpha$  and  $\beta$  function values in the absorber regions (6 input parameters).

We apply a Random Forest regressor to build these surrogate models from simulation data (1200 samples), achieving 98.3 % explained variance in total, on a test set of 300 samples. Figure 2 illustrates the great agreement between predicted and true values obtained from ICOOL simulations performed with corresponding set of input parameters. The lowest prediction error is that of transmission rate (0.05 %), which can be explained with the fact that this output target has the lowest variance. Hence, it is easier for the model to find a general mapping between input and output. The relative emittance reduction is predicted with 1.6 % of relative mean absolute error, and 0.3 %, 0.5 % and 3.2 % for the prediction of the reduction of longitudinal momentum and  $\alpha$  and  $\beta$ -function in absorber, respectively.

The lower prediction accuracy of transverse emittance and  $\beta$ -function compared to the momentum reduction can be explained by the ionization cooling process causing the change of these quantities. While the energy loss comes purely from the interaction between muons and absorber material, the emittance reduction is additionally affected by the multiple scattering, as shown in Fig. 3. In the second cell, the  $\beta$ -function is changed due to the loss of the beam momentum. This makes the construction of mapping function more challenging, hence leading to less accurate prediction of these properties on unseen data. The overall high accuracy demonstrates the possibility to use surrogate models to predict the quantities needed to evaluate the objective function during optimization. Replacing time consuming tracking simulation leads to enormous reduction of the time needed for one optimization step by a factor of 50.

## ANALYSING PARAMETER IMPORTANCE

Exploring the importance of input parameters on the targets prediction helps to better understand the contribution of different beam and lattice properties to the overall cooling performance, to streamline the future models and to identify most critical parameters to be optimized towards desired beam emittances. Random Forest algorithm can naturally provide the ranking of variables importance during the fitting process. The values of each input variable are permuted among the training data and the resulting prediction loss is compared against the error before the permutation, averaging the error over all trees in the ensemble. The permutation breaks the relationship between the input variable and the output target, hence the decrease in the model score indicates the dependence of the model on a particular variable.

Figure 4 illustrates the importance of variables used to predict the transverse emittance reduction: initial kinetic energy of the beam,  $\beta$  at the start of the first cooling cell, average  $\beta$  at absorbers, the absorber density per cell and mean absolute value of  $\alpha$  along the lattice. As expected, the  $\beta$ -function at the location of absorbers has the strongest contribution on the emittance reduction, together with  $\alpha$

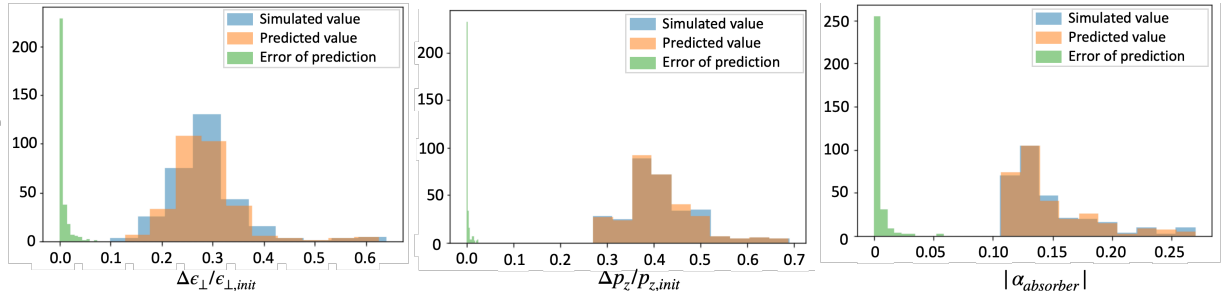


Figure 2: Random Forest model prediction compared to the tracking simulation of transverse emittance reduction, longitudinal momentum reduction and Twiss parameter  $\alpha$  in the absorber regions. Prediction errors are computed as absolute difference between true simulated and predicted values.

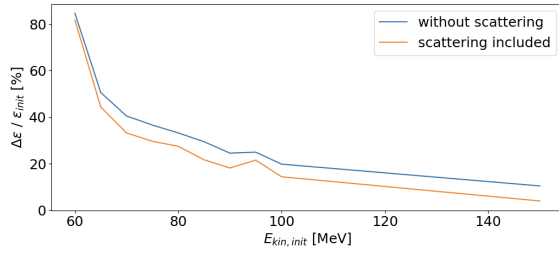


Figure 3: The comparison of simulating the emittance reduction, with and without including the multiple scattering.

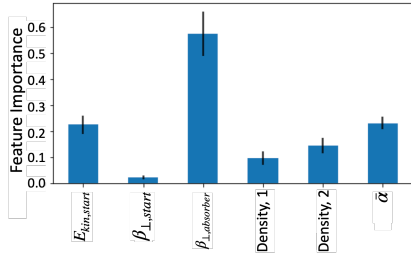


Figure 4: Importance of optimization variables for the prediction of transverse emittance reduction.

and the kinetic energy of the incoming beam since these parameters define the optics of the channel and affect the contribution of the heating term. Moreover, the predicted optics parameters values also reflect the coils configuration which builds the solenoid field inside the cooling cell.

While these results of importance analysis seem to be obvious, they allow an easy interpretation of trained ML model, to compare their prediction with analytical estimates and to ensure that more complex dynamics can be modeled reliably. Thus, the presented concept potentially will help to identify most critical parameters and design bottlenecks in the future.

## INVERSE MODELS

Inverting the model's input and output targets offers the opportunity to predict the required initial beam energy and  $\beta$ -function, absorber densities and solenoid field configuration by providing the desired emittance, momentum reduction and transmission as input. After training the model on 1200 samples, total test accuracy of 97 % could be achieved. To

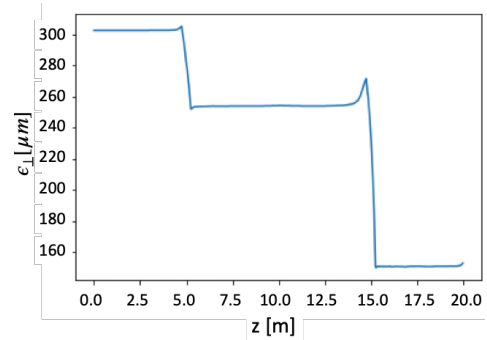


Figure 5: Transverse emittance reduction achieved with predicted simulation parameters.

verify the trained model, we track 1000 particles using the predicted beam and lattice parameters to ensure that the desired cooling performance can be achieved. As an example, providing the relative emittance reduction of 50 % and 98 % transmission rate as input values, the model predicts the lattice and beam parameters which lead to exactly 49.3 % of emittance reduction as shown in Fig. 5 and 98 % transmission according to ICOOL simulation results. This excellent agreement demonstrates that inverted models can provide precise starting values for further optimization.

## CONCLUSIONS

For the first time we demonstrated the concept of applying supervised learning to enhance the optimization within design of the muon collider, specifically for the final cooling system. The results demonstrate a great potential to speed up optimization of cooling cells, estimate the importance of various lattice and beam properties on the cooling performance and to provide precise initial guess for starting parameters in further optimization. First steps towards more complex models are already performed, by collecting the data from simulations including longitudinal beam dynamics, allowing to predict the evolution of longitudinal emittance and tuning radiofrequency parameters. Further improvements are possible by exploring probabilistic approach to include the uncertainty of emittance estimation into surrogate models or with the help of physics-informed neural networks to model more complex beam dynamics.

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