Machine learning enabled fast evaluation of dynamic aperture for storage ring accelerators

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Abstract

For any storage ring-based large-scale scientific facility, one of the most important performance parameters is the dynamic aperture (DA), which measures the motion stability of charged particles in a global manner. To date, long-term tracking-based simulation is regarded as the most reliable method to calculate DA. However, numerical tracking may become a significant issue, especially when a plethora of candidate designs of a storage ring need to be evaluated. In this paper, we present a novel machine learning-based method, which can reduce the computation cost of DA tracking by approximately one order of magnitude, while keeping sufficiently high evaluation accuracy. Moreover, we demonstrate that this method is independent of concrete physical models of a storage ring. This method has the potential to be applied to similar problems of identifying irregular motions in other complex dynamical systems.

1. Introduction

Modern storage-ring accelerators, such as the synchrotron light sources [1] and high-energy colliders [2], have played a key role in a variety of scientific fields like photon sciences [3, 4], nuclear physics [5, 6], material sciences [7, 8], and high-energy physics [9, 10]. A storage ring can be regarded as a complex quasi-Hamiltonian system. The dynamical analysis for motions of charged particles in the storage ring remains an important and active issue in the accelerator field. The concept, dynamic aperture (DA, see details in methods), is widely used to quantitatively measure the region of stable particle motions [11]. DA is important for injection efficiency and beam lifetime [12–14], and is one of the most important performance parameters of a storage ring. In the design of any storage ring, it is necessary to evaluate the DA and further optimize it (often needed) to meet injection and lifetime criterion.

In the last few decades, continuous efforts have been made to accurately predict the DA and to look into the dynamics underlying the DA. Since early 1980s, analytical methods such as Lie algebraic methods [15–17] have been transferred from the domain of nonlinear dynamical systems to DA evaluation and characterization. In the 1990s, numerical analysis methods, e.g., Lyapunov exponents [18] and frequency map analysis [19], were introduced to characterize the stability of particle motions and reveal dangerous resonances limiting the DA. So far, a few analytical formulae (e.g., [20–24]) and numerical tracking programs (e.g., [25–28]) have been developed to evaluate the DA of a storage ring. Analytical approaches are fast, but have only limited accuracy in DA evaluation. Till now, long-term tracking-based method is regarded as the most reliable method to calculate DA. However, numerical tracking may become a significant issue in the cases a plethora of candidate designs (or error models) of a storage ring need to be considered. Finding measures to effectively reduce the computing cost for DA tracking will be very helpful.

To reduce the computational cost, machine learning (ML) techniques have recently inspired a surge of applications to DA evaluation, especially in the time-consuming DA optimization studies [29–33]. These proposals focus mainly on learning the map between the magnetic lattice settings of the storage ring (e.g.,...
the strengths of magnets) and the corresponding DA size. With a supervised ML model trained by existing 
data, the DA size can be predicted in a fraction of a second and thus the DA optimization efficiency can be 
significantly improved. Such an ML-based approach, however, does not always work well. This is because 
that the dynamics underlying the DA is complicated, and there is not explicit dependence between the DA 
and multi-kinds of related factors. Worse still, the available training data in hand is usually insufficient to 
cover a large enough volume in the variable space. As a result, the ML model often predicts accurately for a 
small variation range in the variable space and/or for a small number of control variables. Although this 
limitation can be mitigated to some degree by continuously retraining the ML model with new data samples 
(will take extra computing time) [33], one needs to always concern about the DA prediction accuracy when 
applying the ML model to a new storage ring design, whose lattice settings are away from the distribution of 
the existing training data.

Different from the previous ML-based methods of directly predicting DA from magnetic lattice settings, 
in this paper, we propose a novel ML-based method of predicting DA by learning the motion stability of 
charged particles. In this method, a ML model is trained to predict the long-term motion stability from the 
initial trajectories of charged particles. The training data can be long-term tracking results of sparsely 
sampled initial conditions in the phase space. With this method, the boundary of DA can be reconstructed 
by predicting particles are lost or not from their initial trajectories, and thus the regression problem of 
predicting the DA size of previous ML-based attempts can be reduced to a binary classification problem of 
predicting particle loss. Considering that the conventional DA evaluation calls for the long-term tracking of 
dense enough initial conditions in the phase space, this method allows to reduce the computing cost of 
conventional DA evaluation, based on the fact that it requires to track only sparsely sampled initial 
conditions for sufficiently long time. Taking a fourth generation ring-based light source [1] as an example, 
we demonstrate that this method allows an accurate and fast DA evaluation process, and remains effective 
when the physical model of a storage ring is varied.

2. Methods

2.1. Conventional DA calculation

As a charged particle travels in a storage ring with a specific initial condition, the amplitude of its oscillation 
around the closed orbit [34] may increase over time due to the presence of nonlinearities (e.g., from 
chromatic sextupoles), and in a worse scenario the amplitude exceeds a certain limit (e.g., physical apertures 
of the elements), leading to particle loss. The DA refers to the range of initial conditions of the particles 
whose trajectories stay within the specified limit for a sufficient number of turns. Strictly speaking, to 
represent the DA, one needs to count the initial conditions in 6D phase space, \([x, x', y, y', z, \delta]\), where \(x\) and 
\(y\) (\(x'\) and \(y'\)) are the horizontal and vertical displacements (angular deviations), \(z\) and \(\delta\) are longitudional 
displacements and momentum deviation of the particle relative to a reference particle. However, for the 
sake of illustration, one generally searches for the largest initial amplitudes in transverse coordinate space, 
for which the subsequent trajectories are stable.

For a given lattice of the storage ring, a conventional way to calculate DA is to track particles over a 
range of initial conditions for a specified number of turns (\(\sim 10^5\) turns for lepton machines and 
\(\sim 10^6\) turns for hadron ones). The initial conditions are uniformly sampled along multi-polar directions in transverse 
coordinate space. After checking the stability of subsequent trajectories for all initial conditions, the DA can 
be obtained by connecting the largest amplitudes for stable trajectories in different polar directions. Because 
of the heavy tracking simulation, a single evaluation of DA can take from minutes to days. The situation can 
be far worse in the case of DA optimization, in which one needs to evaluate the DAs for thousands of 
candidate magnetic lattices.

2.2. ML-based scheme

To evaluate DA in a faster manner, supervised ML methods are adopted in this study. A supervised learning 
task concerns to learn the correlations between data feature and label for a set of training data, and to 
predict labels of new data samples based on their data feature. Among various supervised ML methods, we 
select five widely-used methods, which are support vector machine (SVM) [35] based on statistical learning 
theory, random forest (RF) [36] originated from the idea of ensemble learning, Gaussian process (GP) 
classification [37] assuming the data subjected to a joint Gaussian distribution, artificial neural network 
(ANN) [38] simulating the neuronal mechanism of human brain, and eXtreme Gradient Boosting 
(XGBoost) that is a gradient boosting framework [39]. These methods are tested and compared in 
appendix A. It is found that RF shows better performance in this study, and is therefore adopted in this 
study.
Figure 1. Schematic of particles loss prediction from short-term particle trajectories. The surviving particles are assigned a label $+1$ and the lost particles are assigned a label $-1$. $l$ and $u$ are the numbers of labeled and unlabeled samples, respectively, where $l \ll u$. $\{X_1, X_2, \ldots, X_s\}_i$ represents successive particle trajectories of $s$ time intervals starting from the $i$th initial condition $\{X_0\}_i$.

In our DA prediction scheme, the initial conditions of particles are sampled in the same way as in conventional DA calculation. The difference is that particles are tracked for just a few turns (or only one turn). Among the initial conditions, only a small portion (e.g. 10% or lower) of them are randomly selected for long-term tracking. These long-term tracking results are used to train the ML model, where the first few turns’ (or even the first turn’s) trajectories are treated as feature $X$, and the corresponding stability of the trajectories are treated as label $Y$ ($+1$ or $-1$ to represent stable or unstable). The schematic diagram of training is shown in figure 1. The stabilities of trajectories for the other initial conditions with only short-term trajectories tracked, which can be called unlabeled samples, are predicted as stable or unstable by the ML model. After all initial conditions are assigned with labels, the separation curve between the stable and unstable region in the initial condition space can be found, and the DA can be obtained. Apparently, since most of the particles are tracked for only a few turns rather than $10^3$ or even $10^6$ turns, the computation cost can be significantly reduced compared with a conventional DA computation process.

3. Application to DA evaluation for a diffraction-limited storage ring

In this section, taking a 4th-generation storage ring-based light source (4GLS) [1], the high energy photon source (HEPS) [40], as an example, we will investigate the performance of the proposed ML-based DA prediction method. The HEPS is a 4GLS being built in China [41]. The storage ring of the HEPS is designed to store ultra-low-emittance electron beam [42, 43], so as to deliver photon beams of much higher quality than its predecessors and serve tens of users at the same time. The HEPS storage ring comprises 48 seven-bend-achromats that are grouped in 24 super-periods, with a circumference of 1360.4 m and a natural emittance of $\sim 34$ pm. It provides 48 six-meter-long straight sections for insertion devices, producing x-ray radiation with brightness of above $1 \times 10^{22}$ phs mm$^{-2}$ mrad$^{-2}$/0.1%BW. In the design of such a 4GLS, DA optimization is a challenging topic, because the strong sextupoles used for chromaticity correction can lead to highly nonlinear beam dynamics [44]. With various efforts [45–49], the DA for the HEPS storage ring is only of the order of a millimeter, while meeting the requirement of on-axis injection [50] to the storage ring.

In the following we use the conventional computation and the ML-based method to evaluate the on-momentum DA (related to the dynamical acceptance for a particle without any momentum deviation) for the bare lattice (without considering field and alignment errors), and then extend the studies to more practical models of the HEPS storage ring.

First, the on-momentum DA at the center of long straight section is computed with the program AT [28], basically following the conventional calculation process as mentioned above. In the calculation, a total of about 5000 initial conditions of particles are sampled (see figure 2(a)) in the space of $[x, y, \hat{x}, \hat{y} = 0, \hat{z} = 0, \delta = 0]$. A small difference from the calculation procedure mentioned in section 2 is that the initial conditions with larger amplitudes are sampled with a slightly larger density (with a smaller step) to probe the boundary of DA more precisely. The maximum amplitudes of $x$ and $y$ are set to 7 mm, to ensure the area covered by sampled initial conditions is larger than the DA. Particles with different initial conditions are tracked for 1000 turns to see whether the particles survive or get lost, by checking whether their amplitudes exceed a limit of 1 m. The DA obtained from pure long-term particle tracking (hereafter referred to as exact DA) is shown in figure 2(b). The DA calculation takes nearly half an hour on a personal computer.
Then we apply the proposed ML-based method to evaluate the on-momentum DA. For a fair comparison, the same initial conditions as in figure 2(a) are used, for which the particles are tracked for only one turn. Only the initial conditions of surviving particles are recorded in figure 2(c). It appears many particles with large initial amplitudes get lost within the first oscillation period in the ring, suggesting the presence of extremely strong nonlinear magnetic field induced by the sextupoles and octupoles. For those initial conditions left after one turn’s tracking, the period-by-period coordinates are recorded and used as the feature of the samples. The total dimensionality of the ML model’s features is 96, i.e., the 4D trace of the first turn’s period-by-period trajectories. Then, from those initial conditions, 5% of them are randomly selected for long-term tracking (1000 turns), and are assigned with a label (+1 or −1 to represent stable or unstable) based on whether particles survive or get lost after 1000 turns (marked in figure 2(c)). We use the selected samples to train the ML model. The hyper parameter settings of the training are introduced in appendix A. With the trained ML model, the labels of the unlabeled samples (initial conditions with only the first turn’s trajectories) are predicted to be lost or not. Then, the corresponding predicted DA is obtained by extracting the separation curve of the lost and surviving particles, with the results shown in figure 2(d). We perform the whole process, including training, long-term tracking of the labeled particles, and short-term tracking of the unlabeled particles on the same personal computer. The whole process takes about 1 min.

For the convenience of comparison, the predicted DA and the exact DA are plotted together in figure 3(a). It is observed that the boundary of DA can be reconstructed with high accuracy. Some details of the DA, e.g., the small reduction in the vertical DA near x = −1 mm possibly caused by resonance crossing, can be accurately detected by the ML model. Also, the false predictions occur only for the initial conditions close to the boundary of DA. It is probably because the beam dynamics close to the DA boundary (transition between stable and unstable motions) is complicated. When initial amplitudes of the particles are close to the DA boundary, the nonlinear perturbations induce a finite smear of their trajectories. However, the perturbations might not be strong enough to make the particles lost after a sufficiently large number of turns [51], which makes accurate prediction challenging. Considering this challenge and the small ratio of false predictions near the DA boundary, it is reasonable to deduce that the trained model captures most of the underlying correlations between the show-term trajectories of the motions and the corresponding long-term motion stability.

As a further test, we compare the trajectories of particles from two close initial conditions (marked in figure 3(a)), which are within and outside the DA respectively and whose labels are accurately predicted by the ML model. Note that the two selected initial conditions are located in the region where false prediction rarely occurs, which can suggest the best performance of classification of the ML model rather than an average performance. The results are shown in figures 3(b) and (e). Although the difference is apparent between the two trajectories after tracking for more than 100 turns, there is just a little difference between
Figure 3. Comparison of the DAs obtained with pure long-term tracking and the ML-based method. The solid line and the dotted line in (a) represent the exact DA and the predicted DA, respectively. The pink points in (a) represent false predictions of the ML model. (b) and (e) show the turn-by-turn evolution of the transverse amplitudes for two selected initial conditions marked in (a). The first-turn period-by-period trajectories for the two particles are also presented in (c) and (f). The dashed line in (d) represents average predicted DA among 100 repeated tests with different choice of training samples. The shadow in (d) represents the maximum fluctuation among the repeated tests.

the first turn’s period-by-period trajectories (see figures 3(c) and (f)). With the ML model, the short-term trajectories are successfully differentiated and assigned a different label despite the very small difference between them. By contrast, previous experiences (e.g., [52]) indicate that it is very difficult, if not impossible, to accurately judge the stability of motions based on such short-period trajectories.

Furthermore, to avoid the influence associated with the random choice of the training samples, 100 repeated ML-based DA predictions are done, with the results shown in figure 3(d). It shows that the maximum fluctuation of the predicted DAs are comparably small relative to the DA size, suggesting high stability of the ML-based method. The average predicted DA accords with the exact DA, with accuracy of close to 95%. The prediction accuracy is counted by calculating the rate of the number of accurately predicted initial conditions over the number of all unlabeled initial conditions.

For comparison, an alternative method of directly estimating DA based on the same sparsely sampled long-term tracking data is also studied. In this method, we first connect the outermost labeled surviving particles and the innermost labeled lost particles, which suggest an underestimated and an overestimated DA, respectively. The directly estimated boundary of DA is the average of the two connected lines (see details in appendix B). By randomly selecting different ratio of labeled samples, we compare the prediction accuracy of the direct estimation method and the ML-based method in figure 4. It suggests that with a small ratio of labeled samples (e.g., less than 40%), the ML-based method allows higher prediction accuracy, implying that the ML model can provide additional insight to reconstruct the boundary of DA. When the labeled ratio increases, the estimation accuracy of the direct estimation method significantly increases, while the prediction accuracy of the ML-based method increases slowly and saturates at a value of approximately 96%.

Besides random selection of labeled samples, we also try to select labeled samples in a uniform way, i.e., we assign an index to each samples by their polar angles and amplitudes from small to large and uniformly select the labeled samples according to the indices. The results in figure 4 imply that using uniformly selected labeled samples can result in better prediction accuracy of DA than using random selection for both the direct estimation method and the ML-based method, suggesting the importance of the selection of training samples in the DA prediction problem. The prediction accuracy became more stable when the labeled ratio is large with the uniform selection, e.g., when labeled ratio is 30%–65% and 70%–95% for the ML-based method and 40%–65% and 70%–95% for the direct estimation method, the prediction accuracy remains the same. When the labeled ratio is up to 70%, both the direct estimation method and the ML-based method reach their best prediction performance with accuracy of 99% and 100%, respectively.
The direct estimation method cannot reach 100% accuracy because when the particle loss along amplitude is discontinuous, the estimated DA boundary based on the connected lines of the outermost surviving particles and the innermost lost particles will be slightly inaccurate compared to the exact DA. This slight inaccuracy in the estimation may be further improved by removing the edges that contain lost particles from the graph of surviving particles. While with the ML-based method, all particles can be correctly classified. When the labeled ratio is as small as 5%, the prediction accuracy of the ML-based method is about 95%. To obtain the same accuracy (i.e., 95%), the direct estimation method needs a labeled ratio of about 25%, which is five times of the ML-based method. In a single evaluation of DA, the direct estimation method with a labeled ratio of 25% would be a good method to fast predict DA, while in the design stage of a storage ring accelerator needing massive DA evaluations, the ML-based method can further accelerate the computing of DA by a factor of 5. For the ML-based method, a labeled ratio of 5% that can reduce the computing cost of DA by an order of magnitude appears sufficient and promising, which allows a good balance between the calculation cost and prediction performance.

Note that the DA computation results have a strong dependence on the physical model of a storage ring. We test the performance of the ML-based methods with modified lattices of the HEPS storage ring, where certain dynamical effects are included. Specifically, three cases are considered, off-momentum DA, DA in the presence of physical apertures of individual elements instead of a uniform limit of 1 m, and DA in the presence of magnetic field errors, respectively. Figure 5 shows the corresponding exact DAs and the average predicted DAs among 100 repeated tests (with labeled ratio of 5%), respectively. It can be clearly seen the DA size changes as the model is modified. And, in all three cases, the DA prediction accuracy of the ML-based method remains as high as about 95%. It appears that the proposed method is highly independent of the model. Actually, this is also demonstrated in another test, where the strengths of sextupoles and octupoles in the lattice are varied in a large range to search for a larger DA.
Figure 6. Comparison of prediction performance obtained with five ML methods. The trajectory length is defined as the number of super-periodic cells in the HEPS, which represents the length of the data feature in the learning task. A trajectory length of 0 represents only using initial conditions of particles to predict whether they are surviving or lost.

Figure 7. Three methods of directly estimating DA for the bare lattice of the HEPS with a labeled ratio of 5%. The solid green lines in (a)–(c) represent the connected line of the innermost lost particles, the connected line of the outermost surviving particles, and the average of above two connected lines, respectively. The black solid line represents the boundary of the exact DA. The blue and red points represent labeled particles that are surviving and lost after 1000-turn tracking, respectively, which are uniformly selected from particles on specific angles.

4. Conclusion

We have introduced a novel ML-based method of predicting DA, which can accurately predict the stability of massive particle motions in a storage ring, based on only a small amount of long-term particle tracking results together with a huge amount of short-term tracking results. We demonstrate that it is feasible to achieve high accuracy of approximately 95% with only 5%–10% of long-term tracking results. Considering that the computing time for training ML model and short-term particle tracking is negligible compared with the long-term particle tracking, the proposed ML-based method would allow an order of magnitude faster DA evaluation compared to conventional DA computation. Moreover, we show that this method is independent of concrete magnetic lattices of the storage ring and the prediction accuracy of the proposed method remains high as the lattice is modified. This is inherent in the method based on the fact that it concerns only the correlations between the stability of motions and short-term trajectories, which is actually not related to the concrete models of a storage ring.

Extensive DA evaluations are required in many cases, for instances, the error tolerance investigation for a specific storage ring design, and especially lattice and DA optimization in a preliminary design stage of a storage ring based-facility. In the latter case, due to the more efficient and lattice-independent DA
evaluation enabled by this novel method, it would become feasible to systematically explore ultimate performance of a specific lattice structure in a reasonable time, and implement thorough comparisons among different lattice structures to reach an final design with optimal balance among different design objectives.

Determination of motion stability is a fundamental issue not only for accelerator physics, but also among a large area of modern sciences such as celestial mechanics and plasma confinement. Besides the applications to particle accelerators, it is believed this model-independent ML-based method has the potential to be transferred to other similar complex dynamical systems. We have shared a demo for this method on GitHub (https://github.com/wanjinyu/ML_DA) and hope it could be helpful to perform related studies in accelerator physics and other fields.

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Data availability statement

The data generated and/or analysed during the current study are not publicly available for legal/ethical reasons but are available from the corresponding author on reasonable request.

Appendix A. Comparison of multiple ML methods

To explore better DA prediction performance, we compare five supervised ML methods, which are RF, GPC, ANN, SVM, and XGBoost, respectively. The settings of main hyperparameters for above five ML methods are determined by systemized grid search. For RF, the number of decision trees is set to be 300, and the maximum depth of the tree is set to be 7. For GPC, the radial basis function is used as its kernel function, and the maximum iteration number for approximating the posterior during predicting set to be 100. For ANN, a network structure with two hidden layers having 32 and 64 neurons, respectively, is adopted. The rectified linear unit is used as the activation function of the hidden neurons. For SVM, the penalty coefficient is set to be 1 and a radial basis function is used as its kernel function. For XGBoost, the number of boosted classifier is set to be 100, the minimum loss reduction required to make a further partition on a leaf node of the tree is set to be 0.6, and the subsample ratio is set to be 0.8. The random state for RF, GPC, SVM and XGBoost is set to be 0 such that only the choice of training samples can affect the results among the repeated tests. The training of RF, GPC, SVM is implemented on an open source ML library Scikit-Learn [53], and ANN is trained on another open source ML library Keras [54]. For the training of ANN, the maximum number of training iterations is set to be 3000 with a training batch size of 32. The validation ratio is set to be 0.1 to avoid overfitting.

Besides the comparison of using different number of training samples, we also investigate the influence of the length of trajectory that is the data feature on the prediction accuracy. In this scenario, we count the length of trajectory by the number of super-periodic cells that the particle passes through. Figure 6 shows that for RF, the prediction accuracy can be improved by using longer motion trajectories when the trajectory length is less than 10, while further increase can hardly improve the accuracy. It is also observed that the prediction accuracy of GPC may even decrease when more motion information, i.e., longer motion trajectories in the phase space, is provided. This may be because of the sensitivity of its hyper parameter settings to specific learning tasks. To obtain the best performance, the hyper parameter settings may need to be further optimized when the learning task is slightly changed, especially when the length of data feature vector is changed. Nevertheless, with a labeled ratio up to 10%, all tested ML methods imply similar prediction performance. Among the tested methods, RF and ANN show slightly higher prediction accuracy. Considering the training time of ANN is much longer than that of RF, i.e., ~30 s and ~0.1 s, respectively, RF is finally adopted in this study to investigate the nonlinear dynamics of storage ring accelerators.

Appendix B. Direct estimation of DA

Besides the ML-based method, it is also possible to directly estimate the DA from the sparsely sampled long-term tracking results without any aids of ML techniques, which can be called a direct estimation
method. For the purpose of this paper, it is necessary to find a fair baseline of the direct estimation method and to compare the baseline with the proposed ML-based method. Here we test three methods of directly estimating the boundary of DA. The first method is to connect the outermost surviving particles (see figure 7(a)), the second method is to connect the innermost lost particles (see figure 7(b)), and the third method is to take the averaged line of the former two connected lines as the boundary of DA (see figure 7(c)). Note that the results in figure 7 is based on the uniformly selected labeled samples on specific angles, which are 0, π/6, π/3, π/2, 2π/3, 5π/6 and π, respectively. If the labeled samples are randomly selected from all particles, the directly estimated DA boundary would be very jagged. The connected lines of the outermost/innermost surviving/lost particles obviously under-estimate/over-estimate the size of DA. While when the two connected lines are averaged, the estimated DA boundary can be closer to the exact DA boundary. Based on the test results, we choose the averaged line as the directly estimated boundary of DA for comparison.

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