A Literature Review of the Efforts Made for Employing Machine Learning in Synchrotrons

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Significant challenges of new generations of synchrotrons

Data deluge

- The speed of doing experiments and the amount of raw data collected during each experiment is increasing (Wang et al., 2018, 2021)
- Each light source can produce one petabyte of data per day (PHYSICS TODAY, n.d.) or three-petabyte data just in one experiment (Alizadeh & Khaleghi, 2017).
- The manual analysis of such massive data volumes is no longer possible and this prevents the delivery of new science from analyzing many collected raw data (Wang et al., 2018, 2021; PHYSICS TODAY, n.d.)

The new rings drive for significantly lower emittances

- The beam dynamics in the rings become extremely nonlinear, causing smaller dynamic aperture and momentum aperture (Huang et al, 2021).
- The extremely small emittance in rings needs much higher beam stability (Huang et al, 2021)
- In this situation, a good understanding of environmental factors' impacts on the accelerator and beams is essential (Huang et al, 2021)

ML advantages in synchrotrons

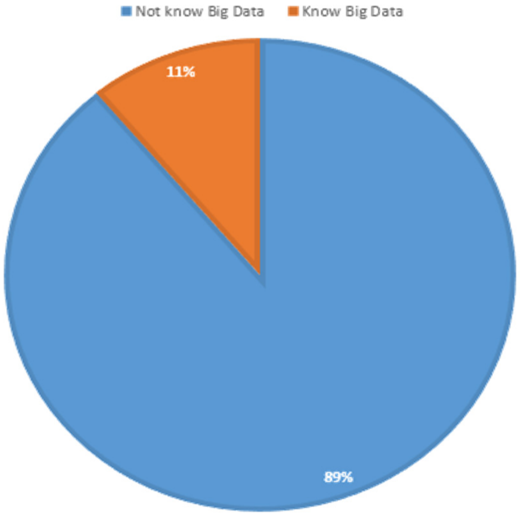
- Reducing unwanted fluctuations in the widths of the electron beams produced that prevent experimental noises obscured measurements (Leemann et al., 2019)
- Stabilizing the photon beam without the need for manual calibrations of measures (Leemann et al., 2019)
- Preventing data deluge (Campbell et al., 2021; Wang et al., 2018, 2021)
- Reducing user-in-the-loop decision-making (Campbell et al., 2021)
- Allowing users to focus on experiments at hand and best use the allocated beam time rather than manual setups and justifications (Campbell et al., 2021)
- Providing instant and straight feedback from speedy physics-based simulations (Campbell et al., 2021)
- Harnessing the brightness of light sources (Campbell et al., 2021)

Challenges of using ML in synchrotrons

- The necessity for long-term data preservation and transfer, as well as the demand for data analysis pipelines (Wang et al., 2018)
- The requirement for instant feedback helping onsite scientific and technical decisions during beamtime (Wang et al., 2018)
- The need for user-friendly software packages to effectively control the extensive data generated in synchrotrons experiments (Wang et al., 2018)
- The lack of remote data analysis workflows and the use of distributed resources for ML purposes. The beamtime required for a particular experiment reaches a limit. Physically visiting the synchrotron is no longer valuable (Hill et al., 2020).

Required solutions

- A cross-domain and cross-facility solution that can accelerate creating a real-time user-friendly, advanced data processing platform at synchrotrons is needed (Wang et al., 2018)
- Some studies reported that a big data center which is termed a super facility is required for data management and processing (Giovannozzi et al., 2021; Wang et al., 2018, 2021)
  - the success of ML can be increased by the explosion in Big Data, advances in computational power, particularly the use of graphics processing units, and the development of more sophisticated ML techniques such as Deep learning (Arpaia et al., 2021; Barrett & Haruna, 2020)
  - 89% of participants were not familiar with big data according to an interview conducted by Alizadeh and Khaleghi (2017) using ten light source facility members



Machine Learning

ML is widely used to make predictions or decisions, a subfield of artificial intelligence and the process of making a mathematical model without being explicitly programmed and using sample data, famous as “training data” (Giovannozzi et al., 2021; National et al., 2018).

Machine learning Techniques

Supervised learning

is valuable when pairs of input and desired output are available. An algorithm can generalize the problem from the given structured data and predict unknown input (Fol et al., 2019).

Unsupervised learning

solve the tasks where only input data is available (Fol et al., 2019)

Reinforcement learning

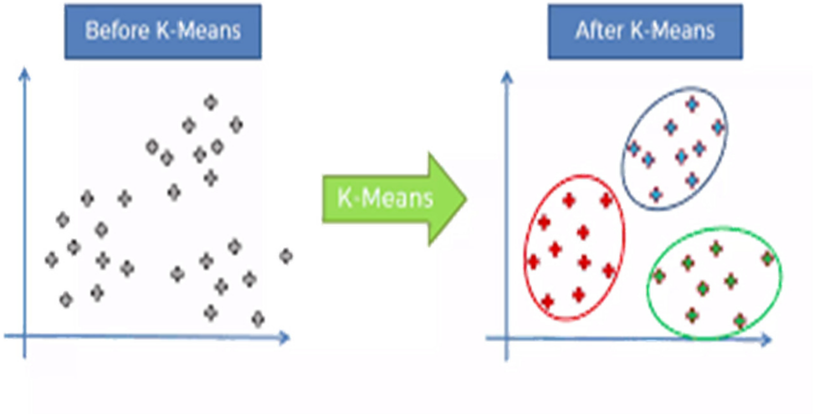
- is based on dynamic environment-agent interaction. The agent starts an action on the environment, and the environment reacts to produce a reward, which the agent uses to learn how to enhance its subsequent actions (Maffettone et al., 2021) .
- does not require a prepared data set consisting of input-output pairs since the agent learns by the continuous interaction with the environment, varying depending on the action and its dynamics (Fol et al., 2019)

Semi-supervised learning

- is halfway between supervised and unsupervised learning. Here, the algorithm is provided with both unlabeled and labeled data (Schmidt, Marques, Botti, & Marques, 2019).
- is instrumental when available data are incomplete and to learn representations (Schmidt, Marques, Botti, & Marques, 2019).

Clustering and Neural Networks (NNs)

- Clustering is categorized as unsupervised learning (needs no labeled data) (Fol et al., 2019).
  - It groups data in some clusters. The similarity between the data within each cluster is maximum, and the dissimilarity between the data assigned to different clusters is minimum (Fol et al., 2019).
- Deep learning now almost synonymous with ML to the public (Reel et al., 2021)
  - uses neural networks composed of hidden layers carrying out different operations to find and explore complex data's representations.
  - improves the performance of classifiers beyond that common ML algorithms offer, especially in the circumstances involving large datasets with high dimensions



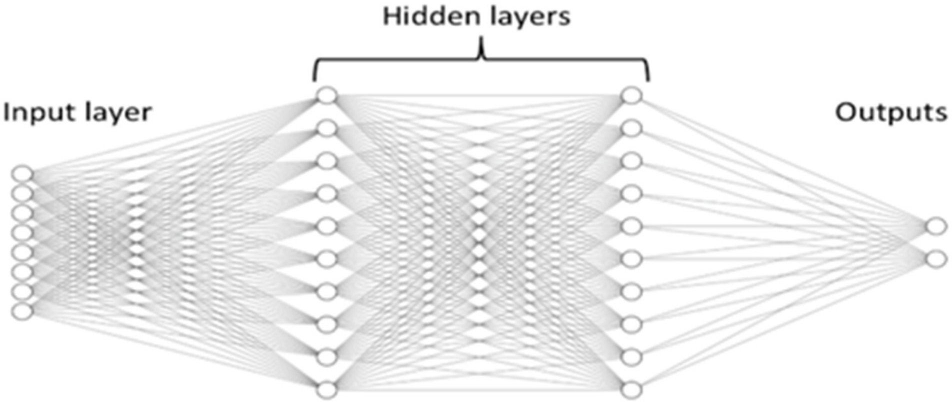


Figure courtesy Alex LeNail

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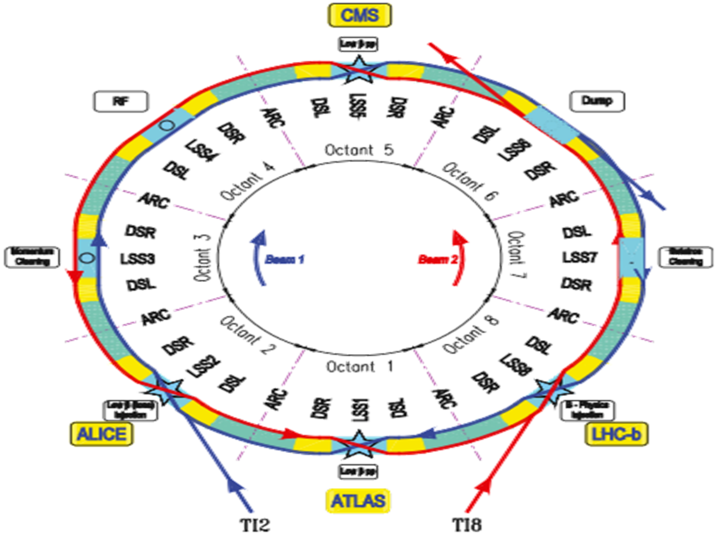
NNs in synchrotrons

- NNs in synchrotrons have attracted particular attention due to their ability to facilitate image-centric big data science and many scientific imaging problems, such as denoising, feature segmentation, image restoration, and super-resolution (Wang et al., 2016; Wang et al., 2018; Liu et al., 2019).
- can explore nonlinear and dynamic behaviors (Reel et al., 2021)
- Image-based diagnostics can be used directly in accelerators both as outputs and inputs (National et al., 2018)
- Produce high-quality output more quickly and reduces the amount of data that must be collected (Liu et al., 2019)
- Can be easily integrated into existing computational pipelines in real time at various synchrotrons (Liu et al., 2019)
- Enable better quality images in the early stages of data acquisition (Liu et al., 2019)

The European Organization for Nuclear Research (CERN) (Arpaia et al., 2021)

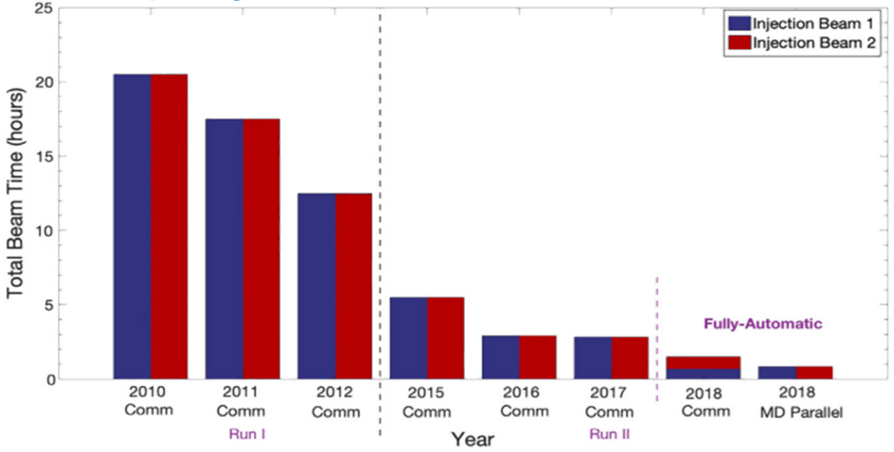
- has mainly focused on applying supervised and unsupervised ML techniques for various domains associated with beam dynamics studies
- The general ideas at CERN to utilize ML include:
  - beam commissioning of the collimation system
  - optimization of beam lifetime and losses
  - detection of collective beam instabilities
  - heating detection from pressure readings
  - numerical simulations of dynamic aperture



The European Organization for Nuclear Research (CERN) is the Large Hadron Collider (LHC) site, the largest and highest-energy particle collider globally

The European Organization for Nuclear Research (CERN) (Arpaia et al., 2021)

- Developing a fully automated software for beam commissioning of the collimation system using ML algorithms.
  - automatic alignment software successfully used throughout 2018 in the LHC operations
  - Using the software as the default software at the LHC in 2021.
  - Decreasing the time to align the collimators at injection by 71.4%, compared to the semi-automatic alignment, namely from 2.8 h to 50 minutes.
  - Incorporating the tool into the angular alignment implementation and successfully decreased the alignment time by 70%, requiring no human intervention.



NSLSII synchrotron (Campbell et al., 2021)

- Developing the Bluesky Suite, a collection of Python libraries for data acquisition and management and mainly to tackle the data “variety” challenge and streaming and real-time data analysis at user facilities
- all data and metadata generated during an experiment can be emitted in real-time to other processes in the form of ‘documents’, Python dictionaries with comprehensible schema.
- The generated documents can be distributed locally or over a network.
- All beamline hardware is accessed via a library called ophyd.
- the access to historical data is through an API called DataBroker.

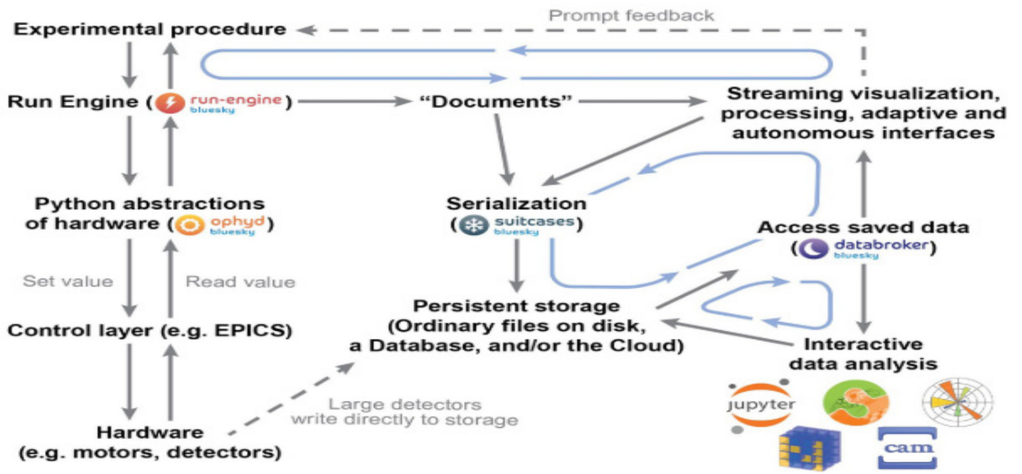
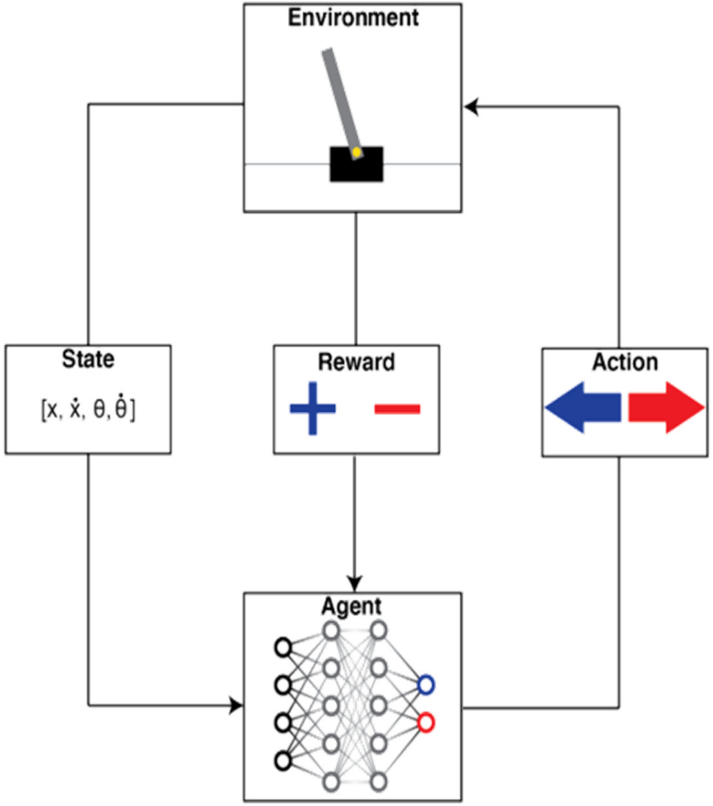


Figure 3. The relationships between the software libraries in Bluesky. Each component is individually useful, and they operate cohesively to leverage scientific Python for data acquisition and analysis. (Courtesy of Brookhaven National Laboratory).

NSLSII synchrotron (Maffettone et al., 2021)

- Used reinforcement learning methods for optimizing beamline operations.
- Python-based Bluesky suite of data acquisition software enables RL applications at a beamline.
  - Demonstrating this functionality by solving a classical RL problem, cartpole, in the Bluesky environment
- Used RL methods to address a prevalent scenario existed on high-throughput beamlines: maximizing data quality across multiple samples of different scattering strength within a limited time window.



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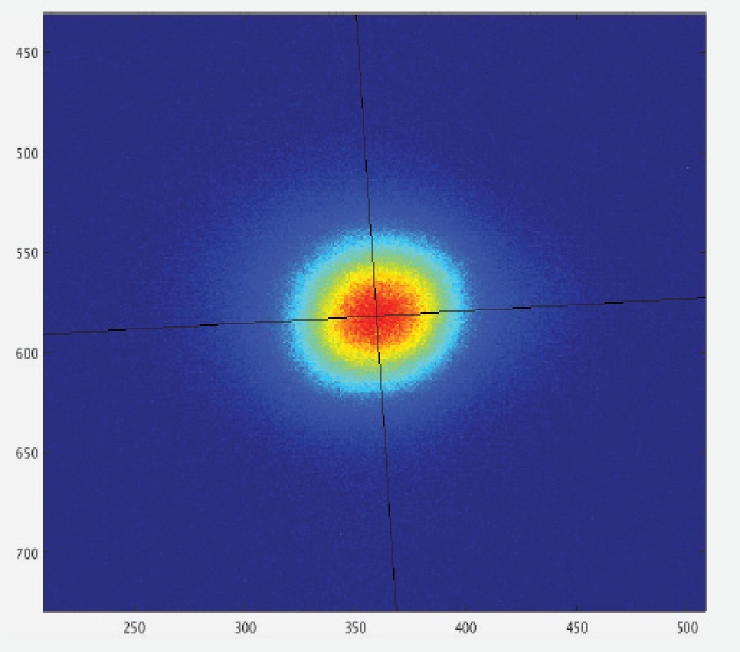
Advanced Light Source (Leemann et al., 2019)

- Simultaneously delivering light to dozens of beamlines is one of the decades-old problems in synchrotron light sources facilities
  - The main side effect of this facet is that the movements of specific insertion devices (IDs), i.e., undulators and wigglers with variable magnetic fields, cause the electron beam’s size to fluctuate.
  - fluctuations affect beamlines' performance.
  - Fluctuations are reduced using corrections based on a combination of static, predetermined physics models and lengthy calibration measurements.

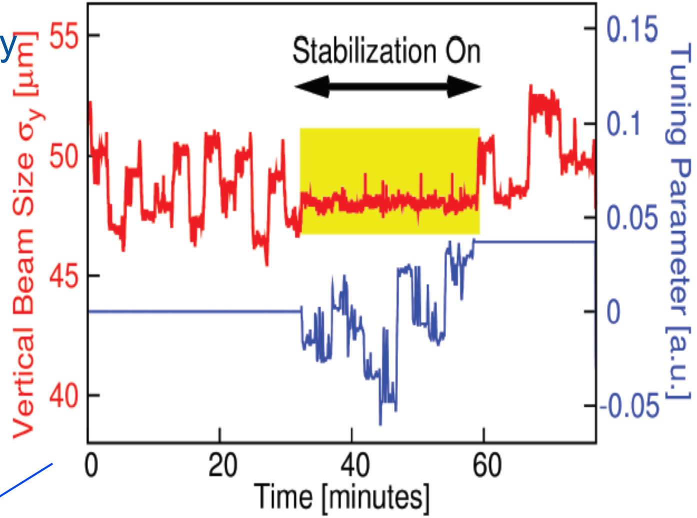


https://als.lbl.gov/machine-learning-helps-stabilize-synchrotron-light/

Advanced Light Source (Leemann et al., 2019)

Showed that NNs algorithms can predict noisy fluctuations in the size of beams generated by light sources

- NNs can correct changes before they occur (feed-forward vs. feed-back correction)
- NNs Significantly help attain order-of-magnitude enhancement instability that fulfils the requirements for different light sources
- The required data for retraining NNs can be obtained constantly, even while the feed-forward system is active
- Continuous retraining allows the neural networks to continually adapt to a drifting machine and changes in ID configurations during run periods, independent of static physics models
- The algorithm learns the complex nonlinear relationships between the ID settings and vertical beam size and made corrections to negate the blips
  - NNs stabilized the vertical beam size at 0.2 µm or 0.4% of the beam size compared to 2–3% without correction



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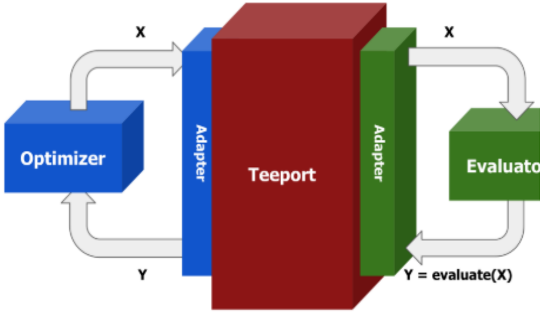
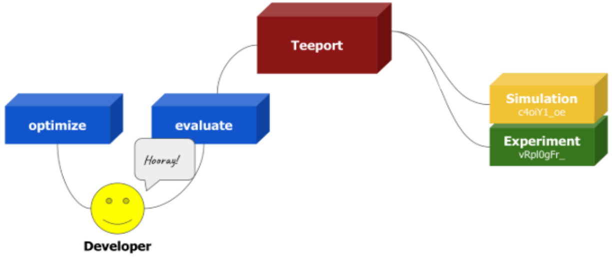
SSRL Light Source (Huang et al., 2021)

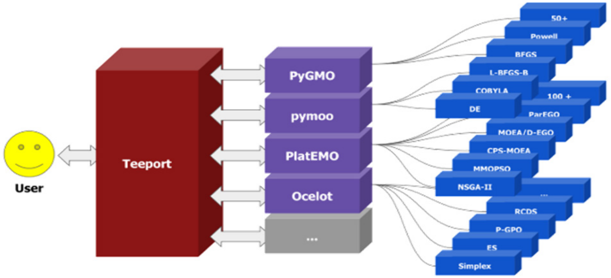
- Developing the Teeport platform to implement online optimizations
  - Teeport decouples the algorithm implementation and the experimental systems by providing a universal middle layer that communicates between the optimizer and the evaluator. They can communicate freely.



The architecture of Teeport



Fast switching between the simulation evaluator and the experimental evaluator



Teeport as a unified interface for the optimization algorithms

- Developing two ML-based global optimization algorithms for storage ring nonlinear beam dynamics optimization
  - Using the multi-generation Gaussian process optimizer (MG-GPO) to solve multiple objective optimization problems
  - Using a neural network-based method to analyze accelerator operation data and study underlying environmental factors' impact on machine performance

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BESSY II Light Source (Ramirez et al., 2019)

- Using supervised learning models trained only with 185 accelerator variables readbacks, i.e., excluding previous lifetime measurements to predict beam lifetime in a time-series fashion
- Implementing the prototypes towards self-tuning of machine parameters in different optimization cases like injection efficiency and orbit correction using deep reinforcement learning agents

Delta synchrotron (Schirmer, 2019)

- Using conventional Feed-Forward neural networks trained on measured orbits to apply local and global beam position corrections to the 1.5–GeV storage ring DELTA.
- ML techniques are an alternative approach for automated orbit correction of the DELTA storage ring.

Work by Fol et al. (2019)

- They identified four main areas that ML algorithms can be helpful, including virtual diagnostics, optimization and operation, beam optics correction, instrumentation fault detection.
- Reinforcement learning is suitable for solving complex control tasks
- Unsupervised learning is helpful for anomaly detection tasks such as detecting instrumentation defects, e.g., using clustering for faulty beam position monitors signal so that these methods can be performed directly without training in accelerator systems.

A Short Synthesis of the Reviewed Articles

Implementing a game-like project defining a reward scheme to train models to optimize a beamline efficiently to advance incorporating ML in synchrotrons
Good works have been done to facilitate data management and computing, but they are ad-hoc based on different beamlines and synchrotrons. These efforts can be converged in a seamlessly integrated platform for diverse beamlines with different requirements to provide impetus to employing ML in different operations of synchrotrons like accelerator design optimization, beam-based optimization, and analysis of accelerator operation data.
Implementing remote data analysis workflows and the use of distributed resources. With the advances in synchrotron technologies, the amount of beamtimes needed for experiments is reduced tremendously. Physically visiting synchrotrons is no longer worthwhile.
Many ML models have been developed in Python. For Python, such as Hypertext Markup Language (HTML), many existing codes are widely available for different use cases. By combining them, standalone platforms can be implemented more easily and rapidly. Some people at accelerator laboratories can be determined to focus on the application of these tools to specific problems. Many libraries for ML purposes have been implemented in Python like Scikit-learn, TensorFlow, Keras, PyTorch, etc. Python is popular among non-computer experts due to its simplicity.
For storing data for ML techniques, mainly supervised algorithms, besides providing large datasets, it is essential to give techniques for tagging data and separating valuable and useful data from less or no useful data. This work reduces the amount of data needed to be stored and improves the efficiency of ML models.

A Short Synthesis of the Reviewed Articles

Deep learning has been considered significantly mainly due to their ability to explore nonlinear and dynamic behaviors and facilitate image-centric big data science.
Less publicly available good and large datasets are available for synchrotrons practices. It can mainly reduce the speed of using ML models in particle accelerators. By providing suitable datasets at cloud-based platforms like Kaggle in a short time, a variety of solutions can be provided for a given problem.
finding the ideal machine configuration using advanced ML online optimization algorithms
Combining big data with ML is already crucial. Storing, managing, and analyzing high-volume data are challenging problems that can be solved using this combination.
In many contexts, usually, it is sufficient to use previously stored data for ML purposes. However, in synchrotrons, it is essential to develop online data streaming and management platforms because real-time usage of ML is vital for us in particle accelerators. Processing and validating data after completing experiments lead to undetected problems and prevent online steering. Online ML algorithms and data processing platforms also can reduce the amount of data needed to be stored.
The existing literature does not provide many direct comparisons between ML techniques using the same publicly available datasets. To choose the best method that suits a given question, an empirical approach investigating different proposed ML methods on the same dataset is recommended.

Conclusion

- The suitability of ML methods has been clearly shown for beam energy, brightness, stability, etc. But much is expected from further application and extension of these approaches to the most diverse beamlines at synchrotrons globally, offering advanced capabilities, exploring the most varied, time-varying, and nonlinear relationships.
- There are many efforts to provide data management platforms for machine learning model. However, these efforts are sparse and heterogeneous based on different beamlines and synchrotrons. Integrating them to propose a more efficient environment for incorporating ML in everyday synchrotron practices is useful.
- Generally, in large experimental facilities such as synchrotron, neutron, and x-ray free-electron laser (XFEL), unifying ML-ready solutions is needed such that they should be general and transferrable to different beamlines and particle accelerators.
- ML algorithms should have the capability to be used online by providing online powerful data analysis platforms. Otherwise, some errors and anomalies may not be detected, and the amount of data that need to be stored will increase.
- Feed-forward correction, evaluation, and optimization (e.g., Feed-Forward Neural Networks) are more beneficial than feedback ones for many synchrotron practices.
- In future research, the aim will be to present a more comprehensive synthesis with more details on how to use the ML in synchrotrons

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Thank You