Accurate & Confident Prediction of Electron Beam Longitudinal Properties using Spectral Virtual Diagnostics

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SLAC NATIONAL ACCELERATOR LABORATORY

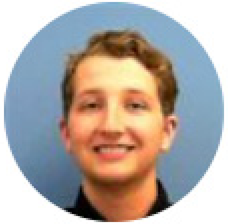
FACET-II Facility for Advanced Accelerator Experimental Tests

LCLS Linac Coherent Light Source

A. Hanuka, Nature Scientific Reports 2021

O. Convery, A. Hanuka, PRAB 2021

Thanks to the wonderful team!



O. Convery
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Outline

1. ML-based virtual diagnostics (VD) – Motivation & Background.

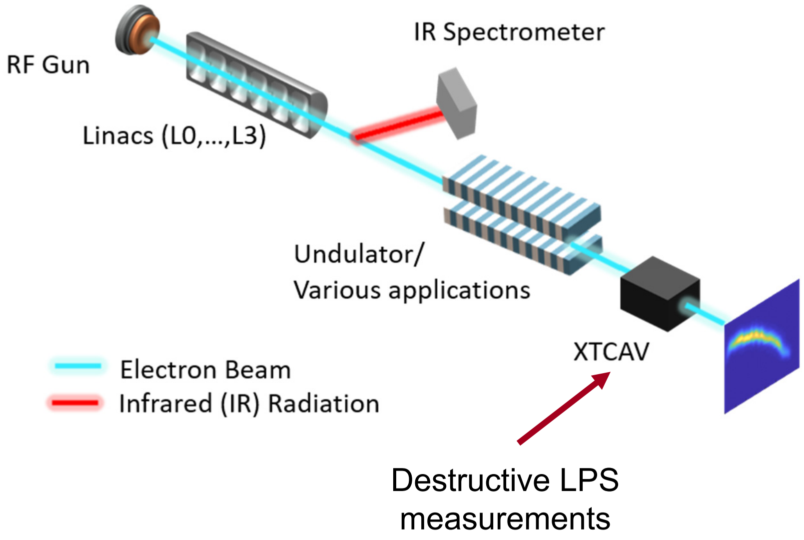
2. Spectral virtual diagnostics – 3 case studies:
    - Improved accuracy over scalar VD (LCLS)
    - Shot-to-shot prediction of fine features (LCLS-II)
    - Going beyond current diagnostic resolution (FACET-II)

3. Incorporating uncertainties – Methods & Results.
    - OOD robustness
    - Latent space interpretability

4. Summary

A. Edelen, et al., Proc NAPAC 2016
C. Emma, et al., PRAB 21, 112802 2018
A. Hanuka, Nature Scientific Reports 2021

Motivation

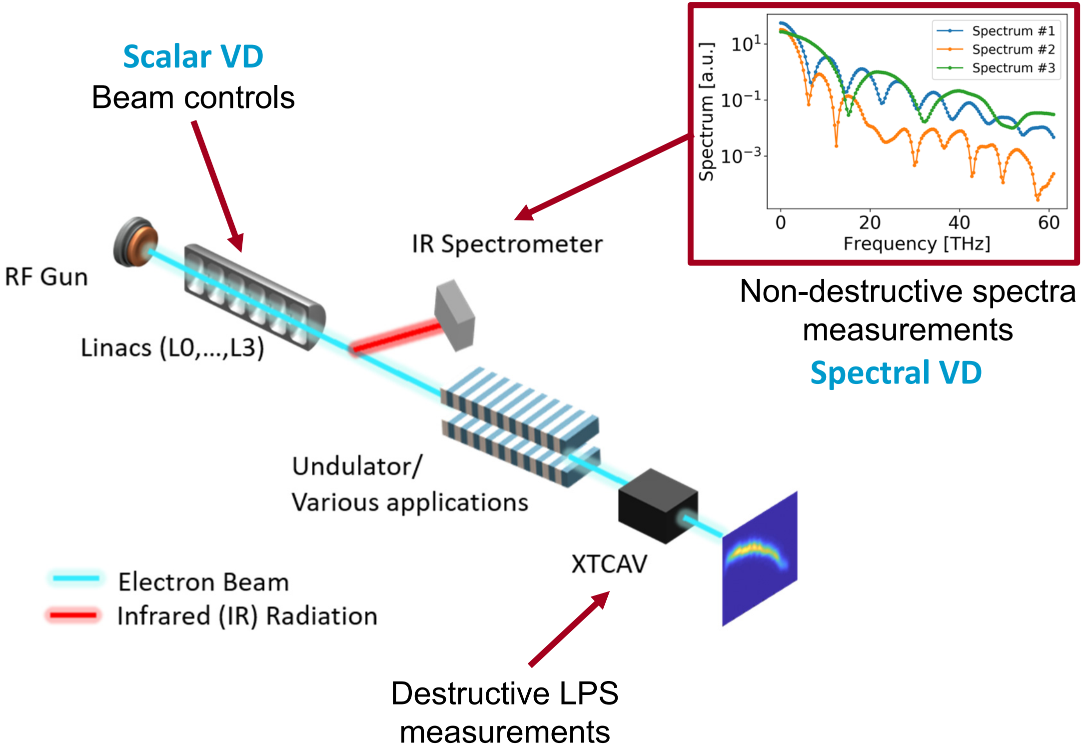


Current diagnostic methods for measuring Longitudinal Phase-space (LPS) are ***destructive***.

Machine learning based diagnostics can predict the beam properties on ***shot-to-shot*** basis ***non-destructively*** during transport and delivery to experiments.

ML-based Virtual Diagnostics (VD)

Goal: Get otherwise unavailable (single-shot) information about the beam non-destructively to improve machine characterization, optimization, and data analysis.

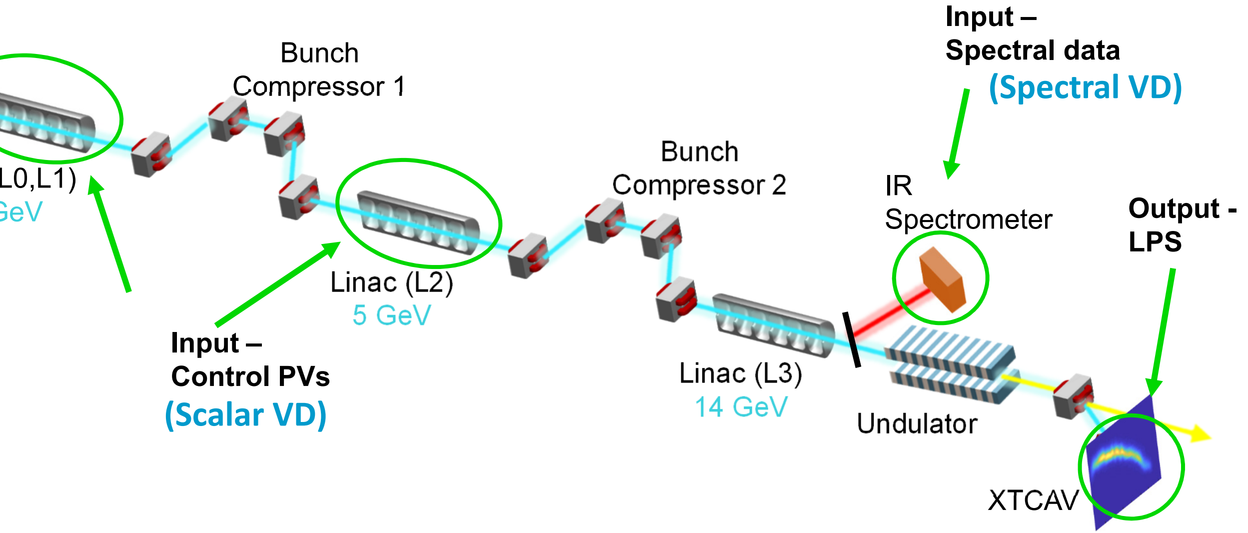


- **Supervised**: pairs of input-output
- Once trained, **fast** to execute!
- Train on measured data and/or (slow) high fidelity simulations.

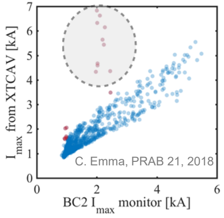
A. Edelen, et al., Proc NAPAC 2016
C. Emma, et al., PRAB 21, 112802 2018

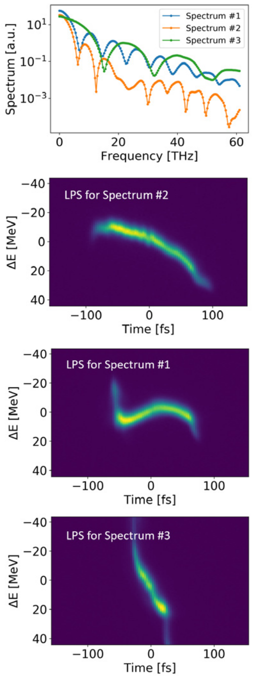
Spectral VD Circumvent the Limitations of Scalar VD

1. Readback scalars are wrong → GIGO!
2. Readback scalars are integrated signals → can not predict shot-to-shot fluctuation effects like microbunching.
3. Bad predictions can result from large discrepancy between diagnostic input (e.g. Bunch Compressor 2 current) and XTCAV current.



Shots with 'bad' prediction circled



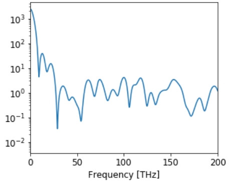


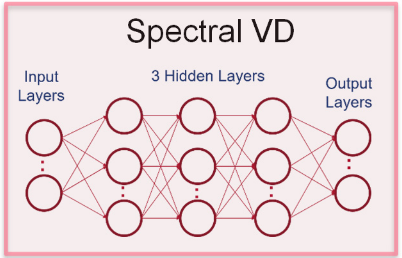
*May be exacerbated in more complicated accelerator operation modes.

Spectral Virtual Diagnostic (VD)

Neural Network – mapping millions of inputs to similarly numerous outputs.

Spectral measurement
(non-destructive)

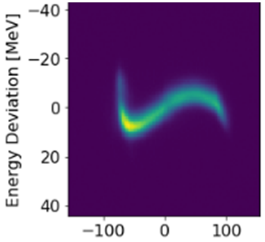




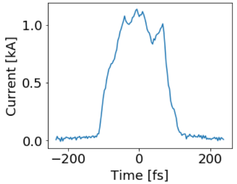
Only train **once!**

Fast prediction of beam

LPS 2D images



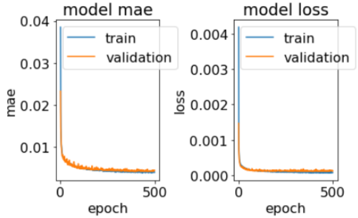
1D Current profile



VD Class in Python is easy to use

```
from VD_class import VD
vd = VD(spectrum, Iz)
Iz_predict = vd.vd_trainer(batch_size=64, epochs=500, mc=False, mbi=False)
```

```
get_model
fit_model
predict_model
```




```
loss:  7.725056511245074e-05
Validation loss:  0.00013231333176889696
Test loss: 9.489419417711619e-05
Test accuracy: 0.004323772620409727
```

https://github.com/adkoo/SpectralVD

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Accurate & Confident Predictions - Case Studies

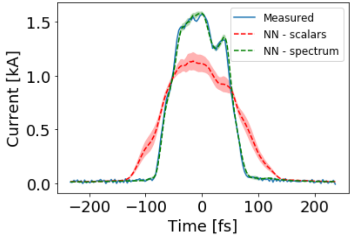
Accuracy would come from designing the neural network architecture & its training.
Confidence would come from various methods depending on the case.

Accuracy

Confidence

LCLS

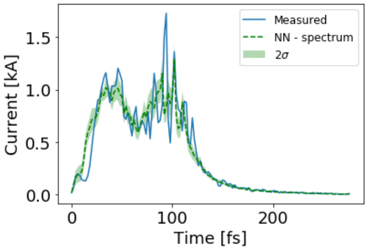
- Experimental
- 1D/2D outputs



Comparing Scalar VD vs Spectral VD

LCLS-II

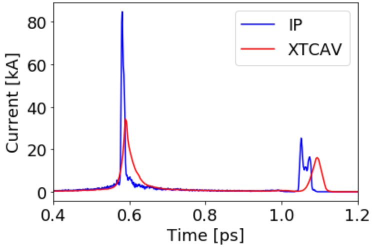
- Microbunching
- Elegant SC SXR simulation



Prediction uncertainty from ensemble

FACET-II

- 2-bunch mode
- Lucretia simulation



Correlating prediction with spectral intensity

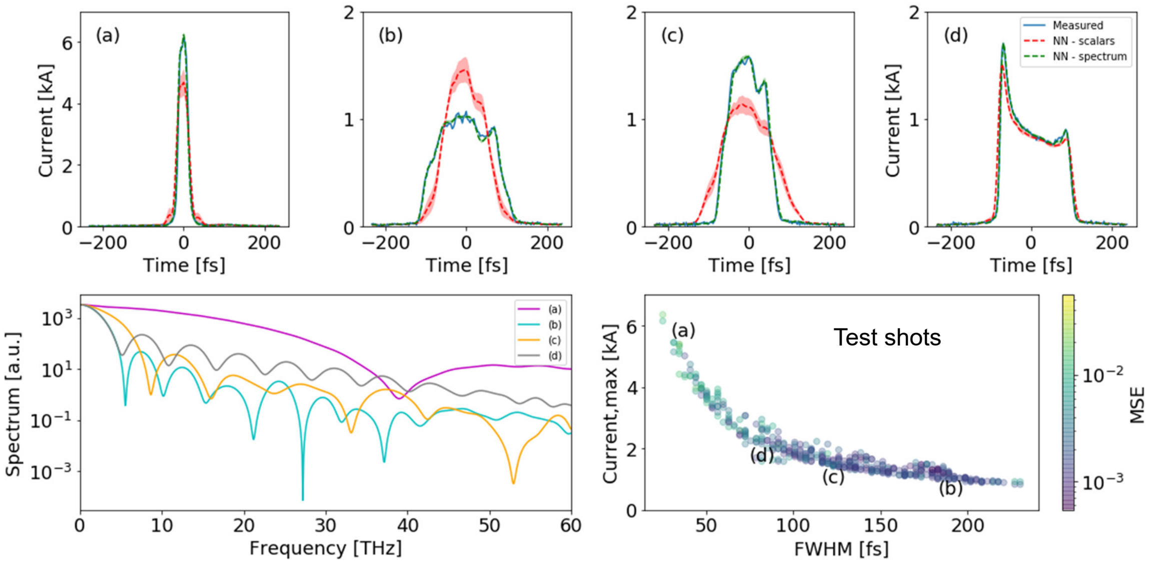
Improved accuracy over scalar VD *(LCLS)*

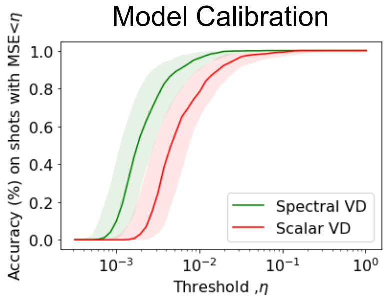
- Train ~4000 examples, Test ~600 examples.
- Scalar VD: optimized NN architecture consistently improved the results by 15%.
- Spectral VD has lower MSE than scalar VD.

LCLS Experiment:

Machine parameters scanned:
L1s phase from -21 to -27.8 deg
BC2 peak current from 1 to 7 kA

Inputs to Scalar VD:
L1s voltage & phase,
L1x voltage, BC1 and BC2 current

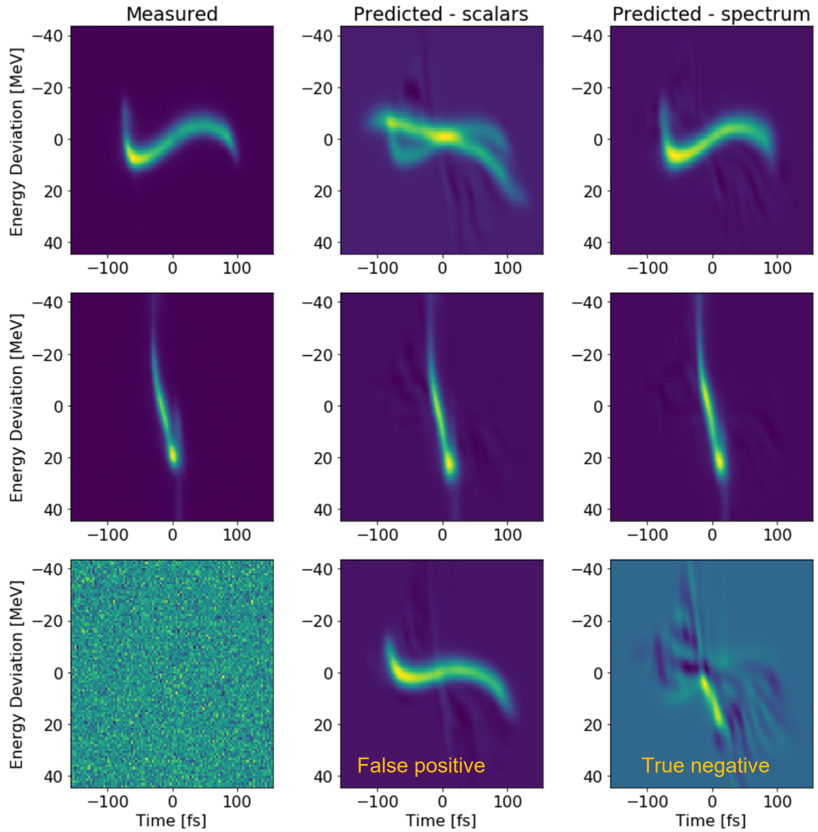




Spectral VD better predicts LPS images *(LCLS)*

- Improved accuracy of the spectral VD*.

- Increased confidence from multiple diagnostic predictions.

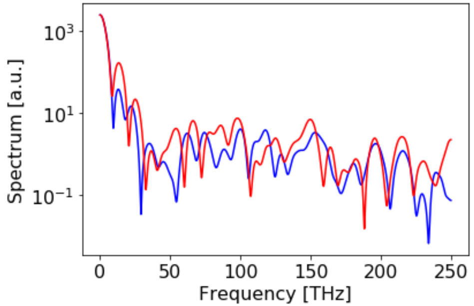


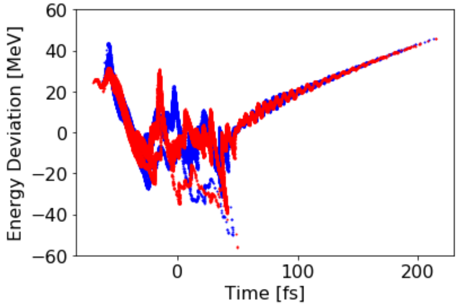
*MSE=0.054,0.079 ; SSIM=0.97,0.96 for spectral, scalars

SSIM=structural similarity index measure [0,1]

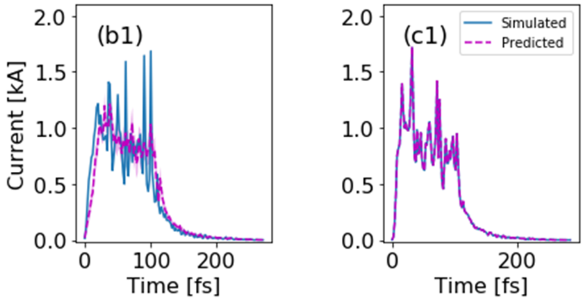
Shot-to-shot prediction of fine features *(LCLS-II)*

- LCLS-II has a 1km bypass line between the linac and the undulator → MBI is especially pronounced → seed the growth of unwanted radiation modes in the FEL.
- Two Simulations of LCLS-II SC SXR – same input, different output → Only Spectral VD can predict!





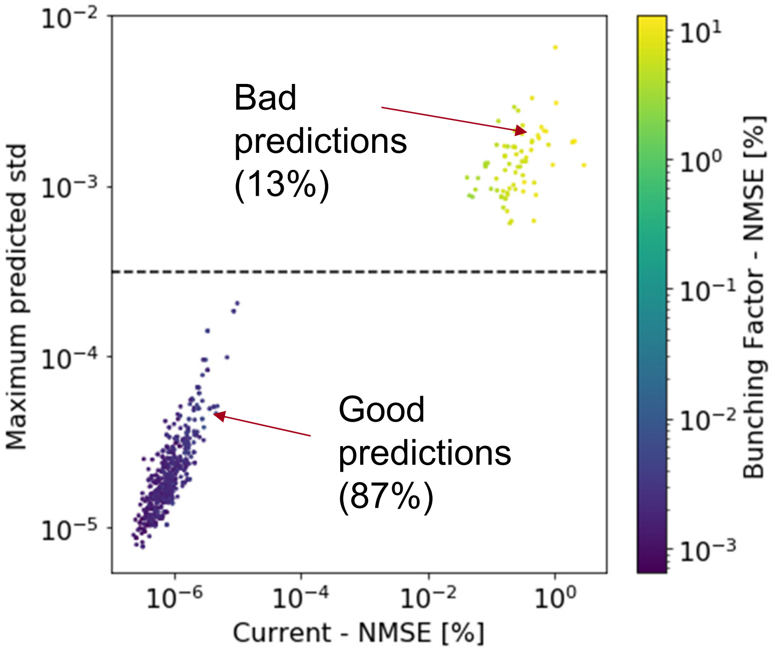
- Ensemble of NN trained on 4000 Elegant simulations → Predict current profile (NMSE=1.1%)

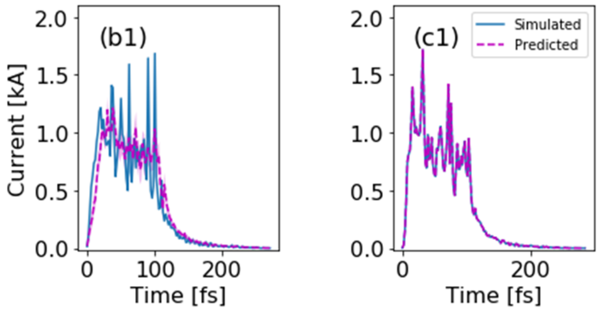


$\mathrm{NMSE}(y, \hat{y}) = \mathrm{MSE}/\sum_{i=0}^{N-1} y_i^2$

Increasing prediction's confidence *(LCLS-II)*

- Correlate max std and mean MSE from ensemble of NN with random initializations.
- Once deployed on the machine, the ground truth will not be available for calculating MSE → we can flag bad shots by setting a threshold (dashed line)

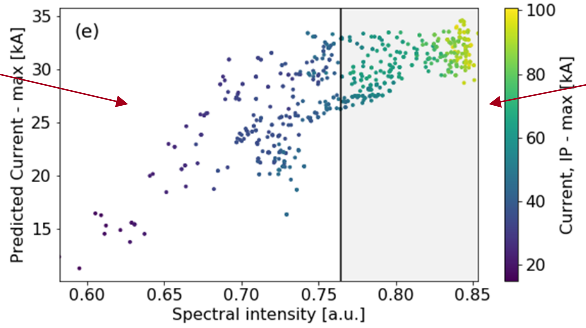




Going beyond current diagnostic resolution *(FACET-II)*

- Spectral VD resolves features that are beyond the TCAV limited resolution.

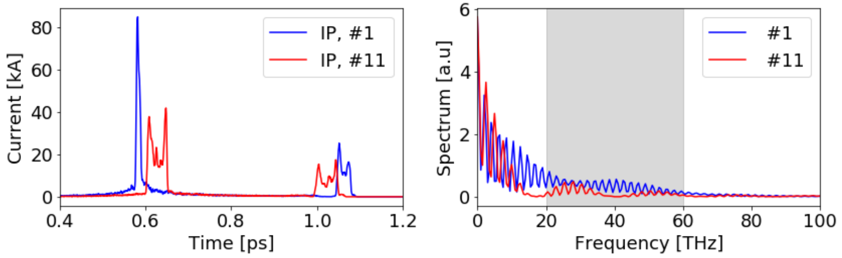
High confidence region (46%)



Shots are beyond the TCAV resolution

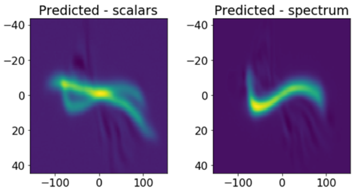
- Optimize the frequency band to distinguish between high peak current (>35 kA) shots to lower ones.

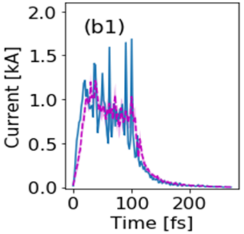
3000 LUCRETIA simulations

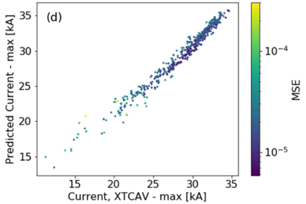


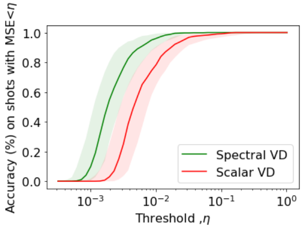
Accurate & Confident Predictions - Summary

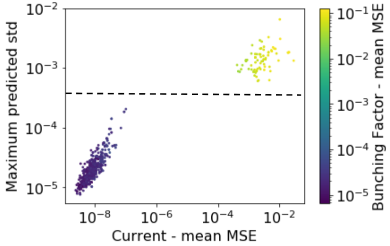
	LCLS	LCLS-II	FACET-II
	• Experimental • 1D/2D outputs	• Microbunching • Elegant SC SXR simulation	• 2-bunch mode • Lucretia simulation
Accuracy	Customized NN architecture.	Wider NN trained longer	Customized NN architecture.
Confidence	Comparing Scalar VD vs Spectral VD	Prediction std from ensemble	Correlating prediction with spectral intensity

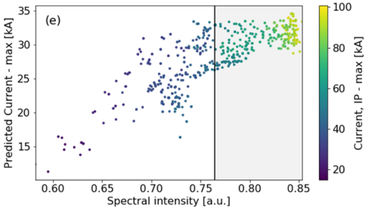












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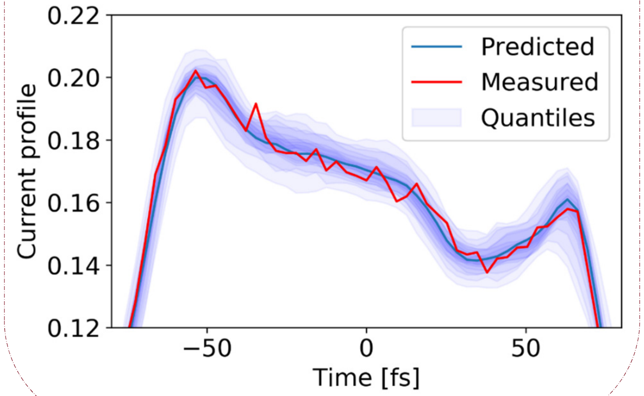
Uncertainty in particle accelerators

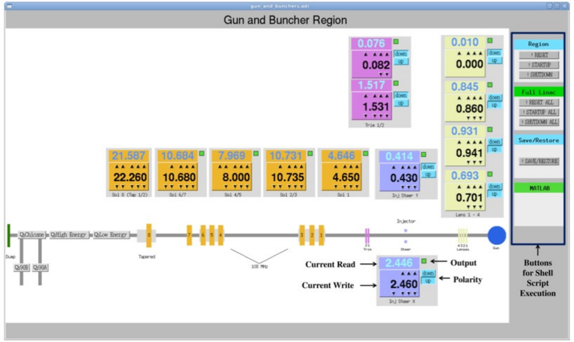
Analysis

- Provide accurate beam information
- UQ captures all possible outputs the machine can produce in a given state



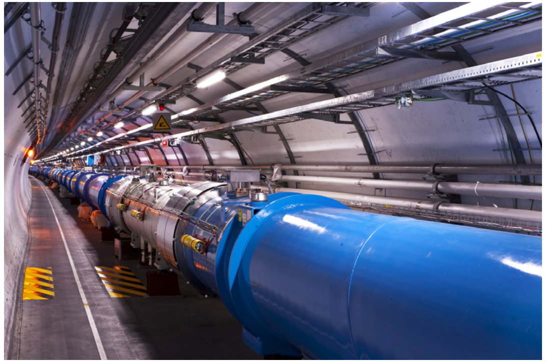
Control

- Tuning loops are often controlled by VD
- Avoiding uncertain state systems can save valuable tuning time

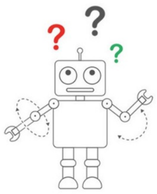


Safety

Avoiding unsafe control actions can lead to costly mistakes (Damage to walls, vacuum state, components)

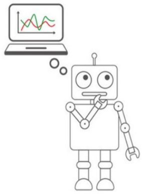


Incorporating Uncertainties – know what we don't know

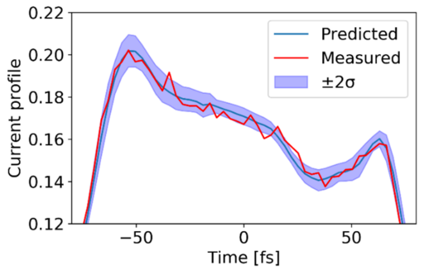


- Neural network is not aware of what it does not know!

- New shots might be out of trained distribution → prediction is unreliable.



Need estimates of std along with prediction mean.



Epistemic uncertainty:
- What the model doesn't know.
- Can be reduced by adding more data.

Aleatoric uncertainty:
- What we can't understand from the data.
- Arises from experimental error or inherent measurement noise.

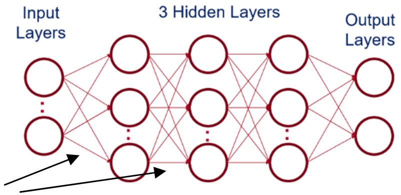
L. Tishby, International Joint Conference on Neural Networks, 1989
L. Smith and Y. Gal, UAI, 2018
B. He, B. Lakshminarayanan, and Y. W. Teh, arXiv:2007 .05864.
Lakshminarayanan, Neurips 2017

Incorporating Uncertainties – Methods

Goal: Quantify how reliable the mean prediction is.

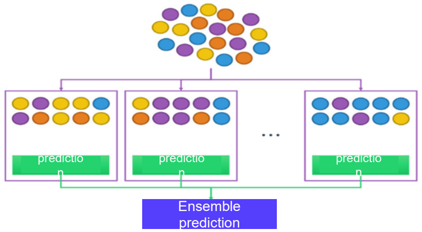
1. **Ensemble methods:** a collection of neural networks

Random initializations



Randomly initialized weights

Random data split



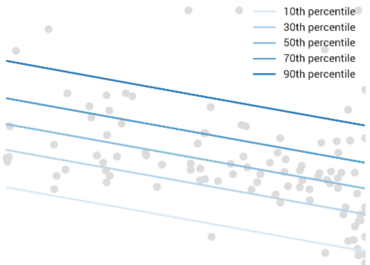
Epistemic uncertainty

2. **Quantile regression:** separate NN to predict each quantile

$$\xi_i = y_i - f(\mathbf{x}_i)$$

$$\mathscr{L}(\xi_i|\alpha) = \begin{cases} \alpha\xi_i & \text{if}\, \xi_i \geq 0, \\ (\alpha - 1)\xi_i & \text{if}\, \xi_i < 0. \end{cases}$$

$$\mathscr{L}(\mathbf{y}, \mathbf{f}|\alpha) = \frac{1}{N}\sum_{i=1}^{N} \mathscr{L}(y_i - f(\mathbf{x}_i)|\alpha)$$



Aleatoric uncertainty

Incorporating Uncertainties – Results

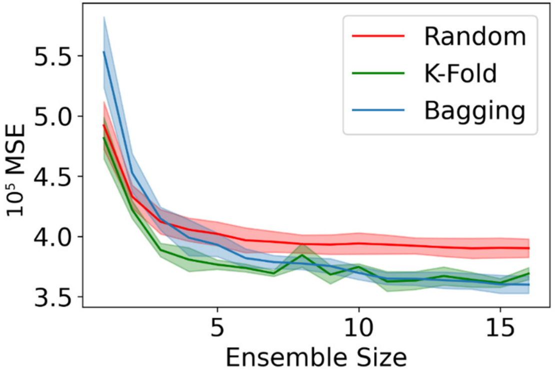
VD:
200,100,50
RELU
Batch 32
500 epochs

- Before exploring the quantified uncertainty, we found which ensemble method yielded the best MSE on the mean prediction.

Random initializations

K-fold = random subsets of data (w/o replacement)

Bagging = random initialization + random "bags" of data (w/ replacement)



Mean Ensemble Prediction:

$$\vec{L}_{\text{predicted}} = M^{-1} \sum_{m=1}^{M} \vec{l}_{\text{predicted},m}$$

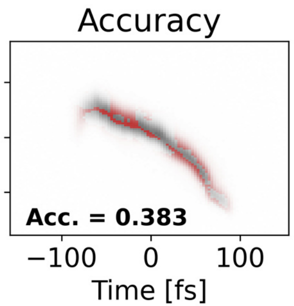
Predictive Standard Deviation:

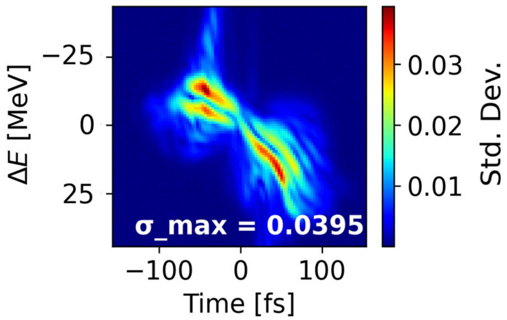
$$\sqrt{M^{-1} \sum_{m=1}^{M} (\vec{l}_{\text{predicted},m} - \vec{L}_{\text{predicted}})^2}$$

- Accuracy evaluates how much of the measured value falls within a $\pm 2\sigma$ bounds

$$\text{Accuracy} = \frac{\sum_{t,e=1}^{T,E} \alpha_{t,e} \cdot L^2_{\text{measured},t,e}}{\sum_{t,e=1}^{T,E} L^2_{\text{measured},t,e}}$$

$$\alpha_t = 1 \text{ if } I_{\text{lower},t} < I_{\text{measured},t} < I_{\text{upper},t}$$



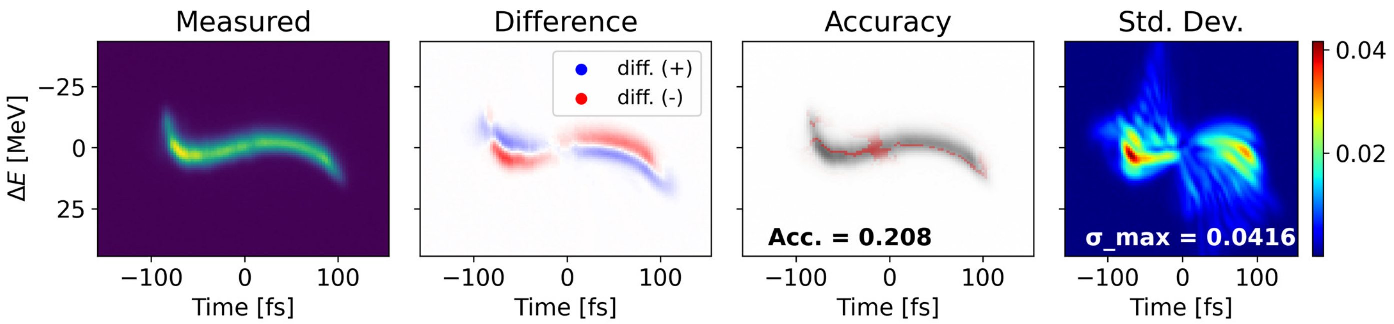


Common prediction errors with LPS images

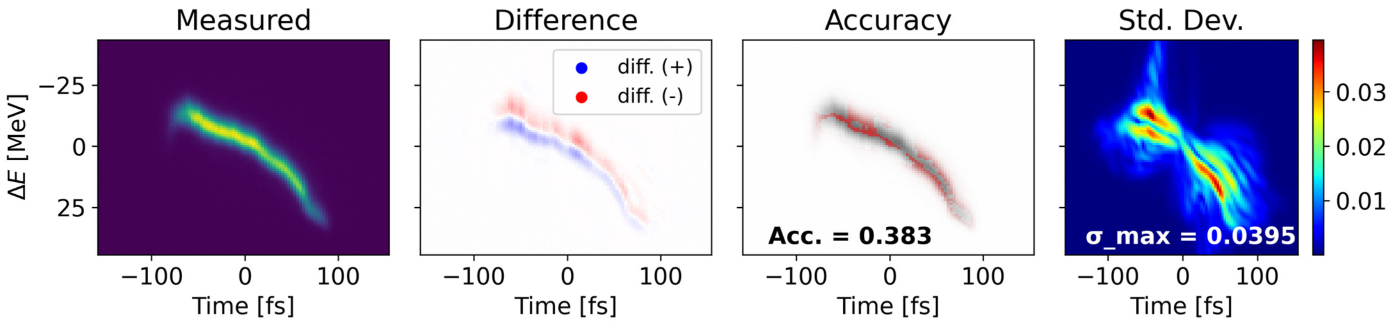
$$\text{Accuracy} = \frac{\sum_{t,e=1}^{T,E} \alpha_{t,e} \cdot L^2_{\text{measured},t,e}}{\sum_{t,e=1}^{T,E} L^2_{\text{measured},t,e}}$$

$$\alpha_t = 1 \text{ if } I_{\text{lower},t} < I_{\text{measured},t} < I_{\text{upper},t}$$

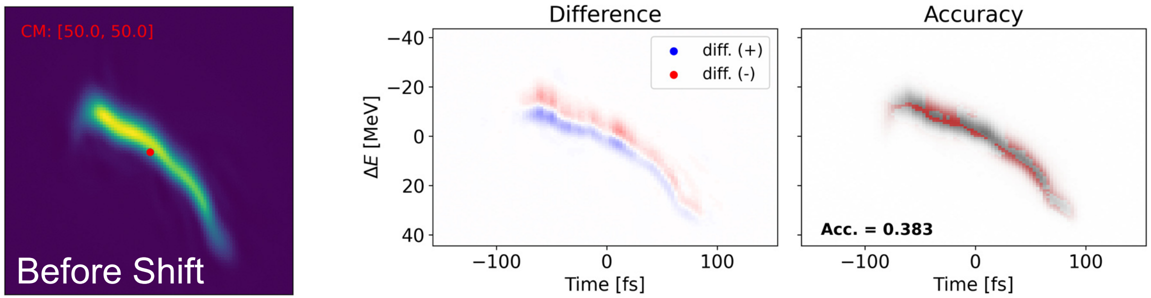
Shape error: the prediction is of the wrong shape



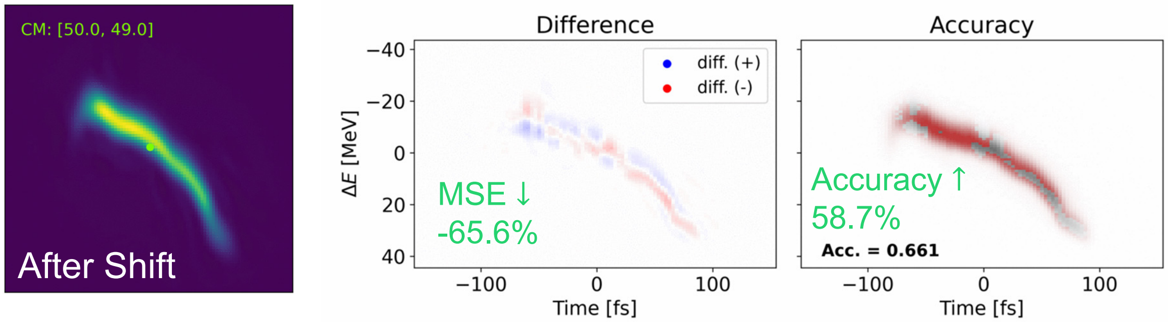
Translational error: the prediction is in the wrong place



Alleviating Translational Error



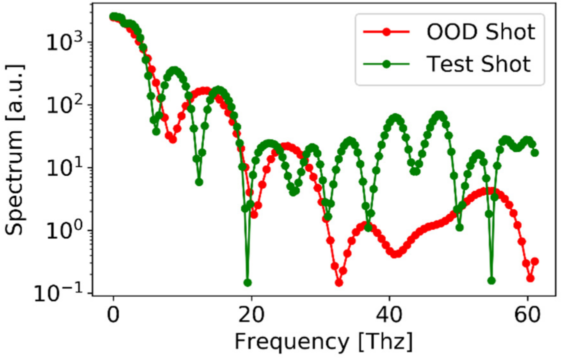
Center of Mass Correction (Prediction → Truth) during training



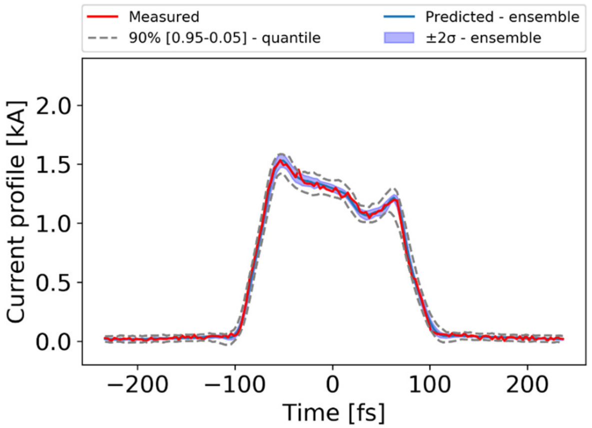
Out-of-distribution (OOD) Robustness

- Evaluate the robustness of the model by predicting an out-of-distribution (OOD) example, e.g. a change in the machine setting.
- Out-of-Distribution → Higher Uncertainty

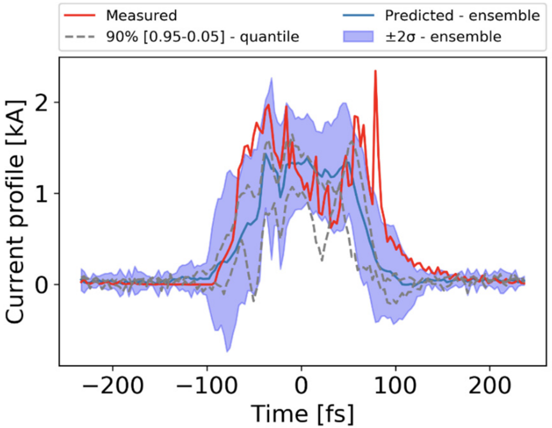
Spectral data



Test shot within the trained distribution

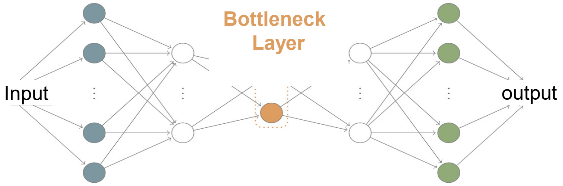


Out-of-distribution



O. Convery, A. Hanuka, PRAB 2021

Latent space interpretability



Bottleneck Layer NN architecture followed by t-SNE Clustering

Latent space of size 64 for each of the 810 test shots is reduced to 2D using t-SNE.

Shots are grouped by shape and maximum current in the latent space.

T-SNE:
- perpelxity = 30
- learning rate = 200
- 1000 iterations
- embedding vector length 64

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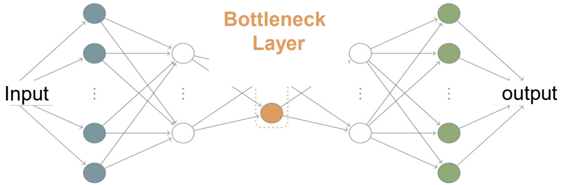

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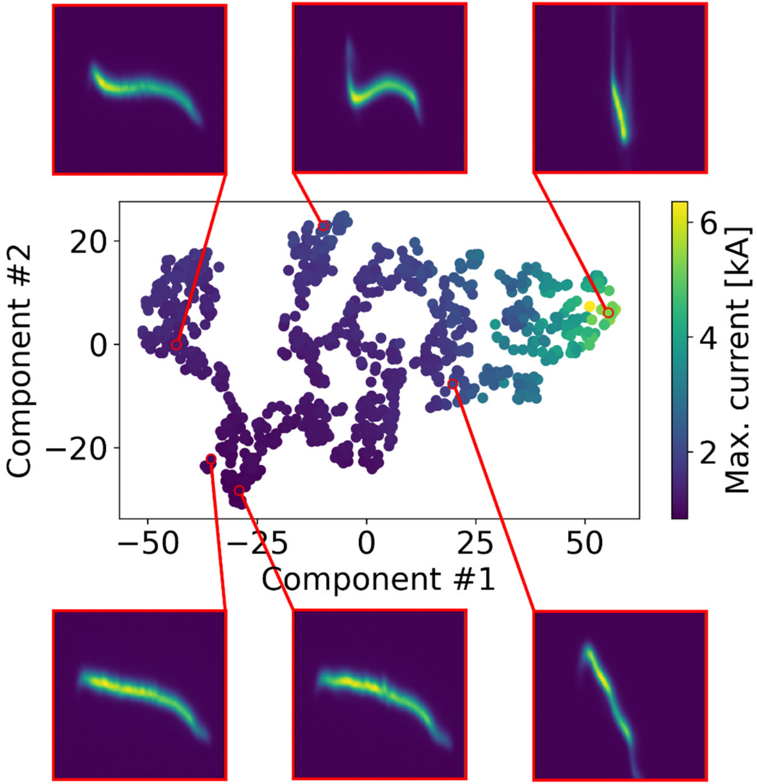

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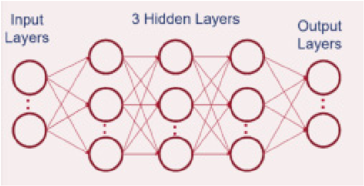
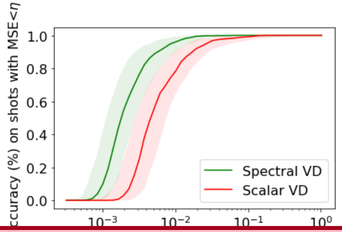
Summary

Non-destructive, shot-to-shot of bunch diagnostic

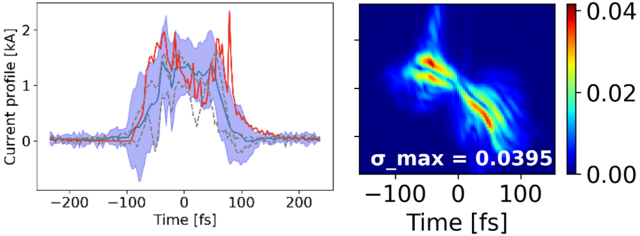


Spectral VD increases confidence & improve accuracy

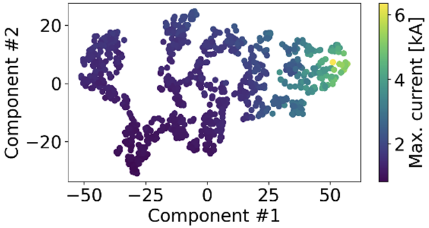


ML-based virtual diagnostic with quantified uncertainties for single shot prediction will provide additional information for analysis, tuning and control.

Quantify prediction robustness (OOD)



Bottleneck architecture to learn an interpretable latent space

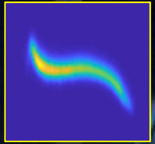


Thank You!

This work was supported by the Department of Energy, Laboratory Directed Research and Development program at SLAC National Accelerator Laboratory, under contract DE-AC02-76SF00515.

https://journals.aps.org/prab/abstract/10.1103/PhysRevAccelBeams.24.074602

https://www.nature.com/articles/s41598-021-82473-0

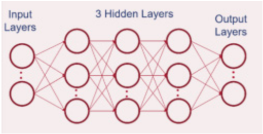


deepart.io

Summary of Virtual Diagnostics

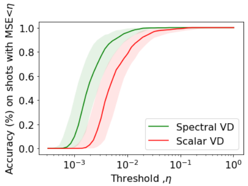
Non-destructive, shot-to-shot of bunch diagnostic during transport and delivery to experiments.

- **Fast & online** – doesn't require convoluted data processing.
- Fill in **missing** information – high peak current, repetition rate, etc.
- Understand **exotic** configs – by combining ML model with simulation.
- **Reverse** engineering of machine settings for a pre-defined current profile.



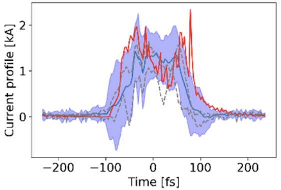
Spectral VD:

- **Increase** confidence – flag bad shots by cross check with scalars VD.
- **Improved** accuracy over scalars VD.
- In some cases is the **only** option! (e.g. microbunching)



Quantify prediction sensitivity:

- Flag **bad** predictions.
- Flag a **change** in the machine – out-of-distribution prediction.

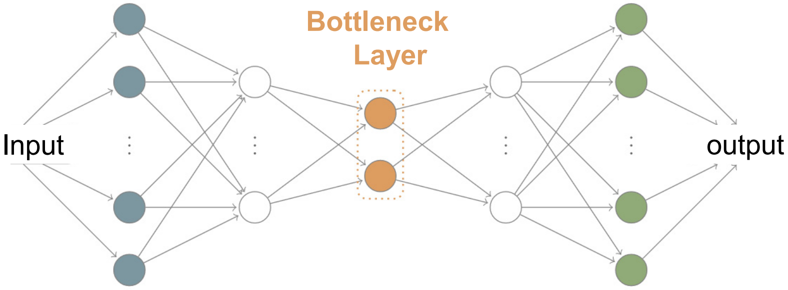


ML-based virtual diagnostic for single shot prediction will provide additional information for users, and a signal for LPS feedback, tuning and control.

Bottleneck architecture to learn important features

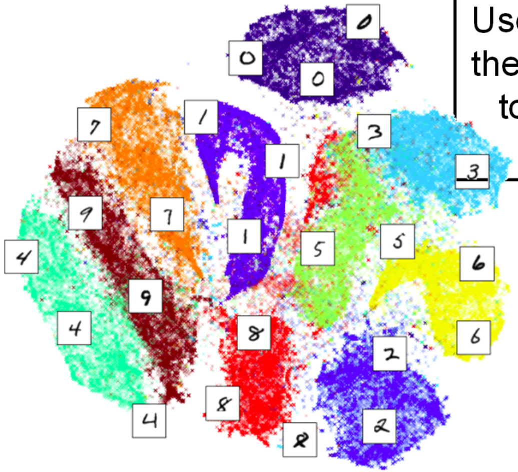
Bottleneck architectures can reduce over-fitting by decreasing the NN complexity.

Condense information about the I/O relation.



t-SNE for dimensionality reduction

T-distributed Stochastic Neighbor Embedding (t-SNE) to visualize high-dimensional space in a 2D-3D space.

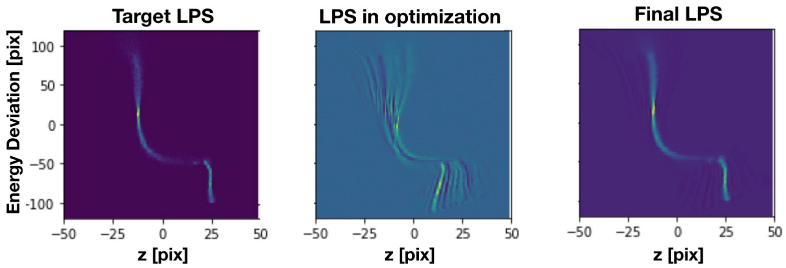


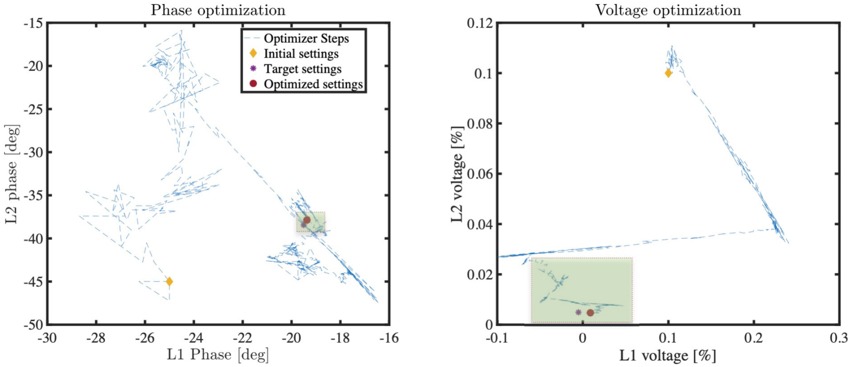
Useful for visualizing the bottleneck layers to find patterns in data.

MNIST images visualized in two dimensions.
Colors indicate the digit of each image.
https://bigsnarf.wordpress.com/2016/11/17/t-sne-attack-data/

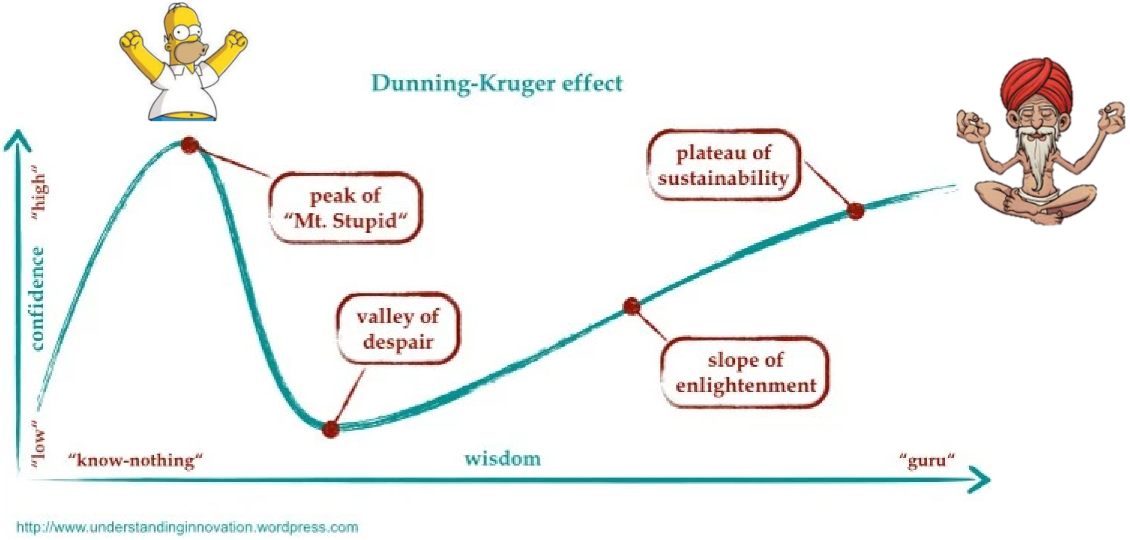
Optimization using LPS virtual diagnostics for two-bunch at FACET-II

- ML prediction of LPS used with conventional optimizer to tune L1-2 phases/voltages for desired LPS.
- Initial settings outside training set of ML model.
- Model shows ability to interpolate within training data.



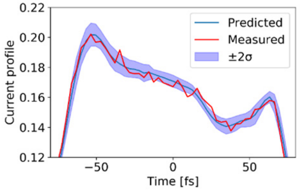


Incorporating Uncertainties – know what we don't know



- Neural network is not aware of what it does not know!
- New shots might be out of trained distribution → prediction is unreliable.

Need estimates of std along with prediction mean.



Summary

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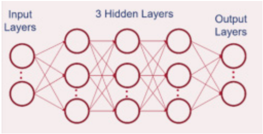

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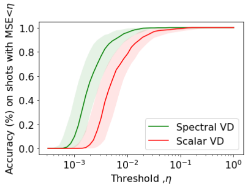

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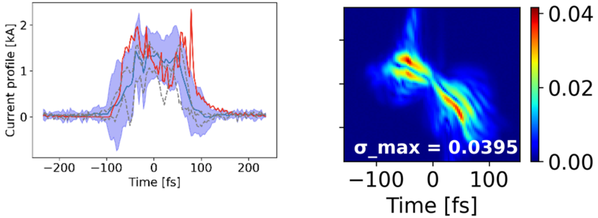
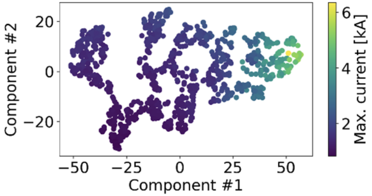


- Bottleneck Architecture to learn latent space



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