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

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FACET-II
Facility for Advanced Accelerator Experimental Tests

LCLS Linac Coherent Light Source

SLAC NATIONAL ACCELERATOR LABORATORY

U.S. DEPARTMENT OF ENERGY
Office of Science

Outline

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

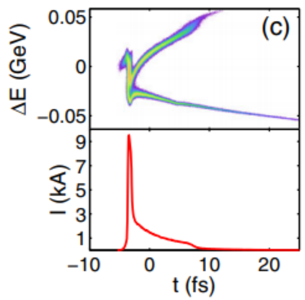
2. Spectral virtual diagnostic – 3 case studies:
    a. Improved accuracy over scalar VD *(LCLS)*
    b. Shot-to-shot prediction of fine features *(LCLS-II)*
    c. Going beyond current diagnostic resolution *(FACET-II)*

3. Incorporating uncertainties - know what we don't know.

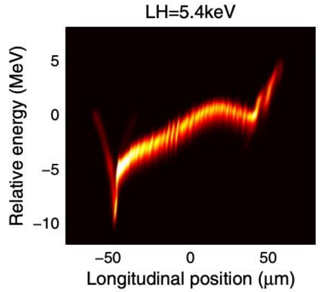
4. Summary

Motivation

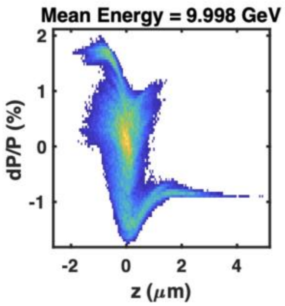
Accurate characterization of beams is required to successfully meet experimental goals.



Huang et al, PRL 119. 154801 2017

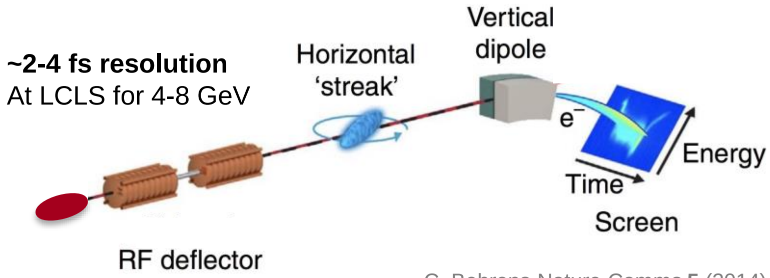


Ratner et al., PRSTAB 18, 030704 (2015)

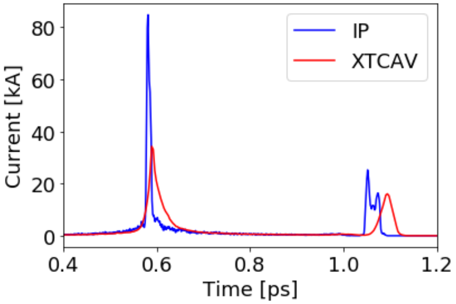


G. White, HEP ABP Workshop #1 2019

Current diagnostic methods for measuring LPS are destructive or have insufficient resolution.



C. Behrens Nature Comms **5** (2014)

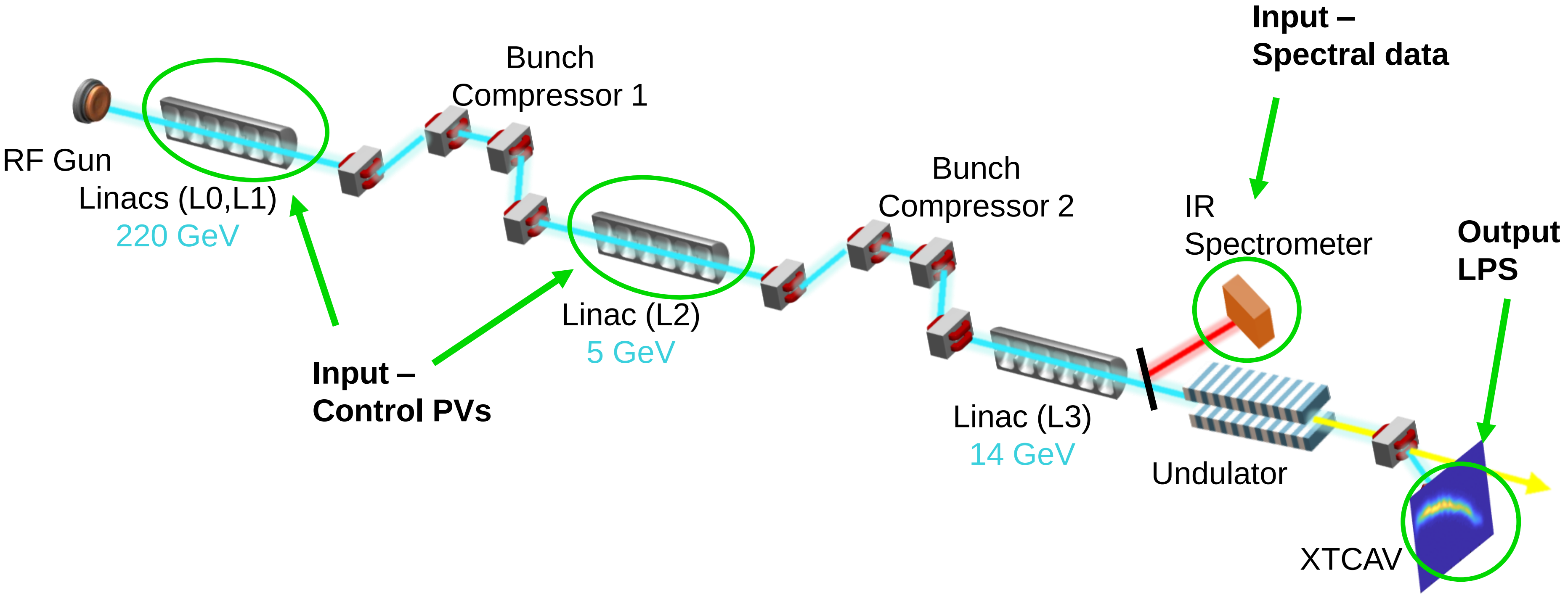


G. White, HEP ABP Workshop #1 2019

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

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



- 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

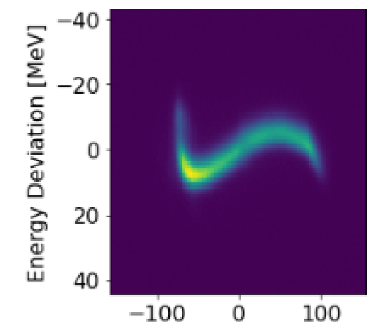
Background: Scalars Virtual Diagnostics (VD)

Measured machine inputs (non-destructive)

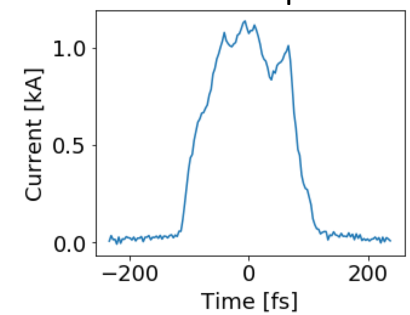
Control PVs (scalars)

Linac phase / amp → Scalars Virtual Diagnostic

LPS 2D images



1D Current profile

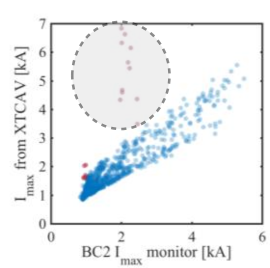


Limitations of Scalar VD:

1. Readback scalars are wrong → GIGO!

2. Readback scalars are integrated signals → cannot predict shot-to-shot fluctuation effects like microbunching.

3. Bad predictions can result from large discrepancy between diagnostic input (e.g. BC2 current) and XTCAV current.



Shots with 'bad' prediction circled

C. Emma, et al., PRAB 21, 112802 (2018)

*May be exacerbated in more complicated accelerator operation modes.

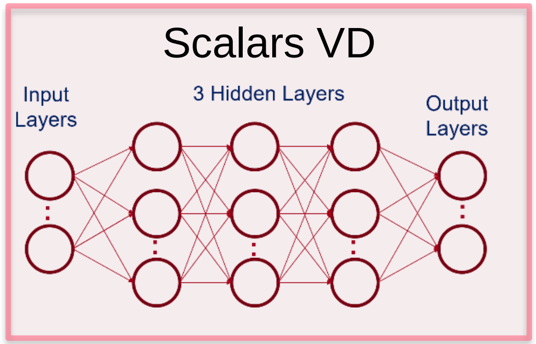
Our Solution: Spectral Virtual Diagnostic (VD)

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

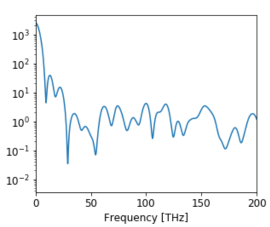
Measured machine inputs (non-destructive)

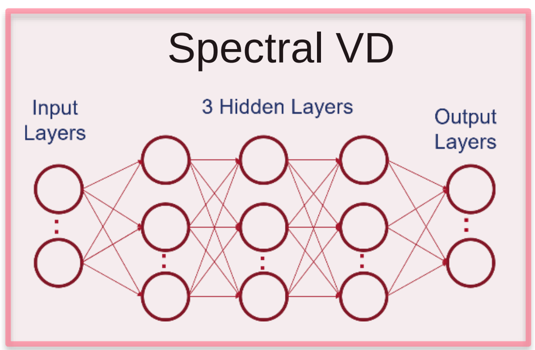
Control PVs (scalars)

Linac phase / amp

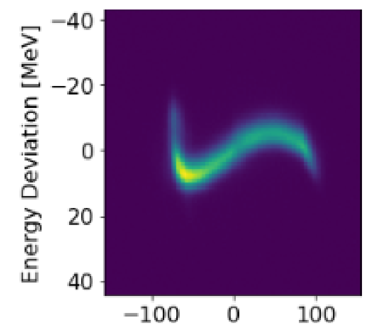


Spectral measurement

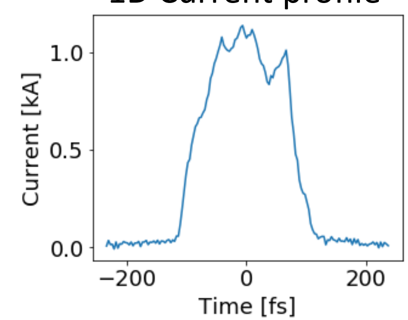




LPS 2D images



1D Current profile



Only train **once!**

Fast prediction of beam

https://github.com/adkoo/SpectralVD

VD Class in Python is easy to use

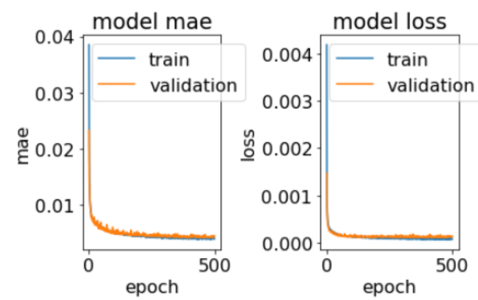
```
from VD_class import VD
vd = VD(spectrum, Iz)
Iz_predict = vd.vd_trainer(batch_size=64, epochs=500, mc=False, mbi=False)
```

get_model

fit_model

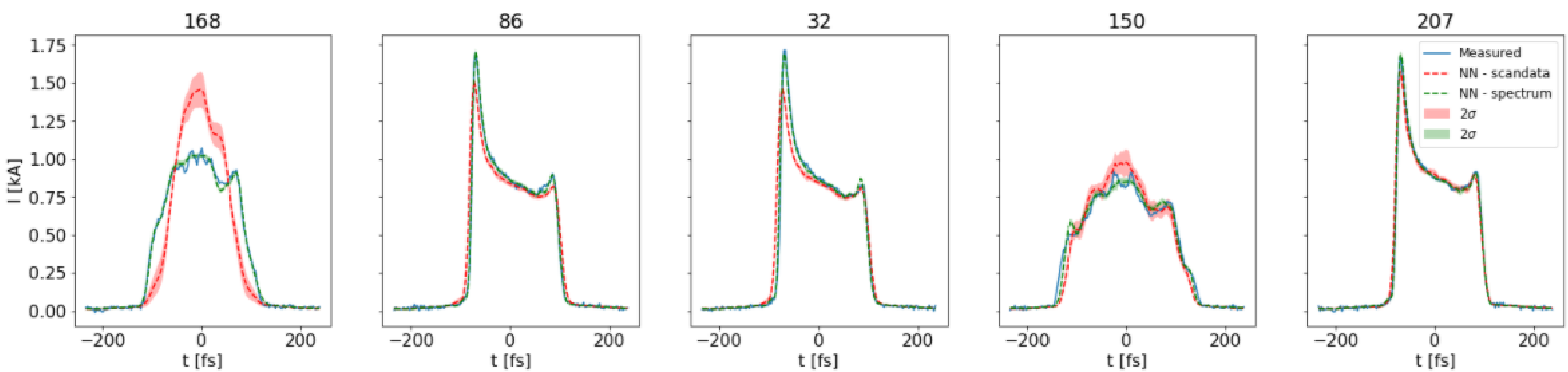
predict_model

```
Model: "model_26"
_________________________________________________________________
Layer (type)                 Output Shape              Param #
=================================================================
input_26 (InputLayer)        (None, 5)                 0
_________________________________________________________________
dense_101 (Dense)            (None, 200)               1200
_________________________________________________________________
dense_102 (Dense)            (None, 100)               20100
_________________________________________________________________
dense_103 (Dense)            (None, 50)                5050
_________________________________________________________________
dense_104 (Dense)            (None, 150)               7650
=================================================================
Total params: 34,000
Trainable params: 34,000
Non-trainable params: 0
_________________________________________________________________
None
Time to perform fit [mins] =  1.140
```




```
loss:  7.725056511245074e-05
Validation loss:  0.0001323133176889696
Test loss: 9.489419417711619e-05
Test accuracy: 0.004323772620409727
```

```
from spec_utils import *
plot_Iz_vs_VDscalar_vs_spec(y_test,y_pred_scalar,y_pred_spec,nrow=nrow,ncol=5, rnd=False, idx=[32,86,150,782,118])
```



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

3. Incorporating uncertainties - know what we don’t know.

4. Summary

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.

LCLS

- Experimental
- 1D/2D outputs

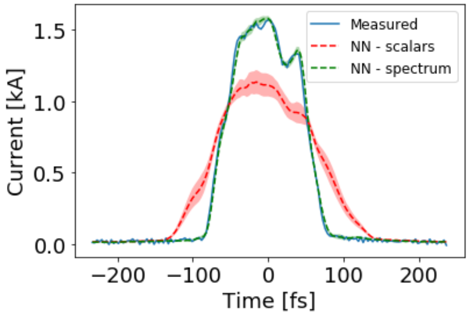
LCLS-II

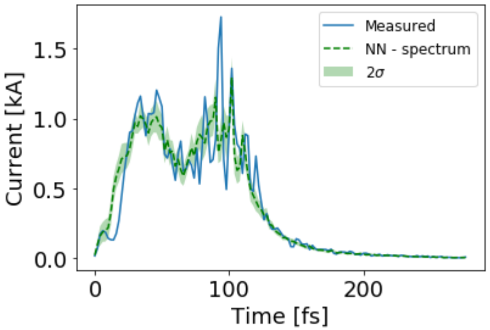
- Microbunching
- Elegant SC SXR simulation

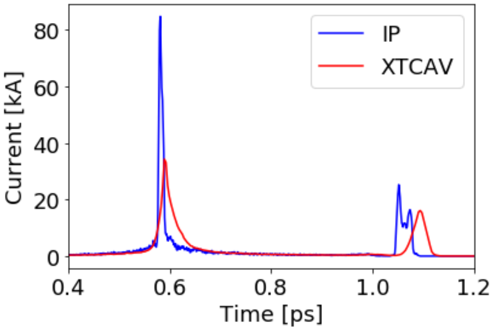
FACET-II

- 2-bunch mode
- Lucretia simulation

Accuracy







Confidence

Comparing Scalar VD vs Spectral VD

Prediction uncertainty from ensemble

Correlating prediction with spectral intensity

Improved accuracy over scalar VD *(LCLS)*

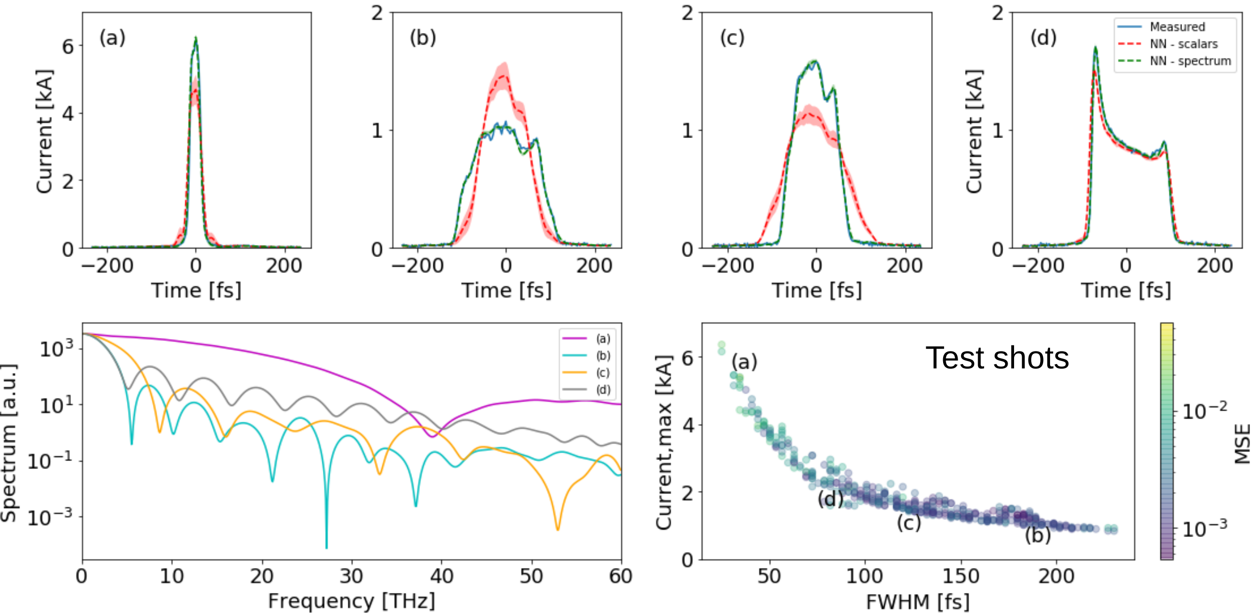
Train on ~4000 examples ; Test on ~600 examples.

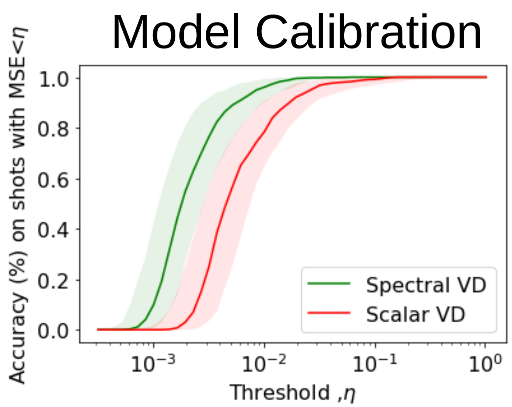
Spectral VD has lower MSE than scalar VD.

LCLS Experiment:

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

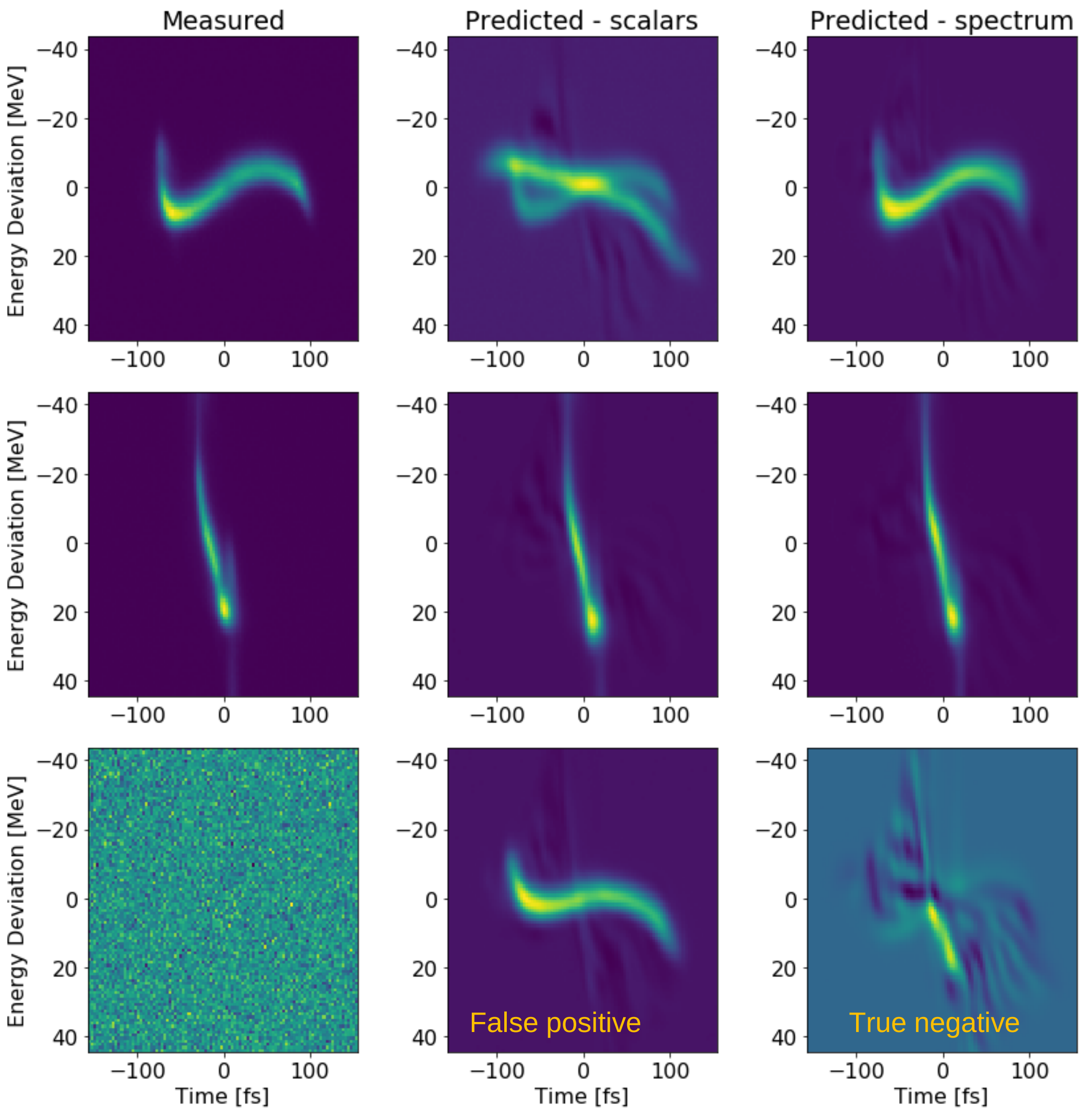
Inputs to Scalar VD:
L1s voltage & phase,
L1x voltage, BC1 and BC2 current





- Scalar VD: Optimized NN architecture compared to prior work - consistently improved by 15%.
- Improved accuracy of the spectral VD.

Spectral VD better predicts LPS images *(LCLS)*



- Improved accuracy of the spectral VD*.
- Increased confidence from multiple diagnostic predictions.

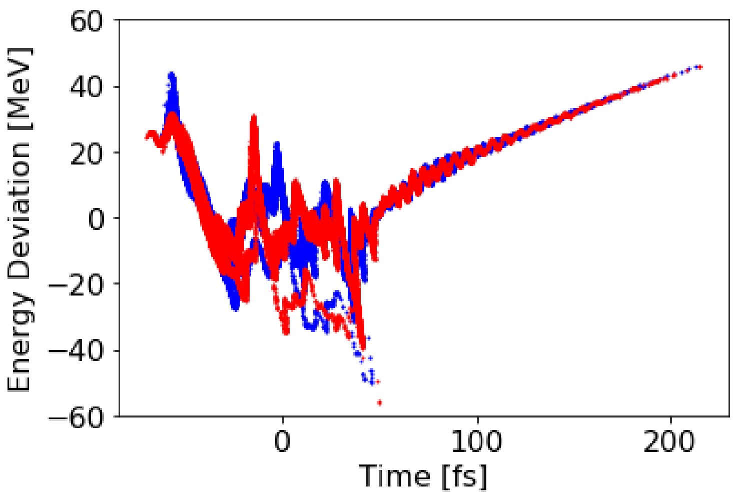
**MSE=0.054,0.079 ; SSIM=0.97,0.96* for *spectral*, *scalars*

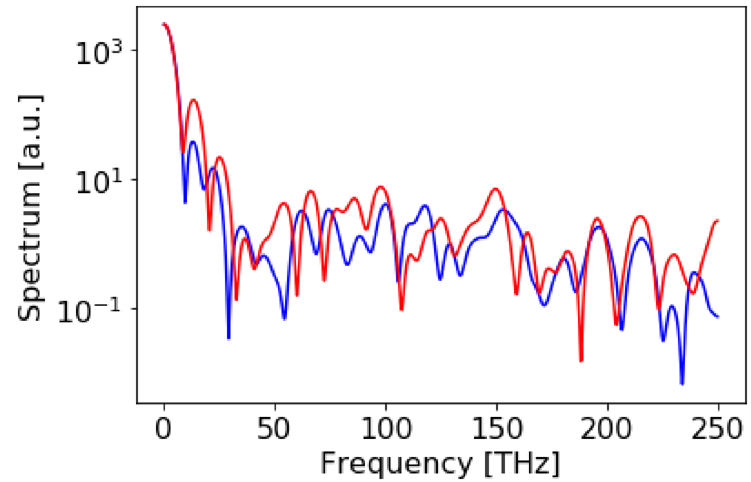
SSIM=structural similarity index measure [0,1]

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

Two Simulations of LCLS-II SC SXR – same input, different output

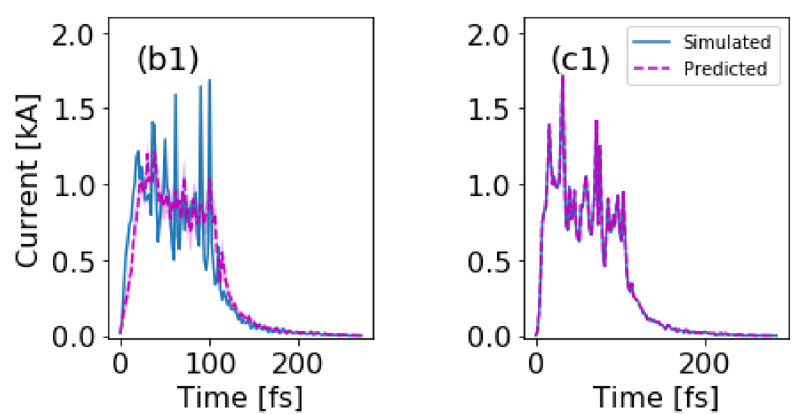
→ Only Spectral VD can be used!





Predict current profile NMSE=1.1%

- 4000 Elegant simulations
- Ensemble of networks to obtain std

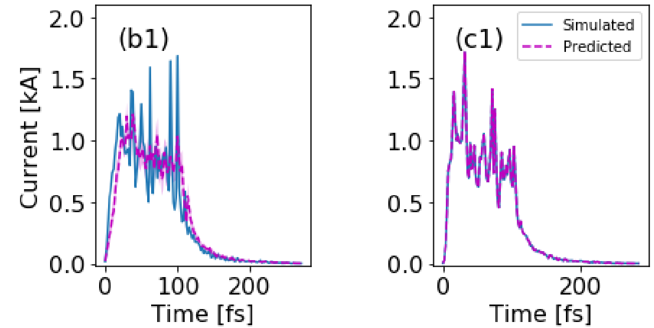


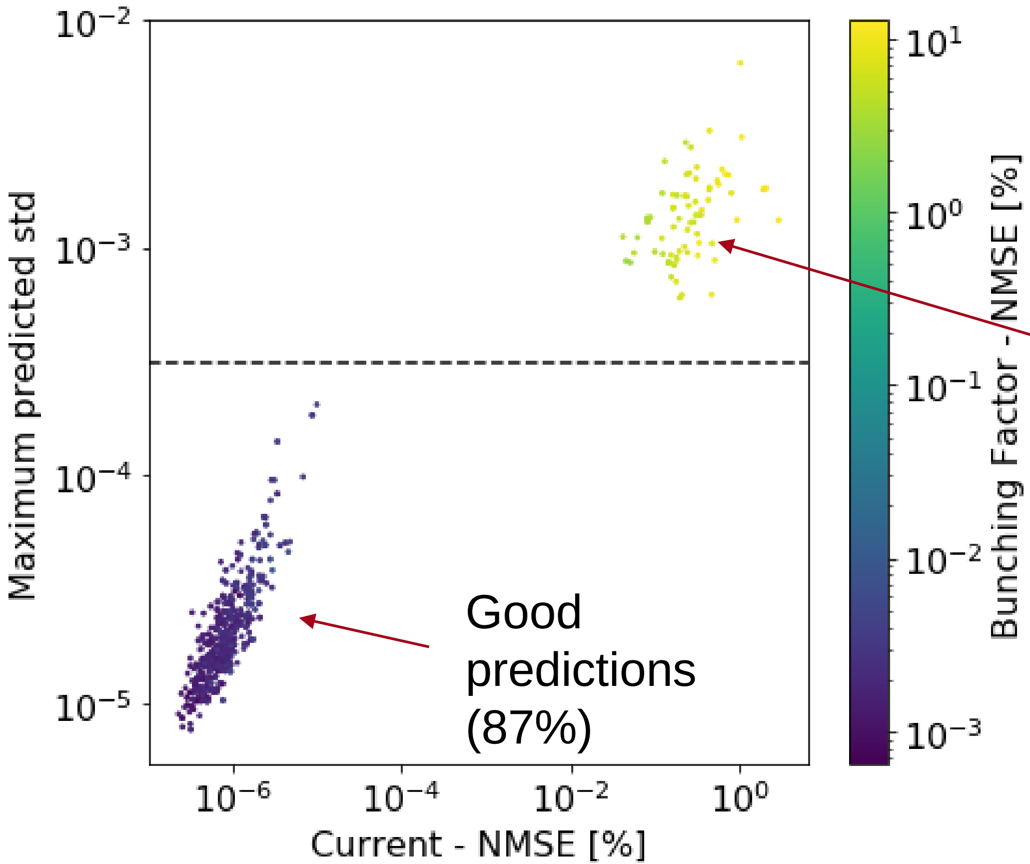
$$\mathrm{NMSE}(y, \hat{y}) = \mathrm{MSE} / \sum_{i=0}^{N-1} y_i^2$$

Increasing prediction’s confidence

(LCLS-II)

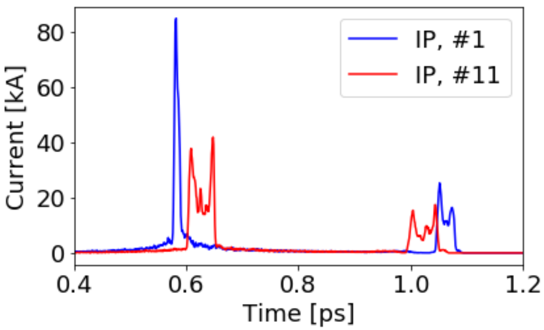
Correlate max std and mean MSE from ensemble of random initializations.

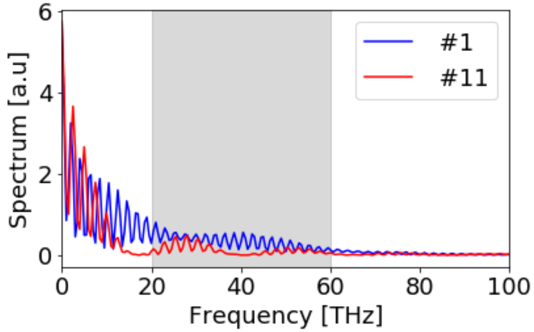




Bad
predictions
(13%)

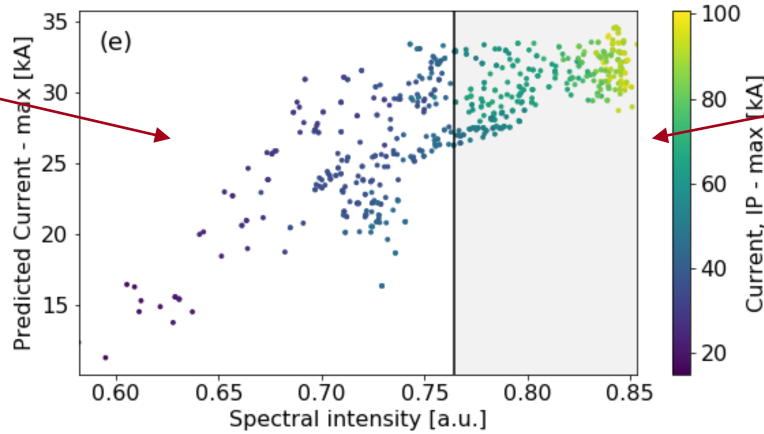
Going beyond current diagnostic resolution *(FACET-II)*





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

High confidence region (46%)



Shots are beyond the TCAV resolution

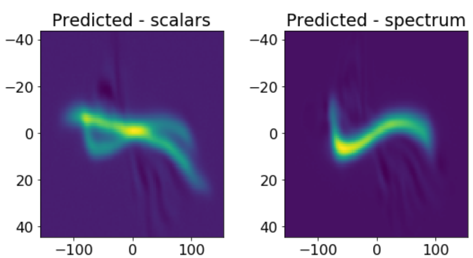
Spectral VD resolves features that are beyond the TCAV limited resolution.

Accurate & Confident Predictions - Summary

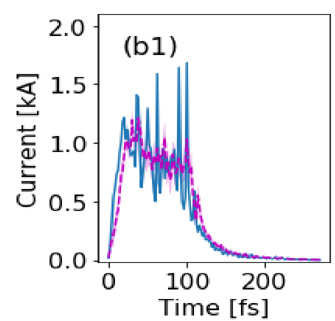
LCLS	LCLS-II	FACET-II
• Experimental • 1D/2D outputs	• Microbunching • Elegant SC SXR simulation	• 2-bunch mode • Lucretia simulation

Accuracy

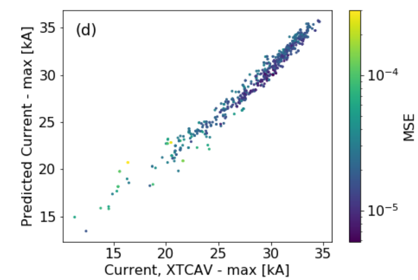
LCLS: Customized the NN architecture.



LCLS-II: Wider NN trained longer

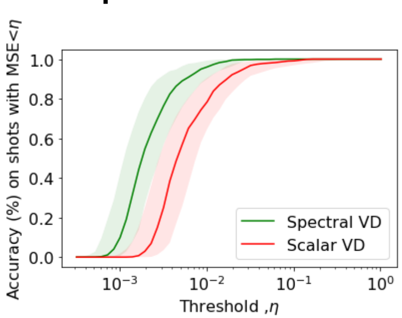


FACET-II: Customized the NN architecture.

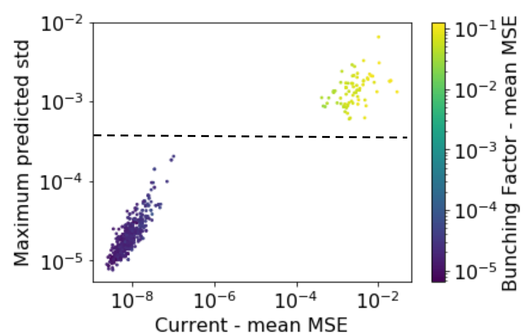


Confidence

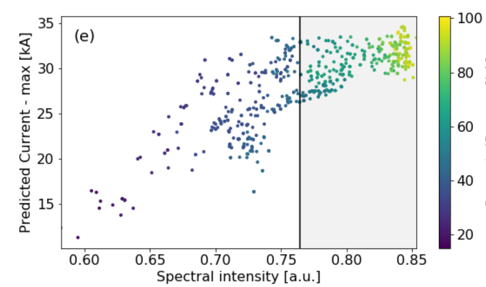
LCLS: Comparing Scalar VD vs Spectral VD



LCLS-II: Prediction std from ensemble



FACET-II: Correlating prediction with spectral intensity



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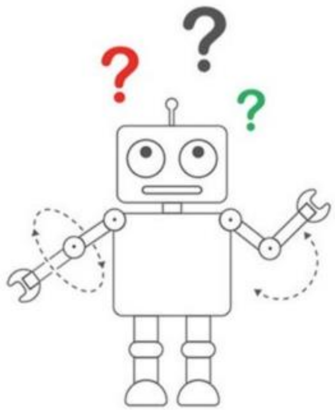
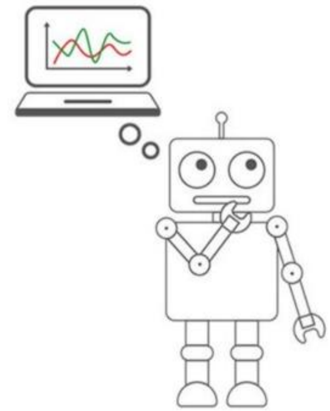
4. Summary

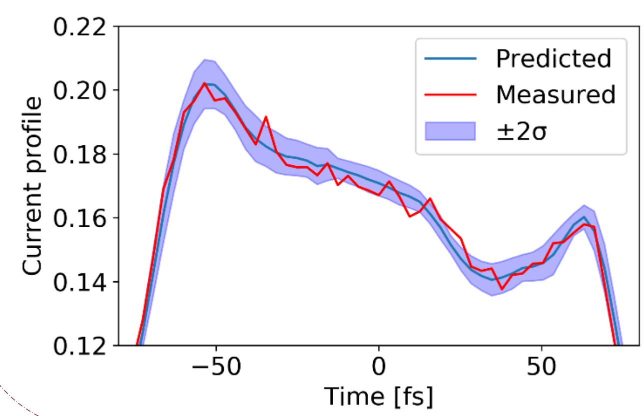
Incorporating Uncertainties – know what we don't know



- 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.

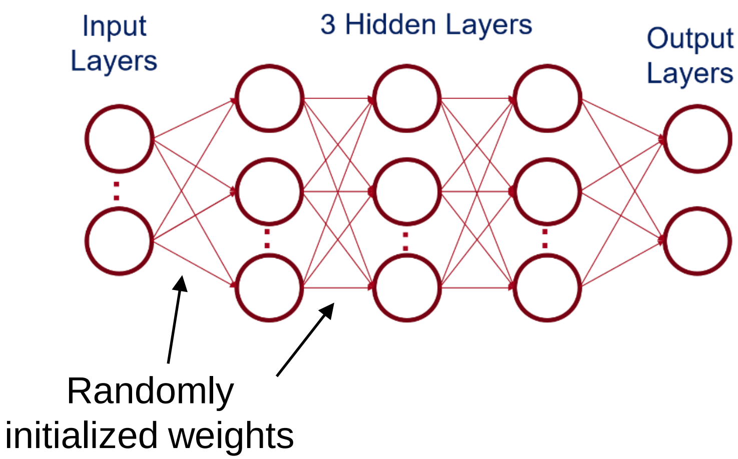


Incorporating Uncertainties – Methods

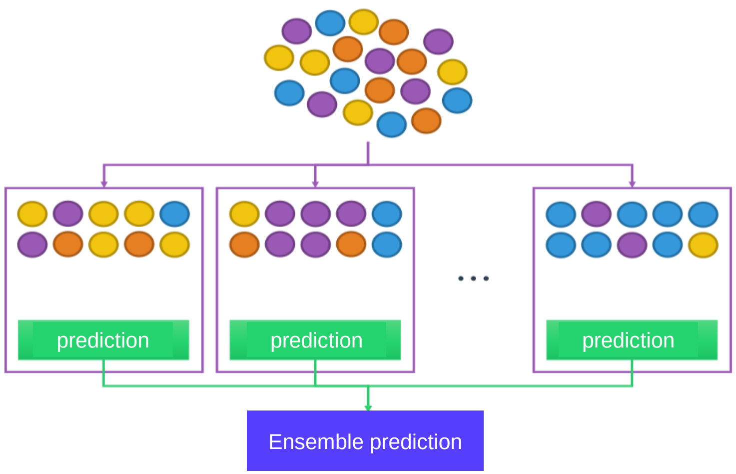
<u>Goal:</u> Prediction sensitivity - quantify how reliable the mean prediction is.

1. Ensemble methods = a collection of neural networks

Random initializations



Random data split

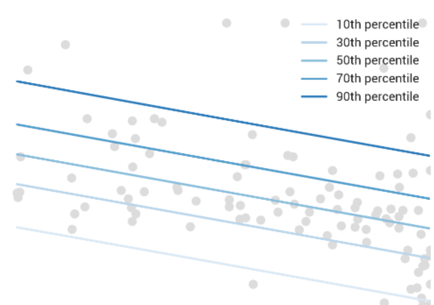


2. Quantile regression:

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

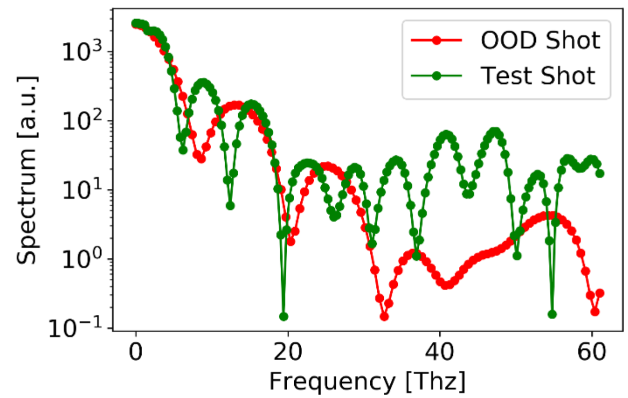
$$\mathcal{L}(\xi_i|\alpha) = \begin{cases} \alpha\xi_i & \text{if } \xi_i \geq 0, \\ (\alpha - 1)\xi_i & \text{if } \xi_i < 0. \end{cases}$$

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

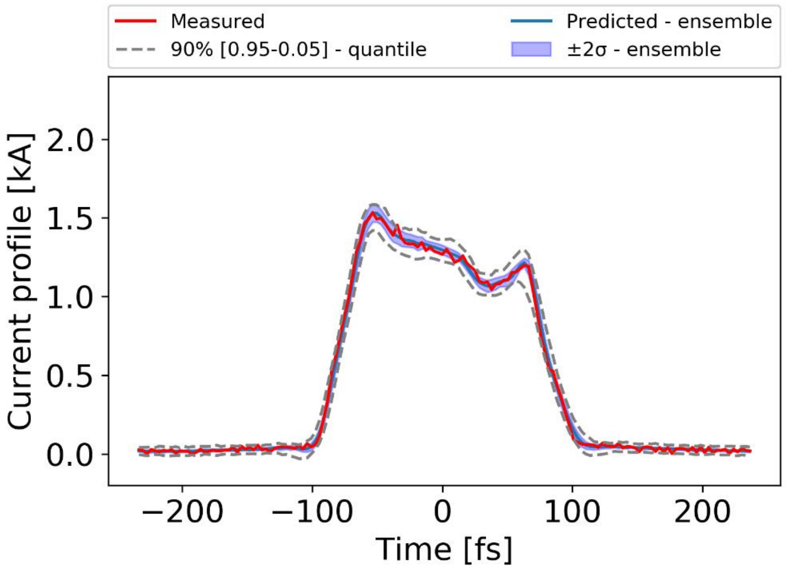


OOD Robustness

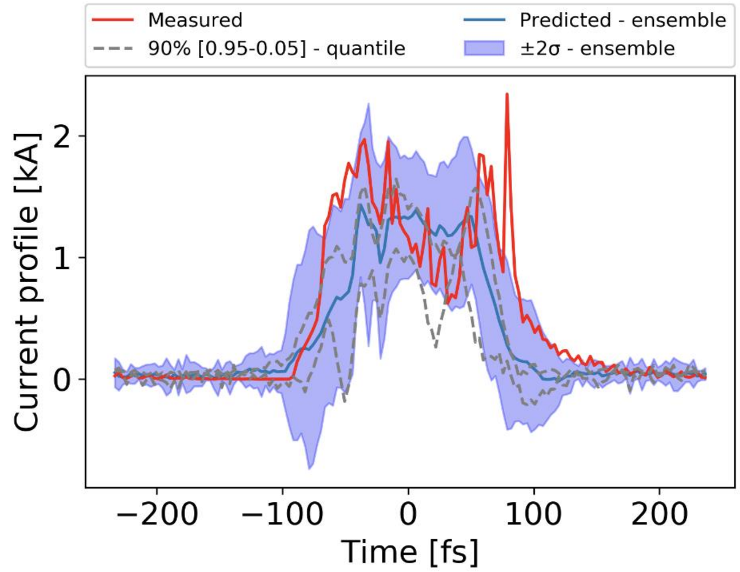
Methods: Ensembles (random initializations, random subset of the data, Bagging), Quantile regression.



Test shot within the trained distribution



Out-of-distribution



Out-of-Distribution → Higher Uncertainty

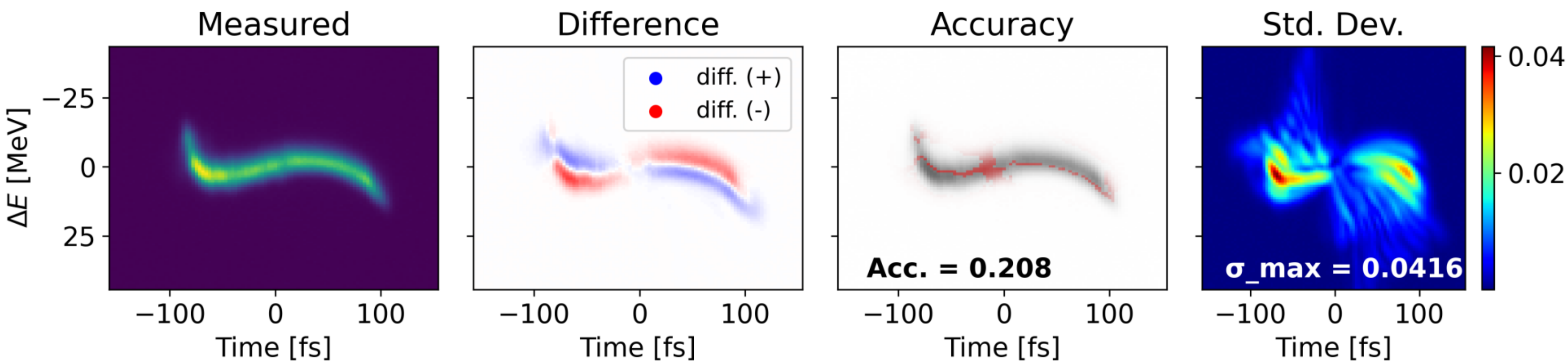
In collaboration with Owen Convery, Lewis Smith and Yarin Gal

Common prediction errors with LPS images

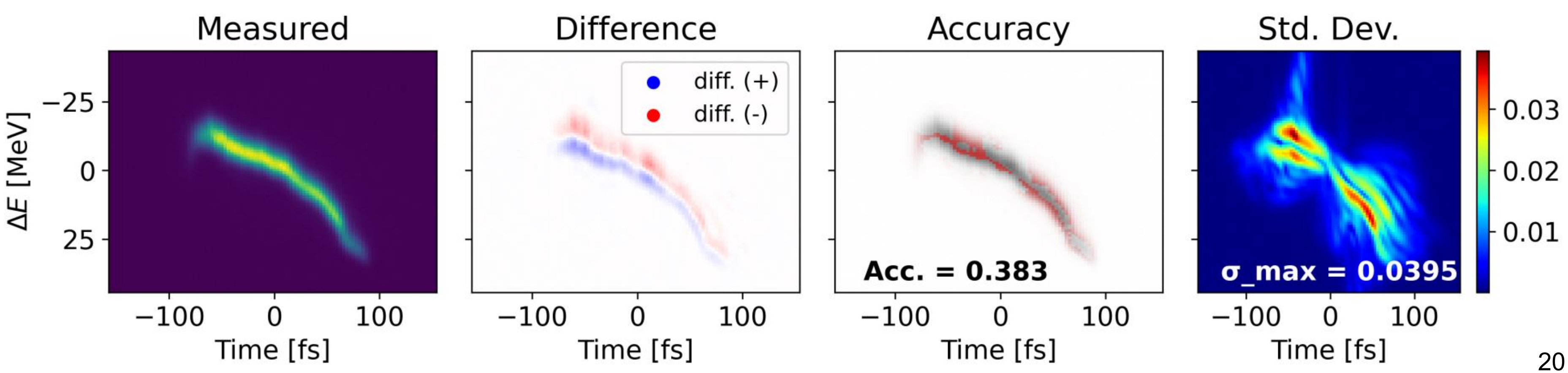
$$\text{Accuracy} = \frac{\sum_{t=1}^{T} \alpha_t \cdot I^2_{\text{measured},t}}{\sum_{t=1}^{T} I^2_{\text{measured},t}}$$

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

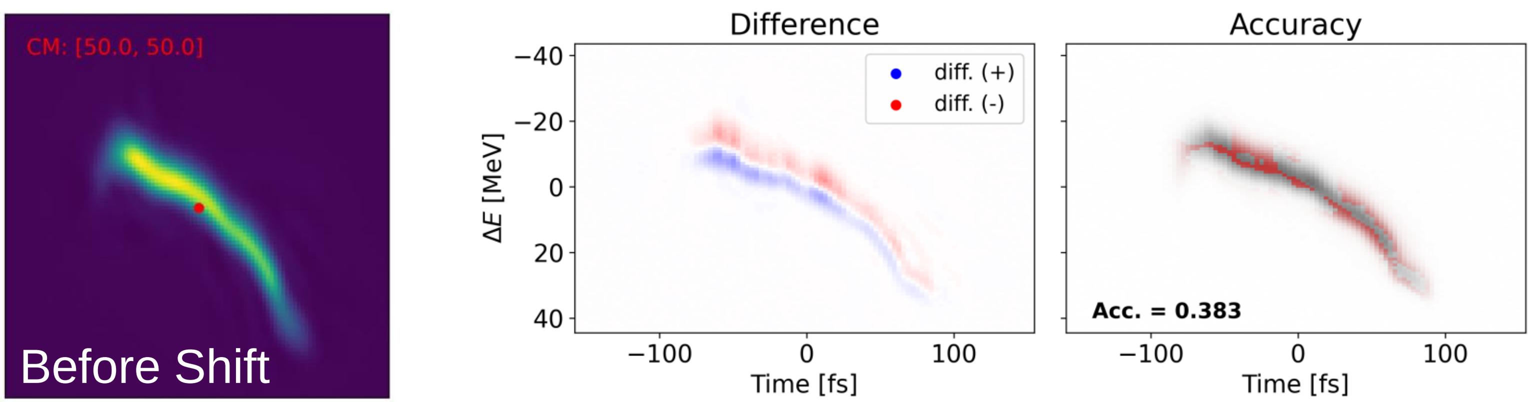
Shot #789 - Shape error: the prediction is of the wrong shape



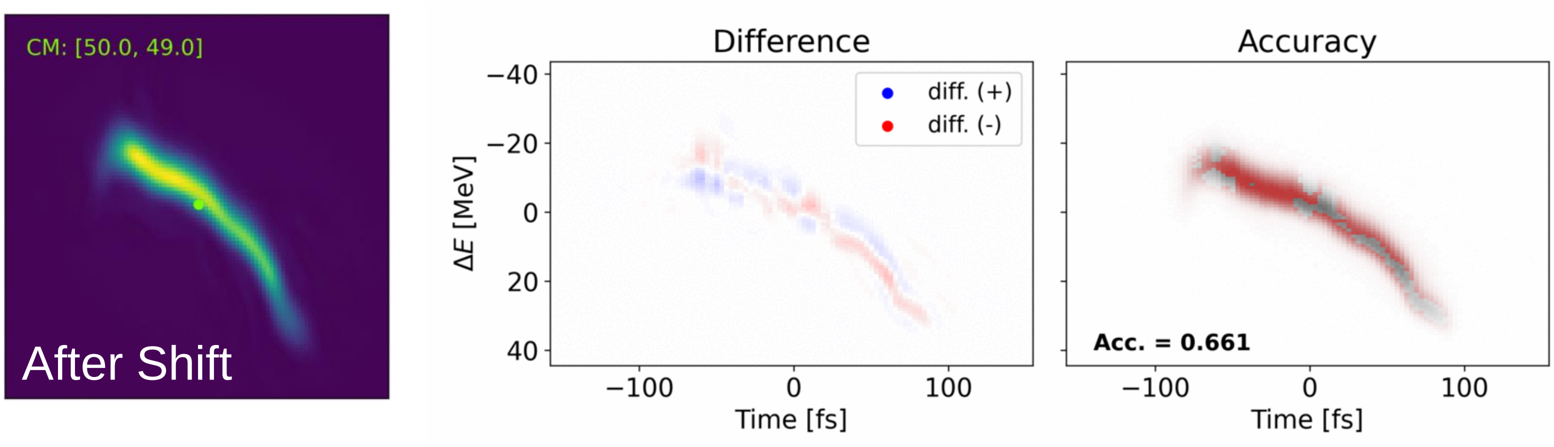
Shot #762 - Translational error: the prediction is in the wrong place



Alleviating Translational Error



Center of Mass Correction (Pred. → Truth)

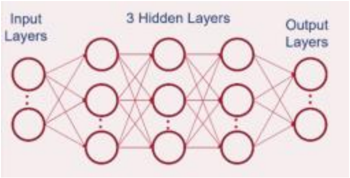


MSE ↓
-65.6%

Accuracy ↑
58.7%

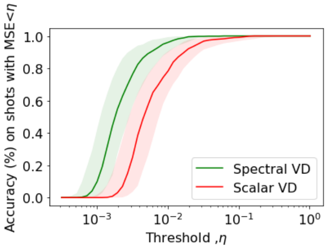
Summary of Virtual Diagnostics

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



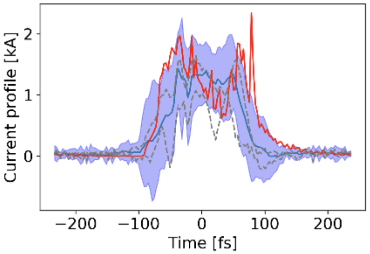
- **Fast & online** – doesn't require convoluted data processing.
- Fill in **missing** information – high peak current, repetition rate, etc.
- Understand **exotic** configs – by combining ML model with simulation.
- **Reverse** engineering of machine settings for a pre-defined current profile.

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.

Thanks to the wonderful team!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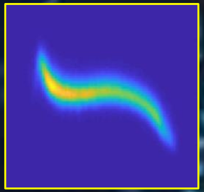
Hanuka, Nature Scientific Reports 11, 2945 (2021)
Convery, arxiv 2105.04654 (2021)

Thank You!



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LCLS Linac Coherent Light Source

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