Machine Learning to Improve the Sensitivity of Soft X-ray Spectroscopy

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BACKGROUND

- Soft XAS probes local atomic structure and electronic properties of specific elements in molecules on surfaces and in solutions. [2]
- FELs add femtosecond time resolution (∴ ultrafast dynamics) and higher peak flux per pulse than synchrotrons. [2]
- SASE X-rays at an FEL have large pulse-to-pulse intensity fluctuations, restricting shot-noise-limited measurements.
- Correcting forthis can recover shot-noise-limited sensitivity.
- This would extend XAS to dilute and radiation-sensitive samples. [3]

OPTICAL DENSITY & REFERENCING

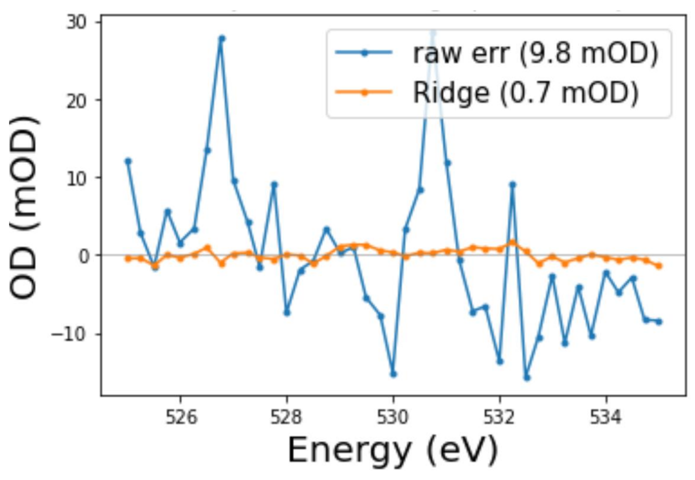
1) I_t Transmitted Beam, I_0 Reference Beam

2) $I_0 \rightarrow$ Sample $\rightarrow I_t$ $\quad \mathrm{OD} = -\log_{10}\left(\frac{I_t}{I_0}\right)$

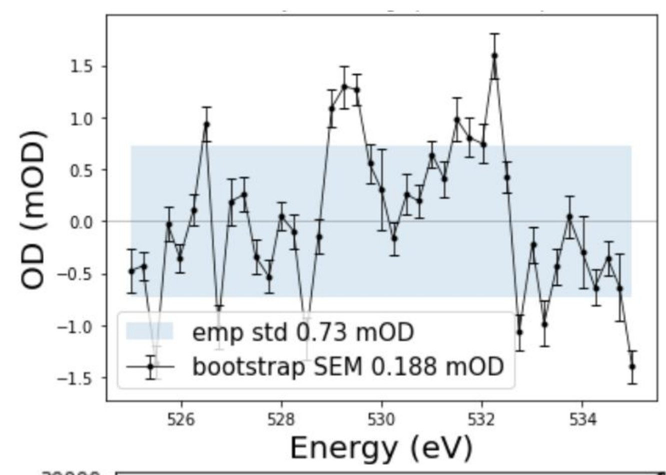
3) $I \rightarrow$ Sample $\rightarrow I_t$, I_0 $\left[\frac{I_t}{I_0}\text{-referencing}\right]$

- Removes common mode noise from shot-shot fluctuations ∴ Get better I_0

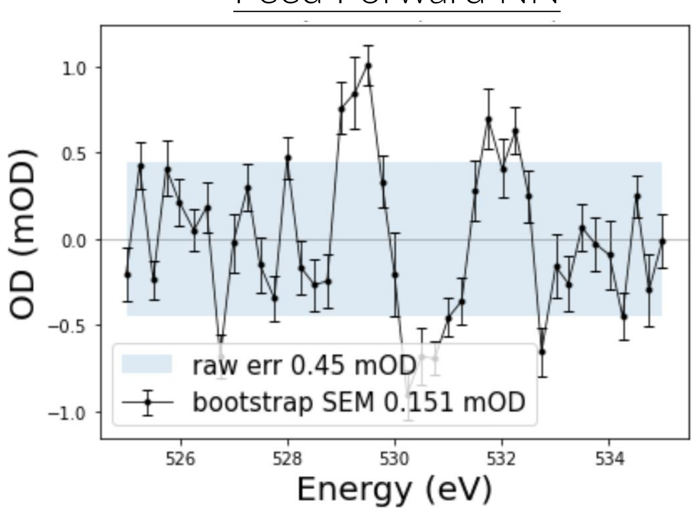
MACHINE LEARNING: No Jet

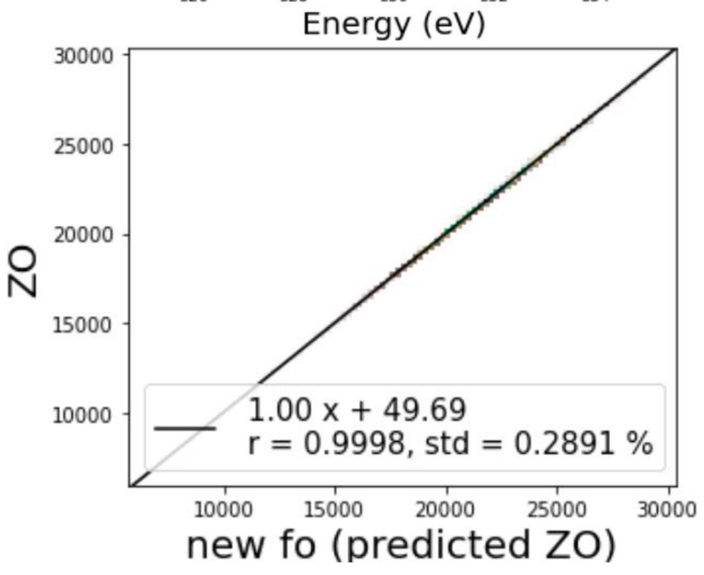


Ridge Regression

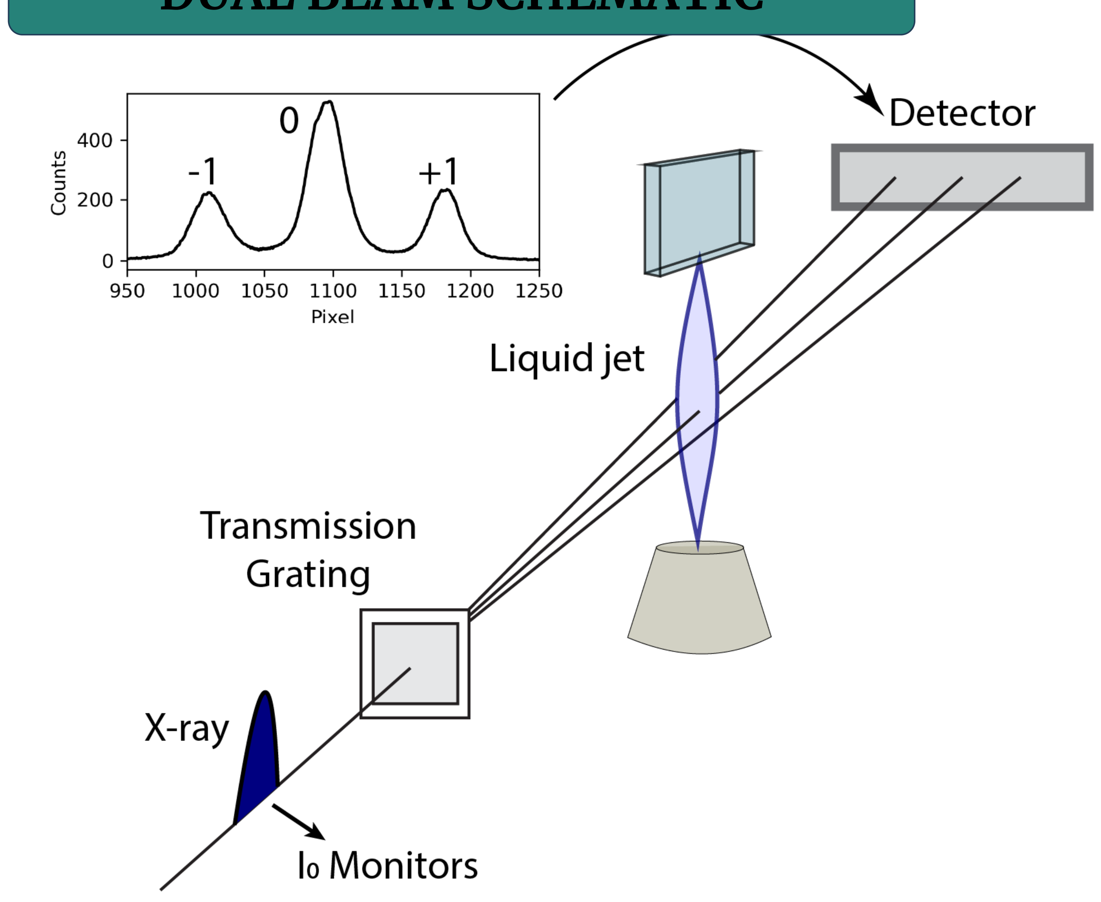


Feed Forward NN



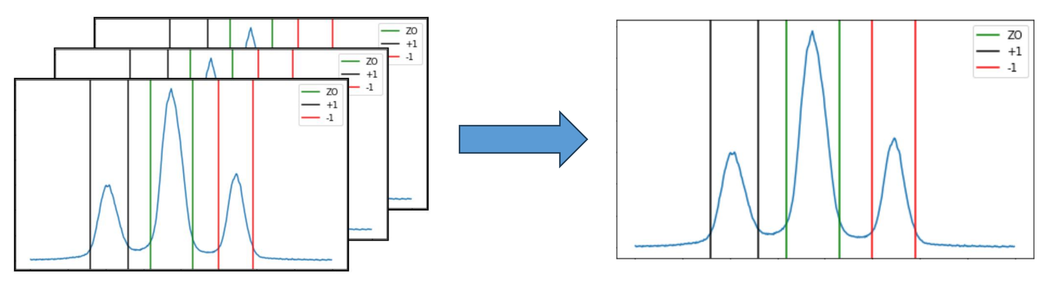


DUAL BEAM SCHEMATIC

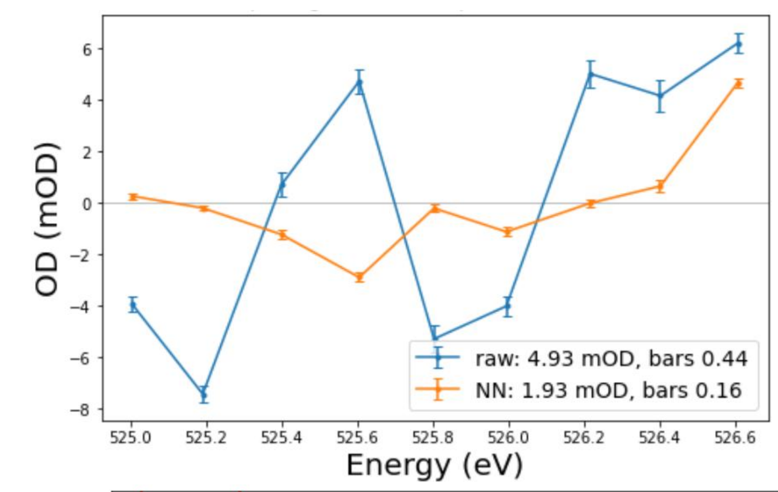


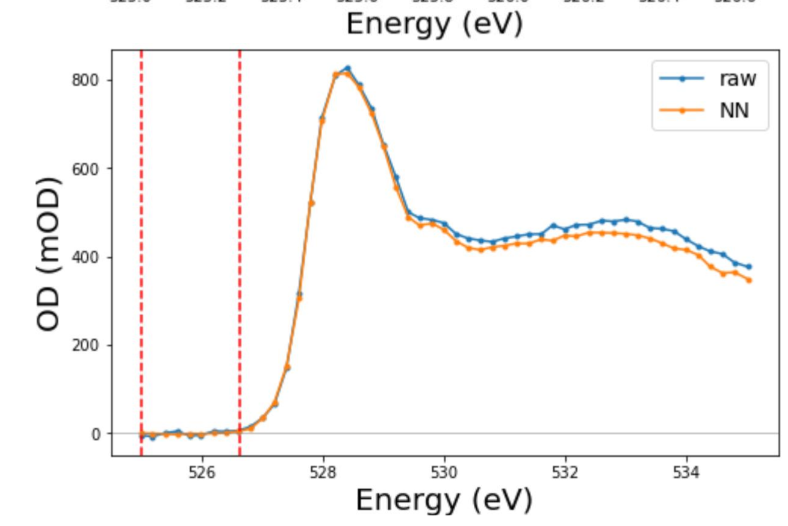
DATA FORMATS

- Single shots
- Integrated/ frame (muttlpe shots)



Static DMSO XAS (Oxygen K edge)

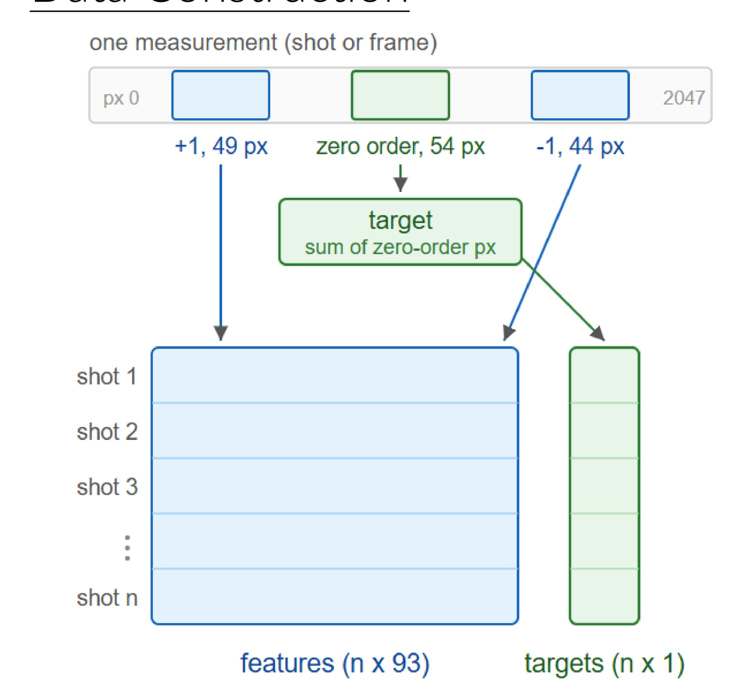


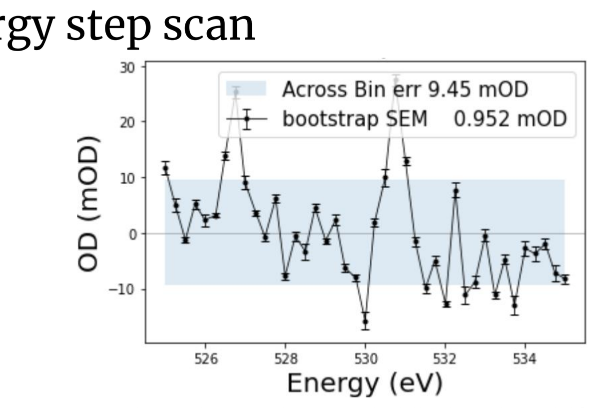


RUN 43

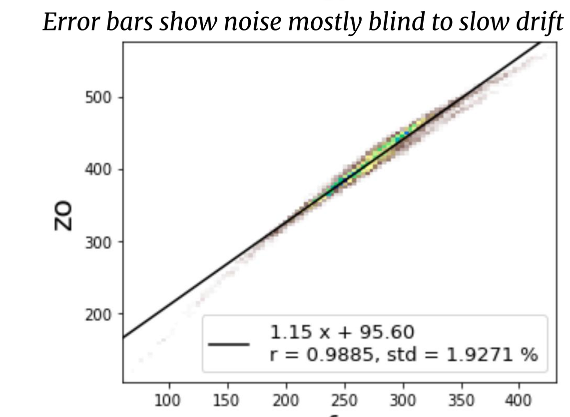
- No-jet monochromatic energy step scan

Data Construction

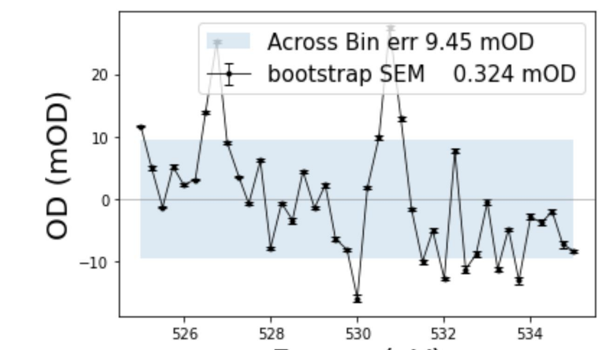




Error bars show noise mostly blind to slow drift



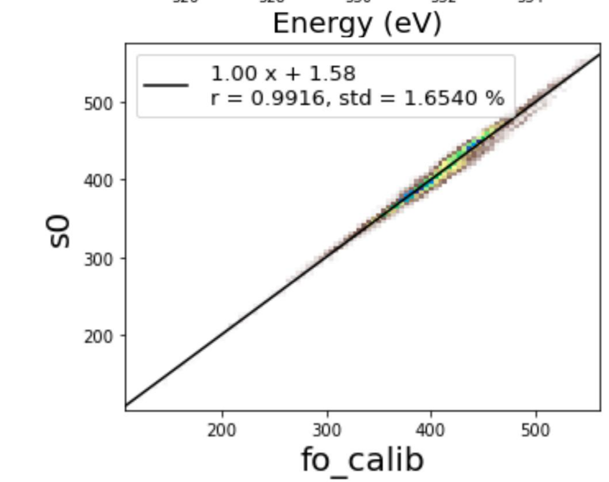
Correlation plot shows ZO-FO nonlinearity



Quadratic Correction

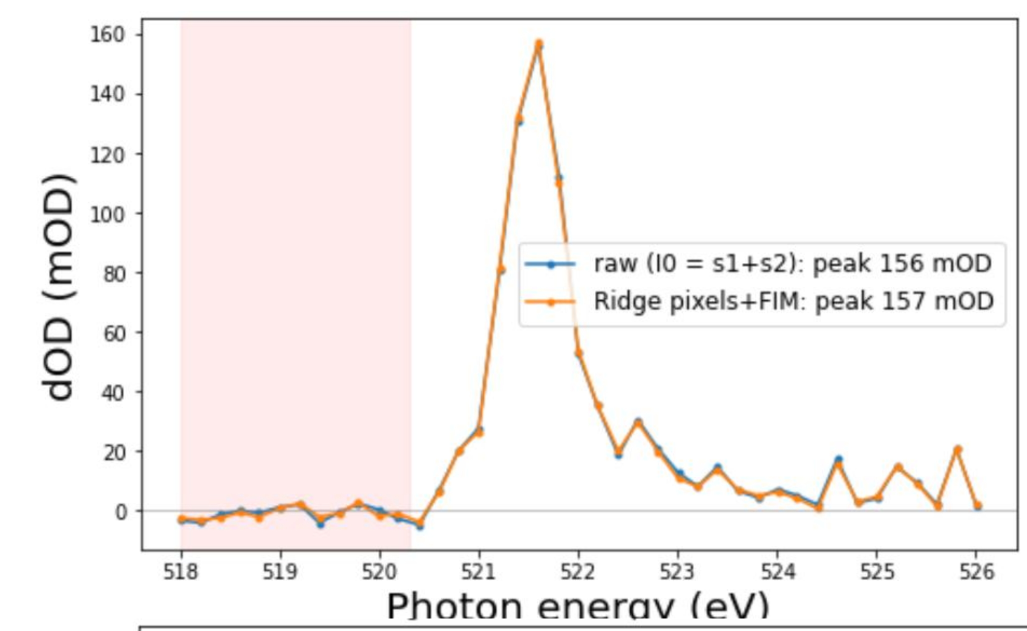
$$I_t = aI_0^2 + bI_0$$

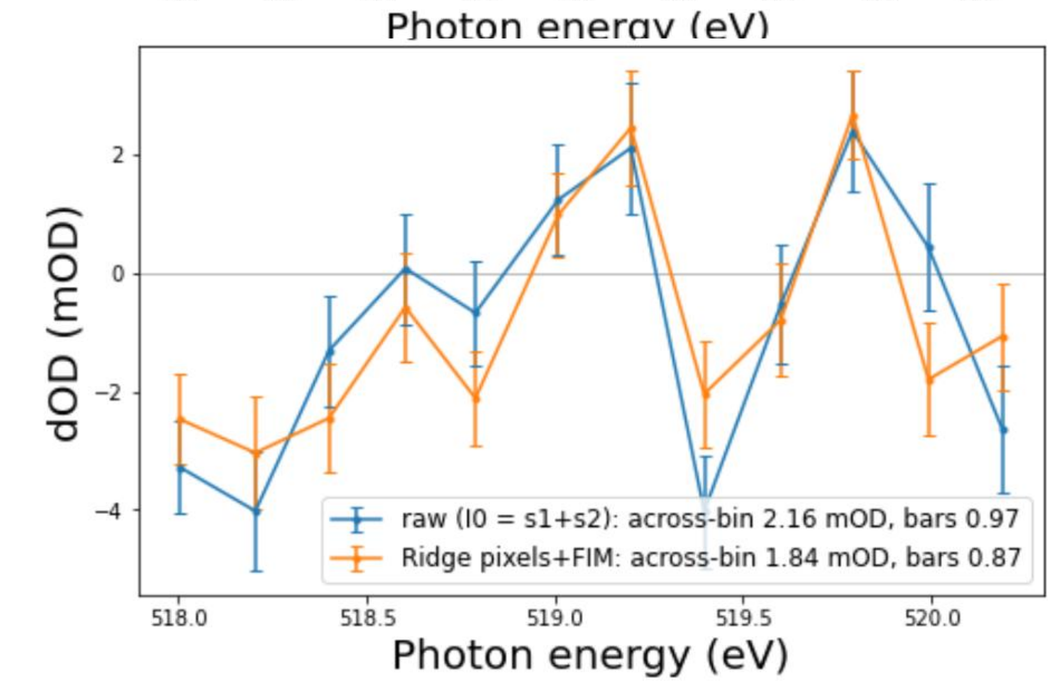
a = -1.416e-05, b = 1.457



1. *Emp noise unchanged*
2. *SEM improved ~3x*
3. *Pearson correlation now 0.9916*
4. *Std ~ 1.17x*

Pump-probe transient absorption scan





RESULTS ANALYSIS

- Ridge Regression improved across bin noise (ABE) 13x on No Jet scan, 11x on static XAS scan, only 1.2x on pump probe scan.
- Pump probe scan's Co filter most likely reduced majority of harmonic contamination.
- SEM 5x No Jet, 3x static XAS, and 1.1x pump probe.
- SEM settled in 0.1mOD - 1mOD range and ABE, 0.5mOD – 2mOD

FUTURE WORKS

- Determine if the already high quality of our pump probe data was sorely due to the CO filter.
- Try to reproduce the same level of improvement seen in the no jet data on the pump probe data.
- Create pipelines for static XAS and pump probe data that automatically implements ML referencing.

ACKNOWLEDGEMENTS

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