Machine-learning-enhanced characterization of x-ray pulses

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FELs of Europe, Topical Workshop on selected problems in FEL physics: from soft x-rays to THz

European XFEL

September 2025

Partially based on Danilo Enoque Ferreira de Lima et al. “Machine-learning-enhanced automatic spectral characterization of x-ray pulses from a free-electron laser”. In: *Communications Physics* 7.1 (Dec. 2024), p. 400. URL: https://doi.org/10.1038/s42005-024-01900-6

Enhancing non-invasive X-ray diagnostics

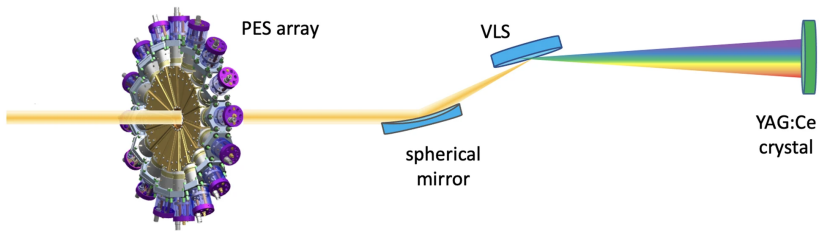
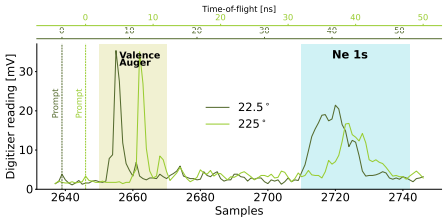


Figure from K. Li et al. 2022. Commun. Phys. 5: 191

Photoelectron spectrometer (PES)

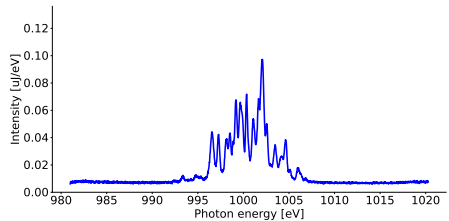
Grating-based spectrometer (GS)

Enhancing non-invasive X-ray diagnostics



Photoelectron spectrometer (PES)

- Non-invasive.
- @ 4.5 MHz.
- Complex calibration.
- Low-resolution.

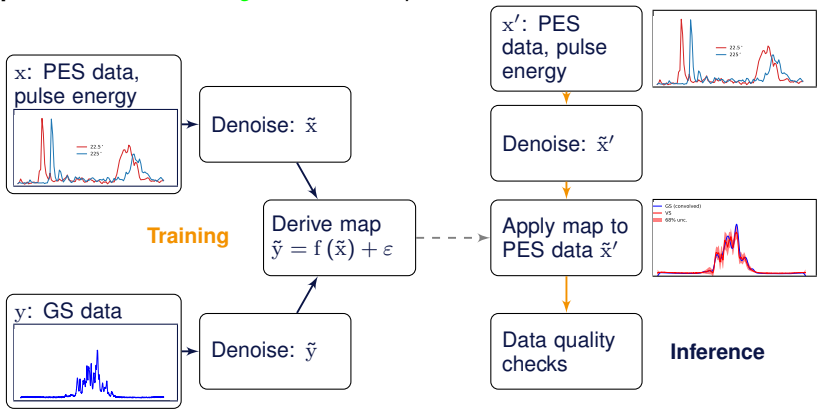


Grating-based spectrometer (GS)

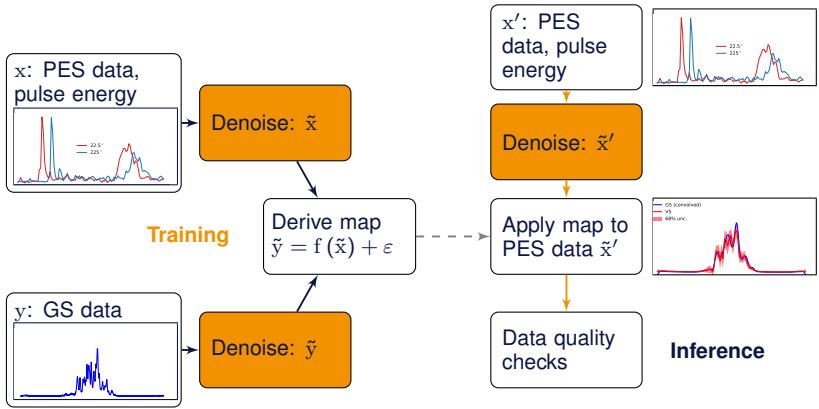
- Invasive.
- @ 10 Hz.
- Simple calibration.
- High-resolution.

Method

Concept. *Profit from advantages of both: map the PES to GS.*

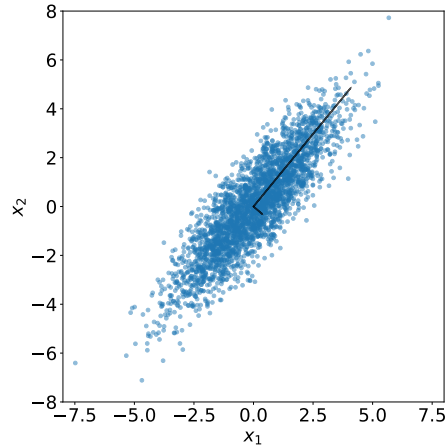


Denoising


x: PES data, pulse energy
Denoise: $\tilde{x}$
Training
Derive map $\tilde{y} = f(\tilde{x}) + \varepsilon$
y: GS data
Denoise: $\tilde{y}$
x′: PES data, pulse energy
Denoise: $\tilde{x}'$
Apply map to PES data $\tilde{x}'$
Data quality checks
Inference

Denoising through representation learning

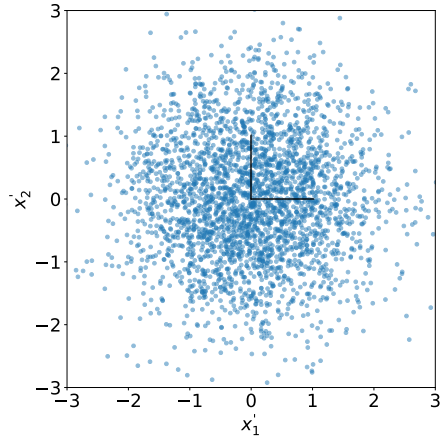
- Principal Component Analysis *decorrelates* and orders latent space variables by *variance*[2].
  - Decorrelates.
  - Ordering principle based on variance.
- We select the highest variance components to mitigate noise.



[2] Karl Pearson F.R.S. “LIII. On lines and planes of closest fit to systems of points in space”. In: *The London, Edinburgh, and Dublin Philosophical Magazine and Journal of Science* 2.11 (1901), pp. 559–572.

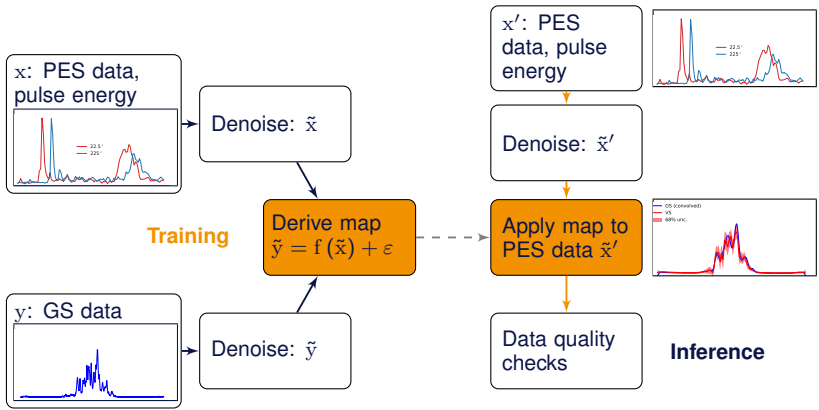
Denoising through representation learning

- Principal Component Analysis *decorrelates* and orders latent space variables by *variance*[2].
  - Decorrelates.
  - Ordering principle based on variance.
- We select the highest variance components to mitigate noise.
- SASE process produces high shot-to-shot variance.



[2] Karl Pearson F.R.S. “LIII. On lines and planes of closest fit to systems of points in space”. In: *The London, Edinburgh, and Dublin Philosophical Magazine and Journal of Science* 2.11 (1901), pp. 559–572.

Fit

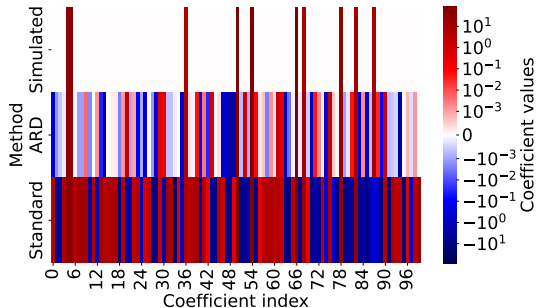

x: PES data, pulse energy
22.5°
22.5°
Denoise: $\tilde{x}$
Training
Derive map $\tilde{y} = f(\tilde{x}) + \varepsilon$
y: GS data
Denoise: $\tilde{y}$
x′: PES data, pulse energy
22.5°
22.5°
Denoise: $\tilde{x}'$
Apply map to PES data $\tilde{x}'$
GS (convolved)
VS
68% unc.
Data quality checks
Inference

Automatic Relevance Determination

- Automatic Relevance Determination (ARD)[3] robust to noise.
- Bayesian procedure → uncertainties!
- Select relevant coefficients based on uncertainties.

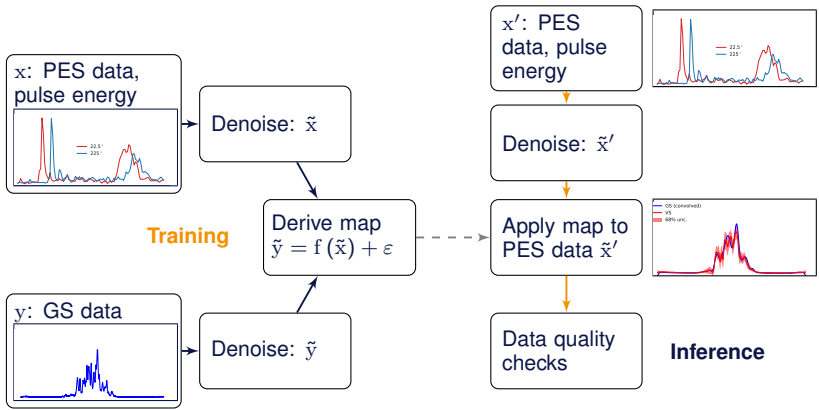
[3] David J. C. MacKay. “Bayesian Non-Linear Modeling for the Prediction Competition”. In: *Maximum Entropy and Bayesian Methods: Santa Barbara, California, U.S.A., 1993*. Ed. by Glenn R. Heidbreder. Dordrecht: Springer Netherlands, 1996, pp. 221–234.

Automatic Relevance Determination’s robustness to noise



(Based on scikit-learn’s ARD example)

Method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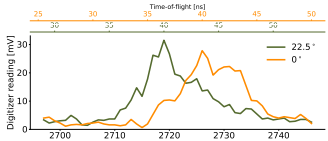
x′: PES data, pulse energy
Denoise: $\tilde{x}'$
Apply map to PES data $\tilde{x}'$
Data quality checks
Inference

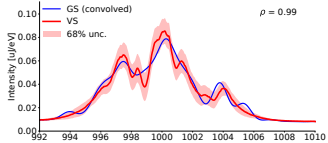
Example

- Left: PES original spectrum.
- Right: Grating spectrum.
- Center: Virtual spectrometer comparison to grating smoothed to the estimated VS resolution.

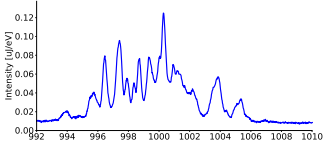
PES spectrum



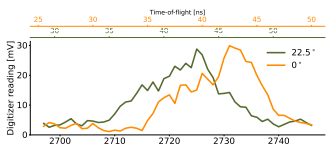
Virtual spectrometer



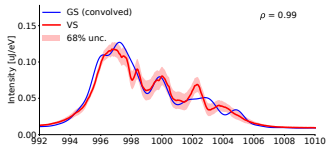
Grating spectrum



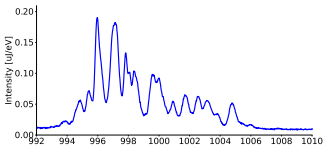
PES spectrum



Virtual spectrometer

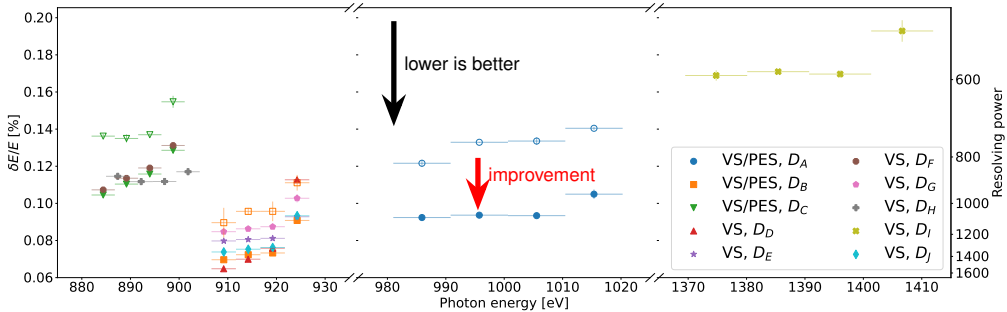


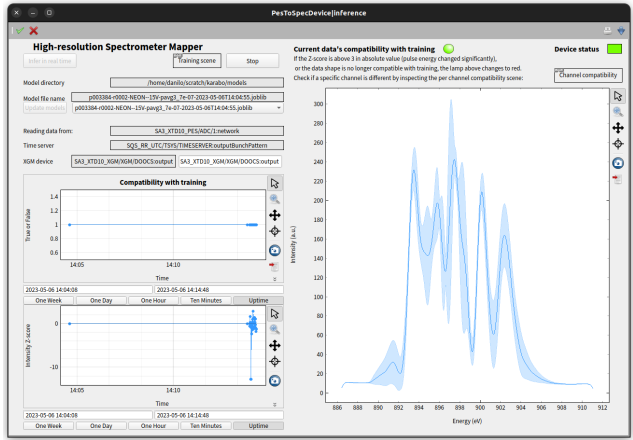
Grating spectrum



Virtual Spectrometer's resolution in real data

- Systematic resolution studies under several conditions done.
- VS (full markers) has better resolution than PES (open symbols).
- Resolution calculated after training to inform scientists.



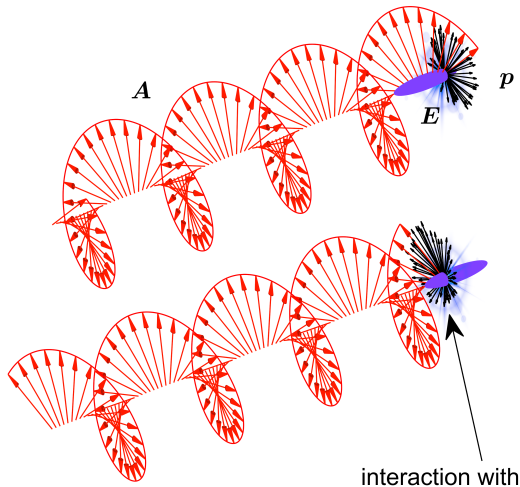

PesToSpecDevice|inference
High-resolution Spectrometer Mapper
Infer in real time
Training scene
Stop
Model directory
/home/danilo/scratch/karabo/models
Model file name
p003384-r0002-NEON--15V-pavg3_7e-07-2023-05-08T14:04:55.joblib
Update models
p003304-r0002-NEON--15V-pavg3_7e-07-2023-05-06T14:04:55.joblib
Reading data from:
SA3_XTD10_PES/ADC/1:network
Time server
SQS_RR_UTC/TSYS/TIMESERVER:outputBunchPattern
XGM device
SA3_XTD10_XGM/XGM/DOOCS:output
SA3_XTD10_XGM/XGM/DOOCS:output
Compatibility with training
True or False
Time
2023-05-06 14:04:08
2023-05-06 14:14:48
One Week
One Day
One Hour
Ten Minutes
Uptime
Intensity Z-score
Current data's compatibility with training
If the Z-score is above 3 in absolute value (pulse energy changed significantly),
or the data shape is no longer compatible with training, the lamp above changes to red.
Check if a specific channel is different by inspecting the per channel compatibility scene:
Channel compatibility
Device status
Intensity (a.u.)
Energy (eV)

High-resolution FEL temporal diagnostics (Work in progress)

Towards ML-enhanced temporal diagnostics

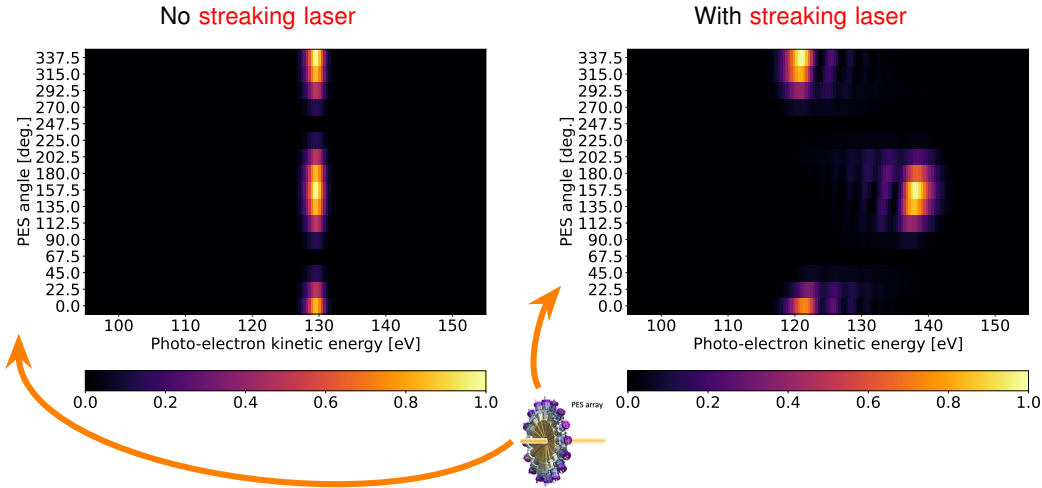
$t = t_1$

$t = t_1 + \Delta t$

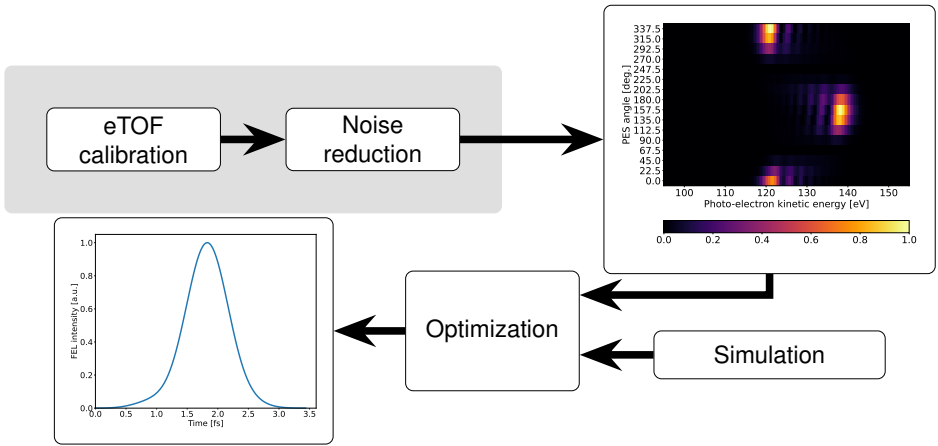


Courtesy of J. Ribbing

Towards ML-enhanced temporal diagnostics

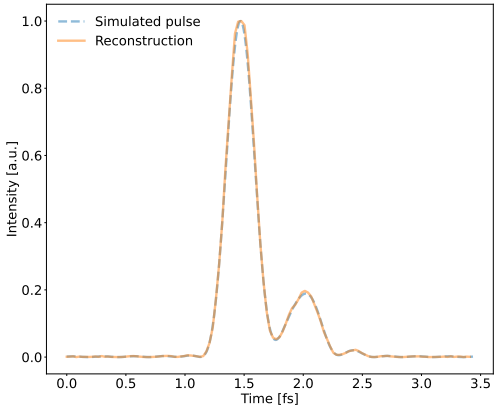


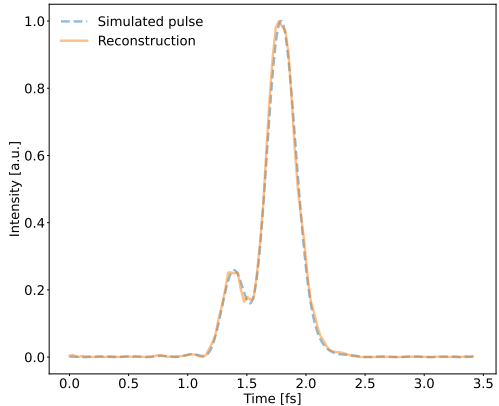
Temporal diagnostics through angular streaking



Instrumental effects

- Critical to consider detector effects.
- ML correction developed based on instrument response improves reconstruction.





Instrumental effects

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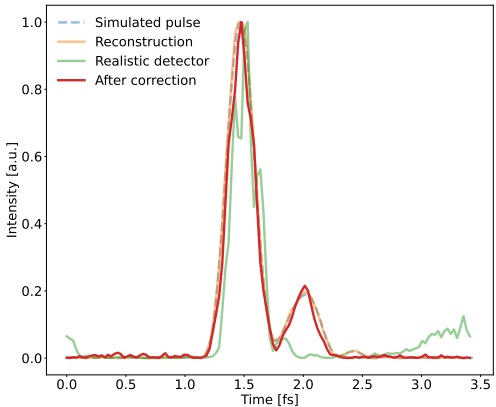
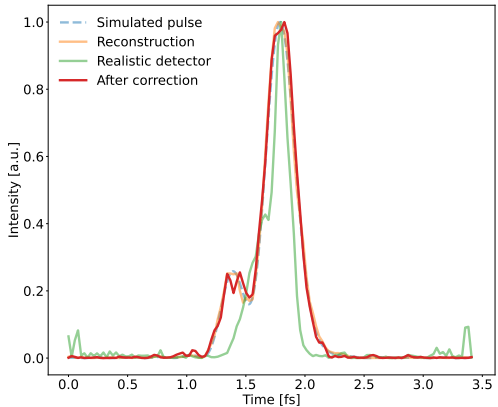




Summary and outlook

Virtual Spectrometer

- Streamlines and automates spectral diagnostics through the PES.
- Enables non-invasive high-resolution full repetition rate spectral properties characterization.

High-resolution temporal diagnostics

- Physics-informed reconstruction of the angular streaking data.
- Instrument effect non-negligible.

Next steps

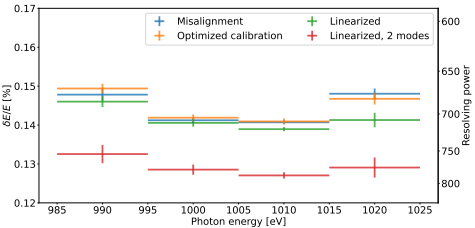
- Extend concepts to higher photon energy diagnostic devices.
- VS: Interpolate over several conditions of the machine and the PES.

Thank you!

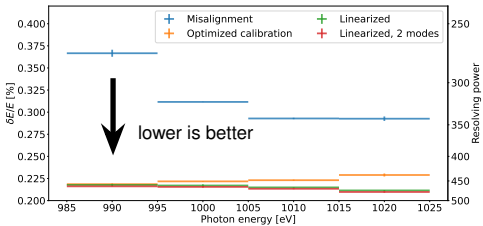
Virtual Spectrometer's resolution in toy model

- Simulated statistical toy model and estimated the resolution.
- Flat and better resolution response with the Virtual Spectrometer, compared to maual optimal PES calibration.
- Misalignments cause further deterioration.

Virtual Spectrometer



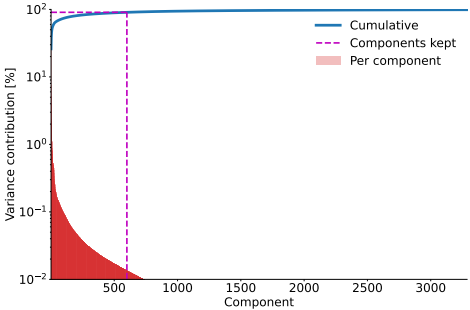
Manual PES calibration



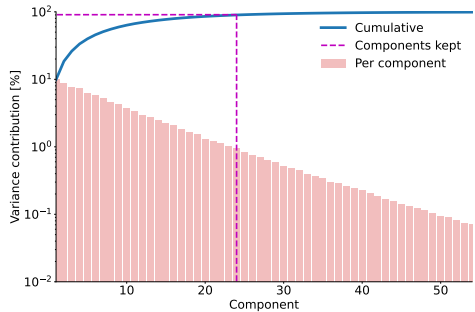
Principal Components

- Fraction of variance taken by the principal components analysed to choose representative components.
- Simplifies problem setting.

PES

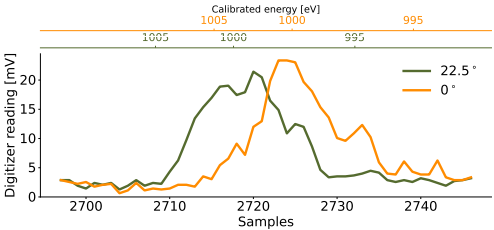


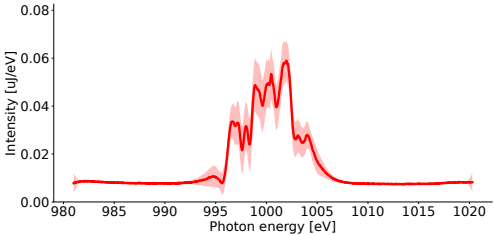
Grating spectrometer



Advantage: automation

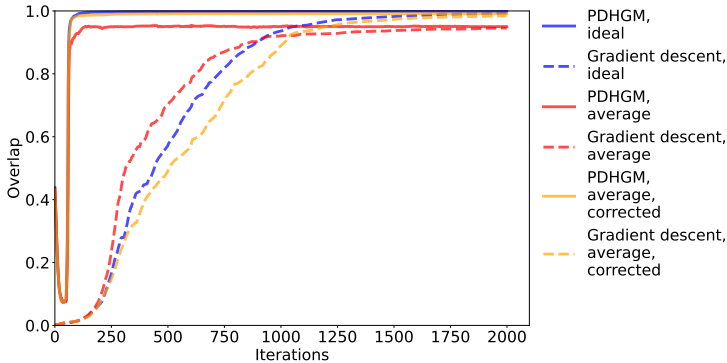
- Both calibration and validation steps are incoporated in the machinery.





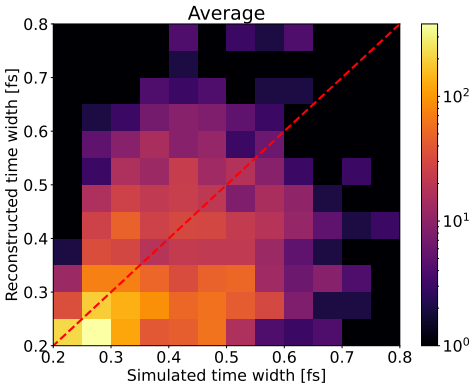
Fast reconstruction for quasi-online monitoring

QUACK performs reconstruction in a fraction of the time of gradient descent.

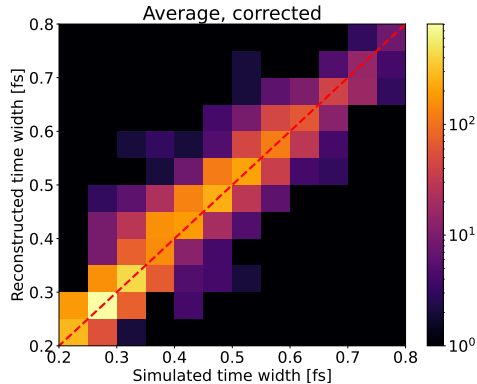


Time width reconstruction

- Simulation: linear chirp, circular polarization.
- Instrumental impact significant $\rightarrow$ rely on high spectral quality.



Simulated instrumental resolution and noise



After instrumental effect correction