XPFS analysis using Convolutional Neural Networks

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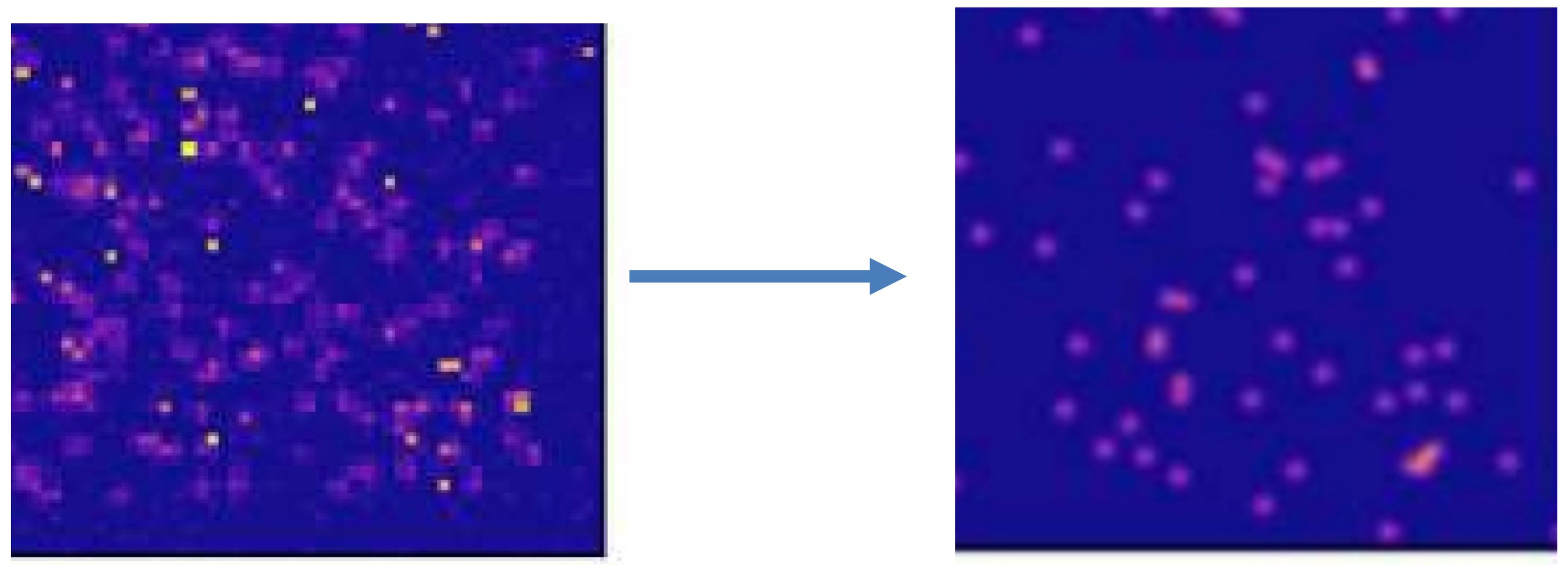
Introduction

- X-ray Photon Fluctuation Spectroscopy is a single photon counting technique used to study ultrafast materials dynamics.
- It is a statistical technique which requires tens of thousands of frames to derive any useful physics.
- To obtain the relevant physics, the experimental data must be denoised and deconvolved to obtain a discrete image which counts the number of incident photons per pixel.

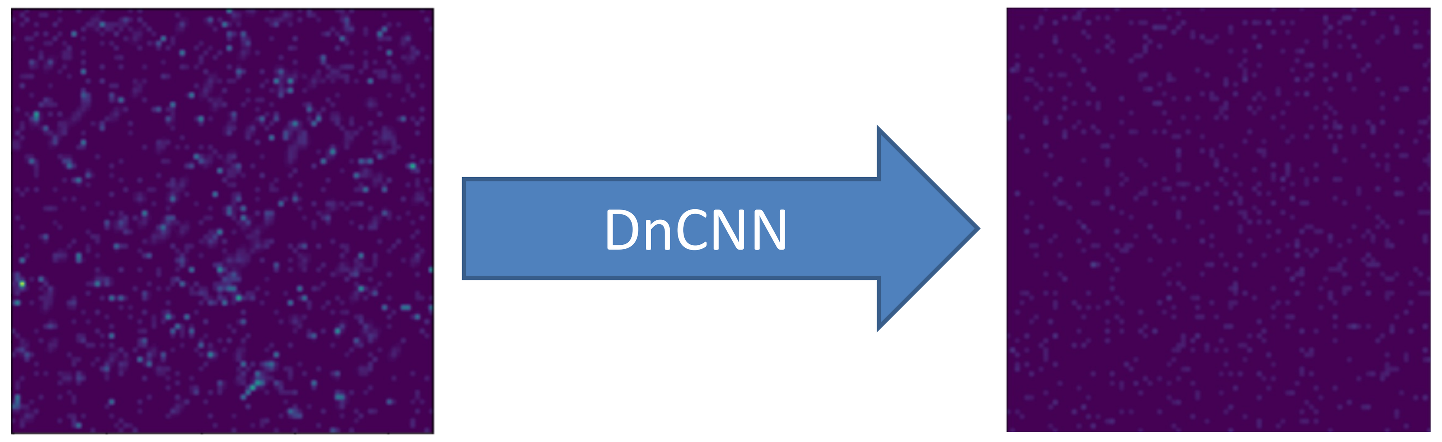


Related Work and Motivation

- Prior methods such as Greedy Guess [2,3] and Greedy Guess - Least Squares [2,3] have been developed for this task, however they are very slow compared to the acquisition speed at LCLS. In addition, these methods often struggle with higher SNR data.
- In this poster, we attempt to analyze XPFS data using convolutional neural networks on data from an accurate experimental simulator [1]. The motivation for this approach is that a supervised pipeline could be **faster** and **more accurate** than conventional approaches.

New Techniques

1. *Background Denoising with a DnCNN* [5]



Noisy Image *Residual Image*

2. *U-net* [6] *+ photon conserving loss function penalty*

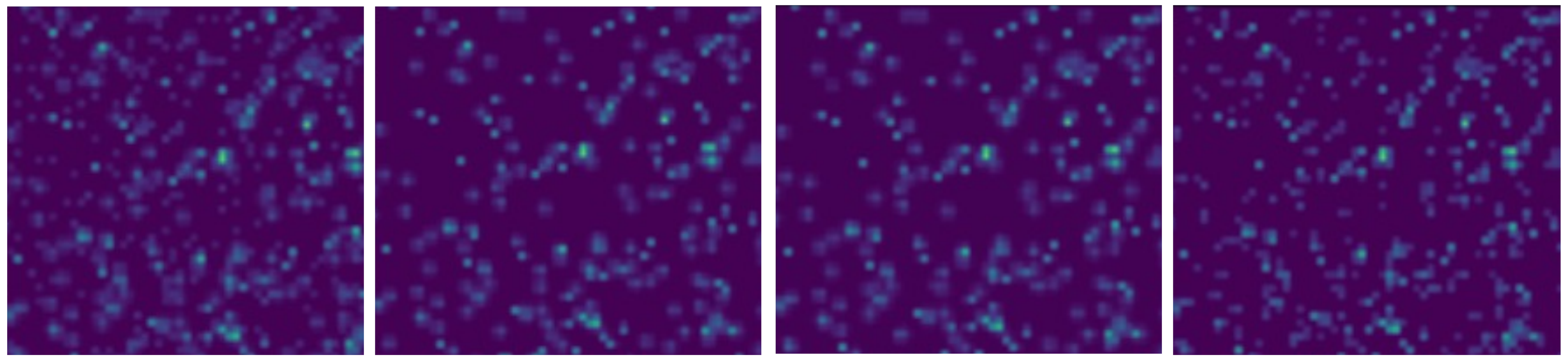
CrossEntropy[true, pred**]** + **MSE[sumPool**(true), **sumPool**(pred)**]**

Standard U-net classification loss

Photon Conserving Term

Simulation Results

1. Background Denoising with a DnCNN



Noisy Image | True Noiseless Image | DcNN Result | Hard Threshold Result

Photon ADU	MAE Ratio: Manual/DnCNN
340	3.23x
170	3.49x
113	5.21x

Takeaway 1: CNN denoising strongly outperforms denoising based on any manual threshold

Takeaway 2: Performance is even more noticeable as the SNR ratio of the data changes – i.e. DnCNN performs better on low signal data.

2. U-net + photon conserving loss function penalty

Method	Macro F1 Score
U-Net	0.67
U-Net + Sample weighting (inverse class prevalence)	0.40
U-Net + 50% SMOTE data	0.67
U-Net + Focal Loss Function [4]	0.46
U-Net + Photon Conserving Loss Penalty (3x)	0.68
U-Net + Photon Conserving Loss Penalty (2x)	0.69

Takeaway 1:Photon Conserving Loss Penalty appears to be helping the sparse prediction issue

Future Work

- Combine different bin sizes for photon conservation constraint
- Add a photon conservation constraint on input space (raw image) in addition to prediction space (discrete photon maps)
- Test generalization of simulation trained DnCNN and U-net on experimental data from LCLS

References

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