Denoising Electron-Microscope Images

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Collaboration with the Crozier lab at ASU (Peter Crozier, Ramon Manzorro, Josh Vincent)

Scientific goal

- We want to understand the atomic structure of catalysts.
- To see the structure, we image them using an electron microscope.

Scientific goal

We want to understand the atomic structure of catalysts.

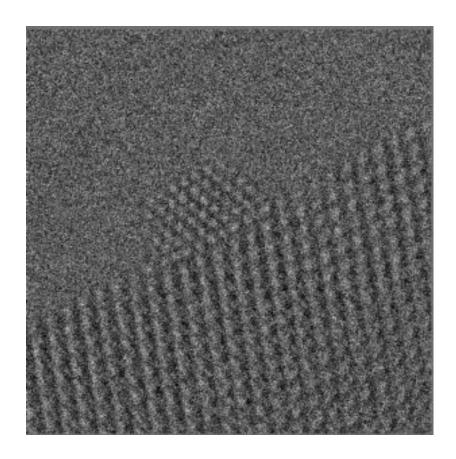
To see the structure, we image them using an electron microscope. Actually,

this guy does the imaging.

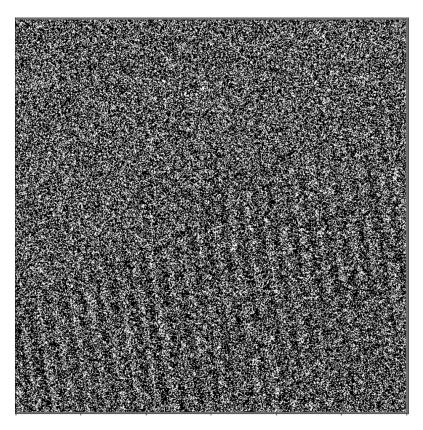
It is estimated that 90% of all manufactured products involve catalytic processes somewhere in their production chain, and such products have considerable impact in energy, healthcare (pharmaceuticals), new - materials (polymers), transport, and the environment (water, air quality, renewable and bio – produced materials)



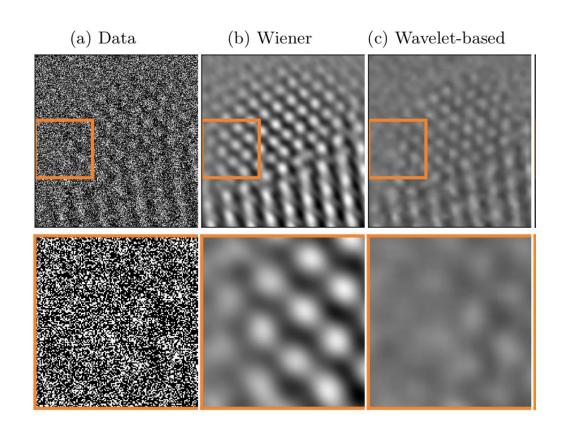
This is what comes out of the microscope:



Single frame



Wiener filtering and wavelet-based method



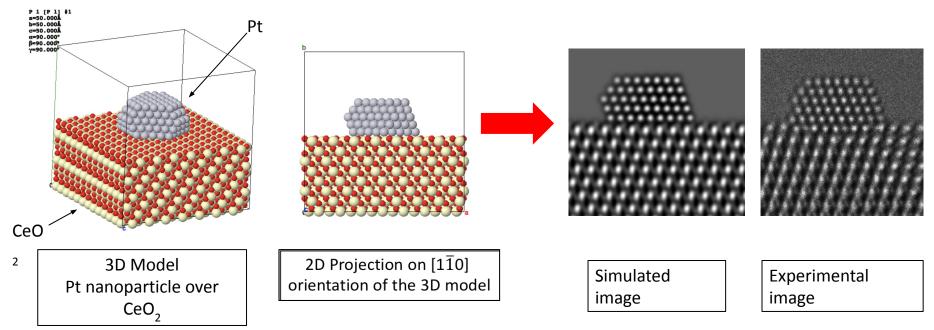
How can we use neural networks to denoise these data?

We need clean image - noisy image pairs to train...

To obtain the clean images we need to denoise!

Simulating electron-microscope images

An atomic model was built to describe the studied system: Pt supported on ceria, CeO₂

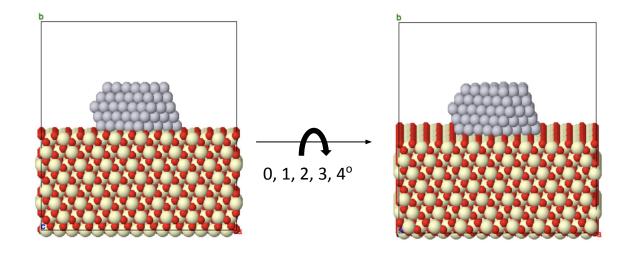


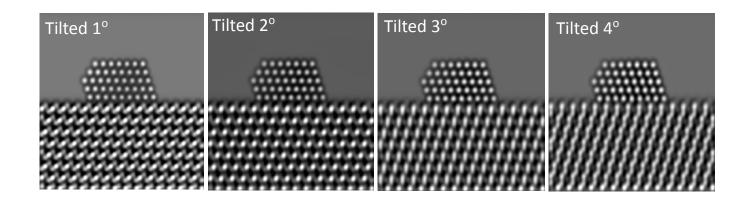
Challenge: The simulation depends on imaging parameters (e. g. tilt, defocus) that are likely to change during the acquisition of experimental data

Thickness

Thickness= 3nm	Thickness= 4nm	Thickness= 5nm	Thickness= 6nm

Tilt

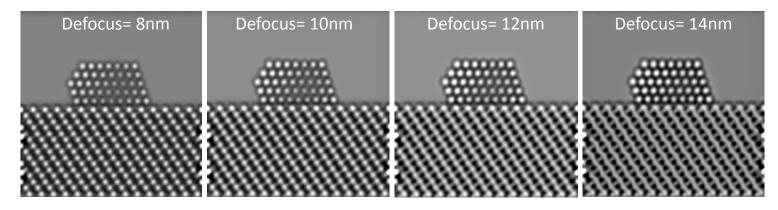




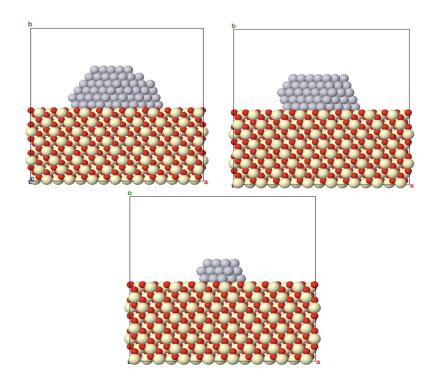
Modulations on intensity: Defocus effect



Variations on the electromagnetic lens lead in modifications of the defocus value

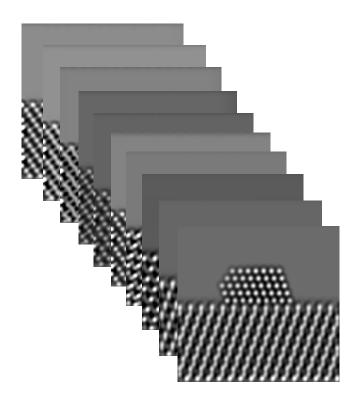


Generation of dataset



Variations in structure (thickness, nanoparticle size, superficial defects) ~1000 atomic models

Variations in imaging parameters

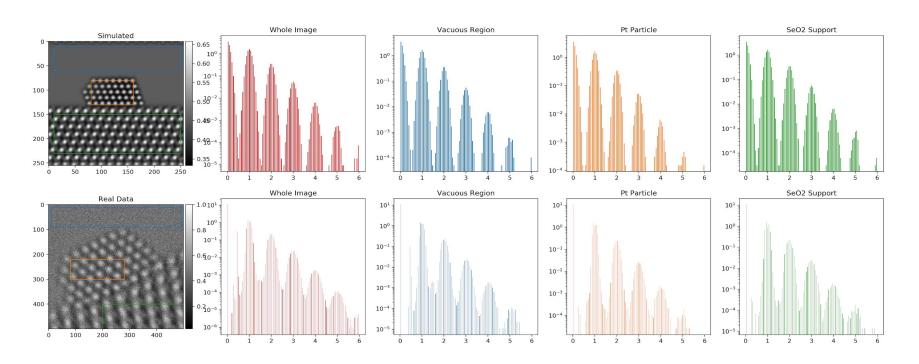


~ 20.000 simulated images

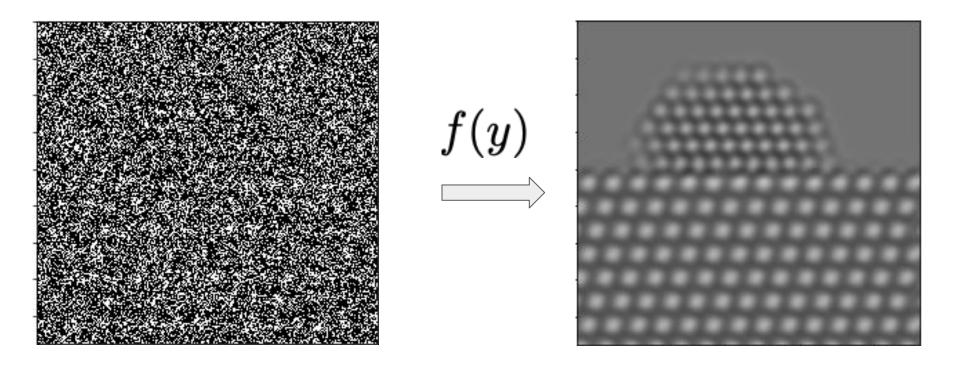
Now we have "clean images" what else do we need?

We need to simulate the noise!

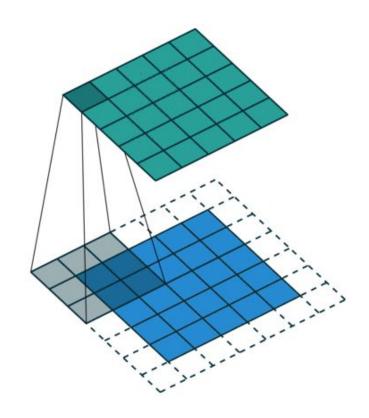
Empirical distribution is well approximated as iid Poisson



Goal: Train convolutional neural network to denoise



Convolutions



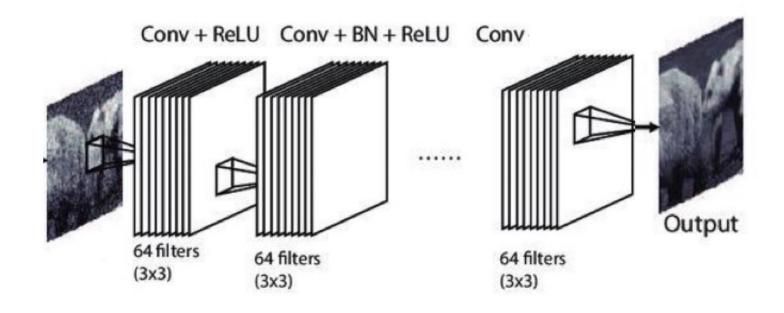
ReLU

9	3	5	-8
-6	2	-3	1
1	3	4	1
3	-4	5	1

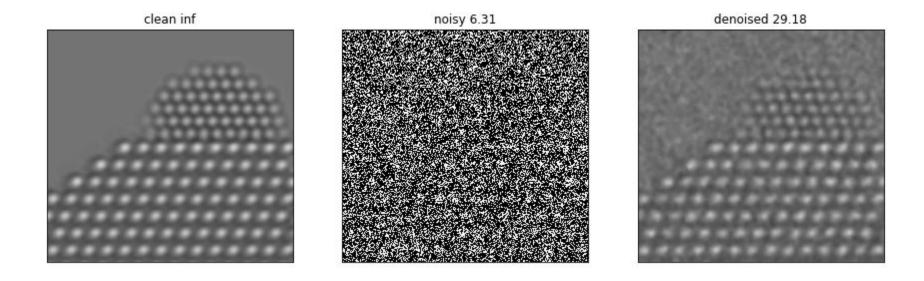


9	3	5	0
0	2	0	1
1	3	4	1
3	0	5	1

DnCNN (Zhang et al, 2017)

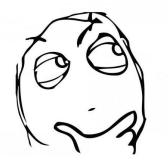


DnCNN

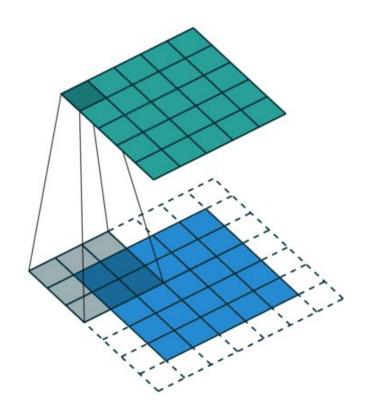




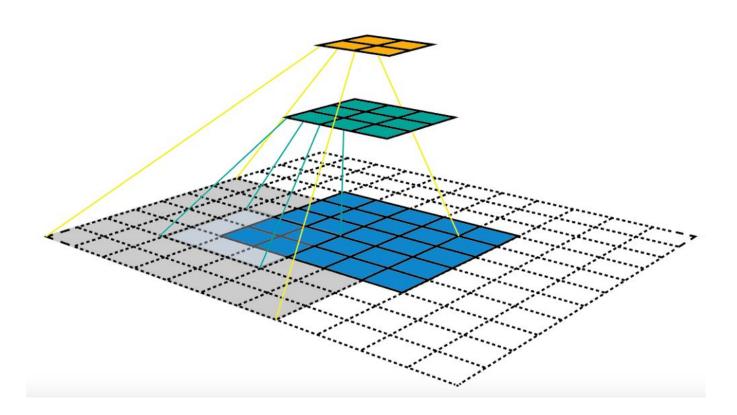
How can we improve it?



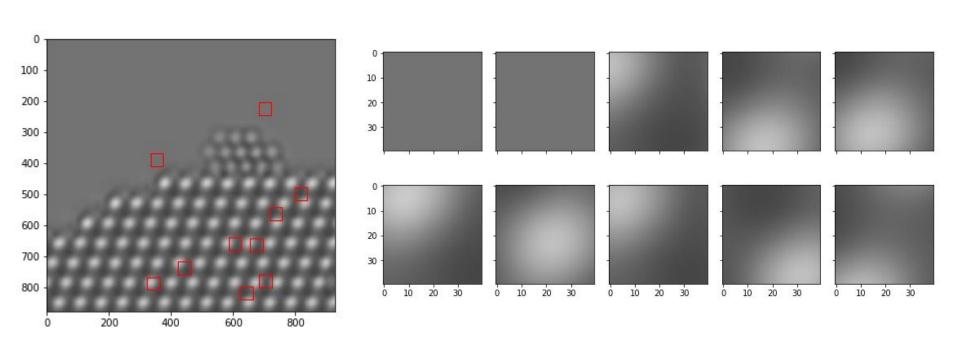
Receptive Field



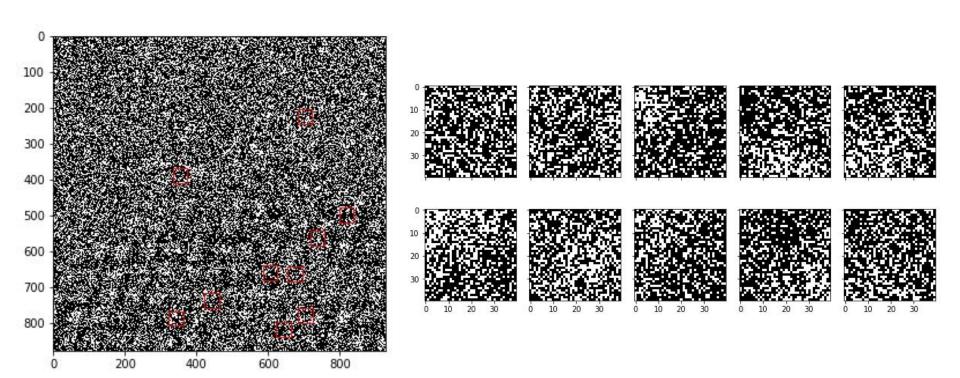
Receptive Field



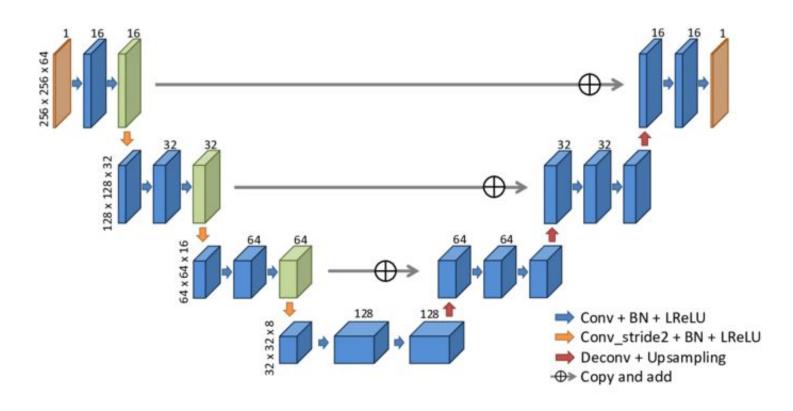
DnCNN has a receptive field of 41 x 41



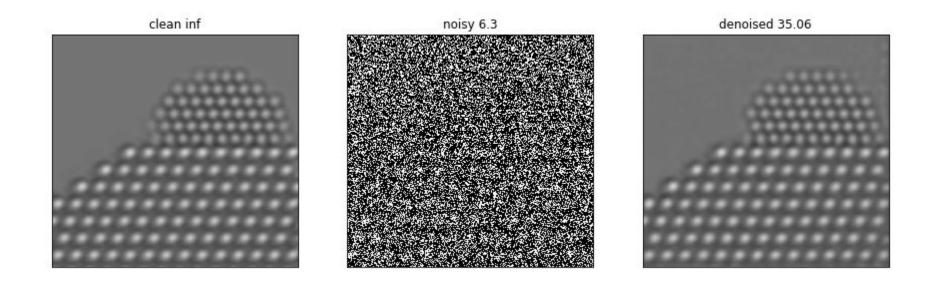
Difficult to see structure in small regions



UNet has large receptive field

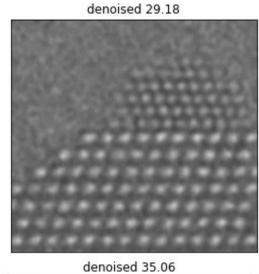


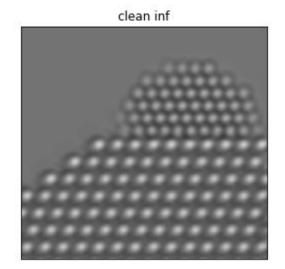
Much better results!

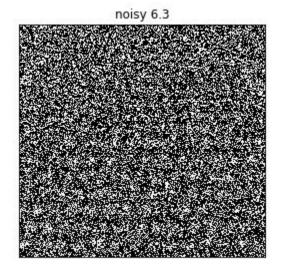


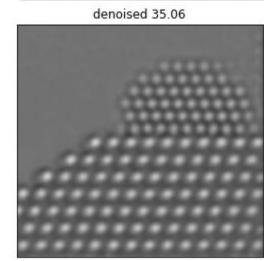
Much better than DnCNN

DnCNN

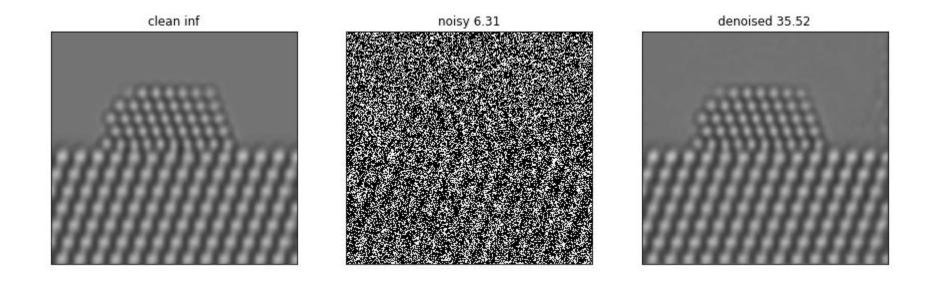






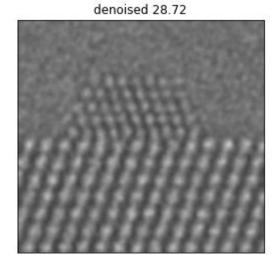


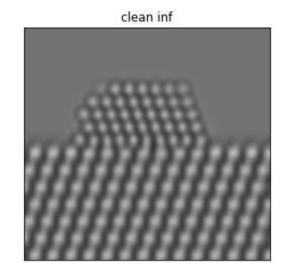
Another example

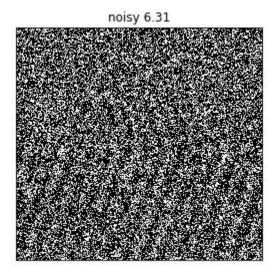


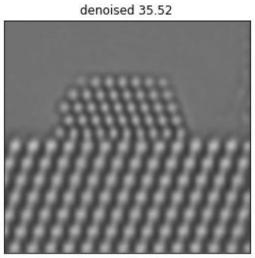
Another example

DnCNN









Increasing field of view

(a	TEM	Images
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Model	Parameters	FoV	PSNR	SSIM
SBD + DnCNN [72]	668K	41×41	30.47 ± 0.64	0.93 ± 0.01
SBD + Small UNet [73]	233K	45×45	30.87 ± 0.56	0.93 ± 0.01
SBD + UNet (32 base channels)	352K	221×221	36.39 ± 0.77	0.98 ± 0.01
SBD + UNet (64 base channels)	1.41 M	221×221	37.24 ± 0.76	0.99 ± 0.01
SBD + UNet (128 base channels)	5.61M	221×221	38.05 ± 0.81	0.99 ± 0.01
SBD + UNet (128 base channels)	70.15M	893×893	42.87 ± 1.45	0.99 ± 0.01

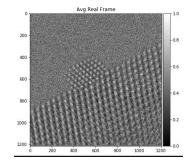
(b) Photographic Images

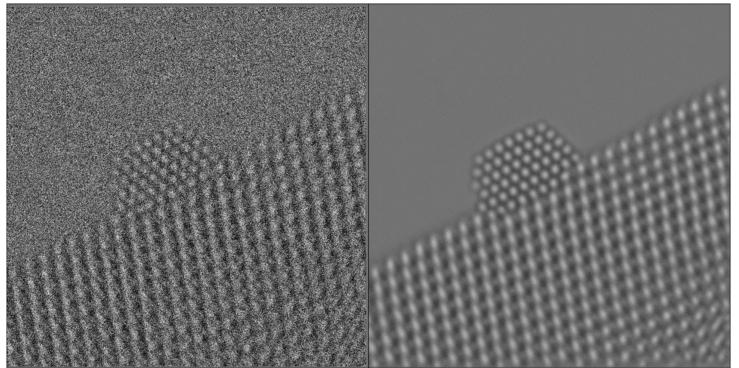
MODEL	Parameters	FoV	PSNR		SS	IM
			$\sigma = 30$	$\sigma = 70$	$\sigma = 30$	$\sigma = 70$
UNet	102K	49 × 49	29.67 ± 2.84	26.16 ± 2.79	0.83 ± 0.06	0.70 ± 0.09
UNet	352K	221×221	29.65 ± 2.76	26.08 ± 2.68	0.83 ± 0.05	0.70 ± 0.08
UNet	4.4M	893×893	29.54 ± 2.82	26.07 ± 2.80	0.83 ± 0.06	0.70 ± 0.09

Ok, what about the real data?

Noisy Movie (Input)

Denoised Movie (Output)





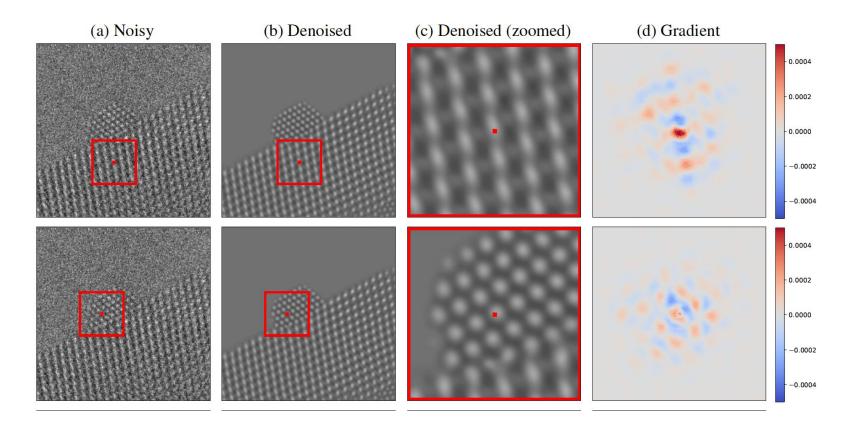
This looks great, but what is this thing doing?



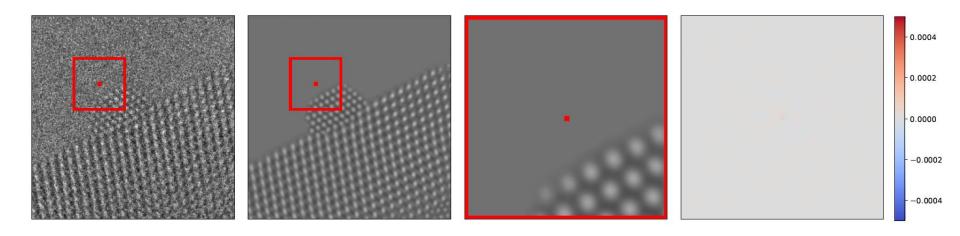
Linear approximation of the learned function

$$f(x) \cong J_x x$$

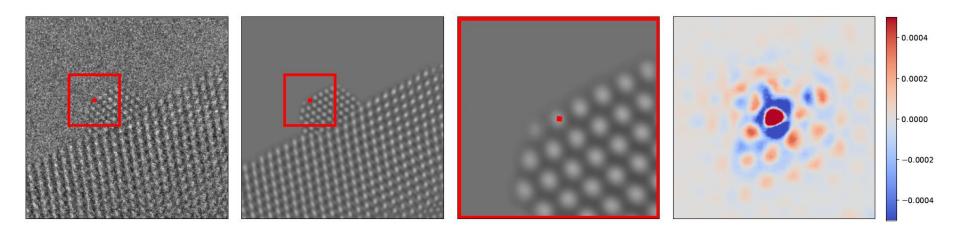
Network looks at neighboring atoms!



In the vacuum



On the surface



For more information

Deep denoising for scientific discovery: A case study in electron microscopy

S. Mohan, R. Manzorro, J. L. Vincent, B. Tang, D. Y. Sheth, D. S. Mattesson, E. P. Simoncelli, P. A. Crozier, C. Fernandez-Granda