Image Processing Pipeline for AI-Driven Nanoparticle Megalibrary Characterization

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Supplemental Information

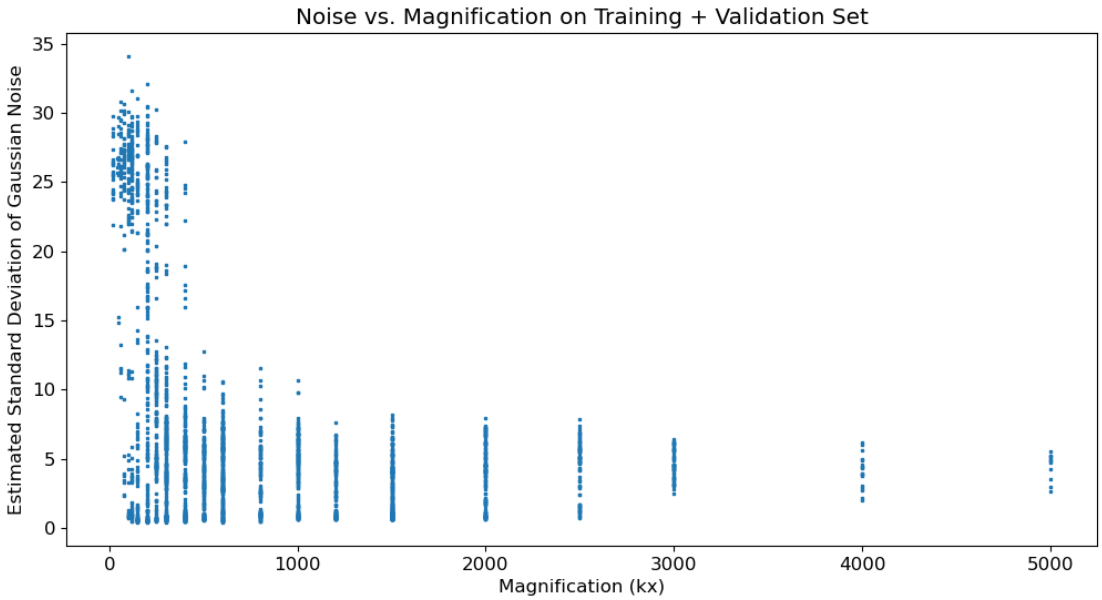

Figure SI 1. Estimated standard deviation of Gaussian noise for images in the training + validation set vs. magnification.

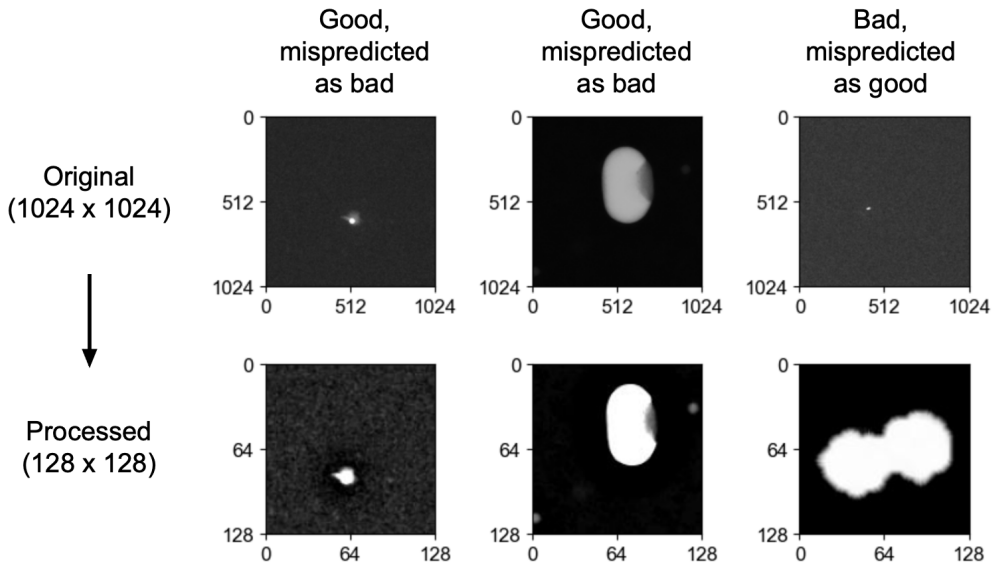

Figure SI 2. Sample original and processed images that were mispredicted by the best-performing model. The pixel resolution of the original images is 1024 x 1024; the processed images have resolutions of 128 x 128. The image on the left is labeled "good" but predicted as "bad;" this may be due to artifacts in the original image that are emphasized after image processing. In the middle image, the image processing pipeline identifies faint background features at the lower left and upper right that are not clearly visible in the original image. In the image to the right, two particles partially overlap, which perhaps accounts for the model's "good" prediction.

Table SI 1. Best Model Decision Performance at Different Pixel Resolutions (Trained on Data1 ∪ Data2 and Tested on Data3); Data from Figure 8.

Pixel Resolution	Accuracy (%)	AUC (%)	$F_{1/3}$ (%)	F_1 (%)	Precision (%)	Recall (%)
	Unprocessed					
16 x 16	57.4	66.0	79.8	65.9	84.2	54.1
32 x 32	57.7	64.1	78.1	67.3	81.4	57.4
64 x 64	70.7	69.9	81.7	80.3	82.0	78.6
128 x 128	75.8	74.2	83.5	84.3	83.3	85.3
	Processed					
16 x 16	86.4	92.8	95.0	90.5	96.2	85.4
32 x 32	80.0	89.2	92.4	85.7	94.3	78.5
64 x 64	87.5	91.1	93.8	91.5	94.4	88.8
128 x 128	88.4	93.5	95.1	92.0	95.9	88.4

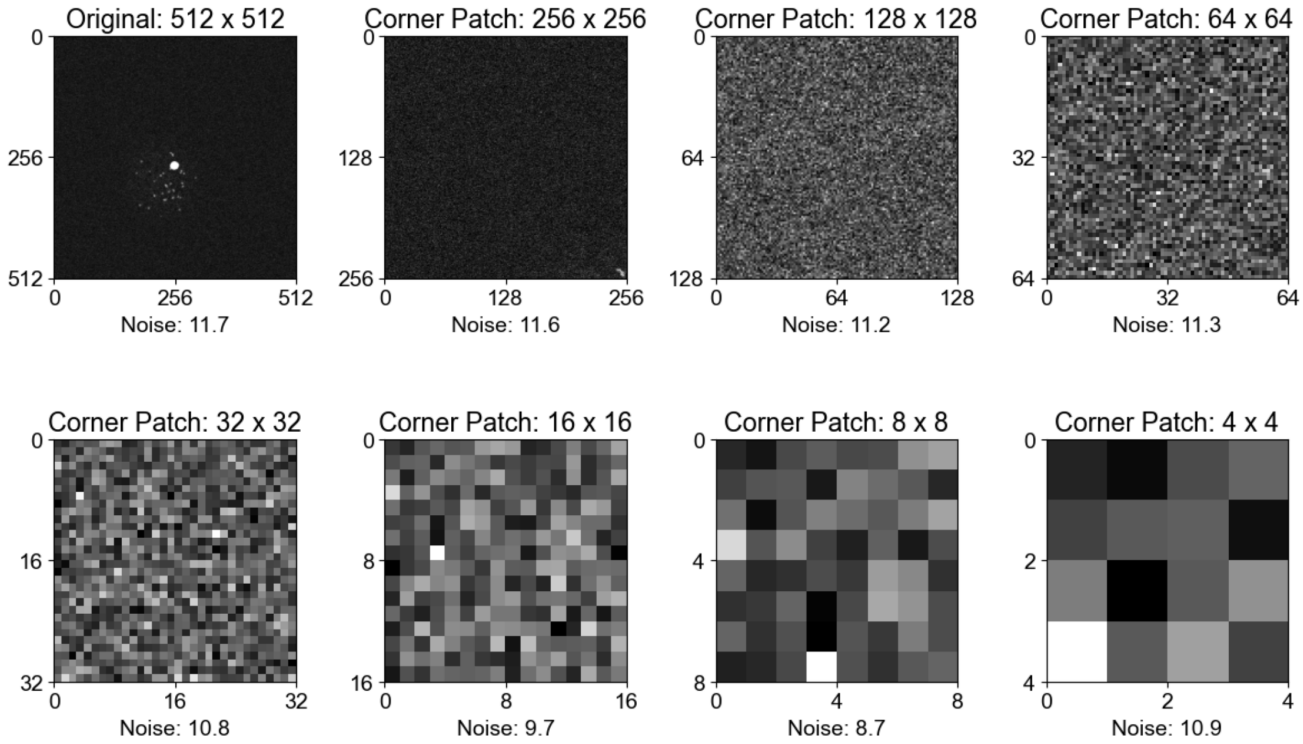

Figure SI 3. Estimating the standard deviation of Gaussian noise for an image using corner patches. The patch dimension appears above each sub-figure and the estimated noise level appears below. Using a corner patch of size 32 x 32 preserved the original noise category in >99.5% of images from the validation set.

Table SI 2. Mispredictions by magnification level on the test set for three different models; data from Figure 9.

Magnification (kx)	Downsizing Only (128 x 128)	Previous Work (512 x 512)	This Work (128 x 128)
50	108	85	55
60	74	68	21
80	70	70	40
100	74	44	36
120	64	34	8
150	45	42	37
200	83	50	62
250	42	50	25
300	63	48	36
400	42	55	18
500	43	47	21
600	42	69	16
800	34	70	11
1000	31	54	12
1200	27	52	11
1500	15	37	5
2000	9	11	4
2500	2	1	0
3000	0	0	0
4000	0	1	0
5000	0	0	0

Table SI 3. Image Processing Time Statistics (ms); Data from Figure 10.

	All Images High Noise	All Images Low Noise	Training + Validation High Noise	Training + Validation Low Noise	Test High Noise	Test Low Noise
Minimum	35.3	13.3	35.3	14.4	43.6	13.3
Median	128.1	59.2	49.3	19.5	129.0	71.1
Maximum	712.4	168.0	712.4	68.7	193.2	168.0

Table SI 4. Inference Time Statistics (ms); Data from Figure 10.

Pixel Resolution	Minimum	Median	Mean	Maximum
128 x 128	0.8	1.0	1.1	32.5
64 x 64	0.6	0.7	0.8	28.0
32 x 32	0.6	0.6	0.7	28.4
16 x 16	0.5	0.6	0.6	30.0