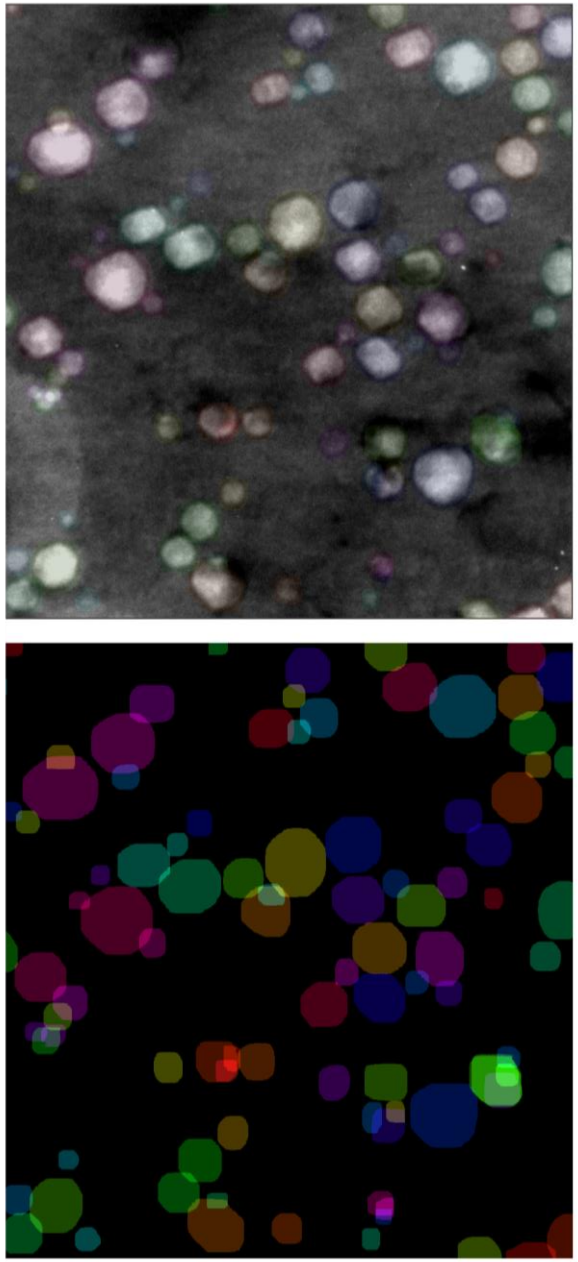
Virtual Summer School: Machine Learning in Electron Microscopy Lecture 13

Examples of DCNN in Electron Microscopy

Tommy Wong

Lecture Github:
github.com/SergeiVKalinin/ML-ElectronMicroscopy-2023/tree/main/Lecture%2013



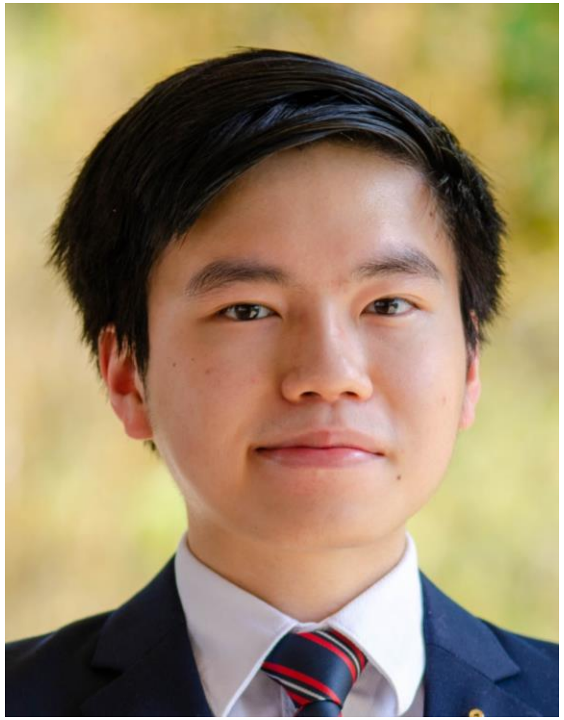
Labeling this image took ~ 1 hr, DL prediction took < 1 min.

About me

Tommy (Chun Yin) Wong

Advisors: Dr. Sergei Kalinin, Dr. Maxim Ziatdinov

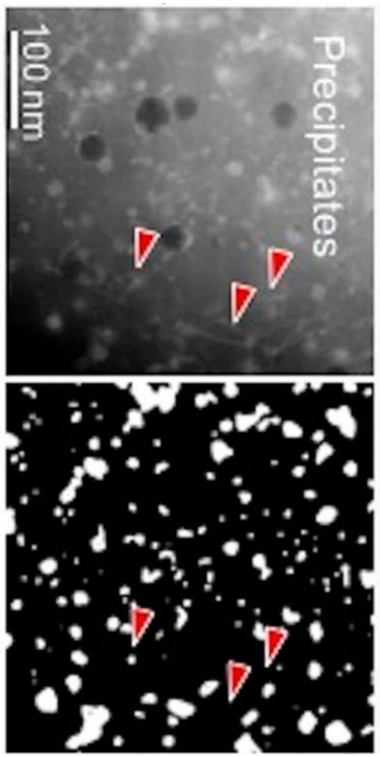
- Research interests: deep learning & computer vision, electron microscopy, radiation damage
- 3rd year Ph.D. student in Energy Science & Engineering, Bredesen Center, University of Tennessee (joint program with ORNL)
- M.S. in Materials Science & Engineering ‘22, University of Tennessee
- B.S.E. in Nuclear Engineering & Radiological Sciences ‘20, University of Michigan



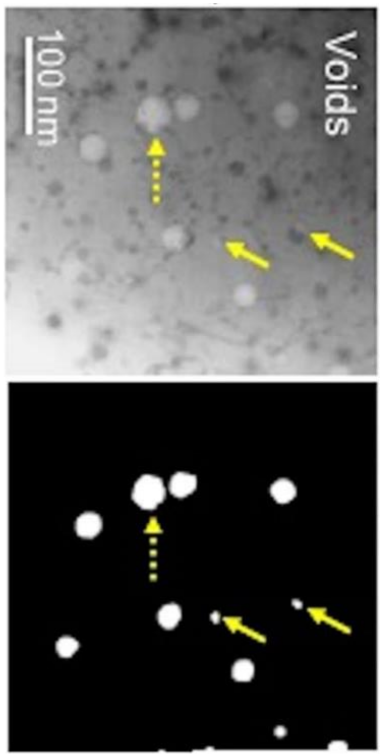
- cwong13@vols.utk.edu
- My Github: github.com/tommycwong

Microstructural defects can be labeled for pixel-wise segmentation

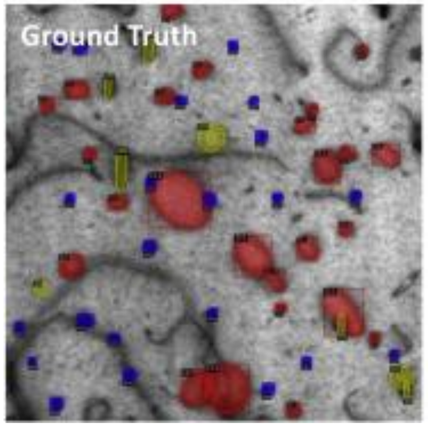
- Segmentation: associating each pixel in an image with a class



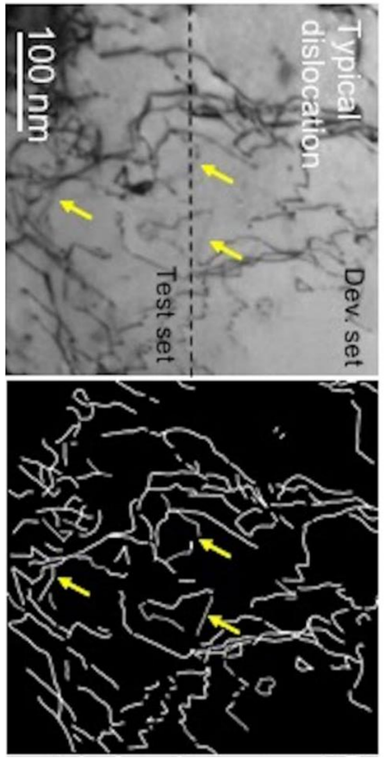
Cavities (bubbles & voids)



Precipitates



Dislocation loops

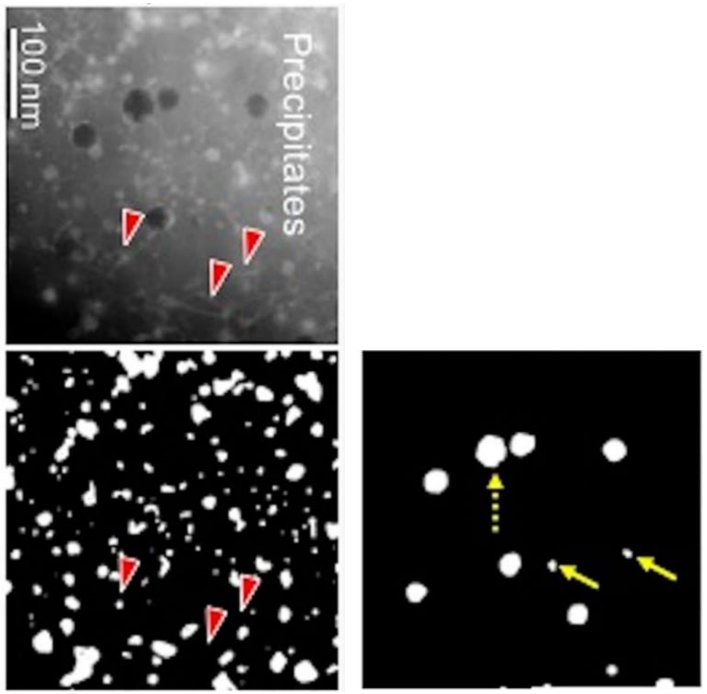


Dislocation lines

Adapted from Roberts et al. 2019 10.1038/s41598-019-49105-0, Jacobs et al. 2022 10.1016/j.xcrp.2022.100876

Different labeling systems are required for different segmentation algorithms

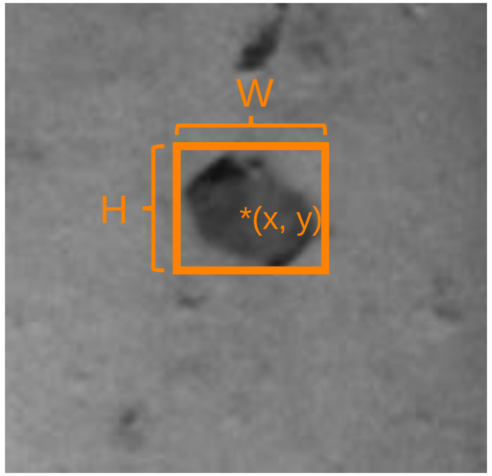
- **Important: labels are usually either 0 or 1**



Precipitates

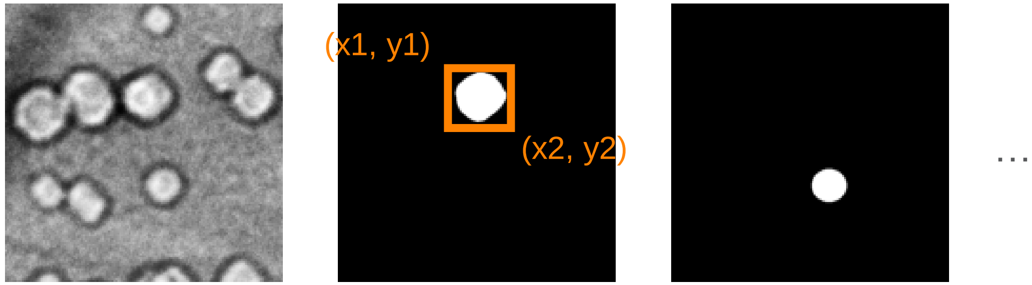
Voids

Semantic segmentation: one-hot encoding (U-Net)



[Class x y W H]

Object identification: bounding box (YOLO)



Dictionary{
‘boxes’: [x1 y1 x2 y2]
‘labels’: class
‘masks’: feature mask
}

Instance segmentation: label encoding (Mask R-CNN)

Adapted from Roberts et al. 2019 10.1038/s41598-019-49105-0, Yang et al. 2011 10.1038/srep00190

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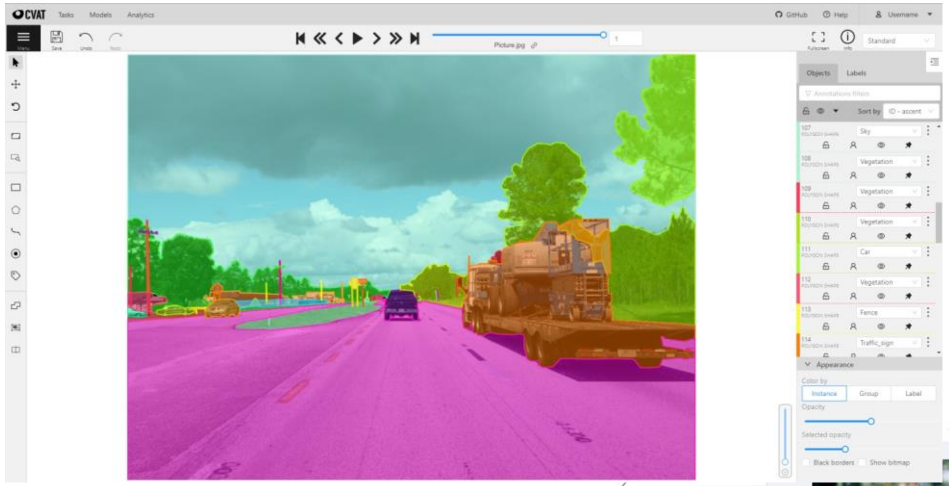
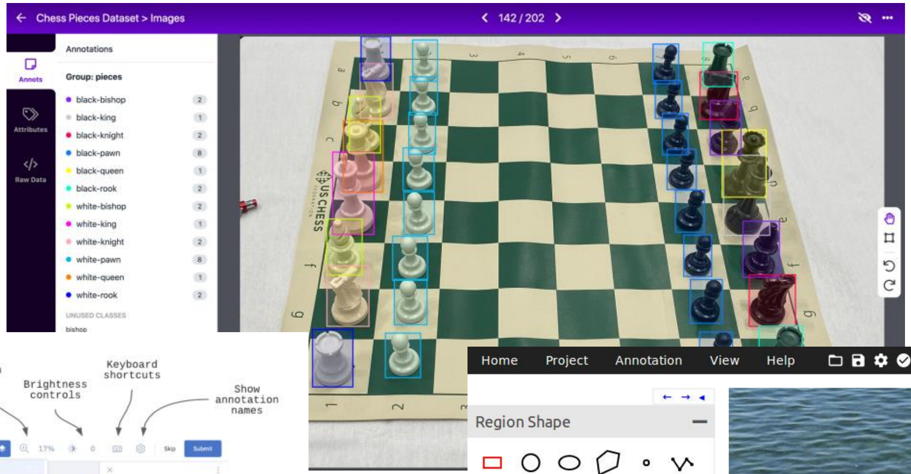
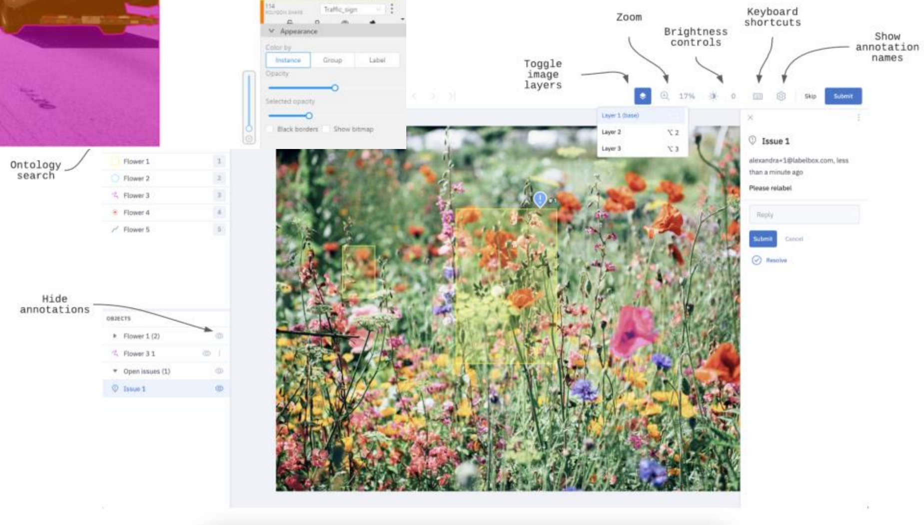
Web-based GUI tools are used for labeling



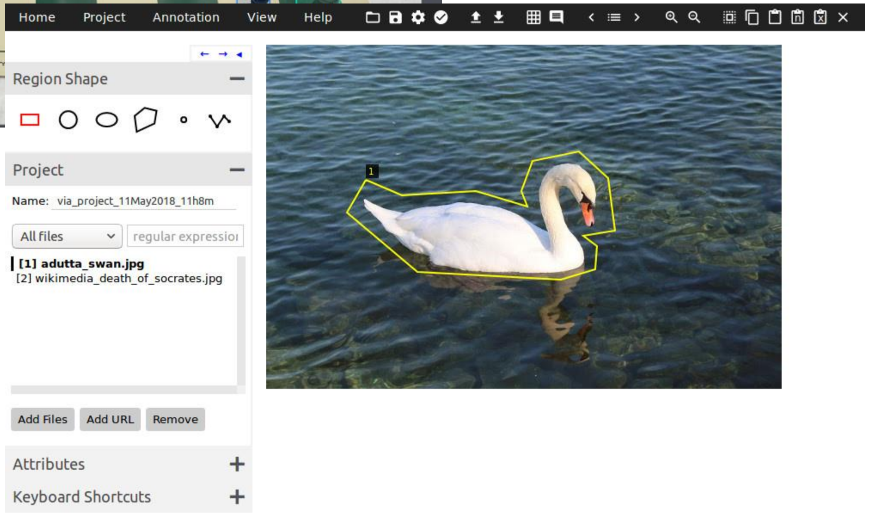
CVAT



Roboflow



Labelbox



VIA

Labeling using Computer Vision Annotation Tool (CVAT)

cvat.ai

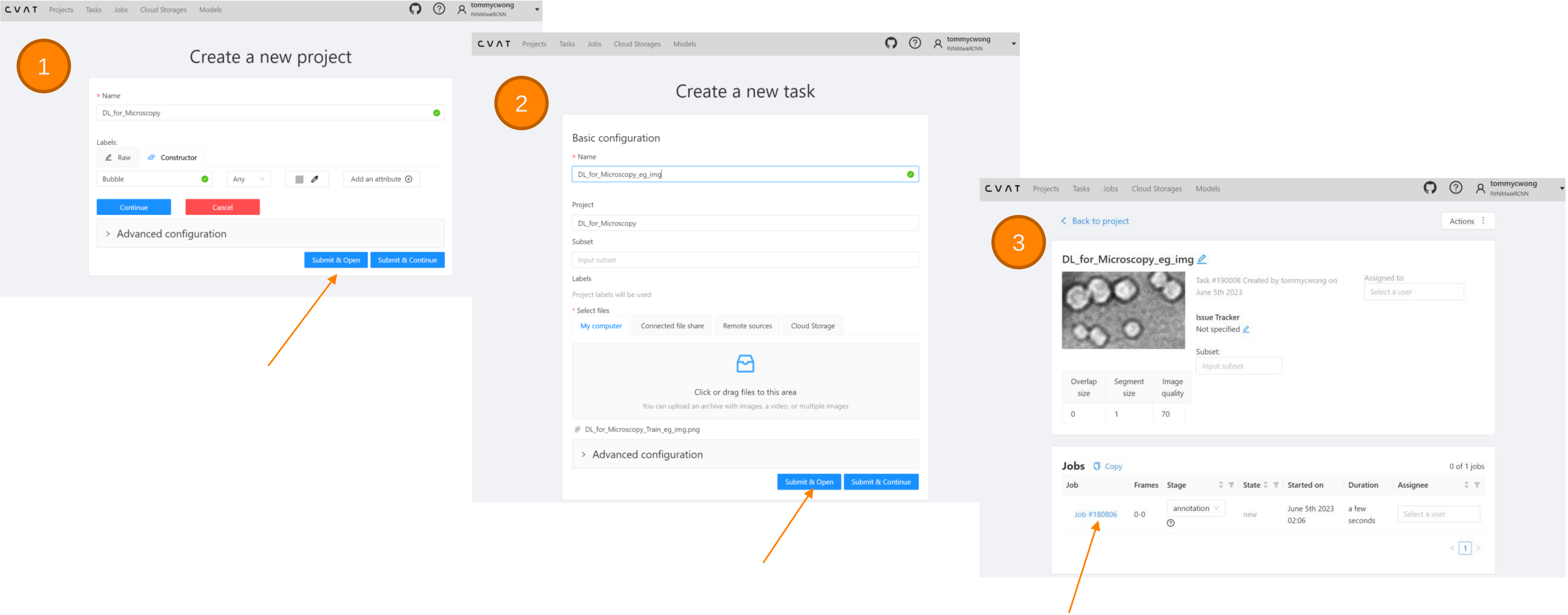
Documentation:
github.com/TaSeeMba/cvat/blob/master/cvat/apps/documentation/user_guide.md

CVAT labeling workflow

Important: before labeling, ensure all image data have the same dimensions e.g. 1024x1024

1. Create project
2. Create tasks
3. Labeling jobs
4. Export labels
5. Parse labels using Python

Creating a project and labeling tasks



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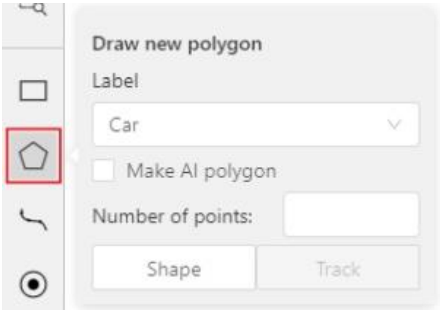
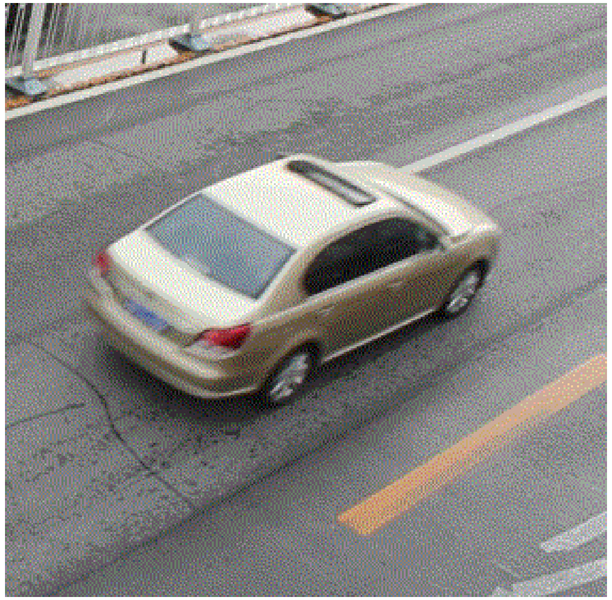
Labeling using polygon and ellipse tools

Remember to click **Save**

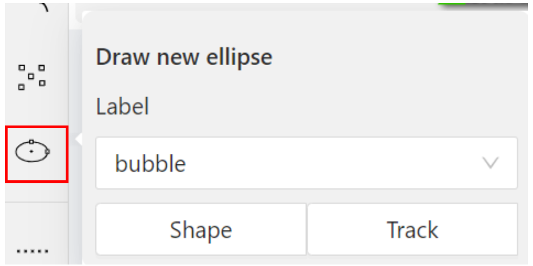
Polygon tool

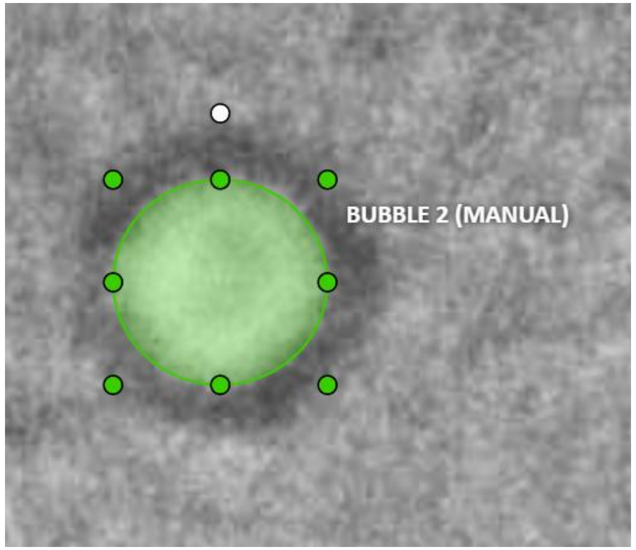
- Hold **Shift** to draw





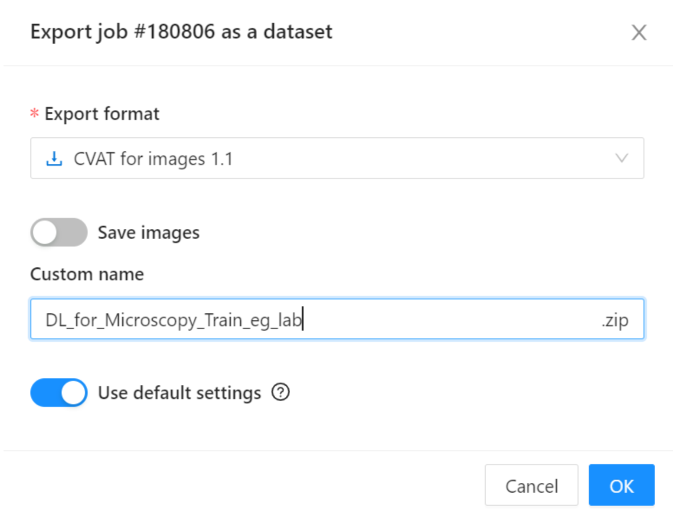
Ellipse tool





Exporting and parsing labels

Export as .xml



Parsing labels using Python

```
get_imgs(train_img_names)

parse_anno_file(xml, train_img_filename)

get_unet_mask(annos)

get_maskrcnn_mask(annos)

get_maskrcnn_dataset(images=train_imgs,
labels=maskRcnn_masks)
```



```xml
<image id="0" name="DL_for_Microscopy_Train_eg_img.png" width="512" height="512">
  <ellipse label="Bubble" source="manual" occluded="0" cx="291.95" cy="334.99" rx="32.35" ry="30.94" z_order="0">
  </ellipse>
  <polygon label="Bubble" source="manual" occluded="0" points="282.22,131.08;289.47,135.54;295.61,142.23;300.07,1
  </polygon>
```

Additional notes on labeling

- Features typically should have a convex mask
  - Concave masks are likely occluded convex masks
- Don’t leave holes between multiple overlapping masks
- Keep in mind output files: different parsing scripts needed for .xml, .json, etc.

Data Augmentation Techniques

Notebook: https://github.com/tommycwong/ML-ElectronMicroscopy-2023/blob/main/Lecture%2013/ML4EM_Summer2023_Data_Augmentation_supp.ipynb

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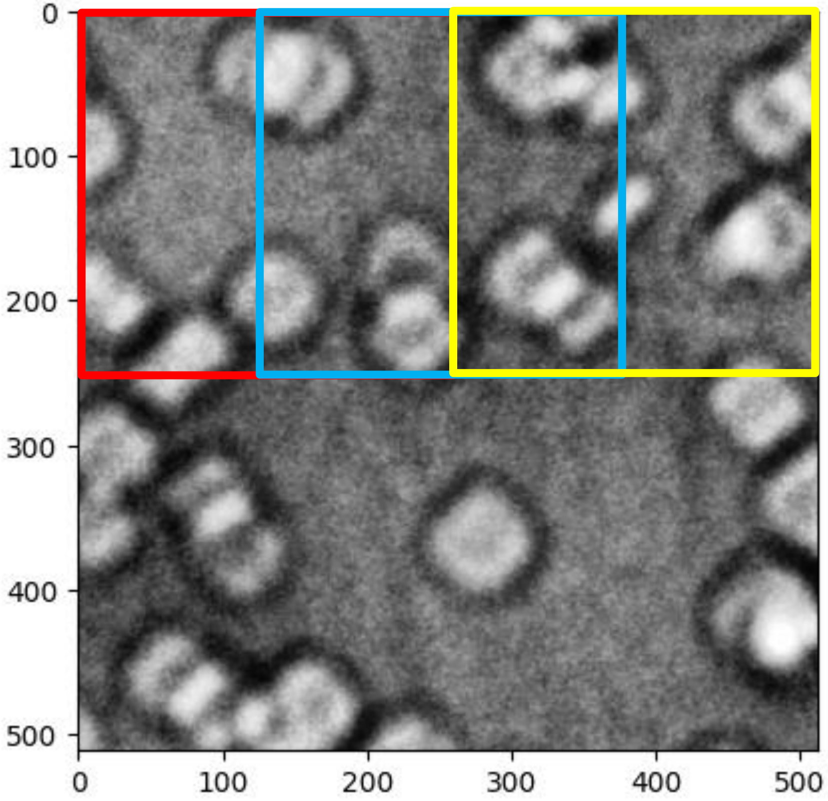
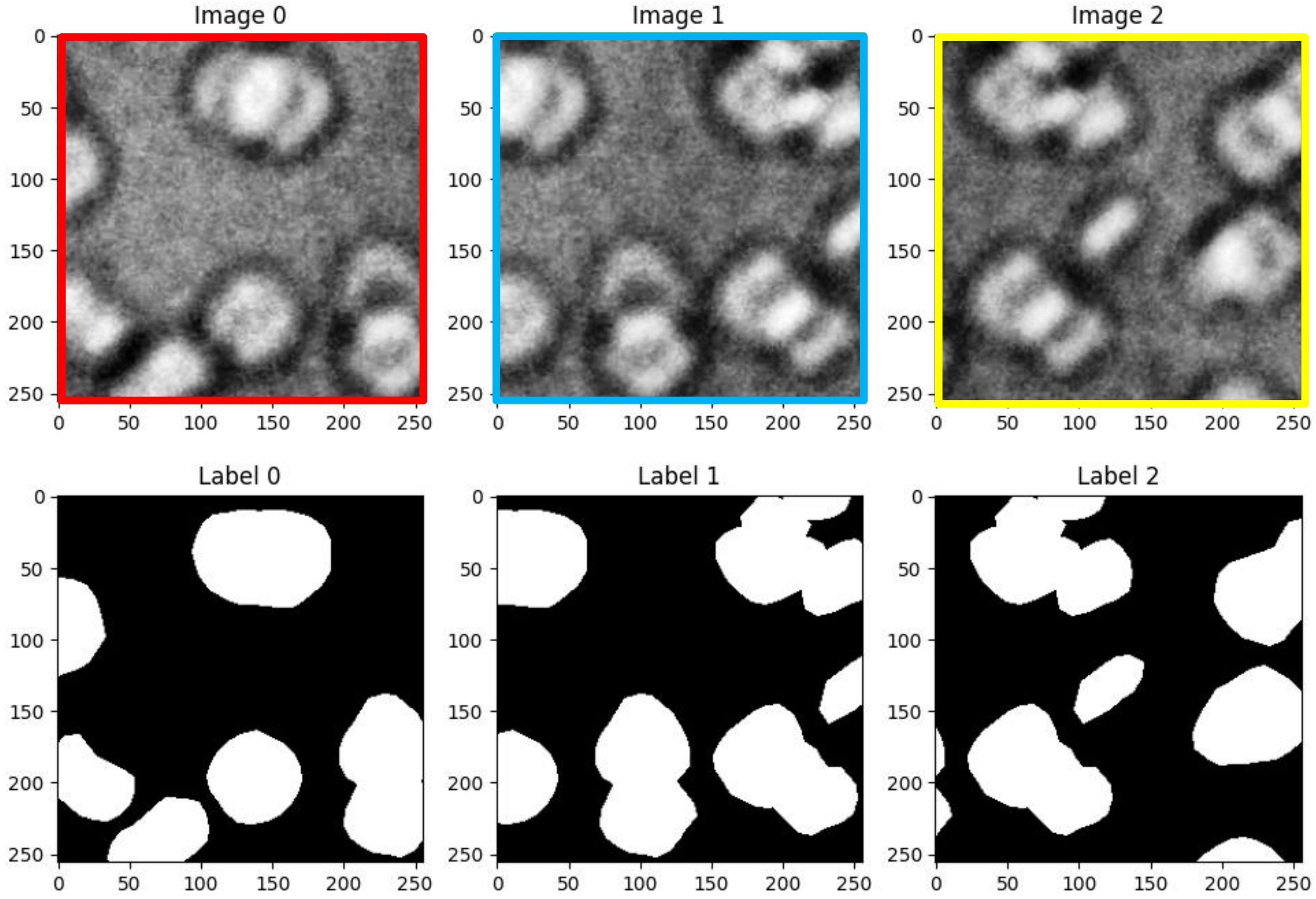
Rationale: more varied data → less overfitting

Electron microscopy experiments yield (relatively) small datasets

∴ requires augmentation

Use a sliding window cropper to enhance the dataset





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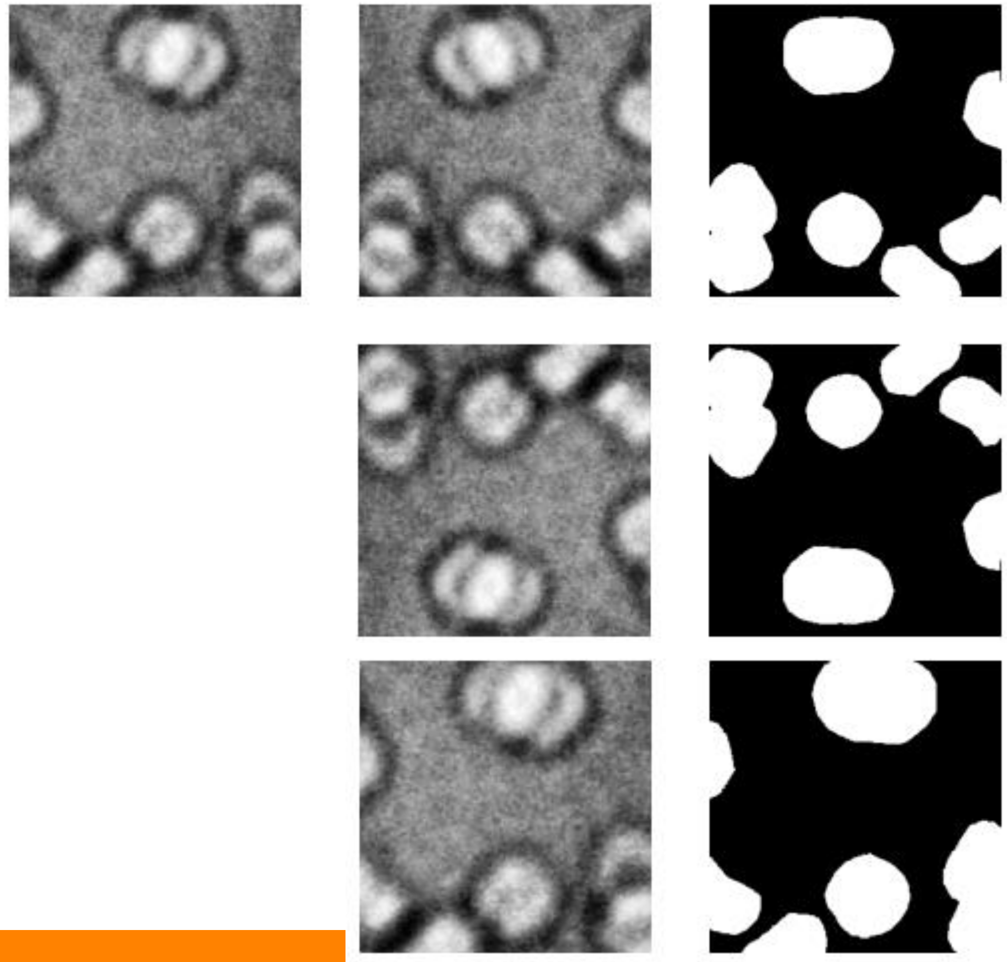
Rotate, flip, resize the image to increase variability

Original



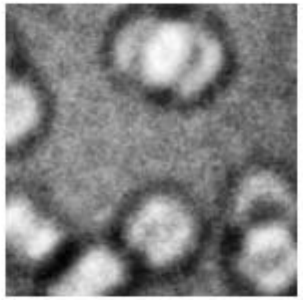
Flipped/Mirrored

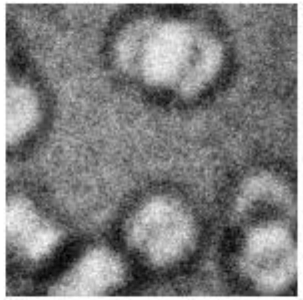
Rotated 180 degrees

Zoomed in

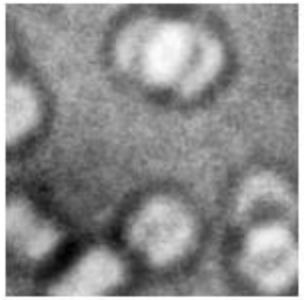
Adding noise to simulate noises during imaging

Original

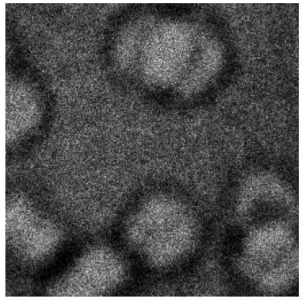




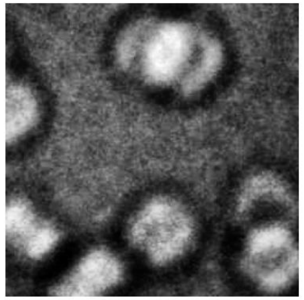
Gaussian



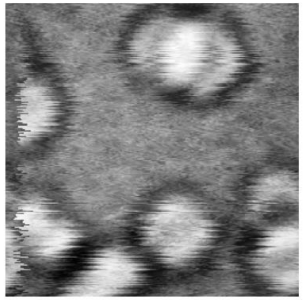
Background noise



Poisson

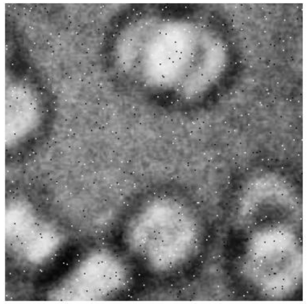


Contrast



Jitter

Blur



Salt & pepper

Convolutional Neural Networks (CNN)

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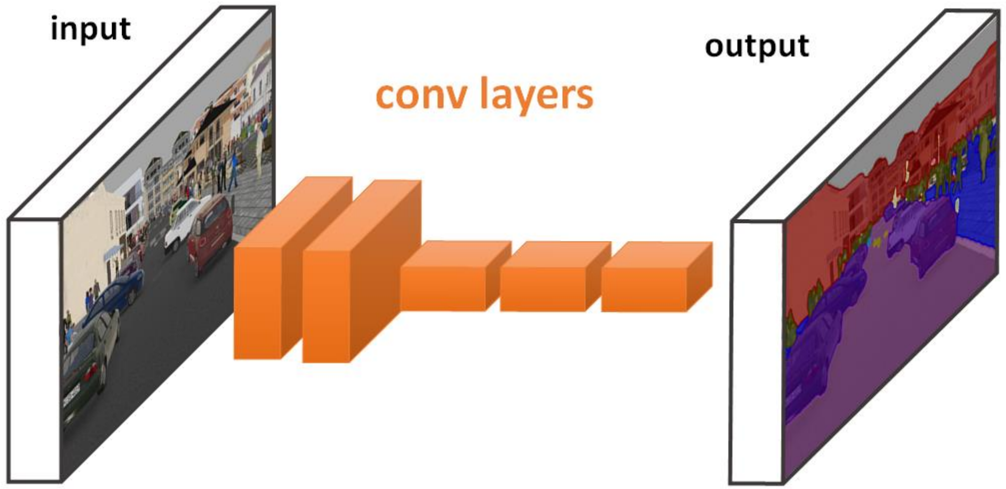
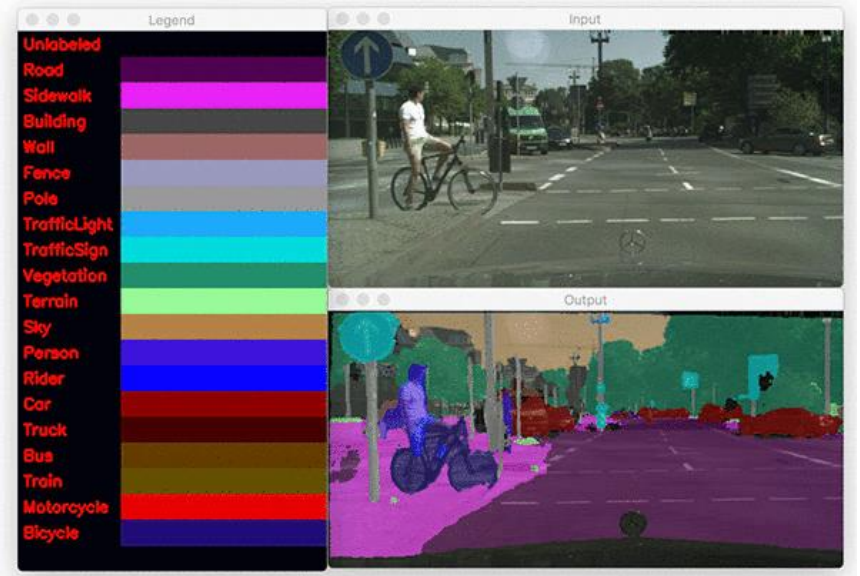
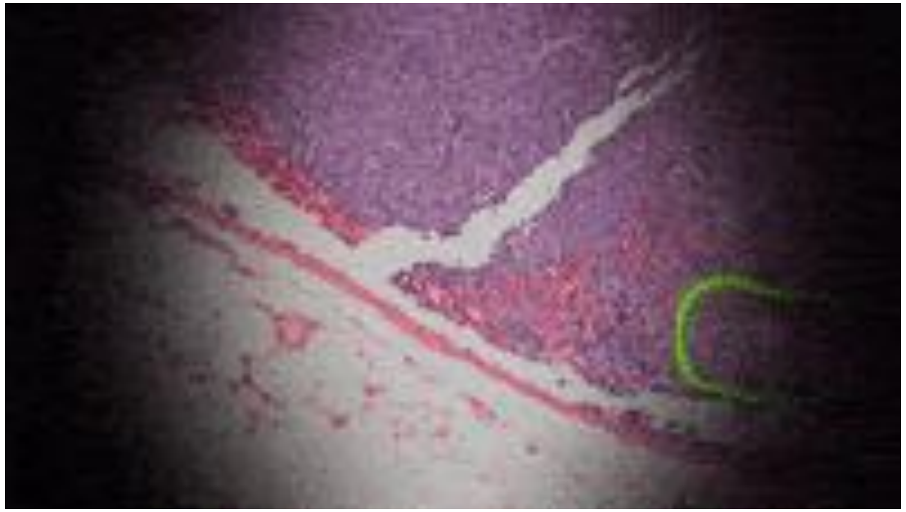


Semantic segmentation assigns class labels to each pixel



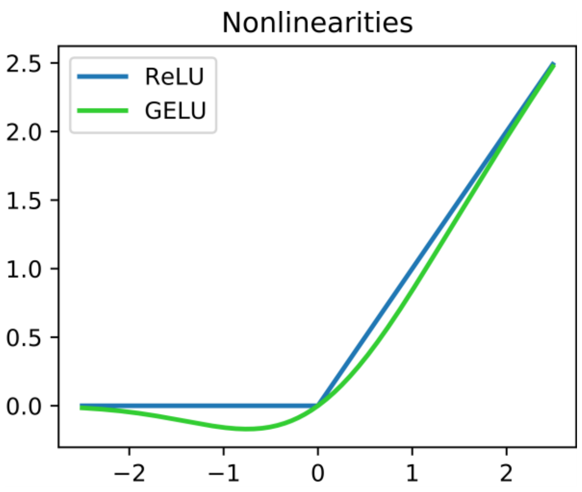
Semantic segmentation of street views *[1], [2]*



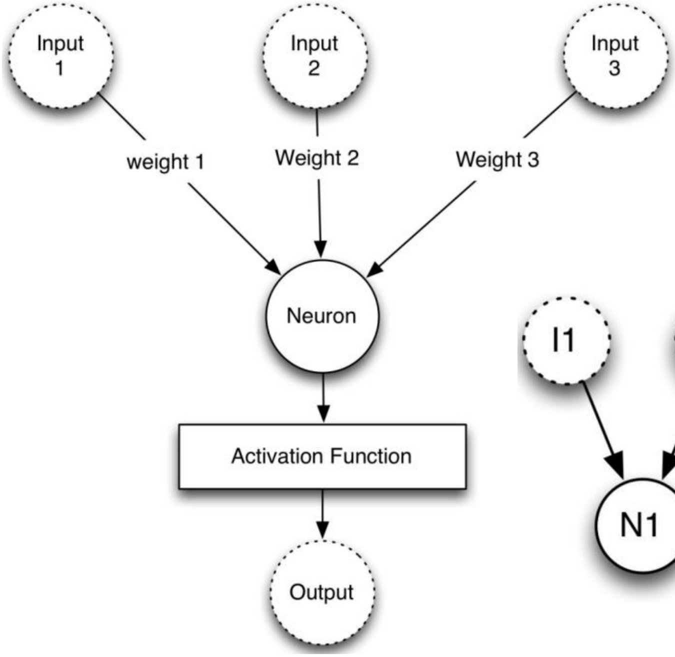
Augmented reality microscope *[3]*

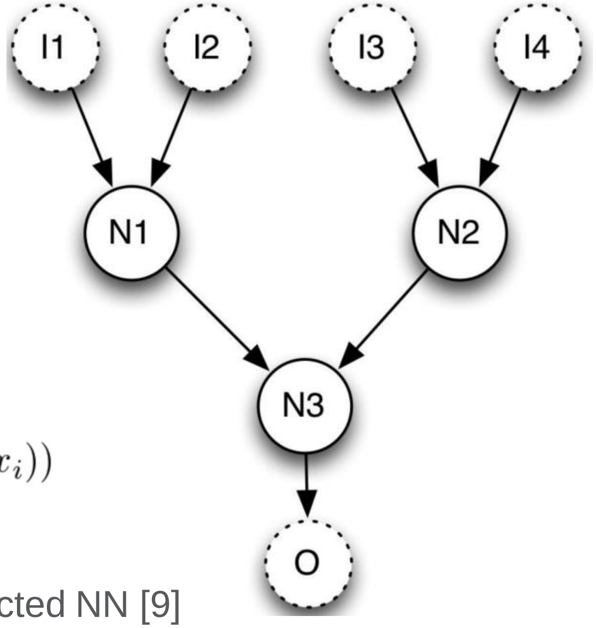
[1] G. Heinrich, “Image Segmentation Using DIGITS 5,” NVIDIA Developer Blog, Nov. 10, 2016. https://developer.nvidia.com/blog/image-segmentation-using-digits-5/ (accessed Feb. 25, 2021).
[2] M. Cordts et al., “The Cityscapes Dataset for Semantic Urban Scene Understanding,” in 2016 IEEE Conference on Computer Vision and Pattern Recognition (CVPR), Las Vegas, NV, USA, Jun. 2016, pp. 3213–3223, doi: 10.1109/CVPR.2016.350.
[3] P.-H. C. Chen et al., “Microscope 2.0: An Augmented Reality Microscope with Real-time Artificial Intelligence Integration,” arXiv:1812.00825 [cs], Dec. 2018, doi: 10.1038/s41591-019-0539-7.

Convolutional Neural Network (CNN)



Activation function: ReLU (Wikipedia)

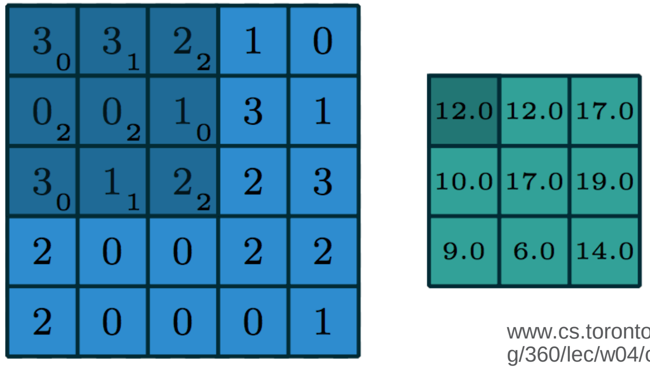




$$f(x_i, w_i) = \phi(\sum_i (w_i \cdot x_i))$$

Artificial neuron and fully connected NN [9]

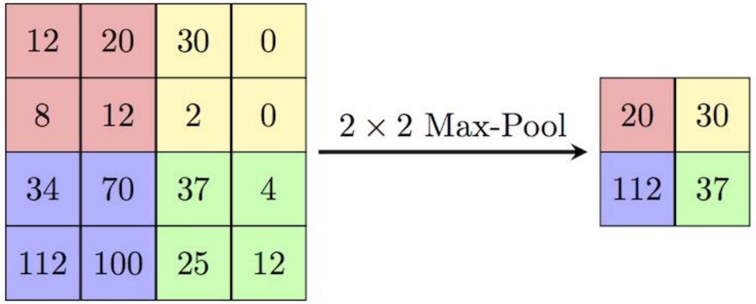
Convolutional Neural Network (CNN)

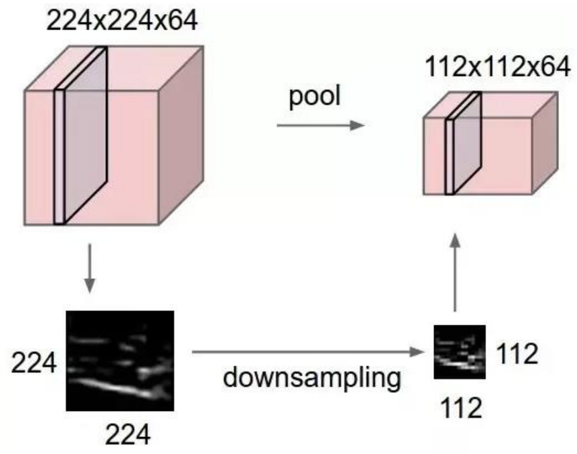


www.cs.toronto.edu/~lczhang/360/lec/w04/convnet.html

Normal convolution kernel

$$
\begin{aligned}
&(3 * 0 + 3 * 1 + 2 * 2) \\
&+ (0 * 2 + 0 * 2 + 1 * 0) \\
&+ (3 * 0 + 1 * 1 + 2 * 2) \\
&= 12
\end{aligned}
$$





Maxpooling

https://computersciencewiki.org/index.php/Max-pooling_/_Pooling

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Deep learning lingo

- Training data—used for training
- Validation data—for predictions *during* training
- Testing data—for predictions *after* training
- Ground truth—actual true labels
- Epoch—1 training cycle
- Batch size—no. of training images each epoch
- Hidden layer—layers between input and output layers
- Learning rate—how big a step an optimizer goes each epoch

Deep learning lingo

Loss function

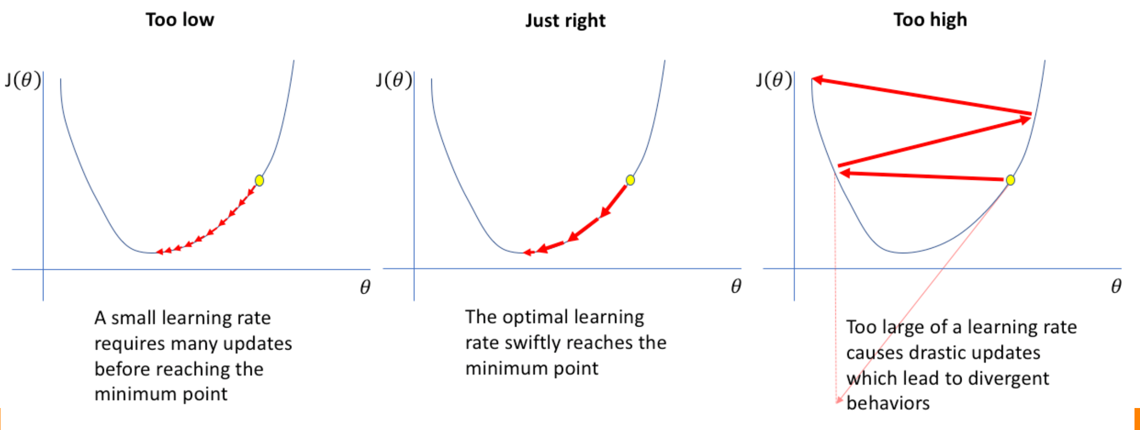
- Evaluates how close the predictions are to the ground truth → Minimize
- Binary cross entropy: (dis)similarity between prediction and GT

$$H_p(q) = -\frac{1}{N}\sum_{i=1}^{N} y_i \cdot log(p(y_i)) + (1 - y_i) \cdot log(1 - p(y_i))$$

https://towardsdatascience.com/understanding-binary-cross-entropy-log-loss-a-visual-explanation-a3ac6025181a

Optimizer

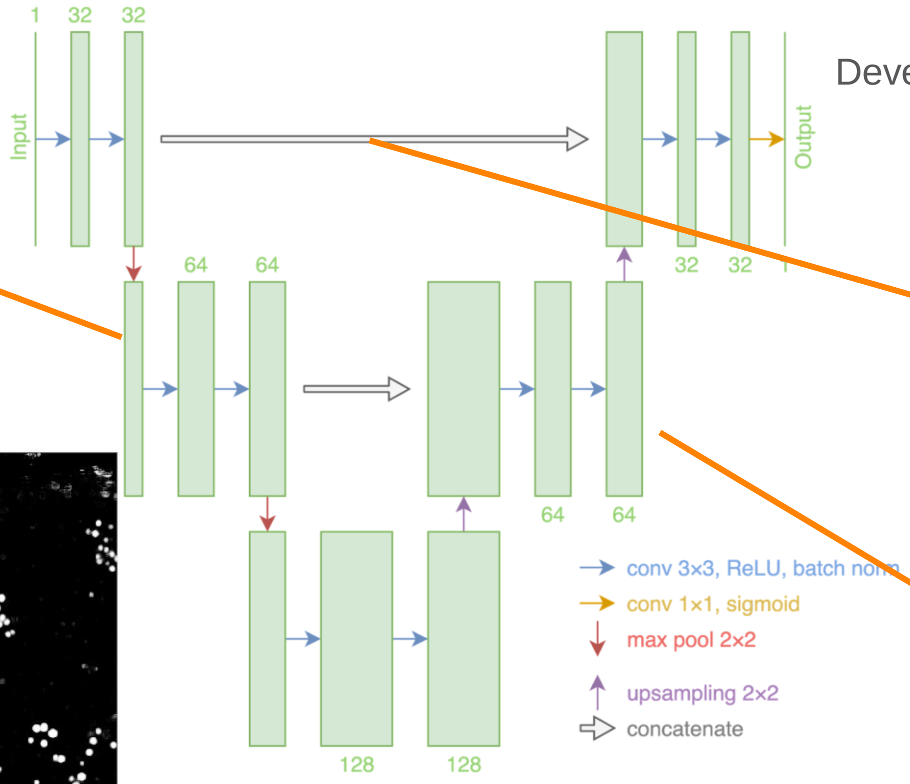
- Controls the *convergence* of a model (by minimizing loss func.)
- Step controlled by learning rate
- Adam optimizer



https://www.jeremyjordan.me/nn-learning-rate/

Semantic segmentation w/ U-Net

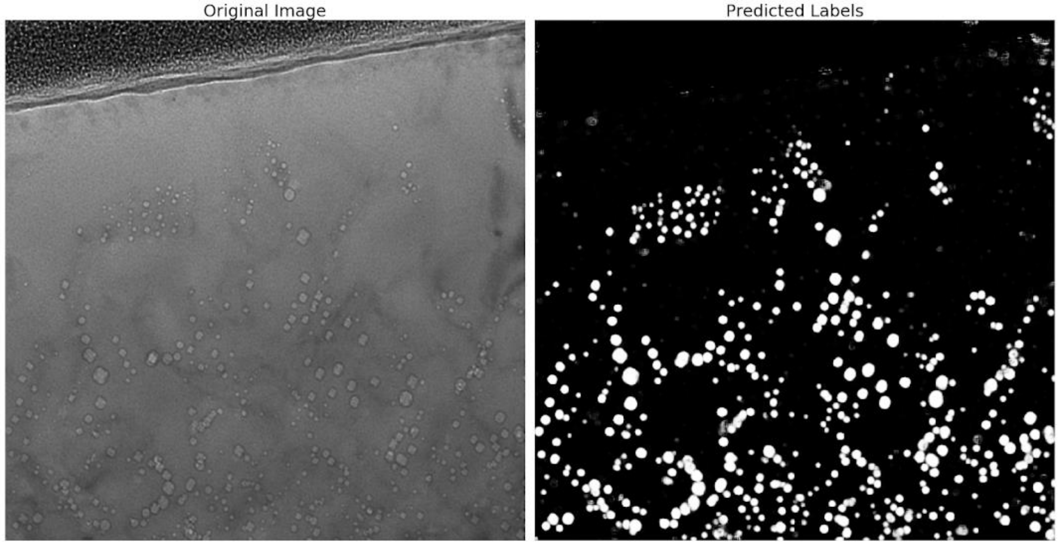
Look for salient features



Developed by Ronneberger et al. (2015) [11]

Preserve “big picture”

Expand back to original size



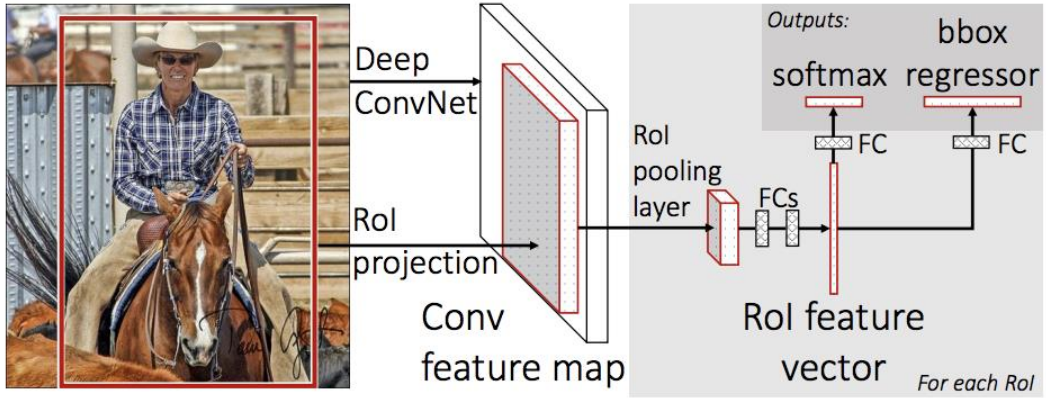
Adapted from Wong et al. (2021) https://doi.org/10.1017/S1431927621007686

U-Net demonstration

https://github.com/tommycwong/ML-ElectronMicroscopy-2023/blob/main/Lecture%2013/ML4EM_Summer2023_U_Net.ipynb

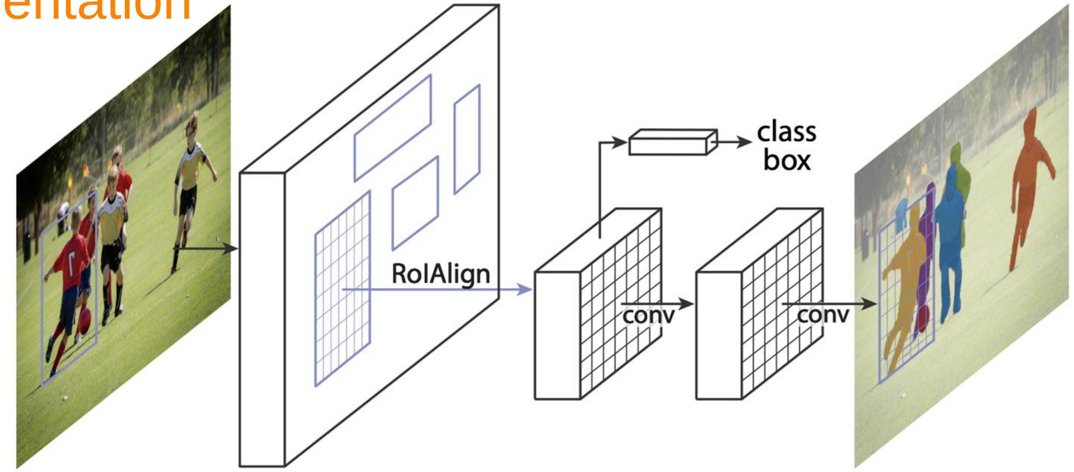
Instance segmentation w/ Mask R-CNN

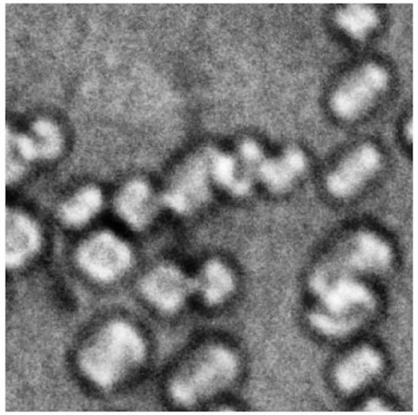
Fast R-CNN

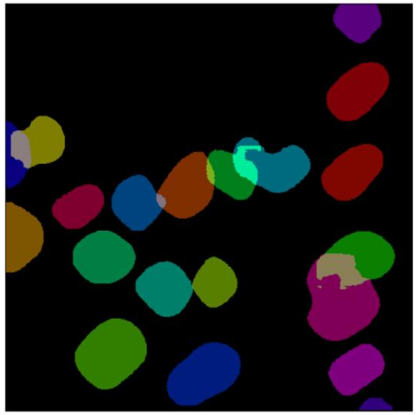


+ segmentation

Mask R-CNN







$$Loss = L_{class} + L_{box} + L_{mask}$$

Adapted from Girschick (2015) https://arxiv.org/abs/1504.08083, He et al. (2018) https://arxiv.org/abs/1703.06870v3

Mask R-CNN demonstration

https://github.com/tommycwong/ML-ElectronMicroscopy-2023/blob/main/Lecture%2013/ML4EM_Summer2023_Mask_R_CNN.ipynb