



Hands on

Machine Learning

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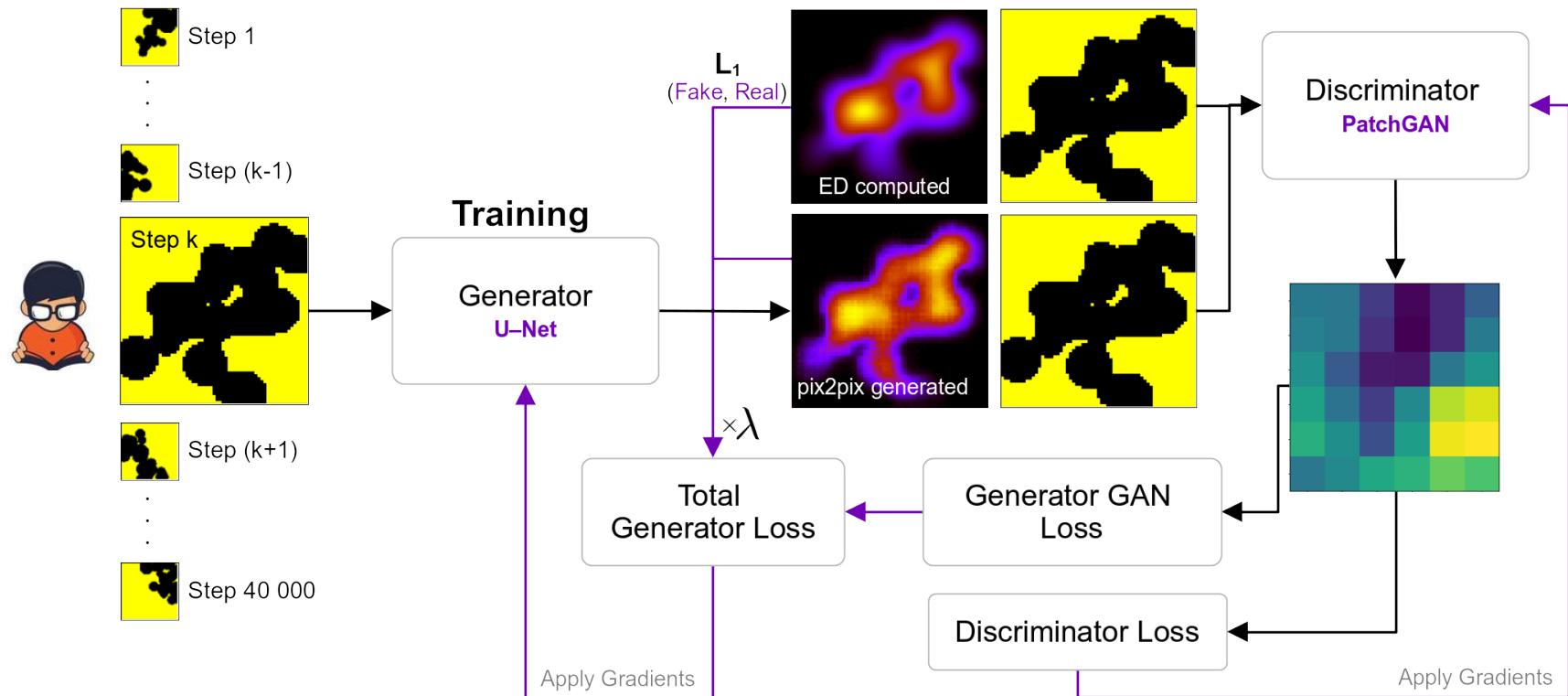


Machine Learning **ML**



Aim: Mapping confinement potential to interacting and non-interacting charge densities, investigating the inverse problem as well.

Architecture of pix2pix



Architecture: Training the pix2pix model. The Generator and Discriminator functions are training simultaneously adversarially.

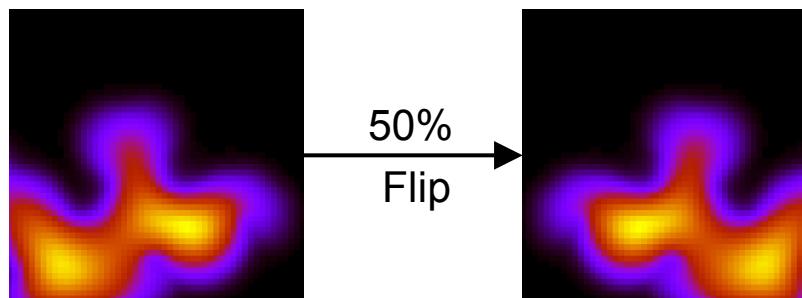
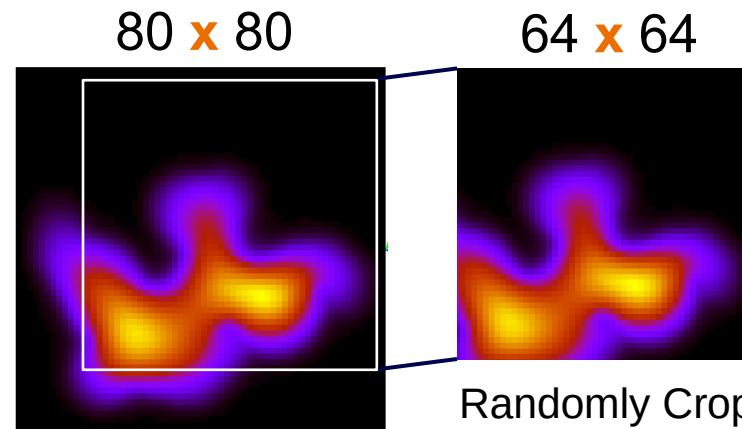
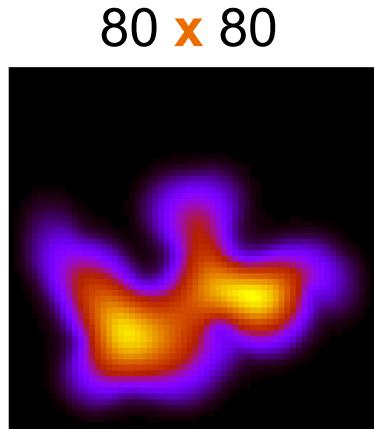
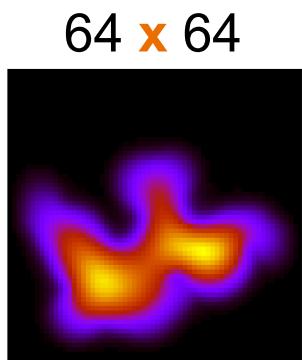
Data preparation

~/WorkML

- Importing Packages
- Check Data
- Split Images
- Resize Images
- Random Crop
- Normalize [-1,1]



Jittering

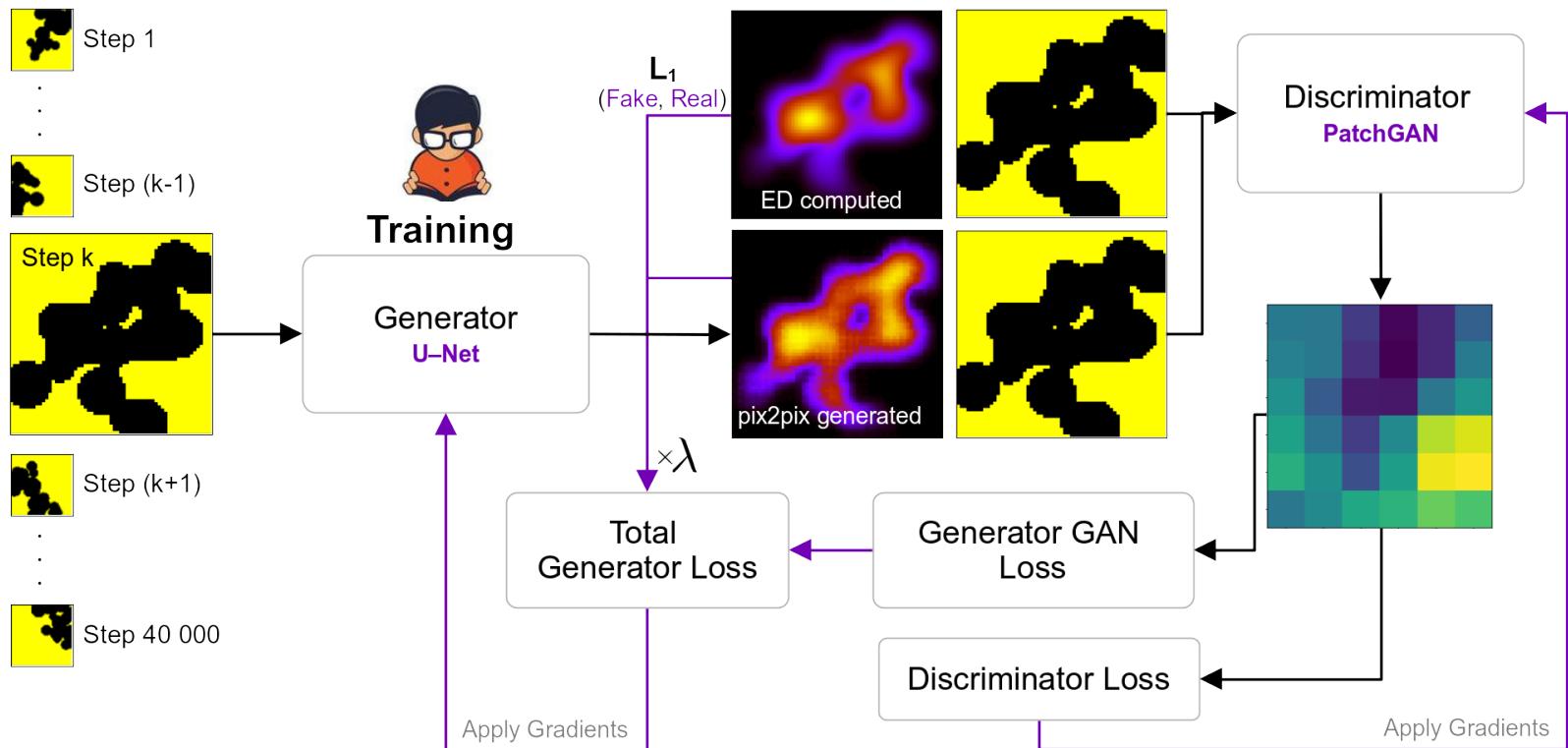


Data preparation

- Process image train
- Process image test
- Load data
 - Load data as numpy
 - Make tensor dataset
- Process test/train
 - Shuffle
 - Batch size



Architecture of pix2pix



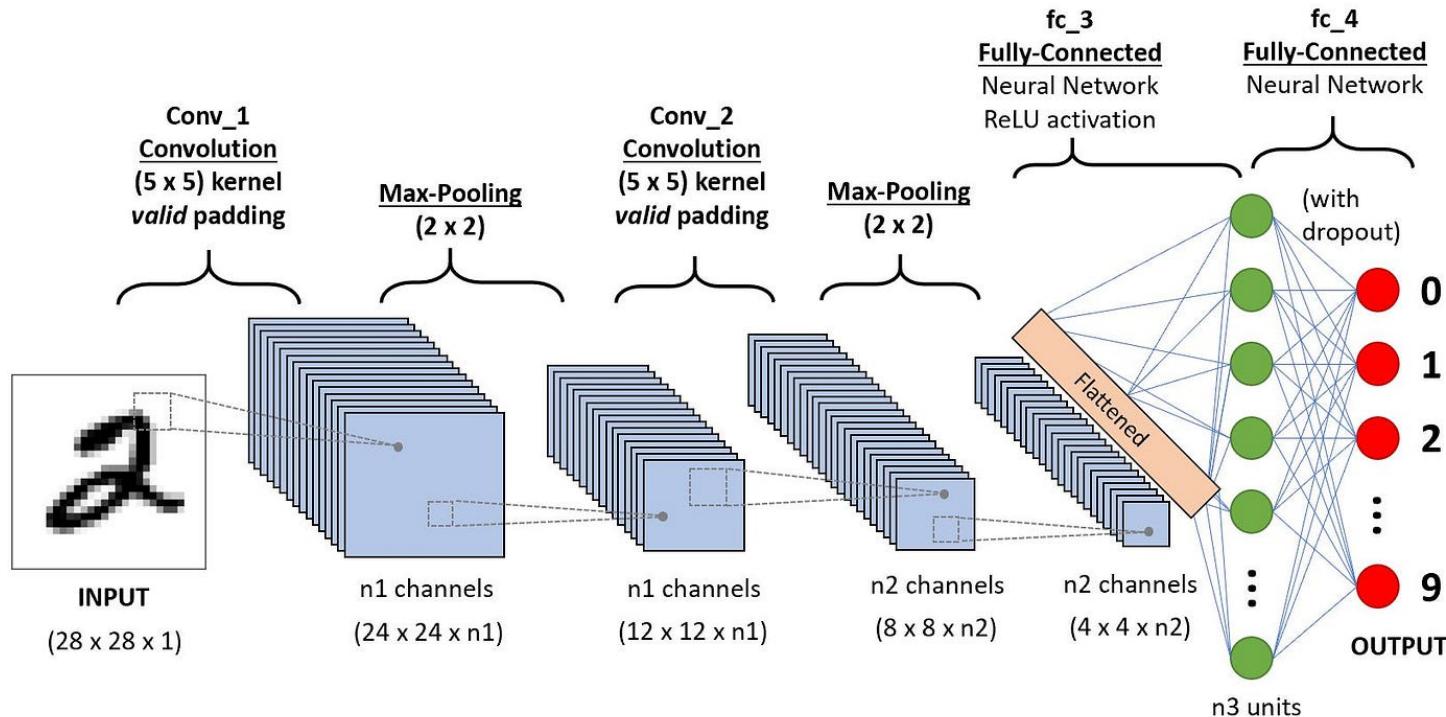
Architecture: Training the pix2pix model. The Generator and Discriminator functions are training simultaneously adversarially.

Kernel Convolution

Visit: [https://en.wikipedia.org/wiki/Kernel_\(image_processing\)](https://en.wikipedia.org/wiki/Kernel_(image_processing))

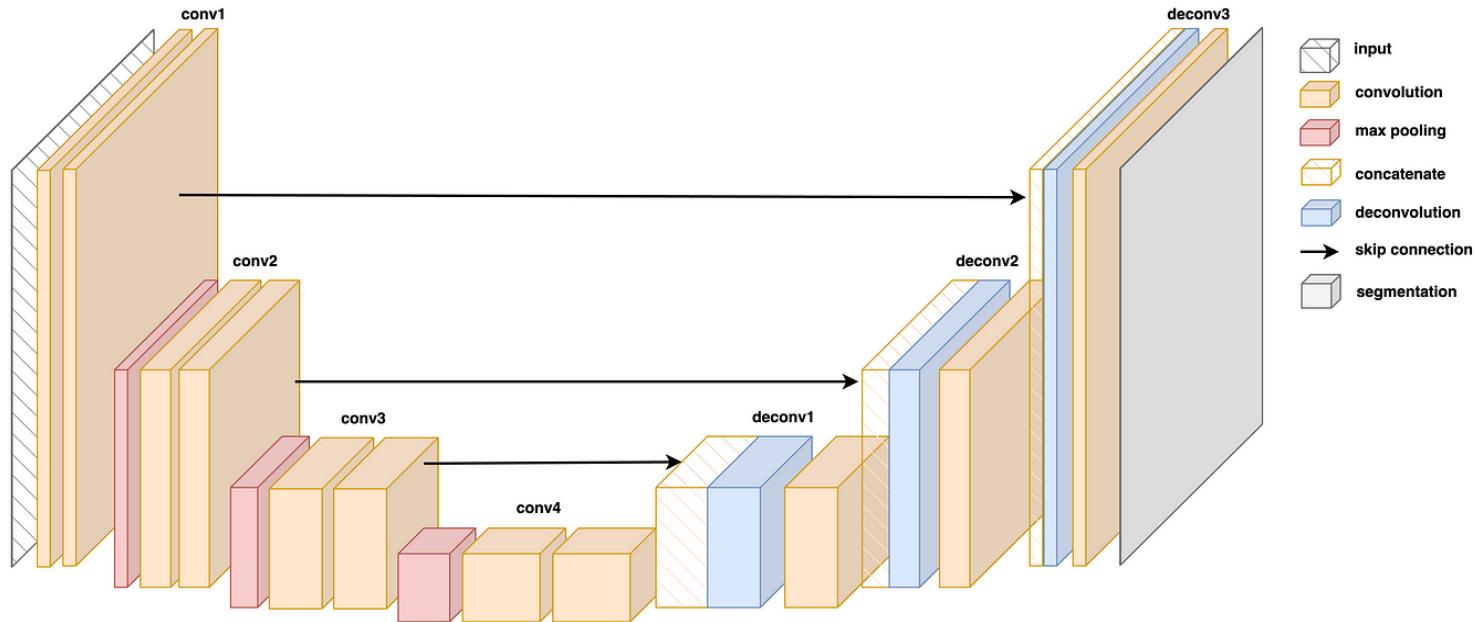
Visit: <https://towardsdatascience.com/types-of-convolution-kernels-simplified-f040cb307c37>

Convolutional Neural Networks **CNNs**



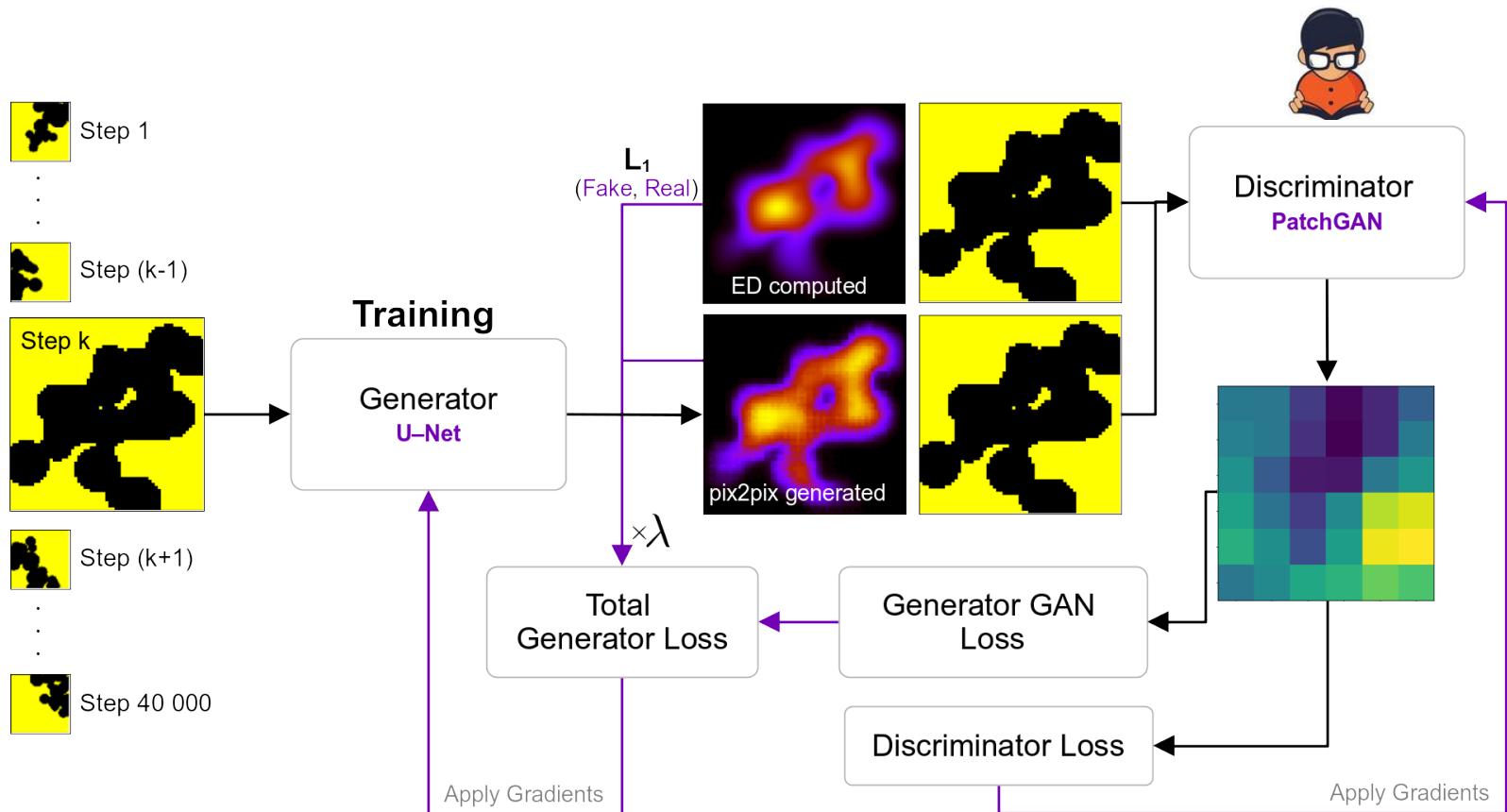
CNNs: By applying successive convolutions to images (i.e **downsampling**), features are identified and served to the network.

Generator U-Net



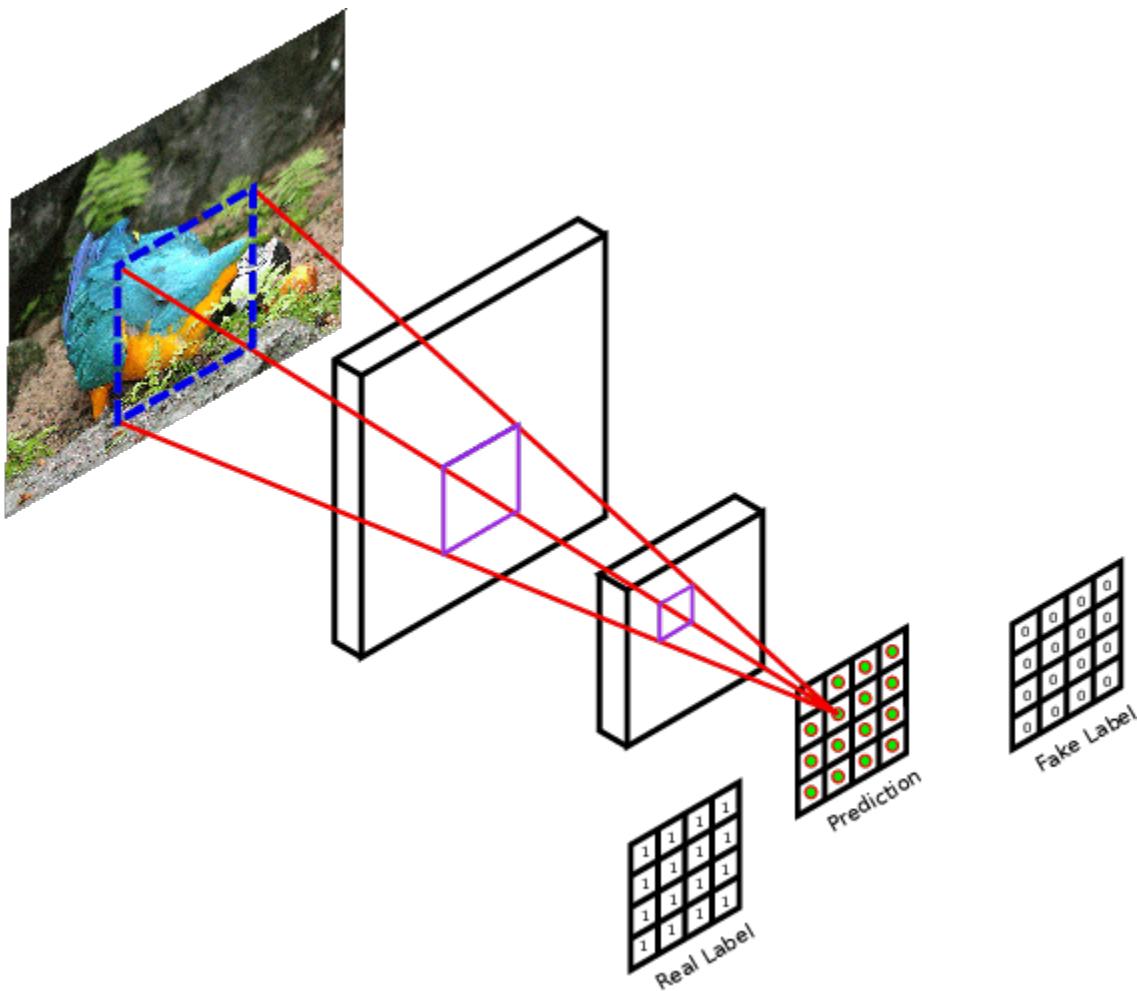
Architecture: Generator is composed of two main procedures, namely the **downsampling** and **upsampling**.

Architecture of pix2pix

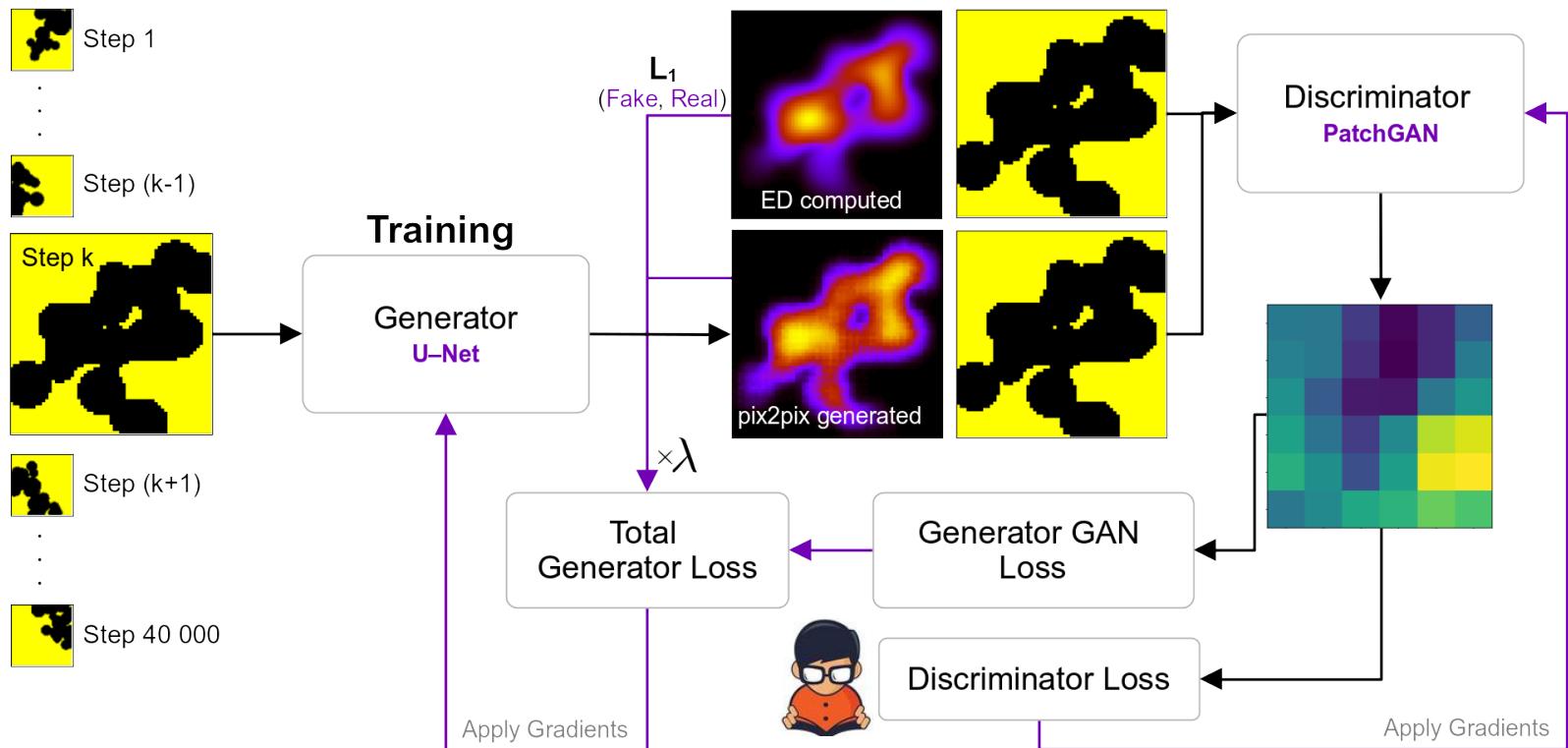


Architecture: Training the pix2pix model. The Generator and Discriminator functions are training simultaneously adversarially.

Discriminator PatchGAN



Architecture of pix2pix



Architecture: Training the pix2pix model. The Generator and Discriminator functions are training simultaneously adversarially.

Error Evaluation

- Errors: L_1 , L_2 , and L_∞

$$L_1 = \frac{1}{N_x \times N_y} \|\beta - \beta_{\text{ref}}\|_1$$

$$L_2 = \frac{1}{\sqrt{N_x \times N_y}} \|\beta - \beta_{\text{ref}}\|_2$$

$$L_\infty = \|\beta - \beta_{\text{ref}}\|_\infty$$

- Matter of fact

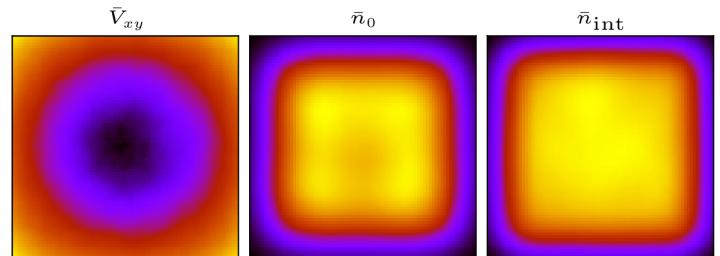
Comparing images is not an easy task, therefore additional error procedures must be considered.

- The R^2 coefficient

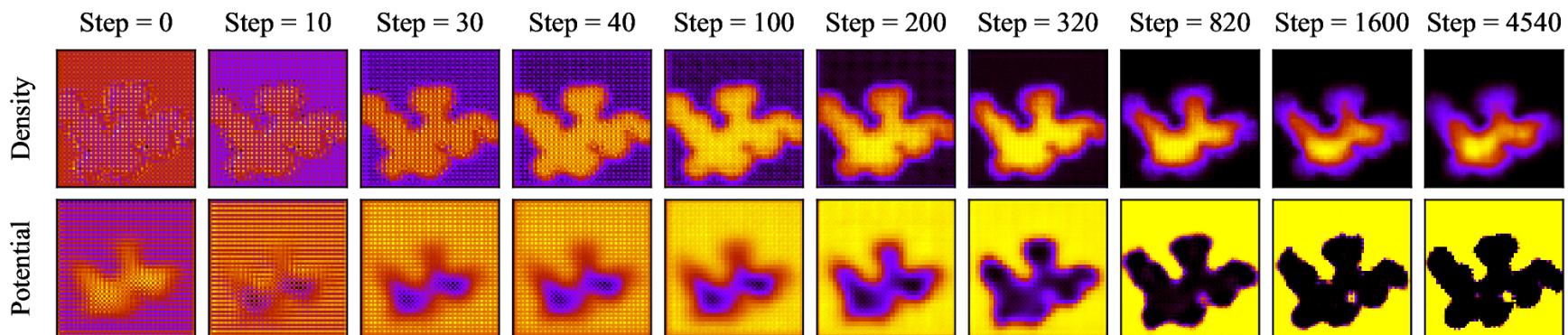
$$R^2 = 1 - \frac{\text{SS}_{\text{res}}}{\text{SS}_{\text{tot}}},$$

$$\text{SS}_{\text{res}} = \sum_{i=1}^{N_{\text{sys}}} \|\beta_i - \beta_{\text{ref},i}\|_2^2$$

$$\text{SS}_{\text{tot}} = \sum_{i=1}^{N_{\text{sys}}} \|\beta_{\text{ref},i} - \bar{\beta}_{\text{ref}}\|_2^2$$



Training Process



Evolution: Training the model when mapping the charge density and the confinement potential

Loss Functions

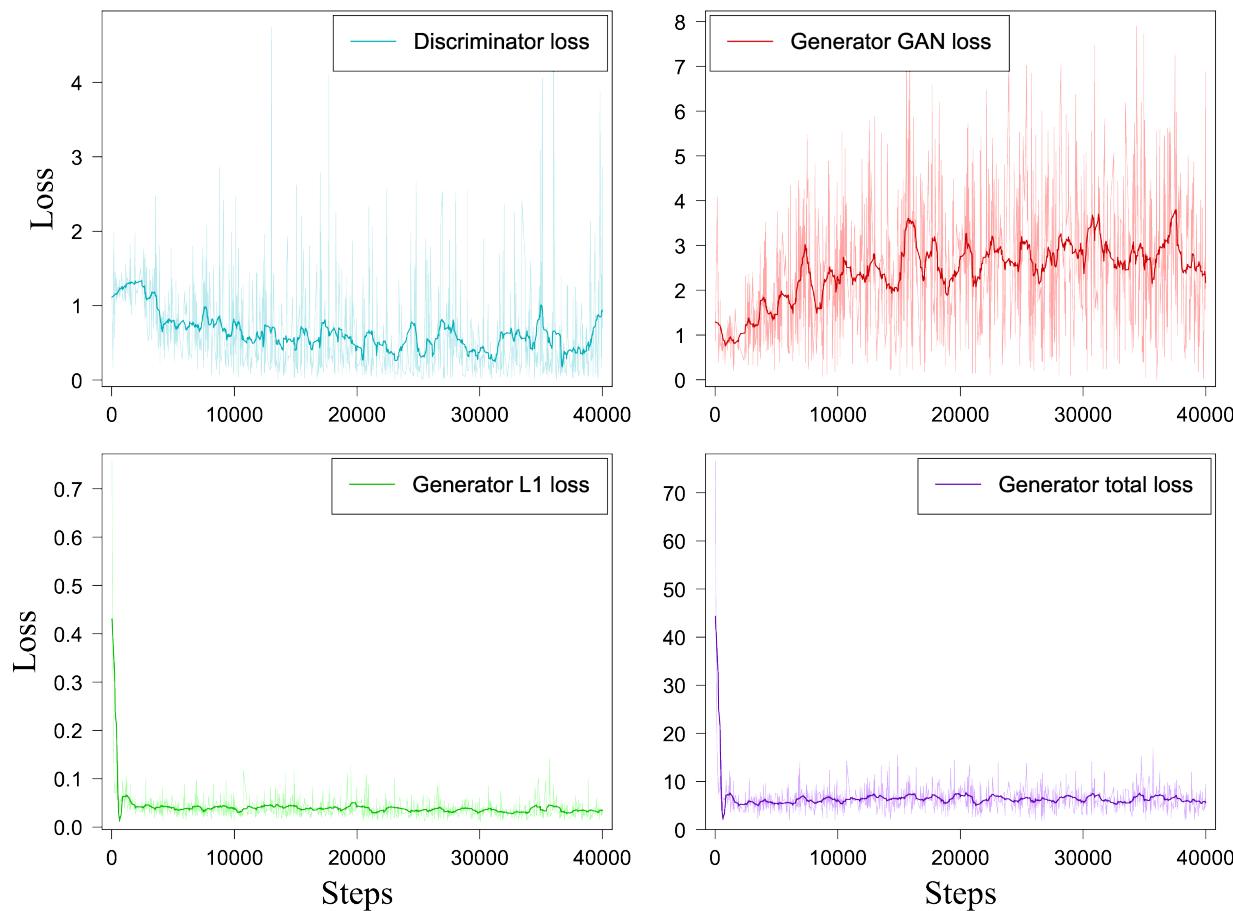


Figure 20: Loss functions for the generator and discriminator. Total generator loss is a linear combination between L_1 and cGAN losses with a scaling factor $\lambda = 100$.

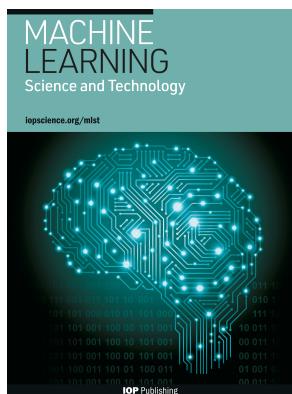
Reference

[1] **Calin-Andrei Pantăș-Simut, Amanda Teodora Preda, Lucian Ion, Andrei Manolescu, George Alexandru Nemnes.** "Mapping confinement potentials and charge densities of interacting quantum systems using conditional generative adversarial networks." Machine Learning: Science and Technology 4.2 (2023): 025023.

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Thank You!

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