

Generative Al with Diffusion Models

Part 2: Denoising Diffusion Probabilistic Models



Agenda

- Part 1: From U-Nets to Diffusion
- Part 2: Denoising Diffusion Probabilistic Models
- Part 3: Optimizations
- Part 4: Classifier-Free Diffusion Guidance
- Part 5: CLIP
- Part 6: Wrap-up & Assessment





Thermodynamic Origins



Deep Unsupervised Learning using Nonequilibrium Thermodynamics

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Abstract

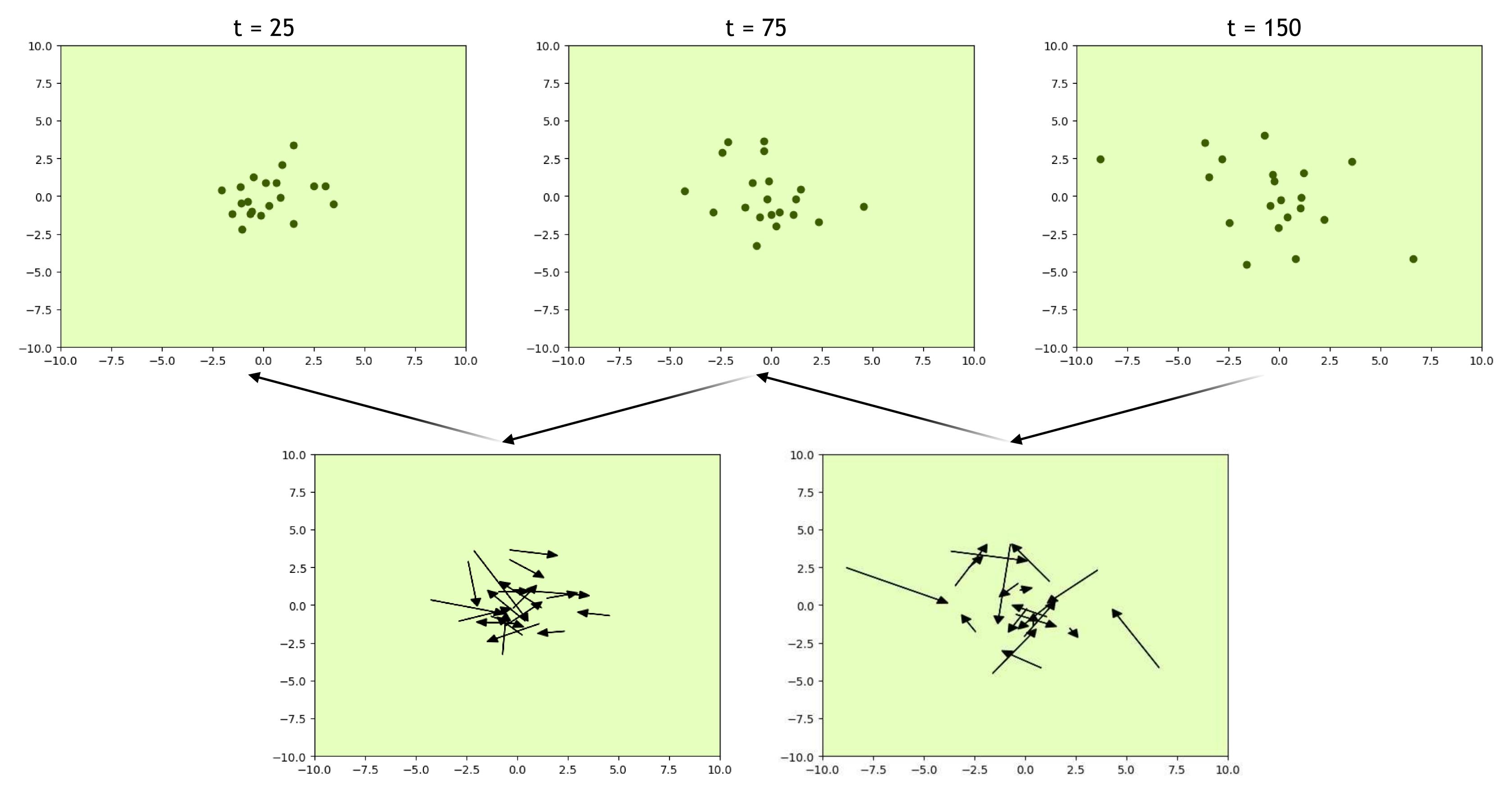
A central problem in machine learning involves modeling complex data-sets using highly flexible families of probability distributions in which learning, sampling, inference, and evaluation

these models are unable to aptly describe structure in rich datasets. On the other hand, models that are *flexible* can be molded to fit structure in arbitrary data. For example, we can define models in terms of any (non-negative) function $\phi(\mathbf{x})$ yielding the flexible distribution $p(\mathbf{x}) = \frac{\phi(\mathbf{x})}{Z}$, where Z is a normalization constant. However, computing this

Green food coloring dissolving in a glass of water



Thermodynamic Origins





Denoising Diffusion Probabilistic Models

Denoising Diffusion Probabilistic Models

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Abstract

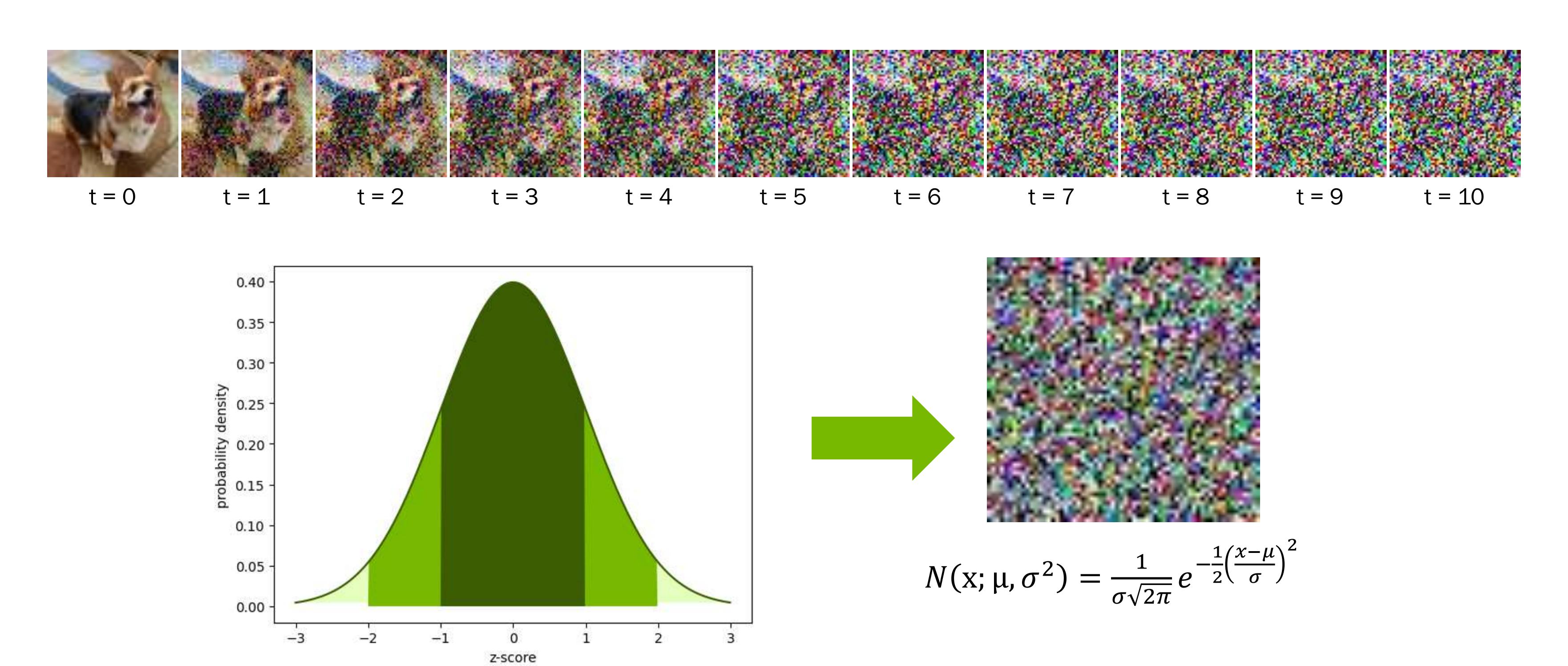
We present high quality image synthesis results using diffusion probabilistic models, a class of latent variable models inspired by considerations from nonequilibrium thermodynamics. Our best results are obtained by training on a weighted variational bound designed according to a novel connection between diffusion probabilistic models and denoising score matching with Langevin dynamics, and our models naturally admit a progressive lossy decompression scheme that can be interpreted as a



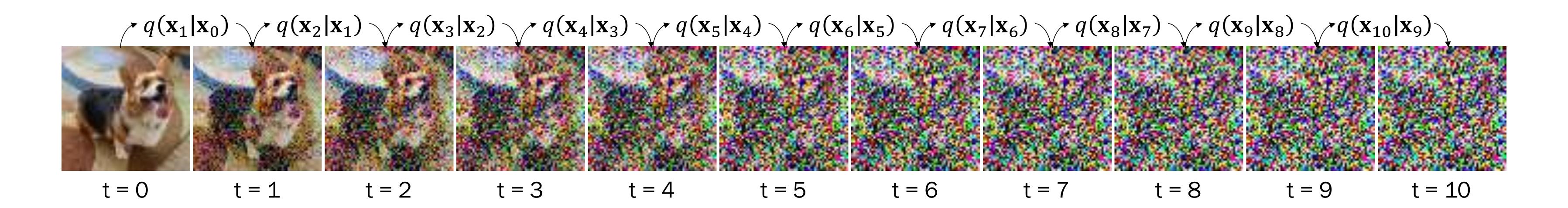




Forward Diffusion



Forward Diffusion



$$\beta = [0.0001, 0.0023, 0.0045, 0.0067, ..., 0.0200]$$
 $t = 0$
 $t = 1$
 $t = 3$
 $t = 4$
 $t = 10$

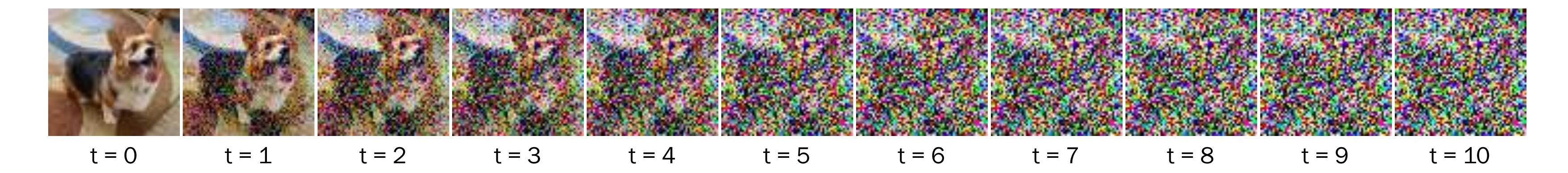
$$T = 10$$

Total number of timesteps

$$\alpha = 1 - \beta$$

Convenient shorthand

Forward Diffusion

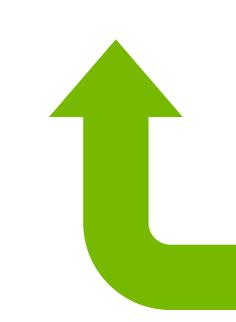


$$q(\mathbf{x}_t|\mathbf{x}_{t-1}) = N(\mathbf{x}_t; \sqrt{1-\beta_t} \cdot \mathbf{x}_{t-1}, \beta_t \cdot \mathbf{I})$$

Code:

noise = torch.randn_like(x_t)
x_t = torch.sqrt(1 - B[t]) * x_t
+ torch.sqrt(B[t]) * noise





Step 2:

- Multiply image at previous step by $\sqrt{1-\beta_t}$
- Add it to the result from step 1

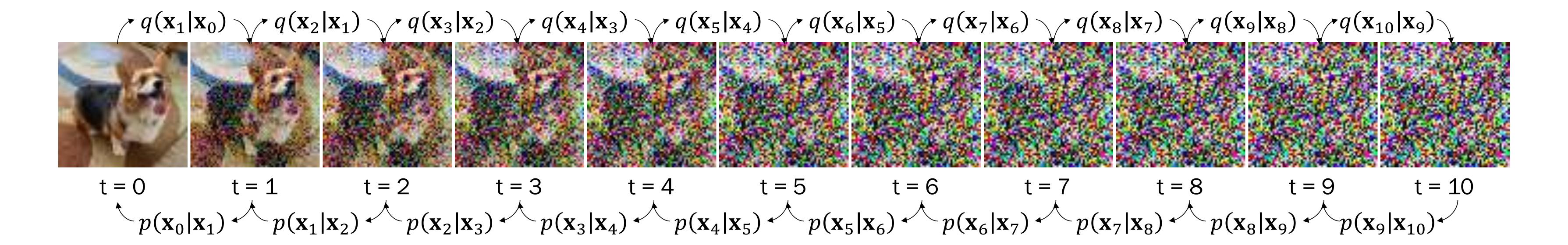
Step 1:

- Generate noise from a standard normal distribution
- Multiply result by $\sqrt{\beta_t}$

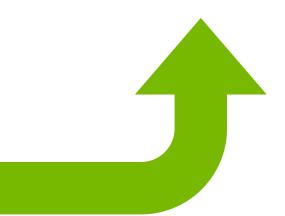


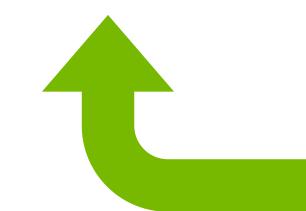


Reverse Diffusion



$$p(\mathbf{x}_{t-1}|\mathbf{x}_t) = N(\mathbf{x}_{t-1}; \boldsymbol{\mu}_{\theta}(\mathbf{x}_t, t), \boldsymbol{\Sigma}_{\theta}(\mathbf{x}_t, t))$$

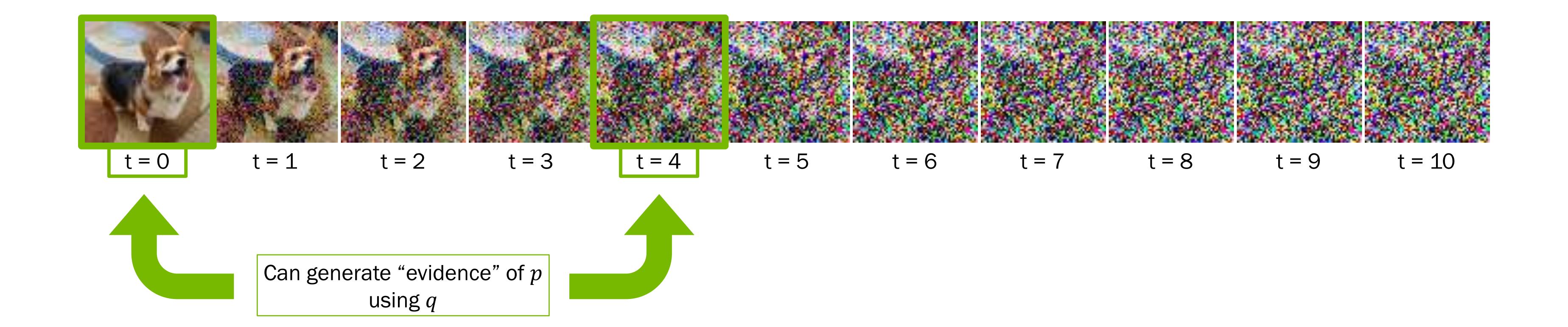




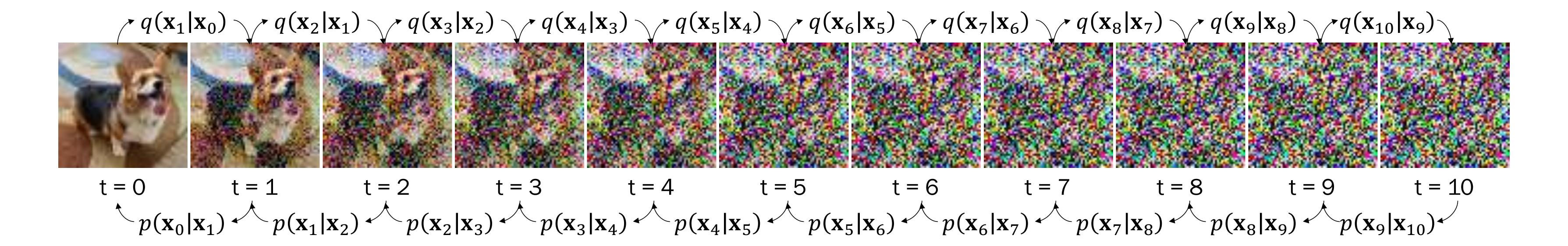
Approximate average used to create \mathbf{x}_t

Difficult to calculate

Reverse Diffusion



Reverse Diffusion



$$p(\mathbf{x}_{t-1}|\mathbf{x}_t) = N(\mathbf{x}_{t-1}; \boldsymbol{\mu}_{\theta}(\mathbf{x}_t, t), \boldsymbol{\Sigma}_{\theta}(\mathbf{x}_t, t))$$

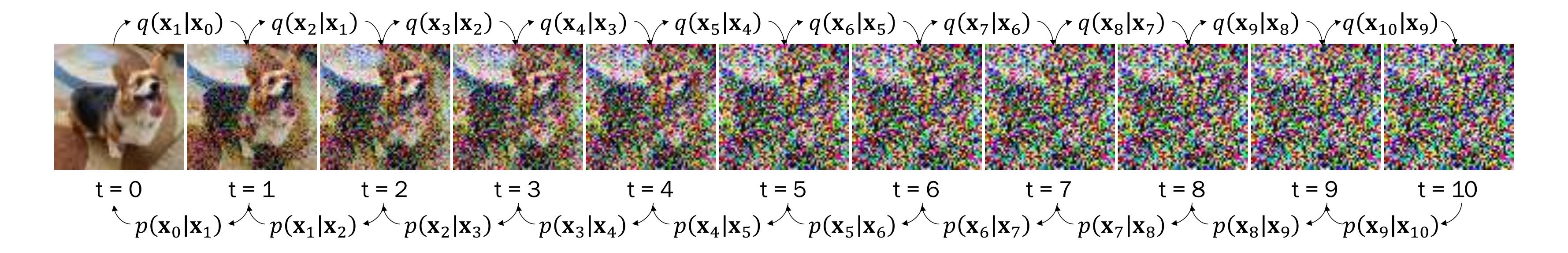
$$q(\mathbf{x}_{t-1}|\mathbf{x}_t,\mathbf{x}_0) = N(\mathbf{x}_{t-1};\widetilde{\boldsymbol{\mu}}(\mathbf{x}_t,\mathbf{x}_0),\widetilde{\beta}_t \cdot \mathbf{I}) \qquad \widetilde{\beta}_t = \frac{1-\overline{\alpha}_{t-1}}{1-\overline{\alpha}_t}\beta_t$$



Use Bayes' Rule and ...



Reverse Diffusion



$$p(\mathbf{x}_{t-1}|\mathbf{x}_t) = N(\mathbf{x}_{t-1}; \boldsymbol{\mu}_{\theta}(\mathbf{x}_t, t), \boldsymbol{\Sigma}_{\theta}(\mathbf{x}_t, t))$$

$$q(\mathbf{x}_{t-1}|\mathbf{x}_t,\mathbf{x}_0) = N(\mathbf{x}_{t-1};\widetilde{\boldsymbol{\mu}}(\mathbf{x}_t,\mathbf{x}_0),\widetilde{\beta}_t \cdot \mathbf{I})$$

$$\widetilde{\mu_t} = \frac{1}{\sqrt{\alpha_t}} \left(x_t - \frac{1 - \alpha_t}{\sqrt{1 - \alpha_t}} \epsilon_t \right) \quad \text{The noise added at time } t$$
 This is what the neural network will estimate





Model Training

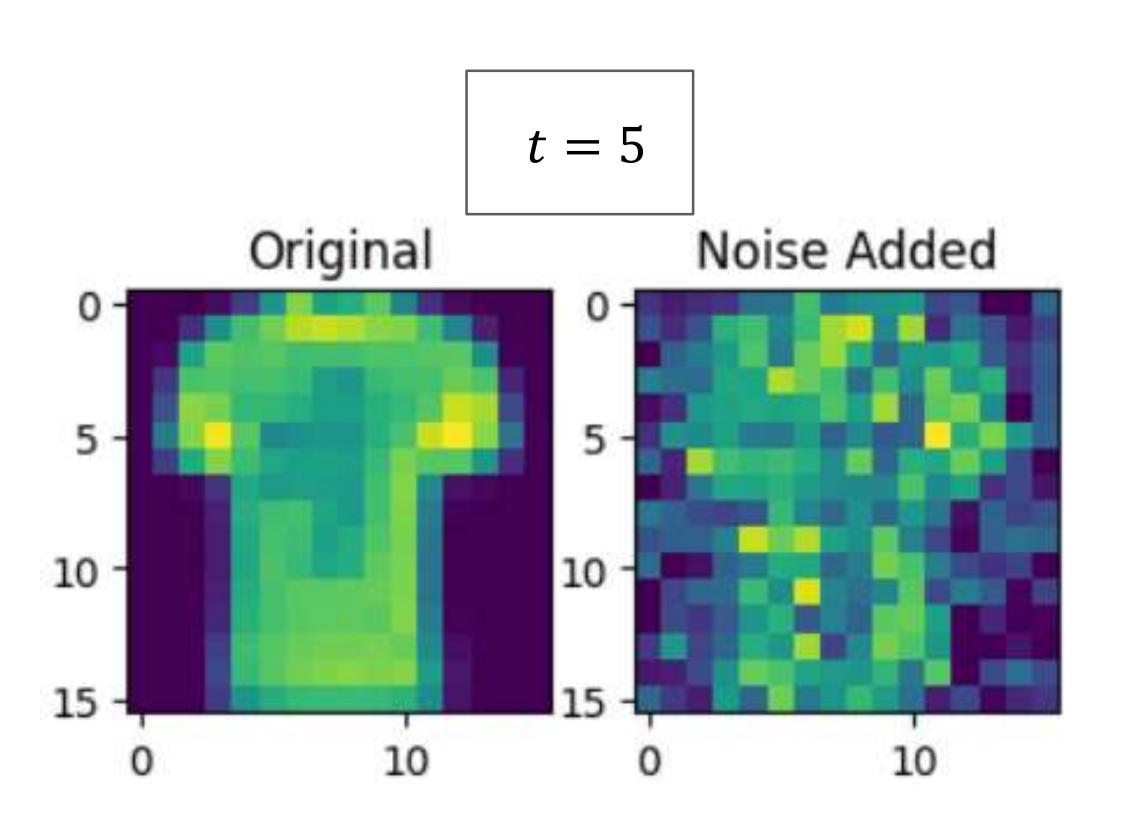
Training Data

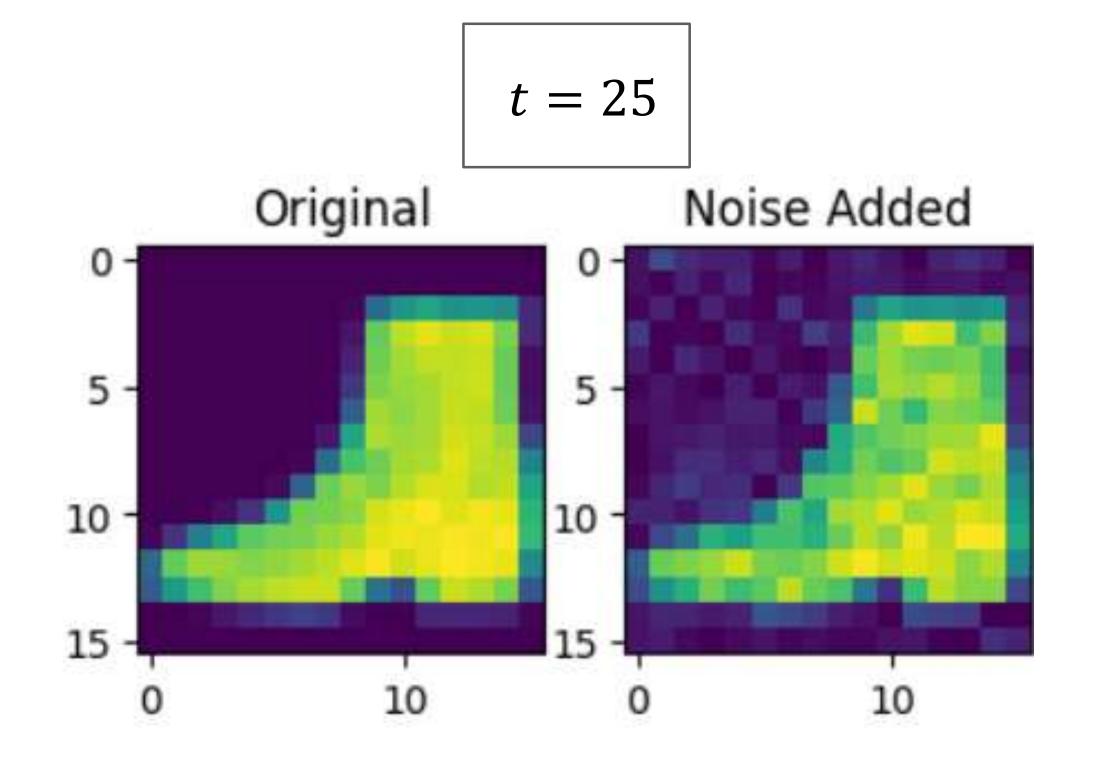
Noisy image at time t

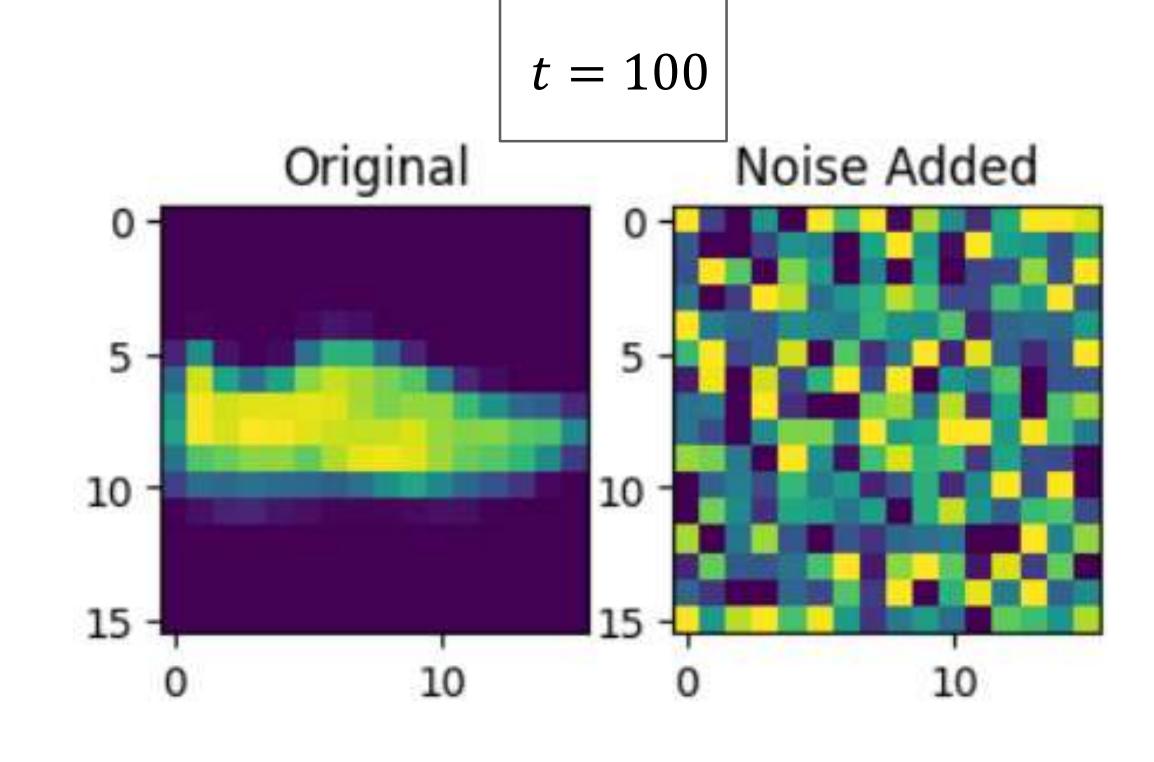
Noise added at time t

$$q(\mathbf{x}_t|\mathbf{x}_0) = N(\mathbf{x}_t; \sqrt{\bar{\alpha}_t} \cdot \mathbf{x}_0, (1 - \bar{\alpha}_t) \cdot \mathbf{I})$$

"Skip ahead" function





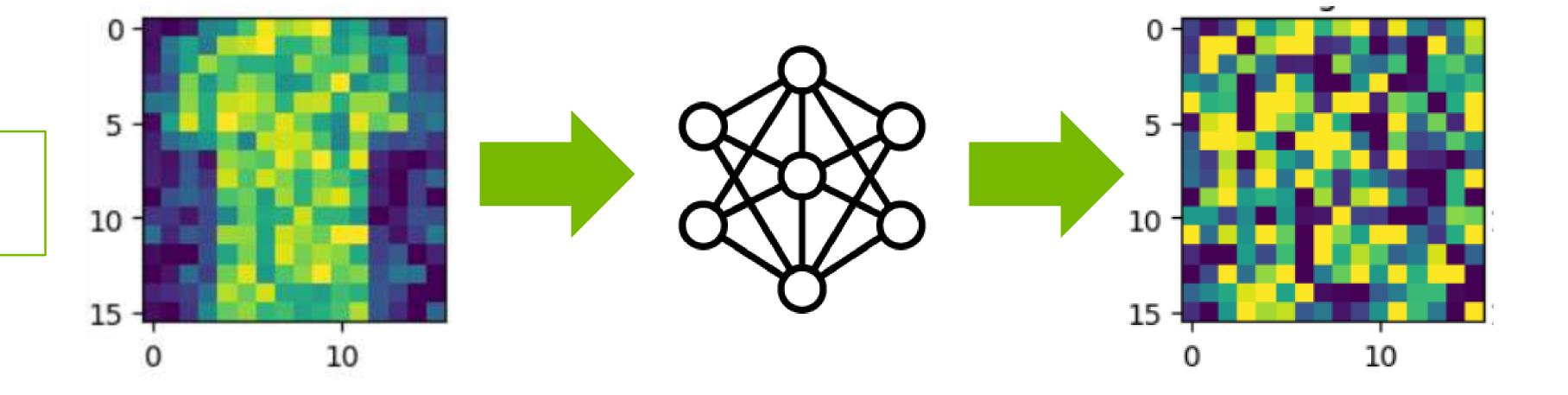




Model Training

ELBO Loss

Noisy image at time t



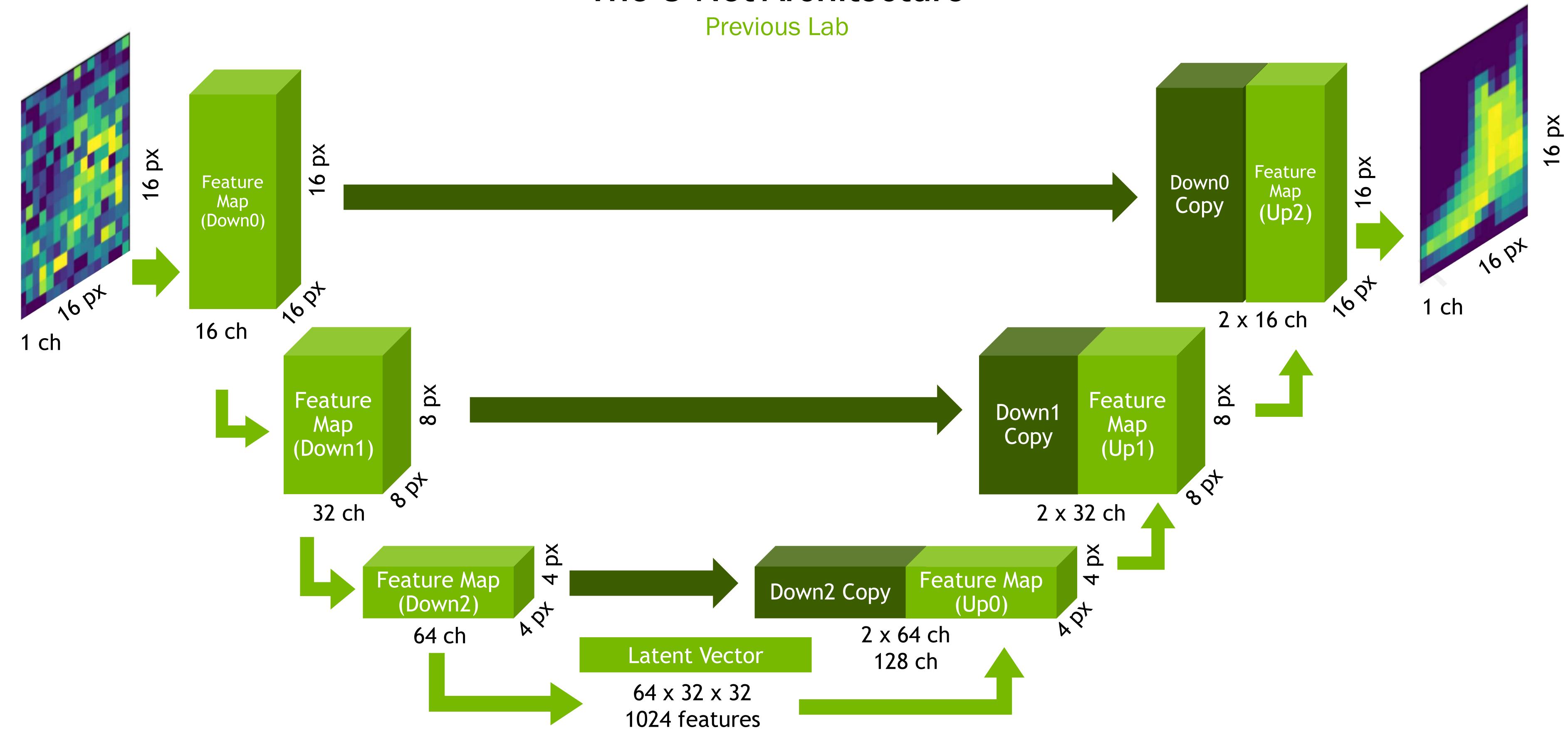
Noise added at time t

$$MSE = \frac{1}{n} \sum_{i=1}^{n} (y_i - \hat{y}_i)^2$$



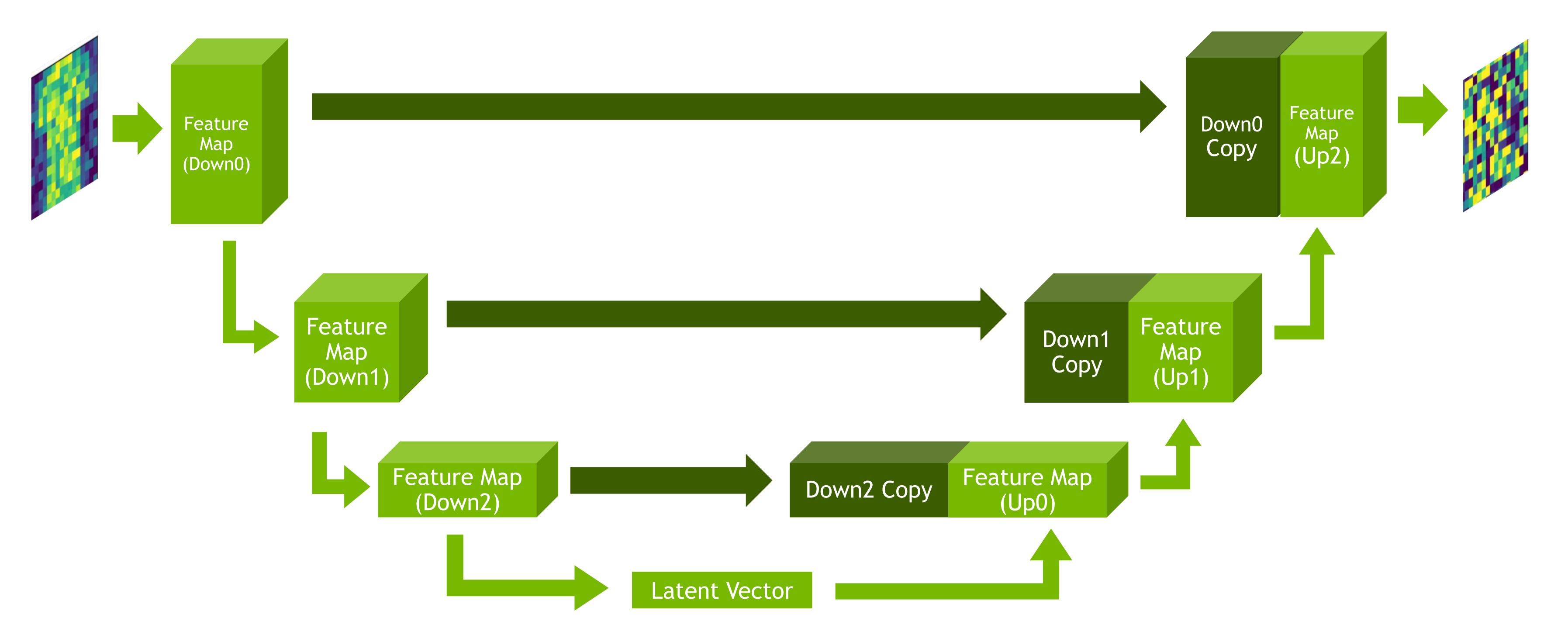


The U-Net Architecture



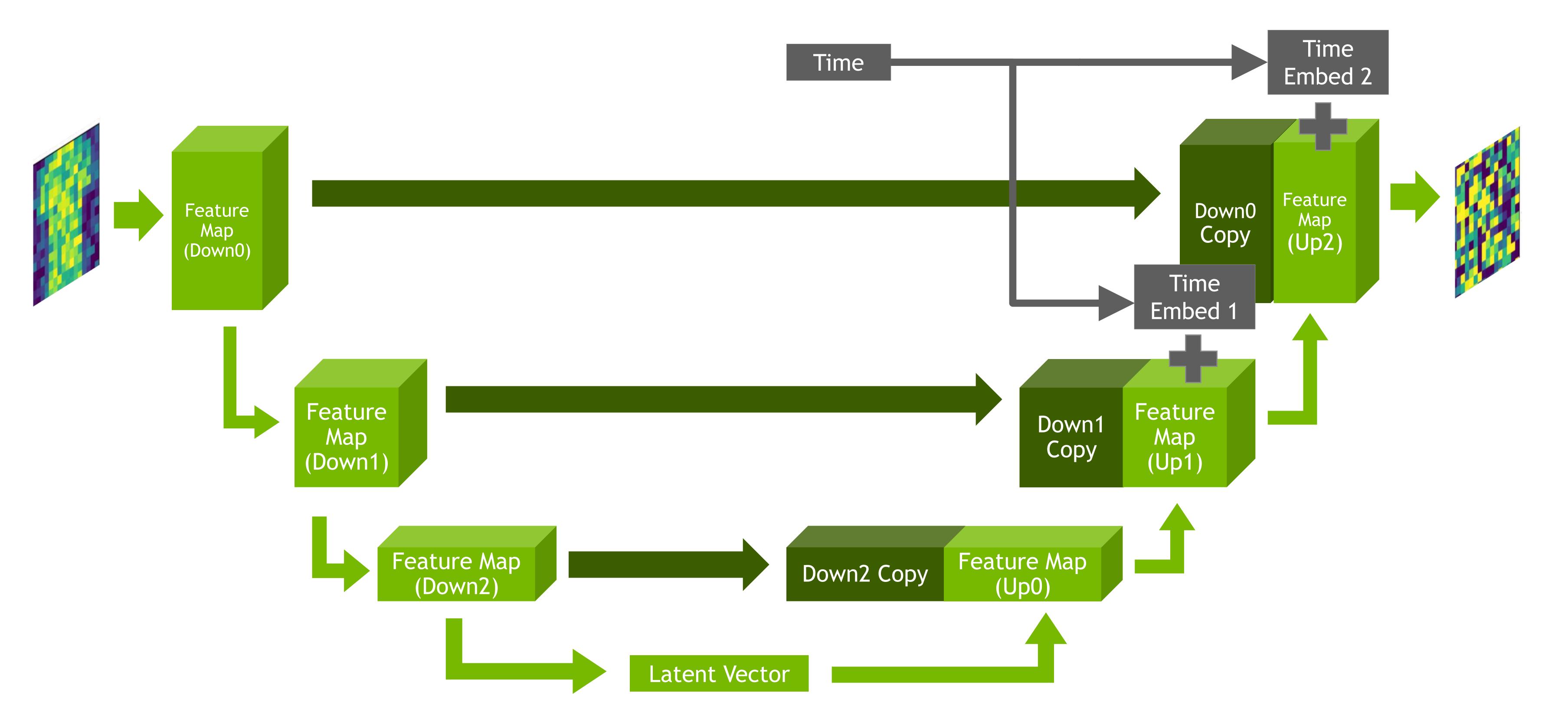
The U-Net Architecture

Next Lab



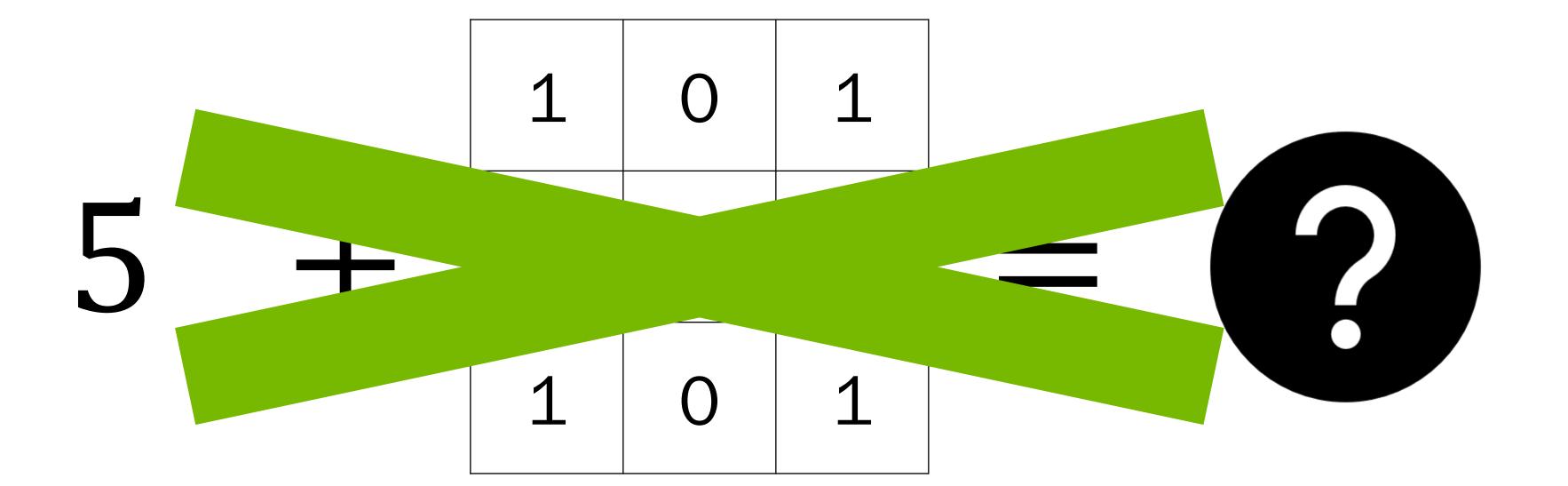


Adding Time





Broadcasting



5

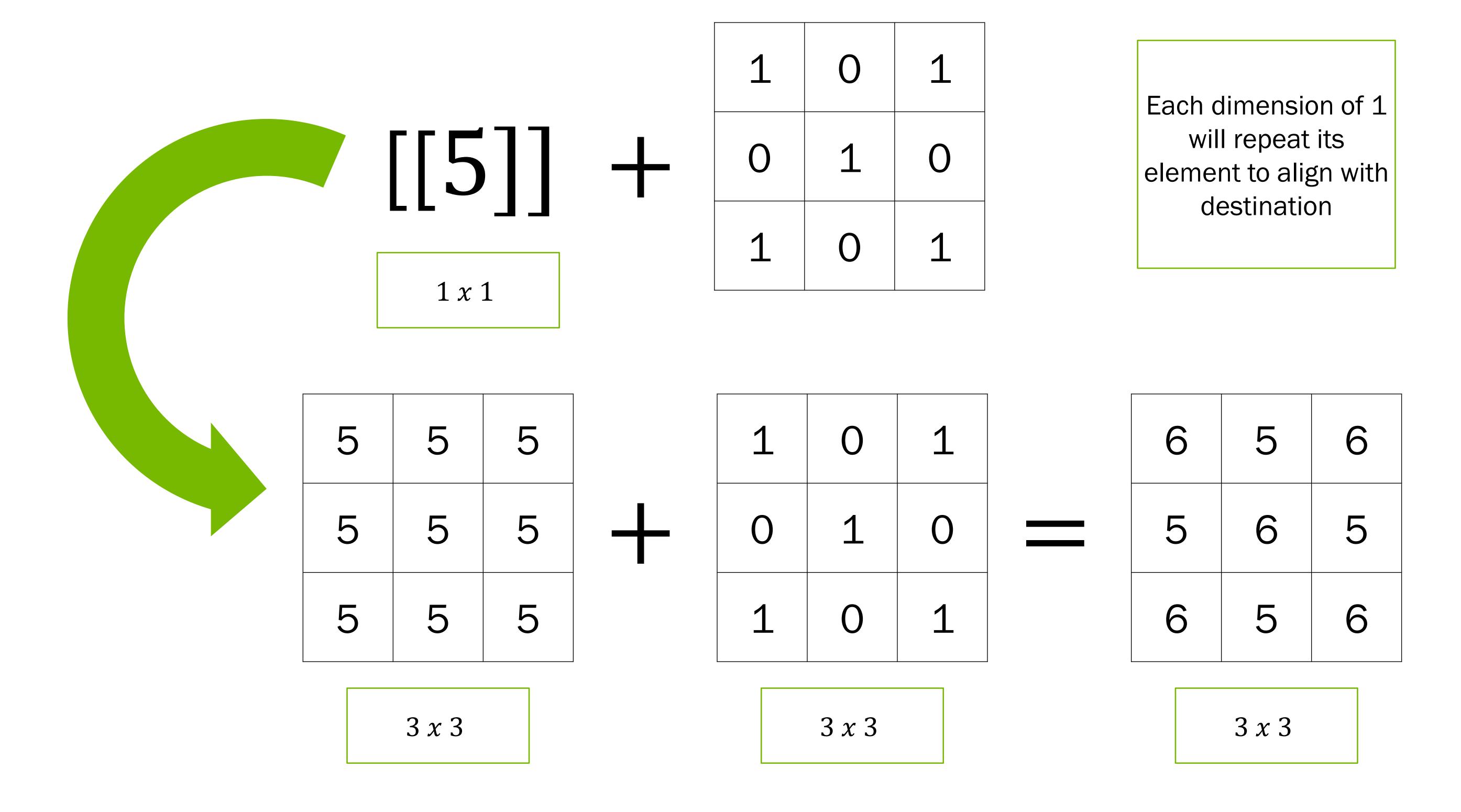
1	0	1
0	1	0
1	0	1

0 or 1

3 *x* 3

Dimensions

Broadcasting



Broadcasting

