CS480/680: Introduction to Machine Learning

Lec 18: Diffusion Models

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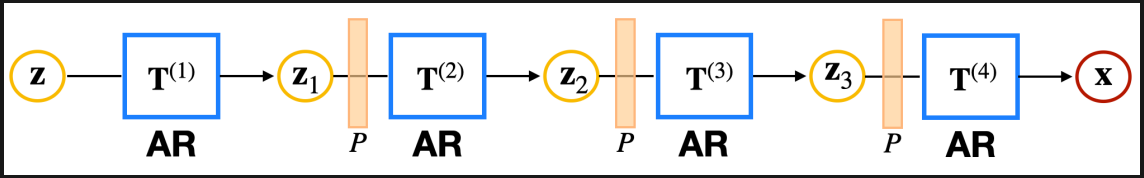
Auto-Regressive (AR) Flow Recalled



$$(\mathbf{T}_{\#}r)(\mathbf{x}) = r(\mathbf{z}) \;/\; \det\left(\nabla \mathbf{T}^{(1)}\mathbf{z}\right) \;/\; \det\left(\nabla \mathbf{T}^{(2)}\mathbf{z}_1\right) \;/\; \det\left(\nabla \mathbf{T}^{(3)}\mathbf{z}_2\right) \;/\; \det\left(\nabla \mathbf{T}^{(4)}\mathbf{z}_3\right)$$

$$x_j = z_j \cdot \exp\left(\alpha_j(z_1, \ldots, z_{j-1})\right) + \mu_j(z_1, \ldots, z_{j-1}) =: T_j(z_1, \ldots, z_{j-1}, z_j)$$

Now let the number of layers approach ∞!

Neural Ordinary Differential Equations (ODE)

$$\mathbf{x}_{t+1} \approx \mathbf{x}_t + \eta_t \cdot \mathbf{f}_t(\mathbf{x}_t) =: \mathbf{T}_t(\mathbf{x}_t)$$
$$\mathrm{d}\mathbf{x}_{t+1} = \mathbf{f}_t(\mathbf{x}_t)\,\mathrm{d}t$$

- Suppose $\mathbf{x}_t \sim p_t$
- Apply change-of-variable-formula we know $\mathbf{x}_{t+1} \sim p_{t+1}$, where

$$\begin{aligned}\log p_{t+1}(\mathbf{x}_{t+1}) &= \log p_t(\mathbf{x}_t) - \log|\det \partial_{\mathbf{x}} \mathbf{T}_t(\mathbf{x}_t)| \\ &= \log p_t(\mathbf{x}_t) - \log|\det[\mathrm{Id} + \eta_t \cdot \partial_{\mathbf{x}} \mathbf{f}_t(\mathbf{x}_t)]| \\ &\approx \log p_t(\mathbf{x}_t) - \eta_t \cdot \langle \partial_{\mathbf{x}}, \mathbf{f}_t(\mathbf{x}_t)\rangle\end{aligned}$$

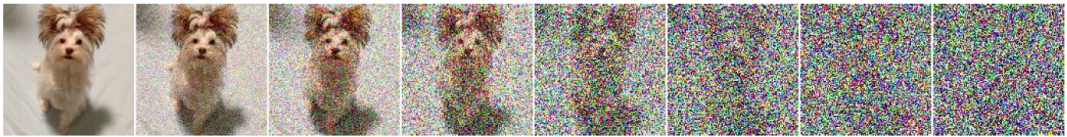
- Continuous change-of-variable formula:

$$\boxed{\frac{\mathrm{d}\log p_t(\mathbf{x}_t)}{\mathrm{d}t} = -\langle \partial_{\mathbf{x}}, \mathbf{f}_t(\mathbf{x}_t)\rangle}$$

T. Q. Chen, Y. Rubanova, J. Bettencourt, and D. K. Duvenaud. "Neural ordinary differential equations". In: *Advances in Neural Information Processing Systems*. 2018, pp. 6572–6583.

Forward SDE (data → noise)

$\mathbf{x}(0)$ — $\mathrm{d}\mathbf{x} = \mathbf{f}(\mathbf{x}, t)\mathrm{d}t + g(t)\mathrm{d}\mathbf{w}$ → $\mathbf{x}(T)$



score function

$\mathbf{x}(0)$ ← $\mathrm{d}\mathbf{x} = \left[\mathbf{f}(\mathbf{x}, t) - g^2(t)\nabla_{\mathbf{x}} \log p_t(\mathbf{x})\right] \mathrm{d}t + g(t)\mathrm{d}\bar{\mathbf{w}}$ — $\mathbf{x}(T)$

Reverse SDE (noise → data)

Y. Song et al. "Score-Based Generative Modeling through Stochastic Differential Equations". In: *International Conference on Learning Representations*. 2021.

Stochastic Differential Equations (SDE)

$$\mathrm{d}\mathbf{x}_{t+1} = \mathbf{f}_t(\mathbf{x}_t)\,\mathrm{d}t + g_t\,\mathrm{d}\mathbf{w}_t$$
$$\mathbf{x}_{t+1} \approx \mathbf{x}_t + \eta_t \cdot \mathbf{f}_t(\mathbf{x}_t) + g_t\sqrt{\eta_t}\cdot\mathbf{z}, \quad \text{where} \quad \mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$$

- Intuitively, $\mathbf{x}_{t+1}$ is now a deformed, noisy version of $\mathbf{x}_t$
  - drift term $\mathbf{f}_t$: the infinitesimal change of $\mathbf{E}[\mathbf{x}_u \mid \mathbf{x}_t]$ when $u \downarrow t$
  - diffusion term g_t: the infinitesimal change of $\mathrm{Var}[\mathbf{x}_u \mid \mathbf{x}_t]$ when $u \downarrow t$
- Kolmogorov forward equation (a.k.a. Fokker-Planck equation):

$$\boxed{\partial_t p_t = -\left\langle \partial_{\mathbf{x}}, p_t \mathbf{f}_t \right\rangle + \tfrac{1}{2} g_t^2 \left\langle \partial_{\mathbf{x}} \partial_{\mathbf{x}}^\top, p_t \right\rangle}, \qquad \mathbf{x}_t \sim p_t$$

- Kolmogorov backward equation (with fixed end time $t > s$):

$$-\partial_s p_s = \left\langle \mathbf{f}_s, \partial_{\mathbf{x}} p_s \right\rangle + \tfrac{1}{2} g_t^2 \partial_{\mathbf{x}} \partial_{\mathbf{x}}^\top p_s$$

ODE $\Leftrightarrow$ SDE

$$\mathrm{d}\mathbf{x}_{t+1} = \mathbf{f}_t(\mathbf{x}_t)\,\mathrm{d}t$$
$$\mathrm{d}\mathbf{x}_{t+1} = \mathbf{f}_t(\mathbf{x}_t)\,\mathrm{d}t + g_t\,\mathrm{d}\mathbf{w}_t$$

- Any ODE is a (trivial) SDE with $g_t \equiv \mathbf{0}$
- Conversely, any SDE is equivalent to an ODE:

$$\boxed{\mathbf{f}_t \leftarrow \mathbf{f}_t - \tfrac{1}{2} g_t^2 \partial_{\mathbf{x}} \log p_t}$$

- The score function plays an important role:

$$\boxed{\mathbf{s}(\mathbf{x}) = \mathbf{s}_p(\mathbf{x}) := \partial_{\mathbf{x}} \log p(\mathbf{x})}$$

Marginal and Conditional Gaussians

- Marginal X and conditional Y | X Gaussian:

$$p(\mathbf{x}) = \mathcal{N}(\mathbf{x} \mid \boldsymbol{\mu}, \Sigma), \qquad i.e., \ \mathsf{X} = \boldsymbol{\mu} + \Sigma^{1/2}\mathsf{Z}_1$$
$$p(\mathbf{y} \mid \mathbf{x}) = \mathcal{N}(\mathbf{y} \mid A\mathbf{x} + \mathbf{b}, S), \ i.e., \ \mathsf{Y} = A\mathsf{X} + \mathbf{b} + S^{1/2}\mathsf{Z}_2,$$

- Equivalent to joint Gaussian:

$$p(\mathbf{x}, \mathbf{y}) = \mathcal{N}\left(\begin{bmatrix} \boldsymbol{\mu} \\ A\boldsymbol{\mu} + \mathbf{b} \end{bmatrix}, \begin{bmatrix} \Sigma & \Sigma A^\top \\ A\Sigma & A\Sigma A^\top + S \end{bmatrix}\right)$$

- Refactorize into marginal Y and conditional X | Y, again Gaussian:

$$p(\mathbf{y}) = \mathcal{N}(\mathbf{y} \mid A\boldsymbol{\mu} + \mathbf{b}, A\Sigma A^\top + S), \quad i.e., \ \mathsf{Y} = A\boldsymbol{\mu} + \mathbf{b} + A\Sigma^{1/2}\mathsf{Z}_1 + S^{1/2}\mathsf{Z}_2$$
$$p(\mathbf{x}|\mathbf{y}) = \mathcal{N}\left(\mathbf{x}|\Xi\big(\Sigma^{-1}\boldsymbol{\mu} + A^\top S^{-1}(\mathbf{y} - \mathbf{b})\big), \Xi\right), \quad \text{where} \quad \Xi = (\Sigma^{-1} + A^\top S^{-1} A)^{-1}$$

- Linear transformation of Gaussian is still Gaussian:

$$[\mathsf{X} - \Sigma A^\top (A\Sigma A^\top + S)^{-1}\mathsf{Y}] \perp\!\!\!\perp \mathsf{Y}$$

  - simply verify the covariance is zero

- Mean and covariance determine a Gaussian:

$$\begin{aligned}
\mathbb{E}[\mathsf{X} \mid \mathsf{Y}] &= \mathbb{E}[\mathsf{X} - \Sigma A^\top (A\Sigma A^\top + S)^{-1}\mathsf{Y} \mid \mathsf{Y}] + \Sigma A^\top (A\Sigma A^\top + S)^{-1}\mathsf{Y} \\
&= \mathbb{E}[\mathsf{X} - \Sigma A^\top (A\Sigma A^\top + S)^{-1}\mathsf{Y}] + \Sigma A^\top (A\Sigma A^\top + S)^{-1}\mathsf{Y} \\
&= \boldsymbol{\mu} - \Sigma A^\top (A\Sigma A^\top + S)^{-1}(A\boldsymbol{\mu} + \mathbf{b}) + \Sigma A^\top (A\Sigma A^\top + S)^{-1}\mathsf{Y} \\
&= \big(\Sigma - \Sigma A^\top (A\Sigma A^\top + S)^{-1} A\Sigma\big)\Sigma^{-1}\mu + \Sigma A^\top (A\Sigma A^\top + S)^{-1}(\mathsf{Y} - \mathbf{b}) \\
\mathrm{Var}[\mathsf{X} \mid \mathsf{Y}] &= \mathrm{Var}[\mathsf{X} - \Sigma A^\top (A\Sigma A^\top + S)^{-1}\mathsf{Y} \mid \mathsf{Y}] \\
&= \mathrm{Var}[\mathsf{X} - \Sigma A^\top (A\Sigma A^\top + S)^{-1}\mathsf{Y}] \\
&= \Sigma - 2\Sigma A^\top (A\Sigma A^\top + S)^{-1} A\Sigma + \Sigma A^\top (A\Sigma A^\top + S)^{-1} A\Sigma \\
&= (\Sigma^{-1} + A^\top S^{-1} A)^{-1}
\end{aligned}$$

  - Sherman-Morrison-Woodbury identity

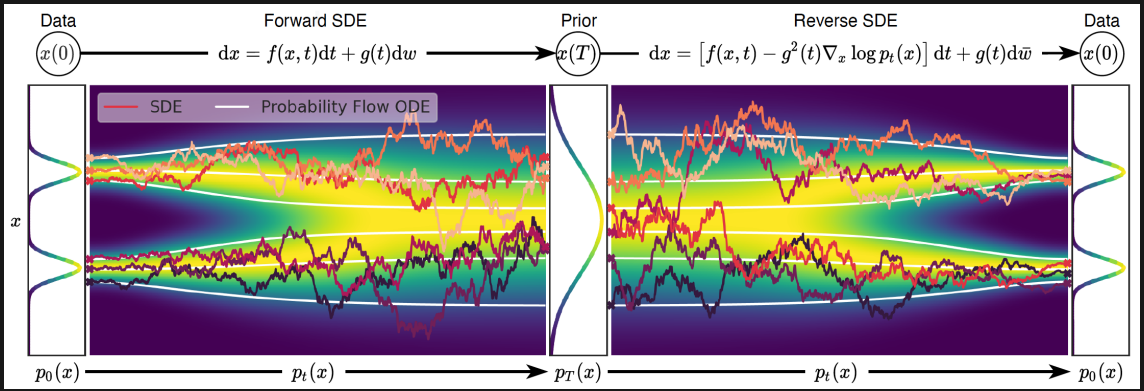
Reverse-time SDE

$$\mathrm{d}\mathbf{x}_{t+1} = \mathbf{f}_t(\mathbf{x}_t)\,\mathrm{d}t + g_t\,\mathrm{d}\mathbf{w}_t$$
$$\mathrm{d}\bar{\mathbf{x}}_{t+1} = \bar{\mathbf{f}}_t(\bar{\mathbf{x}}_t)\,\mathrm{d}t + g_t\,\mathrm{d}\bar{\mathbf{w}}_t, \quad \text{where}$$

$$\boxed{\bar{\mathbf{f}}_t = \mathbf{f}_t - g_t^2\,\partial_{\mathbf{x}} \log p_t}$$

- Time flows backwards for the bar $\overline{\text{quantities}}$
- Forward SDE: diffuses date into noise
- Reverse SDE: molds noise into data
- $\mathbf{f}_t$ and G_t together specify $\bar{\mathbf{f}}_t$: key is to estimate the score $\partial_{\mathbf{x}} \log p_t$

B. D. O. Anderson. "Reverse-time diffusion equation models". *Stochastic Processes and their Applications*, vol. 12, no. 3 (1982), pp. 313–326.



Y. Song et al. "Score-Based Generative Modeling through Stochastic Differential Equations". In: *International Conference on Learning Representations*. 2021.

Score Matching

$$\begin{aligned}\mathbb{F}(p\|q) &:= \tfrac{1}{2}\mathbb{E}_{\mathsf{X}\sim q}\|\partial_{\mathbf{x}}\log p(\mathsf{X}) - \partial_{\mathbf{x}}\log q(\mathsf{X})\|_2^2 \\ &= \mathbb{E}_{\mathsf{X}\sim q}\left[\tfrac{1}{2}\|\mathbf{s}_p(\mathsf{X})\|_2^2 + \langle\partial_{\mathbf{x}}, \mathbf{s}_p(\mathsf{X})\rangle + \tfrac{1}{2}\|\mathbf{s}_q(\mathsf{X})\|_2^2\right] \\ &\approx \hat{\mathbb{E}}_{\mathsf{X}\sim q}\left[\tfrac{1}{2}\|\mathbf{s}_p(\mathsf{X})\|_2^2 + \langle\partial_{\mathbf{x}}, \mathbf{s}_p(\mathsf{X})\rangle\right]\end{aligned}$$

- Under mild conditions, $\mathbb{F}(p\|q) = 0 \iff p \propto q$
- A Convenient way to estimate the score $\mathbf{s}_q$ and hence the density q
- The model score function $\mathbf{s}_p$ can be chosen as a neural net

A. Hyvärinen. "Estimation of Non-Normalized Statistical Models by Score Matching". *Journal of Machine Learning Research*, vol. 6, no. 24 (2005), pp. 695–709.

Denoising Auto-Encoder

- Suppose also have a latent variable Z with joint density $q(\mathbf{x}, \mathbf{z})$
- Exchange differentiation with integration we obtain:

$$\begin{aligned}\mathbb{F}(p\|q) &:= \tfrac{1}{2}\mathbb{E}_{\mathsf{X}\sim q}\|\partial_{\mathbf{x}} \log p(\mathsf{X}) - \partial_{\mathbf{x}} \log q(\mathsf{X})\|_2^2 \\ &= \tfrac{1}{2}\mathbb{E}_{(\mathsf{X},\mathsf{Z})\sim q}[\|\mathbf{s}_p(\mathsf{X}) - \partial_{\mathbf{x}} \log q(\mathsf{X}|\mathsf{Z})\|_2^2 + \|\mathbf{s}_q(\mathsf{X})\|_2^2 - \|\partial_{\mathbf{x}} \log q(\mathsf{X}|\mathsf{Z})\|_2^2] \\ &\approx \tfrac{1}{2}\hat{\mathbb{E}}_{(\mathsf{X},\mathsf{Z})\sim q}\|\mathbf{s}_p(\mathsf{X}) - \partial_{\mathbf{x}} \log q(\mathsf{X}|\mathsf{Z})\|_2^2\end{aligned}$$

- Useful when the conditional density $\partial_{\mathbf{x}} \log q(\mathsf{X}|\mathsf{Z})$ is easy to obtain

P. Vincent. "A Connection Between Score Matching and Denoising Autoencoders". *Neural Computation*, vol. 23, no. 7 (2011), pp. 1661–1674.

Score-based Diffusion Generative Models

$$\mathrm{d}\mathbf{x}_{t+1} = \mathbf{f}_t(\mathbf{x}_t)\,\mathrm{d}t + g_t\,\mathrm{d}\mathbf{w}_t$$
$$\mathbf{x}_{t+1} \approx \mathbf{x}_t + \eta_t \cdot \mathbf{f}_t(\mathbf{x}_t) + g_t\sqrt{\eta_t}\cdot\mathbf{z}, \quad \text{where} \quad \mathbf{z}\sim\mathcal{N}(\mathbf{0},\mathbf{I})$$

- Key is to estimate the score $\mathbf{s}_t(\mathbf{x}) = \partial_{\mathbf{x}}\log p_t$
- Apply denoising auto-encoder score matching:

$$\min_{\boldsymbol{\theta}} \hat{\mathbb{E}}_{t\sim\mu,(\mathsf{X}_t,\mathsf{X}_0)\sim q(\mathbf{x}_t,\mathbf{x}_0)} \lambda_t \|\mathbf{s}_t(\mathsf{X}_t;\boldsymbol{\theta}) - \partial_{\mathbf{x}}\log q(\mathsf{X}_t|\mathsf{X}_0)\|_2^2$$

  - $\mathsf{X}_0 \sim q(\mathbf{x})$, the data density
  - $q(\mathbf{x}_t|\mathbf{x}_0)$ can be derived from the forward SDE, in closed-form if $\mathbf{f}_t$ is affine

Inference After Learning

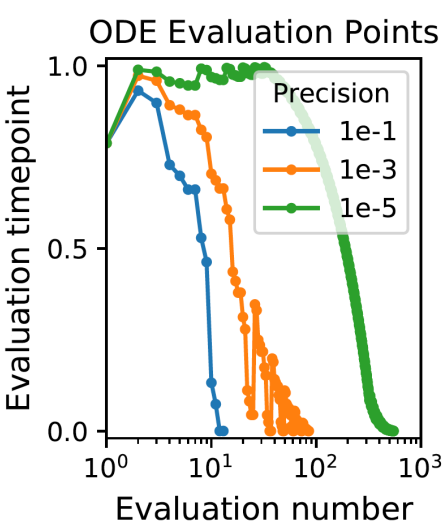
$$\mathrm{d}\mathbf{x}_{t+1} = \mathbf{f}_t(\mathbf{x}_t)\,\mathrm{d}t + g_t\,\mathrm{d}\mathbf{w}_t$$

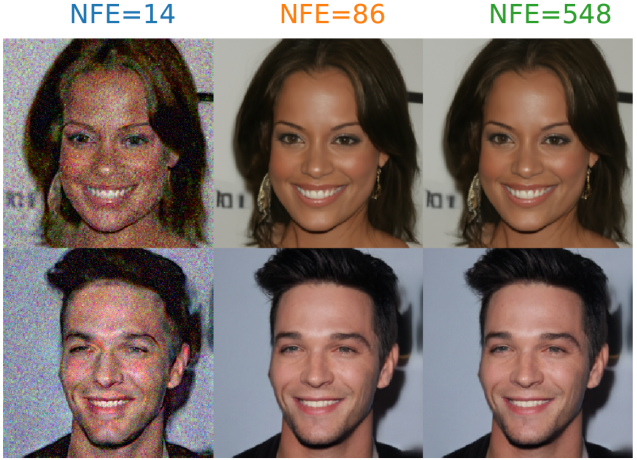
$$\mathrm{d}\bar{\mathbf{x}}_{t+1} = \boxed{\mathbf{f}_t - g_t^2\,\mathbf{s}_t(\bar{\mathbf{x}}_t;\boldsymbol{\theta})}\,\mathrm{d}t + g_t\,\mathrm{d}\bar{\mathbf{w}}_t$$

$$\mathrm{d}\mathbf{x}_{t+1} = \boxed{\mathbf{f}_t - \tfrac{1}{2}g_t^2\,\mathbf{s}_t(\mathbf{x}_t;\boldsymbol{\theta})}\,\mathrm{d}t$$

- Run the reverse SDE or the equivalent ODE
  - sample $\mathbf{x} \sim \mathcal{N}(\mathbf{0}, \mathrm{Id})$
  - apply numerical SDE or ODE solver (e.g., Euler-Maruyama)

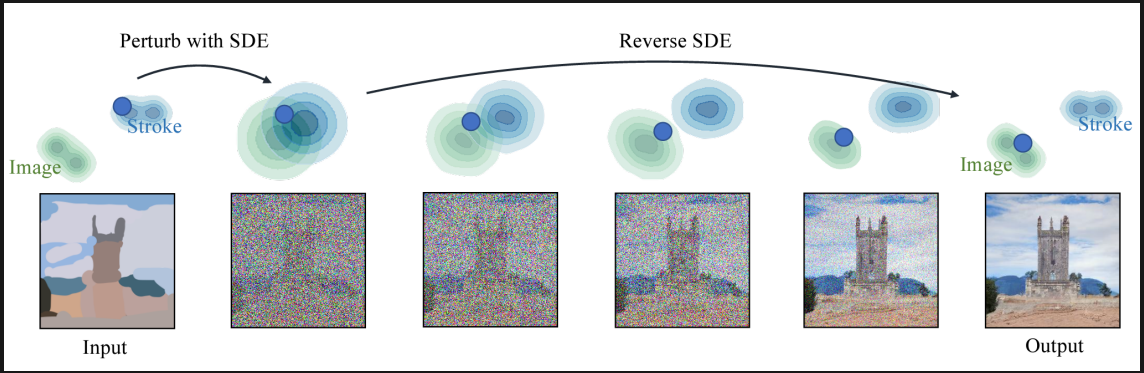
D. J. Higham. "An Algorithmic Introduction to Numerical Simulation of Stochastic Differential Equations". *SIAM Review*, vol. 43, no. 3 (2001), pp. 525–546.





Y. Song et al. "Score-Based Generative Modeling through Stochastic Differential Equations". In: *International Conference on Learning Representations*. 2021.

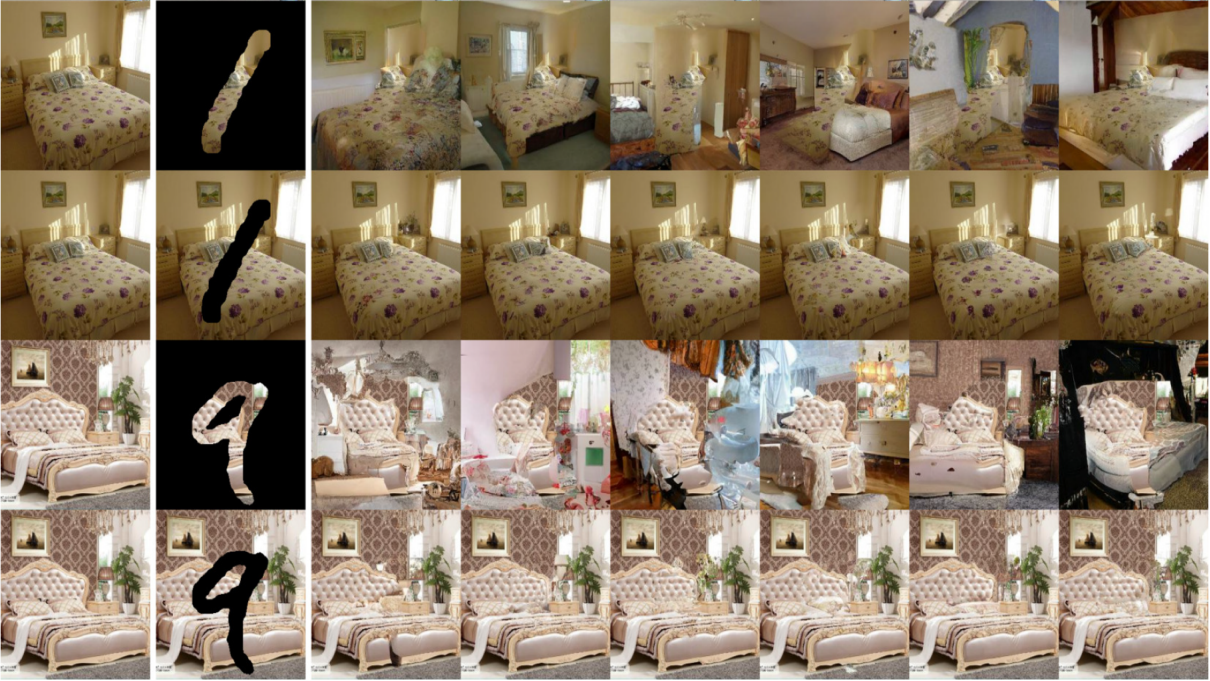
SDEdit



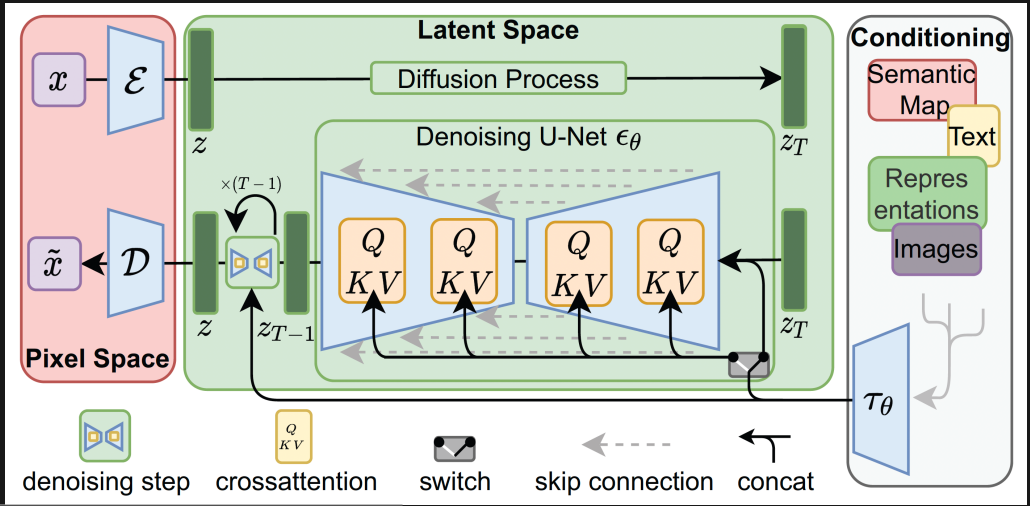
C. Meng et al. "SDEdit: Guided Image Synthesis and Editing with Stochastic Differential Equations". In: *International Conference on Learning Representations*. 2022.

Interpolation

Y. Song et al. "Score-Based Generative Modeling through Stochastic Differential Equations". In: *International Conference on Learning Representations*. 2021.



Stable Diffusion



R. Rombach et al. "High-Resolution Image Synthesis with Latent Diffusion Models". In: *IEEE/CVF Conference on Computer Vision and Pattern Recognition*. 2022, pp. 10674–10685.