Diffusion models for particle physics simulations

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1. **Particle physics simulations**
2. **Diffusion Models**
3. **Equivariant learning**
4. **Appendices**

Particle physics simulations

Collisions

High energy protons

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High energy protons $\xrightarrow{\text{collisions}}$ Non-isolatable elementary particles

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$$\text{High energy protons} \xrightarrow{\text{collisions}} \text{Non-isolatable elementary particles} \xrightarrow{\text{radiate}} \text{Parton shower}$$

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$$\text{Initial particles} \rightarrow \text{Jet constituents}$$

Simulation-based inference

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$$p(\beta|o) = \frac{p(o|\beta)p(\beta)}{\int p(\beta')p(o|\beta')\, d\beta'} p(o|\beta) \quad = \int p(x, \beta|\theta) dz$$

Limitations

- Fit simplified phenomenological models to parton shower, hadronization

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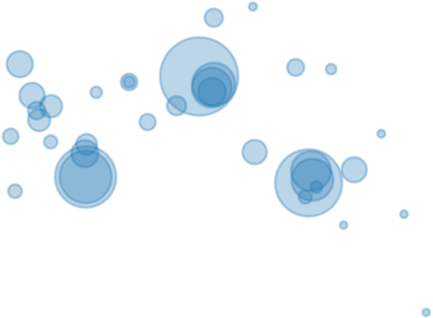
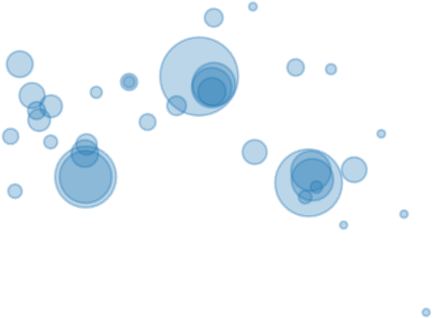
- Slow: 10 s / jet
- One-shot generation: 3-5 OoM speedup!

Representing jets



Gouskos and Qu 2018

Representing jets



Gouskos and Qu 2018

Particle clouds + feature vectors

Diffusion Models

Generative modeling from PDFs

Given: $\mathbf{x}_1, \mathbf{x}_2, \ldots \mathbf{x}_N$ from $p_{\text{data}}(\mathbf{x})$

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$$p_\theta(\mathbf{x}) \quad = \frac{e^{f_\theta(\mathbf{x})}}{Z_\theta}$$

$$Z_\theta = \int e^{f_\theta(\mathbf{x})}\, d\mathbf{x}$$

Score functions

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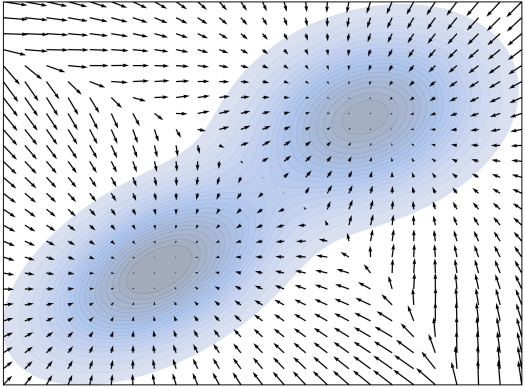
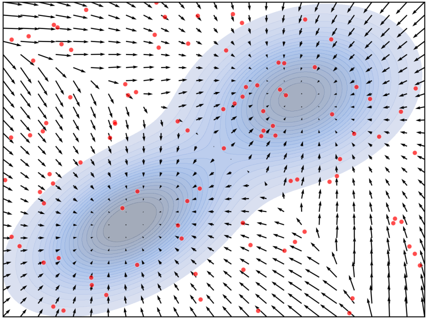


Sampling

$$\mathbf{x}_{t+1} = \mathbf{x}_t + \alpha \cdot s_\theta(\mathbf{x}_t)$$

$$x_0 \sim \pi_{\text{init}}$$

$$t = 0, 1, \ldots T \to \infty$$



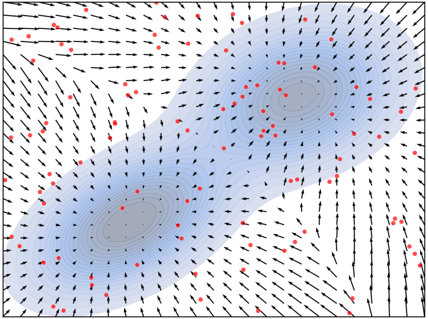
Sampling with Langevin dynamics

$$\mathbf{x}_{t+1} = \mathbf{x}_t + \alpha \cdot s_\theta(\mathbf{x}_t) + \alpha\epsilon \cdot \mathbf{z}_t$$

$$x_0 \sim \pi_{\text{init}}$$

$$\mathbf{z}_t \sim \mathcal{N}(0,1)$$

$$t = 0, 1, \dots T \to \infty$$



Training objective for score

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$$\mathcal{L}_{\mathsf{ESM}}(\theta) = \frac{1}{2}\mathbb{E}_{p_{\mathsf{data}}(\mathbf{x})}\left[||\nabla_{\mathbf{x}} \log p_{\mathsf{data}}(\mathbf{x}) - s_\theta(\mathbf{x})||_2^2\right]$$

$$\iff \mathcal{L}_{\mathsf{ISM}}(\theta) = \frac{1}{2}\mathbb{E}_{p_{\mathsf{data}}(\mathbf{x})}\left[s_\theta(\mathbf{x})^2\right] + \mathbb{E}_{p_{\mathsf{data}}(\mathbf{x})}\left[\nabla_{\mathbf{x}} s_\theta(\mathbf{x})\right]$$

$$\approx \frac{1}{N}\sum_{i=1}^{N}\left[\frac{1}{2}s_\theta(\mathbf{x}_i)^2 + \nabla_{\mathbf{x}_i} s_\theta(\mathbf{x}_i)\right]$$

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Drawbacks

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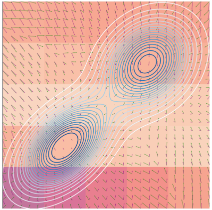
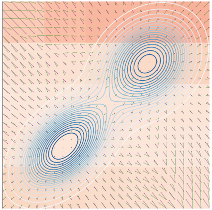
Field in low-density regions





Scaling

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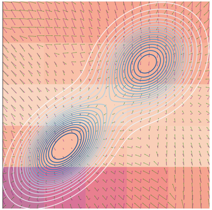

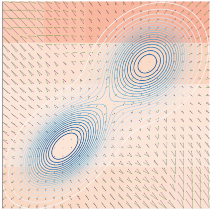

Scaling

$$\frac{1}{2}\mathbb{E}_{p_{\mathsf{data}}(\mathbf{x})}\left[s_\theta(\mathbf{x})^2\right] + \mathbb{E}_{p_{\mathsf{data}}(\mathbf{x})}\left[\nabla_{\mathbf{x}} s_\theta(\mathbf{x})\right]$$

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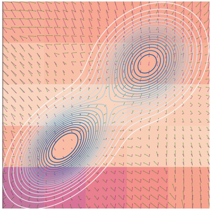
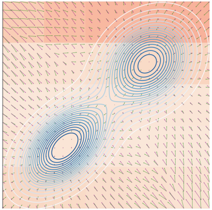




Scaling

$$\frac{1}{2}\mathbb{E}_{p_{\mathsf{data}}(\mathbf{x})}\left[s_\theta(\mathbf{x})^2\right] + \mathbb{E}_{p_{\mathsf{data}}(\mathbf{x})}\left[\nabla_{\mathbf{x}} s_\theta(\mathbf{x})\right]$$

$$\underbrace{\frac{1}{2}\mathbb{E}_{p_{\mathsf{data}}(\mathbf{x})}\left[s_\theta(\mathbf{x})^2\right]}_{\text{Forward propagation}} + \underbrace{\mathbb{E}_{p_{\mathsf{data}}(\mathbf{x})}\left[\mathrm{trace}(\nabla_{\mathbf{x}} s_\theta(\mathbf{x}))\right]}_{\text{Backprops} \propto \dim(\mathbf{x})}$$

Noise perturbation

$$\tilde{\mathbf{x}} = \mathbf{x} + z$$
$$z \sim \mathcal{N}(0, 1)$$
$$q_\sigma(\tilde{\mathbf{x}}|\mathbf{x}) = \mathcal{N}(\mathbf{x}, \sigma^2 I)$$

Denoising objective

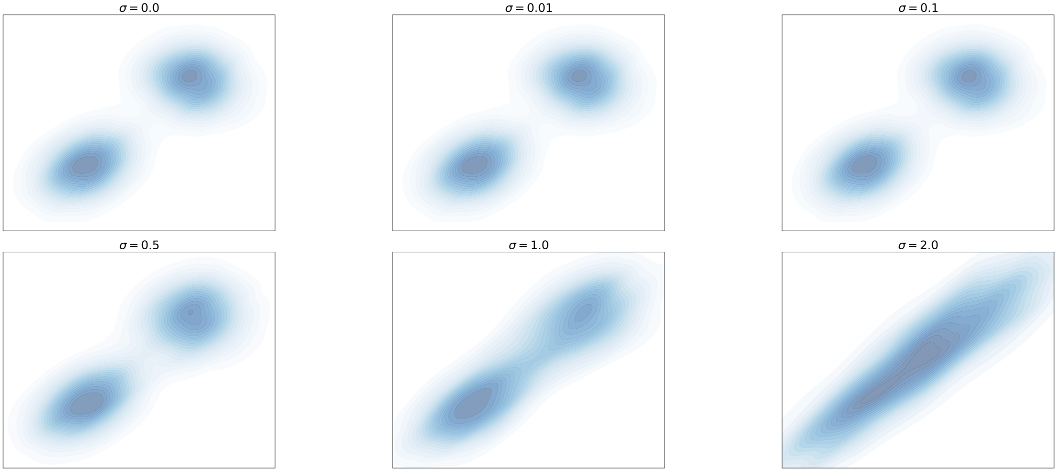
$$\mathcal{L}_{\mathsf{ESM}\sigma}(\theta, \sigma) = \frac{1}{2}\mathbb{E}_{q_\sigma(\tilde{\mathbf{x}})}\left[||s_\theta(\tilde{\mathbf{x}}) - \nabla_{\tilde{\mathbf{x}}} \log q_\sigma(\tilde{\mathbf{x}})||_2^2\right]$$

$$\iff \mathcal{L}_{\mathsf{ISM}\sigma}(\theta, \sigma) = \frac{1}{2}\mathbb{E}_{q_\sigma(\tilde{\mathbf{x}}, \mathbf{x})}\left[||s_\theta(\tilde{\mathbf{x}}) - \nabla_{\tilde{\mathbf{x}}} \log q_\sigma(\tilde{\mathbf{x}}|\mathbf{x})||_2^2\right]$$

Gradient of the corrupted distribution

$$
\begin{aligned}
\nabla_{\tilde{\mathbf{x}}} \log q_\sigma(\tilde{\mathbf{x}}|\mathbf{x}) &= \nabla_{\tilde{\mathbf{x}}} \log \frac{1}{(2\pi)^{\frac{d}{2}}\sigma^d} e^{-\frac{1}{2\sigma^2}||\tilde{\mathbf{x}}-\mathbf{x}||^2} \\
&= \nabla_{\tilde{\mathbf{x}}} \log e^{-\frac{1}{2\sigma^2}||\tilde{\mathbf{x}}-\mathbf{x}||^2} - \nabla_{\tilde{\mathbf{x}}} \log(2\pi)^{\frac{d}{2}}\sigma^d \\
&= -\nabla_{\tilde{\mathbf{x}}} \frac{1}{2\sigma^2}||\tilde{\mathbf{x}}-\mathbf{x}||^2 \\
&= \frac{||\tilde{\mathbf{x}}-\mathbf{x}||}{\sigma^2} \\
\therefore \mathcal{L}_{\mathsf{ISM}\sigma}(\theta,\sigma) &= \frac{1}{2}\mathbb{E}_{q_\sigma(\tilde{\mathbf{x}},\mathbf{x})}\left[||s_\theta(\tilde{\mathbf{x}}) - \frac{||\tilde{\mathbf{x}}-\mathbf{x}||}{\sigma^2}||_2^2\right]
\end{aligned}
$$

Multiple noise levels



Multiple noise levels

$$\mathcal{L}(\theta, \{\sigma_i\}_{i=1}^{L}) = \frac{1}{L}\sum_{i=1}^{L} \lambda(\sigma_i)\mathbb{E}_{q_{\sigma_i}(\tilde{\mathbf{x}},\mathbf{x})}\left[|| s_\theta(\tilde{\mathbf{x}}, \sigma_i) - \frac{||\tilde{\mathbf{x}} - \mathbf{x}||}{\sigma^2} ||_2^2 \right]$$

Sampling with annealed Langevin dynamics

$$\tilde{\mathbf{x}}_0 \sim \pi_{\mathsf{init}}$$

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From $i = 1, 2, \dots L$ with $\frac{\sigma_1}{\sigma_2} = \cdots = \frac{\sigma_{L-1}}{\sigma_L} > 1$

Sampling with annealed Langevin dynamics

$$\tilde{\mathbf{x}}_0 \sim \pi_{\text{init}}$$

From $i = 1, 2, \ldots L$ with $\frac{\sigma_1}{\sigma_2} = \cdots = \frac{\sigma_{L-1}}{\sigma_L} > 1$

$$\alpha_i = \gamma \frac{\sigma_i^2}{\sigma_L^2}$$
$$\tilde{\mathbf{x}}_t = \tilde{\mathbf{x}}_{t-1} + \alpha_i s_\theta(\tilde{\mathbf{x}}_{t-1}, \sigma_i) + \epsilon \alpha_i \mathbf{z}_t$$
$$\mathbf{z}_t \sim \mathcal{N}(0, 1)$$

Conditional generation

$$p(\mathbf{x}|\mathbf{y}) = \frac{p(\mathbf{y}|\mathbf{x})p(\mathbf{x})}{\color{red}{p(\mathbf{y})}}$$

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$$\begin{aligned}
\nabla_{\mathbf{x}} \log p(\mathbf{x}|\mathbf{y}) &= \nabla_{\mathbf{x}} \log p(\mathbf{y}|\mathbf{x}) + \nabla_{\mathbf{x}} \log p(\mathbf{x}) - \nabla_{\mathbf{x}} \log p(\mathbf{y}) \\
&= \nabla_{\mathbf{x}} \log p(\mathbf{x}) + \nabla_{\mathbf{x}} \log p(\mathbf{y}|\mathbf{x}) \\
&= {\color{teal} s_\theta(\mathbf{x})} + {\color{olive}\gamma} \nabla_{\mathbf{x}} \log p(\mathbf{y}|\mathbf{x})
\end{aligned}$$

Single model for guidance

$$
\begin{aligned}
p(\mathbf{y}|\mathbf{x}) &= \nabla_{\mathbf{x}} \log p(\mathbf{x}|\mathbf{y}) - \nabla_{\mathbf{x}} \log p(\mathbf{x}) \\
\implies \nabla_{\mathbf{x}} \log p(\mathbf{x}|\mathbf{y}) &= \nabla_{\mathbf{x}} \log p(\mathbf{x}) + \gamma \nabla_{\mathbf{x}} \log p(\mathbf{x}|\mathbf{y}) - \gamma \nabla_{\mathbf{x}} \log p(\mathbf{x}) \\
&= \gamma \nabla_{\mathbf{x}} \log p(\mathbf{x}|\mathbf{y}) + (\gamma - 1) \nabla_{\mathbf{x}} \log p(\mathbf{x}) \\
&\approx \gamma s_\theta(\mathbf{x}, \mathbf{y}) - (\gamma - 1) s_\theta(\mathbf{x}, \phi)
\end{aligned}
$$

Equivariant learning

- Equivariant: $f(g(I)) = g'(f(I))$, $g \in G, g' \in G'$

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- Images: translation, rotation, reflection
- Graphs, sets: permutation

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- Images: translation, rotation, reflection
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Inductive biases

In ML

1. Data augmentation

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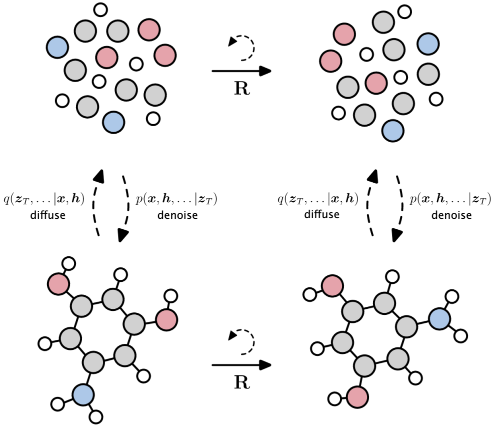
2. Model architecture

Equivariant diffusion models



$$p(\boldsymbol{x}, \boldsymbol{h}) = p(\mathbf{R}\boldsymbol{x}, \boldsymbol{h})$$

Hoogeboom et al. 2022

Lorentz equivariance in diffusion?

Lorentz equivariance in diffusion?

$$\text{eg.} \begin{pmatrix} \gamma & -\gamma\beta & 0 & 0 \\ -\gamma\beta & \gamma & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

(relative velocity $\beta = \frac{v}{c}$, boost factor $\gamma = \frac{1}{(1-\beta^2)^2}$)

Appendices

Derivation of divergence objective for score

$$\frac{1}{2}\mathbb{E}_{p_{\text{data}}(\mathbf{x})}\left[||\nabla_{\mathbf{x}} \log p_{\text{data}}(\mathbf{x}) - s_\theta(\mathbf{x})||_2^2\right]$$

$$= \frac{1}{2}\int p_{\text{data}}(\mathbf{x})\left(\nabla_{\mathbf{x}} \log p_{\text{data}}(\mathbf{x}) - \nabla_{\mathbf{x}} f_\theta(\mathbf{x})\right)^2 \, d\mathbf{x}$$

$$= \frac{1}{2}\int p_{\text{data}}(\mathbf{x})\left(\nabla_{\mathbf{x}} \log p_{\text{data}}(\mathbf{x})\right)^2 \, d\mathbf{x} + \frac{1}{2}\int p_{\text{data}}(\mathbf{x})\left(\nabla_{\mathbf{x}} f_\theta(\mathbf{x})\right)^2 \, d\mathbf{x} - \int p_{\text{data}}(\mathbf{x})\nabla_{\mathbf{x}} \log p_{\text{data}}(\mathbf{x}) \cdot \nabla_{\mathbf{x}}$$

Constant in training

Use $\nabla_{\mathbf{x}} \log p_{\text{data}}(\mathbf{x}) = \frac{\nabla_{\mathbf{x}} p_{\text{data}}(\mathbf{x}}{p_{\text{data}}(\mathbf{x})}$

$$= C + \frac{1}{2}\int p_{\text{data}}(\mathbf{x})\left(\nabla_{\mathbf{x}} f_\theta(\mathbf{x})\right)^2 \, d\mathbf{x} - \int \nabla_{\mathbf{x}} p_{\text{data}}(\mathbf{x}) \cdot \nabla_{\mathbf{x}} f_\theta(\mathbf{x}) \, d\mathbf{x}$$

Integrate by parts

$$= C + \frac{1}{2}\int p_{\text{data}}(\mathbf{x})\left(\nabla_{\mathbf{x}} f_\theta(\mathbf{x})\right)^2 \, d\mathbf{x} - p_{\text{data}}(\mathbf{x})\nabla_x f_\theta(\mathbf{x})\big|_{-\infty}^{\infty} + \int p_{\text{data}}(\mathbf{x})\nabla_{\mathbf{x}}\nabla_{\mathbf{x}} f_\theta(\mathbf{x}) d\mathbf{x}$$

Boundary values $\rightarrow$ 0

$$= C + \frac{1}{2}\mathbb{E}_{p_{\text{data}}(\mathbf{x})}\left[\nabla_{\mathbf{x}} f_\theta(\mathbf{x})^2\right] + \mathbb{E}_{p_{\text{data}}(\mathbf{x})}\left[\nabla_{\mathbf{x}}^2 f_\theta(\mathbf{x})\right] = C + \frac{1}{2}\mathbb{E}_{p_{\text{data}}(\mathbf{x})}\left[s_\theta(\mathbf{x})^2\right] + \mathbb{E}_{p_{\text{data}}(\mathbf{x})}\left[\nabla_{\mathbf{x}} s_\theta(\mathbf{x})\right]$$

Derivation of noise-perturbed divergence objective

$$\frac{1}{2}\mathbb{E}_{q_\sigma(\tilde{\mathbf{x}})}\left[||s_\theta(\tilde{\mathbf{x}}) - \nabla_{\tilde{\mathbf{x}}} \log q_\sigma(\tilde{\mathbf{x}})||_2^2\right]$$

$$= \frac{1}{2}\mathbb{E}_{q_\sigma(\tilde{\mathbf{x}})}\left[s_\theta(\tilde{\mathbf{x}})^2\right] - \int q_\sigma(\tilde{\mathbf{x}}) s_\theta(\tilde{\mathbf{x}}) \nabla_{\tilde{\mathbf{x}}} \log q_\sigma(\tilde{\mathbf{x}})\, d\tilde{\mathbf{x}} + \frac{1}{2}\int q_\sigma(\tilde{\mathbf{x}})(\nabla_{\tilde{\mathbf{x}}} \log q_\sigma(\tilde{\mathbf{x}}))^2\, d\tilde{\mathbf{x}}$$

Use $\nabla_{\tilde{\mathbf{x}}} \log q_\sigma(\tilde{\mathbf{x}}) = \frac{\nabla_{\tilde{\mathbf{x}}} q_\sigma(\tilde{\mathbf{x}})}{q_\sigma(\tilde{\mathbf{x}})}$ Constant in training

$$\int s_\theta(\tilde{\mathbf{x}}) \nabla_{\tilde{\mathbf{x}}} q_\sigma(\tilde{\mathbf{x}})\, d\tilde{\mathbf{x}}$$

Use $q_\sigma(\tilde{\mathbf{x}}) = \int p_{\text{data}}(x) p_\sigma(\tilde{\mathbf{x}}|bx)$

$$= \int s_\theta(\tilde{\mathbf{x}}) \nabla_{\tilde{\mathbf{x}}} \left(\int p_{\text{data}}(\mathbf{x}) q_\sigma(\tilde{\mathbf{x}}|\mathbf{x})\, d\mathbf{x}\right) d\tilde{\mathbf{x}}$$

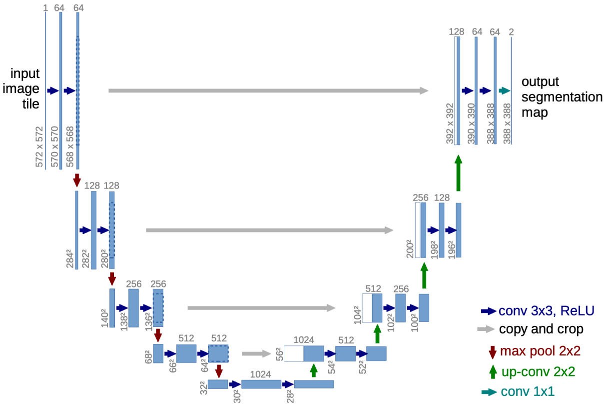
Differentiation under integral

$$= \int s_\theta(\tilde{\mathbf{x}}) \left(\int p_{\text{data}}(\mathbf{x}) \nabla_{\tilde{\mathbf{x}}} q_\sigma(\tilde{\mathbf{x}}|\mathbf{x})\, d\mathbf{x}\right) d\tilde{\mathbf{x}} = \int\int s_\theta(\tilde{\mathbf{x}}) p_{\text{data}}(\mathbf{x}) q_\sigma(\tilde{\mathbf{x}}|\mathbf{x}) \nabla_{\tilde{\mathbf{x}}} \log q_\sigma(\tilde{\mathbf{x}}|\mathbf{x})\, d\mathbf{x}\, d\tilde{\mathbf{x}}$$

Use $\nabla_{\tilde{\mathbf{x}}} q_\sigma(\tilde{\mathbf{x}}|\mathbf{x}) = q_\sigma(\tilde{\mathbf{x}}|\mathbf{x}) \nabla_{\tilde{\mathbf{x}}} \log q_\sigma(\tilde{\mathbf{x}}|\mathbf{x})$

$$= \mathbf{E}_{q_\sigma(\tilde{\mathbf{x}},\mathbf{x})}\left[s_\theta(\tilde{\mathbf{x}}) \nabla_{\tilde{\mathbf{x}}} \log q_\sigma(\tilde{\mathbf{x}}|\mathbf{x})\right]$$

U-Net



Source: Ronneberger et al. (2015)