Diffusion models for particle physics simulations

Arjun Sharma

May 15, 2025

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

Particle physics simulations

Collisions

High energy protons

Collisions

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

Collisions

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

Collisions

$$\text{High energy protons} \xrightarrow{\text{collisions}} \text{Non-isolatable elementary particles} \xrightarrow{\text{radiate}} \text{Parton shower} \xrightarrow[\text{hadronization}]{\text{cooling}} \text{Jet}$$

Collisions

$$\text{High energy protons} \xrightarrow{\text{collisions}} \text{Non-isolatable elementary particles} \xrightarrow{\text{radiate}} \text{Parton shower} \xrightarrow[\text{hadronization}]{\text{cooling}} \text{Jet}$$

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

Simulation-based hypothesis testing

Simulation-based hypothesis testing

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

Simulation-based hypothesis testing

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

- Input: z_0, β

Simulation-based hypothesis testing

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

- Input: z_0, β
- Latent states: $z_i \sim p_i(z_i|\beta, z_{<i})$

Simulation-based hypothesis testing

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

- Input: z_0, β
- Latent states: $z_i \sim p_i(z_i|\beta, z_{<i})$
- Output: $o \sim p(o|\beta, z)$

Simulation-based hypothesis testing

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

- Input: z_0, β
- Latent states: $z_i \sim p_i(z_i|\beta, z_{<i})$
- Output: $o \sim p(o|\beta, z)$

$$p(o|\beta) = \int p(x, \beta|\theta) dz$$

Limitations

Limitations

- Fit simplified phenomenological models to parton shower, hadronization

Limitations

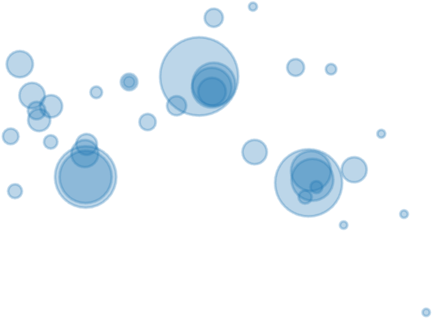
- Fit simplified phenomenological models to parton shower, hadronization
- Slow: 10 s / jet

Limitations

- Fit simplified phenomenological models to parton shower, hadronization
- Slow: 10 s / jet
- One-shot generation: 3-5 OoM speedup!

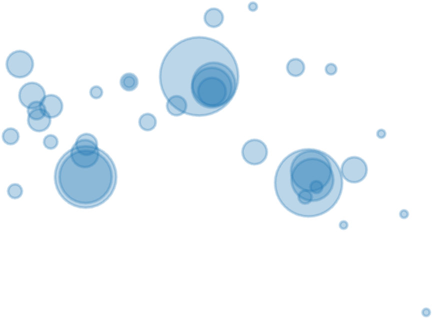
Representing jets

Representing jets



Gouskos and Qu 2018

Representing jets



Gouskos and Qu 2018

Particle clouds + feature vectors

Diffusion Models

Generative modeling

Generative modeling

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

Generative modeling

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

Learn f_θ s.t.

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

Generative modeling

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

Learn f_θ s.t.

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

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

Score functions

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

Score functions

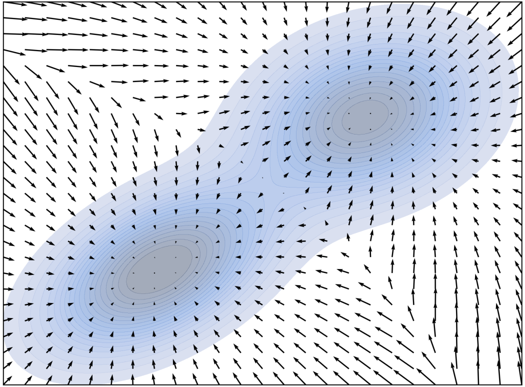
$$p_\theta(\mathbf{x}) = \frac{e^{f_\theta(\mathbf{x})}}{Z_\theta}$$

$$\begin{aligned}
\nabla_\mathbf{x} \log p_\theta(\mathbf{x}) &= \nabla_\mathbf{x} f_\theta(\mathbf{x}) - \nabla_\mathbf{x} \log Z_\theta \\
&= \nabla_\mathbf{x} f_\theta(\mathbf{x}) = s_\theta(\mathbf{x})
\end{aligned}$$

Score functions

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

$$\begin{aligned}\nabla_{\mathbf{x}} \log p_\theta(\mathbf{x}) &= \nabla_{\mathbf{x}} f_\theta(\mathbf{x}) - \nabla_{\mathbf{x}} \log Z_\theta \\ &= \nabla_{\mathbf{x}} f_\theta(\mathbf{x}) = s_\theta(\mathbf{x})\end{aligned}$$

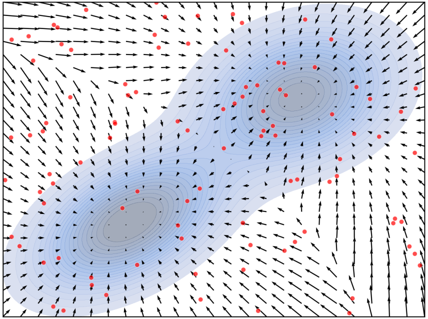


Sampling

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

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

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



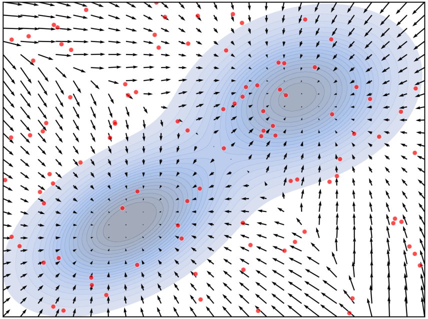
Sampling with Langevin dynamics

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

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

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

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



Training objective for score

Training objective for score

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

Training objective for score

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

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

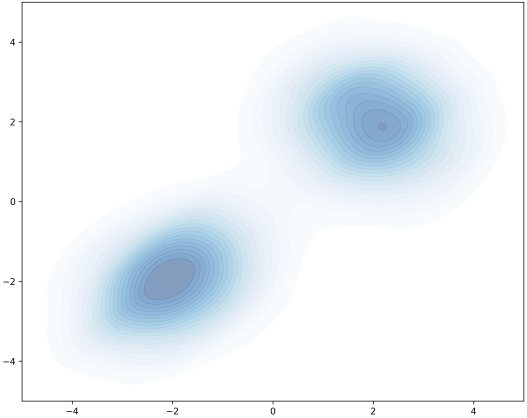
Training objective for score

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

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

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

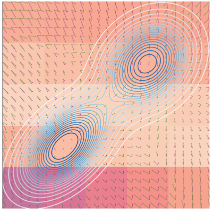
Training

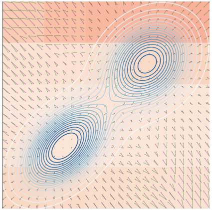


Drawbacks

Drawbacks

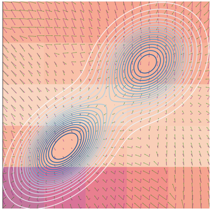
Field in low-density regions

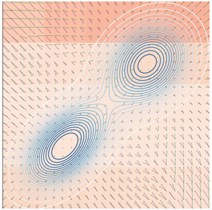




Drawbacks

Field in low-density regions

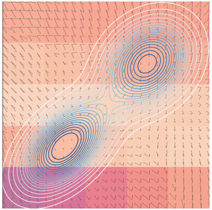


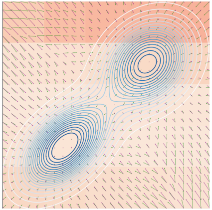


Scaling

Drawbacks

Field in low-density regions



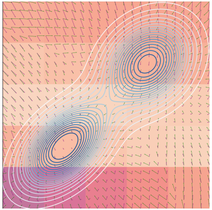


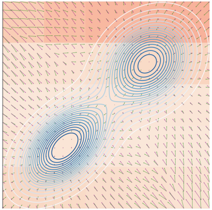
Scaling

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

Drawbacks

Field in low-density regions





Scaling

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

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

Noise perturbation

Noise perturbation

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

Denoising objective

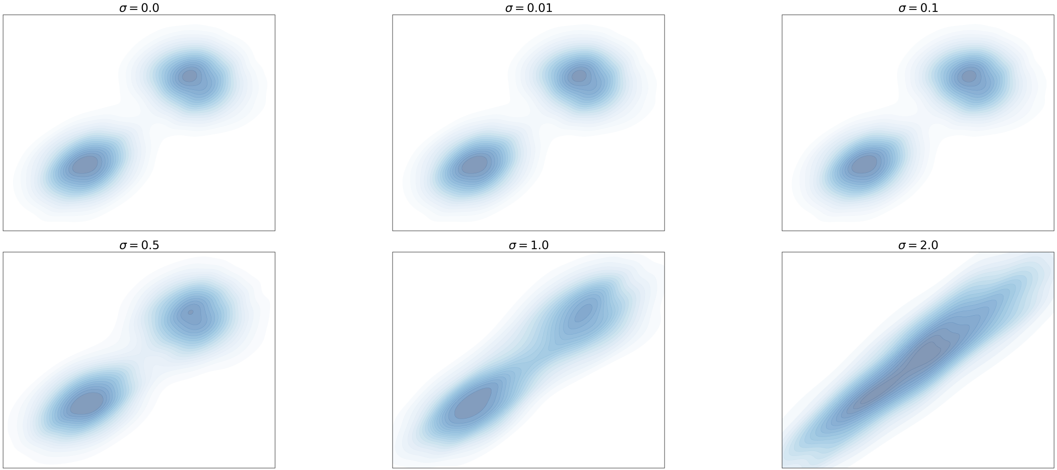
$$\mathcal{L}_{\mathsf{ESM}\sigma}(\theta, \sigma) = \frac{1}{2}\mathbb{E}_{q_\sigma(\tilde{\mathbf{x}})}\left[||s_\theta(\tilde{\mathbf{x}}) - \nabla_{\tilde{\mathbf{x}}} \log q_\sigma(\tilde{\mathbf{x}})||_2^2\right]$$

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

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

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

Sampling with annealed Langevin dynamics

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

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

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

Conditional generation

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

Conditional generation

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

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

Single model for guidance

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

Final score model

$$s_theta(\mathbf{x}, \mathbf{y}, \beta)$$

Equivariant learning

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

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

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

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

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

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

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

Inductive biases

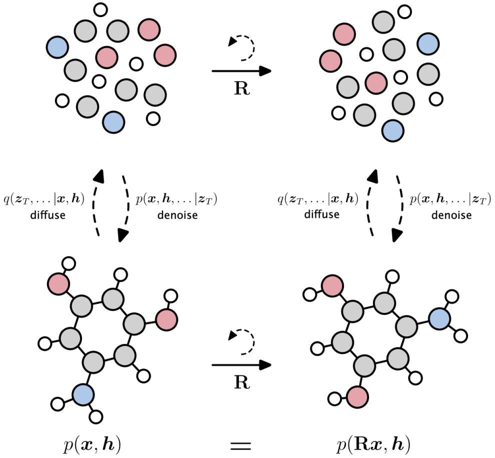
In ML

1. Data augmentation

In ML

1. Data augmentation
2. Model architecture

Equivariant diffusion models



Hoogeboom et al. 2022

Lorentz equivariance in diffusion?

Lorentz equivariance in diffusion?

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

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

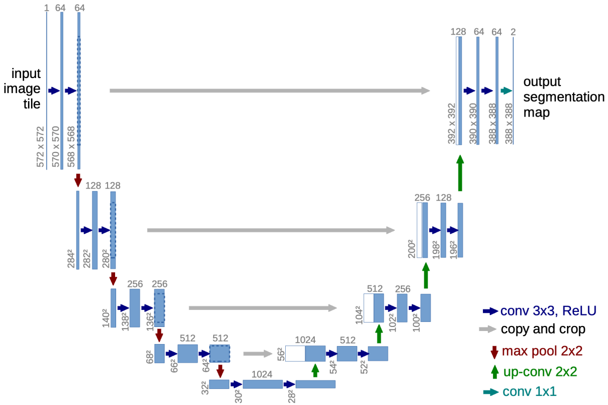
Differentiation under integral

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

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)