Generative Networks; Diffusion Models

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Denoising Diffusion Probabilistic Models

$\mathbf{x}_0 \sim q(\mathbf{x}_0) \rightarrow$ data

$p_\theta(\mathbf{x}_0) := \int p_\theta(\mathbf{x}_{0:T})\, d\mathbf{x}_{1:T}$

$$p_\theta(\mathbf{x}_{0:T}) := p(\mathbf{x}_T)\prod_{t=1}^{T} p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t) \rightarrow \text{reverse process}$$

$p(\mathbf{x}_T) = \mathcal{N}(\mathbf{x}_T; \mathbf{0}, \mathbf{I})$

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

$\boldsymbol{\Sigma}_\theta(\mathbf{x}_t, t) = \sigma_t^2\mathbf{I} \rightarrow$ untrained time dependent constants

$$\boldsymbol{\mu}_\theta(\mathbf{x}_t, t) = \frac{1}{\sqrt{\alpha_t}}\left(\mathbf{x}_t - \frac{\beta_t}{\sqrt{1-\bar{\alpha}_t}}\boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t)\right)$$

$\boldsymbol{\epsilon}_\theta \rightarrow$ function approximator

Algorithm 2 Sampling

1: $\mathbf{x}_T \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
2: **for** $t = T, \ldots, 1$ **do**
3: $\quad \mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ if $t > 1$, else $\mathbf{z} = \mathbf{0}$
4: $\quad \mathbf{x}_{t-1} = \frac{1}{\sqrt{\alpha_t}}\left(\mathbf{x}_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}}\boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t)\right) + \sigma_t\mathbf{z}$
5: **end for**
6: **return** $\mathbf{x}_0$

$$q(\mathbf{x}_{1:T}|\mathbf{x}_0) := \prod_{t=1}^{T} q(\mathbf{x}_t|\mathbf{x}_{t-1}) \rightarrow \text{approximate posterior (forward process or diffusion process)}$$

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

$\beta_1, \ldots, \beta_T \rightarrow$ variance schedule (hyperparameters)

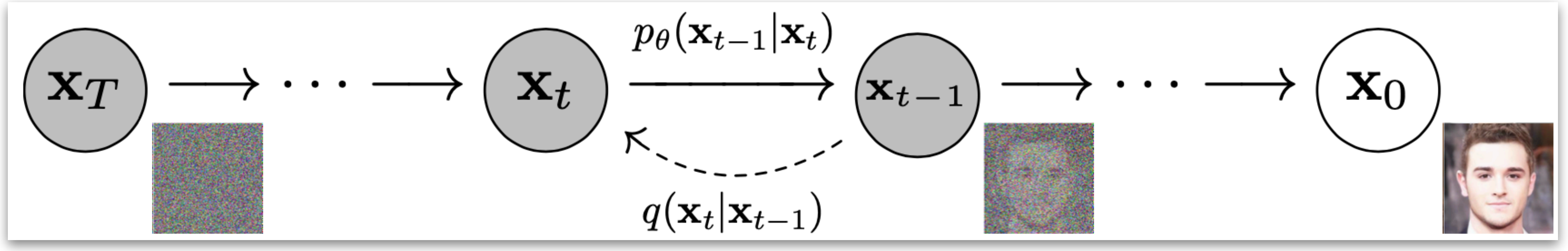
variational bound on negative log likelihood

$$\mathbb{E}\left[-\log p_\theta(\mathbf{x}_0)\right] \le \mathbb{E}_q\left[-\log\frac{p_\theta(\mathbf{x}_{0:T})}{q(\mathbf{x}_{1:T}|\mathbf{x}_0)}\right] = \mathbb{E}_q\left[-\log p(\mathbf{x}_T) - \sum_{t\ge1}\log\frac{p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)}{q(\mathbf{x}_t|\mathbf{x}_{t-1})}\right] =: L$$

$q(\mathbf{x}_t|\mathbf{x}_0) = \mathcal{N}(\mathbf{x}_t; \sqrt{\bar{\alpha}_t}\mathbf{x}_0, (1-\bar{\alpha}_t)\mathbf{I}) \rightarrow$ sampling at an arbitrary timestep

$\alpha_t := 1 - \beta_t$ and $\bar{\alpha}_t := \prod_{s=1}^{t}\alpha_s$

$\sigma_t^2 = \tilde{\beta}_t = \frac{1-\bar{\alpha}_{t-1}}{1-\bar{\alpha}_t}\beta_t$



Rewriting L

$$\mathbb{E}_q\Bigg[\underbrace{D_{\mathrm{KL}}(q(\mathbf{x}_T|\mathbf{x}_0)\,\|\,p(\mathbf{x}_T))}_{L_T} + \sum_{t>1}\underbrace{D_{\mathrm{KL}}(q(\mathbf{x}_{t-1}|\mathbf{x}_t,\mathbf{x}_0)\,\|\,p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t))}_{L_{t-1}}\underbrace{-\log p_\theta(\mathbf{x}_0|\mathbf{x}_1)}_{L_0}\Bigg]$$

L_T is a constant during training and can be ignored

$q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0) = \mathcal{N}(\mathbf{x}_{t-1}; \tilde{\boldsymbol{\mu}}_t(\mathbf{x}_t, \mathbf{x}_0), \tilde{\beta}_t\mathbf{I}) \rightarrow$ forward process posteriors

$$\tilde{\boldsymbol{\mu}}_t(\mathbf{x}_t, \mathbf{x}_0) := \frac{\sqrt{\bar{\alpha}_{t-1}}\beta_t}{1-\bar{\alpha}_t}\mathbf{x}_0 + \frac{\sqrt{\alpha_t}(1-\bar{\alpha}_{t-1})}{1-\bar{\alpha}_t}\mathbf{x}_t$$

$$L_{t-1} = \mathbb{E}_q\left[\frac{1}{2\sigma_t^2}\|\tilde{\boldsymbol{\mu}}_t(\mathbf{x}_t, \mathbf{x}_0) - \boldsymbol{\mu}_\theta(\mathbf{x}_t, t)\|^2\right] + C$$

$$\boxed{L_{\text{simple}}(\theta) := \mathbb{E}_{t,\mathbf{x}_0,\boldsymbol{\epsilon}}\left[\left\|\boldsymbol{\epsilon} - \boldsymbol{\epsilon}_\theta(\sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon}, t)\right\|^2\right]}$$

$L_0 \rightarrow$ see the paper

Algorithm 1 Training

1: **repeat**
2: $\quad \mathbf{x}_0 \sim q(\mathbf{x}_0)$
3: $\quad t \sim \mathrm{Uniform}(\{1, \ldots, T\})$
4: $\quad \boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
5: $\quad$ Take gradient descent step on
$\qquad \nabla_\theta \left\|\boldsymbol{\epsilon} - \boldsymbol{\epsilon}_\theta(\sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon}, t)\right\|^2$
6: **until** converged

Ho, Jonathan, Ajay Jain, and Pieter Abbeel. "Denoising diffusion probabilistic models." *Advances in Neural Information Processing Systems* 33 (2020): 6840-6851.

Questions?