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## 1. 项目进展

### 1.1. 使用神经网络学习生命游戏的演化动力学

### 1.2. 微型抗癌机器人在血液中的动力学

# 2. 文献阅读

## 2.1. Denoising Diffusion Probabilistic Models

Jonathan He, Ajay Jain and Pieter Abbeel | https://arxiv.org/abs/2006.11239

有关加噪过程中的权重推导

$$
\begin{aligned}
\boldsymbol{x}_t &= \sqrt{1-\beta_t}\boldsymbol{x}_{t-1} + \sqrt{\beta_t}\varepsilon_t, & \varepsilon_t \sim N(0,I) \\
&= \sqrt{1-\beta_t}\left[\sqrt{1-\beta_{t-1}}\boldsymbol{x}_{t-2} + \sqrt{\beta_{t-1}}\varepsilon_{t-1}\right] + \sqrt{\beta_t}\varepsilon_t, & \varepsilon_{t-1} \sim N(0,I) \\
&= \sqrt{(1-\beta_t)(1-\beta_{t-1})}\boldsymbol{x}_{t-2} + \sqrt{(1-\beta_t)\beta_{t-1}}\varepsilon_{t-1} + \sqrt{\beta_t}\varepsilon_t \\
&= \sqrt{(1-\beta_t)(1-\beta_{t-1})}\boldsymbol{x}_{t-2} + \sqrt{(1-\beta_t)\beta_{t-1} - (1-\beta_t) + 1}\bar{\varepsilon}_t \\
&= \sqrt{(1-\beta_t)(1-\beta_{t-1})}\boldsymbol{x}_{t-2} + \sqrt{1-(1-\beta_t)(1-\beta_{t-1})}\bar{\varepsilon}_t \\
&\ \ \vdots \\
&= \sqrt{\prod_{s=1}^{t}(1-\beta_s)\boldsymbol{x}_0} + \sqrt{1-\prod_{s=1}^{t}(1-\beta_s)\bar{\varepsilon}_t} = \sqrt{\bar{\alpha}_t}\boldsymbol{x}_0 + \sqrt{1-\bar{\alpha}_t}\bar{\varepsilon}_t
\end{aligned}
$$

负对数似然函数的变分上界

$$
\begin{aligned}
\mathbb{E}_{p_\theta}[-\log p_\theta(\boldsymbol{x}_0)] &= \mathbb{E}_{p_\theta}\left[-\log p_\theta(\boldsymbol{x}_0)\int q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)\mathrm{d}\boldsymbol{x}_{1:T}\right] \\
&= \mathbb{E}_{p_\theta}\left[-\int q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)\log p_\theta(\boldsymbol{x}_0)\mathrm{d}\boldsymbol{x}_{1:T}\right] \\
&= -\mathbb{E}_{p_\theta(\boldsymbol{x}_0),q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}\left[\log\frac{p_\theta(\boldsymbol{x}_0)p_\theta(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}{p_\theta(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}\right] \\
&= -\mathbb{E}_{p_\theta(\boldsymbol{x}_0),q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}\left[\log\frac{p_\theta(\boldsymbol{x}_{0:T})q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}{p_\theta(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}\right] \\
&= -\mathbb{E}_{p_\theta(\boldsymbol{x}_0),q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}\left[\log\frac{p_\theta(\boldsymbol{x}_{0:T})}{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}\right] - \mathbb{E}_{p_\theta(\boldsymbol{x}_0),q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}\left[\log\frac{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}{p_\theta(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}\right] \\
&= -\mathbb{E}_{p_\theta(\boldsymbol{x}_0),q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}\left[\log\frac{p_\theta(\boldsymbol{x}_{0:T})}{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}\right] - \underbrace{\mathbb{E}_{p_\theta(\boldsymbol{x}_0)}[D_{\mathrm{KL}}[q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0) \mid p_\theta(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)]]}_{\geqslant 0} \\
&\leqslant \mathbb{E}_q\left[\log\frac{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}{p_\theta(\boldsymbol{x}_{0:T})}\right] =: L
\end{aligned}
$$

将变分上界写成三项 KL 散度之和

$$
\begin{aligned}
L &= \mathbb{E}_q\left[\log \frac{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}{p_\theta(\boldsymbol{x}_{0:T})}\right] \\
&= \mathbb{E}_q\left[\log \frac{q(\boldsymbol{x}_T|\boldsymbol{x}_0)\prod_{t=2}^T q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t,\boldsymbol{x}_0)}{p_\theta(\boldsymbol{x}_T)\prod_{t=1}^T p_\theta(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t)}\right] \\
&= \mathbb{E}_q\left[\log \frac{q(\boldsymbol{x}_T|\boldsymbol{x}_0)}{p_\theta(\boldsymbol{x}_T)} + \sum_{t=2}^T \frac{q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t,\boldsymbol{x}_0)}{p_\theta(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t)} + \log \frac{1}{p_\theta(\boldsymbol{x}_0|\boldsymbol{x}_1)}\right] \\
&= \mathbb{E}_q\left[D_{\mathrm{KL}}[q(\boldsymbol{x}_T|\boldsymbol{x}_0)|p_\theta(\boldsymbol{x}_T)] + \sum_{t=2}^T D_{\mathrm{KL}}[q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t,\boldsymbol{x}_0)|p_\theta(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t)] - \log p_\theta(\boldsymbol{x}_0|\boldsymbol{x}_1)\right] \\
&= \mathbb{E}_q\left[L_T + \sum_{t=2}^T L_{t-1} - L_0\right].
\end{aligned}
$$

$q(\boldsymbol{x}_{t-1} \mid \boldsymbol{x}_t, \boldsymbol{x}_0)$ 的计算

$$
\begin{aligned}
q(\boldsymbol{x}_{t-1} \mid \boldsymbol{x}_t, \boldsymbol{x}_0) &= q(\boldsymbol{x}_t \mid \boldsymbol{x}_{t-1}, \boldsymbol{x}_0)\frac{q(\boldsymbol{x}_{t-1} \mid \boldsymbol{x}_0)}{q(\boldsymbol{x}_t \mid \boldsymbol{x}_0)} \\
&= q(\boldsymbol{x}_t \mid \boldsymbol{x}_{t-1})\frac{q(\boldsymbol{x}_{t-1} \mid \boldsymbol{x}_0)}{q(\boldsymbol{x}_t \mid \boldsymbol{x}_0)} \\
&\propto \exp\left\{-\frac{1}{2}\left[\frac{\left\|\boldsymbol{x}_t - \sqrt{\alpha_t}\boldsymbol{x}_{t-1}\right\|^2}{\beta_t} + \frac{\left\|\boldsymbol{x}_t - \sqrt{\bar{\alpha}_{t-1}}\boldsymbol{x}_0\right\|^2}{1-\bar{\alpha}_{t-1}} - \frac{\left\|\boldsymbol{x}_t - \sqrt{\alpha_t}\boldsymbol{x}_{t-1}\right\|^2}{1-\bar{\alpha}_t}\right]\right\}
\end{aligned}
$$

参考资料

1.

## 2.2. Sliced Score Matching: A Scalable Approach to Density and Score Estimation

Yang Song, Sahaj Garg, Jiaxin Shi, Stefano Ermon | https://arxiv.org/abs/1905.07088

# 3. 学习进度

## 3.1. 随机过程

首先复习回顾了有关于尾部概率的诸不等式。

## 3.2. 随机微分方程

本周学习了 Itô 积分的链式法则、和乘积法则。

## 3.3. Gray-Scott 系统

参考资料

# 4. 问题解决记录

## 4.1. Typst 相关

## 4.2. 推导相关

# 5. 下周计划

论文阅读

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项目进度

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理论学习

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