

Low-Dose Continuous SDE

Low-Dose continuous SDE, or LDSDE for short, formulates low-dose to high-dose (quantum-noise-wise) breast CT image synthesis problem into standard continuous SDE problem suitable for diffusion network. The complete math derivation and implementation detail can be found below

Sampling

Suppose we have a perfect projection without any noise, \mathbf{x}_{-1} , which is also normalized, we can get initial ($t = 0$) high-dose scan and prior ($t = 1$) low-dose scan using the simple addition of quantum and electronic noise. [All projections are normalized by I_0 , the high dose]

$$\begin{aligned}
 &\text{denote } \sigma_q^2 = \frac{\mathbf{x}_{-1}}{I_0} \\
 &\mathbf{x}_0 \sim \mathcal{N}(\mathbf{x}_{-1}, \sigma_q^2 + \sigma_e^2) \\
 &\mathbf{x}_0 = \mathbf{x}_{-1} + \sqrt{\sigma_q^2 + \sigma_e^2} \epsilon \\
 &\text{And, with } \alpha_t = \frac{I_t}{I_0} \\
 &\mathbf{x}_t \sim \mathcal{N}(\alpha_t \mathbf{x}_{-1}, \alpha_t \sigma_q^2 + \sigma_e^2) \\
 &\mathbf{x}_t = \alpha_t \mathbf{x}_{-1} + \sqrt{\alpha_t \sigma_q^2 + \sigma_e^2} \epsilon
 \end{aligned} \tag{38}$$

Note that the sampling of \mathbf{x}_0 is equivalent if we define $\alpha_0 = 1$, which is true

Continuous Low Dose SDE Derivation

From LDP [Wang 2014], transition between $\mathbf{x}_{t+\Delta t}$ and \mathbf{x}_t can be formulated as follows:

$$\begin{aligned}
 &\text{Define: } \alpha'_t = \frac{\alpha_{t+\Delta t}}{\alpha_t} \\
 &\mathbf{x}_{t+\Delta t} = \alpha'_t \mathbf{x}_t + \sigma_{q, inj} \epsilon + \sigma_{e, inj} \epsilon
 \end{aligned} \tag{39}$$

To match the noise variance for both quantum noise and electronic noise:

$$\begin{aligned}
 \sigma_{q, target}^2 &= \alpha_{t+\Delta t} \sigma_q^2 = \alpha_t'^2 \sigma_{q, x_t}^2 + \sigma_{q, inj}^2 \\
 &= \alpha_t'^2 \alpha_t \sigma_q^2 + \sigma_{q, inj}^2
 \end{aligned} \tag{40}$$

$$\begin{aligned}
\sigma_{e,target}^2 &= \sigma_e^2 = \alpha_t'^2 \sigma_{e,x_t}^2 + \sigma_{e,inj}^2 \\
&= \alpha_t'^2 \sigma_e^2 + \sigma_{e,inj}^2
\end{aligned} \tag{41}$$

The injected noise variance:

$$\sigma_{q,inj}^2 = (\alpha_{t+\Delta t} - \alpha_t'^2 \alpha_t) \sigma_q^2 \tag{42}$$

$$\sigma_{e,inj}^2 = (1 - \alpha_t'^2) \sigma_e^2 \tag{43}$$

Now, we can write the transition from \mathbf{x}_t to $\mathbf{x}_{t+\Delta t}$ as follows:

$$\mathbf{x}_{t+\Delta t} = \alpha_t' \mathbf{x}_t + \sqrt{(\alpha_{t+\Delta t} - \alpha_t'^2 \alpha_t) \sigma_q^2} \boldsymbol{\epsilon} + \sqrt{(1 - \alpha_t'^2) \sigma_e^2} \boldsymbol{\epsilon} \tag{44}$$

Subtract both sides of \mathbf{x}_t

$$\mathbf{x}_{t+\Delta t} - \mathbf{x}_t = (\alpha_t' - 1) \mathbf{x}_t + \sqrt{(\alpha_t' - \alpha_t'^2) \frac{\mathbf{x}_{-1}}{I_0}} \boldsymbol{\epsilon} + \sqrt{(1 - \alpha_t'^2) \sigma_e^2} \boldsymbol{\epsilon} \tag{45}$$

For the \mathbf{x}_t term

$$\begin{aligned}
(\alpha_t' - 1) \mathbf{x}_t &= \frac{\alpha_{t+\Delta t} - \alpha_t}{\alpha_t} \mathbf{x}_t \\
&= \frac{\alpha_{t+\Delta t} - \alpha_t}{\Delta t} \frac{\mathbf{x}_t}{\alpha_t} \Delta t
\end{aligned} \tag{46}$$

Take limit $\lim_{\Delta t \rightarrow 0}$

$$\lim_{\Delta t \rightarrow 0} (\alpha_t' - 1) \mathbf{x}_t = \frac{d\alpha_t}{dt} \frac{\mathbf{x}_t}{\alpha_t} dt \tag{47}$$

For the Quantum noise term

$$\begin{aligned}
\sqrt{(\alpha_{t+\Delta t} - \alpha_t'^2 \alpha_t) \sigma_q^2} \boldsymbol{\epsilon} &= \sqrt{(\alpha_t' \alpha_t - \alpha_t'^2 \alpha_t) \sigma_q^2} \boldsymbol{\epsilon} \\
&= \sqrt{\alpha_t \alpha_t' (1 - \alpha_t') \sigma_q^2} \boldsymbol{\epsilon} \\
&= \sqrt{\alpha_t} \sqrt{\alpha_t' (1 - \alpha_t') \sigma_q^2} \boldsymbol{\epsilon}
\end{aligned} \tag{48}$$

$$\begin{aligned}
\sqrt{\alpha_t} \sqrt{\alpha_t' (1 - \alpha_t')} &= \sqrt{\alpha_t} \sqrt{\alpha_t' \frac{\alpha_t - \alpha_{t+\Delta t}}{\alpha_t}} \\
&= \sqrt{\alpha_t} \sqrt{\frac{\alpha_t'}{\alpha_t} \frac{\alpha_t - \alpha_{t+\Delta t}}{\Delta t} \Delta t} \\
&= \sqrt{\alpha_t} \sqrt{\frac{\alpha_{t+\Delta t}}{\alpha_t^2}} \sqrt{\frac{\alpha_t - \alpha_{t+\Delta t}}{\Delta t}} \sqrt{\Delta t} \\
&= \sqrt{\frac{\alpha_{t+\Delta t}}{\alpha_t}} \sqrt{\frac{\alpha_t - \alpha_{t+\Delta t}}{\Delta t}} \sqrt{\Delta t}
\end{aligned} \tag{49}$$

$$\begin{aligned}
\sqrt{(\alpha_{t+\Delta t} - \alpha_t'^2 \alpha_t) \sigma_q^2} \epsilon &= \sqrt{\frac{\alpha_{t+\Delta t}}{\alpha_t}} \sqrt{\frac{\alpha_t - \alpha_{t+\Delta t}}{\Delta t}} \sqrt{\Delta t} \sqrt{\sigma_q^2} \epsilon \\
&= \sqrt{\frac{\alpha_{t+\Delta t}}{\alpha_t}} \sigma_q \sqrt{\frac{\alpha_t - \alpha_{t+\Delta t}}{\Delta t}} \sqrt{\Delta t} \epsilon
\end{aligned} \tag{50}$$

For the Electronic noise term

$$\sqrt{(1 - \alpha_t'^2) \sigma_e} \epsilon = \sqrt{(1 + \alpha_t')(1 - \alpha_t')} \sigma_e \epsilon \tag{51}$$

$$\begin{aligned}
\sqrt{(1 + \alpha_t')(1 - \alpha_t')} &= \sqrt{(1 + \alpha_t') \frac{\alpha_t - \alpha_{t+\Delta t}}{\alpha_t}} \\
&= \sqrt{\frac{(1 + \alpha_t')}{\alpha_t} \frac{\alpha_t - \alpha_{t+\Delta t}}{\Delta t} \Delta t} \\
&= \sqrt{\frac{\alpha_t + \alpha_{t+\Delta t}}{\alpha_t^2}} \sqrt{\frac{\alpha_t - \alpha_{t+\Delta t}}{\Delta t}} \sqrt{\Delta t}
\end{aligned} \tag{52}$$

$$\begin{aligned}
\sqrt{(1 - \alpha_t'^2) \sigma_e} \epsilon &= \sqrt{\frac{\alpha_t + \alpha_{t+\Delta t}}{\alpha_t^2}} \sqrt{\frac{\alpha_t - \alpha_{t+\Delta t}}{\Delta t}} \sqrt{\Delta t} \sigma_e \epsilon \\
&= \sqrt{\frac{\alpha_t + \alpha_{t+\Delta t}}{\alpha_t^2}} \sigma_e \sqrt{\frac{\alpha_t - \alpha_{t+\Delta t}}{\Delta t}} \sqrt{\Delta t} \epsilon
\end{aligned} \tag{53}$$

Adding equation (13) and (16) together:

$$\left(\sqrt{\frac{\alpha_{t+\Delta t}}{\alpha_t}} \sigma_q + \sqrt{\frac{\alpha_t + \alpha_{t+\Delta t}}{\alpha_t^2}} \sigma_e \right) \sqrt{\frac{\alpha_t - \alpha_{t+\Delta t}}{\Delta t}} \sqrt{\Delta t} \epsilon \tag{54}$$

Then take $\lim_{\Delta t \rightarrow 0}$:

Using Taylor expansion $\lim_{a \rightarrow 0} \frac{f(x+a)}{f(x)} = 1$ and $\lim_{a \rightarrow 0} \frac{f(x+a) - f(x)}{a} = f'(x)$

$$\left(\sigma_q + \sqrt{\frac{2}{\alpha_t}} \sigma_e \right) \sqrt{-\frac{d\alpha_t}{dt}} \sqrt{dt} \epsilon = \left(\sqrt{\alpha_t} \sigma_q + \sqrt{2} \sigma_e \right) \sqrt{-\frac{1}{\alpha_t} \frac{d\alpha_t}{dt}} \sqrt{dt} \epsilon \tag{55}$$

Now, with $\lim_{\Delta t \rightarrow 0} \mathbf{x}_{t+\Delta t} - \mathbf{x}_t = d\mathbf{x}$, the whole SDE becomes:

$$\begin{aligned}
d\mathbf{x} &= \frac{d\alpha_t}{dt} \frac{\mathbf{x}_t}{\alpha_t} dt + \left(\sqrt{\alpha_t} \sigma_q + \sqrt{2} \sigma_e \right) \sqrt{-\frac{1}{\alpha_t} \frac{d\alpha_t}{dt}} \sqrt{dt} \epsilon \\
&= \frac{A(t)}{\alpha(t)} \mathbf{x}_t dt + \left(\sqrt{\alpha_t} \sigma_q + \sqrt{2} \sigma_e \right) \sqrt{-\frac{A(t)}{\alpha(t)}} d\mathbf{w} \\
&= D(t) \mathbf{x}_t dt + \left(\sqrt{\alpha_t} \sigma_q + \sqrt{2} \sigma_e \right) \sqrt{-D(t)} d\mathbf{w}
\end{aligned} \tag{56}$$

Where we define

$$\text{Tube Output Scaling Factor: } \alpha(t) \equiv \alpha_t = \frac{I_t}{I_0} \quad (57)$$

$$A(t) = \frac{d\alpha(t)}{dt} \quad (58)$$

$$\text{Dose Scheduling: } D(t) = \frac{A(t)}{\alpha(t)} \quad (59)$$

$$d\mathbf{w} = \sqrt{dt}\epsilon \quad (60)$$

The final standard SDE from

$$d\mathbf{x} = \mathbf{f}(\mathbf{x}, t)dt + \mathbf{g}(t)d\mathbf{w} \quad (61)$$

Where

$$\mathbf{f}(\mathbf{x}, t) = D(t)\mathbf{x}_t \quad (62)$$

$$\mathbf{g}(t) = \left(\sqrt{\alpha_t}\sigma_q + \sqrt{2}\sigma_e \right) \sqrt{-D(t)} \quad (63)$$

Reverse Low-Dose SDE

Follow the similar derivation in Fourier Diffusion SDE [Tivnan, 2023]

Reverse SDE

$$d\mathbf{x} = [\mathbf{f}(\mathbf{x}, t) - \mathbf{g}^2(t)\nabla_{\mathbf{x}_t} \log p(\mathbf{x}_t|\mathbf{x}_{-1})]dt + \mathbf{g}(t)d\mathbf{w} \quad (64)$$

The main point is then to approximate the score function $\nabla_{\mathbf{x}_t} \log p(\mathbf{x}_t|\mathbf{x}_{-1})$ with neural network $\mathbf{s}_\theta(\mathbf{x}_t, t)$. However, the important thing is to get the ground truth score function.

Recall that

$$\begin{aligned} \mathbf{x}_t &= \alpha_t \mathbf{x}_{-1} + \sqrt{\alpha_t \sigma_q^2 + \sigma_e^2} \epsilon \\ \mathbf{x}_t &\sim \mathcal{N}(\alpha_t \mathbf{x}_{-1}, \alpha_t \sigma_q^2 + \sigma_e^2) \end{aligned} \quad (65)$$

with $\sigma = \sqrt{\alpha_t \sigma_q^2 + \sigma_e^2}$, score function is

$$\begin{aligned} \mathbf{u}(\mathbf{x}_t) &= \nabla_{\mathbf{x}_t} \log p(\mathbf{x}_t|\mathbf{x}_{-1}) = \frac{1}{p(\mathbf{x}_t|\mathbf{x}_{-1})} \frac{\partial p(\mathbf{x}_t|\mathbf{x}_{-1})}{\partial \mathbf{x}_t} \\ p(\mathbf{x}_t|\mathbf{x}_{-1}) &= \frac{1}{\sigma \sqrt{2\pi}} e^{-\frac{1}{2} \left(\frac{\mathbf{x}_t - \alpha_t \mathbf{x}_{-1}}{\sigma} \right)^2} \\ \frac{\partial p(\mathbf{x}_t|\mathbf{x}_{-1})}{\partial \mathbf{x}_t} &= \frac{-(\mathbf{x}_t - \alpha_t \mathbf{x}_{-1})}{\sigma^2} p(\mathbf{x}_t|\mathbf{x}_{-1}) \\ \nabla_{\mathbf{x}_t} \log p(\mathbf{x}_t|\mathbf{x}_{-1}) &= \mathbf{u}(\mathbf{x}_t) = \frac{-(\mathbf{x}_t - \alpha_t \mathbf{x}_{-1})}{\sigma^2} \end{aligned} \quad (66)$$

Then, the loss function is

$$\begin{aligned}\mathcal{L}(\theta; \sigma) &= \left| \mathbf{s}_\theta(\mathbf{x}_t, t) + \frac{(\mathbf{x}_t - \alpha_t \mathbf{x}_{-1})}{\sigma^2} \right|^2 \\ \mathcal{L}(\theta; \sigma) &= \left| \mathbf{s}_\theta(\mathbf{x}_t, t) + \frac{(\mathbf{x}_t - \alpha_t \mathbf{x}_{-1})}{\alpha_t \sigma_q^2 + \sigma_e^2} \right|^2\end{aligned}\tag{67}$$

However, the major problem is that even after the network is fully learned, we still have \mathbf{x}_{-1} term in $\mathbf{g}(t)$ in order to go the reverse SDE. The solution to this is provided below

Improved Loss And Removal of Need for \mathbf{x}_{-1}

Notice that if we expand the score function

$$\nabla_{\mathbf{x}_t} \log p(\mathbf{x}_t | \mathbf{x}_{-1}) = \frac{-(\mathbf{x}_t - \alpha_t \mathbf{x}_{-1})}{\sigma^2} = \frac{-(\sqrt{\alpha_t \sigma_q^2 + \sigma_e^2} \epsilon)}{(\sqrt{\alpha_t \sigma_q^2 + \sigma_e^2})^2} = \frac{-\epsilon}{\sqrt{\alpha_t \sigma_q^2 + \sigma_e^2}} = \frac{-\epsilon}{\sigma}\tag{68}$$

Which means, we can train the network to predict $-\epsilon$ instead, we can also use the prior image \mathbf{x}_T as conditioning

$$\mathcal{L}(\theta; \sigma) = |\mathbf{s}_\theta(\mathbf{x}_t, \mathbf{x}_T, t) + \epsilon|^2\tag{69}$$

Once fully trained, we can use the network as follows:

using \mathbf{x}_T as approximation of \mathbf{x}_{-1}

$$\begin{aligned}\mathbf{x}_{-1} &\approx \mathbf{x}_T / \alpha_T \\ \sigma_q^2 &= \frac{\mathbf{x}_{-1}}{I_0} \\ \sigma &= \sqrt{\alpha_t \sigma_q^2 + \sigma_e^2} \\ \mathbf{f}(\mathbf{x}, t) &= D(t) \mathbf{x}_t \\ \mathbf{g}(t) &= \left(\sqrt{\alpha_t} \sigma_q + \sqrt{2} \sigma_e \right) \sqrt{-D(t)} \\ \nabla_{\mathbf{x}_t} \log p(\mathbf{x}_t | \mathbf{x}_{-1}) &= \frac{-\epsilon}{\sigma} \approx \frac{\mathbf{s}_\theta(\mathbf{x}_t, \mathbf{x}_T, t)}{\sigma} \\ d\mathbf{x} &= [\mathbf{f}(\mathbf{x}, t) - \mathbf{g}^2(t) \nabla_{\mathbf{x}_t} \log p(\mathbf{x}_t | \mathbf{x}_{-1})] dt + \mathbf{g}(t) d\mathbf{w}\end{aligned}\tag{70}$$

Dose Scheduling (Linear)

To obtain the dose scheduling term $D(t)$, we start with

$$\begin{aligned}I_0 &: \text{Initial High Dose} \\ I_{min} &: \text{Target Low Dose} \\ t &\in [0, 1] \\ I_0 &\rightarrow I_{min} \text{ is linear of } t \\ I(t) &= (I_{min} - I_0)t + I_0\end{aligned}\tag{71}$$

Recall that by definition

$$\begin{aligned}\alpha(t) &= \frac{I(t)}{I_0} \\ \alpha(t) &= \frac{(I_{min} - I_0)t + I_0}{I_0} = 1 + \left(\frac{I_{min}}{I_0} - 1 \right)t\end{aligned}\tag{72}$$

Therefore, by definition of $A(t)$

$$A(t) = \frac{d\alpha(t)}{dt} = \left(\frac{I_{min}}{I_0} - 1 \right)\tag{73}$$

Subsequently,

$$D(t) = \frac{A(t)}{\alpha(t)} = \frac{\frac{I_{min}}{I_0} - 1}{1 + \left(\frac{I_{min}}{I_0} - 1 \right)t} = \frac{I_{min} - I_0}{I_0 + (I_{min} - I_0)t}\tag{74}$$