

# A Note on Diffusion NFT

Qiang Liu

DiffusionNFT [1] can be viewed as learning a reward-tilted update around a pretrained velocity field. Let  $v_t^0(x) = \mathbb{E}[X_1 - X_0 \mid X_t = x]$  be a pretrained velocity field trained on pairs  $(X_0, X_1) \sim \pi_0 \times \pi_1$ , with the standard linear interpolation  $X_t = (1-t)X_0 + tX_1$ . Assume we have an additional reward  $r(x) \geq 0$ , and we are interested in steering  $v_t^0$  to reflect the preference of  $r$ .

DiffusionNFT introduces a learnable field  $\mu_t(\cdot)$  and forms two symmetric perturbations around  $v_t^0$ :

$$\mu_t^+(x) := v_t^0(x) + \beta(\mu_t(x) - v_t^0(x)), \quad \mu_t^-(x) := v_t^0(x) - \beta(\mu_t(x) - v_t^0(x)),$$

where  $\beta > 0$ . Then it fits  $\mu$  by a reward-weighted regression:

$$L(\mu) := \mathbb{E} \left[ r(X_1) \|\mu_t^+(X_t) - (X_1 - X_0)\|^2 + (1 - r(X_1)) \|\mu_t^-(X_t) - (X_1 - X_0)\|^2 \right].$$

Here the expectation is over  $(X_0, X_1) \sim \gamma$  (a coupling of  $\pi_0$  and  $\pi_1$ ) and over  $t \sim p(t)$  supported on  $[0, 1]$ , with  $X_t = (1-t)X_0 + tX_1$ . Intuitively, high-reward samples pull the policy toward  $v_t^+$ , while low-reward samples pull it toward  $v_t^-$ .

Let  $v_t^*$  be the minimum of  $L(\mu)$ , and  $v_t^{*\pm}$  the corresponding perturbations. After training, we may sample from either  $v_t^*$  or the positive perturbation  $v_t^{*+}$ .

What distribution does DiffusionNFT sample from? There is generally no closed-form expression for the resulting distributions, and the learned velocity field does not correspond exactly to the rectified-flow (RF) field of an explicit tilted target distribution.

But here we give two interpretations.

**DiffusionNFT as Extrapolation** We can rewrite DiffusionNFT into

$$v_t^*(x) = v_t^0(x) + \frac{2}{\beta} \hat{m}_t^r(x)(\hat{v}_t^r(x) - v_t^0(x)), \quad v_t^{*\pm}(x) = v_t^0(x) \pm 2\hat{m}_t^r(x)(\hat{v}_t^r(x) - v_t^0(x)),$$

where

$$\hat{v}_t^r(x) = \frac{\mathbb{E}[r(X_1)(X_1 - X_0) \mid X_t = x]}{\mathbb{E}[r(X_1) \mid X_t = x]}, \quad \hat{m}_t^r(x) = \mathbb{E}[r(X_1) \mid X_t = x].$$

Here  $\hat{v}_t^r$  is the rectified flow vector field of the reward-tilted distribution: This is reweighting by  $r(x)$  (not exponential tilting).

$$\hat{\pi}_1(x) = \frac{\pi_1(x)r(x)}{Z}, \quad Z = \int \pi_1(x)r(x)dx.$$

Here,  $v_t^*$  and  $v_t^{*+}$  are extrapolation of the original  $v_t^0$  and the  $\hat{v}_t^r$ , with a magnitude weighted by  $\hat{m}_t^r$ . Note that  $\hat{m}_t^r(x) = \mathbb{E}[r(X_1) \mid X_t = x]$  is the conditional expected reward at the bridge state  $X_t = x$ .

**DiffusionNFT as Taylor Approximation** Alternatively, let us consider the exponential-tilted distribution:

$$\tilde{\pi}_1^\alpha(x) = \frac{\pi_1(x) \exp(\alpha r(x))}{\tilde{Z}_\alpha}, \quad \tilde{Z}_\alpha = \int \pi_1(x) \exp(\alpha r(x)) dx.$$

Here  $\alpha \in \mathbb{R}$  is a scalar inverse temperature; as  $\alpha$  changes from 0 to 1, the distribution  $\tilde{\pi}_1^\alpha$  changes from  $\tilde{\pi}_1^0 = \pi_1$  to  $\tilde{\pi}_1^1$ . This exponential tilting differs from the  $r$ -reweighted distribution  $\hat{\pi}_1 \propto \pi_1 r$ ; we connect them via a first-order linearization at  $\alpha = 0$ .

It would be interesting to estimate the derivative of  $\tilde{v}_t^\alpha$  w.r.t.  $\alpha$ , where  $\tilde{v}_t^\alpha$  denotes the RF velocity field associated with  $\tilde{\pi}_1^\alpha$ . We can show that

$$\begin{aligned} \partial_\alpha \tilde{v}_t^\alpha(x) |_{\alpha=0} &= \text{cov}(X_1 - X_0, r(X_1) | X_t = x) \\ &= \hat{m}_t^r(x)(\hat{v}_t^r(x) - v_t^0(x)). \end{aligned}$$

Hence,  $v_t^*$  and  $v_t^{*\pm}$  can be viewed as Taylor approximating  $\tilde{v}_t^\alpha$  from  $\alpha = 0$ :

$$\begin{aligned} v_t^*(x) &= v_t^0(x) + \frac{2}{\beta} \partial_\alpha \tilde{v}_t^\alpha(x) |_{\alpha=0} \approx \tilde{v}_t^{2/\beta}(x), \\ v_t^{*\pm}(x) &= v_t^0(x) \pm 2 \partial_\alpha \tilde{v}_t^\alpha(x) |_{\alpha=0} \approx \tilde{v}_t^{\pm 2}(x). \end{aligned}$$

## 1 Proofs

### 1.1 Formula of DiffusionNFT Solution

**Theorem 1.1.** *Following the set up above, and assume  $v_t^0(x) = \mathbb{E}[X_1 - X_0 | X_t = x]$ . We have the following equivalent expressions of  $v_t^*(x)$  from DiffusionNFT:*

$$\begin{aligned} v_t^*(x) &= v_t^0(x) + \frac{2}{\beta} (\hat{m}_t^r(x)(\hat{v}_t^r(x) - v_t^0(x))) \\ &= v_t^0(x) + \frac{2}{\beta} \text{cov}(2r(X_1) - 1, X_1 - X_0 | X_t = x) \\ &= v_t^0(x) + \frac{2}{\beta} \partial_\alpha \tilde{v}_t^\alpha(x) |_{\alpha=0}, \end{aligned}$$

Similar expression holds for  $v_t^{*\pm}(x)$  if  $\frac{2}{\beta}$  is replaced by  $\pm 2$ .

*Proof.* Using Lemma 1.2 below, we can rewrite the loss  $L(\mu)$  as:

$$L(\mu) = \mathbb{E}[\|\beta \mu_t(X_t) - \beta v_t^0(X_t) - (2r(X_1) - 1)(X_1 - X_0 - v_t^0(X_t))\|^2] + \text{const.}$$

Hence, the optimal solution is

$$v_t^*(x) = v_t^0(x) + \frac{1}{\beta} \mathbb{E}[(2r(X_1) - 1)(X_1 - X_0 - v_t^0(X_t)) | X_t = x].$$

Plugging  $v_t^0(x) = \mathbb{E}[X_1 - X_0 | X_t = x]$  into the above yields

$$\begin{aligned} v_t^*(x) &= v_t^0(x) + \frac{1}{\beta} \mathbb{E}[(2r(X_1) - 1)(X_1 - X_0 - \mathbb{E}[X_1 - X_0 | X_t = x]) | X_t = x] \\ &= v_t^0(x) + \frac{2}{\beta} (\mathbb{E}[r(X_1)(X_1 - X_0) | X_t = x] - \mathbb{E}[r(X_1) | X_t = x] \mathbb{E}[X_1 - X_0 | X_t = x]) \\ &= v_t^0(x) + \frac{2}{\beta} (\hat{m}_t^r(x)(\hat{v}_t^r(x) - v_t^0(x))) \\ &= v_t^0(x) + \frac{2}{\beta} \text{cov}(2r(X_1) - 1, X_1 - X_0 | X_t = x) \\ &= v_t^0(x) + \frac{2}{\beta} \partial_\alpha \tilde{v}_t^\alpha(x)|_{\alpha=0}, \end{aligned}$$

where we used Theorem 1.3.

Plugging  $v_t^{*\pm}(x) = v_t^0(x) \pm 2\partial_\alpha \tilde{v}_t^\alpha(x)|_{\alpha=0}$  into the above yields the formula for  $v_t^{*\pm}(x)$ .

□

**Lemma 1.2.** Let  $\mu^\pm = \mu \pm \beta(\mu - v)$ , and

$$\ell(\mu) = r \|\mu^+ - y\|^2 + (1 - r) \|\mu^- - y\|^2,$$

where  $\mu, v, y \in \mathbb{R}^d$ ,  $r \in \mathbb{R}$ . Then, we can rewrite  $\ell(\mu)$  into

$$\ell(\mu) = \|\beta\mu - \beta v - (2r - 1)(y - v)\|^2 + \text{const},$$

where *const* is a term that does not depend on  $\mu$ .

Hence, the minimum of  $\ell(\mu)$  is achieved at

$$\mu^* = v + \frac{1}{\beta}(2r - 1)(y - v).$$

*Proof.* Expand the loss:

$$\begin{aligned} \ell(\mu) &= r \|\mu^+ - y\|^2 + (1 - r) \|\mu^- - y\|^2 \\ &= r \|(1 - \beta)v + \beta\mu - y\|^2 + (1 - r) \|(1 + \beta)v - \beta\mu - y\|^2 \\ &= \beta^2 \mu^2 + 2\beta\mu(r(1 - \beta)v - ry + (1 - r)y - (1 - r)(1 + \beta)v) + \text{const} \\ &= \beta^2 \mu^2 + 2\beta\mu(-\beta v + (1 - 2r)(y - v)) + \text{const} \\ &= \|\beta\mu - \beta v - (2r - 1)(y - v)\|^2 + \text{const}. \end{aligned}$$

Hence, the minimum is achieved at

$$\mu^* = \frac{1}{\beta}(\beta v - (1 - 2r)(y - v)) = v + \frac{1}{\beta}(2r - 1)(y - v).$$

□

## 1.2 Derivative of RF Velocity Field

We give the formula for the derivative  $\partial_\alpha v_t^\alpha(x)$  of the RF velocity field  $v_t^\alpha(x)$  w.r.t. a general parameter  $\alpha$  of the target distribution.

Let  $X_0 \sim \pi_0$  be a base distribution and  $X_1 \sim \pi_1^\alpha$  be a target distribution depending on a scalar parameter  $\alpha$ . Define the linear interpolation  $X_t = (1-t)X_0 + tX_1$ , and the rectified flow velocity field

$$v_t^\alpha(x) = \mathbb{E}_{(X_0, X_1) \sim \gamma^\alpha} [X_1 - X_0 \mid X_t = x], \quad t \in [0, 1],$$

where  $(X_0, X_1)$  is a coupling of  $\pi_0$  and  $\pi_1^\alpha$  with a joint density  $\gamma^\alpha(x_0, x_1)$  that is differentiable in  $\alpha$ . Typically,  $(X_0, X_1)$  is the independent coupling  $\gamma(x_0, x_1) = \pi_0(x_0) \times \pi_1^\alpha(x_1)$ .

**Theorem 1.3** (Derivative of the RF velocity via conditional score). *Assume  $\log \gamma^\alpha$  is differentiable in  $\alpha$  and differentiation can be exchanged with integration and conditioning. Then*

$$\partial_\alpha v_t^\alpha(x) = \text{Cov}_{\gamma^\alpha} \left( X_1 - X_0, \partial_\alpha \log \gamma^\alpha(X_0, X_1) \mid X_t = x \right).$$

In particular, in the case of independent coupling  $\gamma^\alpha(x_0, x_1) = \pi_0(x_0) \pi_1^\alpha(x_1)$ , we have

$$\partial_\alpha v_t^\alpha(x) = \text{Cov}_{\gamma^\alpha} \left( X_1 - X_0, \partial_\alpha \log \pi_1^\alpha(X_1) \mid X_t = x \right).$$

Further, for the exponential-tilted family  $\tilde{\pi}_1^\alpha(x) = \frac{\pi_1(x) \exp(\alpha r(x))}{\tilde{Z}_\alpha}$  with  $\tilde{Z}_\alpha = \int \pi_1(x) \exp(\alpha r(x)) dx$ , and the corresponding RF velocity field  $\tilde{v}_t^\alpha$  under  $\tilde{\gamma}^\alpha(x_0, x_1) = \pi_0(x_0) \tilde{\pi}_1^\alpha(x_1)$ , we have

$$\partial_\alpha \tilde{v}_t^\alpha(x) = \text{Cov}_{\tilde{\gamma}^\alpha} \left( X_1 - X_0, r(X_1) \mid X_t = x \right).$$

*Proof.* Fix  $t \in [0, 1]$  and  $x$ . Note

$$v_t^\alpha(x) = \frac{m_t^\alpha(x) - x}{1 - t}, \quad m_t^\alpha(x) = \mathbb{E}[X_1 \mid X_t = x].$$

So it suffices to differentiate  $m_t^\alpha(x)$ .

Note that

$$m_t^\alpha(x) = \int x_1 p_t^\alpha(x_1 \mid x) dx_1,$$

where  $p_t^\alpha(x_1 \mid x)$  denotes the conditional density of  $X_1$  given  $X_t = x$ , defined in terms of the joint density  $\gamma^\alpha(x_0, x_1)$ . By applying the change of variables  $X_0 = \frac{x - tx_1}{1-t}$ , we obtain

$$p_t^\alpha(x_1 \mid x) = \frac{\gamma^\alpha\left(\frac{x - tx_1}{1-t}, x_1\right) \cdot \frac{1}{1-t}}{\rho_t^\alpha(x)}, \quad \rho_t^\alpha(x) = \int \gamma^\alpha\left(\frac{x - tx_1}{1-t}, x_1\right) \cdot \frac{1}{1-t} dx_1.$$

Differentiate under the integral:

$$\partial_\alpha m_t^\alpha(x) = \int x_1 \partial_\alpha p_t^\alpha(x_1 \mid x) dx_1 = \int x_1 p_t^\alpha(x_1 \mid x) \partial_\alpha \log p_t^\alpha(x_1 \mid x) dx_1 = \mathbb{E}[X_1 \partial_\alpha \log p_t^\alpha(X_1 \mid x) \mid X_t = x].$$

Now expand the conditional score. Up to an  $\alpha$ -independent constant,

$$\log p_t^\alpha(x_1 \mid x) = \log \gamma^\alpha\left(\frac{x - tx_1}{1-t}, x_1\right) - \log \rho_t^\alpha(x) + \text{const.}$$

Hence

$$\partial_\alpha \log p_t^\alpha(x_1 \mid x) = \partial_\alpha \log \gamma^\alpha\left(\frac{x - tx_1}{1 - t}, x_1\right) - \partial_\alpha \log \rho_t^\alpha(x).$$

Using the Fisher identity for the marginal  $\rho_t^\alpha(x)$ ,

$$\partial_\alpha \log \rho_t^\alpha(x) = \mathbb{E}\left[\partial_\alpha \log \gamma^\alpha(X_0, X_1) \mid X_t = x\right].$$

So

$$\partial_\alpha \log p_t^\alpha(X_1 \mid x) = \partial_\alpha \log \gamma^\alpha(X_0, X_1) - \mathbb{E}\left[\partial_\alpha \log \gamma^\alpha(X_0, X_1) \mid X_t = x\right].$$

Plugging back,

$$\begin{aligned} \partial_\alpha m_t^\alpha(x) &= \mathbb{E}\left[X_1 \left( \partial_\alpha \log \gamma^\alpha(X_0, X_1) - \mathbb{E}[\partial_\alpha \log \gamma^\alpha(X_0, X_1) \mid X_t = x] \right) \mid X_t = x\right] \\ &= \text{Cov}\left(X_1, \partial_\alpha \log \gamma^\alpha(X_0, X_1) \mid X_t = x\right). \end{aligned}$$

Hence,

$$\begin{aligned} \partial_\alpha v_t^\alpha(x) &= \frac{1}{1-t} \partial_\alpha m_t^\alpha(x) \\ &= \frac{1}{1-t} \text{Cov}\left(X_1, \partial_\alpha \log \gamma^\alpha(X_0, X_1) \mid X_t = x\right) \\ &= \text{Cov}\left(\frac{X_1 - x}{1-t}, \partial_\alpha \log \gamma^\alpha(X_0, X_1) \mid X_t = x\right) \\ &= \text{Cov}\left(X_1 - X_0, \partial_\alpha \log \gamma^\alpha(X_0, X_1) \mid X_t = x\right), \end{aligned}$$

where we note that  $X_1 - X_0 = \frac{X_1 - x}{1-t}$  conditioned on  $X_t = x$ .

Finally, for the exponential-tilted family  $\tilde{\pi}_1^\alpha$ , we have

$$\partial_\alpha \log \tilde{\pi}_1^\alpha(X_1) = r(X_1) - \partial_\alpha \log \tilde{Z}_\alpha.$$

Hence,

$$\begin{aligned} \partial_\alpha \tilde{v}_t^\alpha(x) &= \frac{1}{1-t} \text{Cov}\left(X_1, r(X_1) - \partial_\alpha \log \tilde{Z}_\alpha \mid X_t = x\right) \\ &= \text{Cov}\left(X_1 - X_0, r(X_1) \mid X_t = x\right), \end{aligned}$$

where  $\partial_\alpha \log \tilde{Z}_\alpha$  is dropped as it is a deterministic constant and does not influence the conditional covariance.  $\square$

## References

- [1] Zheng, K., Chen, H., Ye, H., Wang, H., Zhang, Q., Jiang, K., Su, H., Ermon, S., Zhu, J., and Liu, M.-Y. (2025). Diffusionnft: Online diffusion reinforcement with forward process. *arXiv preprint*.