

DiffusionNFT as Taylor Approximation

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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 μ by a reward-weighted regression:

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

Here the expectation is over $(X_0, X_1) \sim \gamma$ (a coupling of π_0 and π_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 there are two interpretations.

DiffusionNFT as Extrapolation As show in the paper, 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-weighted distribution:

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

where we reweight the density by $r(x)$ (not exponential tilting that we have below).

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 α 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 $\hat{\pi}_1 \propto \pi_1 r$.

Let \tilde{v}_t^α be the RF velocity field associated with $\tilde{\pi}_1^\alpha$. As shown in Theorem 1.3 below, we can express the derivative of \tilde{v}_t^α w.r.t. α as a conditional covariance:

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

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

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

$$v_t^{\pm}(x) = v_t^0(x) \pm 2 \partial_\alpha \tilde{v}_t^\alpha(x) |_{\alpha=0} \approx \tilde{v}_t^{\pm 2}(x).$$

This perspective suggests a multi step variant of DiffusionNFT: instead of taking a single update based on the linearization at $\alpha = 0$, we can take multiple Euler steps along the α direction, repeatedly re linearizing around the current α , to better track \tilde{v}_t^α for larger values of α .

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:*

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

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

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

where we used Theorem 1.3.

Plugging $v_t^{*\pm}(x) = v_t^0(x) \pm 2\partial_\alpha \tilde{v}_t^\alpha(x) \big|_{\alpha=0}$ 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 μ .

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 α 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 α . 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 π_0 and π_1^α with a joint density $\gamma^\alpha(x_0, x_1)$ that is differentiable in α . 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 α and differentiation can be exchanged with integration and conditioning. Then*

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

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

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

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^α under $\tilde{\gamma}^\alpha(x_0, x_1) = \pi_0(x_0)\tilde{\pi}_1^\alpha(x_1)$, we have

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

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 α -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

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

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

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

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*.