Temporal Difference Flows (Farebrother et al., 2025)

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July 13, 2025

Outline

1. Motivation
2. Flow Matching
3. Application to Reinforcement Learning

Variational inference with normalizing flows (Rezende & Mohamed)

Given data $\mathcal{X} \sim p(\mathbf{x})$. Want to learn $p(\mathbf{x})$.

- Assume there exists some joint $p(\mathbf{x}, \mathbf{z})$, $\mathbf{z} \sim p(\mathbf{z})$ is latent (no samples of $\mathbf{z}$). (we choose $p(\mathbf{z})$ i.e. $\mathcal{N}(0, 1)$).
- Maximize log-likelihood $\log p_\theta(\mathbf{x})$ via ELBO:

$$\log p_\theta(\mathbf{x}) \geq \mathbb{D}_{\mathrm{KL}}[q_\phi(\mathbf{z} \mid \mathbf{x}) \mid\mid p(\mathbf{z})] + \mathbb{E}_q[\log p_\theta(\mathbf{x} \mid \mathbf{z})]. \quad \text{(ELBO)}$$

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Problem. Recall $q_{\phi^*} = \arg\max_\phi \mathrm{ELBO}(\phi) = p_\theta(z \mid x)$.

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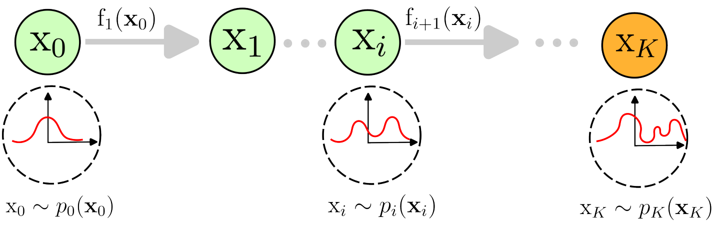
- Rarely the case.

How do we create a more expressive family that we can still optimize?

Given target distribution $p(\mathbf{x})$. Pick some initial distribution p_0, where we can sample $\mathbf{x}_0 \sim p_0$.

Idea. *Learn sequence of functions $f_1, f_2, \ldots, f_K$, such that*

$$(f_K \circ f_{K-1} \cdots \circ f_1)(\mathbf{x}_0) \sim p$$



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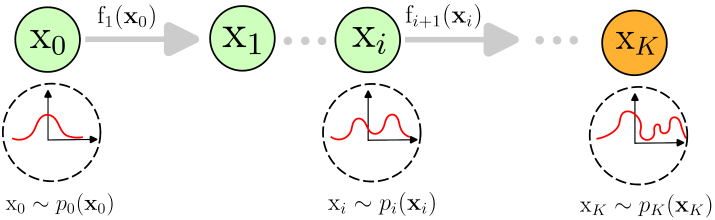
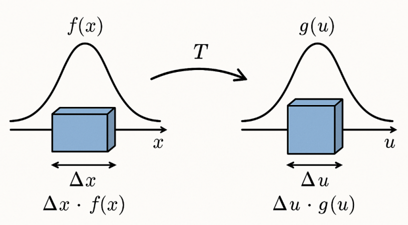


How do we learn such a sequence of functions f_i?

Given **invertible**, **smooth both ways** function $T : \mathbb{R}^d \to \mathbb{R}^d$.

Change of variables theorem. For $X, Y \subset \mathbb{R}^d$, $T : X \to Y$

$$\int_X p_0(\mathbf{x}) d\mathbf{x} = \int_{T^{-1}(Y)} p_0(T^{-1}(\mathbf{y})) \left|\det \frac{\partial T}{\partial y}\right|^{-1} d\mathbf{y}.$$



$$\Rightarrow f_1(\mathbf{x}_0) \sim p_0(\mathbf{x}_0) \left|\det \frac{\partial f_1}{\partial \mathbf{x}}\right|^{-1}$$

$$\Rightarrow \log p_K(\mathbf{x}_k) = \log p_0(\mathbf{x}_0) - \sum_{k=1}^K \left|\det \frac{\partial f_k}{\partial \mathbf{x}_{k-1}}\right|^{-1}$$

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Why not take $K \to \infty$...

Neural Ordinary Differential Equations (Chen et al.)

Replace $\mathbf{x}_{t+1} = f_t(\mathbf{x}_t)$ with the **ODE**

$$\frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t} = f_t(\mathbf{x}_t).$$

Remark. *Instantaneous COV*

$$\frac{\partial \log p_t(\mathbf{x}_t)}{\partial t} = -\operatorname{tr}\left(\frac{df}{d\mathbf{x}_t}\right)$$

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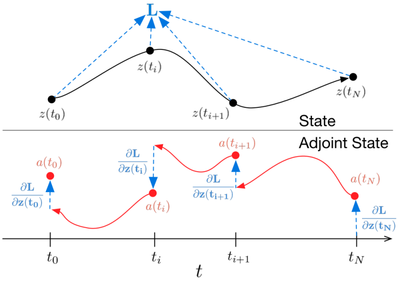
- Requires **exact** ODE solve for unbiased gradient.



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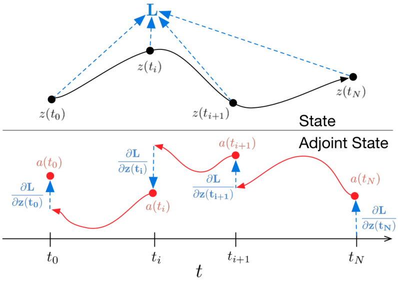
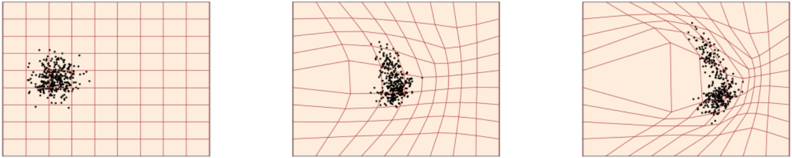


Can we learn f_t without backprop through an ODE?

Disclaimer. f_t will now often be referred to as the *flow*.

Book keeping. We say the *flow* f_t *generates* a probability path p_t if $X_t = f_t(X_0) \sim p_t$. Equivalently,

$$p_t(x) = [f_{t\sharp}p_0](x) \triangleq p_0(f_t^{-1}(y)) \left|\det \partial_y f_t^{-1}(y)\right| .$$



Key Idea. Do **not** learn the *flow* f_t, learn the **velocity** of the flow.

Def. This velocity is a *vector field* $u_t : \mathbb{R}^d \to \mathbb{R}^d$, such that

$$\frac{\mathrm{d}f_t(\mathbf{x})}{\mathrm{d}t} = u_t(f_t(\mathbf{x})).$$

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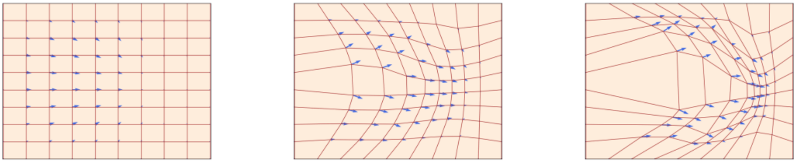
To sample, solve ODE at **sample time** i.e.

$$f_{t+\Delta t}(\mathbf{x}) \approx f_t(\mathbf{x}) + \Delta t \cdot u_t(f_t(\mathbf{x})) \qquad \text{(Euler method)}$$

By uniqueness of ODE, (vector field u_t) $\leftrightarrow$ (flow f_t).



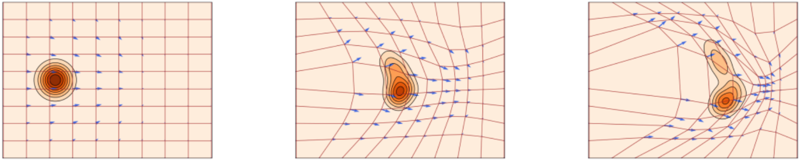
Def. A *vector field* u_t *generates* a probability path p_t if its corresponding flow f_t *generates* p_t.

Thm. A *vector field* u_t *generates* a probability path p_t if and only if it satisfies the *continuity equation*.

Continuity Equation.

$$\frac{\mathrm{d}}{\mathrm{d}t}p_t(x) + \mathrm{div}(p_t u_t)(x) = 0,$$

where $\mathrm{div}(v)(x) = \sum_{i=1}^{d} \partial_{x^i} v^i(x)$, and $v(x) = (v^1(x), \ldots, v^d(x))$.



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Proof: (If people care)

$$\frac{d}{dt}\mathbb{E}f(X_t) = \frac{d}{dt}\int_{\mathbb{R}^d} f(x)p_t(x)dx = \int_{\mathbb{R}^d} f(x)\partial_t p_t(x)dx,$$

$$\begin{aligned} \mathbb{E}\frac{d}{dt}f(X_t) &= \int_{\mathbb{R}^d} \left(\nabla f(x_t)\cdot v_t(x_t)\right) p_t(x_t)dx_t \\ &= 0 - \int_{\mathbb{R}^d} f(x_t)\mathrm{div}(v_t(x_t)p_t(x_t))dx_t \qquad \text{(IBP)} \\ &= \int_{\mathbb{R}^d} -f(x)\mathrm{div}(v_t(x)p_t(x))dx.. \end{aligned}$$

The result follows from fundamental lemma of calculus of variations.

How do we actually learn the vector field u_t?

Flow Model Loss.

$$\mathcal{L}_{\text{FM}}(\theta) = \mathbb{E}_{t,p_t(x)} \|v_t(x;\theta) - u_t(x)\|^2$$

- $p_t : \mathcal{X} \to [0,1]$: probability density path.
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1. How to choose p_t?
2. Given p_t need to solve continuity equation for u_t, which is a **PDE** likely without close-form.

Key Idea. *Given the endpoint X_1, we can easily construct a path between X and X_1.*

Ex: *Consider*

$$f_t(x \mid x_1) = (1-t)x + tx_1$$

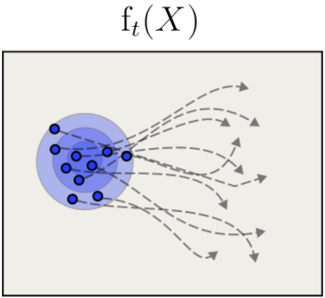

Figure: Without target **how** do we construct p_t, f_t?

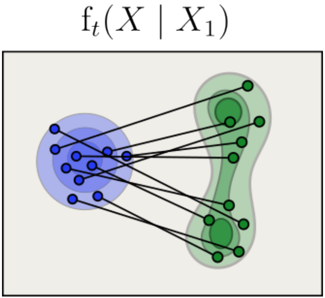

Figure: With target, make f_t **line** to known x_1.

What does the conditional flow being nice have to do with our problem?

Idea 1: Given target data distribution q, approximate q by marginalizing "nice" conditionals by q i.e.

$$p_t(\mathbf{x}) = \int p_t(\mathbf{x} \mid \mathbf{x}_1) q(\mathbf{x}_1) \mathrm{d}\mathbf{x}_1. \qquad \text{(Marginal Density)}$$

For $p_1(\mathbf{x} \mid \mathbf{x}_1) \sim N(x_1, \sigma_1)$, with $\sigma_1 \ll 1$, $p_1(\mathbf{x}) \approx q(\mathbf{x})$.

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Idea 2: Use this to define an approximate vector field

$$u_t(\mathbf{x}) = \int u_t(\mathbf{x} \mid \mathbf{x}_1) \frac{p_t(\mathbf{x} \mid \mathbf{x}_1) q(\mathbf{x}_1)}{p_t(\mathbf{x})} \mathrm{d}\mathbf{x}_1. \quad \text{(Marginal Vector Field)}$$

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Thm. *The marginal vector field u_t generates the marginal probability path p_t.* (Check continuity equation)

Conditional Flow Model Loss.

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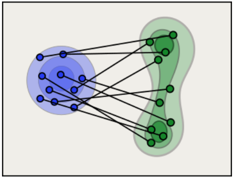
Thm. *Up to a constant independent of θ, $\mathcal{L}_{\text{FM}}(\theta) = \mathcal{L}_{\text{CFM}}(\theta)$. In particular, $\nabla\mathcal{L}_{\text{FM}}(\theta) = \nabla\mathcal{L}_{\text{CFM}}(\theta)$.*

Batch *i*



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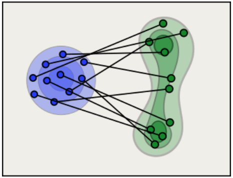
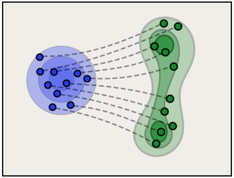


$\mathbb{E}$[**Batch**]



How do we actually use this?

Example: Optimal Transport

For $x \sim \mathcal{N}(0, 1)$,

$$f_t(x) = \mu_t(x_1) + x\sigma_t(x_1) \implies f_t(x) \sim \mathcal{N}(\mu_t(x), \sigma_t(x)).$$

Consider

$$\mu_t = tx_1, \quad \sigma_t(x) = 1 - (1 - \sigma_{\text{min}})t,$$

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Recall

$$\frac{\mathrm{d}}{\mathrm{d}t} f_t(x) = u(f_t(x) \mid x_1) \implies u(x \mid x_1) = \frac{\mathrm{d}}{\mathrm{d}t} f_t(f_t^{-1}(x)).$$

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Diffusion Meets Flow Matching: Two Sides of the Same Coin (Gao et al., 2024)

Recall that instead of an ODE, in diffusion, we have a **SDE**

$$\mathrm{d}\mathbf{x}_t = f_t(\mathbf{x}_t)\mathrm{d}t + \sigma(\mathbf{x}_t)\mathrm{d}B_t.$$

However, for *OU* process, we can actually absorb Brownian motion term and get vector field

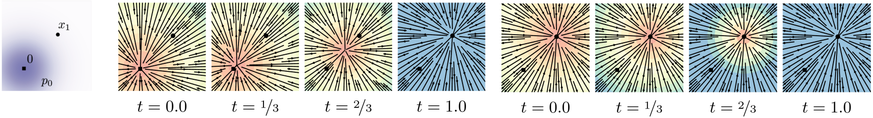
$$u_t(\mathbf{x}_t) = -(\mathbf{x}_t + \nabla \ln p_t(\mathbf{x}_t)).$$

Similarly, learning the score function $\nabla \ln p_t(\mathbf{x}_t)$ can be rewritten as the flow matching objective for certain choices of p_t see (Lipman et al., 2024).

Why Flows?

Anecdotally.

- *The OT path's conditional vector field has constant direction in time and is arguably simpler to fit with a parametric model. (Lipman et al., 2023)*
- *The deterministic nature of ODEs equips flow-matching methods with simpler learning objectives and faster inference speed (Zheng et al., 2025)*



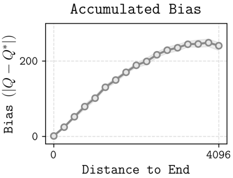
Conditional score

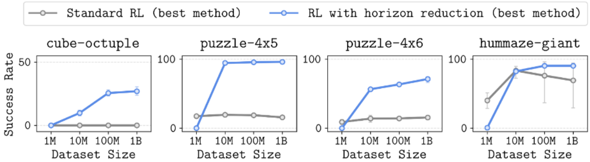
Conditional vector field

Q learning is not yet scalable (Park, 2025)

Long horizon problems are hard.

$$\mathbb{E}_{(s,a,r,s')\sim\mathcal{D}}\left[\left(Q_\theta(s,a) - \underbrace{\left(r + \gamma \max_{a'} Q_{\bar{\theta}}(s',a')\right)}_{\texttt{Biased}}\right)^2\right].$$





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Def. We define the *successor measure* as

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Recall. The *successor measure* is the unique fix point to the *Bellman* equation

$$\begin{aligned} m^\pi(\cdot \mid s, a) &= (\mathcal{T}^\pi m^\pi)(\cdot \mid s, a) \\ &:= (1-\gamma)P(\cdot \mid s, a) + \gamma(P^\pi m^\pi)(\cdot \mid s, a), \end{aligned}$$

where

$$(P^\pi m)(\mathrm{d}x \mid s, a) = \int_{s'} P(\mathrm{d}s' \mid s, a) m(\mathrm{d}x \mid s', \pi(s')).$$

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Can we learn from offline one-step transitions (S, A, S')?

Leverage **recursive** structure of Bellman equation i.e.

$$X_0 \sim p_0$$
$$Z = X_1 \sim (1-\gamma)\delta_{S'} + \gamma\delta_{\tilde{f}_1(X_0 \mid S', \pi(S'))}. \qquad \text{(TD-CFM)}$$

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- With probability $(1-\gamma)$, $X_1 = S'$
- With probability γ, sample from $\tilde{m}^\pi$ by integrating $\tilde{f}_t$.

Can we do better?

Lemma. Let v_t^1 and v_t^2 be vector fields that generate the probability paths p_t^1 and p_t^2, respectively. Then, for any $\gamma \in [0, 1]$, the mixture probability path $p_t = (1-\gamma)p_t^1 + \gamma p_t^2$ is generated by the vector field.

$$v_t := \frac{(1-\gamma)p_t^1 v_t^1 + \gamma p_t^2 v_t^2}{(1-\gamma)p_t^1 + \gamma p_t^2}.$$

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Idea. Learn v_t for $p_t^1 = P(\cdot \mid S,A)$, $p_t^2 = (P^\pi m)(\cdot \mid S,A)$

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How do we get v_t^1 and v_t^2? Conditioning trick **separately!**

Case 1. $\mathcal{L}_{\text{OS}}, S' \sim P(\cdot \mid S, A)$

1. Our dataset (S, A, S') has plenty of samples $S' \sim P(\cdot \mid S, A)$
2. $\vec{u}_t(\cdot \mid Z), \vec{p}_t(\cdot \mid Z)$ can be chosen as done before in **traditional** flow matching

$$\vec{v}_t(x \mid s, a) = \int \vec{u}_t(x \mid x_1) \frac{\vec{p}_t(x \mid x_1) P(\mathrm{d}x_1 \mid s, a)}{\vec{p}_t(x \mid s, a)},$$

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$$\mathcal{L}_{COS}(\theta) = \mathbb{E}_{\rho,t,Z,\vec{X}_t}\left[\left\|\tilde{v}_t(\vec{X}_t \mid S, A; \theta) - \vec{u}_t(\vec{X}_t \mid Z)\right\|^2\right],$$

$$\text{where } Z = X_1 \sim P(\cdot \mid S, A),\ \vec{X}_t \sim \vec{p}_t(\cdot \mid Z)$$

Case 2. $\mathcal{L}_{\text{GHM}}$, $S' \sim (P^\pi m)(\cdot \mid S, A)$

Assume. probability path m_t, such that $m_0 = m_0$ and $m_1 = m_1$.

Recall. We want a *marginal* distribution, such that

$$(P^\pi m_t)(\cdot \mid S, A) \approx \int_{S'} p_t(\cdot \mid S', A') q(S' \mid S, A)$$

for some p_t and q.

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Note. Taking $p_t(\cdot \mid S')$ to be $N(S', \sigma)$ and q to be the desired distribution was just one choice. Need following criteria:

1. $p_t(\cdot \mid S', A')$ can be sampled from,
2. The conditional vector field $u_t(\cdot \mid S', A')$ that generates $p_t(\cdot \mid S', A')$ can be easily computed,
3. Marginal $p_1 \approx P^\pi m_1 = P^\pi m$.

Case 2. $\mathcal{L}_{\text{GHM}}$, $S' \sim (P^\pi m)(\cdot \mid S, A)$

By definition,

$$(P^\pi m)(\cdot \mid S, A) \approx \int_{S'} m(\cdot \mid S', A') P(S' \mid S, A).$$

In particular,

$$(P^\pi m)(\cdot \mid S, A) \approx \int_{S'} m_1(\cdot \mid S', A') P(S' \mid S, A)$$

and m_t satisfies (1),(2),(3)!

Chicken or the egg: How do we compute the vector field that generates m_t?

Case 2. $\mathcal{L}_{\text{GHM}}$, $S' \sim (P^\pi m)(\cdot \mid S, A)$

Lemma. If $v_t^{(n+1)} = \arg\max \mathcal{L}_{\text{OS+GHM}}(v_t^{(n)})$ then $v_t^{(n+1)}$ generates $m_t^{(n+1)}$ and $m_t^{(n+1)} = \mathcal{T}^\pi m_t^{(n)}$.

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Implication. Use $v_t^{(n+1)}(\cdot|S', A')$ in **CFM** loss $\implies$ will converge to vector field that generates $P^\pi m_t$.

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$$\mathcal{L}_{CGHM}(\theta) = \mathbb{E}_{\rho,t,\widehat{X}_t}\left[\left\|\tilde{v}_t(\widehat{X}_t \mid S, A; \theta) - \tilde{v}_t^{(n)}(\widehat{X}_t \mid S', \pi(S')\right\|^2\right],$$

where $X_0 \sim p_0$, $S' \sim P(\cdot \mid S, A)$, $\widehat{X}_t = \widetilde{f}_t^{(n)}(X_0 \mid S', \pi(S'))$, Now we just combine the **objectives**!!

$$\mathcal{L}_{COS}(\theta) = \mathbb{E}_{\rho,t,Z,\vec{X}_t}\left[\left\|\tilde{v}_t(\vec{X}_t \mid S, A; \theta) - \vec{u}_t(\vec{X}_t \mid Z)\right\|^2\right],$$

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$$+$$

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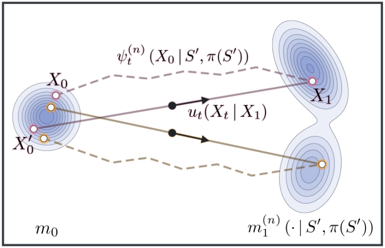
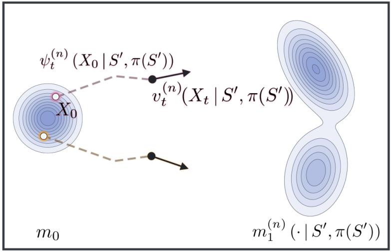
where $X_0 \sim p_0$, $S' \sim P(\cdot \mid S, A)$, $\widehat{X}_t = \widetilde{f}_t^{(n)}(X_0 \mid S', \pi(S'))$,

$$\mathcal{L}_{\mathrm{TD^2-CFM}}(\theta) = (1-\gamma)\mathcal{L}_{COS}(\theta) + \gamma\mathcal{L}_{CGHM}(\theta) \implies \text{Lower Var}\,(\nabla\mathcal{L}).$$

TD-CFM

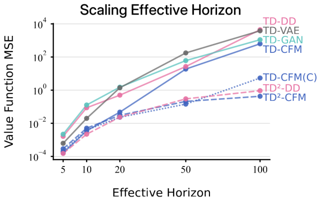


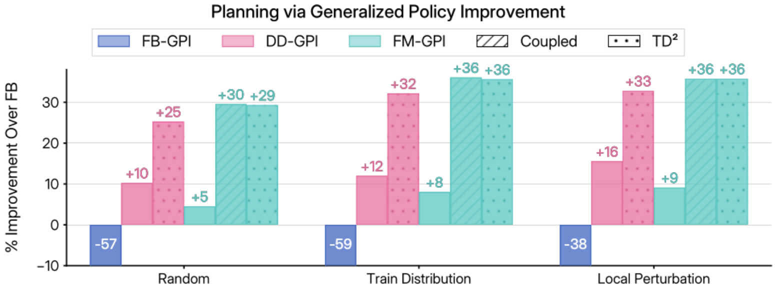
TD²-CFM



GPI:

- Train π_w with Forward backward.
- Do GPI as $w_t \in \arg\max_{w \sim D(W)} \underbrace{(1-\gamma)^{-1}\mathbb{E}_{X\sim m^{\pi_w}(\cdot|s_t,\pi_w(s_t))}[r(X)]}_{Q^{\pi_w}(s_t,\pi_w(s_t))}$.
- Averaged over 128 samples.





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