Temporal Difference Flows [FPT+25]

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July 10, 2025

Outline

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

Variational inference with normalizing flows [RM]

- Want to maximize log-likelihood $\log p_\theta(\mathbf{x})$. Introduce latent $\mathbf{z} \sim p$.

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

- Simultaneously learn q_ϕ and p_θ

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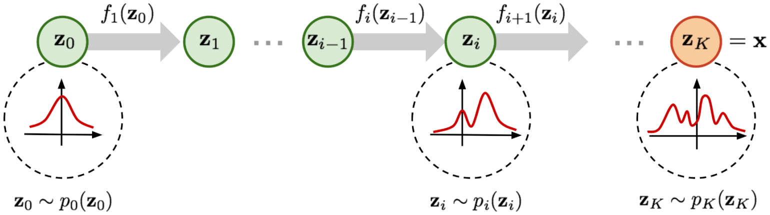
- Rarely the case.

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

Given target distribution q. Pick some initial distribution p_0, where we can sample $\mathbf{z}_0 \sim p_0$.

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

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



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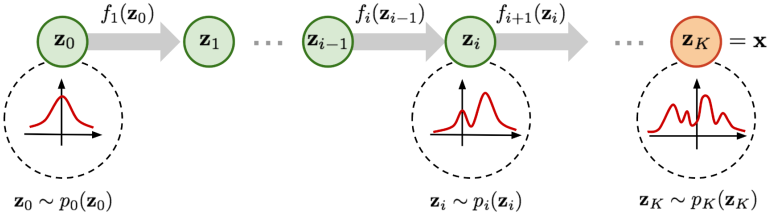
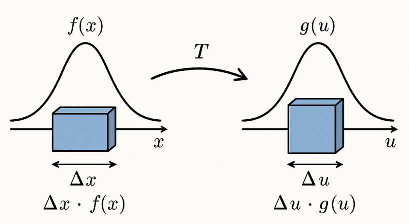


How do we learn such a sequence of functions f_i?

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

Change of variables theorem

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



$\Rightarrow$ Density of $f_1(\mathbf{z}_0) = p_0(\mathbf{z}_0) \left| \det \frac{\partial f_1}{\partial \mathbf{z}} \right|^{-1}$

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

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Need to pick **simple** transformations i.e.

$$f(\mathbf{z}) = \mathbf{z} + \mathbf{u}h(\mathbf{w}^\top \mathbf{z} + b).$$

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

Neural Ordinary Differential Equations [CRBD]

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

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

Remark. *Instantaneous COV*

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

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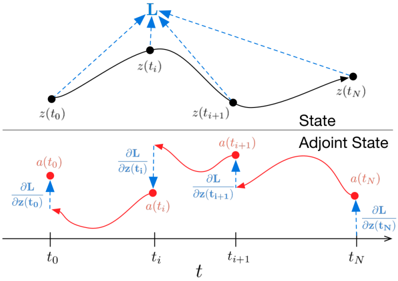
Given $\mathbf{x}^{(i)}$ from dataset, now must compute $\mathbf{x}_0^{(i)} = \int_1^0 f_t^{-1}(\mathbf{x}_t^{(i)})dt$

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



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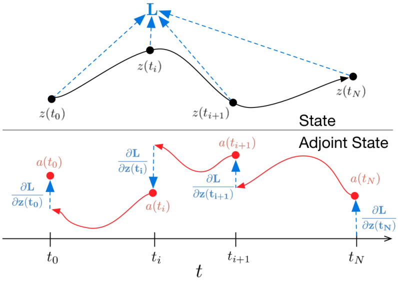


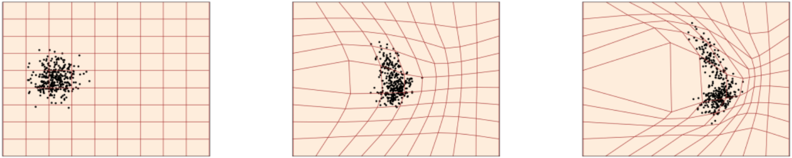
Can we learn f_t without backprop through an ODE?

Flow Matching for Generative Modeling [LCB+23]

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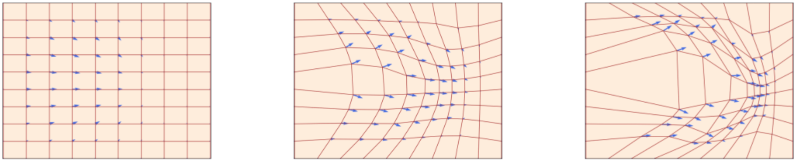
To sample, solve ODE at **sample time** i.e.

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

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



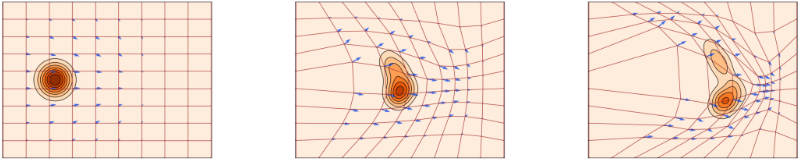
Def. A *vector field* u_t *generates* a probability path p_t if its corresponding flow f_t *generates* p_t.

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)

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

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

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.
- $u_t : \mathbb{R}^d \to \mathbb{R}^d$: vector field that *generates* p_t.

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Intractable.

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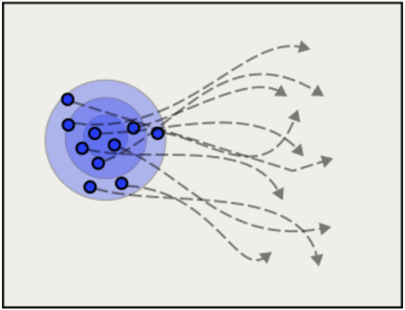
1. How to choose p_t?
2. Given p_t need to solve continuity equation for u_t, which is a **PDE** likely without close-form.

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

Ex: *Consider*

$$f_t(x \mid x_1) = tx_1 + (1 - (1 - \sigma_{\text{min}})t)x$$

$\mathrm{f}_t(X)$



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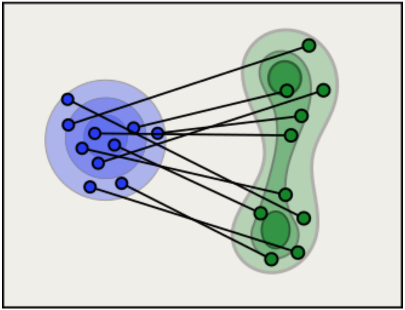

What does the conditional flow being nice have to do with our problem?

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

$$\mathcal{L}_{\text{CFM}}(\theta) = \mathbb{E}_{t,q(x_1),p_t(x|x_1)} \|v_t(x;\theta) - u_t(x \mid x_1)\|^2$$

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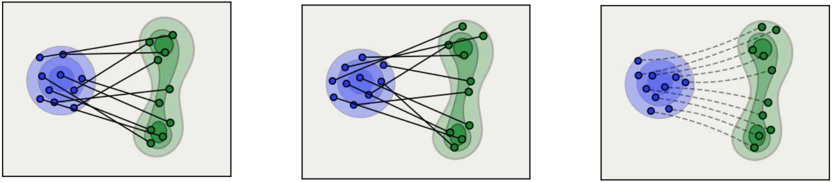
Thm. *Up to a constant independent of θ, $\mathcal{L}_{FM}(\theta) = \mathcal{L}_{CFM}(\theta)$. In particular, $\nabla \mathcal{L}_{FM}(\theta) = \nabla \mathcal{L}_{CFM}(\theta)$.*

Batch i | **Batch** j | $\mathbb{E}[$**Batch**$]$



How do we actually use this?

Example: Optimal Transport

For $f_t(x) = \mu_t(x_1) + x\sigma_t(x_1)$, we consider

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

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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 [GHH+24]

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

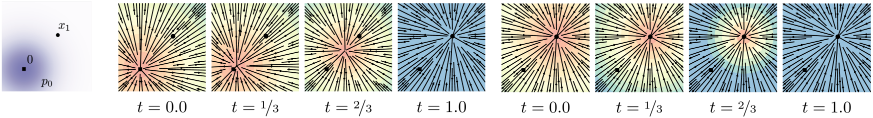
$$u_t(\mathbf{x}_t) = -(\mathbf{x}_t + \nabla \ln p_t(\mathbf{x}_t)).$$

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 [LHH+24].

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. [LCB+23]*
- *The deterministic nature of ODEs equips flow-matching methods with simpler learning objectives and faster inference speed [ZPLE25]*



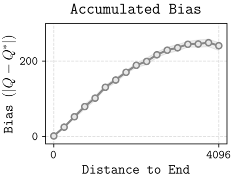
Conditional score

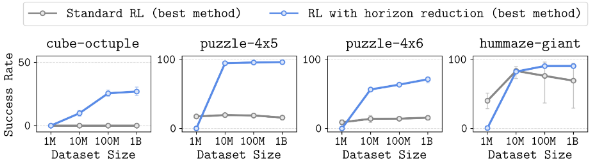
Conditional vector field

Q learning is not yet scalable [Par25]

Long horizon problems are hard.

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





Temporal Difference Flows [FPT+25]

Idea: Apply flow matching to learn the *successor measure* of an MDP.

Def. We define the *successor measure* as

$$m^\pi(\mathsf{X} \mid s, a) = (1-\gamma) \sum_{k=0}^{\infty} \gamma^k \Pr(S_{k+1} \in \mathsf{X} \mid S_0 = s, A_0 = a, \pi),$$

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

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

The most straightforward idea is to just substitute m^{π} for q in flow matching i.e.

$$\mathcal{L}_{\text{MC-CFM}}(\theta) = \mathbb{E}_{\rho,t,Z,X_t}\left[\left\|\tilde{v}_t(X_t \mid S, A; \theta) - u_t(X_t \mid Z)\right\|^2\right],$$

where $Z = X_1 \sim m^{\pi}(\cdot \mid S, A), X_t \sim p_t(\cdot \mid Z)$.

Here we just use the optimal transport conditional vector field and corresponding probability density path.

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where $Z = X_1 \sim m^\pi(\cdot \mid S, A), X_t \sim p_t(\cdot \mid Z)$.

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

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

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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?

Case 1: We sample S'

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

$$\boxed{\begin{gathered} \vec{\mathcal{L}}(\theta) = \mathbb{E}_{\rho, t, Z, \vec{X}_t}\left[\left\|\tilde{v}_t(\vec{X}_t \mid S, A; \theta) - \vec{u}_t(\vec{X}_t \mid Z)\right\|^2\right], \\ \text{where } Z = X_1 \sim P(\cdot \mid S, A),\ \vec{X}_t \sim \vec{p}_t(\cdot \mid Z) \end{gathered}}$$

Lemma. Assuming $v_t^{(n+1)} = \arg\min_v \mathcal{L}_{\mathrm{TD}^2-\mathrm{CFM}}$ (TBD), then $v_t^{(n+1)}$ induces a probability path $m_t^{(n+1)}$ such that $m_0^{(n+1)} = m_0$ and $m_1^{(n+1)} = \mathcal{T}^\pi m_1^{(n)}$.

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Case 2: We sample future state

$$\widehat{v}_t^{(n)}(x \mid s, a) = \int v_t^{(n)}(x \mid s', a') \frac{m_t^{(n)}(x \mid s', a') P(\mathrm{d}s' \mid s, a)}{\widehat{p}_t^{(n)}(x \mid s, a)},$$

where $\widehat{p}_t^{(n)}(x \mid s, a) = \int m_t^{(n)}(x \mid s', a') P(\mathrm{d}s' \mid s, a)$, and $a' = \pi(s')$.

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

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

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

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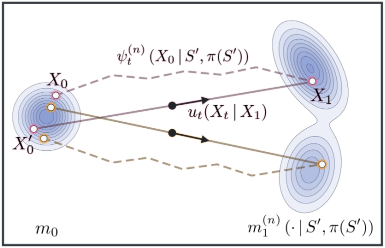
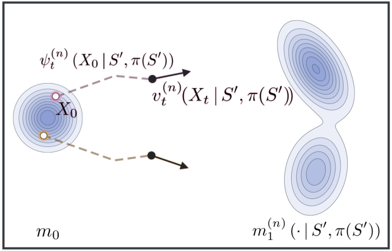
where $X_0 \sim p_0, S' \sim P(\cdot \mid S, A), \widehat{X}_t = \widetilde{f}_t^{(n)}(X_0 \mid S', \pi(S'))$,

$\mathcal{L}_{\mathrm{TD}^2-\mathrm{CFM}}(\theta) = (1-\gamma)\vec{\mathcal{L}}(\theta) + \gamma\widehat{\mathcal{L}}(\theta) \implies$ Lower variance gradient.

TD-CFM

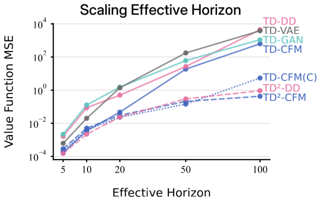


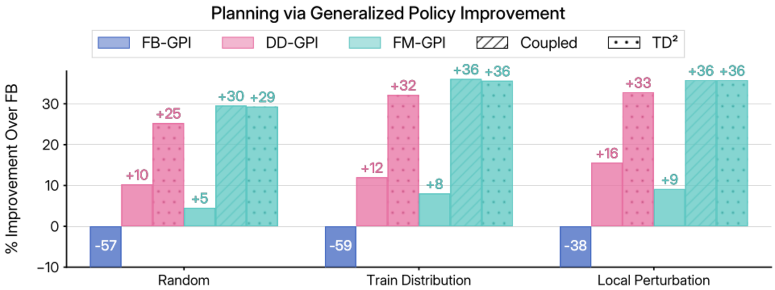
TD²-CFM



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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