北京大學 PEKING UNIVERSITY
西安交通大學
華中科技大學
Microsoft
北京中关村学院 Zhongguancun Academy

Quotient-Space Diffusion Models

Yixian Xu=

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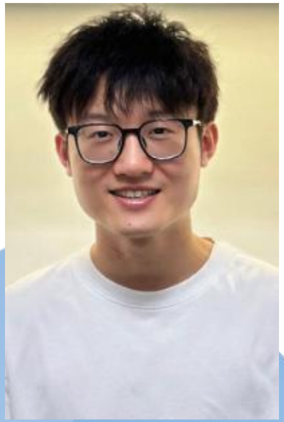
Shengjie Luo

Kaiyuan Gao

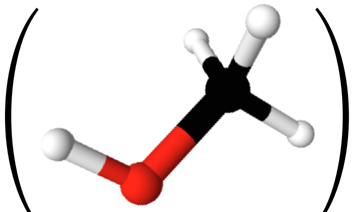


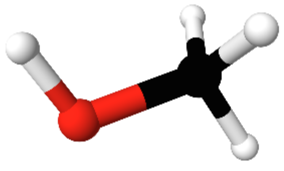
Tianyu He

Di He*

Chang Liu*

Symmetry under Group ($\mathcal{G}$) Actions

$p\Bigg($  $\Bigg)$

$= p\Bigg($  $\Bigg)$

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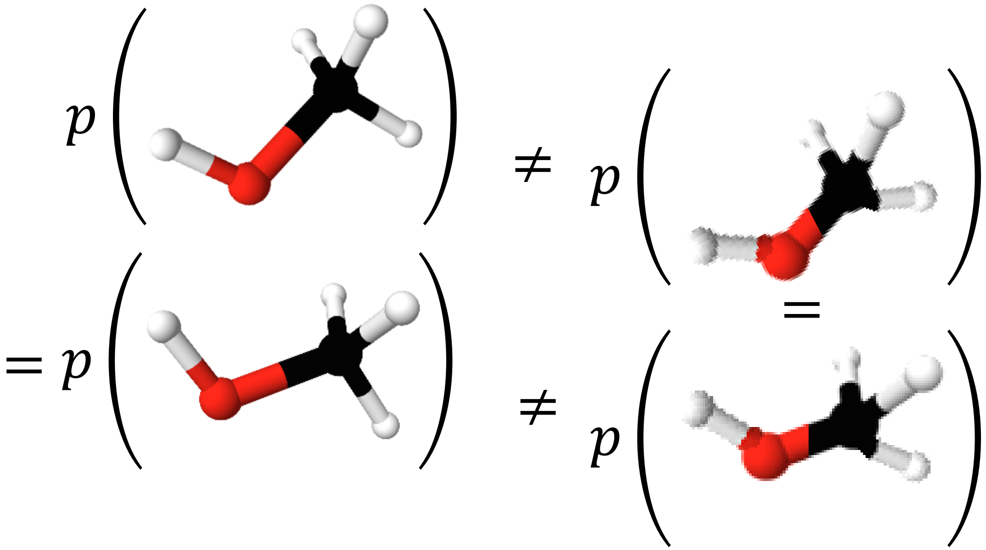

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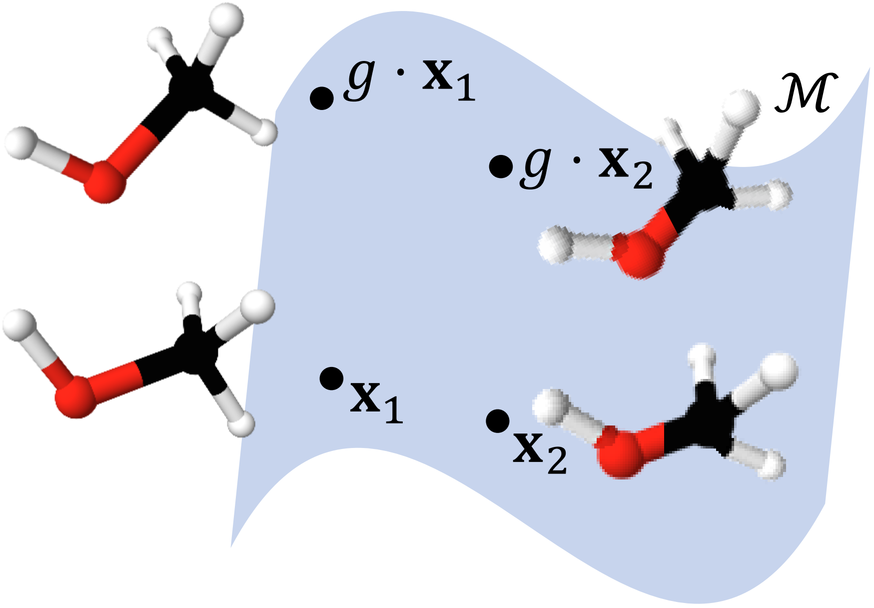

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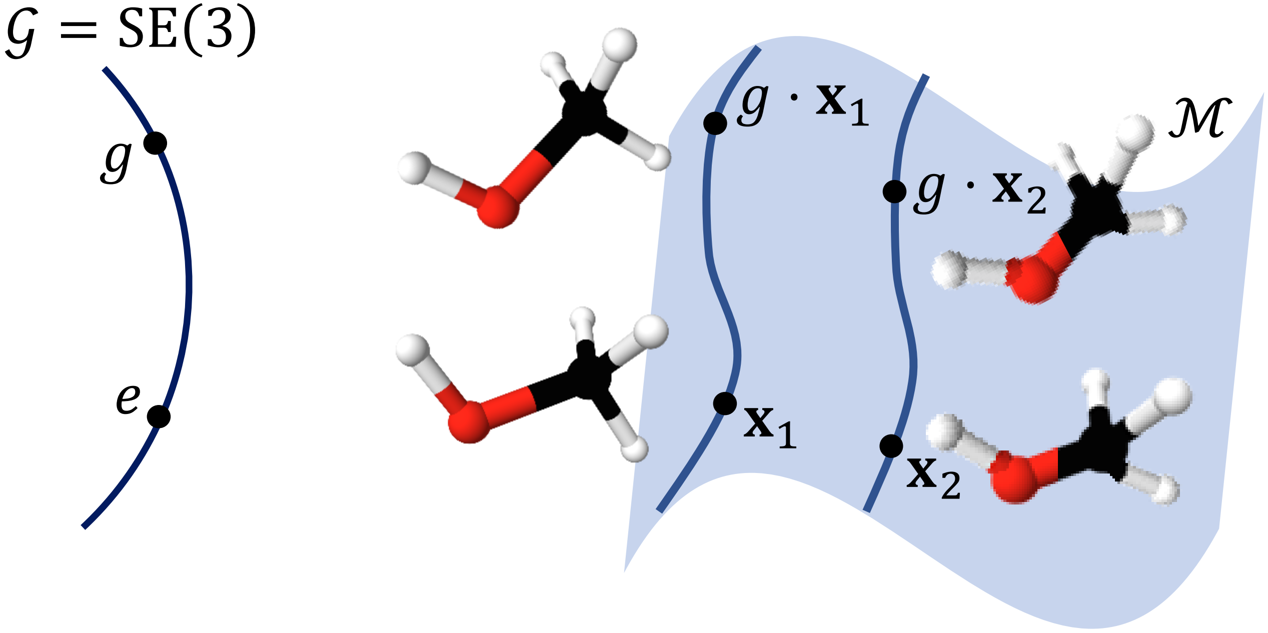
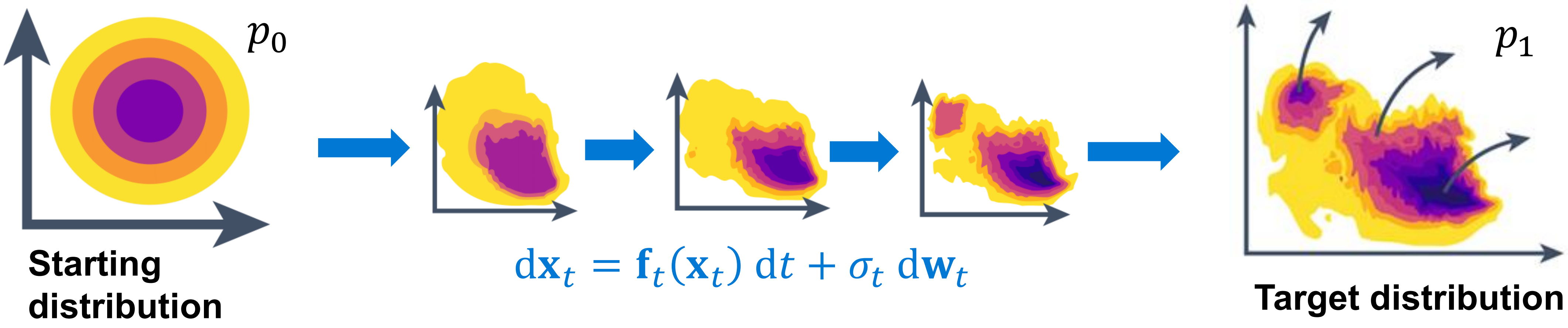


Equivariant Diffusion Models



$$\mathrm{d}\mathbf{x}_t = \mathbf{f}_t(\mathbf{x}_t)\,\mathrm{d}t + \sigma_t\,\mathrm{d}\mathbf{w}_t$$

Generation:

- Invariant start $p_0(\mathbf{x}_0) = p_0(g \cdot \mathbf{x}_0)$
- Equivariant process[1] $(g\,\cdot)_* \mathbf{f}_t(\mathbf{x}_t) = \mathbf{f}_t(g \cdot \mathbf{x}_t)$

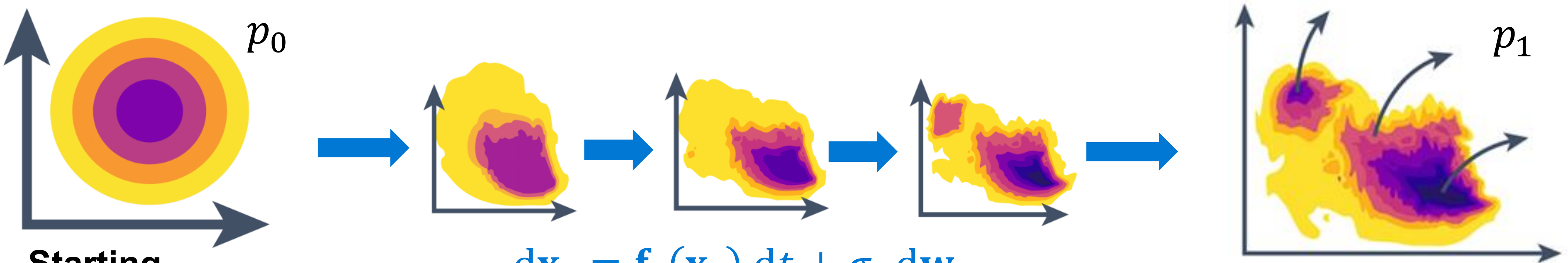
➔

✅ Invariant target $p_1(\mathbf{x}_1) = p_1(g \cdot \mathbf{x}_1)$

---

[1]: $\mathbf{w}_t$ is invariant if the group action is isometric.

Equivariant Diffusion Models



Starting distribution

$$\mathrm{d}\mathbf{x}_t = \mathbf{f}_t(\mathbf{x}_t)\,\mathrm{d}t + \sigma_t\,\mathrm{d}\mathbf{w}_t$$

Target distribution

Generation:

- Invariant start $p_0(\mathbf{x}_0) = p_0(g \cdot \mathbf{x}_0)$
- Equivariant process[1] $(g\,\cdot)_* \mathbf{f}_t(\mathbf{x}_t) = \mathbf{f}_t(g \cdot \mathbf{x}_t)$

➔

✅ Invariant target $p_1(\mathbf{x}_1) = p_1(g \cdot \mathbf{x}_1)$

Training:

$$\mathbf{f}_{\theta,t}(\mathbf{x}_t) = \mathrm{coeff1}_t\,\mathbf{x}_t + \mathrm{coeff2}_t\,\mathbf{D}_{\theta,t}(\mathbf{x}_t),$$

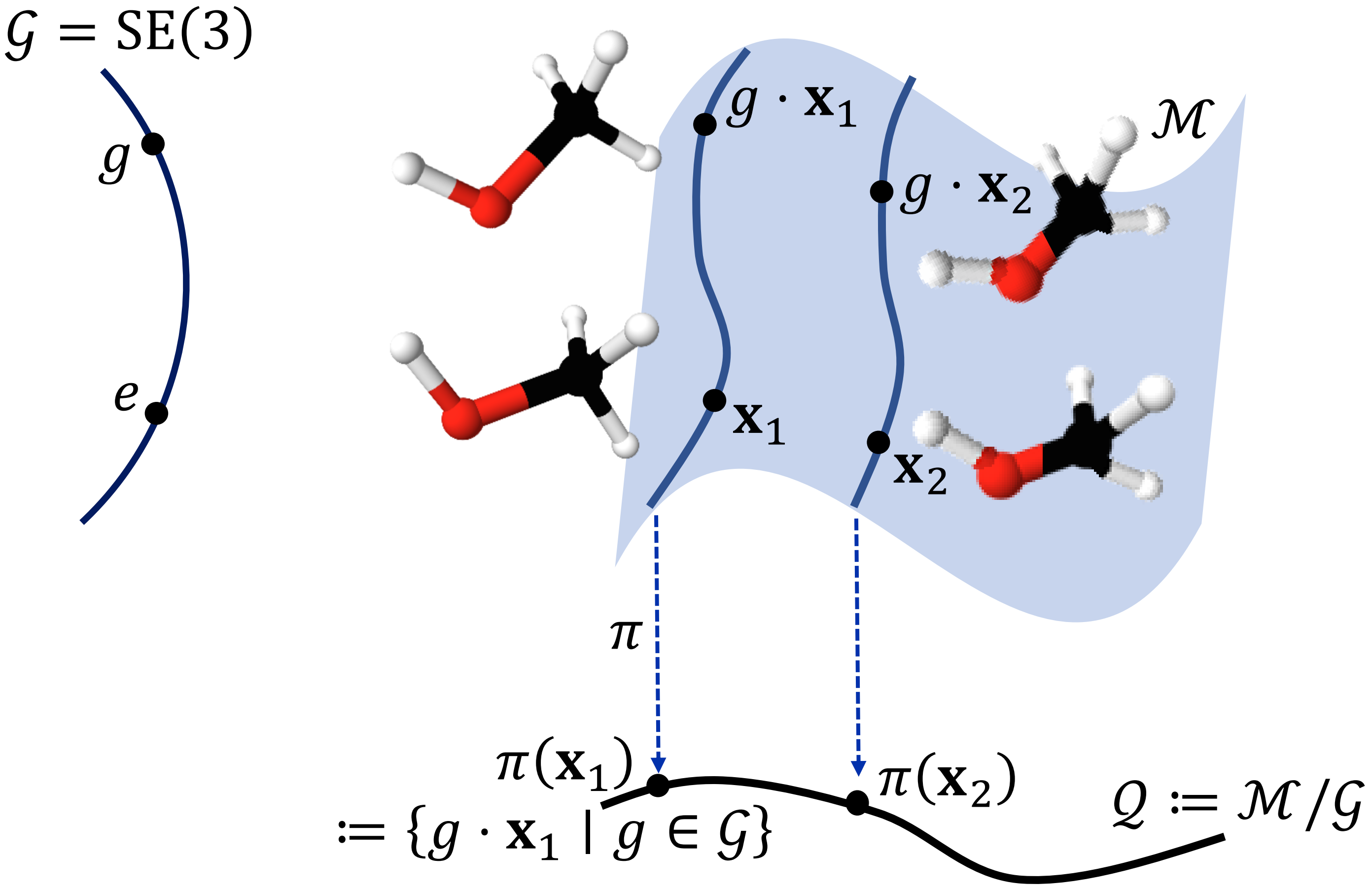
where $\min_{\theta} \mathbb{E}_{p(\mathbf{x}_1,\mathbf{x}_t)} \left\| \mathbf{D}_{\theta,t}(\mathbf{x}_t) - \mathbf{x}_1 \right\|^2.$

❓ $\mathbf{D}_{\theta,t}(\mathbf{x}_t)$ still learns a full mapping: Can we leverage *symmetry* to reduce learning difficulty?

---

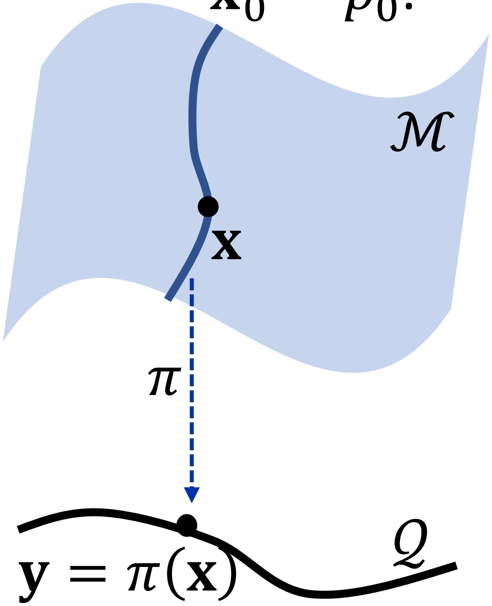
[1]: $\mathbf{w}_t$ is invariant if the group action is isometric.

The View under Quotient Space



Quotient-Space Diffusion Process

$$\mathrm{d}\mathbf{x}_t = \mathbf{f}_t(\mathbf{x}_t)\,\mathrm{d}t + \sigma_t\,\mathrm{d}\mathbf{w}_t,$$
$$\mathbf{x}_0 \sim p_0.$$



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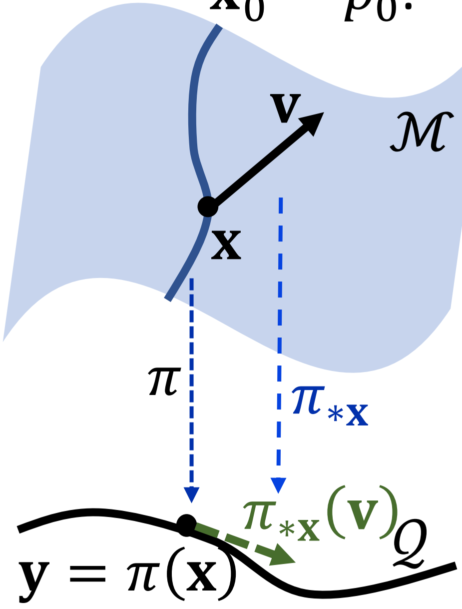

For characterizing intrinsic move

$$\mathrm{d}\mathbf{y}_t = (\pi_*\mathbf{f}_t)(\mathbf{y}_t)\,\mathrm{d}t - \frac{\sigma_t^2}{2}\underbrace{\mathbf{h}(\mathbf{y}_t)}\,\mathrm{d}t + \sigma_t\,\mathrm{d}\boldsymbol{\omega}_t,$$
$$\mathbf{y}_0 \sim \pi_\# p_0.$$

“**mean curvature vector field**”:

effect of volume change across equivalence classes

Quotient-Space Diffusion Process

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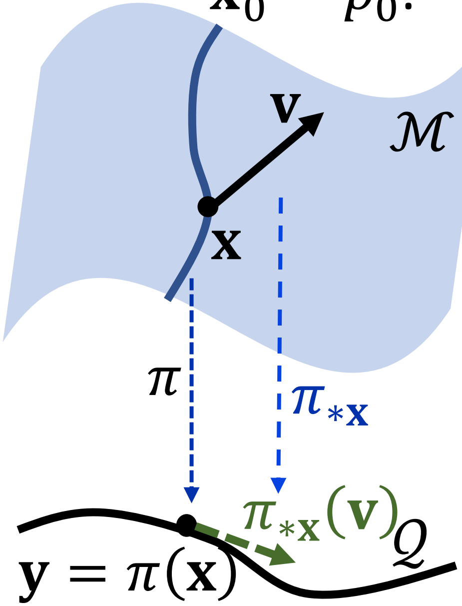
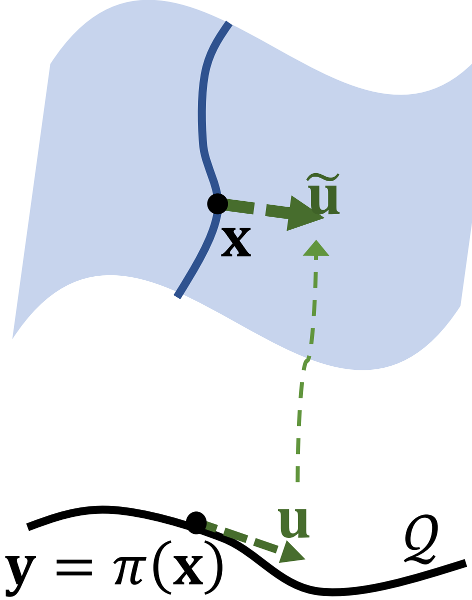


For characterizing intrinsic move

For easier simulation



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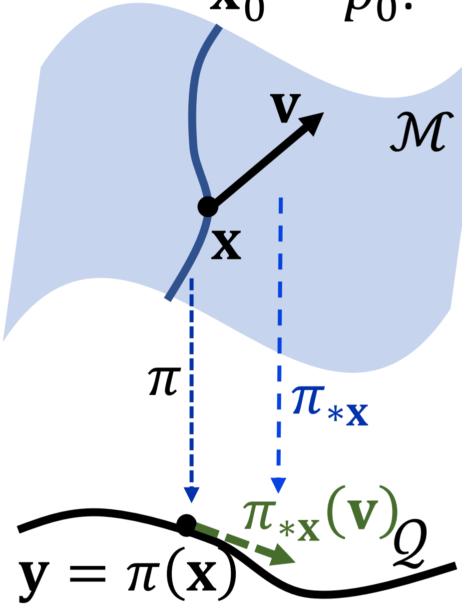

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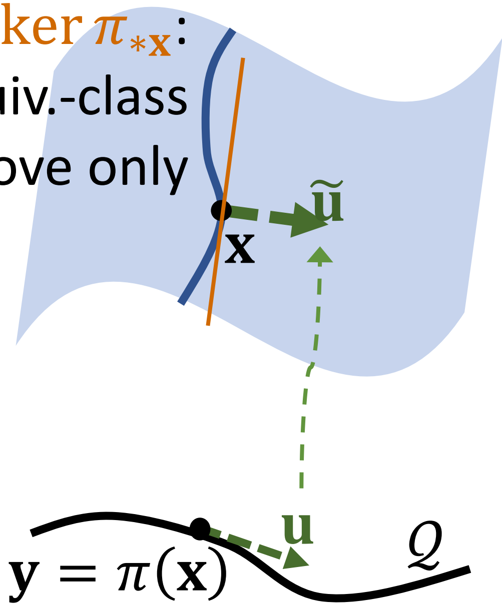
effect of volume change across equivalence classes

$\mathcal{V}_{\mathbf{x}} \coloneqq \ker \pi_{*\mathbf{x}}$:

intra-equiv.-class

move only



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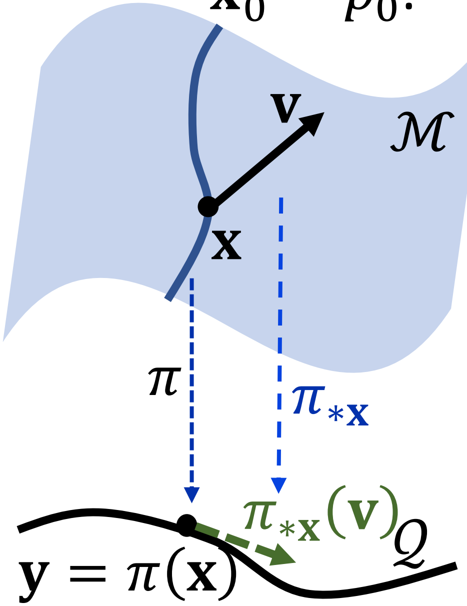

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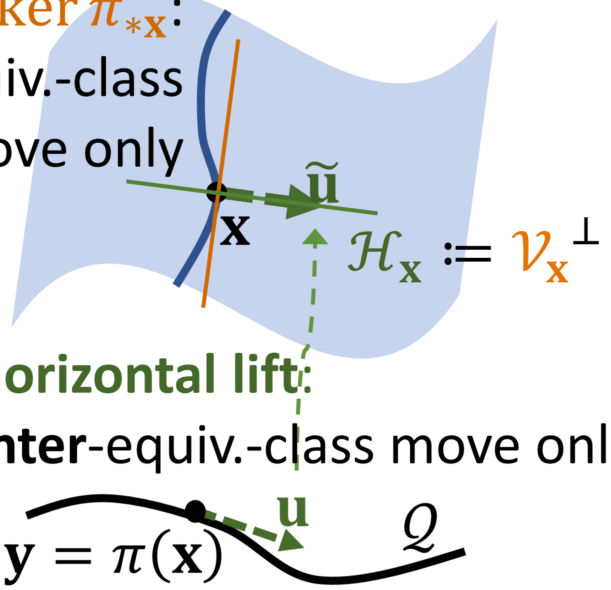

horizontal lift:
inter-equiv.-class move only

$$\mathrm{d}\mathbf{y}_t = (\pi_*\mathbf{f}_t)(\mathbf{y}_t)\,\mathrm{d}t - \frac{\sigma_t^2}{2}\underbrace{\mathbf{h}(\mathbf{y}_t)}\,\mathrm{d}t + \sigma_t\,\mathrm{d}\boldsymbol{\omega}_t,$$
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Quotient-Space Diffusion Process

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$$\mathrm{d}\mathbf{x}_t = P_{\mathbf{x}_t}\big(\mathbf{f}_t(\mathbf{x}_t)\big)\,\mathrm{d}t - \frac{\sigma_t^2}{2}\tilde{\mathbf{h}}(\mathbf{x}_t)\,\mathrm{d}t + \sigma_t P_{\mathbf{x}_t}\,\mathrm{d}\mathbf{w}_t,$$
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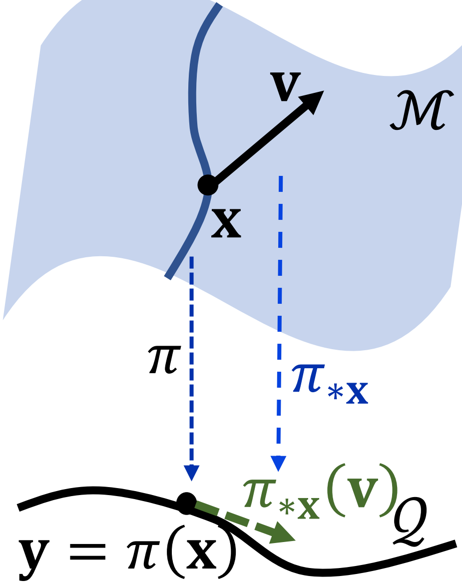

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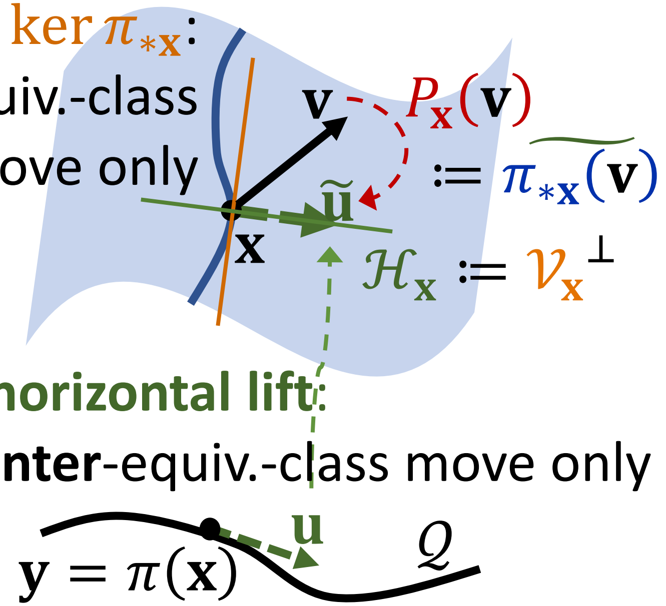

$\mathcal{V}_{\mathbf{x}} := \ker \pi_{*\mathbf{x}}$: **intra**-equiv.-class move only

$P_{\mathbf{x}}(\mathbf{v}) := \widetilde{\pi_{*\mathbf{x}}(\mathbf{v})}$

$\mathcal{H}_{\mathbf{x}} := \mathcal{V}_{\mathbf{x}}^{\perp}$

horizontal lift:

inter-equiv.-class move only

$$\mathrm{d}\mathbf{y}_t = (\pi_*\mathbf{f}_t)(\mathbf{y}_t)\,\mathrm{d}t - \frac{\sigma_t^2}{2}\underbrace{\mathbf{h}(\mathbf{y}_t)}\,\mathrm{d}t + \sigma_t\,\mathrm{d}\boldsymbol{\omega}_t,$$
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Quotient-Space Diffusion Process

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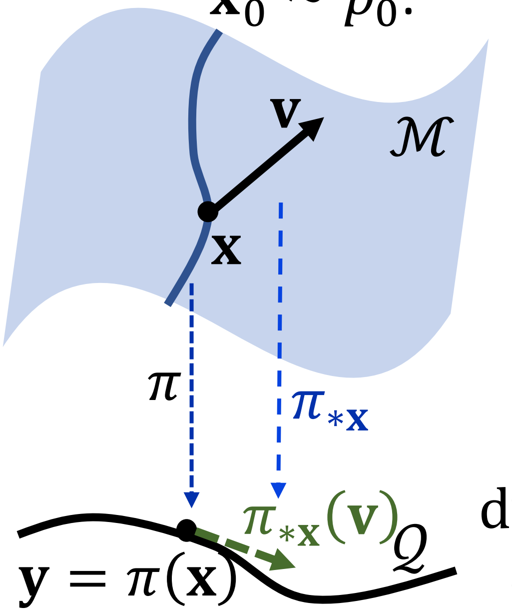

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“mean curvature vector f

effect of volume change across equ

$$\mathrm{d}\mathbf{x}_t = P_{\mathbf{x}_t}\big(\mathbf{f}_t(\mathbf{x}_t)\big)\,\mathrm{d}t - \frac{\sigma_t^2}{2}\tilde{\mathbf{h}}(\mathbf{x}_t)\,\mathrm{d}t + \sigma_t P_{\mathbf{x}_t}\,\mathrm{d}\mathbf{w}_t,$$

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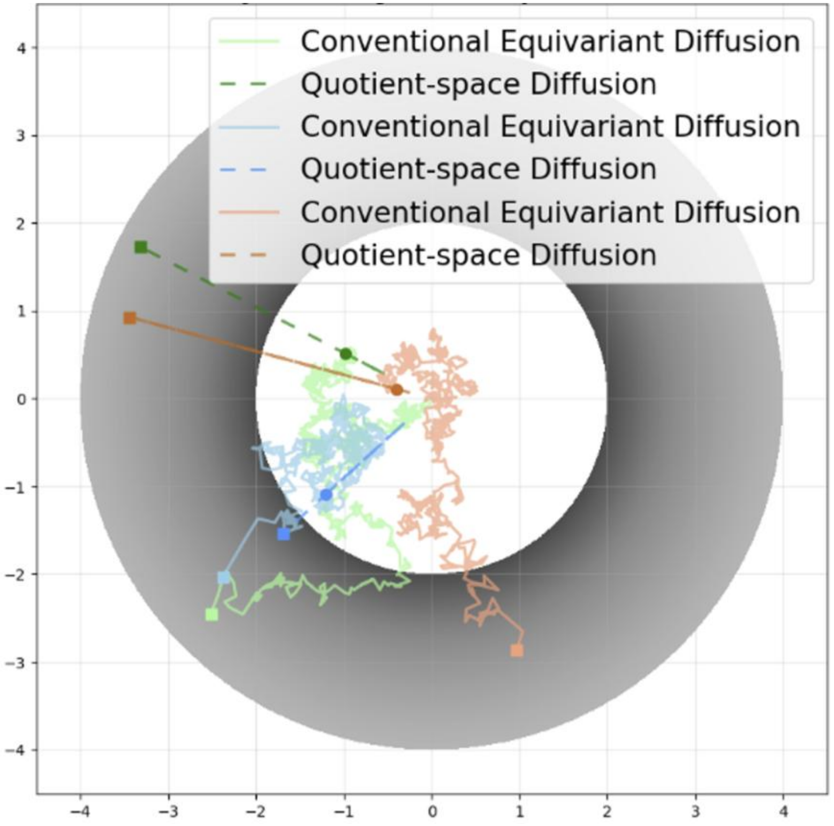

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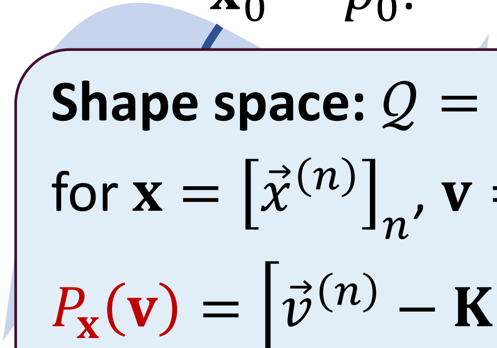


Shape space: $\mathcal{Q} = \mathbb{R}^{3N}_{\mathrm{CoM}}/\mathrm{SO}(3)$:

for $\mathbf{x} = \left[\vec{x}^{(n)}\right]_n$, $\mathbf{v} = \left[\vec{v}^{(n)}\right]_n$,

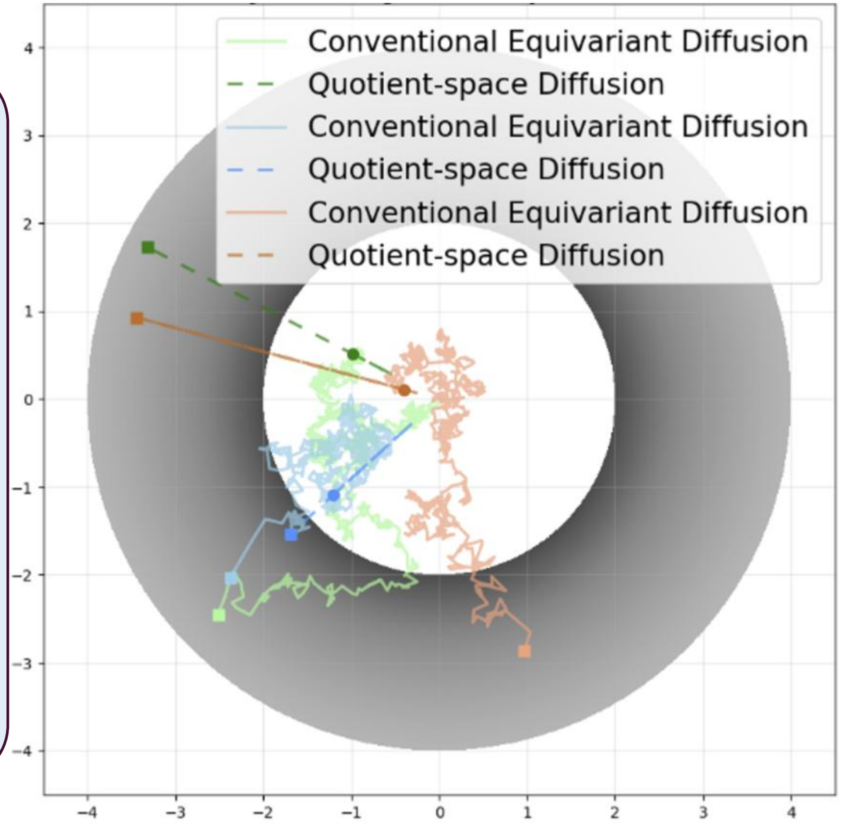
$$P_{\mathbf{x}}(\mathbf{v}) = \left[\vec{v}^{(n)} - \mathbf{K}(\mathbf{x})^{-1}\left(\sum_{n'=1}^{N} \vec{x}^{(n')} \times \vec{v}^{(n')}\right) \times \vec{x}^{(n)}\right]_n,$$

$$\tilde{\mathbf{h}}(\mathbf{x}) = \left[\left(\mathbf{K}(\mathbf{x})^{-1} - \mathrm{tr}\left(\mathbf{K}(\mathbf{x})^{-1}\right)\mathbf{I}\right) \vec{x}^{(n)}\right]_n,$$

where $\mathbf{K}(\mathbf{x}) \coloneqq \sum_{n=1}^{N} \left\|\vec{x}^{(n)}\right\|^2 \mathbf{I} - \sum_{n=1}^{N} \vec{x}^{(n)}\, \vec{x}^{(n)\top} \in \mathbb{R}^{3\times 3}$.

Removes total/rigid-body angular momentum!

Leaves only deformation (change of shape)!



Quotient-Space Diffusion Process

Generation guarantee:

Same $(p_t)_t$!

$$\mathrm{d}\mathbf{x}_t = \mathbf{f}_t(\mathbf{x}_t)\,\mathrm{d}t + \sigma_t\,\mathrm{d}\mathbf{w}_t, \quad \mathbf{x}_0 \sim p_0. \quad \Longleftrightarrow \quad \mathrm{d}\mathbf{x}_t = P_{\mathbf{x}_t}\big(\mathbf{f}_t(\mathbf{x}_t)\big)\,\mathrm{d}t - \frac{\sigma_t^2}{2}\tilde{\mathbf{h}}(\mathbf{x}_t)\,\mathrm{d}t + \sigma_t P_{\mathbf{x}_t}\,\mathrm{d}\mathbf{w}_t, \quad \mathbf{x}_0 \sim p_0.$$

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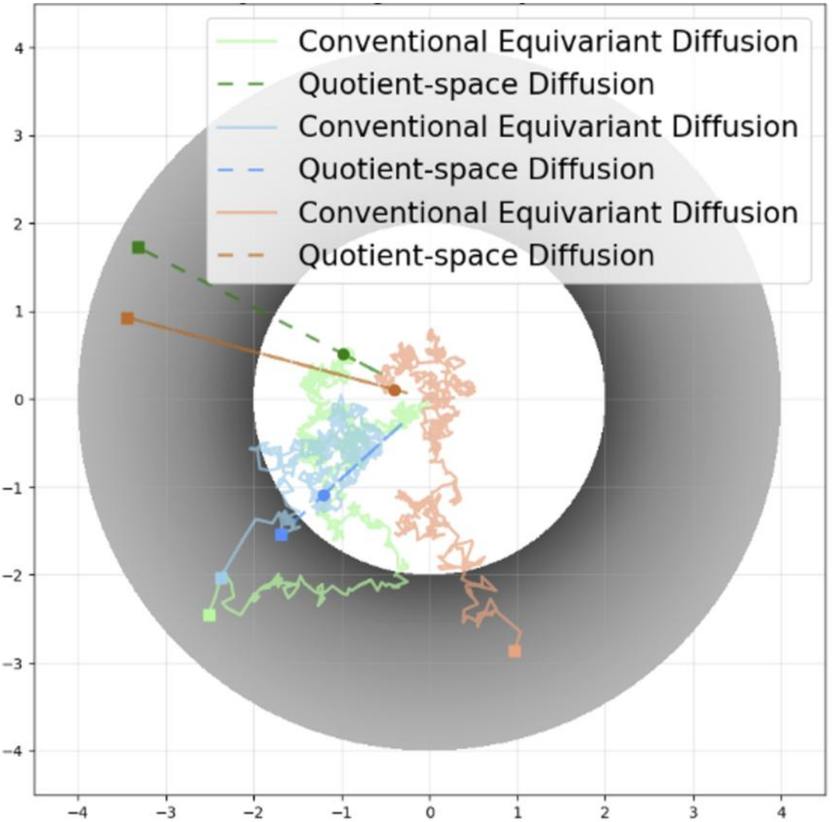
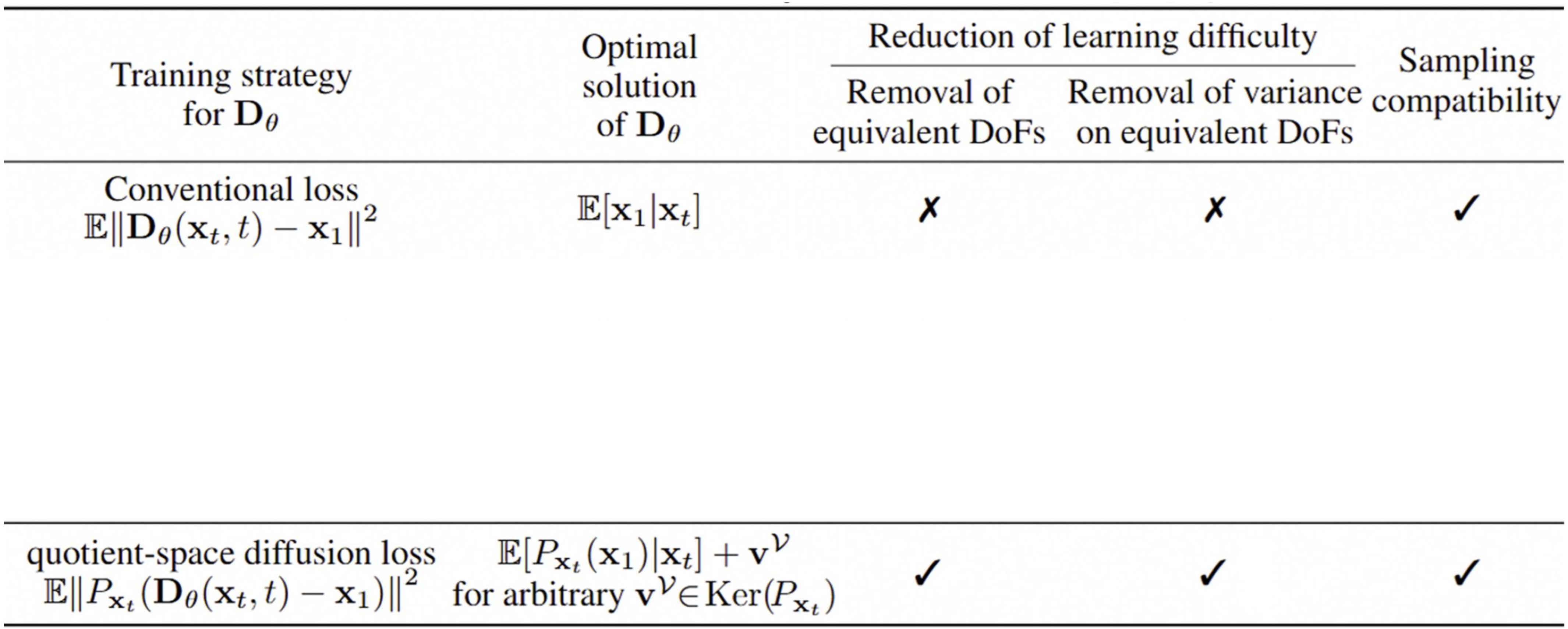


Reduction of Learning Difficulty

Training convenience: $\mathbb{E}\left\|\mathbf{D}_{\theta,t}(\mathbf{x}_t)-\mathbf{x}_1\right\|^2$ ➔ $\mathbb{E}\left\|P_{\mathbf{x}_t}\left(\mathbf{D}_{\theta,t}(\mathbf{x}_t)-\mathbf{x}_1\right)\right\|^2$:
no need to learn anything corresponding to **intra**-equiv.-class movement!



Training strategy for $\mathbf{D}_\theta$	Optimal solution of $\mathbf{D}_\theta$	Reduction of learning difficulty		Sampling compatibility
		Removal of equivalent DoFs	Removal of variance on equivalent DoFs	
Conventional loss $\mathbb{E}\|\mathbf{D}_\theta(\mathbf{x}_t,t)-\mathbf{x}_1\|^2$	$\mathbb{E}[\mathbf{x}_1\|\mathbf{x}_t]$	✗	✗	✓
quotient-space diffusion loss $\mathbb{E}\|P_{\mathbf{x}_t}(\mathbf{D}_\theta(\mathbf{x}_t,t)-\mathbf{x}_1)\|^2$	$\mathbb{E}[P_{\mathbf{x}_t}(\mathbf{x}_1)\|\mathbf{x}_t]+\mathbf{v}^{\mathcal{V}}$ for arbitrary $\mathbf{v}^{\mathcal{V}}\in\mathrm{Ker}(P_{\mathbf{x}_t})$	✓	✓	✓

Reduction of Learning Difficulty

Training convenience: $\mathbb{E}\left\Vert\mathbf{D}_{\theta,t}(\mathbf{x}_t)-\mathbf{x}_1\right\Vert^2$ ➔ $\mathbb{E}\left\Vert P_{\mathbf{x}_t}\left(\mathbf{D}_{\theta,t}(\mathbf{x}_t)-\mathbf{x}_1\right)\right\Vert^2$:
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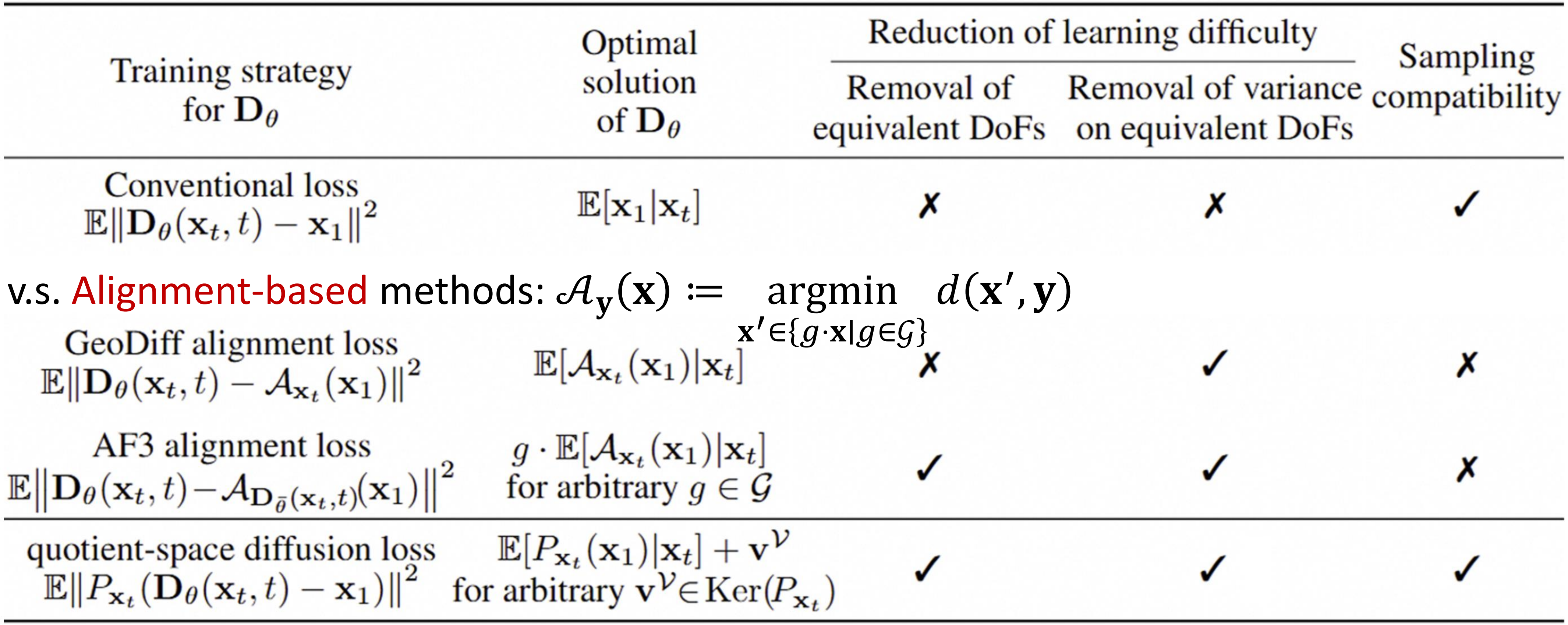
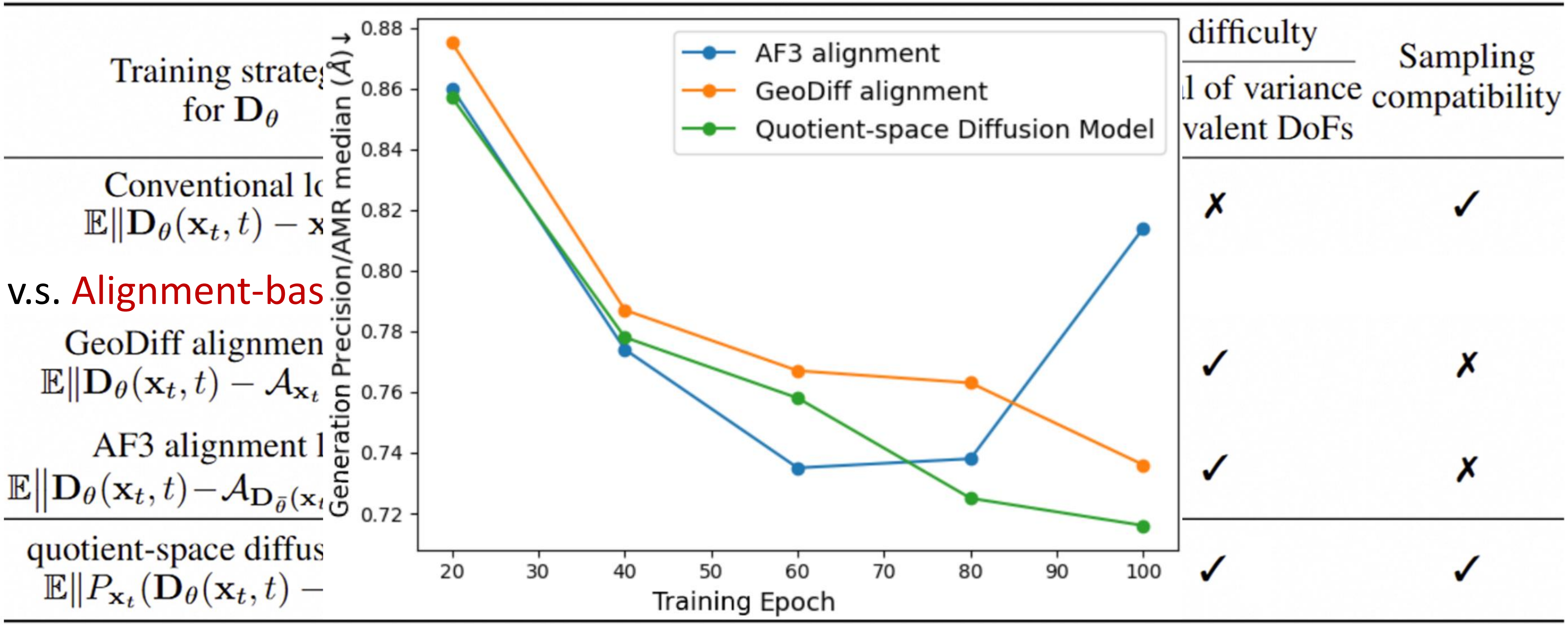


		Reduction of learning difficulty		
Training strategy for $\mathbf{D}_\theta$	Optimal solution of $\mathbf{D}_\theta$	Removal of equivalent DoFs	Removal of variance on equivalent DoFs	Sampling compatibility
Conventional loss $\mathbb{E}\Vert\mathbf{D}_\theta(\mathbf{x}_t,t)-\mathbf{x}_1\Vert^2$	$\mathbb{E}[\mathbf{x}_1\mid\mathbf{x}_t]$	✗	✗	✓
GeoDiff alignment loss $\mathbb{E}\Vert\mathbf{D}_\theta(\mathbf{x}_t,t)-\mathcal{A}_{\mathbf{x}_t}(\mathbf{x}_1)\Vert^2$	$\mathbb{E}[\mathcal{A}_{\mathbf{x}_t}(\mathbf{x}_1)\mid\mathbf{x}_t]$	✗	✓	✗
AF3 alignment loss $\mathbb{E}\left\Vert\mathbf{D}_\theta(\mathbf{x}_t,t)-\mathcal{A}_{\mathbf{D}_{\bar\theta}(\mathbf{x}_t,t)}(\mathbf{x}_1)\right\Vert^2$	$g\cdot\mathbb{E}[\mathcal{A}_{\mathbf{x}_t}(\mathbf{x}_1)\mid\mathbf{x}_t]$ for arbitrary $g\in\mathcal{G}$	✓	✓	✗
quotient-space diffusion loss $\mathbb{E}\Vert P_{\mathbf{x}_t}(\mathbf{D}_\theta(\mathbf{x}_t,t)-\mathbf{x}_1)\Vert^2$	$\mathbb{E}[P_{\mathbf{x}_t}(\mathbf{x}_1)\mid\mathbf{x}_t]+\mathbf{v}^{\mathcal{V}}$ for arbitrary $\mathbf{v}^{\mathcal{V}}\in\mathrm{Ker}(P_{\mathbf{x}_t})$	✓	✓	✓

v.s. Alignment-based methods: $\mathcal{A}_{\mathbf{y}}(\mathbf{x}) \coloneqq \operatorname*{argmin}_{\mathbf{x}'\in\{g\cdot\mathbf{x}\mid g\in\mathcal{G}\}} d(\mathbf{x}',\mathbf{y})$

Reduction of Learning Difficulty

Training convenience: $\mathbb{E}\left\|\mathbf{D}_{\theta,t}(\mathbf{x}_t) - \mathbf{x}_1\right\|^2$ ➔ $\mathbb{E}\left\|P_{\mathbf{x}_t}\left(\mathbf{D}_{\theta,t}(\mathbf{x}_t) - \mathbf{x}_1\right)\right\|^2$:
no need to learn anything corresponding
to **intra**-equiv.-class movement!

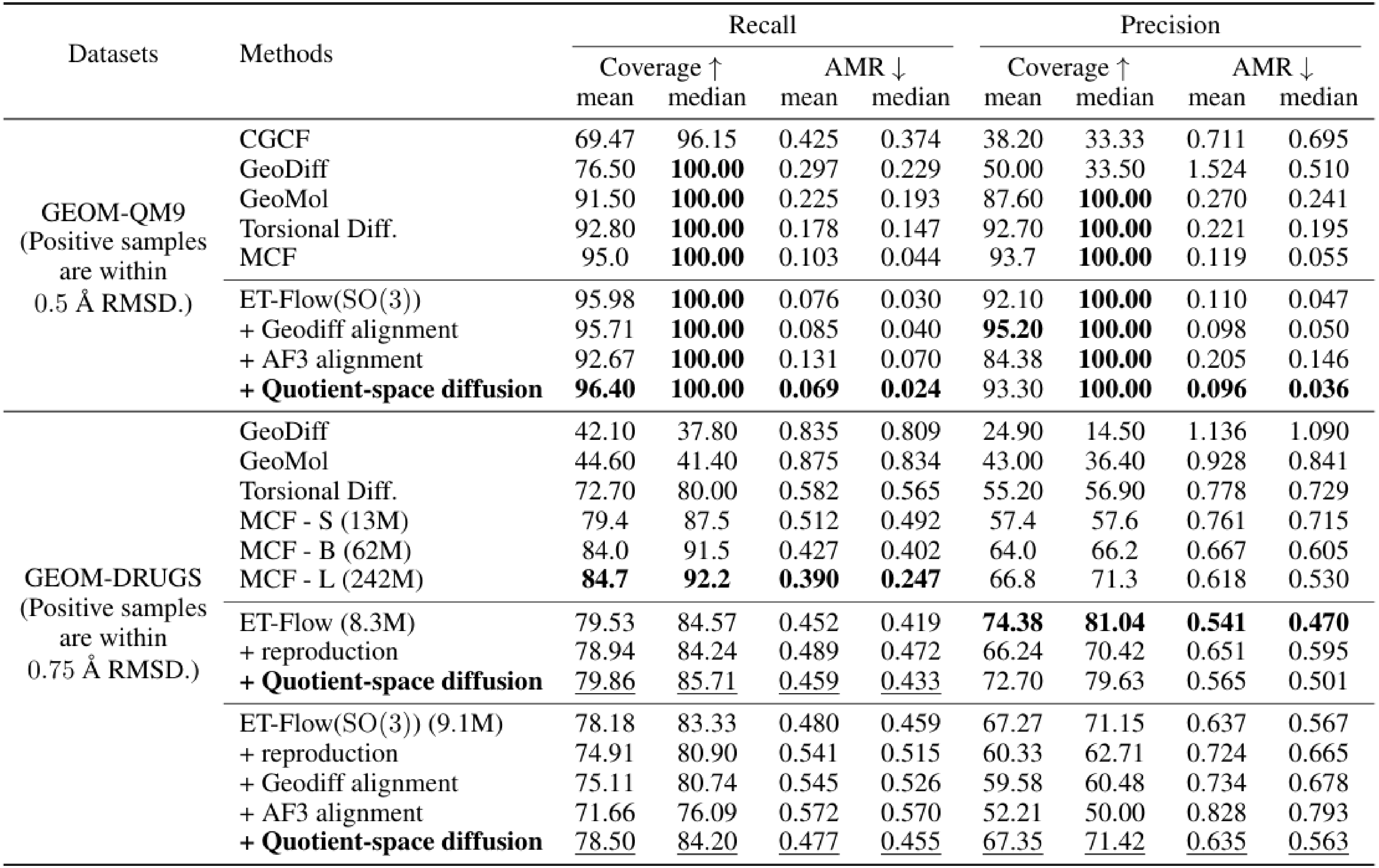


Training strate for $\mathbf{D}_\theta$	difficulty l of variance valent DoFs	Sampling compatibility
Conventional l $\mathbb{E}\|\mathbf{D}_\theta(\mathbf{x}_t, t) - \mathbf{x}$	✗	✓

v.s. Alignment-bas

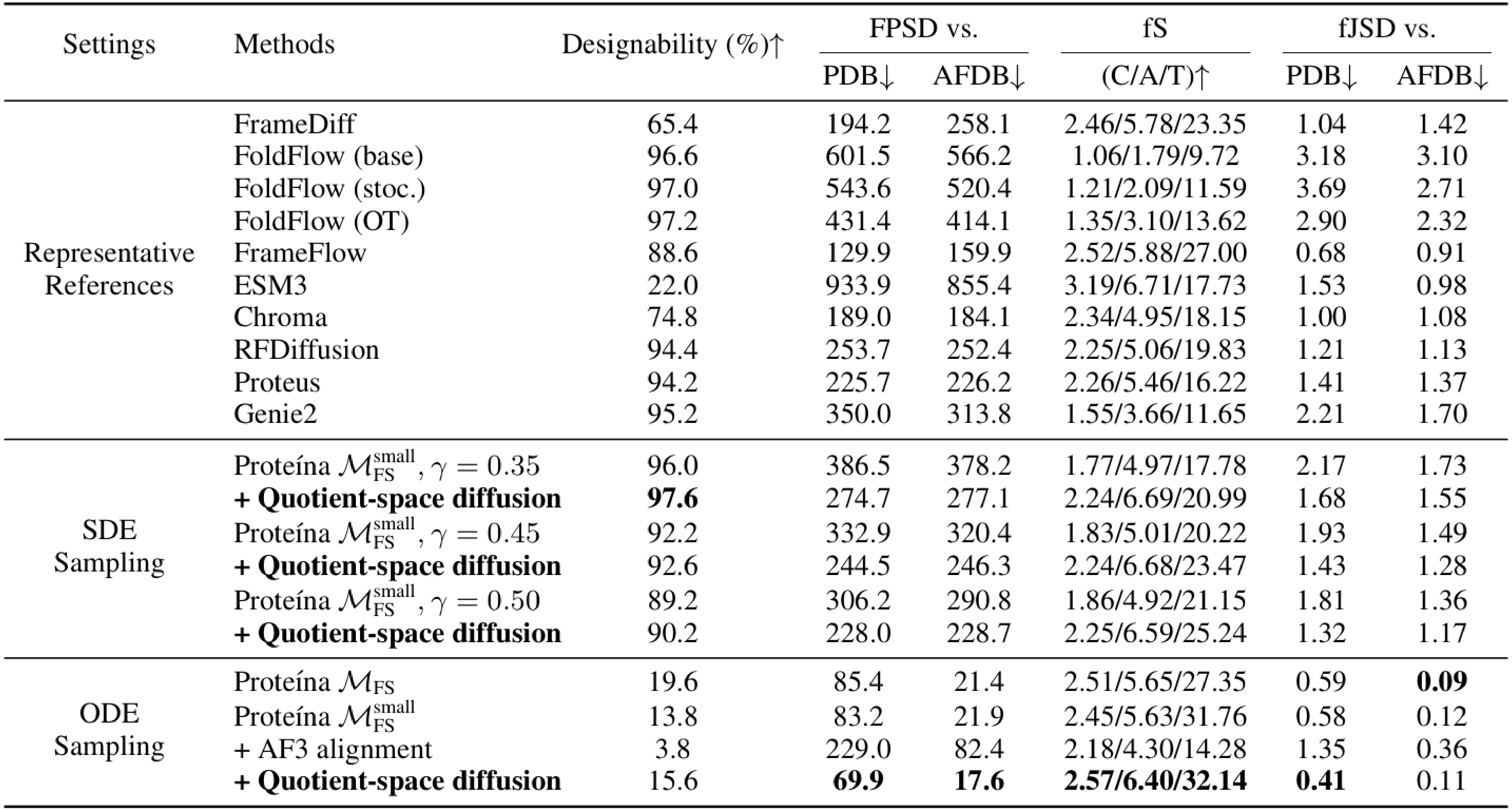
GeoDiff alignmen $\mathbb{E}\|\mathbf{D}_\theta(\mathbf{x}_t, t) - \mathcal{A}_{\mathbf{x}_t}$	✓	✗
AF3 alignment l $\mathbb{E}\|\mathbf{D}_\theta(\mathbf{x}_t, t) - \mathcal{A}_{\mathbf{D}_{\bar{\theta}}(\mathbf{x}_t}$	✓	✗
quotient-space diffus $\mathbb{E}\|P_{\mathbf{x}_t}(\mathbf{D}_\theta(\mathbf{x}_t, t) -$	✓	✓

Results: Molecular Structure Generation



Datasets	Methods	Recall				Precision			
		Coverage ↑		AMR ↓		Coverage ↑		AMR ↓	
		mean	median	mean	median	mean	median	mean	median
GEOM-QM9 (Positive samples are within 0.5 Å RMSD.)	CGCF	69.47	96.15	0.425	0.374	38.20	33.33	0.711	0.695
	GeoDiff	76.50	**100.00**	0.297	0.229	50.00	33.50	1.524	0.510
	GeoMol	91.50	**100.00**	0.225	0.193	87.60	**100.00**	0.270	0.241
	Torsional Diff.	92.80	**100.00**	0.178	0.147	92.70	**100.00**	0.221	0.195
	MCF	95.0	**100.00**	0.103	0.044	93.7	**100.00**	0.119	0.055
	ET-Flow(SO(3))	95.98	**100.00**	0.076	0.030	92.10	**100.00**	0.110	0.047
	+ Geodiff alignment	95.71	**100.00**	0.085	0.040	**95.20**	**100.00**	0.098	0.050
	+ AF3 alignment	92.67	**100.00**	0.131	0.070	84.38	**100.00**	0.205	0.146
	+ Quotient-space diffusion	**96.40**	**100.00**	**0.069**	**0.024**	93.30	**100.00**	**0.096**	**0.036**
GEOM-DRUGS (Positive samples are within 0.75 Å RMSD.)	GeoDiff	42.10	37.80	0.835	0.809	24.90	14.50	1.136	1.090
	GeoMol	44.60	41.40	0.875	0.834	43.00	36.40	0.928	0.841
	Torsional Diff.	72.70	80.00	0.582	0.565	55.20	56.90	0.778	0.729
	MCF - S (13M)	79.4	87.5	0.512	0.492	57.4	57.6	0.761	0.715
	MCF - B (62M)	84.0	91.5	0.427	0.402	64.0	66.2	0.667	0.605
	MCF - L (242M)	**84.7**	**92.2**	**0.390**	**0.247**	66.8	71.3	0.618	0.530
	ET-Flow (8.3M)	79.53	84.57	0.452	0.419	**74.38**	**81.04**	**0.541**	**0.470**
	+ reproduction	78.94	84.24	0.489	0.472	66.24	70.42	0.651	0.595
	+ Quotient-space diffusion	79.86	85.71	0.459	0.433	72.70	79.63	0.565	0.501
	ET-Flow(SO(3)) (9.1M)	78.18	83.33	0.480	0.459	67.27	71.15	0.637	0.567
	+ reproduction	74.91	80.90	0.541	0.515	60.33	62.71	0.724	0.665
	+ Geodiff alignment	75.11	80.74	0.545	0.526	59.58	60.48	0.734	0.678
	+ AF3 alignment	71.66	76.09	0.572	0.570	52.21	50.00	0.828	0.793
	+ Quotient-space diffusion	78.50	84.20	0.477	0.455	67.35	71.42	0.635	0.563

Results: Protein Structure Generation



Settings	Methods	Designability (%)↑	FPSD vs.		fS	fJSD vs.	
			PDB↓	AFDB↓	(C/A/T)↑	PDB↓	AFDB↓
Representative References	FrameDiff	65.4	194.2	258.1	2.46/5.78/23.35	1.04	1.42
	FoldFlow (base)	96.6	601.5	566.2	1.06/1.79/9.72	3.18	3.10
	FoldFlow (stoc.)	97.0	543.6	520.4	1.21/2.09/11.59	3.69	2.71
	FoldFlow (OT)	97.2	431.4	414.1	1.35/3.10/13.62	2.90	2.32
	FrameFlow	88.6	129.9	159.9	2.52/5.88/27.00	0.68	0.91
	ESM3	22.0	933.9	855.4	3.19/6.71/17.73	1.53	0.98
	Chroma	74.8	189.0	184.1	2.34/4.95/18.15	1.00	1.08
	RFDiffusion	94.4	253.7	252.4	2.25/5.06/19.83	1.21	1.13
	Proteus	94.2	225.7	226.2	2.26/5.46/16.22	1.41	1.37
	Genie2	95.2	350.0	313.8	1.55/3.66/11.65	2.21	1.70
SDE Sampling	Proteína $\mathcal{M}_{\text{FS}}^{\text{small}}, \gamma = 0.35$	96.0	386.5	378.2	1.77/4.97/17.78	2.17	1.73
	+ Quotient-space diffusion	**97.6**	274.7	277.1	2.24/6.69/20.99	1.68	1.55
	Proteína $\mathcal{M}_{\text{FS}}^{\text{small}}, \gamma = 0.45$	92.2	332.9	320.4	1.83/5.01/20.22	1.93	1.49
	+ Quotient-space diffusion	92.6	244.5	246.3	2.24/6.68/23.47	1.43	1.28
	Proteína $\mathcal{M}_{\text{FS}}^{\text{small}}, \gamma = 0.50$	89.2	306.2	290.8	1.86/4.92/21.15	1.81	1.36
	+ Quotient-space diffusion	90.2	228.0	228.7	2.25/6.59/25.24	1.32	1.17
ODE Sampling	Proteína $\mathcal{M}_{\text{FS}}$	19.6	85.4	21.4	2.51/5.65/27.35	0.59	**0.09**
	Proteína $\mathcal{M}_{\text{FS}}^{\text{small}}$	13.8	83.2	21.9	2.45/5.63/31.76	0.58	0.12
	+ AF3 alignment	3.8	229.0	82.4	2.18/4.30/14.28	1.35	0.36
	+ Quotient-space diffusion	15.6	**69.9**	**17.6**	**2.57/6.40/32.14**	**0.41**	0.11

Thanks!

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