ReQFlow: Rectified Quaternion Flow for Efficient and High-Quality Protein Backbone Generation

Angxiao Yue, Zichong Wang, Hongteng Xu

Renmin University of China

高瓴人工智能学院
Gaoling School of Artificial Intelligence

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Background & Contributions

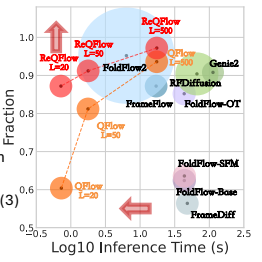
Task: Protein backbone generation

Previous works:

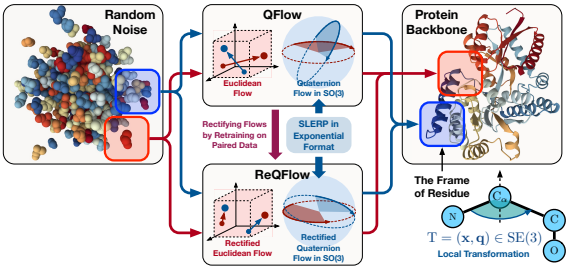
- Low generation designability
- Long inference time

Highlight of our method:

- Use unit **quaternions** to represent rotations
- Construct SO(3) flow with **SLERP** in an exponential format (QFlow)
- **First paper** explores **ReFlow** in SO(3) to accelerate inference (**ReQFlow**)
- **SOTA** on designability, **37×faster** than RFDiffusion and **62× faster** than Genie2 when best tradeoff



Our Method



Train: $\boldsymbol{q} = \exp\left(\frac{1}{2}\boldsymbol{\omega}\right) = \left[\cos\frac{\phi}{2}, \sin\frac{\phi}{2}\boldsymbol{u}^\top\right]^\top \in \mathbb{S}^3$ $\Rightarrow$ $\boldsymbol{\omega}_{\theta,t} = \frac{2\log(\boldsymbol{q}_t^{-1} \otimes \boldsymbol{q}_{\theta,1})}{1-t}$

$\boldsymbol{q}_t = \boldsymbol{q}_0 \otimes \exp(t \log(\boldsymbol{q}_0^{-1} \otimes \boldsymbol{q}_1))$ $\quad \mathcal{L}_{SO(3)} = \mathbb{E}_{t,\mathcal{Q}_0,\mathcal{Q}_1}[\|\boldsymbol{\omega} - \boldsymbol{\omega}_{\theta,t}\|^2]$

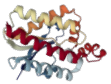
Inference: $\boldsymbol{q}_{t+\Delta t} = \boldsymbol{q}_t \otimes \exp\left(\frac{1}{2}\Delta t \cdot \gamma e^{-\gamma t}\boldsymbol{\omega}_{\theta,t}\right)$ $\Rightarrow$ **ReFlow**

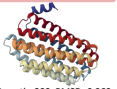
Experiment

Paper

Code


Length=100, RMSD=0.969


Length=200, RMSD=1.322


Length=300, RMSD=0.960

Method	Efficiency		Designability		Diversity	Novelty
	Step	Time(s)	Fraction↑	scRMSD↓	TM↓	TM↓
RFDiffusion	50	66.23	0.904	$1.102_{\pm 1.617}$	0.382	0.527
Genie2	1000	112.93	0.908	$1.132_{\pm 1.389}$	0.370	**0.475**
	500	55.86	0.000	$18.169_{\pm 5.963}$	-	-
FrameDiff	500	48.12	0.564	$2.936_{\pm 3.093}$	0.441	0.591
FoldFlow$_{\text{Base}}$	500	43.52	0.624	$3.080_{\pm 3.449}$	0.469	0.645
FoldFlow$_{\text{SFM}}$	500	43.63	0.636	$3.031_{\pm 3.589}$	0.411	0.604
FoldFlow$_{\text{OT}}$	500	43.35	0.852	$1.760_{\pm 2.593}$	0.434	0.617
FoldFlow2	50	6.35	0.952	$1.083_{\pm 1.308}$	0.373	0.527
	20	2.63	0.644	$3.060_{\pm 3.210}$	0.339	0.492
FrameFlow	500	17.05	0.872	$1.380_{\pm 1.392}$	0.346	0.562
	200	6.77	0.864	$1.542_{\pm 1.889}$	0.348	0.564
	100	3.46	0.708	$2.167_{\pm 2.373}$	0.332	0.560
	50	1.73	0.704	$2.639_{\pm 3.079}$	0.334	0.536
	20	0.71	0.436	$4.652_{\pm 4.390}$	0.319	0.501
	10	0.37	0.180	$7.343_{\pm 5.125}$	0.317	0.482
QFlow	500	17.37	0.936	$1.163_{\pm 0.938}$	0.356	0.635
	200	7.10	0.864	$1.400_{\pm 1.259}$	**0.344**	0.620
	100	3.48	0.916	$1.342_{\pm 1.364}$	0.348	0.614
	50	1.77	0.812	$1.785_{\pm 1.551}$	**0.344**	0.571
	20	0.73	0.604	$3.090_{\pm 3.374}$	0.325	0.537
	10	0.38	0.332	$5.032_{\pm 4.303}$	0.313	0.528
ReQFlow	500	17.42	**0.972**	$\mathbf{1.071}_{\pm \mathbf{0.482}}$	0.377	0.645
	200	6.94	0.932	$1.160_{\pm 0.782}$	0.384	0.648
	100	3.58	0.928	$1.245_{\pm 1.059}$	0.369	0.629
	50	1.78	0.912	$1.254_{\pm 0.915}$	0.369	0.608
	20	0.72	0.872	$1.418_{\pm 0.998}$	0.355	0.581
	10	0.38	0.676	$2.443_{\pm 2.382}$	0.337	0.540