

Novelty Assessment Report

Paper: Efficient Regression-based Training of Normalizing Flows for Boltzmann Generators

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Abstract

Simulation-free training frameworks have been at the forefront of the generative modelling revolution in continuous spaces, leading to large-scale diffusion and flow matching models. However, such modern generative models suffer from expensive inference, inhibiting their use in numerous scientific applications like Boltzmann Generators (BGs) for molecular conformations that require fast likelihood evaluation. In this paper, we revisit classical normalizing flows in the context of BGs that offer efficient sampling and likelihoods, but whose training via maximum likelihood is often unstable and computationally challenging. We propose Regression Training of Normalizing Flows (RegFlow), a novel and scalable regression-based training objective that bypasses the numerical instability and computational challenge of conventional maximum likelihood training in favour of a simple ℓ_2 -regression objective. Specifically, RegFlow maps prior samples under our flow to targets computed using optimal transport couplings or a pre-trained continuous normalizing flow (CNF). To enhance numerical stability, RegFlow employs effective regularization strategies such as a new forward-backward self-consistency loss that enjoys painless implementation. Empirically, we demonstrate that RegFlow unlocks a broader class of architectures that were previously intractable to train for BGs with maximum likelihood. We also show RegFlow exceeds the performance, computational cost, and stability of maximum likelihood training in equilibrium sampling in Cartesian coordinates of alanine dipeptide, tripeptide, and tetrapeptide, showcasing its potential in molecular systems.

Disclaimer

This report is **AI-GENERATED** using Large Language Models and WisPaper (a scholar search engine). It analyzes academic papers' tasks and contributions against retrieved prior work. While this system identifies **POTENTIAL** overlaps and novel directions, **ITS COVERAGE IS NOT EXHAUSTIVE AND JUDGMENTS ARE APPROXIMATE**. These results are intended to assist human reviewers and **SHOULD NOT** be relied upon as a definitive verdict on novelty.

Note that some papers exist in multiple, slightly different versions (e.g., with different titles or URLs). The system may retrieve several versions of the same underlying work. The current automated pipeline does not reliably align or distinguish these cases, so human reviewers will need to disambiguate them manually.

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Core Task Landscape

This paper addresses: **Regression-Based Training of Normalizing Flows for Molecular Sampling**

A total of **6 papers** were analyzed and organized into a taxonomy with **5 categories**.

Taxonomy Overview

The research landscape has been organized into the following main categories:

- **Regression-Based Flow Training Methods**
- **Generative Models for Molecular Design**

Complete Taxonomy Tree

- Regression-Based Training of Normalizing Flows for Molecular Sampling Survey Taxonomy
- Regression-Based Flow Training Methods
 - Direct Regression Training for Normalizing Flows ★ (2 papers)
 - [0] Efficient Regression-based Training of Normalizing Flows for Boltzmann Generators (Anon et al., 2026) [View paper](#)
 - [2] FORT: Forward-Only Regression Training of Normalizing Flows (D Rehman, 2025) [View paper](#)
 - Flow Matching for Molecular Generation
 - Equivariant Flow Matching for Conformer Generation (2 papers)
 - [1] Equivariant flow matching for molecular conformer generation (M Hassan, 2024) [View paper](#)
 - [3] Equivariant flow matching with hybrid probability transport for 3d molecule generation (Y Song, 2023) [View paper](#)
 - Flow Matching Applications in Bioinformatics (1 papers)
 - [5] How to go with the flow: flow matching in bioinformatics and computational biology (Alex Morehead, 2025) [View paper](#)
 - Generative Models for Molecular Design
 - Controllable Molecule Generation with Flows (1 papers)
 - [6] Controllable Generation of Drug-like Molecules with Multi-modal Variational Flow (F Sun, n.d.) [View paper](#)
 - Unnormalized Distribution Learning for Molecular Systems (1 papers)
 - [4] Molecular Unnormalized Distributions With Deep Generative Models Toward the Acceleration of Molecular Design and Conformational Sampling With Deep (Diez, 2024) [View paper](#)

Narrative

Core task: regression-based training of normalizing flows for molecular sampling. The field divides into two main branches that reflect complementary perspectives on generative modeling for molecules. The first branch, Regression-Based Flow Training Methods, focuses on how to train normalizing flows without relying on maximum likelihood or adversarial objectives, instead using direct regression or forward-only schemes to match target distributions. The second branch, Generative Models for Molecular Design, encompasses a broader set of architectures and problem settings—ranging from equivariant flow matching to controllable generation—that address the unique geometric and chemical constraints of molecular data. Together, these branches illustrate a shift from classical likelihood-based training toward more flexible regression frameworks, while also highlighting the domain-specific challenges of sampling from high-dimensional molecular conformations and unnormalized Boltzmann distributions.

Several active lines of work reveal key trade-offs between training efficiency, sample quality, and physical interpretability. Some studies explore hybrid probability transport schemes (Hybrid Probability Transport[3]) or methods that handle unnormalized target densities directly (Molecular Unnormalized Distributions[4]), addressing the difficulty of computing partition functions in molecular systems. Others investigate equivariant architectures (Equivariant Flow Matching[1]) or domain-specific applications (Flow in Bioinformatics[5], Controllable Drug Generation[6]) that respect molecular symmetries and enable goal-directed design. Within this landscape, Boltzmann

Generators[0] sits squarely in the Direct Regression Training cluster, closely aligned with Forward Only Regression[2]. Both emphasize training flows via regression objectives rather than likelihood maximization, but Boltzmann Generators[0] specifically targets equilibrium sampling from Boltzmann distributions, whereas Forward Only Regression[2] explores a more general forward-pass training paradigm. This positioning underscores an emerging theme: leveraging regression-based objectives to bypass expensive likelihood computations while maintaining the invertibility and exact sampling guarantees that normalizing flows provide.

Related Works in Same Category

The following **1 sibling papers** share the same taxonomy leaf node with the original paper:

1. FORT: Forward-Only Regression Training of Normalizing Flows

Authors: D Rehman, O Davis, J Lu, J Tang, M Bronstein | **Year/Venue:** 2025 | **URL:** [View paper](#)

Abstract

Sampling of molecular systems. In this paper, we revisit classical TRAINING (FORT), a novel regression-based training can train the normalizing flow solely based on samples from the

△ Similarity Notice

These papers appear to be the same work or very close variants. Both papers share an identical title ('Efficient Regression-based Training of Normalizing Flows for Boltzmann Generators'), nearly identical abstracts describing the REGFLOW method, and the same core technical contributions including regression-based training objectives, forward-backward self-consistency regularization, and experiments on alanine dipeptide/tripeptide/tetrapeptide. The candidate paper appears to be a later version with minor formatting differences and potentially updated results (e.g., Table 2 shows slight numerical variations), but the fundamental methodology, approach, and contributions are essentially identical.

Contributions Analysis

Overall novelty summary. The paper proposes RegFlow, a regression-based training objective for normalizing flows applied to Boltzmann Generators for molecular conformations. It sits in the 'Direct Regression Training for Normalizing Flows' leaf, which contains only two papers total. This is a sparse research direction within the broader taxonomy of seven papers across five leaf nodes, suggesting the specific combination of regression training and normalizing flows for molecular sampling remains relatively unexplored compared to adjacent areas like flow matching or diffusion-based methods.

The taxonomy reveals neighboring work in flow matching for molecular generation, which includes equivariant flow matching for conformer generation and broader bioinformatics applications. These adjacent branches emphasize continuous normalizing flows trained via vector field regression, whereas the paper's leaf focuses specifically on discrete normalizing flows with regression objectives that avoid maximum likelihood. The taxonomy explicitly excludes flow matching from this category, positioning the work as an alternative training paradigm that retains invertibility guarantees while bypassing likelihood computation challenges inherent in classical normalizing flow training.

Among twenty-five candidates examined, the analysis identifies limited prior work overlap. The core RegFlow objective examined ten candidates with one appearing to provide overlapping prior work, as does the forward-backward self-consistency regularization. The energy-free targeted free energy perturbation method examined five candidates with none clearly refuting it. These statistics reflect a focused semantic search rather than exhaustive coverage, suggesting that within the examined scope, the regression training framework and regularization strategies show moderate novelty, while the free energy perturbation component appears less contested by prior literature.

Based on the limited search scope of top-twenty-five semantic matches, the work appears to occupy a relatively sparse position in the taxonomy, with only one sibling paper in its immediate category. The contribution-level analysis suggests the core training objective has some precedent among examined candidates, while the free energy method shows less overlap. However, these findings are constrained by the search methodology and do not constitute an exhaustive assessment of all relevant prior work in regression-based flow training or molecular sampling.

This paper presents **3 main contributions**, each analyzed against relevant prior work:

Contribution 1: REGFLOW: Regression-based training objective for normalizing flows

Description: The authors introduce REGFLOW, a new training framework for classical normalizing flows that replaces maximum likelihood estimation with a simple regression objective. This approach maps prior samples to targets computed using optimal transport couplings or a pre-trained continuous normalizing flow, avoiding the numerical instability and computational expense of traditional MLE training.

This contribution was assessed against **10 related papers** from the literature. Papers with potential prior art are analyzed in detail with textual evidence; others receive brief assessments.

1. Normalizing Flows for Conformal Regression

URL: [View paper](#)

Brief Assessment

Conformal Regression Flows[15] focuses on conformal prediction for uncertainty estimation using normalizing flows to optimize calibration metrics. This is fundamentally different from REGFLOW's regression-based training framework that replaces MLE with l_2 -regression objectives for learning invertible mappings in generative modeling contexts.

2. Normalizing Flow as a Flexible Fidelity Objective for Photo-Realistic Super-resolution

URL: [View paper](#)

Brief Assessment

Photo Realistic Superresolution[19] applies normalizing flows to image super-resolution tasks with adversarial training, not to general regression-based training frameworks that replace maximum likelihood estimation for normalizing flows in scientific applications like Boltzmann generators.

3. On Learning the Tail Quantiles of Driving Behavior Distributions via Quantile Regression and Flows

URL: [View paper](#)

Brief Assessment

Tail Quantiles Driving[20] focuses on quantile regression and autoregressive quantile flows for predicting driver behavior distributions in autonomous driving scenarios, not on general regression-based training frameworks for normalizing flows that avoid maximum likelihood estimation.

4. Human pose regression with residual log-likelihood estimation

URL: [View paper](#)

Brief Assessment

Residual Log Likelihood[14] focuses on human pose estimation using normalizing flows to model output distributions for regression tasks, not on training normalizing flows themselves as generative models for molecular systems or general distribution matching.

5. Beyond Squared Error: Exploring Loss Design for Enhanced Training of Generative Flow Networks

URL: [View paper](#)

Brief Assessment

GFlowNet Loss Design[18] focuses on regression losses for generative flow networks (GFlowNets), which are designed to sample from unnormalized distributions. This is fundamentally different from REGFLOW's regression-based training for classical normalizing flows that avoids maximum likelihood estimation.

6. FORT: Forward-Only Regression Training of Normalizing Flows

URL: [View paper](#)

Prior Art Analysis

Forward Only Regression[2] demonstrates that a regression-based training objective for normalizing flows that avoids maximum likelihood estimation was already proposed. Both papers introduce regression objectives that map prior samples to targets, bypassing MLE training's numerical instability. The candidate paper explicitly describes training normalizing flows using a simple ℓ_2 -regression objective that maps prior samples to pre-computed targets, which is the same core approach claimed as novel in the original paper.

Evidence

Evidence 1 - **Rationale:** Both papers describe the same core contribution: a regression-based training objective for normalizing flows using ℓ_2 -regression that maps prior samples to pre-computed targets, avoiding MLE training. - **Original:** we propose regression training of normalizing flows (regflow), a novel and scalable regression-based training objective that bypasses the numerical instability and computational challenge of conventional maximum likelihood training in favor of a simple ℓ_2 -regression objective. specifically, regflow... - **Candidate:** we introduce regression training of normalizing flows (regflow), a novel regression-based training objective for classical normalizing flows that marks a significant departure from the well-established mle training objective. our key insight is that access to coupled samples from any invertible map is s...

Evidence 2 - **Rationale:** The mathematical formulation of the regression objective is identical in both papers, showing that the same training approach was already described in Forward Only Regression[2]. - **Original:** $l(\theta) = \mathbb{E}_{x_0, x_1} \mathbb{E}_h \|f_{1, \theta}(x_0) - f^{-1}(x_0)\|_2^2 + \lambda r$ where $r = \mathbb{E}_{x_0, x_1} \|x_1 - x_0\|_2^2 + \lambda r$, where r is a regularization strategy and $\lambda r \in \mathbb{R}^+$ is the strength of regularization. explicit in eq. (5) is the need to procure one-step targets $x_1 = f^{-1}(x_0)$ from a known invertible mapping f^{-1} . - **Candidate:** $l(\theta) = \mathbb{E}_{x_0, x_1} \mathbb{E}_h \|f_{1, \theta}(x_0) - f^{-1}(x_0)\|_2^2 + \lambda r$ where $r = \mathbb{E}_{x_0, x_1} \|x_1 - x_0\|_2^2 + \lambda r$, (5) where r is a regularization strategy and $\lambda r \in \mathbb{R}^+$ is the strength of regularization. explicit in eq. (5) is the need to procure one-step targets $x_1 = f^{-1}(x_0)$ from a known invertible mapping f^{-1} .

Evidence 3 - **Rationale:** Both papers propose the same two target generation strategies (CNF-based and OT-based), indicating that this approach was already established in Forward Only Regression[2]. - **Original:** we propose endpoint targets that are either: (1) outputs of a larger pretrained cnf; or (2) the solution to a pre-computed ot map done offline as a pre-processing step. - **Candidate:** we propose endpoint targets that are either: (1) outputs of a larger pretrained cnf; or (2) the solution to a pre-computed ot map done offline as a pre-processing step.

7. Improving and generalizing flow-based generative models with minibatch optimal transport

URL: [View paper](#)

Brief Assessment

Minibatch Optimal Transport[12] focuses on conditional flow matching for continuous normalizing flows (CNFs), not classical normalizing flows. The candidate's regression objective is designed for CNFs with simulation-free training, while REGFLOW targets classical normalizing flows to avoid MLE instability and enable one-step exact likelihoods without numerical ODE simulation.

8. High-order flow matching: Unified framework and sharp statistical rates

URL: [View paper](#)

Brief Assessment

High Order Matching[16] focuses on flow matching models with high-order trajectory derivatives for improved expressiveness, not on regression-based training of classical normalizing flows to avoid MLE instability.

9. Autoregressive Quantile Flows for Predictive Uncertainty Estimation

URL: [View paper](#)

Brief Assessment

Autoregressive Quantile Flows[17] focuses on a scoring rule-based objective for quantile flows that avoids Jacobian determinants, but targets predictive uncertainty estimation rather than the general regression-based training framework for classical normalizing flows proposed in the original paper. The candidate does not demonstrate prior work on mapping flows to optimal transport couplings or pre-trained CNF targets.

10. Normalizing Flow Regression for Bayesian Inference with Offline Likelihood Evaluations

URL: [View paper](#)

Brief Assessment

Offline Likelihood Flows[13] focuses on Bayesian inference with offline likelihood evaluations for posterior approximation, while REGFLOW addresses generative modeling with regression objectives to avoid MLE instability in normalizing flows training.

Contribution 2: Forward-backward self-consistency regularization

Description: The authors propose a novel forward-backward self-consistency regularizer that ensures invertibility at the output level without requiring computation of the Jacobian determinant. This regularization strategy enhances numerical stability during training and opens possibilities for less constrained architectures.

This contribution was assessed against **10 related papers** from the literature. Papers with potential prior art are analyzed in detail with textual evidence; others receive brief assessments.

1. Neural encoding and decoding with a flow-based invertible generative model

URL: [View paper](#)

Prior Art Analysis

Flow Encoding Decoding[23] demonstrates prior work on forward-backward self-consistency regularization for ensuring invertibility in normalizing flows. The candidate paper explicitly proposes a 'forward-backward self-consistency regularizer' that ensures invertibility at

the output level without requiring Jacobian determinant computation, which directly addresses the same technical challenge as the original paper's contribution. Both papers use this regularization to maintain numerical stability and invertibility during training of flow-based models.

Evidence

Evidence 1 - **Rationale:** While the candidate uses 'jacobian clamping' terminology, the implementation shows a forward-backward consistency approach that ensures invertibility through regularization, similar to the original paper's claimed contribution. - **Original:** to enhance numerical stability, regflow employs effective regularization strategies such as a new forward-backward self-consistency loss that enjoys painless implementation - **Candidate:** the regularization is implemented as $l_{jc} = (\max(q, \lambda +) - \lambda +)^2 + (\min(q, \lambda -) - \lambda -)^2$ to control the change ratio q to lie within $[\lambda -, \lambda +]$. we can adjust the interval to make $\|g_{x \rightarrow s}(x_f) - g_{x \rightarrow s}(x' f)\|$ small when $\|x_f - x' f\|$ is small. therefore, the jacobian clamping can facilitate synchronous conv...

Evidence 2 - **Rationale:** The candidate paper implements forward-backward consistency through reconstruction losses that ensure the model can map forward and backward while maintaining consistency, which is the core principle of the original paper's claimed contribution. - **Original:** the second regularizer is a new forward-backward self-consistency regularizer that ensures invertibility at the output level, but at double the computational cost. however, interestingly, since it does not require the jacobian, it opens up potential directions for less constrained architectures. - **Candidate:** constraints are imposed on x and \hat{x} of the image domain, x_f and \hat{x}_f of the feature domain, and s and \hat{s} of the neural activity domain. concretely, the following three losses are added to the holistic loss: $l_x = \|\hat{x} - x\|_2^2$, $l_{x_f} = \|\hat{x}_f - x_f\|_2^2$, $l_s = \|\hat{s} - s\|_2^2$

2. BiCAPT: Bidirectional Computer-Assisted Pronunciation Training with Normalizing Flows

URL: [View paper](#)

Brief Assessment

BiCAPT[27] focuses on computer-assisted pronunciation training using normalizing flows for mispronunciation detection and correction. The paper does not discuss forward-backward self-consistency regularization or training stability techniques for normalizing flows.

3. Koopman Invertible Autoencoder: Leveraging Forward and Backward Dynamics for Temporal Modeling

URL: [View paper](#)

Brief Assessment

Koopman Invertible Autoencoder[25] focuses on temporal modeling in dynamical systems using Koopman operator theory with invertible neural networks for bidirectional dynamics. The original paper's forward-backward self-consistency regularizer is designed specifically for normalizing flows to ensure invertibility without Jacobian determinant computation, which is a different technical context and application domain than temporal sequence modeling.

4. Bidirectional Modeling and Analysis of Brain Aging with Normalizing Flows

URL: [View paper](#)

Brief Assessment

Brain Aging Flows[29] focuses on bidirectional brain aging modeling using conditional normalizing flows for age prediction and template generation, not on training stability or invertibility regularization techniques for normalizing flows.

5. SyMOT-Flow: Learning optimal transport flow for two arbitrary distributions with maximum mean discrepancy

URL: [View paper](#)

Brief Assessment

SyMOT Flow[26] uses symmetric forward-backward loss for distribution matching in optimal transport, not for ensuring invertibility in normalizing flow training as a regularization strategy to avoid Jacobian computation.

6. Bidirectional consistency models

URL: [View paper](#)

Brief Assessment

Bidirectional Consistency Models[21] focuses on bidirectional traversal along probability flow ODEs for diffusion models, not on invertibility regularization for normalizing flows. The technical contexts and applications differ fundamentally.

7. Semi-Supervised Learning for Anomaly Traffic Detection via Bidirectional Normalizing Flows

URL: [View paper](#)

Brief Assessment

Anomaly Traffic Detection[24] focuses on semi-supervised anomaly detection in network traffic using bidirectional normalizing flows for data transformation, not on training stability or architectural constraints in normalizing flows for generative modeling.

8. A Normalizing Flow-Based Bidirectional Mapping Residual Network for Unsupervised Defect Detection

URL: [View paper](#)

Brief Assessment

Bidirectional Defect Detection[28] focuses on anomaly detection using normalizing flows for defect detection in images, not on training stability or invertibility regularization for normalizing flows in general applications like Boltzmann generators.

9. Reliable Event Generation With Invertible Conditional Normalizing Flow

URL: [View paper](#)

Brief Assessment

Invertible Event Generation[22] focuses on event stream generation using normalizing flows with intensity-guided conditional mechanisms, not on forward-backward self-consistency regularization for general normalizing flow training stability.

10. Invertible Modeling of Bidirectional Relationships in Neuroimaging With Normalizing Flows: Application to Brain Aging.

URL: [View paper](#)

Brief Assessment

Invertible Brain Aging[30] applies normalizing flows to neuroimaging for brain aging modeling, not to training stability or architectural constraints in flow-based generative models. The technical domains and objectives differ fundamentally.

Contribution 3: Energy-free targeted free energy perturbation method

Description: The authors develop a new approach to Targeted Free Energy Perturbation that trains normalizing flows using only samples from metastable states, eliminating the need for costly energy function evaluations during training. This represents a distinct capability compared to traditional MLE-trained normalizing flows.

This contribution was assessed against **5 related papers** from the literature. Papers with potential prior art are analyzed in detail with textual evidence; others receive brief assessments.

1. Targeted Free Energy Perturbation Revisited: Accurate Free Energies from Mapped Reference Potentials.

URL: [View paper](#)

Brief Assessment

Targeted Free Energy[9] focuses on mapping reference potentials for quantum mechanical free energy calculations in molecular systems, not on training normalizing flows without energy evaluations for Boltzmann generators in the context described by the original paper.

2. FreeFlow: Latent Flow Matching for Free Energy Difference Estimation

URL: [View paper](#)

Brief Assessment

FreeFlow[11] focuses on estimating free energy differences between molecular systems using flow matching in latent space, not on training normalizing flows without energy evaluations for targeted free energy perturbation as described in the original paper's contribution.

3. Multimap targeted free energy estimation

URL: [View paper](#)

Brief Assessment

Multimap Free Energy[8] focuses on computing free energies at QM level from molecular simulations using multiple configuration maps, not on training normalizing flows without energy evaluations for general Boltzmann generators.

4. Accurate Free Energy Estimations of Molecular Systems Via Flow-based Targeted Free Energy Perturbation

URL: [View paper](#)

Brief Assessment

Flow Targeted Perturbation[10] focuses on molecular free energy calculations using normalizing flows trained on metastable state samples, but does not address the specific training methodology of normalizing flows without energy evaluations during training as described in the original paper's RegFlow framework.

5. Lattice free energies of molecular crystals using normalizing flow

URL: [View paper](#)

Brief Assessment

Lattice Free Energies[7] focuses on targeted free energy perturbation (TFEP) for molecular crystal polymorphs using normalizing flows trained on MD data, but still requires energy evaluations during inference for free energy calculations. The original paper's contribution is training normalizing flows without energy evaluations during training for Boltzmann generators in molecular conformations, which is a distinct application and methodology.

Appendix: Text Similarity Detection

Textual similarity detection checked 25 papers and found 4 similarity segment(s) across 2 paper(s).

The following **2 paper(s)** were detected to have high textual similarity with the original paper. These may represent different versions of the same work, duplicate submissions, or papers with substantial textual overlap. Readers are advised to verify these relationships independently.

1. FORT: Forward-Only Regression Training of Normalizing Flows

Detected in: Core Task (sibling), Contribution: contribution_1

△ **Note:** This paper shows substantial textual similarity with the original paper. It may be a different version, a duplicate submission, or contain significant overlapping content. Please review carefully to determine the nature of the relationship.

2. Multimap targeted free energy estimation

Detected in: Contribution: contribution_3

△ **Note:** This paper shows substantial textual similarity with the original paper. It may be a different version, a duplicate submission, or contain significant overlapping content. Please review carefully to determine the nature of the relationship.

References

- [0] Efficient Regression-based Training of Normalizing Flows for Boltzmann Generators [View paper](#)
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- [3] Equivariant flow matching with hybrid probability transport for 3d molecule generation [View paper](#)
- [4] $\hat{\mu}$: Molecular Unnormalized Distributions With Deep Generative Models Toward the Acceleration of Molecular Design and Conformational Sampling With Deep $\hat{\mu}$ [View paper](#)
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- [10] Accurate Free Energy Estimations of Molecular Systems Via Flow-based Targeted Free Energy Perturbation [View paper](#)
- [11] FreeFlow: Latent Flow Matching for Free Energy Difference Estimation [View paper](#)
- [12] Improving and generalizing flow-based generative models with minibatch optimal transport [View paper](#)
- [13] Normalizing Flow Regression for Bayesian Inference with Offline Likelihood Evaluations [View paper](#)
- [14] Human pose regression with residual log-likelihood estimation [View paper](#)
- [15] Normalizing Flows for Conformal Regression [View paper](#)

- [16] High-order flow matching: Unified framework and sharp statistical rates [View paper](#)
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