Adaptive Quantization in GFN for Probabilistic Sequential Prediction

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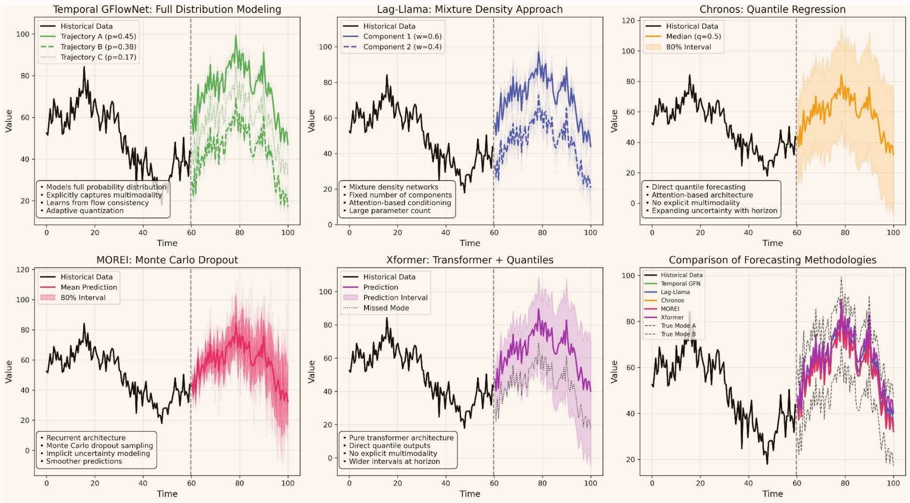
Overview of Temporal GFN

1. Methodology
2. Core Innovation
3. Key Takeaway
4. Experiments and results



What Happens During Training?

Temporal GFN learns to generate **sequences of forecasted values** by taking actions (predicting quantized values) step by step. The key goals are:

1. **Sample high-reward future trajectories** (matching the ground truth),
2. **Adapt the quantization resolution** over time based on model performance,
3. **Train a forward policy** (and optionally backward policy) using **Trajectory Balance loss** with gradients propagated through **Straight-Through Estimators (STE)**.

GFN for Time Series: A forecast Cursor

Goal: Construct initial GFN state from the time series history (context window).

- Given a dataset with time series samples $x_{1:T}$, we split each into:
  - **Context window** $x_{1:C}$ → used as input ("observed history").
  - **Forecast horizon** $x_{C+1:C+H}$ → ground truth to evaluate the prediction.
- The **initial state** s_0 is constructed as:

$$s_0 = \mathrm{Encoder}(x_{1:C})$$

  where the encoder could be an LSTM, Transformer encoder, or sliding-window patch embedding layer. This produces a fixed-length latent representation that the GFN policy can condition on.
- The state representation includes:
  - Latent embedding of the history window,
  - A **forecast cursor** (step counter $t = 0$),
  - Possibly a cache of previously sampled outputs if needed for autoregression.

Discrete Action Space via Quantization

Goal: Convert continuous forecast space into discrete tokens/actions.

- The normalized range of values $[v_{\min}, v_{\max}]$ is partitioned into K bins:

$$\{q_1, q_2, \dots, q_K\}, \quad q_k = v_{\min} + (k - 0.5) \cdot \Delta, \quad \Delta = \frac{v_{\max} - v_{\min}}{K}$$

- These **quantized centers** q_k act as tokens. At each forecasting step t, the GFN **chooses one token** q_k as the predicted value for x_{C+t+1}.
- **Each GFN action** is selecting one of these bins:

$$a_t \in \{q_1, q_2, \dots, q_K\}$$

- The quantized value is appended to the state, updating the forecast:

$$s_{t+1} = s_t \cup \{a_t\}$$

Trajectory Construction via Forward Policy

Goal: Build a full trajectory $\tau = (a_0, \ldots, a_{H-1})$ of quantized forecasts using a learned policy.

At each time step $t \in [0, H-1]$:

1. **Forward Policy Sampling:**
   - Compute logits $\mathbf{z}_t = f_\theta(s_t) \in \mathbb{R}^K$
   - Convert to probabilities over actions:

$$P_F(a_t = q_k | s_t) = \mathrm{softmax}(z_{t,k})$$

2. **Action Selection via STE:**
   - **Hard forward action:** sample or take argmax over P_F → yields discrete token $a_t^{\mathrm{hard}} = q_k$
   - **Soft value for gradient:** compute expected value:

$$a_t^{\mathrm{soft}} = \sum_k q_k \cdot P_F(a_t = q_k \mid s_t)$$

3. **State Update:**
   - Append discrete a_t^{hard} to current sequence.
   - Update s_{t+1} with new time step's embedding (can use a positional encoding or RNN hidden state update).
   - Repeat for H steps to get complete trajectory $\tau = (a_0, \ldots, a_{H-1})$

Reward Computation

Goal: Evaluate trajectory quality by comparing with true future values.

Let true future be $y = x_{C+1:C+H}$, predicted quantized values $z = (a_0, ..., a_{H-1})$

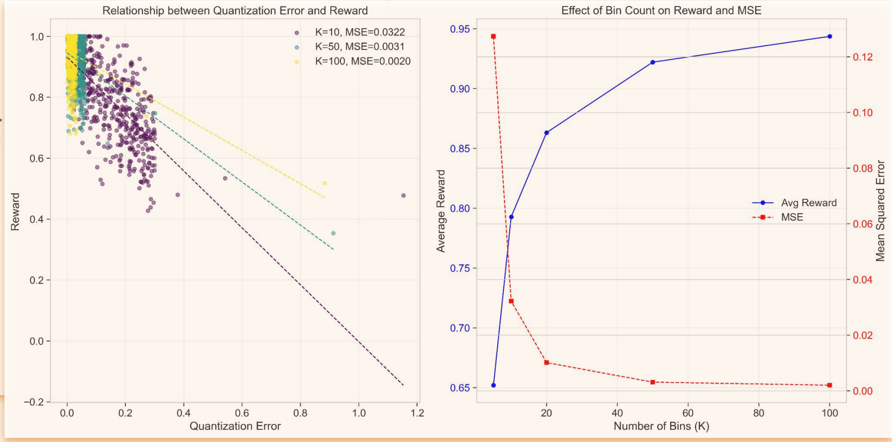
- Define **normalized squared error**:

$$\mathrm{NSE}(z, y) = \frac{1}{H} \sum_{t=1}^{H} \frac{(z_t - y_t)^2}{(v_{\max} - v_{\min})^2}$$

- Define **exponential reward**:

$$R(\tau) = \exp(-\beta \cdot \mathrm{NSE}(z, y))$$

where β is a scaling constant (e.g., 5–20).



Adaptive Quantization Update

Goal: Adjust number of bins K based on model learning progress.

After each epoch:

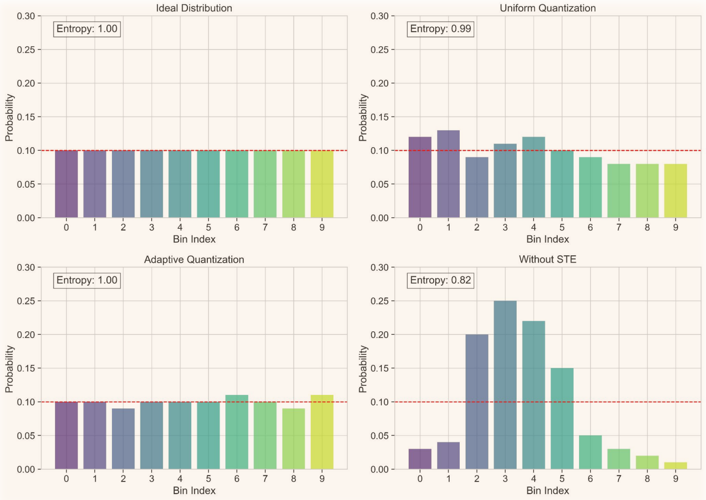
1. **Track:**
   - Recent average reward improvement ΔR_e
   - Policy entropy $H_e = \mathbb{E}_t[H(P_F(a_t|s_t))] \in [0, 1]$
2. **Update factor:**

$$\eta_e = 1 + \lambda \left(\frac{\max(0, \epsilon - \Delta R_e)}{\epsilon} + (1 - H_e) \right)$$

3. **New bin count:**

$$K_e = \min(K_{\max}, \lfloor K_{e-1} \cdot \eta_e \rfloor)$$

4. **Re-quantize bins:**
   - Uniformly repartition $[v_{\min}, v_{\max}]$ into new K_e bins.
   - Optionally interpolate soft logits from old K to new K if needed.



Loss and training Objective

Goal: Train forward policy (and optionally backward policy) to match desired sampling distribution $P^*(\tau) \propto R(\tau)$

Trajectory Balance Loss:

For trajectory $\tau = (s_0 \to s_1 \to \cdots \to s_H)$:

$$\mathcal{L}_{TB} = \left(\log Z + \sum_{t=0}^{H-1} \log P_F(a_t \mid s_t) - \sum_{t=1}^{H} \log P_B(s_{t-1} \mid s_t) - \log R(\tau) \right)^2$$

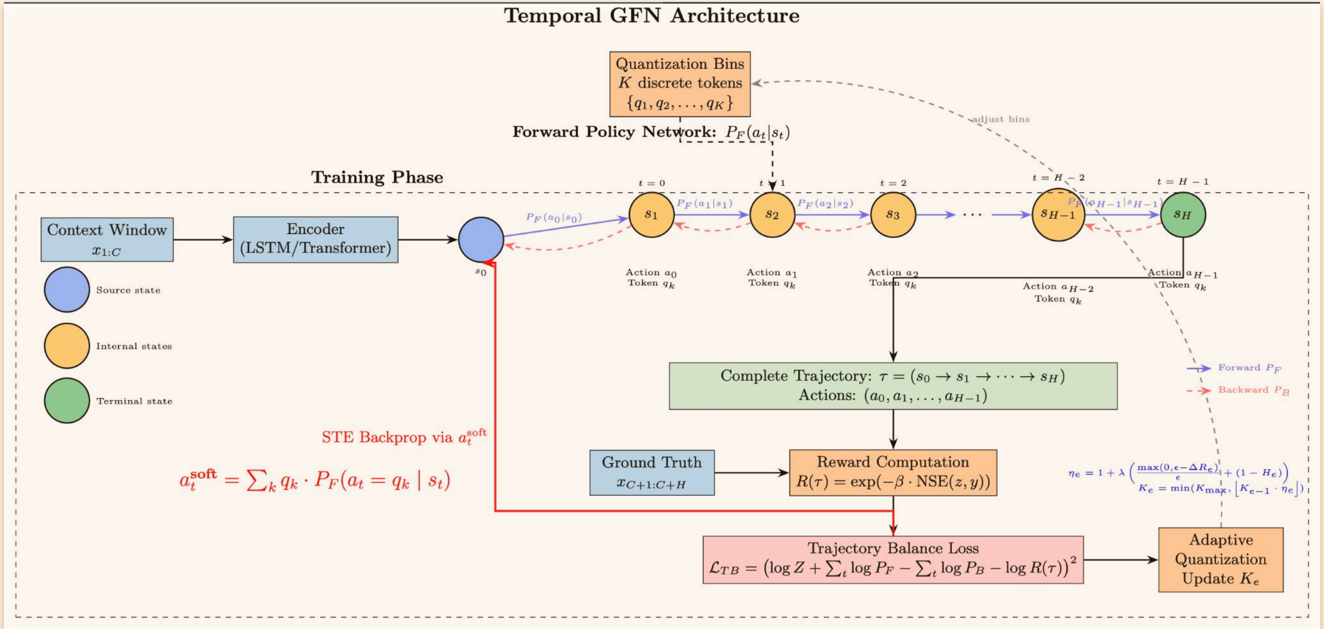
- **Optional entropy regularization:**

$$\mathcal{L}_{\text{entropy}} = -\lambda_H \sum_{t=0}^{H-1} H(P_F(\cdot|s_t))$$

- **Total loss:**

$$\mathcal{L}_{\text{total}} = \mathcal{L}_{TB} + \mathcal{L}_{\text{entropy}}$$

GFN Architecture



Experiments and results

Table 1: Aggregated Relative Performance vs. RL/MCMC on Benchmark I.

Method	CRPS (↓)	WQL (↓)	MASE (↓)	Avg. Improv. (%)
Temporal GFN (Adaptive K20)	0.1674	0.2273	**0.8938**	-
Temporal GFN (Fixed K20)	0.1781	0.2401	0.9363	-5.9%
Temporal GFN (Learned Pol. Adapt K10)	**0.1453**	**0.2137**	1.0345	+6.0%*
PPO	0.2299	0.3013	1.1759	-25.1%
SAC	0.2423	0.3227	1.2491	-29.5%
MCMC	0.2673	0.3522	1.3523	-35.5%

*Avg. Improv. for Learned Policy calculated based on CRPS/WQL vs Adaptive K20.

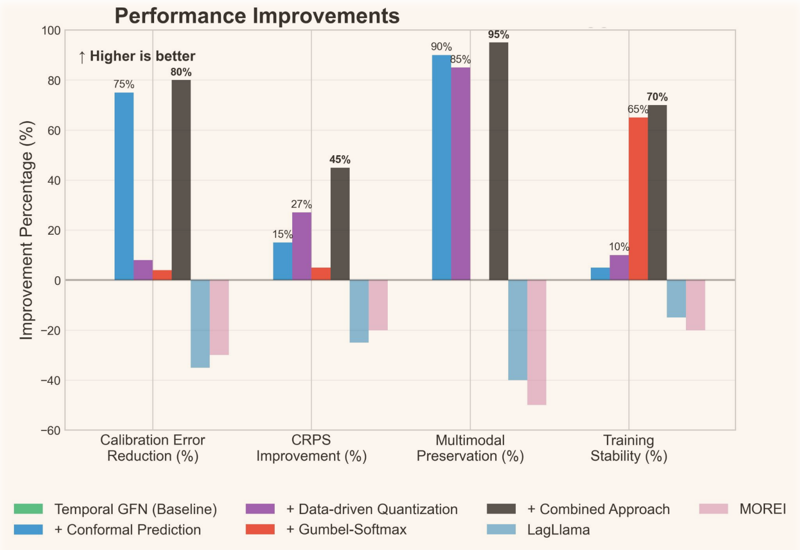
Table 2: Aggregated Relative Performance vs. SOTA Models (In-Domain / Zero-Shot).

Model	Eval Setting	CRPS (↓)	WQL (↓)	MASE (↓)	Calib. Err. (↓)	Multimod. (↑)
Temporal GFN	Zero-Shot / In-Domain	**0.1542**	**0.2158**	**0.9378**	**0.0348**	**0.8762**
Lag-Llama	Zero-Shot / Pretrained	0.1675	0.2401	0.9532	0.0623	0.7234
Chronos (Base)	Zero-Shot / Pretrained	0.1731	0.2534	1.0273	0.0571	0.6957
MOREI (Base)	Task-Specific Trained	0.1859	0.2678	1.0871	0.0745	0.6182
TimeFM	Task-Specific Trained	0.2076	0.2846	1.1258	0.1183	0.3012
Temporal GFN (Learned Pol.)	In-Domain	0.1453	0.2137	1.0345	-	-

Main Temporal GFN results reflect strong performance across settings. Calib. Err. & Multimod. primarily from healthcare/extended benchmarks. Task-Specific models trained per dataset. Learned Policy results from Table 3.

Table 3: Ablation Study Configurations and Main Results.

Experiment Config	Quantization	Start K	Policy Type	CRPS	WQL	MASE
Fixed K=10	fixed	10	uniform	0.1546	0.2346	1.1946
Fixed K=20	fixed	20	uniform	0.1921	0.2521	0.9721
Adaptive K=10	adaptive	10	uniform	0.1688	0.2408	1.1048
Adaptive K=20	adaptive	20	uniform	0.1845	0.2385	**0.9532**
Learned Policy (Adapt K10)	adaptive	10	learned	**0.1453**	**0.2137**	1.0345



Thank You !