[논문 리뷰] Distribution-Free Multivariate Density Forecast

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1. DAN-NFN [1] 2. JDAN-NFN [2]

DAN-NFN

■ Problem Description of Density Forecast

- □ A positive-weighted ANN, named distribution approximation network (DAN)
- □ The other ANN, named network forecast network (NFN), is built as the forecaster of DAN
- □ DAN-NFN is trained through maximum likelihood estimation (MLE)

$$
f(y_{t+k}|X_t) = \begin{cases} w_0 \cdot \delta(y_{t+k}), & y_{t+k} = 0 \\ \bar{f}(y_{t+k}), & y_{t+k} \in (0,1) \\ w_1 \cdot \delta(y_{t+k-1}), & y_{t+k} = 1 \end{cases} \quad \mathbf{\Lambda} = \begin{cases} w_{0k} = [0,1], & w_{0k} = [0,1], \\ w_{0k} = w_1 \in [0,1], & y_{0k} = [0,1], \\ \bar{f}(y_{t+k}), & y_{t+k} = 1 \end{cases} \quad \mathbf{\Lambda} = \begin{cases} w_{0k} = [0,1], & w_{0k} = [0,1], \\ \bar{f}(y_{t+k}), & y_{t+k} = [0,1], \\ \int_{0}^{1} \bar{f}(y_{t+k}), & y_{t+k} = 0 \end{cases} \quad \mathbf{\Lambda} = \begin{cases} w_0, & y_{t+k} = 0 \\ w_0 + w_1 \in [0,1], & y_{t+k} = [0,1], \\ \int_{0}^{1} \bar{f}(y_{t+k}), & y_{t+k} = 0 \\ w_0 + w_1 \in [0,1], & y_{t+k} = [0,1], \\ w_0 + w_1 \in [0,1], & y_{t+k} = [0,1], \\ \lim_{y \to 0} \bar{F}(y) = 0, & y_{t+k} = [0,1], \\ \lim_{y \to 0} \bar{F}(y) = 0, & y_{t+k} = [0,1], \\ \lim_{y \to 0} \bar{F}(y_{t+k}), & y_{t+k} = 1 \end{cases} \quad \mathbf{\Lambda} = \begin{cases} w_0 \in [0,1], & w_1 \in [0,1], \\ w_0 + w_1 \in [0,1], & y_{t+k} = [0,1], \\ \lim_{y \to 0} \bar{F}(y) = 0, & y_{t+k} = [0,1], \\ \lim_{y \to 0} \bar{F}(y) = 1 - w_0 - w_1, & y_{t+k} = [0,1], \\ \lim_{y \to 0} \bar{F}(y_{t+k}), & y_{t+k} = 1 \end{cases} \quad \mathbf{\Lambda} = \begin{cases} w_0 \in [0,1], & w_1 \in [0,1], \\ w_0 + w_1 \in [0,1], & y_{t+k} = [0,1], \\ \lim_{y \to 0} \bar{F}(y) =
$$

▣ Framework of DAN-NFN

□ NFN 에서 DAN의 W^+ , B, n_0 , n_1 출력, DAN에서 입력 받은 weight를 이용하여 monotone non-decreasing CDF로 활용

$$
\overline{\Gamma}_D(y; \mathbf{W}^+, \mathbf{B}) = \frac{\Gamma_D(y; \mathbf{W}^+, \mathbf{B}) - \Gamma_D(L_y; \mathbf{W}^+, \mathbf{B})}{\Gamma_D(U_y; \mathbf{W}^+, \mathbf{B}) - \Gamma_D(L_y; \mathbf{W}^+, \mathbf{B})}
$$
(16)

▣ Framework of DAN-NFN

□ CDF를 PDF로 변환 가능하고, 이를 MLE기반 NLL을 통해 최적화

 \Box $NLL = \sum^{T} -ln\hat{f}(y_{t+k}|X_t)$

PDF
\n
$$
\hat{f}(y_{t+k}|X_t) = \begin{cases}\nn_0 \cdot n_1 \cdot \delta(y_{t+k}), & y_{t+k} = 0 \\
(1 - n_0) \overline{\Gamma'_D}(y_{t+k}; \mathbf{W}^+, \mathbf{B}), y_{t+k} \in (0,1) \\
n_0 \cdot (1 - n_1) \cdot \delta(y_{t+k} - 1), & y_{t+k} = 1\n\end{cases}
$$

$$
\frac{y_{t+k}^* - Loss from \{X_t, y_{t+k}^*\} \text{ and optimizer}}{\frac{\left[\prod_{\theta_{k+k}}^{H} y_{t+k}^* = 0, loss_t = -\ln(\widehat{w}_0) = -\ln(n_0 \cdot n_1), \right]}{\sqrt{\sigma_{\theta_N} loss_t = \frac{\partial[-\ln(n_0 \cdot n_1)]}{\partial n_0} \cdot \nabla_{\theta_N} n_0 + \frac{\partial[-\ln(n_0 \cdot n_1)]}{\partial n_1} \cdot \nabla_{\theta_N} n_1}} \cdot \frac{\text{optimize}}{\text{softmax}}{\text{Adam}(\nabla_{\theta_N} loss_t]} \text{H} \frac{y_{t+k}^* \in (0,1), loss_t = -\ln[\widehat{f}(y_{t+k}^* | X_t)] = -\ln[(1 - n_0) \cdot \overline{\Gamma}_D'(y_{t+k}^*; \mathbf{W}^+, \mathbf{B})], \right]}}{\left[\nabla_{\theta_N} loss_t = \left[\nabla_{\mathbf{W}^+}\{-\ln[(1 - n_0) \cdot \overline{\Gamma}_D'(y_{t+k}^*; \mathbf{W}^+, \mathbf{B})]\}\right]^T \cdot \nabla_{\theta_N} \mathbf{W}^+ + \right]} \frac{\left[\nabla_{\mathbf{B}}\{-\ln[(1 - n_0) \cdot \overline{\Gamma}_D'(y_{t+k}^*; \mathbf{W}^+, \mathbf{B})]\}\right]^T \cdot \nabla_{\theta_N} \mathbf{B}}{\frac{\partial \{(-\ln[(1 - n_0) \cdot \overline{\Gamma}_D'(y_{t+k}^*; \mathbf{W}^+, \mathbf{B})]\}}{\frac{\partial n_0}{\partial n_0}} \cdot \nabla_{\theta_N} n_0}} \cdot \nabla_{\theta_N} n_0}
$$

▣ Architecture of DAN-NFN

X

Shorted

layers

 (a)

□ Time series를 다를 수 있도록 LSTM Layer 사용

 $\mathbf{c}_{\tau-1}$

 $\mathbf{h}_{\tau-1}$

□ Gradient diffusion을 방지하기 위한 residual architecture

 $\rightarrow \odot \rightarrow \oplus$

 σ

 $tanh$

 \mathbf{h}_{τ}

 \mathbf{h}_{τ}

Fig. 2. Residual architecture and LSTM. (a) Structure of the residual network. (b) Information flow in LSTM. (c) LSTM layer.

 (b)

 $\mathbf{c}_{\mathcal{I}}$ $\left[\mathbf{x}_{t-d+1},...,\mathbf{x}_{t}\right]$

LSTM

layer, M

 $[\mathbf{h}_{t-d+1},...,\mathbf{h}_{t}]$

 (c)

Fig. 3. Structures of NFN and DAN. (a) NFN. (b) DAN.

■ Problem Description of Multivariate Density Forecast

- □ A joint distribution approximation network (JDAN) is a generic framework for approximating real continuous joint CDFs through a deep NN
- □ NFN outputs all parameters of JDAN
- □ JDAN-NFN is trained through maximum likelihood estimation (MLE)

Let $y_{t+\tau}$ be a *D*-dimensional random vector, then $f(\cdot)$ should satisfy the following conditions:

$$
\begin{cases}\nf(\cdot) \text{ is nonnegative and bounded,} \\
\int_{-\infty}^{+\infty} \cdots \int_{-\infty}^{+\infty} f(y) dy^1 \cdots dy^D = 1.\n\end{cases}
$$
\n(1)\n
$$
\begin{cases}\n(i) \ F(\cdot) \text{ is continuously differentiable,} \\
(ii) \ \frac{\partial^D(F(y))}{\partial y^1 \cdots \partial y^D} |_{y=y_{t+\tau}} \ge 0,\n\end{cases}
$$
\n(3)\n
$$
F(y_{t+\tau}) = \int_{-\infty}^{y_{t+\tau}^1} \cdots \int_{-\infty}^{y_{t+\tau}^D} f(y) dy^1 \cdots dy^D. \qquad (2)\n\begin{cases}\n(i) \ F(\cdot) \text{ is continuously differentiable,} \\
(ii) \ \frac{\partial^D(F(y))}{\partial y^1 \cdots \partial y^D} |_{y=y_{t+\tau}} \ge 0,\n\end{cases}
$$
\n(3)

JDAN-NFN

▣ Framework of JDAN-NFN

- □ NFN은 JDAN의 parameters인 W⁺, B, C 출력
- □ JDAN은 Tensor W⁺, B 으로 D차원의 CDFs 생성
- □ 각각 CDFs에 대한 correlation term을 $C\left(\frac{D}{2}\right)$ $\binom{D}{2}$ dim)로 표현 (time-variant correlation)
- □ JDAN-NFN 의 Ψ 는 DAN-NFN의 Γ 와 동일한 의미 $\mathbf{\Psi}^{\mathcal{C}} = \frac{1}{\binom{D}{2}} \cdot \sum_{i>d}^{D} \sum_{d=1}^{D-1} [\mathbf{C}_{di} \cdot (1 - \overline{\mathbf{\Psi}}^d) \cdot (1 - \overline{\mathbf{\Psi}}^i) + 1], \quad (10)$ $\mathbf{\Psi}_{\mathcal{J}}(\boldsymbol{y}_{t+\tau}; \mathbf{W}^+, \mathbf{B}, \mathbf{C}) = \mathbf{\Psi}^{\mathcal{C}} \cdot \prod_{i=1}^D \overline{\mathbf{\Psi}}^d.$ (11)

Loss function $L(\boldsymbol{\theta}_N, \boldsymbol{X}_t, \boldsymbol{y}_{t+\tau}^*) = -\ln[\widehat{f}(\boldsymbol{y}_{t+\tau}^*|\boldsymbol{X}_t)],$

Constraints of JDAN-NFN ▣

CDF of JDAN-NQF \Box

$$
\mathbf{\Psi}^{\mathcal{C}} = \frac{1}{\binom{D}{2}} \cdot \sum_{i>d}^{D} \sum_{d=1}^{D-1} [\mathbf{C}_{di} \cdot (1 - \overline{\mathbf{\Psi}}^d) \cdot (1 - \overline{\mathbf{\Psi}}^i) + 1], \quad (10)
$$

$$
\Psi_{\mathcal{J}}(\boldsymbol{y}_{t+\tau}; \mathbf{W}^+, \mathbf{B}, \mathbf{C}) = \Psi^{\mathcal{C}} \cdot \prod_{d=1}^{D} \overline{\Psi}^d.
$$
 (11)

$$
\mathbf{\Psi}_{\mathcal{J}}^{1,2} = \overline{\mathbf{\Psi}}^1 \cdot \overline{\mathbf{\Psi}}^2 \cdot [\mathbf{C}_{12} \cdot (1 - \overline{\mathbf{\Psi}}^1) \cdot (1 - \overline{\mathbf{\Psi}}^2) + 1]. \tag{40}
$$

$$
\frac{\partial^2 (\mathbf{\Psi}_{\mathcal{J}}^{1,2})}{\partial y^1 \partial y^2} = \frac{\partial \overline{\mathbf{\Psi}}^1}{\partial y^1} \cdot \frac{\partial \overline{\mathbf{\Psi}}^2}{\partial y^2} \cdot \left[\mathbf{C}_{12} \cdot (1 - 2\overline{\mathbf{\Psi}}^1) \cdot (1 - 2\overline{\mathbf{\Psi}}^2) + 1 \right].
$$
\n(41)

Limits of JDAN-NQF \Box $\lim_{\boldsymbol{y}_{t+\tau}\rightarrow+\infty}\boldsymbol{\Psi}_{\mathcal{J}}(\boldsymbol{y}_{t+\tau};\mathbf{W}^{+},\mathbf{B},\mathbf{C})$ $\mathbf{v} = \lim_{\boldsymbol{y}_{t+\tau} \to +\infty} \boldsymbol{\Psi}^{\mathcal{C}} \cdot \left(\prod_{d=1}^D \lim_{y_{t+\tau}^i \to +\infty} \overline{\boldsymbol{\Psi}}^d \right) = 1,$ (13) $\lim_{y_{t+\tau}^d \to -\infty} \Psi_{\mathcal{J}}(\mathbf{y}_{t+\tau}; \mathbf{W}^+, \mathbf{B}, \mathbf{C}) = 0, \forall d \in [1, D].$ (14)

JDAN-NFN

■ Evaluation measure

$$
\Box \quad \text{Reliability} \qquad \qquad b^{\alpha_{j,\,d}}_{\tau} = \alpha_{j,\,d} - \frac{1}{N} \sum_{i=1}^{N} H(\hat{q}^{\alpha_{j,\,d}}_{i+\tau|i} - y^{d*}_{i+\tau}),
$$

□ Sharpness

$$
\delta_{\tau}^{\alpha_{j,d}} = \frac{1}{N} \sum_{i=1}^{N} (\hat{q}_{i+\tau|i}^{1-\alpha_{j,d}/2} - \hat{q}_{i+\tau|i}^{\alpha_{j,d}/2}),
$$

$$
\Box \quad \text{Skill score} \qquad \qquad S_{t+\tau|t}^d = \sum_{j=1}^J \{ [H(\hat{q}_{t+\tau|t}^{\alpha_{j,d}} - y_{t+\tau}^{d*}) - \alpha_{j,d}] (y_{t+\tau}^{d*} - \hat{q}_{t+\tau|t}^{\alpha_{j,d}}) \},
$$

□ Variogram score

$$
VS_{t+\tau|t} = \sum_{i=1}^{D} \sum_{j=1}^{D} w_{ij} (|y_{t+\tau}^{i*} - y_{t+\tau}^{j*}|^{p} - E_{\widehat{\Phi}} |Y_i - Y_j|^{p})^2
$$

$$
\approx \sum_{i=1}^D \sum_{j=1}^D w_{ij} (|y^{i*}_{t+\tau}-y^{j*}_{t+\tau}|^p - \frac{1}{m}\sum_{k=1}^m |Y_i^{(k)}-Y_j^{(k)}|^p)^2,
$$

\Box **Dataset**

TABLE I DETAILS OF THE THREE DATA SETS

Results \Box

TABLE III PERFORMANCE DEMONSTRATION

denotes parametric approaches; denotes nonparametric approaches

[1] Hu, T., Guo, Q., Li, Z., Shen, X., & Sun, H. (2019). Distribution-free probability density forecast through deep neural networks. IEEE transactions on neural networks and learning systems, 31(2), 612-625.

[2] Meng, Z., Guo, Y., Tang, W., & Sun, H. (2022). Nonparametric multivariate probability density forecast in smart grids with deep learning. IEEE Transactions on Power Systems, 38(5), 4900-4915.