Normalizing Flow to Augmented Posterior: Conditional Density Estimation with Interpretable Dimension Reduction for High Dimensional Data

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Abstract : The conditional density characterizes the distribution of a response variable y given other predictor x and plays a key role in many statistical tasks, including classification and outlier detection. Although there has been abundant work on the problem of Conditional Density Estimation (CDE) for a low-dimensional response in the presence of a high-dimensional predictor, little work has been done for a high-dimensional response such as images. The promising performance of normalizing flow (NF) neural networks in unconditional density estimation acts as a motivating starting point. In this work, the authors extend NF neural networks when external x is present. Specifically, they use the NF to parameterize a one-to-one transform between a high-dimensional y and a latent z that comprises two components $[z_p, z_n]$. The z_p component is a low-dimensional subvector obtained from the posterior distribution of an elementary predictive model for x, such as logistic/linear regression. The z_n component is a high-dimensional independent Gaussian vector, which explains the variations in y not or less related to x. Unlike existing CDE methods, the proposed approach coined Augmented Posterior CDE (AP-CDE) only requires a simple modification of the common normalizing flow framework while significantly improving the interpretation of the latent component since z_p represents a supervised dimension reduction. In image analytics applications, AP-CDE shows good separation of \Box -related variations due to factors such as lighting condition and subject id from the other random variations. Further, the experiments show that an unconditional NF neural network based on an unsupervised model of z, such as a Gaussian mixture, fails to generate interpretable results.

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