

Normalising Flows for Conditional Density Estimation

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Conditional Density Estimation

Figure 1: QR code for CDE animation

Conditional density estimation (CDE) is a form of supervised learning with methods in statistics, machine learning and deep learning. It is a generalisation of regression. Instead of predicting a point estimate \hat{y} and generating a confidence or credible interval $\hat{y} \pm CI$, the task is to predict the full conditional density $p(y|x)$ of the data for a given query point x , an improved form of **uncertainty quantification (UQ)**.

Figure 2 shows kernel CDE [1] [2] using the faithful geyser data via the `hdrcde` R package, demonstrating an improvement in UQ by using CDE instead of intervals. Early CDE methods included Kernel-CDE, Mixture Density Networks [3] and discretisation of the target variable via class probability estimators [4] (Figure 1). Modern methods for CDE include Random Forest-CDE [5] and Bottleneck Conditional Density Estimation, a variation on Conditional-VAEs [6].

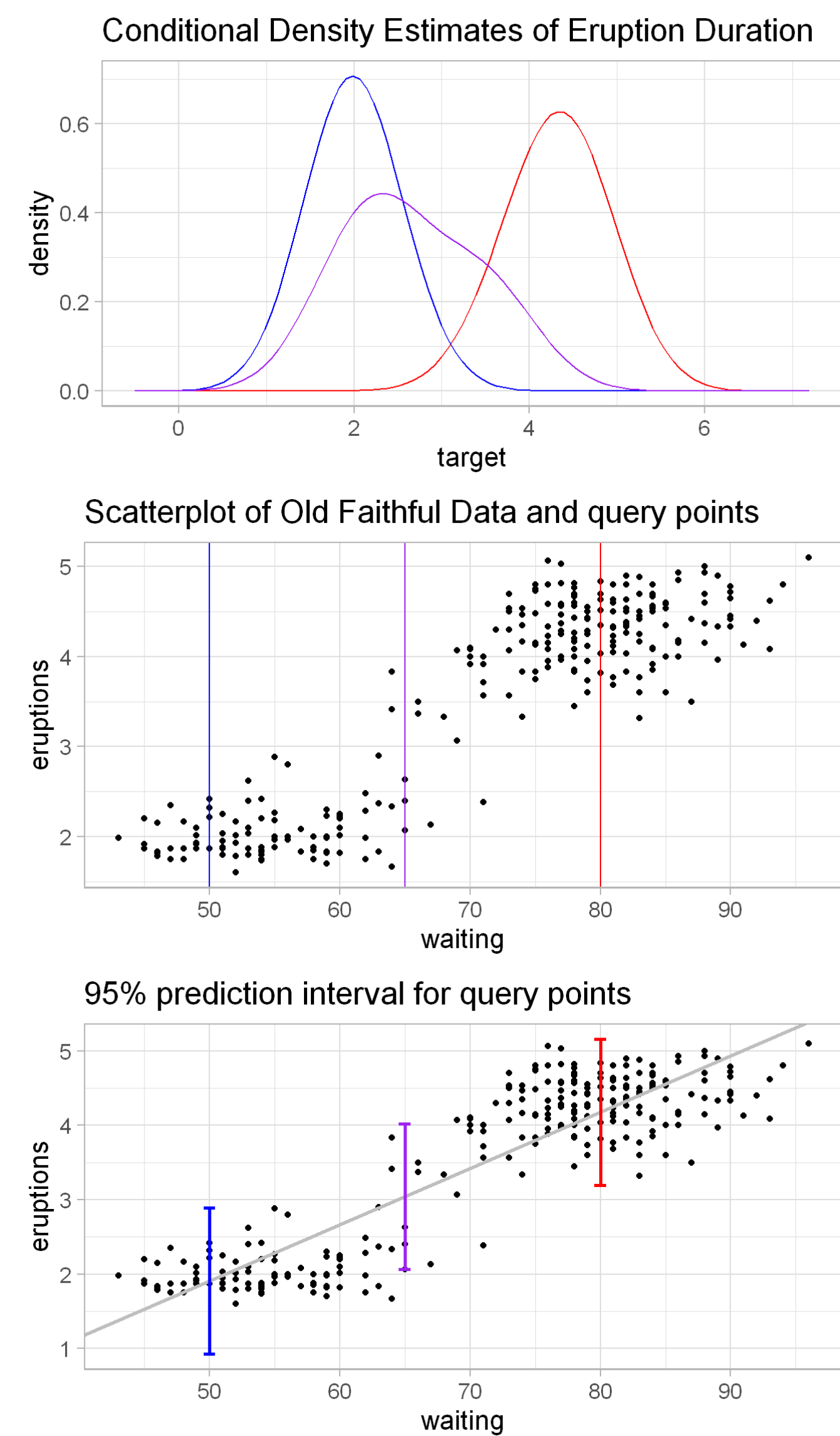


Figure 2: Demonstration of estimation using KCDE vs Simple Linear Regression & Prediction Intervals

Normalising Flows

Normalising flows (NFs) are sequences of invertible, differentiable, transformations (bijections) on a base probability distribution (often a simple Gaussian) to approximate the true density, which may be skewed, multi-modal or complex (even discontinuous) [7]. NFs were proposed as a density estimation procedure [8], then for use as approximate posteriors in variational inference (VI) [9]. They came to prominence for efficiency and expressiveness in both sampling (generative direction) and density evaluation (normalising direction). NFs fit alongside VAEs and GANs as recent DL generative models, however, VAEs and GANs are not efficient for density evaluation.

By the term *normalising flows* people mean *bijections which are convenient to compute, invert, and calculate the determinant of their Jacobian* [7].

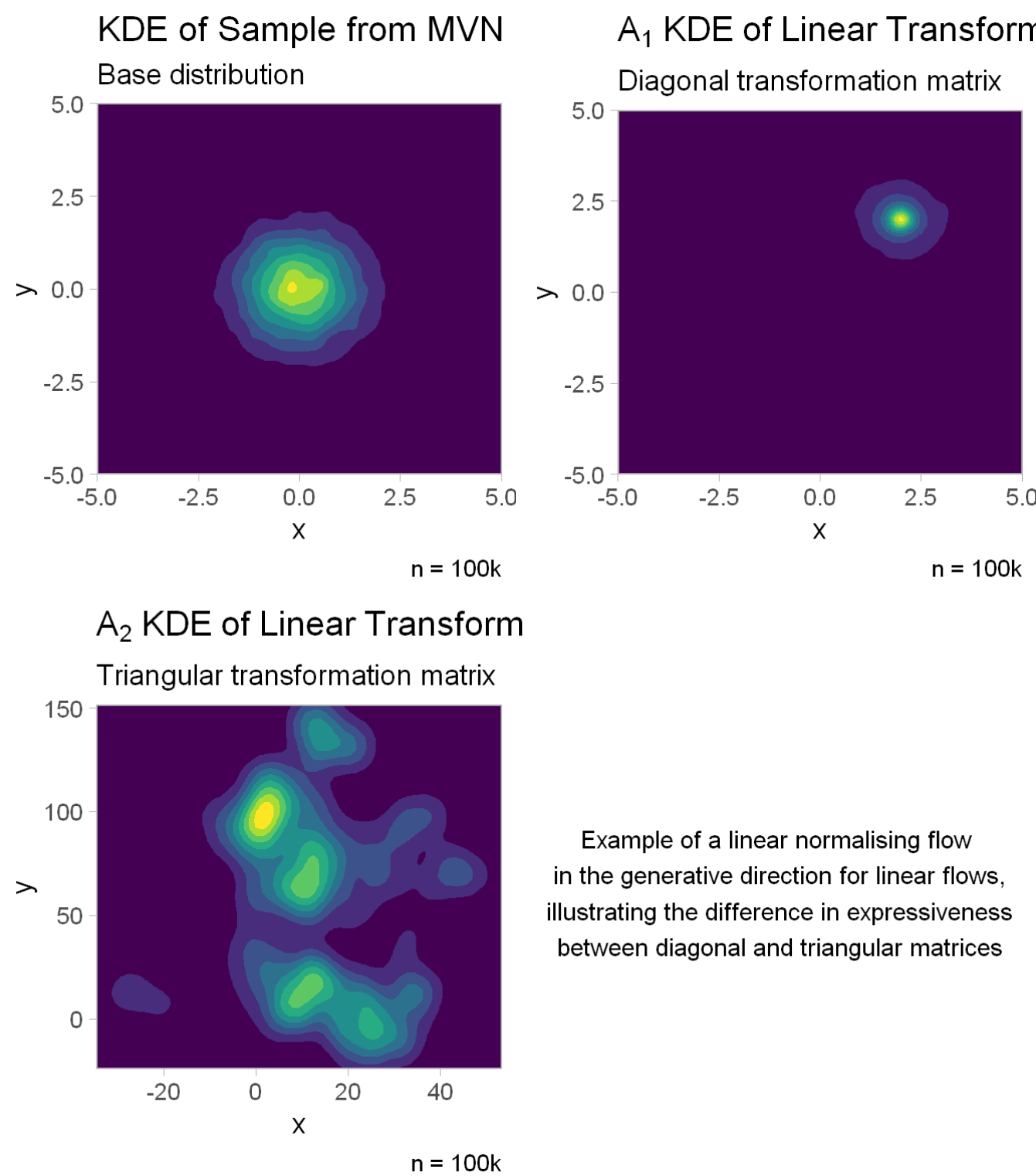


Figure 3: Expressiveness varies by choice of flow

Normalising flows are trained by maximising log-likelihood via SGD, or minimising KL-divergence when VI is used. Three properties are important for NFs [7]:

- Efficiency
- Expressiveness
- Invertibility

The number of layers and class of model both influence the expressiveness of the trained distribution. Figure 3 shows a sample from a MVN: $\mathbf{x} \sim \mathcal{N}(u, \Sigma)$ transformed using two simple linear ($g(x) = \mathbf{A}\mathbf{x} + b$) flows, where $A_1 := \text{diag}(v)$, $A_2 := \text{tri}(v)$, $v \sim U(0, 3)$ and $b \sim U(-3, 3)$, $\mathbf{x} \in \mathbb{R}^2$. For A_1 and A_2 , positive entries on the diagonal ensure invertibility.

Practical NF models often use **coupling** functions (NICE, RealNVP, Neural Spline Flows, Glow). Coupling functions split the input into disjoint partions, applying an arbitrarily complex conditioning function (e.g. an invertible NN) to one. Other models use coupling functions where the conditioner is **autoregressive** (MAFs, IAFs, NAFs). Recent developments include continuous NFs using neural ordinary differential equations (e.g. FFJORD), work on ordinal data and on manifold learning [7].

NFs for CDE

Normalising flows (NFs) find applications in conditional class probability estimation, conditional image generation and multivariate time series prediction. Work on CDE with NFs is limited. This includes Bayesian NFs, with a framework for priors over CDE estimators using BNNs with VI [10]. CDE using MAFs and Real NVP by conditioning each term in the chain rule of probability with the inclusion of y at every layer was proposed in 2017 [11]. This was explored while introducing noise regularisation for CDE in 2019 [12]. Conditional NFs for structured prediction have also been developed [13]. Progress in using NFs for CDE has been limited by the following factors:

- Computational difficulty of scaling NFs to large data sets - newer continuous NF models are restricted to usage on small image benchmark sets [14].
- Deep learning focus is often in areas of traditional strength, e.g. image data.

Figure 4 demonstrates using NFs to create CDEs of rainfall & soil moisture (data source: NIWA, 10 months). We scale the data, train the flow, and condition on two levels of rainfall $[-1, 1]$ to show the conditional densities. Note the separate estimates have different modality, which could reflect a differing seasonal effect. Other climatological variables and spatio-temporal factors would be extra sources of variation not considered. The marginals are simulated well while the joint is poorly approximated (and

noisy). The probabilistic programming libraries `pyro` and `tensorflow probability` both implement NFs.

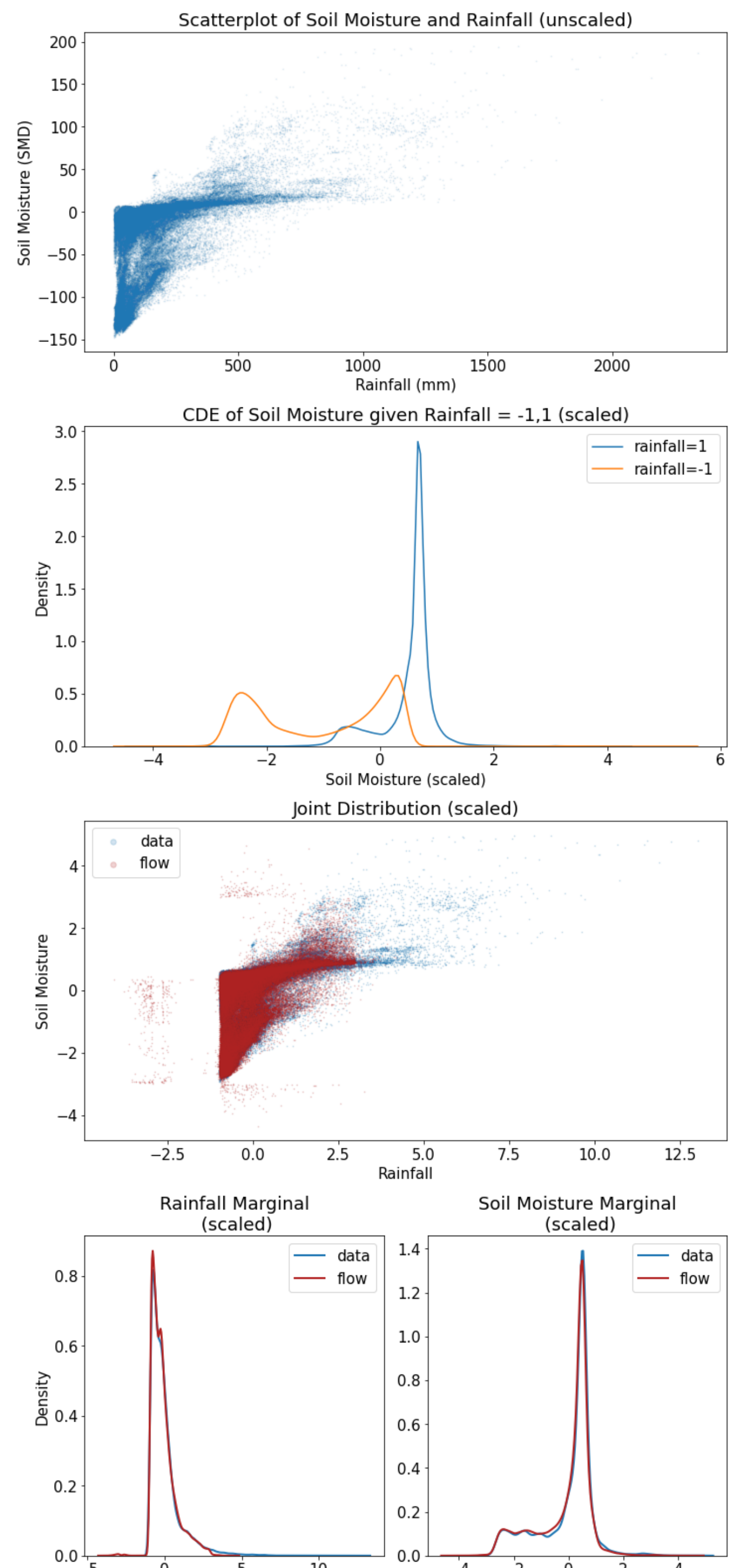


Figure 4: Training NFs for CDE with climatological data

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1. Poster produced via the *posterdown* package. The code to reproduce this poster is at https://github.com/MattSkiff/nf_cde_poster.