Deep Learning - Foundations and Concepts

Chapter 18. Normalizing Flows

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Outline

Normalizing flows

- We define a distribution $p_z(z)$ over a latent variable z.
- And we use a deep neural network architecture to define an invertible function $x = f(z; w)$ that transforms the latent space into the data space.
- We can ensure that the overall function is invertible if we make each layer of the network invertible:
  - $x = f^A(f^B(f^C(z)))$.
  - $z = g^C(g^B(g^A(x)))$.

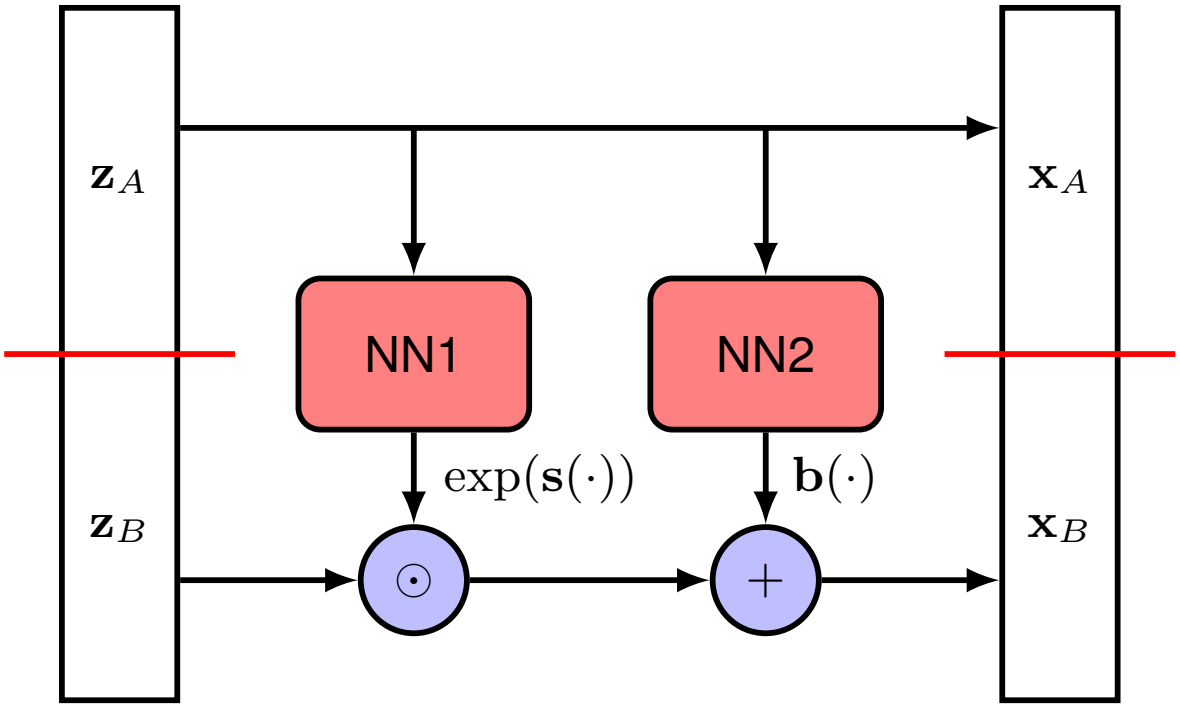
Normalizing flows

This approach to modelling a flexible distribution is called a normalizing flow because:

- The transformation of a probability distribution through a sequence of mappings is somewhat analogous to the flow of a fluid.
- The effect of the inverse mapping is to transform the complex data distribution into a normalized form, typically a Gaussian distribution.

Real NVP

Figure: A single layer of the real NVP normalizing flow model



Real NVP

Real-valued non-volume-preserving (real NVP) partitions the latent variable $z \in \mathbb{R}^D$ and the output vector $x \in \mathbb{R}^D$ into two parts: $z = (z_A, z_B)$ and $x = (x_A, x_B)$, where $z_A, x_A \in \mathbb{R}^d$. The transformation function is given by:

$$
\begin{aligned}
x_A &= z_A \\
x_B &= \exp(s(z_A; w)) \odot z_B + b(z_A; w)
\end{aligned}
$$

where $s(z_A; w)$ and $b(z_A; w)$ are the real-valued outputs of neural networks, and $\odot$ denotes element-wise multiplication of the two vectors.

Real NVP

The overall transformation is easily invertible:

$$
\begin{aligned}
z_A &= x_A \\
z_B &= \exp(-s(x_A; w)) \odot (x_B - b(x_A; w))
\end{aligned}
$$

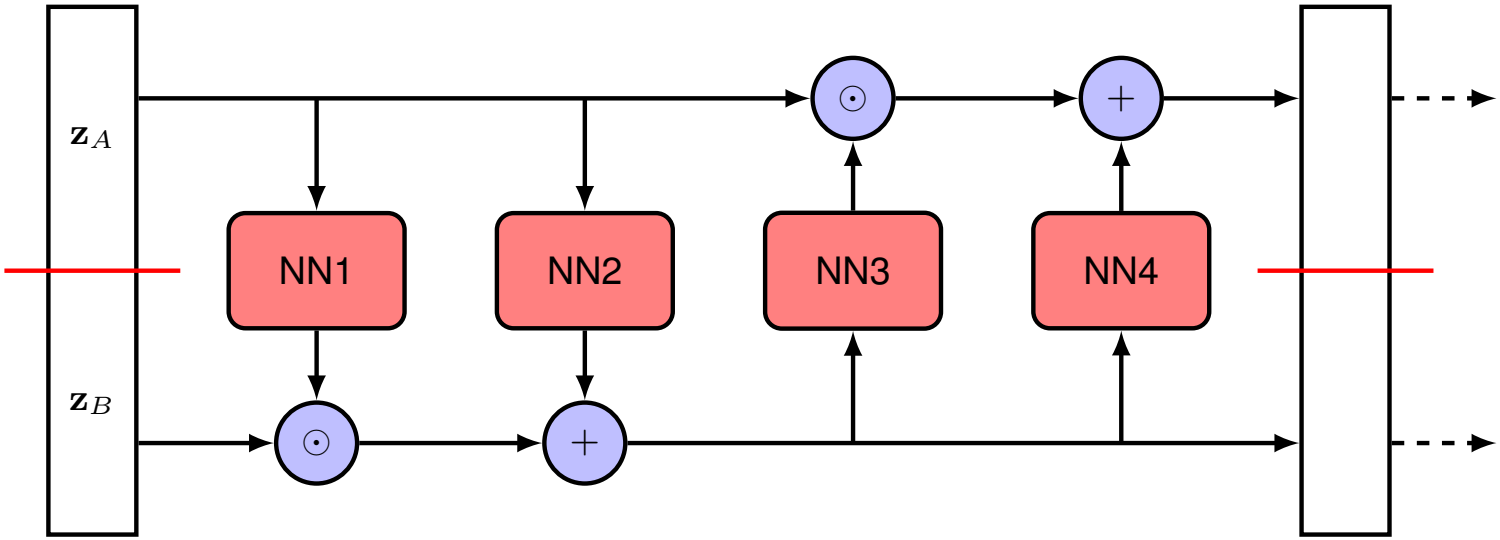
The Jacobian matrix of this inverse mapping is given by:

$$
J = \begin{pmatrix} I_d & 0 \\ \frac{\partial z_B}{\partial x_A} & \operatorname{diag}(\exp(-s(x_A; w))) \end{pmatrix}
$$

We see that the Jacobian matrix is a lower triangular matrix, and its determinant is simply given by the product of the elements of $\exp(-s(x_A; w))$.

Real NVP

Figure: A double-layer structure where the roles of z_A and z_B are reversed in the second layer



Coupling flows

The real NVP model belongs to a broad class of normalizing flows called coupling flows:

$$x_A = z_A$$
$$x_B = h(z_B, g(z_A; w))$$

where:

- $h(z_B, g)$ is a function of z_B that is efficiently invertible for any given value of g and is called the coupling function.
- The function $g(z_A; w)$ is called a conditioner and is typically represented by a neural network.

Masked autoregressive flows

In masked autoregressive flows (MAFs), the transformation function from the latent space into the data space is given by:

$$x_d = h(z_d, g_d(x_{1:d-1}; w_d))$$

where:

- h is the coupling function, which is chosen to be easily invertible with respect to z_d.
- g_d is the conditioner, which is typically represented by a deep neural network.
- $x_{1:d-1}$ denotes $x_1, \ldots, x_{d-1}$.

Masked autoregressive flows

The overall transformation is easily invertible:

$$z_d = h^{-1}(x_d, g_d(x_{1:d-1}; w_d))$$

- The inverse can be performed efficiently on modern hardware since $z_1, \ldots, z_D$ can be evaluated in parallel.
- The Jocobian matrix is a lower-triangular matrix whose determinant can also be evaluated efficiently.
- However, sampling from this model must be done sequentially because the values of $x_1, \ldots, x_{d-1}$ must be evaluated before x_d can be computed.

Inverse autoregressive flows

To avoid this inefficient sampling, we can instead define an inverse autoregressive flow (IAF) given by:

$$x_d = h(z_d, \tilde{g}_d(z_{1:d-1}; w_d))$$

The inverse is given by:

$$z_d = h^{-1}(x_d, \tilde{g}_d(z_{1:d-1}; w_d))$$

We see that:

- Sampling is now efficient since the evaluation of the elements $x_1, \ldots, x_D$ can be performed in parallel.
- The Jocobian matrix is again a lower-triangular matrix whose determinant can be evaluated efficiently.
- The inverse calculations are intrinsically sequential and slow.