4. Normalizing Flows

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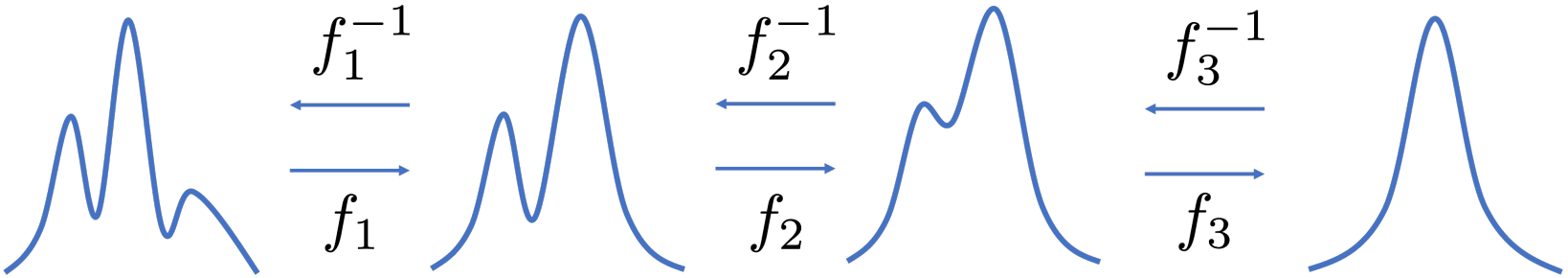
AI Summer School @ KAUST

Normalizing Flows: intuition

*Family of neural networks that can learn to **warp a simple density function** (e.g., gaussian) **into a complex one** (the one of interest). Provide tractable maximum likelihood estimation.*



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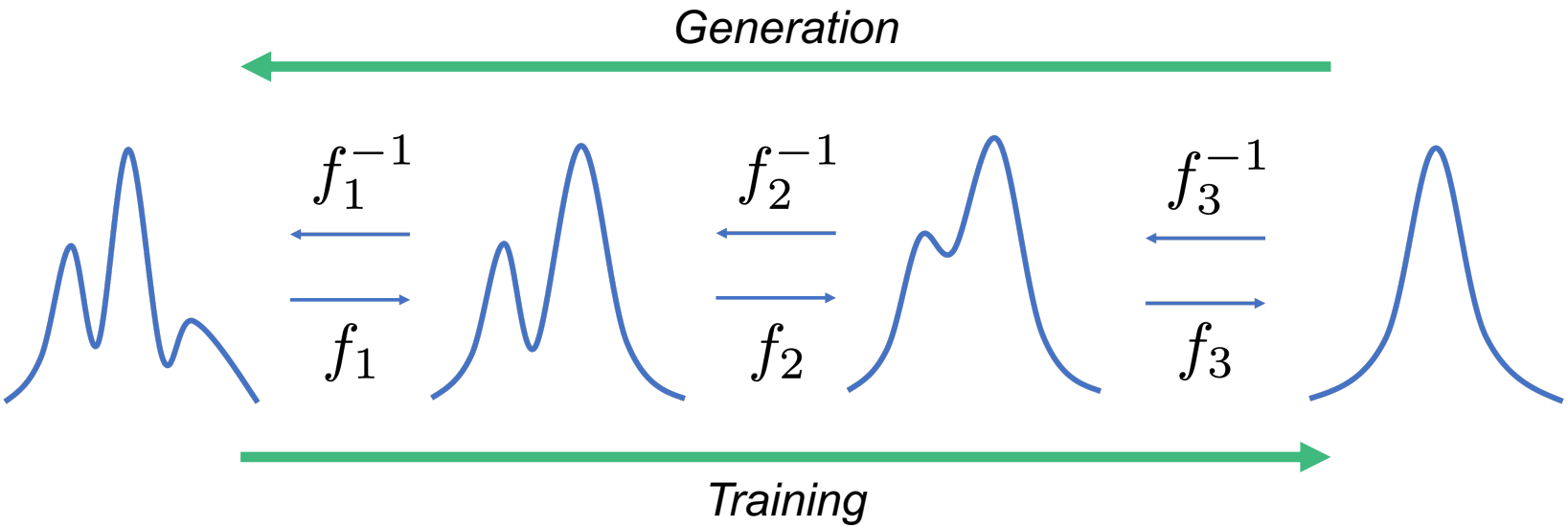
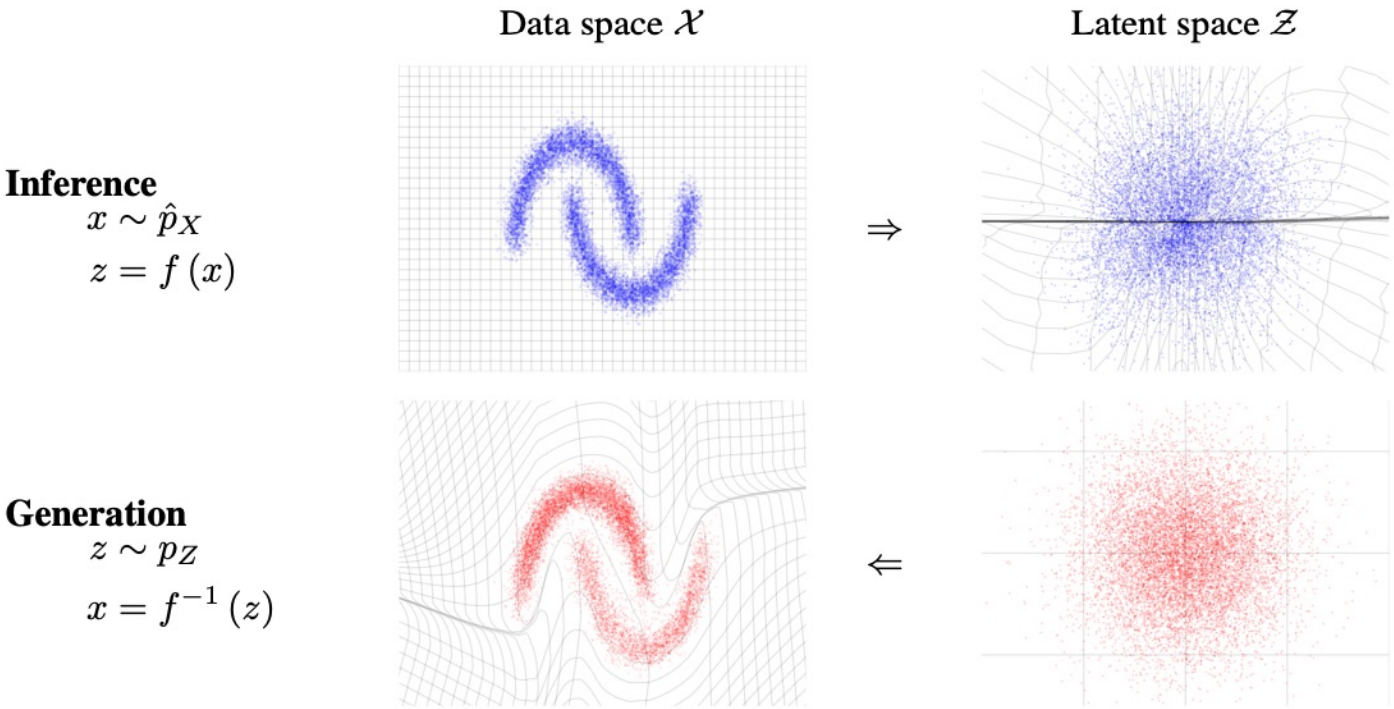


Normalizing Flows: intuition

Family of neural networks that can learn to warp a simple density function (e.g., gaussian) into a complex one (the one of interest). Provide ***tractable maximum likelihood estimation.***

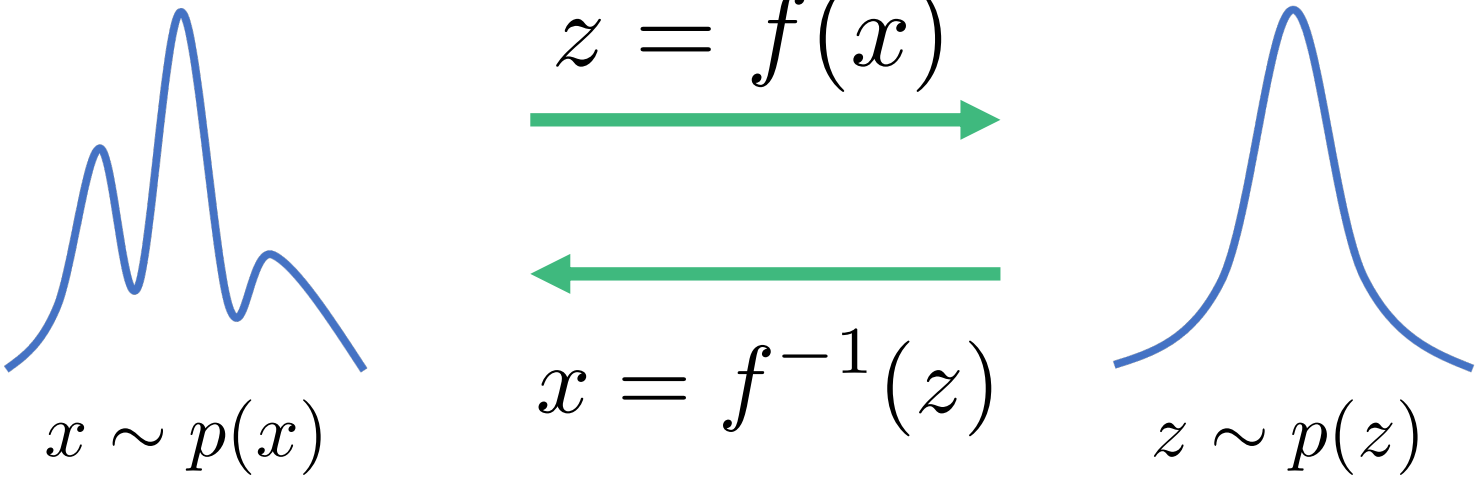
$$\underset{\theta}{\operatorname{argmax}}\ p_\theta(\mathbf{x})$$ *is feasible without approximations*

Normalizing Flows: intuition

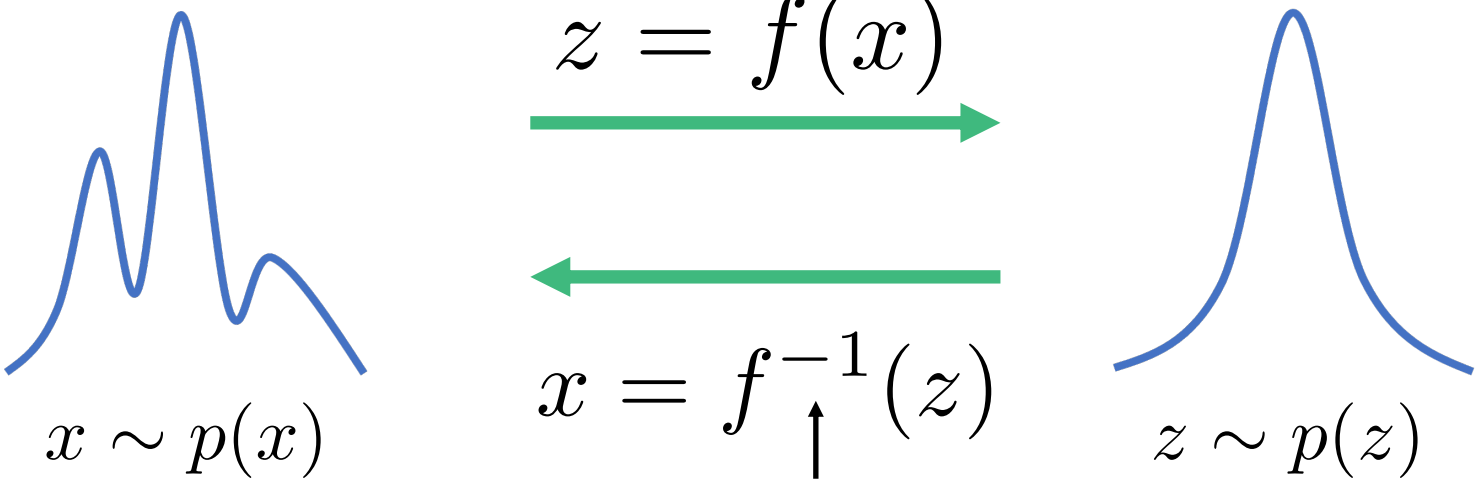


Dinh et al. (2014)

Normalizing Flows: basic principle



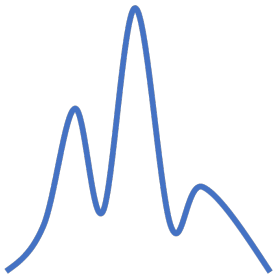
Normalizing Flows: basic principle



Design an invertible function: we will need to introduce **Invertible NNs**

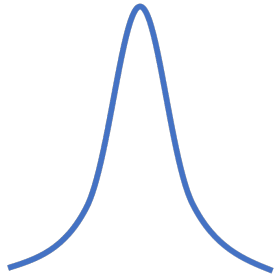
Normalizing Flows: basic principle

In practice multiple transformations are required:



$$f = f_3 \circ f_2 \circ f_1$$

$$f^{-1} = f_1^{-1} \circ f_2^{-1} \circ f_3^{-1}$$

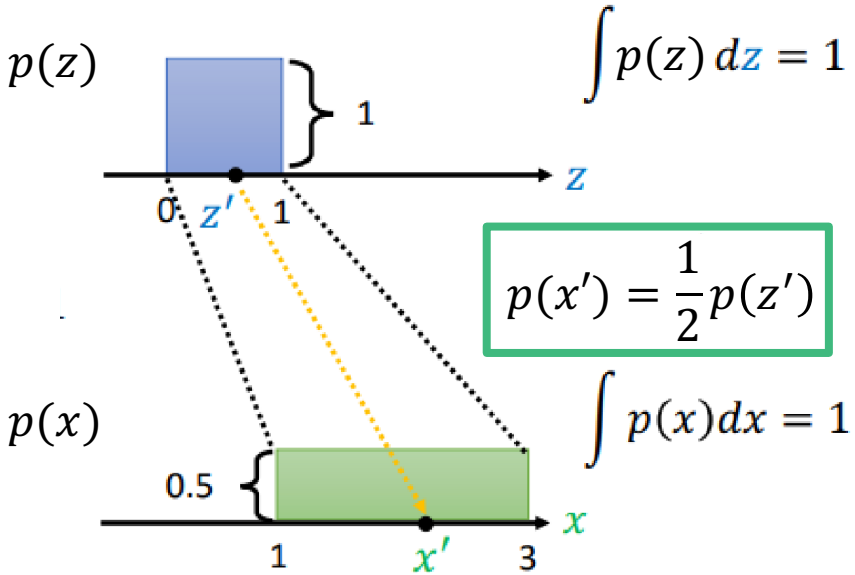


Change of variable theorem

Define density of a random variable that is a deterministic transformation of another variable → **ensures still sums to 1!**

$$z = f(x) = \frac{x-1}{2}$$

$$x = f^{-1}(z) = 2z + 1$$



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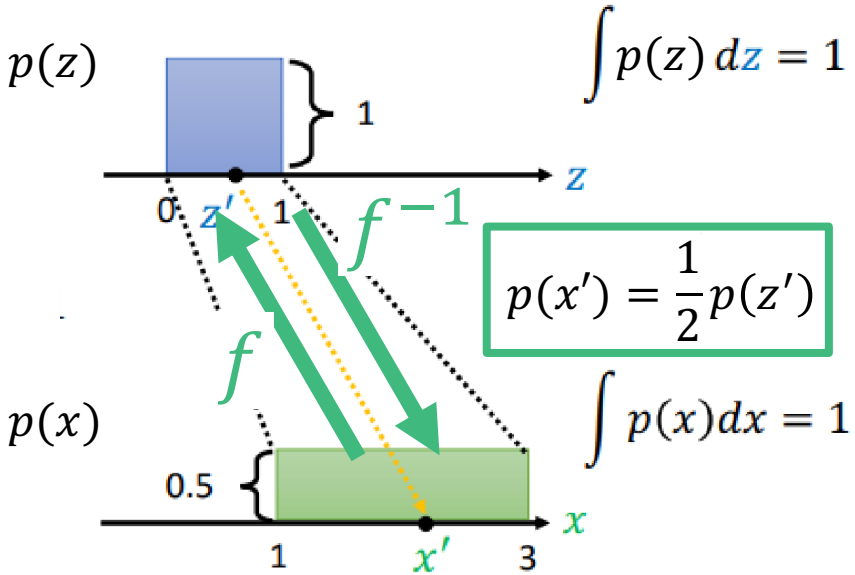

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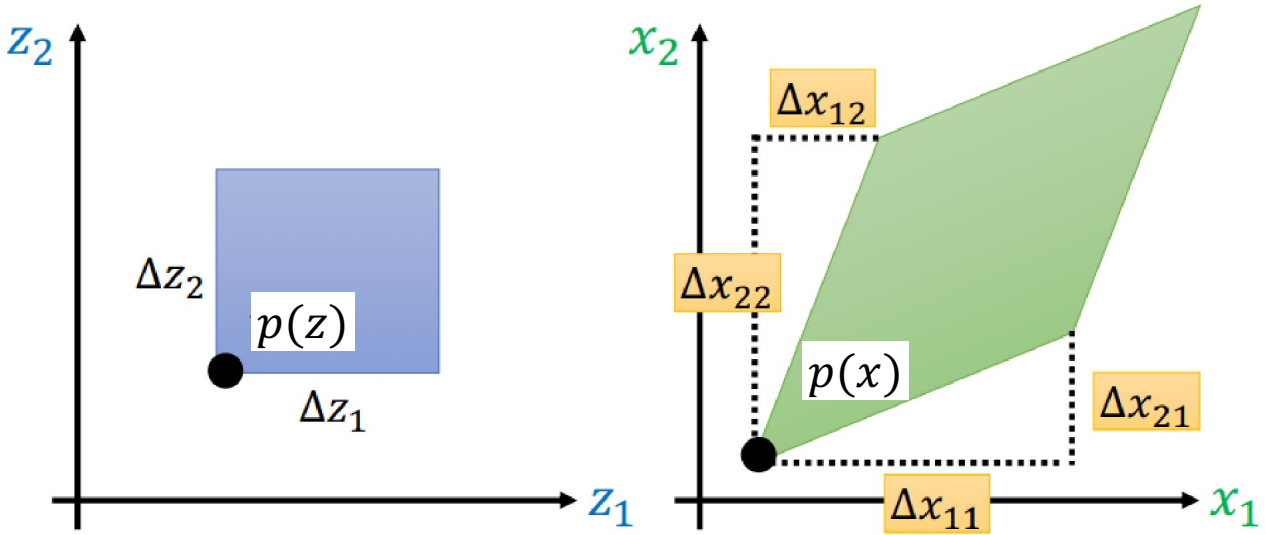


Change of variable theorem

Given $x \in \mathbb{R}^N$ and $z \in \mathbb{R}^N$ (must be same dimensionality!), we get:

$$p_X(x) = p_Z(f(x)) \left| \det \frac{\partial f(x)}{\partial x} \right|$$

Change of variable theorem

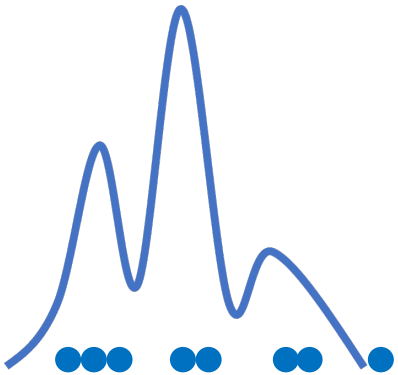
Given $x \in \mathbb{R}^N$ and $z \in \mathbb{R}^N$ (must be same dimensionality!), we get:

$$p_X(x) = p_Z(f(x)) \left| \det \; J_f \right|$$

Jacobian matrix $\in \mathbb{R}^{NxN}$

Normalizing Flows: learning process

Change of variable theorem allows direct maximum-likelihood for NFs:



Training samples

$x \sim p(x)$

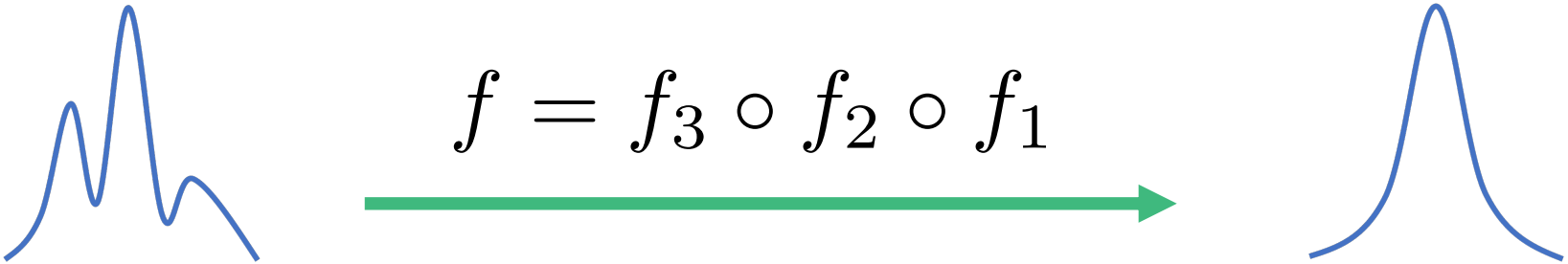
$$\underset{\theta}{\operatorname{argmax}}\, p_X(x) =$$

$$\underset{\theta}{\operatorname{argmax}}\, p_Z(f_\theta(x))\left|\det J_{f_\theta}\right|$$

$$\underset{\theta}{\operatorname{argmin}}\; -logp_Z(f_\theta(x)) - log\left|\det J_{f_\theta}\right|$$

Normalizing Flows: learning process

In practice multiple transformations are required:



$$\underset{\theta}{\operatorname{argmin}} \; -logp_Z(f_\theta(x)) - \sum_i log|\det J_{f_{i,\theta}}|$$

Normalizing Flows in practice

Training Algorithm

1. Select a batch of training samples and feed to network (f_θ)
2. Compute the loss: 1) Evaluate the probability of each output ($p_Z(f_\theta(x))$). This is easy to do as p_Z is chosen to be a simple distribution with analytical pdf (eg gaussian). 2) Compute the log-determinant of the Jacobian + backprop.

Inference Algorithm

1. Randomly sample a value from the distribution p_Z
2. Feed this sample into the inverse transformation f_θ^{-1} to obtain a sample x of p_X
3. Optional: feed the sample into the network and evaluate its probability via the change of variable formula.

Why Normalizing Flows?

Normalizing: *the change of variables formula gives a normalized density after applying an invertible transformation.*

Flow: *multiple invertible transformations can be composed with each other to create more complex invertible transformations*.

Computational issues with NFs

Computing the log-determinant of Jacobian can be expensive!

$$\sigma(x) = \frac{1}{1 + e^{-Wx-b}}$$

Very simple MLP network

$$J_{\sigma(x)} = \left[\frac{e^{-Wx-b}}{(1+e^{-Wx-b})^2} \odot w_1, \ldots, \frac{e^{-Wx-b}}{(1+e^{-Wx-b})^2} \odot w_n \right]$$

Dense matrix, determinant roughly as expensive as inverting J

Computational issues with NFs

Computing the log-determinant of Jacobian can be expensive!

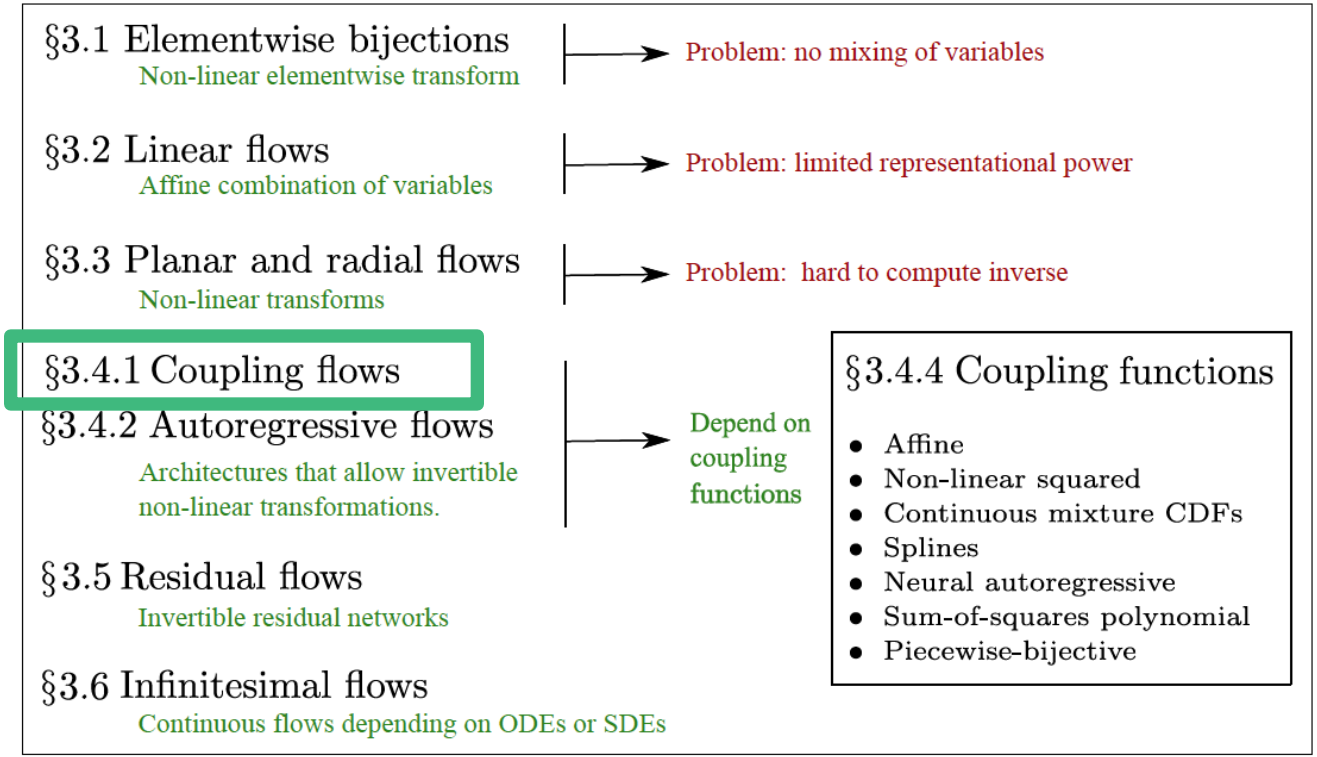
Solution

Design **invertible** transformations whose **Jacobian has special structure**
→ eg. lower triangular (determinant = product of diag. elements)

↓

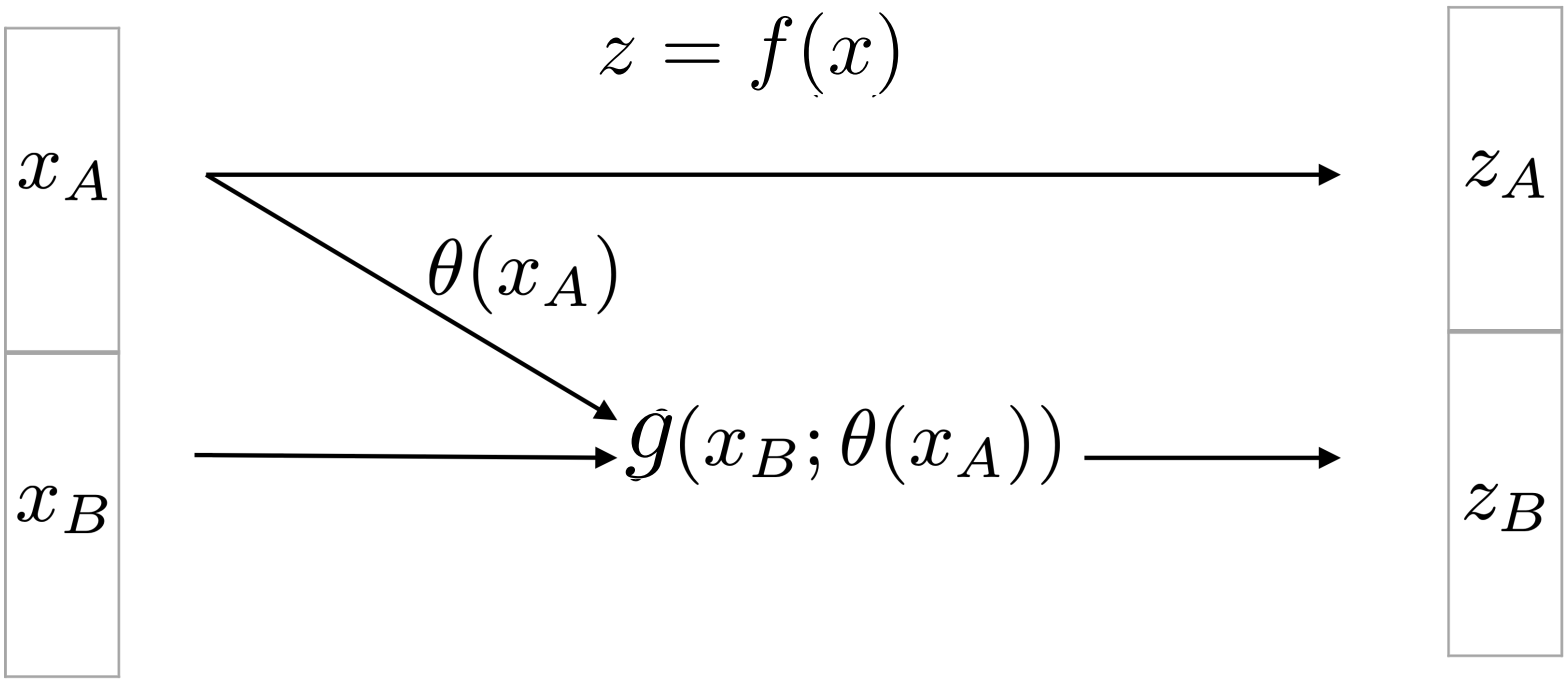
Coupling layers/flows

Computational issues with NFs

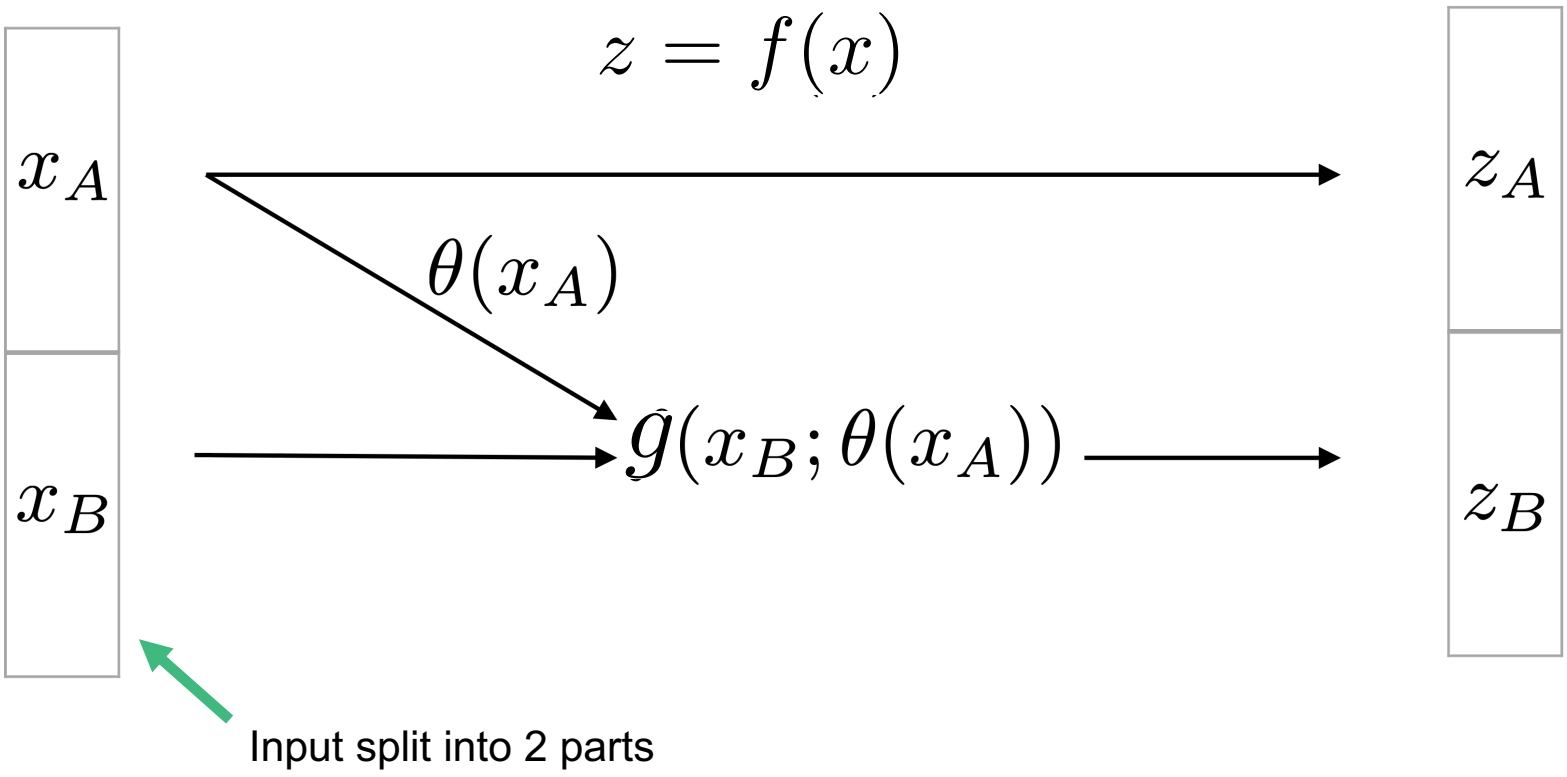


From Normalizing Flows: An Introduction and Review of Current Methods. I. Kobyzev, S.J.D. Prince, and M.A. Brubaker

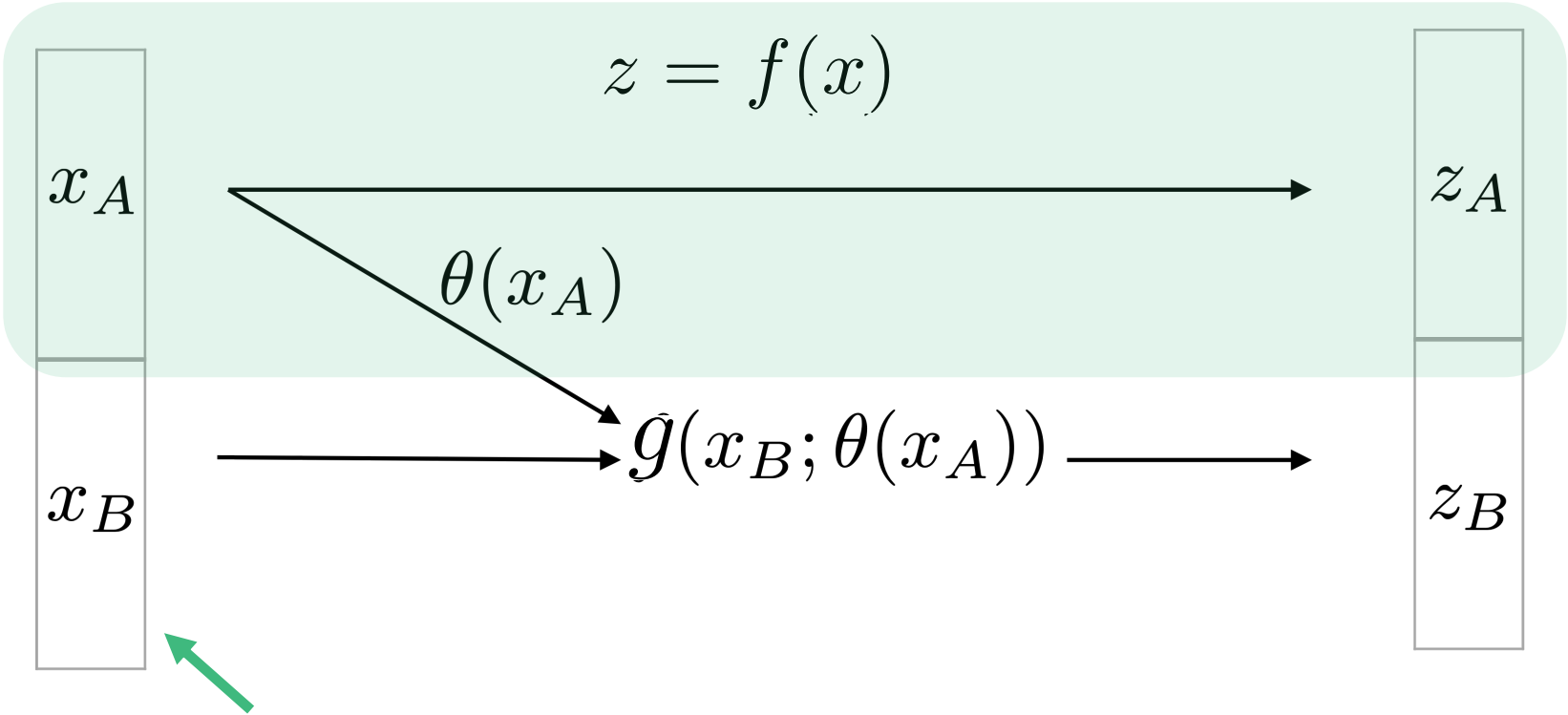
Coupling layers/flows



Coupling layers/flows

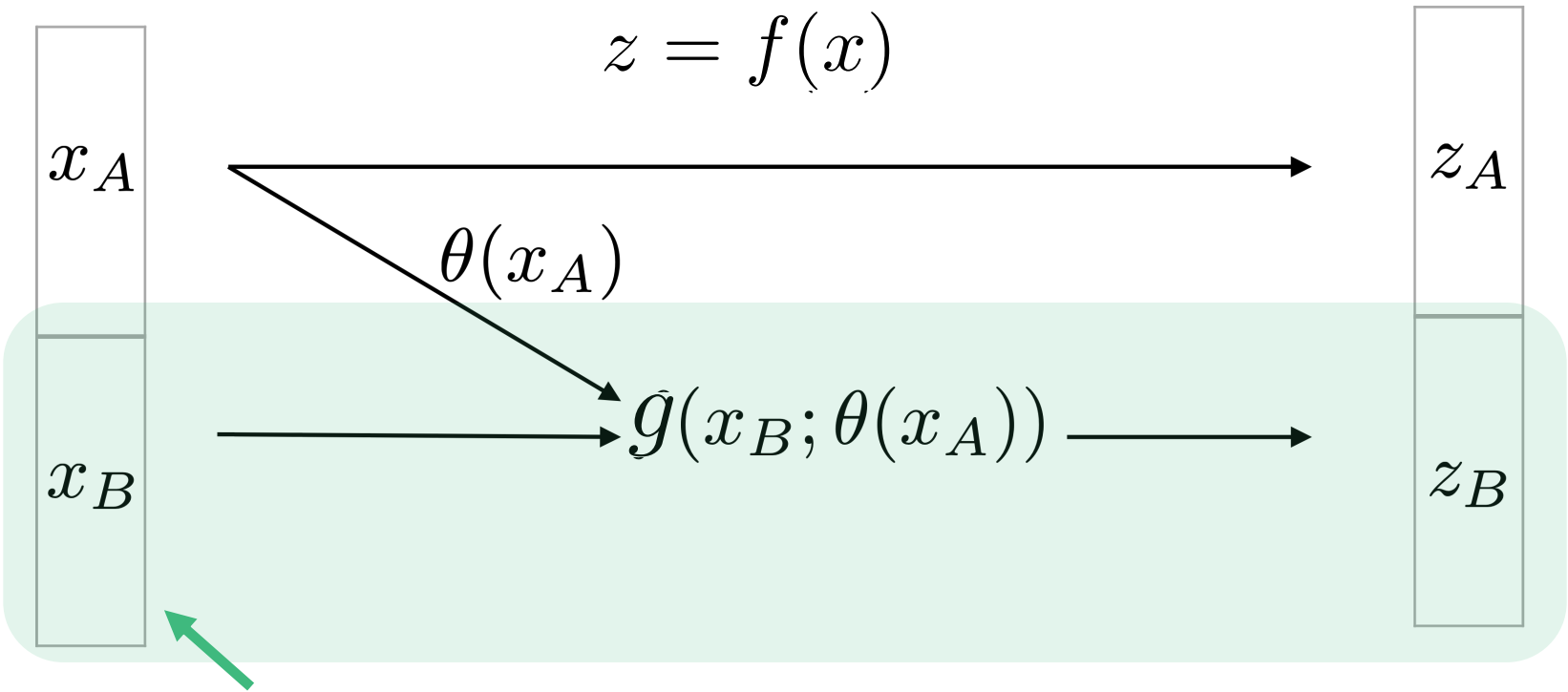


Coupling layers/flows



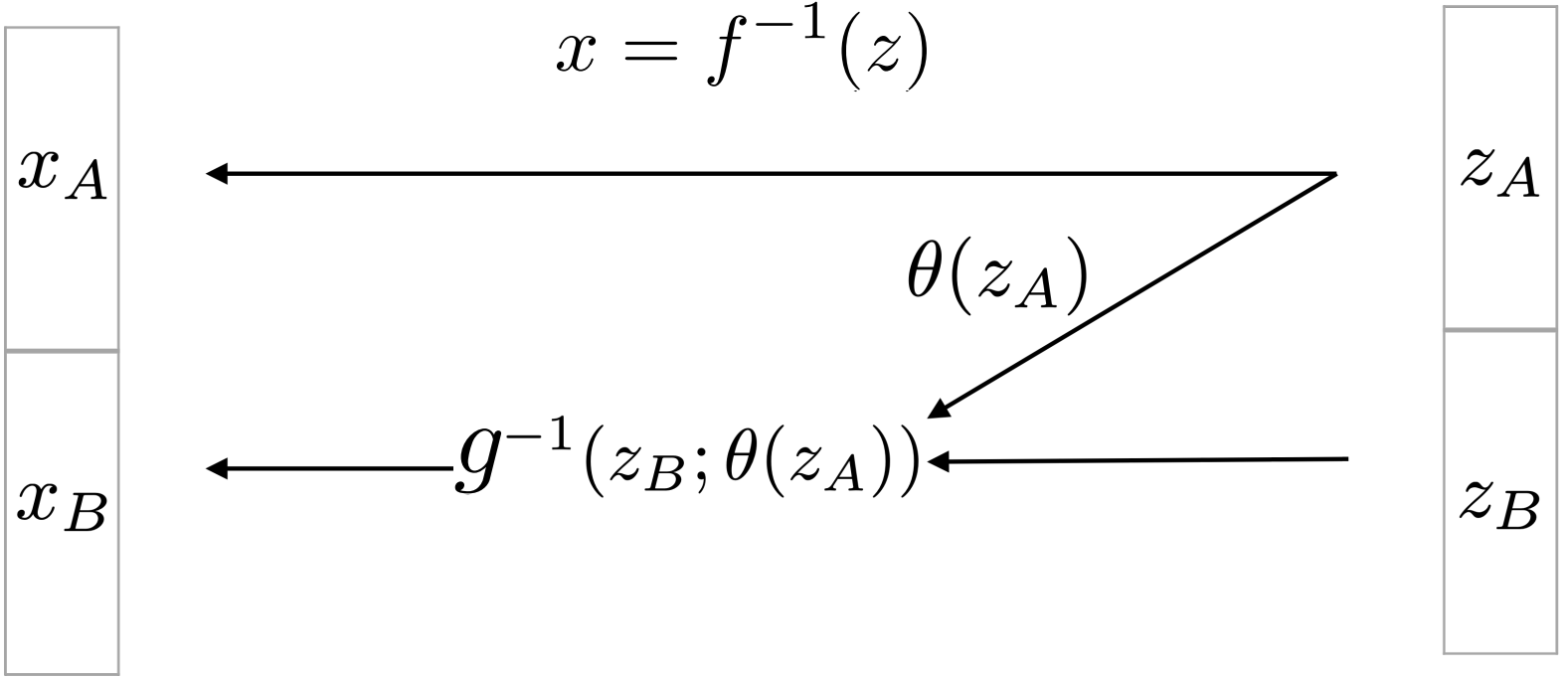
Input split into 2 parts: half **directly mapped to output** ($z_A = x_A$)

Coupling layers/flows



Input split into 2 parts: other half combined with top half in an **invertible way**

Coupling layers/flows



The flow designed like this is invertible **for any choice of θ!**

Coupling layers/flows

Forward:

$$z_A = x_A$$
$$z_B = g(x_B; \theta(x_A))$$

Inverse:

$$x_A = z_A$$
$$x_B = g^{-1}(z_B; \theta(z_A))$$

Coupling layers/flows

Choice of g:

- NICE (Dinh et al., 2014): Additive coupling function

$$z_B = x_B + \theta(x_A)$$

- REAL NVP (Dinh et al., 2016): Affine coupling function

$$z_B = x_B \odot e^{s(x_A)} + t(x_A)$$

Scale and Transformation: Can be NNs

Coupling layers/flows: inverse and Jacobian

Let's consider first the first scenario (i.e., additive coupling):

$$z_A = x_A \qquad\qquad x_A = z_A$$
$$z_B = x_B + \theta(x_A) \quad \rightarrow \quad x_B = z_B - \theta(x_A)$$

$$J_f = \begin{bmatrix} \partial z_A/\partial x_A & \partial z_A/\partial x_B \\ \partial z_B/\partial x_A & \partial z_B/\partial x_B \end{bmatrix} = \begin{bmatrix} I & 0 \\ \partial\theta(x_A)/\partial x_A & I \end{bmatrix}$$

Irrelevant..

$$detJ_f = 1$$

Coupling layers/flows: inverse and Jacobian

Let's consider first the second scenario (i.e., affine coupling):

$$z_A = x_A$$
$$z_B = x_B \odot e^{s(x_A)} + t(x_A)$$

$$x_A = z_A$$
$$x_B = (z_B - t(x_A)) \odot e^{-s(x_A)}$$

$$J_f = \begin{bmatrix} \partial z_A/\partial x_A & \partial z_A/\partial x_B \\ \partial z_B/\partial x_A & \partial z_B/\partial x_B \end{bmatrix} = \begin{bmatrix} I & 0 \\ \partial z_B/\partial x_A & diag\{e^{s(x_A)}\} \end{bmatrix}$$

$$detJ_f = \prod_i e^{s(x_A)_i}$$

Irrelevant..

Coupling layers/flows

Choice of $\boldsymbol{\theta}$:

- NICE (Dinh et al., 2014): MLP with ReLU
- REAL NVP (Dinh et al., 2016): Convolution residual layer
- Glow (Kingma et al., 2018): 3-layer CNN with ReLU
- …

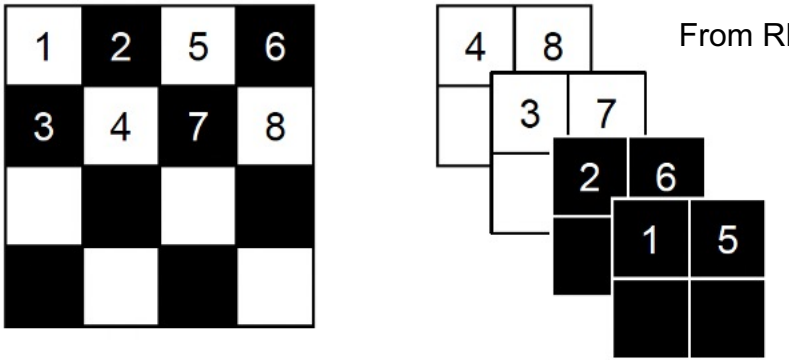
Split functions

What is the most effective way to partition x?

- Separating the input in half and passing the first half untouched leads to **poor expressivity!**
- Use some sort of **shuffling** before separating → better…
- More structured ways:
    - REAL NVP (Dinh et al., 2016): Masking
    - Glow (Kingma et al., 2018): 1x1 Conv.

Split functions

What is the most effective way to partition x?



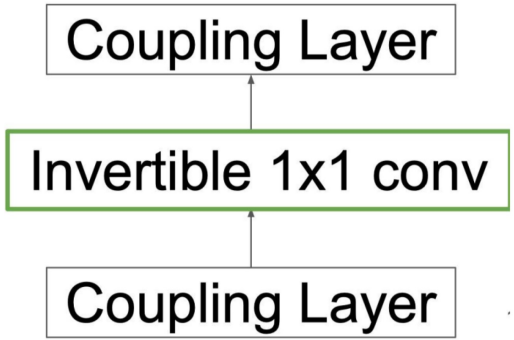
From REAL NVP (Dinh et al., 2016)

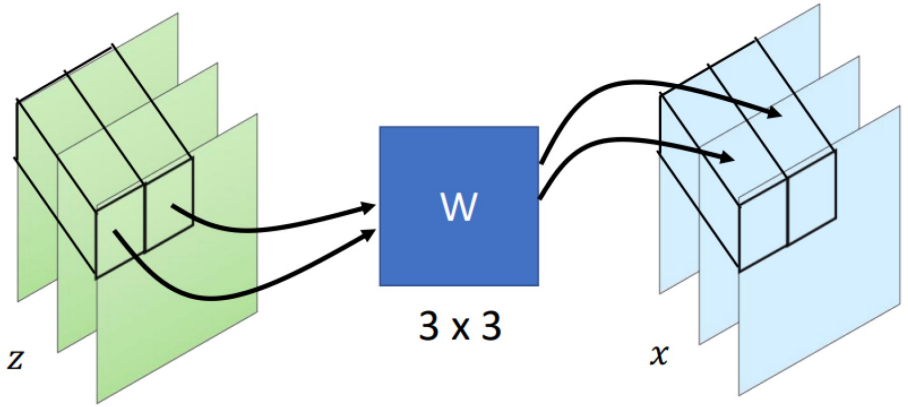
Figure 3: Masking schemes for affine coupling layers. On the left, a spatial checkerboard pattern mask. On the right, a channel-wise masking. The squeezing operation reduces the $4 \times 4 \times 1$ tensor (on the left) into a $2 \times 2 \times 4$ tensor (on the right). Before the squeezing operation, a checkerboard pattern is used for coupling layers while a channel-wise masking pattern is used afterward.

Split functions

What is the most effective way to partition x?

From Glow (Kingma et al., 2018)





W can shuffle the channels.

If W is invertible, it is easy to compute W^{-1}.

3		0	0	1	1
1	=	1	0	0	2
2		0	1	0	3

NFs in action

MNIST from NICE

NFs in action

Generation from RealNVP

NFs in action

Generation from Glow