EE-559 – Deep learning

9.4. Non-volume preserving networks

François Fleuret

https://fleuret.org/ee559/

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ÉCOLE POLYTECHNIQUE
FÉDÉRALE DE LAUSANNE

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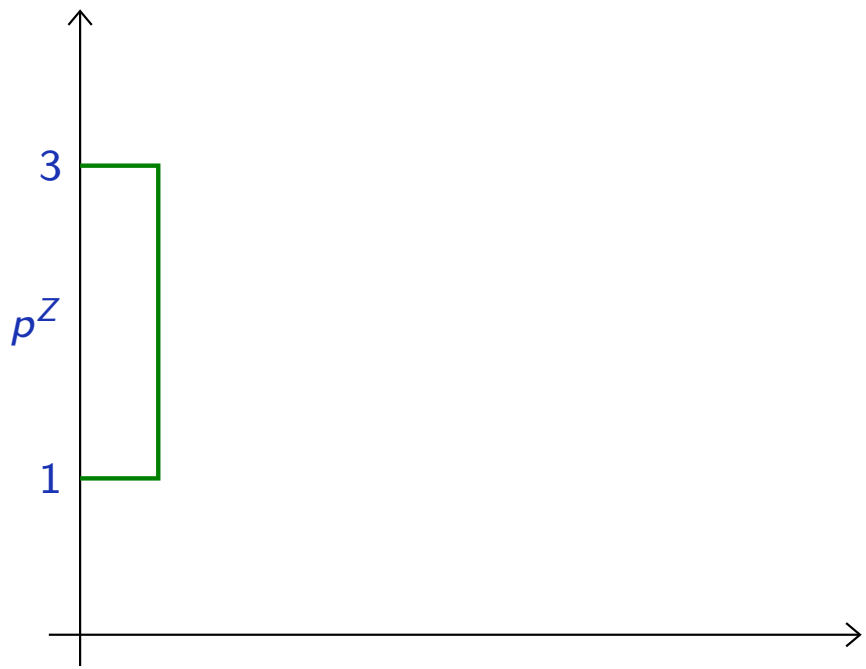

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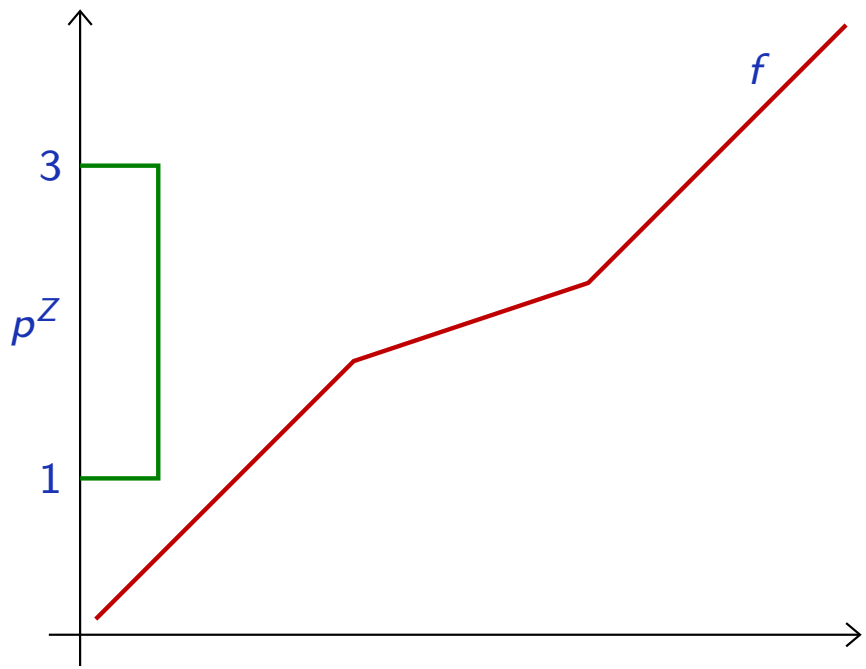

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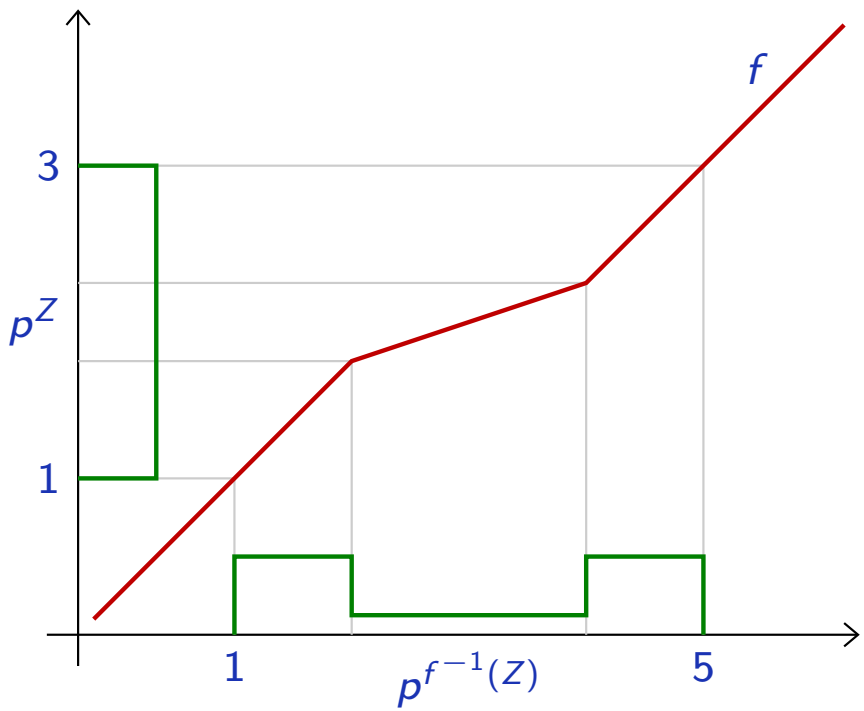

From this equality, if f is a parametric function such that we can compute [and differentiate]

$$p^Z(f(x))$$

and

$$|J_f(x)|$$

then, we can make the distribution of $f^{-1}(Z)$ fits the data by optimizing

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If we are able to do so, then we can synthesize a new X by sampling $Z \sim \mathcal{N}(0, 1)$ and computing $f^{-1}(Z)$.

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And remember that if f is is a composition of functions

$$f = f^{(K)} \circ \cdots \circ f^{(1)}$$

we have

$$J_f(x) = \prod_{k=1}^{K} J_{f^{(k)}}\left(f^{(k-1)} \circ \cdots \circ f^{(1)}(x)\right),$$

so

$$\log|J_f(x)| = \sum_{k=1}^{K} \log\left|J_{f^{(k)}}\left(f^{(k-1)} \circ \cdots \circ f^{(1)}(x)\right)\right|.$$

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Dinh et al. (2014) introduced the **coupling layers** to address both issues.

The resulting Non-Volume Preserving network (NVP) is an example of a **Normalizing flow** (Rezende and Mohamed, 2015).

We use here the formalism from Dinh et al. (2016).

Given a dimension d, a Boolean vector $b \in \{0,1\}^d$ and two mappings

$$s : \mathbb{R}^d \to \mathbb{R}^d$$
$$t : \mathbb{R}^d \to \mathbb{R}^d,$$

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we define a [fully connected] coupling layer as the transformation

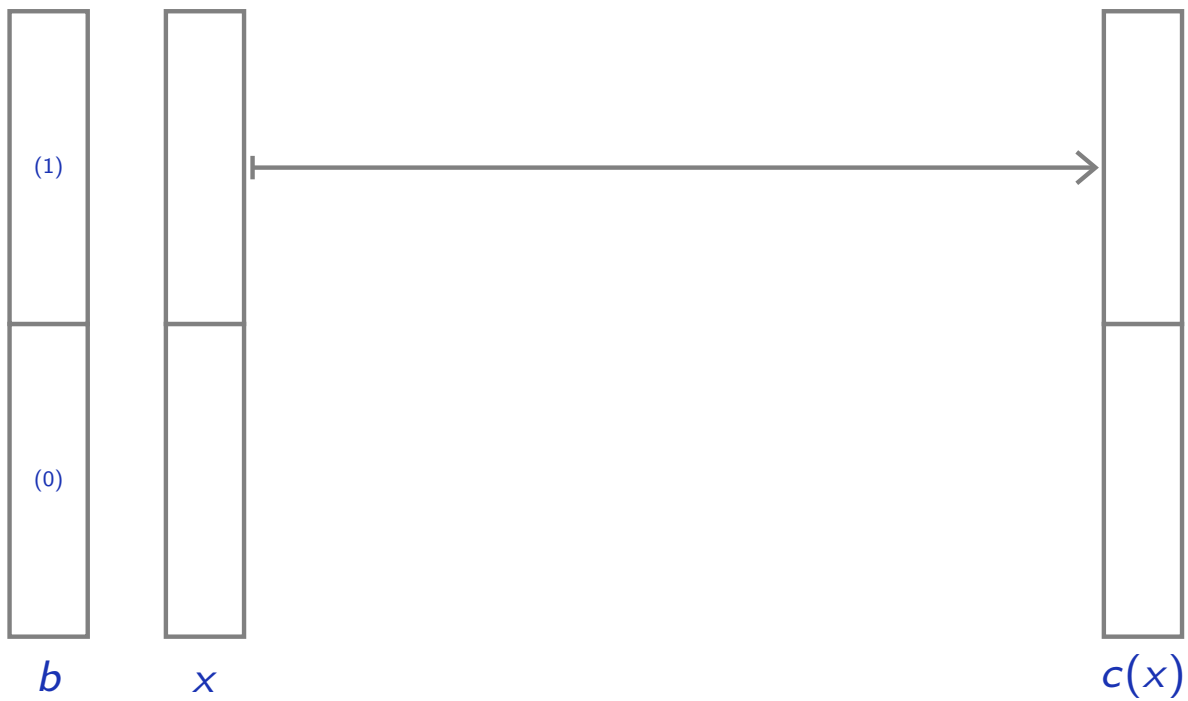
$$\begin{aligned} c : \mathbb{R}^d &\to \mathbb{R}^d \\ x &\mapsto b \odot x + (1 - b) \odot \Big(x \odot \exp(s(b \odot x)) + t(b \odot x) \Big) \end{aligned}$$

where exp is component-wise, and $\odot$ is the Hadamard component-wise product.

The expression

$$c(x) = b \odot x + (1 - b) \odot \Big(x \odot \exp(s(b \odot x)) + t(b \odot x) \Big)$$

can be understood as: forward $b \odot x$ unchanged,



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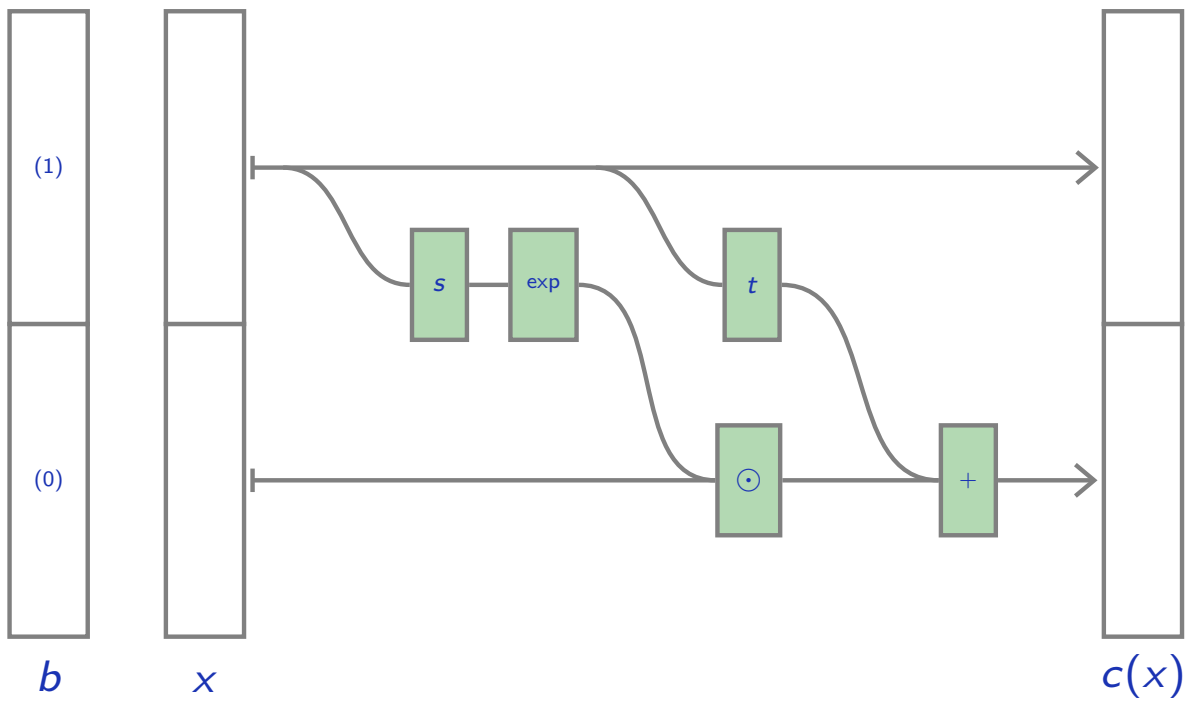
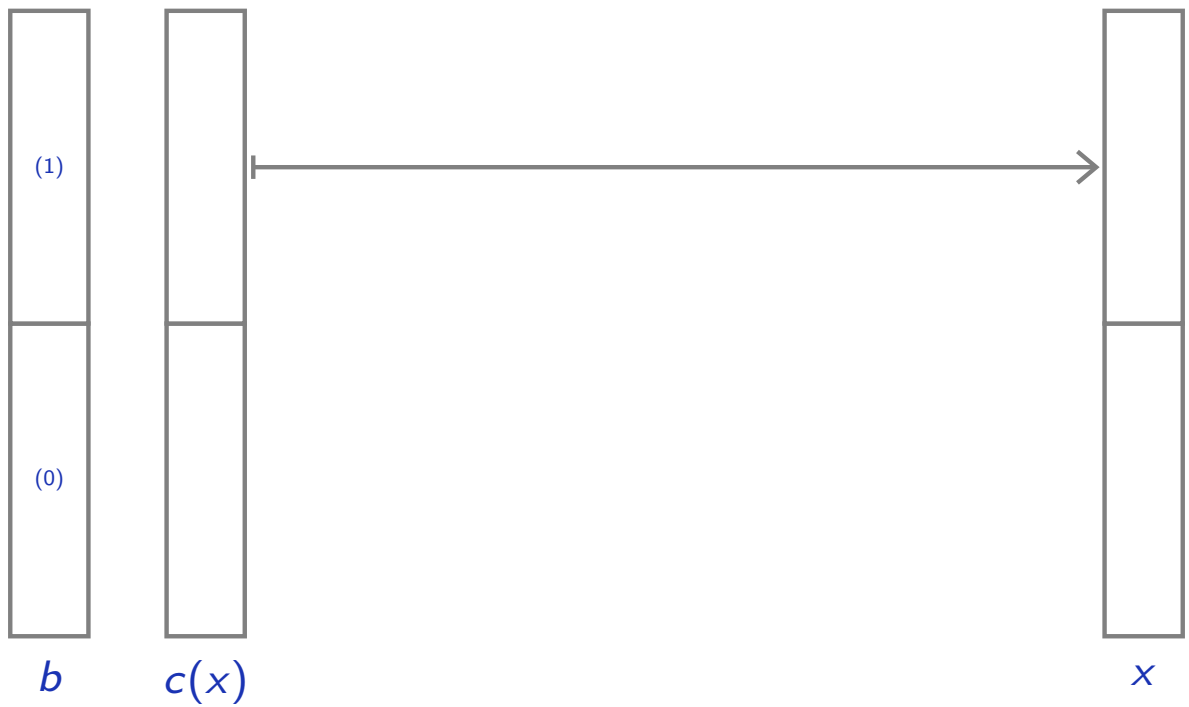
can be understood as: forward $b \odot x$ unchanged, and apply to $(1 - b) \odot x$ an invertible transformation parametrized by $b \odot x$.



The consequence is that c is invertible, and if $y = c(x)$

$$x = b \odot y + (1 - b) \odot \Big(y - t(b \odot y)\Big) \odot \exp(-s(b \odot y)).$$



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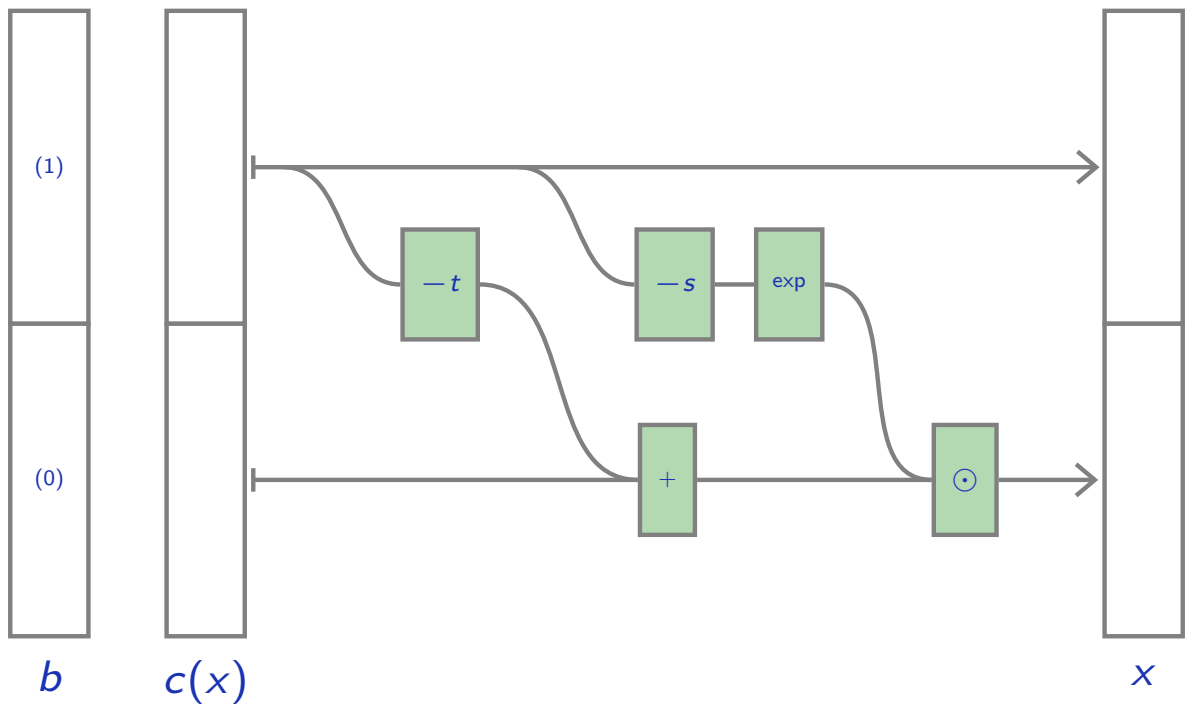

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$$c_i(x) = b_i \odot x_i + (1 - b_i) \odot \Big(x_i \odot \exp(s_i(b \odot x)) + t_i(b \odot x) \Big)$$

we have, $\forall i, j, x$,

$$\begin{aligned} b_i = 1 \quad &\Rightarrow \quad c_i(x) = x_i \\ &\Rightarrow \quad \frac{\partial c_i}{\partial x_j} = 1_{\{i=j\}} \end{aligned}$$

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Hence $\frac{\partial c_i}{\partial x_j}$ can be non-zero only if $i = j$, or $(1 - b_i)b_j = 1$.

If we re-order both the rows and columns of the Jacobian to put first the non-zeros entries of b, and then the zeros, it becomes lower triangular

$$J_c(x) = \left(\begin{array}{c|c} \begin{matrix} 1 & & \\ & \ddots & \\ & & 1 \end{matrix} & (0) \\ \hline (\neq 0) & \begin{matrix} \exp(s_k(x \odot b)) & & \\ & \ddots & \\ & & \exp(s_{k'}(x \odot b)) \end{matrix} \end{array}\right)$$

its determinant remains unchanged, and we have

$$\begin{aligned} \log |J_{f^{(k)}}(x)| &= \sum_{i:b_i=0} s_i(x \odot b) \\ &= \sum_i \left((1-b) \odot s\left(x \odot b\right)\right)_i . \end{aligned}$$

```
dim = 6

x = torch.empty(1, dim).normal_().requires_grad_()
b = torch.zeros(1, dim)
b[:,:dim//2] = 1.0

s = nn.Sequential(nn.Linear(dim, dim), nn.Tanh())
t = nn.Sequential(nn.Linear(dim, dim), nn.Tanh())

c = b * x + (1 - b) * (x * s(b * x).exp() + t(b * x))

j = torch.cat([torch.autograd.grad(c_k, x, retain_graph=True)[0] for c_k in c[0]])

print(j)
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```
tensor([[ 1.0000,  0.0000,  0.0000,  0.0000,  0.0000,  0.0000],
        [ 0.0000,  1.0000,  0.0000,  0.0000,  0.0000,  0.0000],
        [ 0.0000,  0.0000,  1.0000,  0.0000,  0.0000,  0.0000],
        [ 0.6073,  0.3393,  0.0282,  0.9897,  0.0000,  0.0000],
        [-0.3223, -0.0081,  0.1224,  0.0000,  1.4373,  0.0000],
        [ 0.0301,  0.3185,  0.0665,  0.0000,  0.0000,  1.0295]])
```

To recap, with $f^{(k)}, k = 1, \ldots, K$ coupling layers,

$$f = f^{(K)} \circ \cdots \circ f^{(1)},$$

and $x_n^{(0)} = x_n$ and $x_n^{(k)} = f^{(k)}\left(x_n^{(k-1)}\right)$,

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$$\mathscr{L}(f) = \sum_n \left(-\frac{1}{2}\left(\left\| x_n^{(K)} \right\|^2 + d \log 2\pi \right) + \sum_{k=1}^{K} \log \left| J_{f^{(k)}}\left(x_n^{(k-1)}\right) \right| \right),$$

with

$$\log \left| J_{f^{(k)}}(x) \right| = \sum_i \left(\left(1 - b^{(k)}\right) \odot s^{(k)}\left(x \odot b^{(k)}\right) \right)_i.$$

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$$\log \left| J_{f^{(k)}}(x) \right| = \sum_i \left(\left(1 - b^{(k)}\right) \odot s^{(k)}\left(x \odot b^{(k)}\right) \right)_i.$$

And to sample we just need to generate $Z \sim \mathcal{N}(0, I)$ and compute $f^{-1}(Z)$.

A coupling layer can be implemented with

```
class NVPCouplingLayer(nn.Module):
    def __init__(self, map_s, map_t, b):
        super(NVPCouplingLayer, self).__init__()
        self.map_s = map_s
        self.map_t = map_t
        self.b = b.clone().unsqueeze(0)

    def forward(self, x_and_logdetjac):
        x, logdetjac = x_and_logdetjac
        s, t = self.map_s(self.b * x), self.map_t(self.b * x)
        logdetjac += ((1 - self.b) * s).sum(1)
        y = self.b * x +  (1 - self.b) * (torch.exp(s) * x + t)
        return (y, logdetjac)

    def invert(self, x):
        s, t = self.map_s(self.b * x), self.map_t(self.b * x)
        return self.b * x + (1 - self.b) * (torch.exp(-s) * (x - t))
```

The `forward` here computes both the image of x and the update on the accumulated determinant of the Jacobian, *i.e.*

$$(x, u) \mapsto (f(x), u + |J_f(x)|) .$$

We can then define a complete network with one-hidden layer tanh MLPs for the s and t mappings

```
class NVPNet(nn.Module):
    def __init__(self, dim, hidden_dim, depth):
        super(NVPNet, self).__init__()
        b = torch.empty(dim)
        self.layers = nn.ModuleList()
        for d in range(depth):
            if d%2 == 0:
                i = torch.randperm(b.numel())[0:b.numel() // 2]
                b.zero_()[i] = 1
            else:
                b = 1 - b
            map_s = nn.Sequential(nn.Linear(dim, hidden_dim), nn.Tanh(),
                                  nn.Linear(hidden_dim, dim))
            map_t = nn.Sequential(nn.Linear(dim, hidden_dim), nn.Tanh(),
                                  nn.Linear(hidden_dim, dim))
            self.layers.append(NVPCouplingLayer(map_s, map_t, b))

    def forward(self, x_and_logdetjac):
        for m in self.layers: x_and_logdetjac = m(x_and_logdetjac)
        return x_and_logdetjac

    def invert(self, x):
        for m in reversed(self.layers): x = m.invert(x)
        return x
```

And the log-proba of individual samples of a batch

```
def LogProba(x_and_logdetjac):
    (x, logdetjac) = x_and_logdetjac
    log_p = logdetjac - 0.5 * x.pow(2).add(math.log(2 * math.pi)).sum(1)
    return log_p
```

Training is achieved by maximizing the mean log-proba

```
batch_size = 100

model = NVPNet(dim = 2, hidden_dim = 2, depth = 4)
optimizer = optim.Adam(model.parameters(), lr = 1e-2)

for e in range(args.nb_epochs):

    acc_loss = 0

    for b in range(0, nb_train_samples, batch_size):
        output = model((input[b:b+batch_size], 0))
        loss = - LogProba(output).mean()
        acc_loss = acc_loss + loss.item()
        model.zero_grad()
        loss.backward()
        optimizer.step()
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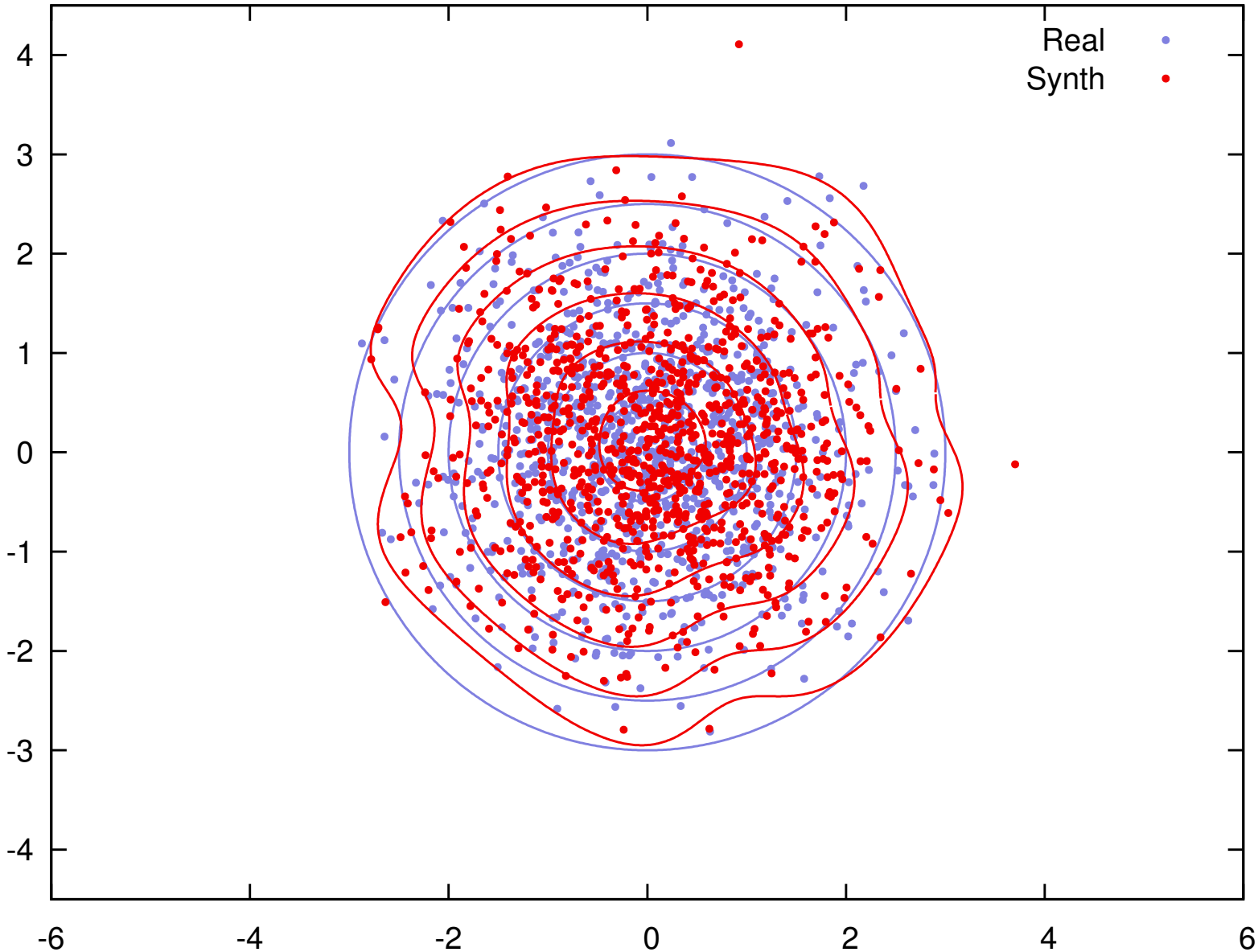
Finally, we can sample according to $p_{f^{-1}(Z)}$ with

```
z = torch.empty(nb_train_samples, 2).normal_()
x = model.invert(z)
```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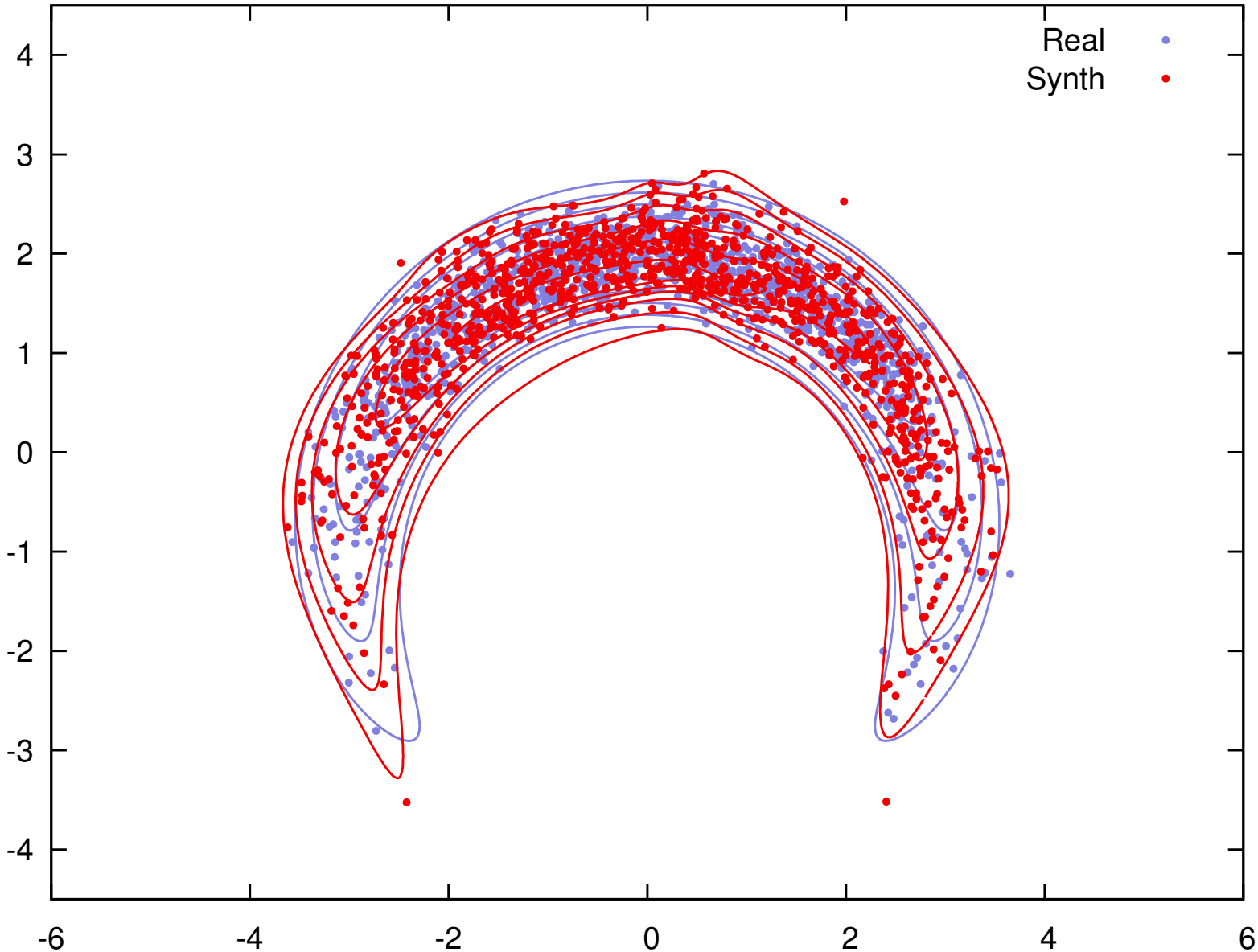
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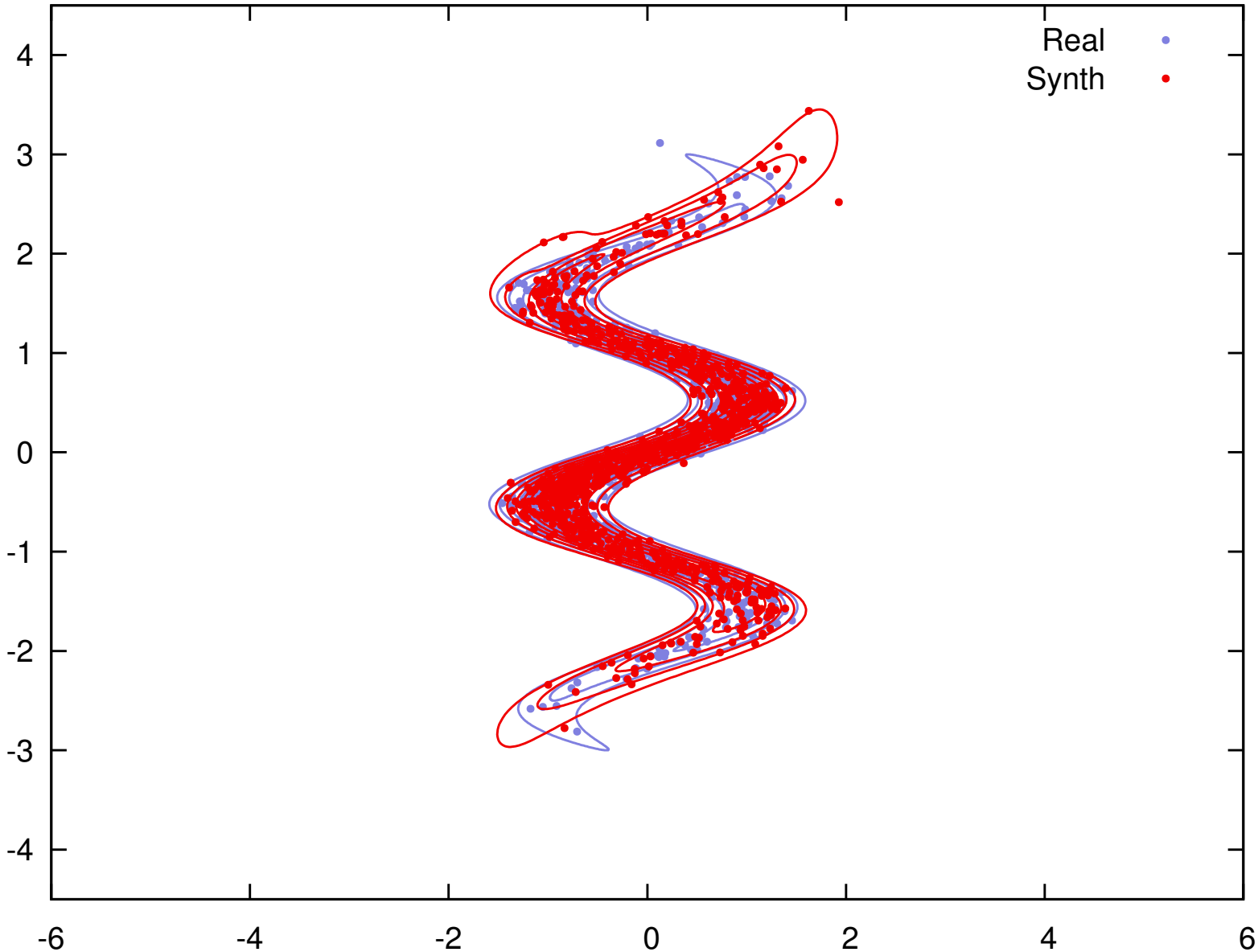
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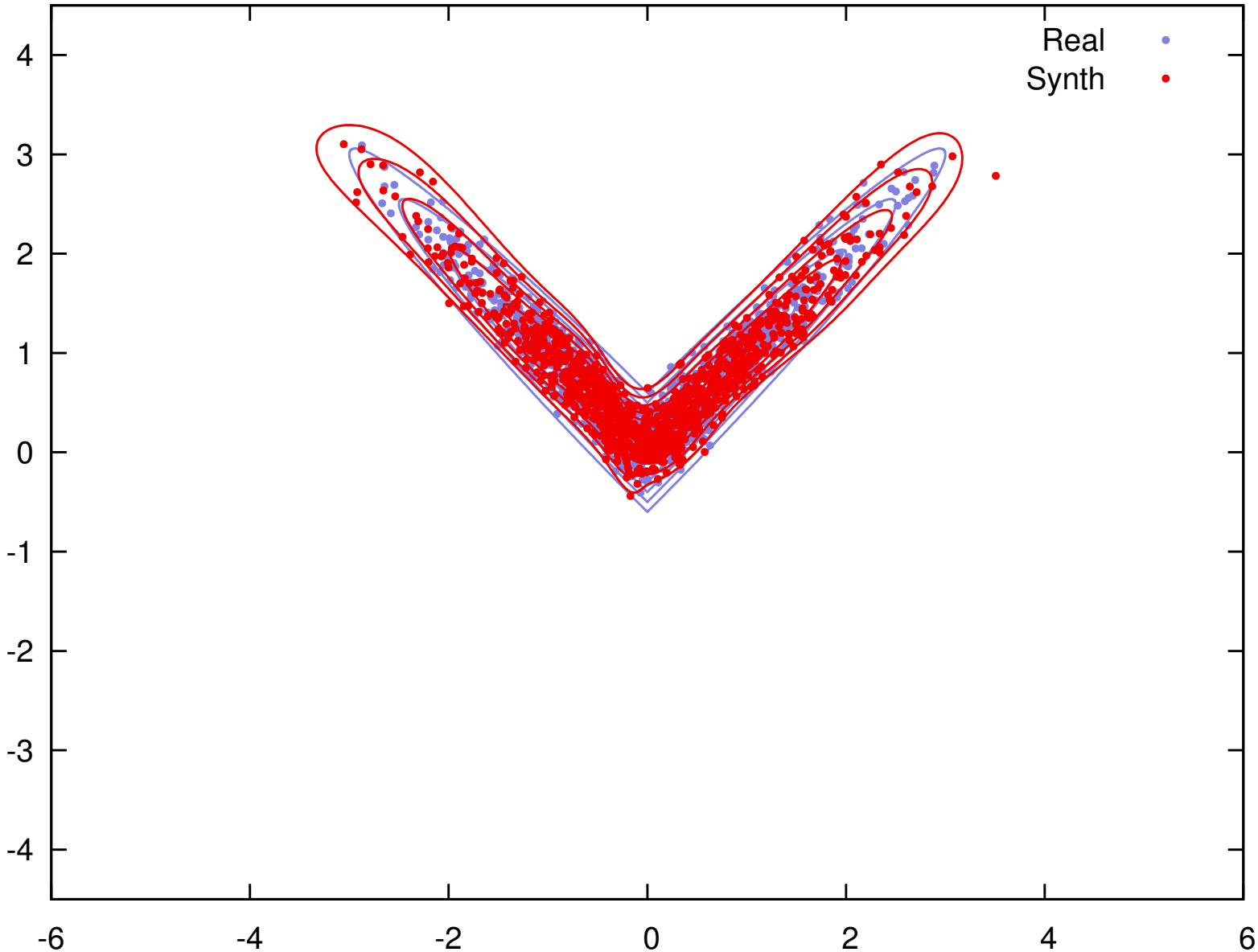
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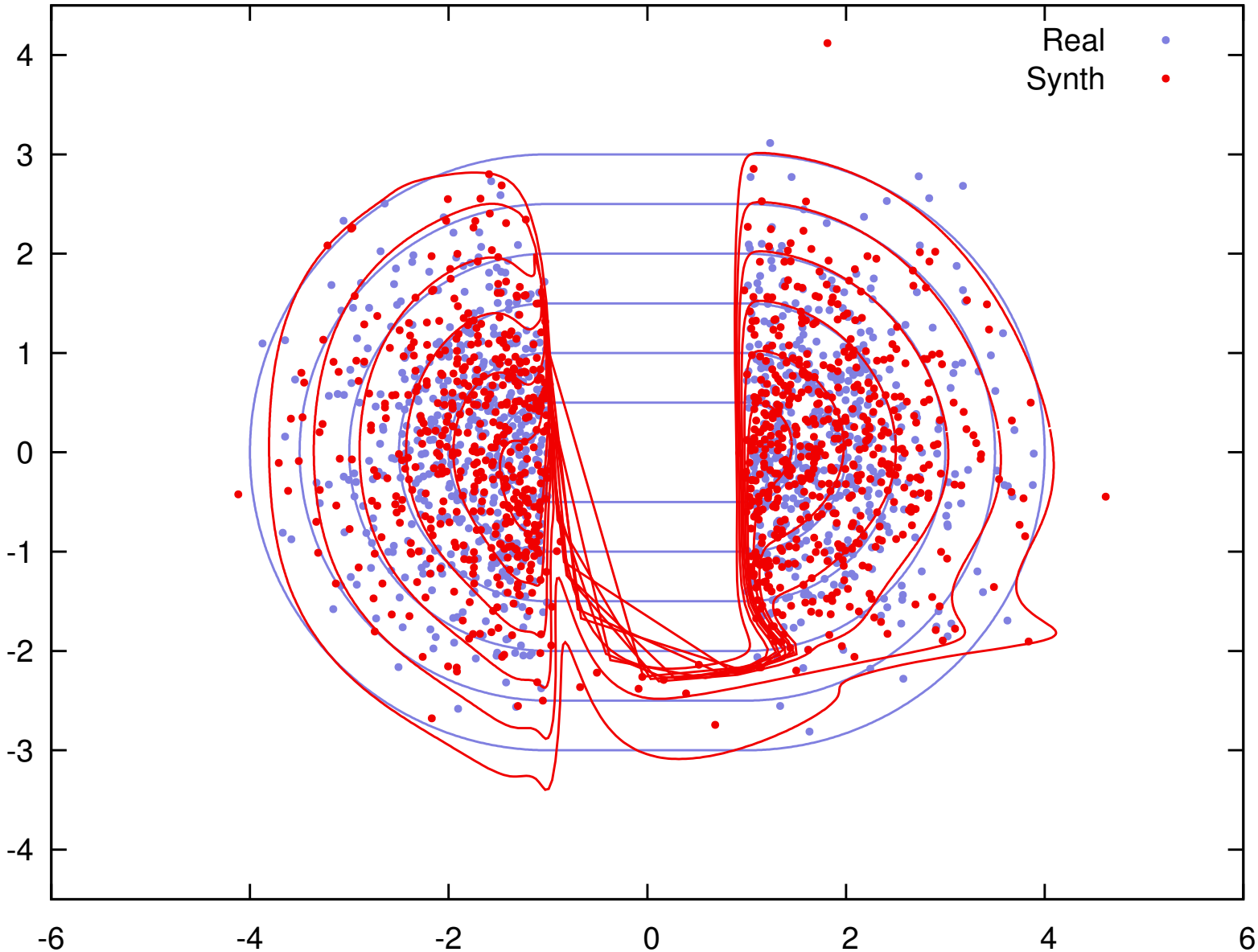
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Dinh et al. (2016) apply this approach to convolutional layers by using bs consistent with the activation map structure, and reducing the map size while increasing the number of channels.

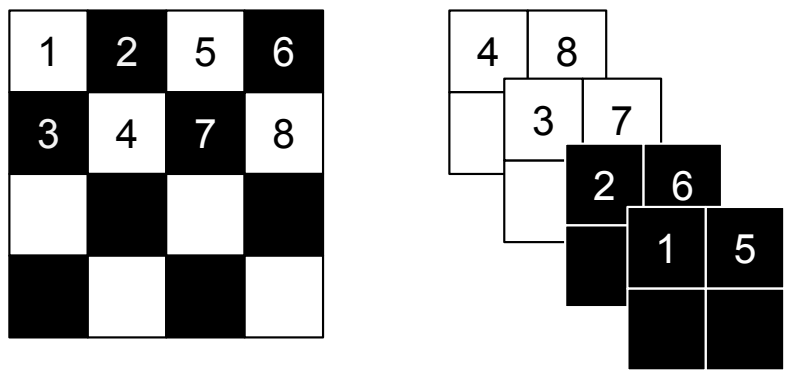
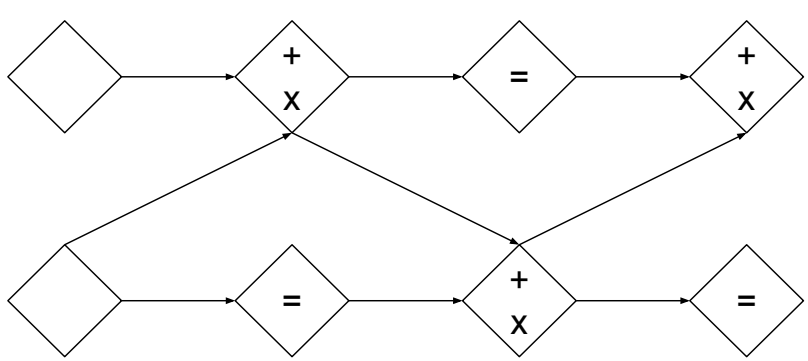


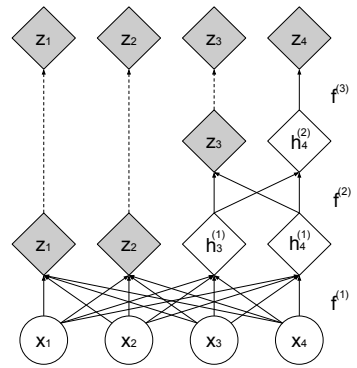
Figure 3: Masking schemes for affine coupling layers. On the left, a spatial checkerboard pattern mask. On the right, a channel-wise masking. The squeezing operation reduces the $4 \times 4 \times 1$ tensor (on the left) into a $2 \times 2 \times 4$ tensor (on the right). Before the squeezing operation,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

(Dinh et al., 2016)

They combine these layers by alternating masks, and branching out half of the channels at certain points to forward them unchanged.



(a) In this alternating pattern, units which remain identical in one transformation are modified in the next.



(b) Factoring out variables. At each step, half the variables are directly modeled as Gaussians, while the other half undergo further transformation.

Figure 4: Composition schemes for affine coupling layers.

(Dinh et al., 2016)

The structure for generating images consists of

- $\times 2$ stages
  - $\times 3$ checkerboard coupling layers,
  - a squeezing layer,
  - $\times 3$ channel coupling layers,
  - a factor-out layer.
- $\times 1$ stage
  - $\times 4$ checkerboard coupling layers
  - a factor-out layer.

The s and t mappings get more complex in the later layers.

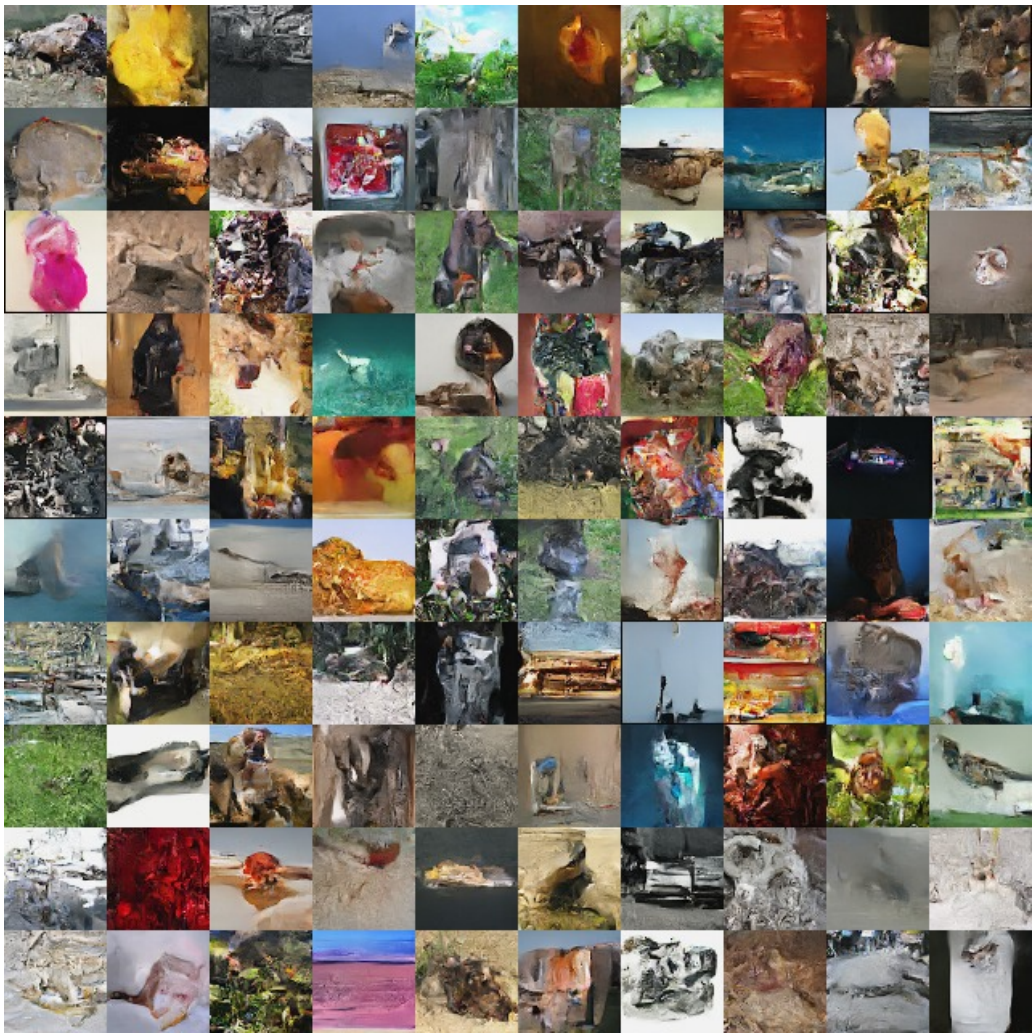


Figure 7: Samples from a model trained on *Imagenet* (64×64).

(Dinh et al., 2016)

Figure 8: Samples from a model trained on *CelebA*.

(Dinh et al., 2016)

Figure 9: Samples from a model trained on *LSUN* (*bedroom* category).

(Dinh et al., 2016)

Figure 10: Samples from a model trained on *LSUN* (*church outdoor* category).

(Dinh et al., 2016)

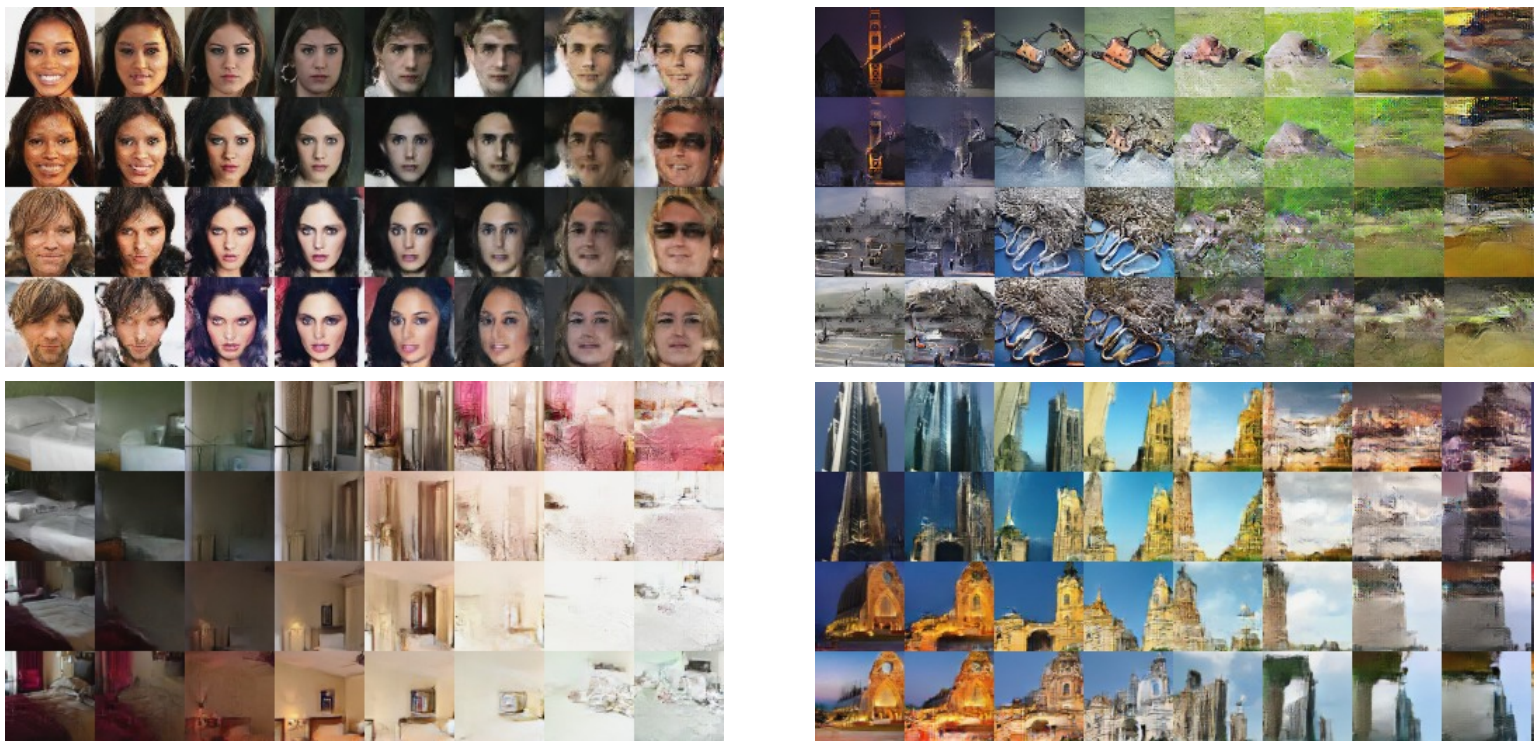


Figure 6: Manifold generated from four examples in the dataset. Clockwise from top left: CelebA, Imagenet (64×64), LSUN (tower), LSUN (bedroom).

(Dinh et al., 2016)

The end

References

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