Deep learning

10.3. Non-volume preserving networks

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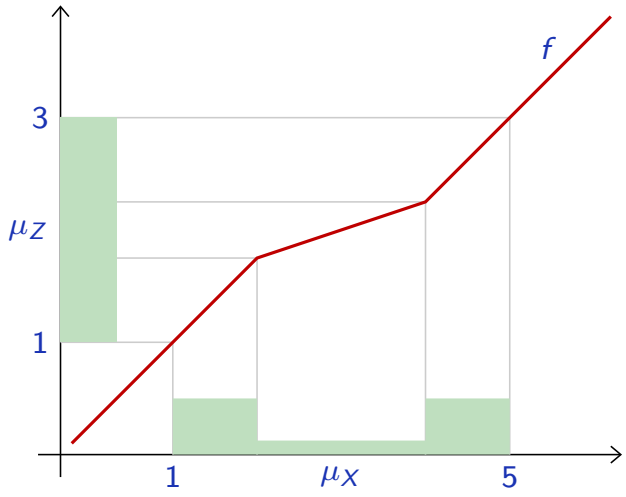
A standard result of probability theory is that if f is continuous, invertible and [almost everywhere] differentiable, and $X = f^{-1}(Z)$, then

$$\forall x,\ \mu_X(x) = \mu_Z(f(x))\,|J_f(x)|\,.$$



The term $|J_f(x)|$ accounts for the local "stretching" of the space.

Notes

Another strategy to model high dimension data densities is to train a model to transform the data density into a fixed "normalized" one. The resulting mapping is called a normalizing flow.
Those methods rely on a standard result of probability theory. If f is continuous, invertible, and [almost everywhere] differentiable, and $X = f^{-1}(Z)$, then the density μ_X of X at a certain point x is equal to the density of Z at the image point $f(x)$ multiplied by the determinant of f's Jacobian at x that reflects the local expansion of the space.

This formula shows that the density of X is proportional to how likely it was for Z to be $f(x)$, and how much f is "stretching" locally the space there.
Here we take Z uniform on $[1, 3]$, and f monotonically increasing with three linear pieces, the first and last ones with a slope of 1, and the middle one with a slop lesser than 1. When the slope is 1, we have the exact same density in the two domains. When the slope is smaller, the corresponding density from Z is expanded on a broader domain for X.

Since

$$\mu_X(x) = \mu_Z(f(x))\,|J_f(x)|\,,$$

if f is a parametric function such that we can compute [and differentiate]

$$\mu_Z(f(x)) \quad \text{and} \quad |J_f(x)|\,,$$

given $x_1, \ldots, x_N$ i.i.d $\sim \mu$, we can make μ_X fit the data by maximizing

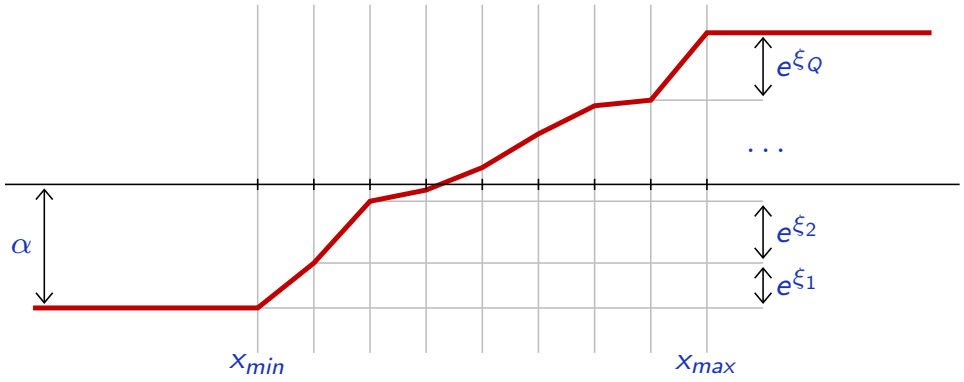
$$\sum_n \log \mu_X(x_n) = \sum_n \log \mu_Z(f(x_n)) + \log |J_f(x_n)|\,.$$

If $Z \sim \mathcal{N}(0, I)$,

$$\log \mu_Z\left(f(x_n)\right) = -\frac{1}{2}\left(\|f(x_n)\|^2 + d \log 2\pi\right).$$

We aim at $f(X) \sim \mathcal{N}(0, I)$, hence at f **normalizing** the distribution.

Consider an increasing piece-wise linear mapping with parameters $\alpha, \xi_1, \ldots, \xi_Q$.



Notes

To illustrate this on a simple example, we consider an increasing piece-wise affine model:

- $f(x) = \alpha$ for $x \leq x_{min}$,
- $[x_{min}, x_{max}]$ is split in N intervals in each of which f is affine and increases by e^{ξ_q},
- f is constant for $x \geq x_{max}$, and hence equal to $\alpha + \sum_q e^{\xi_q}$.

The quantities N, x_{min}, and x_{max} will be fixed, while α and the ξ_qs are the parameters of f that will be optimized during training.

```
class PiecewiseLinear(nn.Module):
    def __init__(self, nb, xmin, xmax):
        super().__init__()
        self.xmin = xmin
        self.xmax = xmax
        self.nb = nb
        self.alpha = nn.Parameter(torch.tensor([xmin], dtype = torch.float))
        mu = math.log((xmax - xmin) / nb)
        self.xi = nn.Parameter(torch.empty(nb + 1).normal_(mu, 1e-4))

    def forward(self, x):
        y = self.alpha + self.xi.exp().cumsum(0)
        u = self.nb * (x - self.xmin) / (self.xmax - self.xmin)
        n = u.long().clamp(0, self.nb - 1)
        a = (u - n).clamp(0, 1)
        x = (1 - a) * y[n] + a * y[n + 1]
        return x
```

Notes

We initialize the model so that f behaves like the identity on $[x_{min}, x_{max}]$.
`forward` operates on a batch of values. The variable `y` holds f's values at the changes of slope, `n` the index of the interval for each input value, and `a` the relative position in the interval.

For $f : \mathbb{R} \to \mathbb{R}$ increasing, we have

$$|J_f(x_n)| = f'(x_n)$$

so we should minimize

$$\sum_n \frac{1}{2}\left(f(x_n)^2 + \log 2\pi\right) - \log f'(x_n).$$

To work with batches of samples, we have to compute $(f'(x_1), \ldots, f'(x_N))$ with autograd.

With

$$\Phi(x_1, \ldots, x_N) = f(x_1) + \cdots + f(x_N)$$

we have

$$\nabla\Phi(x_1, \ldots, x_n) = \big(f'(x_1), \ldots, f'(x_N)\big)\,.$$

$$\mathscr{L}(f) = \frac{1}{N} \sum_n \frac{1}{2} \left(f(x_n)^2 + \log 2\pi \right) - \log f'(x_n).$$

```
for input in train_input.split(batch_size):
    input.requires_grad_()
    output = model(input)

    derivatives, = autograd.grad(
        output.sum(), input,
        retain_graph = True, create_graph = True
    )

    loss = ( 0.5 * (output**2 + math.log(2*pi)) - derivatives.log() ).mean()

    optimizer.zero_grad()
    loss.backward()
    optimizer.step()
```

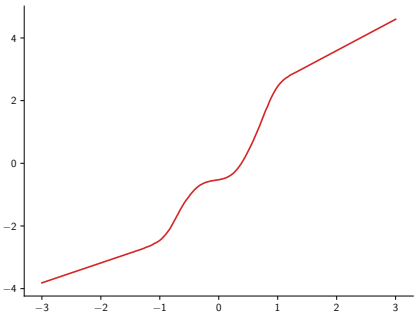
Notes

We need the derivative of f w.r.t. its input, so specify `requires_grad_()`, and compute the gradient of `output.sum()` to get $(f'(x_1), \ldots, f'(x_N))$.

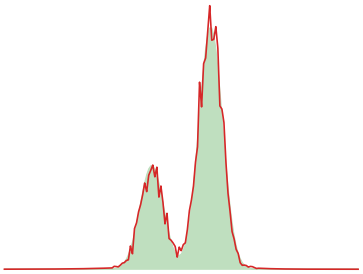
Since PyTorch by default allows to use the autograd graph only once, we specify `retain_graph=True` when computing the f' to be able to use it a second time to compute the gradient of the loss. And since the loss depends on the f', we also state `create_graph = True`.

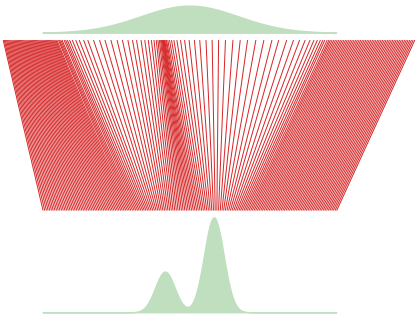
Target distribution μ

Resulting mapping $\hat{f}$



μ_X with $X = \hat{f}^{-1}(Z)$ and $Z \sim \mathcal{N}(0, 1)$





Notes

As a toy example, we use a mixture of two Gaussian distributions as the data distribution (top left), and train a `PiecewiseLinear` model with 1000 intervals to map this distribution normal distribution of zero mean and unit variance.
The empirical distribution (red curve, bottom left) is estimated by taking regularly spaced points on the interval, and computing for each of these x the log of the normal density at $f(x)$, and $f'(x)$.
The bottom right image shows how f is contracting or expanding the space to properly fit the normal distribution. The mapping from x to $f(x)$ is depicted by the red lines. In particular, the "hole" between the two Gaussians in the mixture gets contracted to fit the normal part, which the middle of the Gaussians are expanded. The tails are just shifted.

Non-Volume Preserving networks

To apply the same idea to high dimension signals, we have to compute and differentiate $|J_f(x)|$. And to use that approach for synthesis, we can sample $Z \sim \mathcal{N}(0, I)$ and compute $f^{-1}(Z)$.

However, for standard layers:

- computing $f^{-1}(z)$ is impossible, and
- computing $|J_f(x)|$ is intractable.

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

The resulting Non-Volume Preserving network (NVP) is one form of **normalizing flow** among many techniques (Papamakarios et al., 2019).

Notes

In the toy example of the first part, computing $|J_f|$ could be done with autograd since we were in 1d. This does not scale to real-world high dimension signals.

Remember that if f is a composition

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

we have

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

hence

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

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

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

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.

For clarity in what follows, b has all 1s first, follows by 0s, but this is not required.

$$b = (\underbrace{1, 1, \ldots, 1}_{\Delta}, \underbrace{0, 0, \ldots, 0}_{d-\Delta})$$

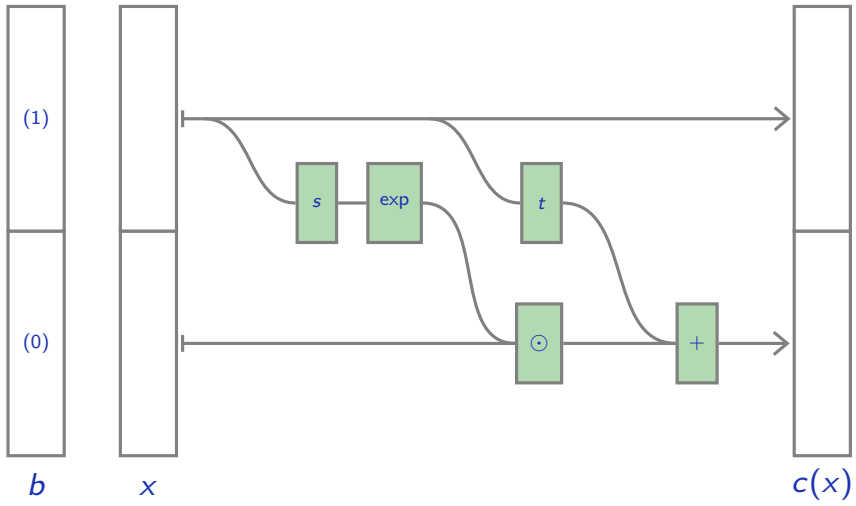
Notes

The quantities t and s stand respectively for translation and scale.
Such a "coupling layer" keeps the components for which the corresponding b_i is 1 unchanged, modifies the other components in an invertible way that only depends on the unchanged ones.

The expression

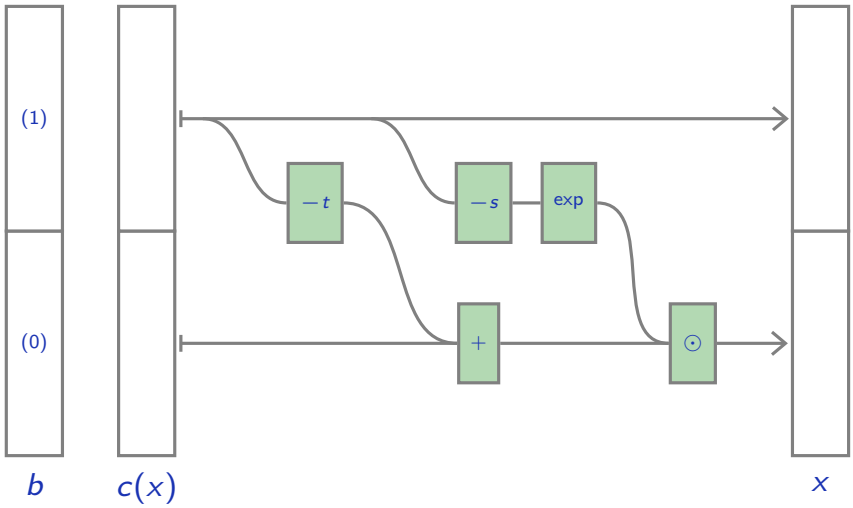
$$c(x) = b \odot x + (1 - b) \odot \Big(x \odot \exp(s(b \odot x)) + t(b \odot x) \Big)$$

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



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

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



The second property of this mapping is the simplicity of its Jacobian.

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

and we have

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

Notes

Remember that for the sake of simplicity we make the assumption that all the 1s in b appear consecutively first.
For any pair i, j such that $b_i = 1, b_j = 1$, we have

$$\frac{\partial c_i}{\partial x_j} = \frac{\partial x_i}{\partial x_j} = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{otherwise} \end{cases},$$

which gives us a diagonal of ones in the top left part of the Jacobian.
For any pair i, j such that $b_i = 0, b_j = 0$, we have

$$\begin{aligned} \frac{\partial c_i}{\partial x_j} &= \frac{\partial}{\partial x_j}\left(x_i e^{\overbrace{s_i(b \odot x)}^{\substack{\text{does not depend} \\ \text{on } x_j \text{ because } b_j=0}}} + \overbrace{t_i(b \odot x)}^{\substack{\text{constant} \\ \text{w. r. t. } x_j}}\right) \\ &= \begin{cases} \exp(s_i(b \odot x)) & \text{if } i = j \\ 0 & \text{otherwise} \end{cases}, \end{aligned}$$

so the bottom right part of the Jacobian is a diagonal with terms $\exp(s_i(x \odot b))$.

```
dim = 6

x = torch.randn(1, dim).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 * torch.exp(s(b * x)) + t(b * x))

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

print(j)
```

prints

```
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],
        [ 0.4001, -0.3774, -0.9410,  1.0074,  0.0000,  0.0000],
        [-0.1756,  0.0409,  0.0808,  0.0000,  1.2412,  0.0000],
        [ 0.0875, -0.3724, -0.1542,  0.0000,  0.0000,  0.6186]])
```

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 $x_n^{(k)} = f^{(k)}\left(x_n^{(k-1)}\right)$, we train by minimizing

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

with

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

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

Notes

Since all coupling layers are invertible, f^{-1} can be computed. So at generation time, we draw a sample $Z \sim \mathcal{N}(0, I)$ and compute $X = f^{-1}(Z)$

A coupling layer can be implemented with

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

    def forward(self, x, ldj): # ldj for log det Jacobian
        s, t = self.map_s(self.b * x), self.map_t(self.b * x)
        ldj = ldj + ((1 - self.b) * s).sum(1)
        y = self.b * x + (1 - self.b) * (torch.exp(s) * x + t)
        return y, ldj

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

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

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

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().__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.clone()))

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

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


Notes

Masks b are made in such a way that $b^{(2n)}$ are generated at random, while $b^{(2n+1)} = 1 - b^{(2n)}$. It assures that all the components of the input are changed. This is one out of many strategies that can be used to ensure that the components are modified.

And the log-proba of individual samples of a batch

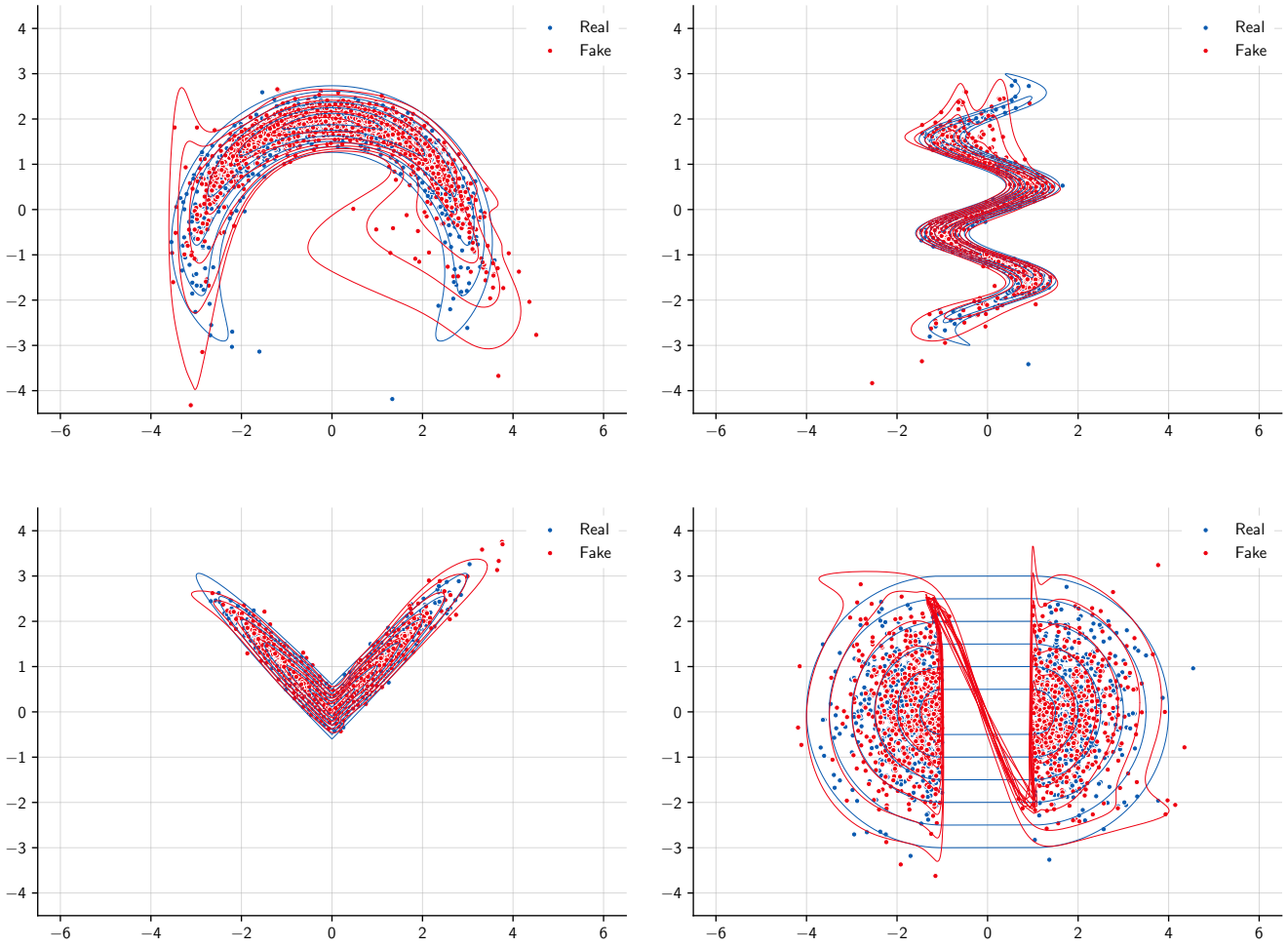
```
def LogProba(x, ldj):
    log_p = - 0.5 * (x**2 + math.log(2*pi)).sum(1) + ldj
    return log_p
```

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):

    for input in train_input.split(batch_size):
        output, ldj = model(input, 0)
        loss = - LogProba(output, ldj).mean()
        model.zero_grad()
        loss.backward()
        optimizer.step()
```

Finally, we can sample according to μ_X with

```
z = torch.randn(nb_generated_samples, 2)
x = model.invert(z)
```



Notes

We test this model on 2d synthetic distributions. On each graph:

- the blue dots are sampled training points,
- the blue lines are circles deformed by the "true" f,
- the red lines are circles deformed by the trained model,
- The red dots are points sampled according to the trained model.

The true density at the bottom-right is discontinuous. It is obtained by sampling according to a normal, and adding 1 if the x coordinate is positive, and -1 otherwise. This is challenging for the model which is continuous.

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.

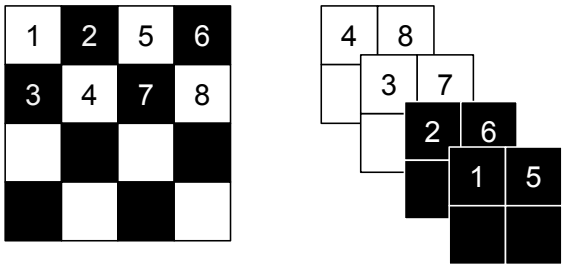
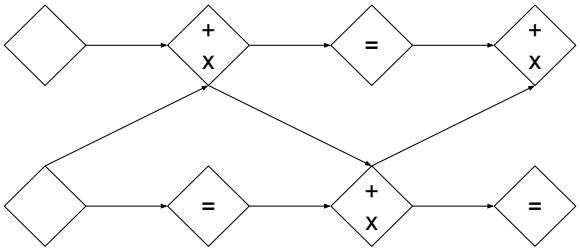


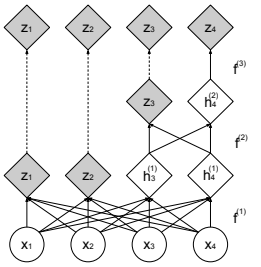
Figure 3: Masking schemes for affine coupling layers. On the left, a spatial checkerboard pattern mask. On the right, a channel-wise masking. The squeezing operation reduces the $4 \times 4 \times 1$ tensor (on the left) into a $2 \times 2 \times 4$ tensor (on the right). Before the squeezing operation,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

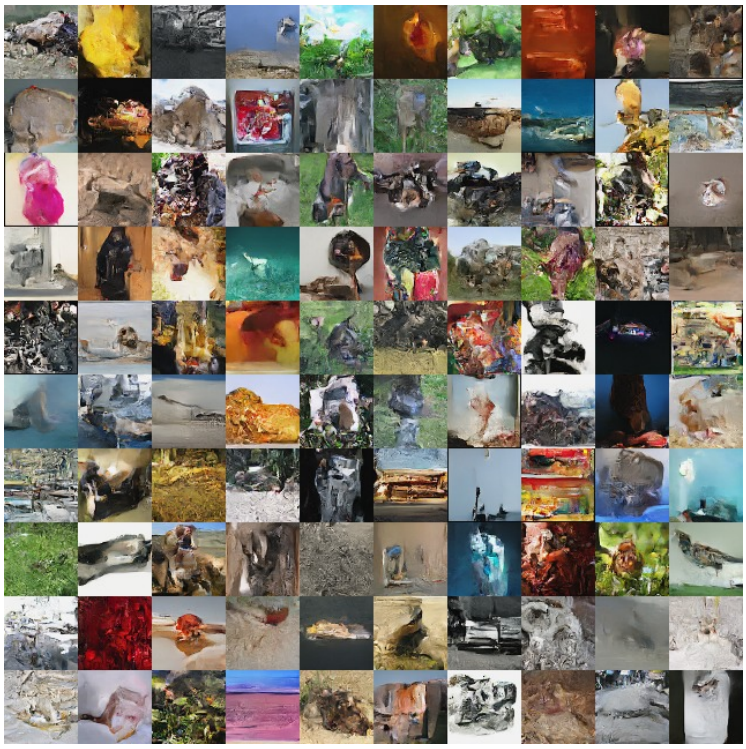


Figure 7: Samples from a model trained on *Imagenet* (64×64).

(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)

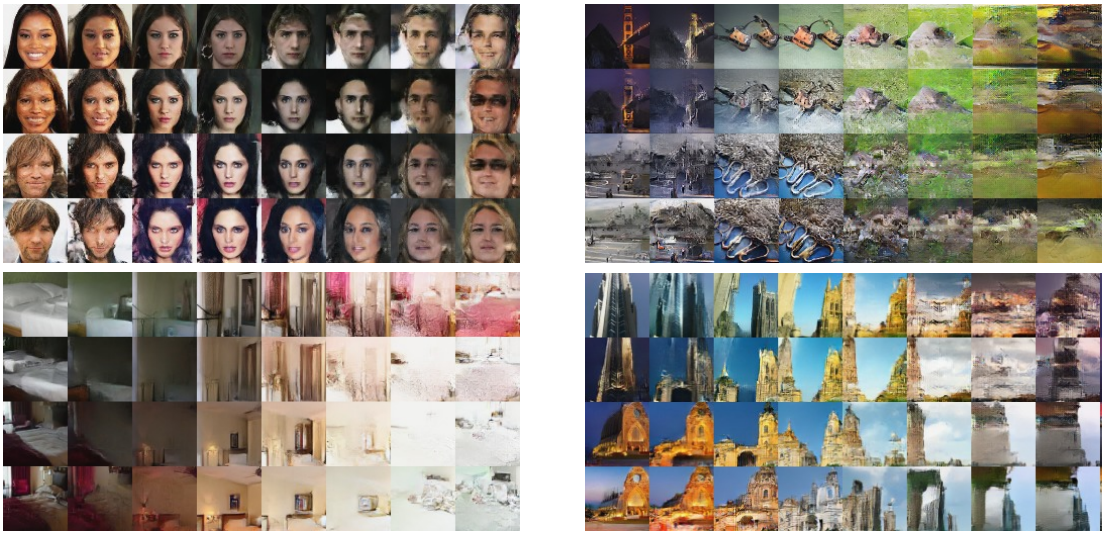


Figure 6: Manifold generated from four examples in the dataset. Clockwise from top left: CelebA, Imagenet (64×64), LSUN (tower), LSUN (bedroom).

(Dinh et al., 2016)

References

L. Dinh, D. Krueger, and Y. Bengio. **NICE: non-linear independent components estimation**. CoRR, abs/1410.8516, 2014.

L. Dinh, J. Sohl-Dickstein, and S. Bengio. **Density estimation using real NVP**. CoRR, abs/1605.08803, 2016.

G. Papamakarios, E. Nalisnick, D. Rezende, S. Mohamed, and B. Lakshminarayanan. **Normalizing flows for probabilistic modeling and inference**. CoRR, abs/1912.02762, 2019.