Lecture 15: Unsupervised Deep Learning (III)

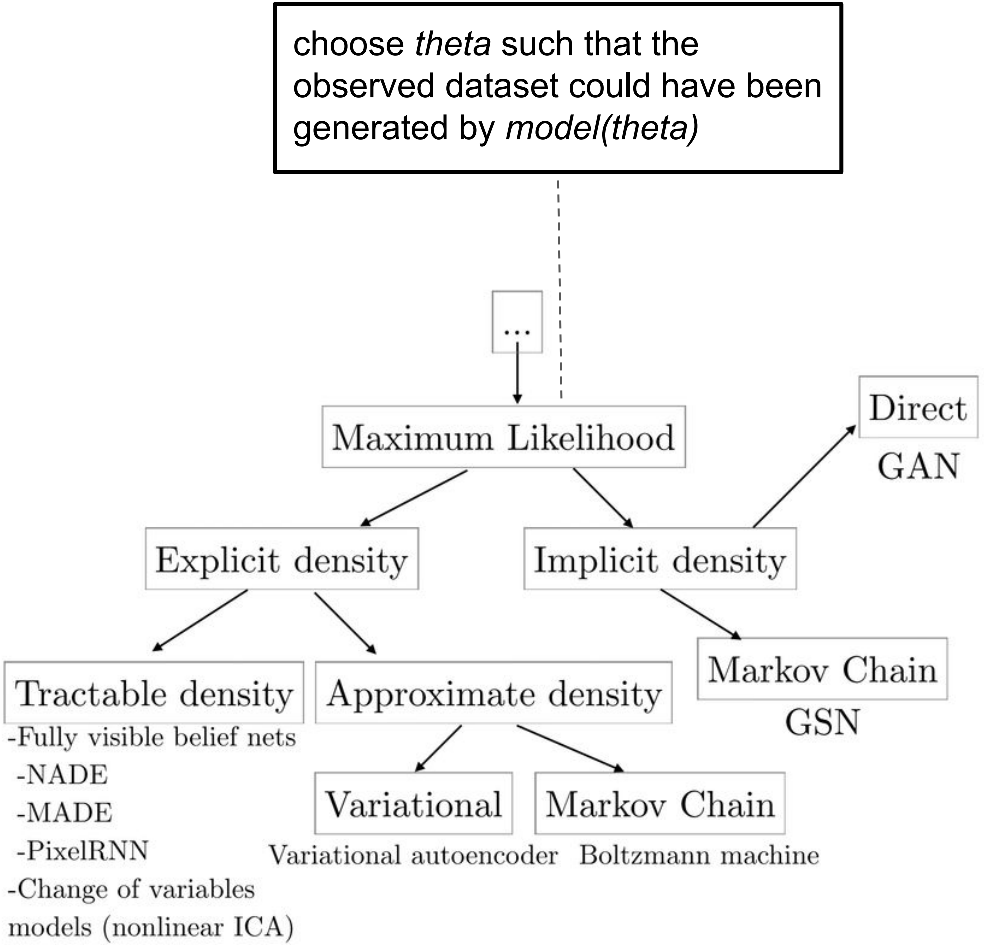
Applications of Generative Models; Normalizing Flows

Outline

1. **Some applications of convolutional autoencoders and GAN**
   a. Image-to-Image Translation with Conditional Adversarial Nets
   b. Unpaired Image-to-Image Translation using Cycle-Consistent Adversarial Networks
   c. PuppetGAN: Cross-Domain Image Manipulation by Demonstration

2. Normalizing Flows
   a. Change of variable formula
   b. Planar and radial flows
   c. Real NVP
   d. GLOW
   e. FFJORD
   f. Likelihood vs probability

Recap: GANs



choose *theta* such that the observed dataset could have been generated by *model(theta)*
...
Maximum Likelihood
Explicit density
Implicit density
Direct
GAN
Markov Chain
GSN
Tractable density
-Fully visible belief nets
-NADE
-MADE
-PixelRNN
-Change of variables models (nonlinear ICA)
Approximate density
Variational
Variational autoencoder
Markov Chain
Boltzmann machine

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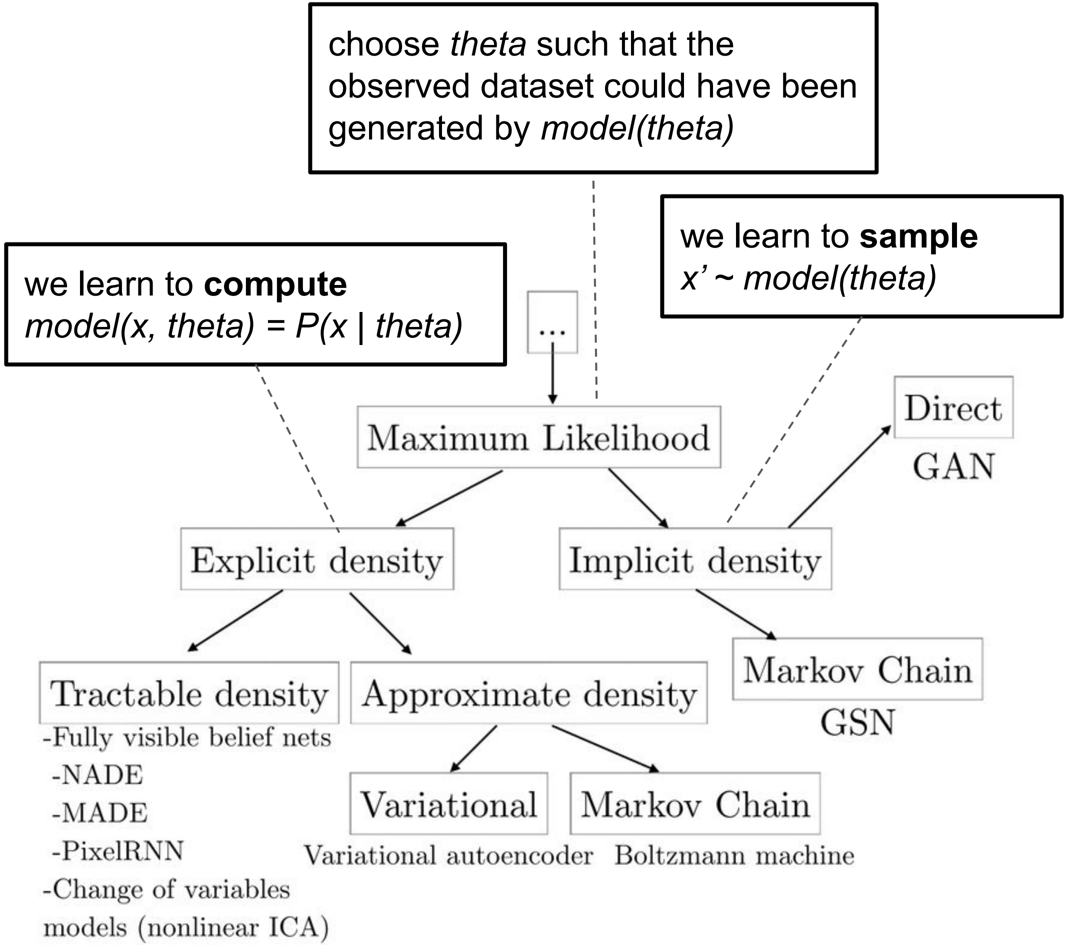

choose *theta* such that the observed dataset could have been generated by *model(theta)*
we learn to **compute** *model(x, theta) = P(x | theta)*
we learn to **sample** *x' ~ model(theta)*
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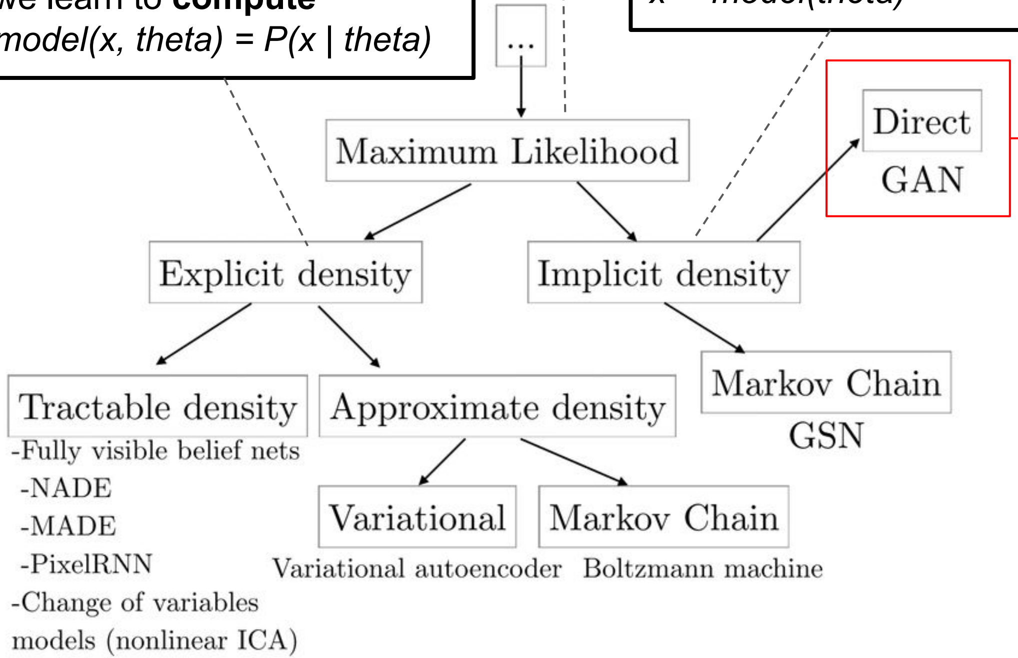
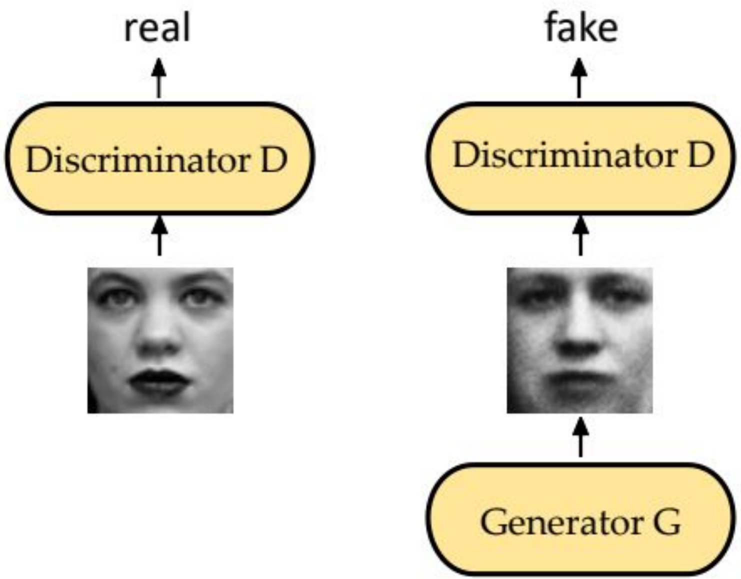
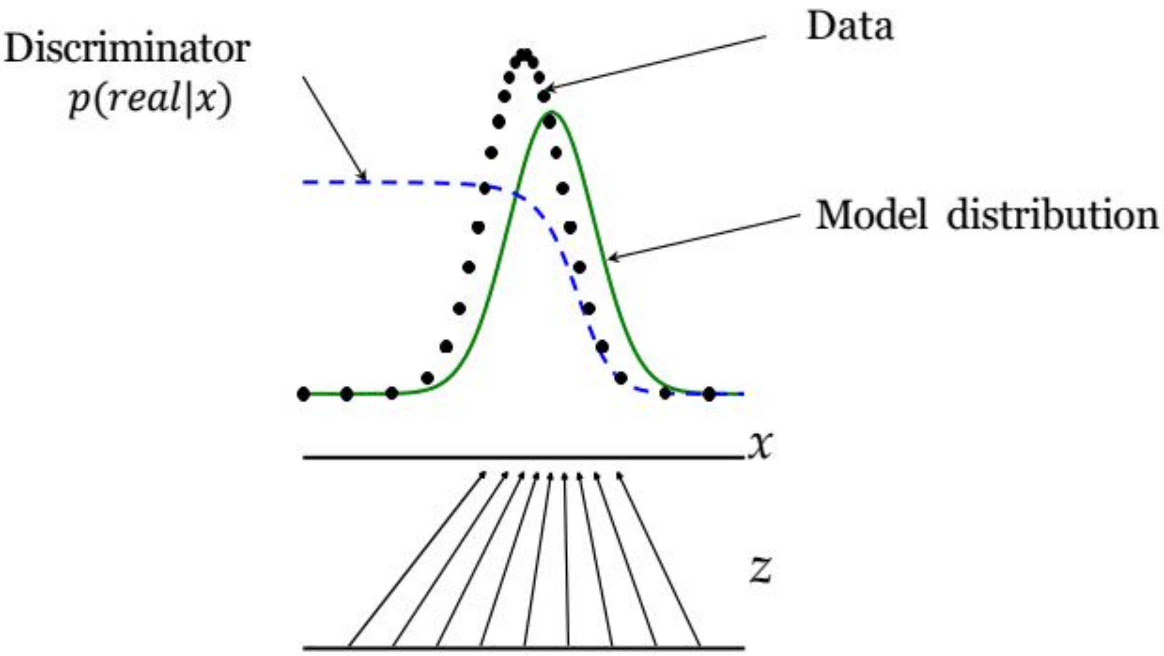


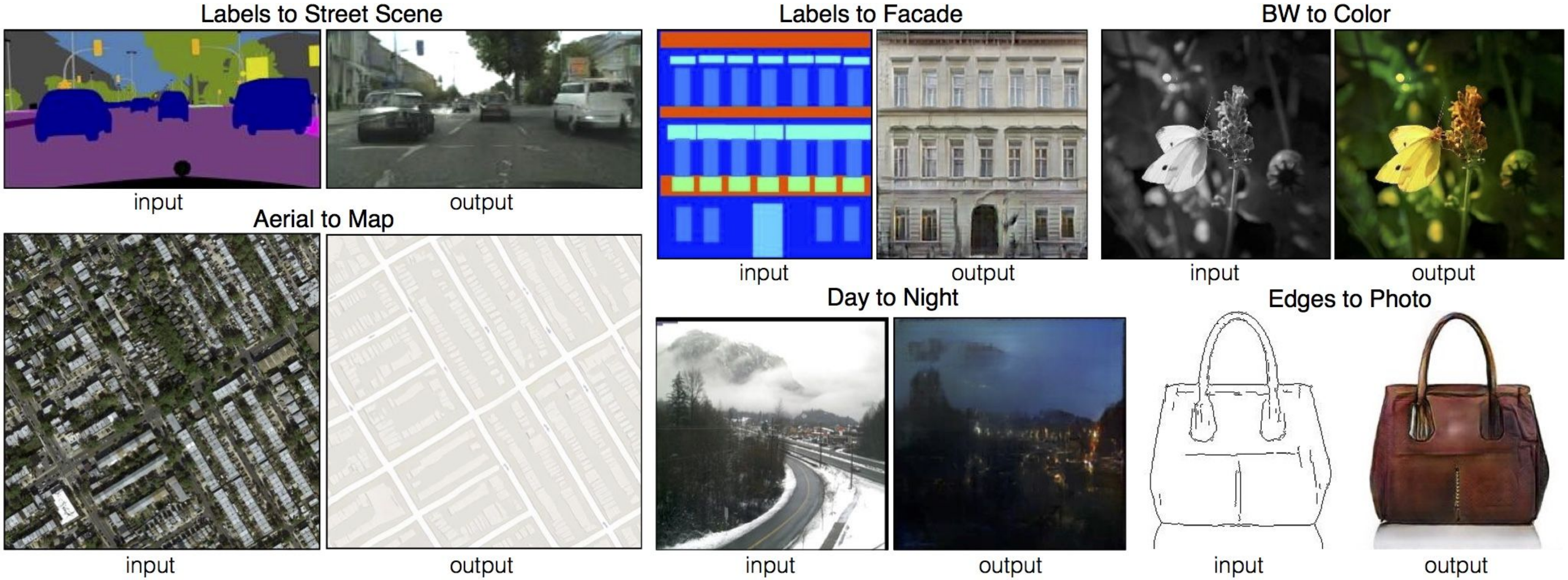


train G “to fool” D,
train D “to catch” G

Recap: GANs



Example Application 1:
Improving outputs of **supervised** image-to-image models



“Image-to-Image Translation with Conditional Adversarial Nets” [Phillip Isola, Jun-Yan Zhu, Tinghui Zhou, Alexei A. Efros]

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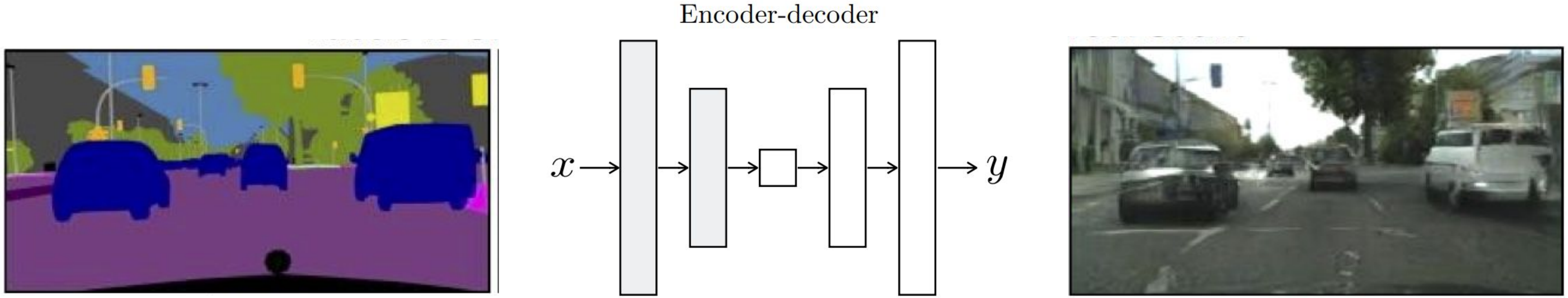

Q: This is a regression model: why not just use a simple supervised loss? (L1, L2)

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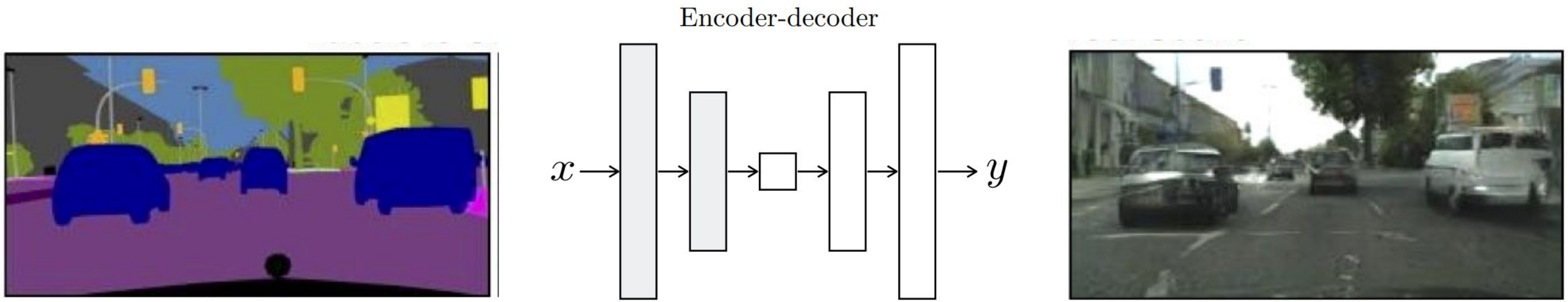

Q: This is a regression model: why not just use a simple supervised loss? (L1, L2)
A: These losses assume that multiple outputs are independent.

$$Y_i = f(X, theta) + e_i \quad e_i \sim \mathrm{N}(0, \mathrm{I}) \quad => \quad \text{L2 loss}$$

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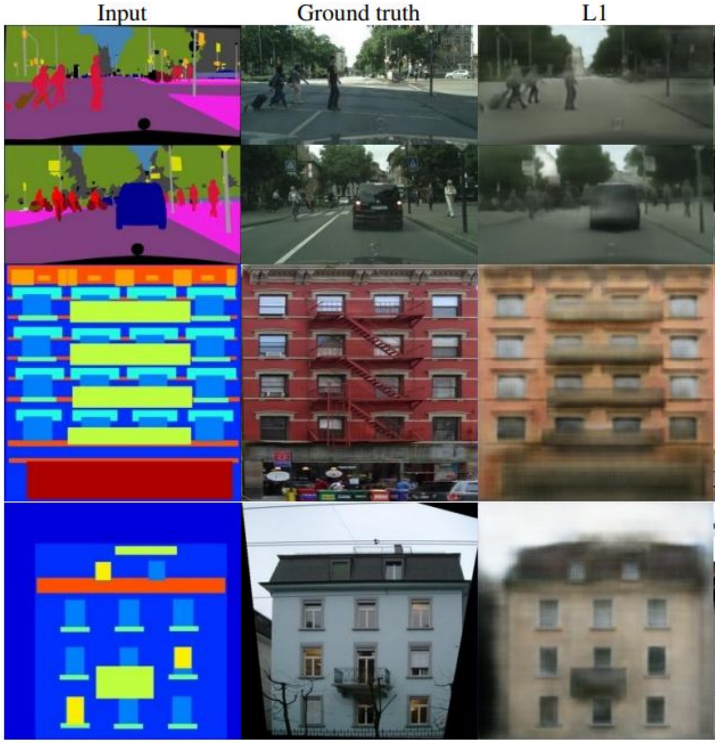

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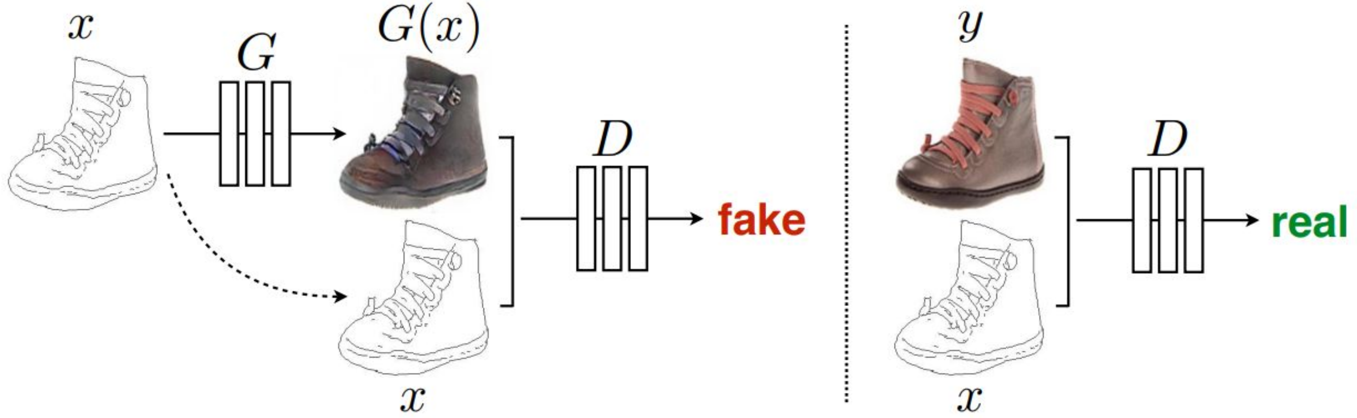

Figure 2: Training a conditional GAN to map edges→photo. The discriminator, D, learns to classify between fake (synthesized by the generator) and real {edge, photo} tuples. The generator, G, learns to fool the discriminator. Unlike an unconditional GAN, both the generator and discriminator observe the input edge map.

Example Application 1:
Improving outputs of **supervised** image-to-image models

Takeaway:

if the output domain has some structure (i.e. an image)
adversarial losses force the model to follow that structure

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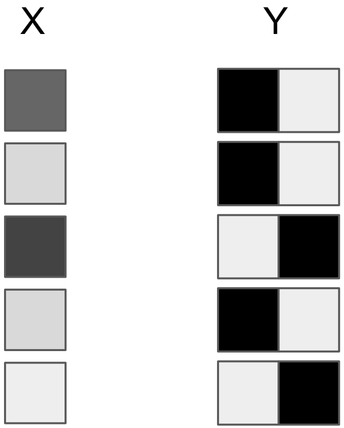
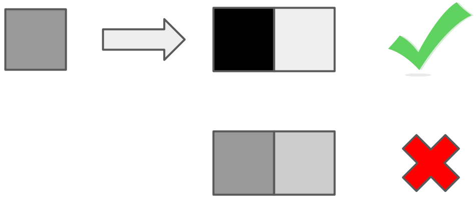
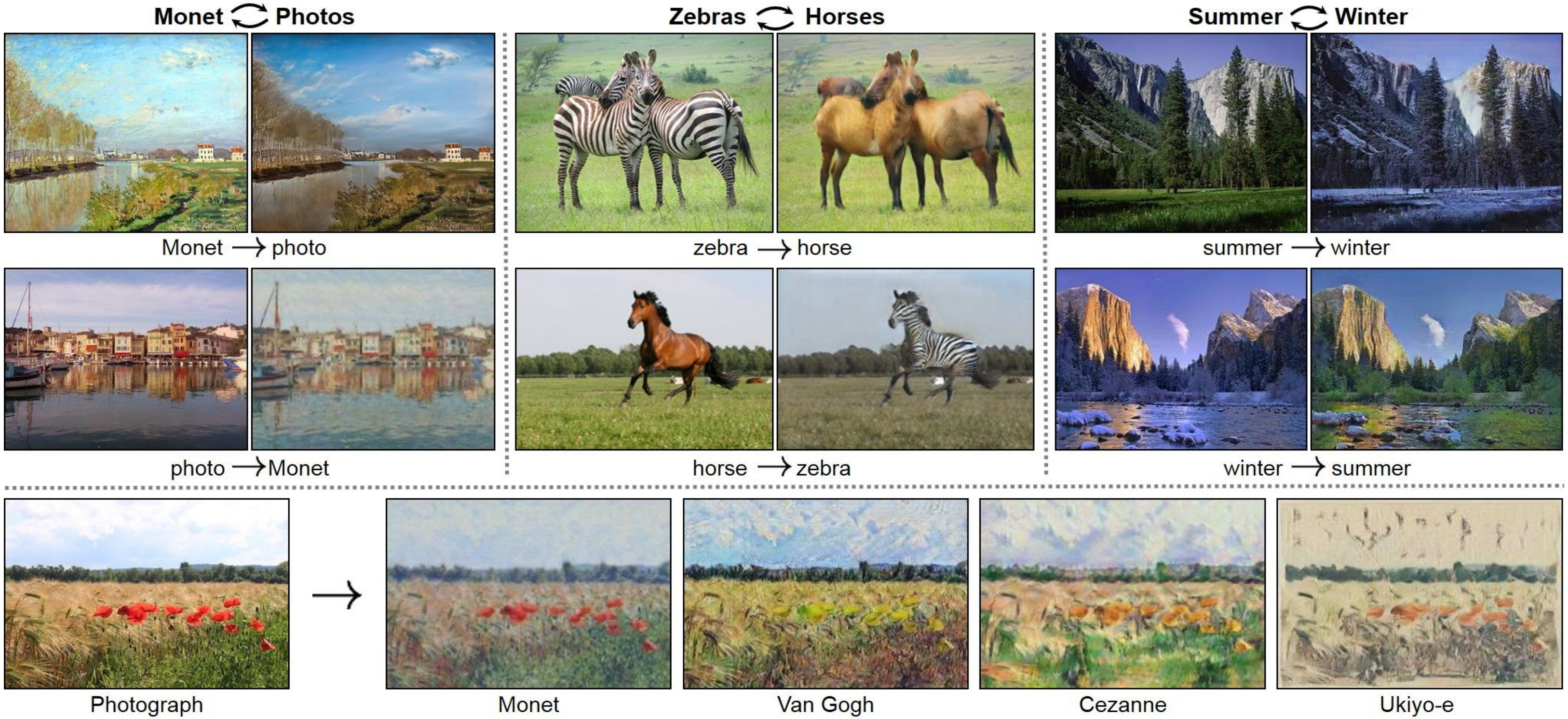


plain regression model is encouraged to “interpolate” outputs if uncertain

adversarial losses explicitly penalise outputs that look “too different from outputs in the training set”



Example Application 2:
Enabling **unsupervised** image-to-image training



“Unpaired Image-to-Image Translation using Cycle-Consistent Adversarial Networks” [Jun-Yan Zhu, Taesung Park, Phillip Isola, Alexei A. Efros]

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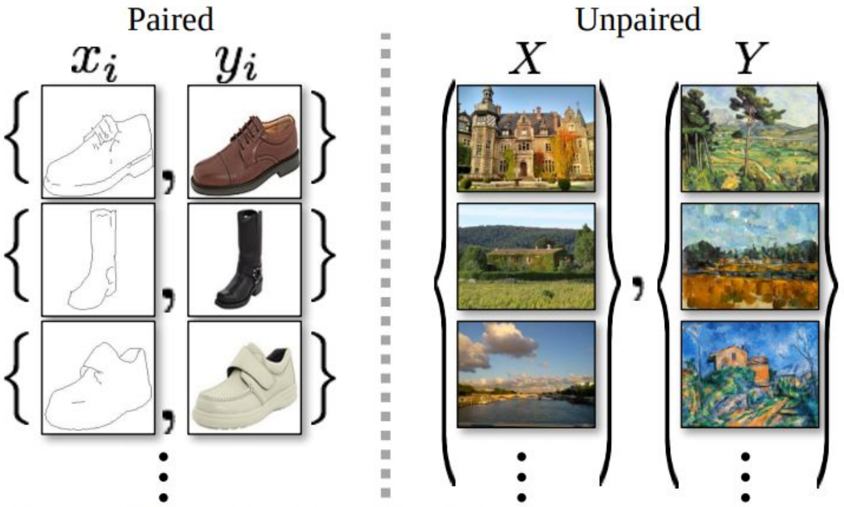

Figure 2: *Paired* training data (left) consists of training examples $\{x_i, y_i\}_{i=1}^N$, where the correspondence between x_i and y_i exists [22]. We instead consider *unpaired* training data (right), consisting of a source set $\{x_i\}_{i=1}^N$ ($x_i \in X$) and a target set $\{y_j\}_{j=1}$ ($y_j \in Y$), with no information provided as to which x_i matches which y_j.

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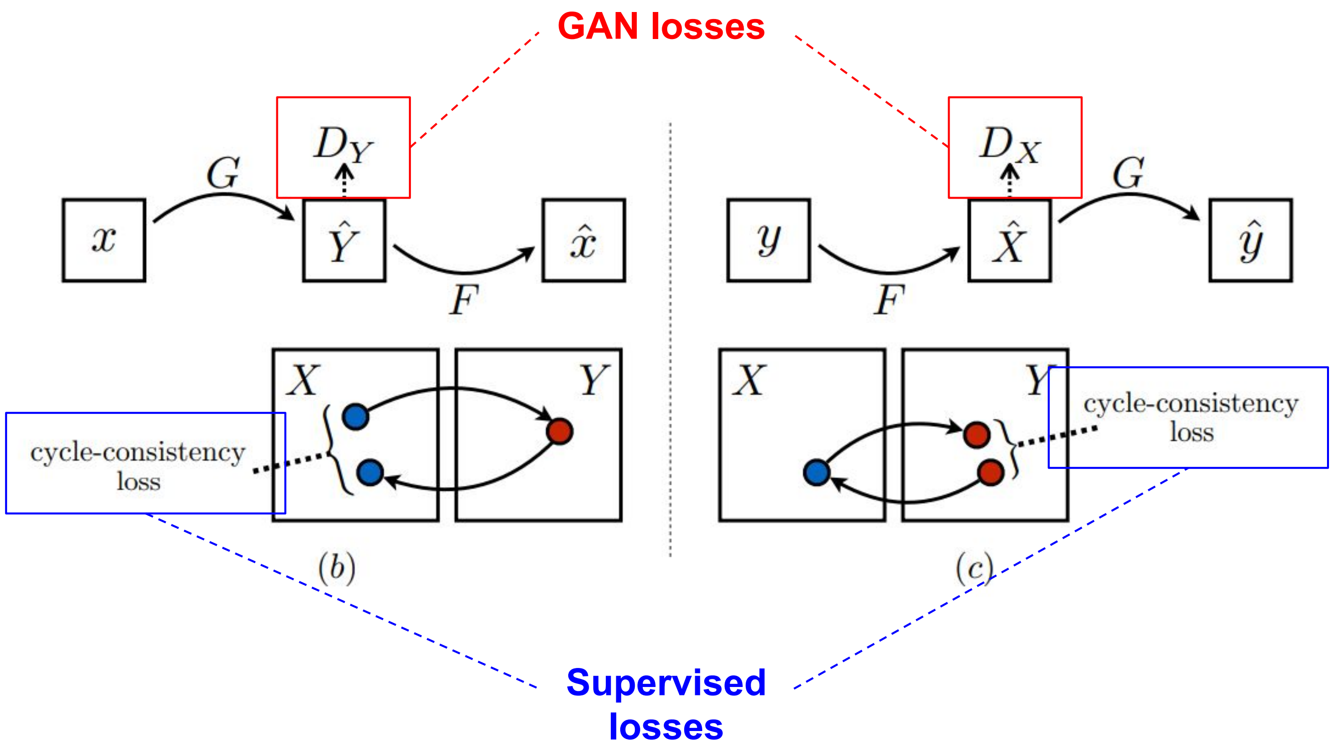

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Example Application 2:
Enabling **unsupervised** image-to-image training

Takeaway:

adversarial losses enable discovery of latent correspondances in the structure of two datasets

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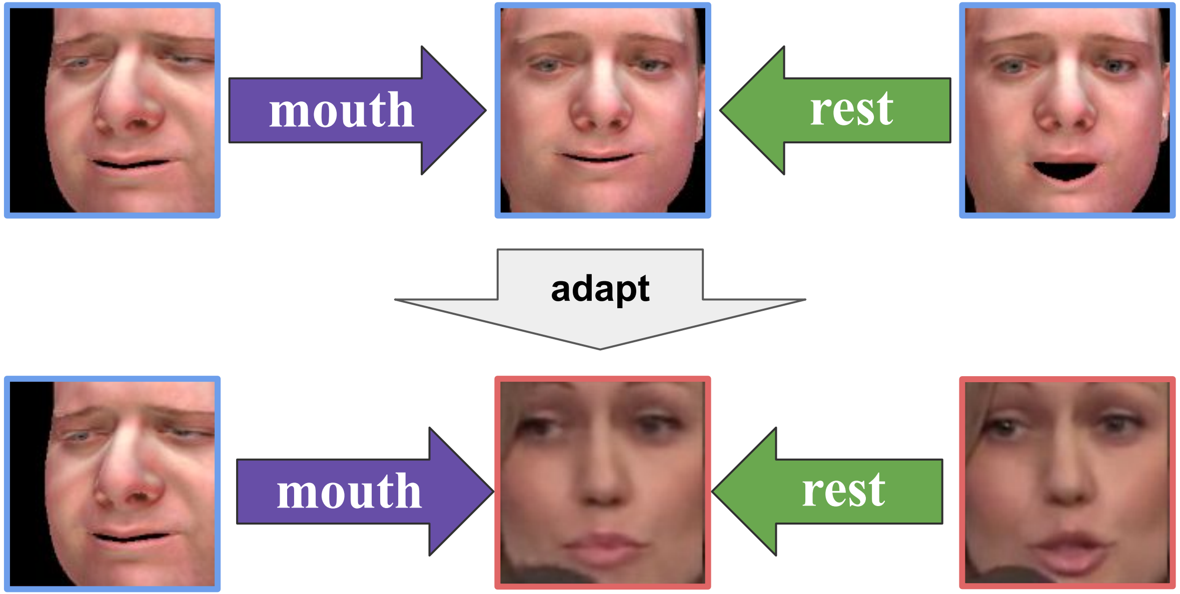
Example Application 3:
Cross-domain attribute manipulation



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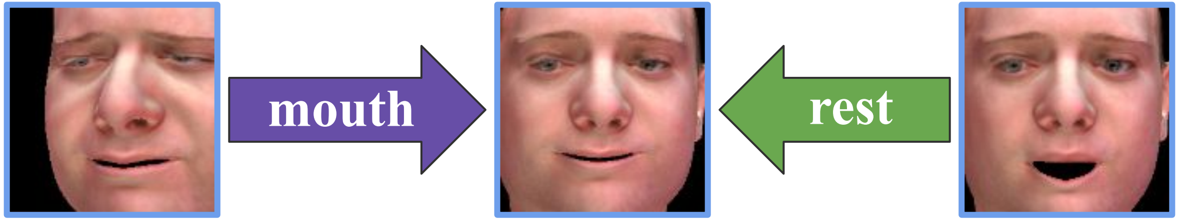

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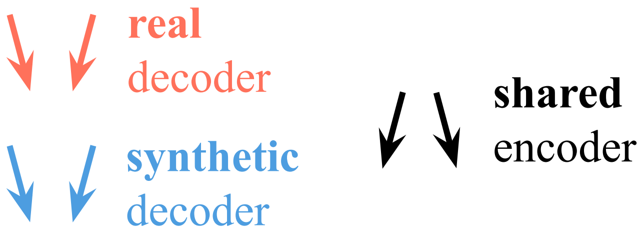
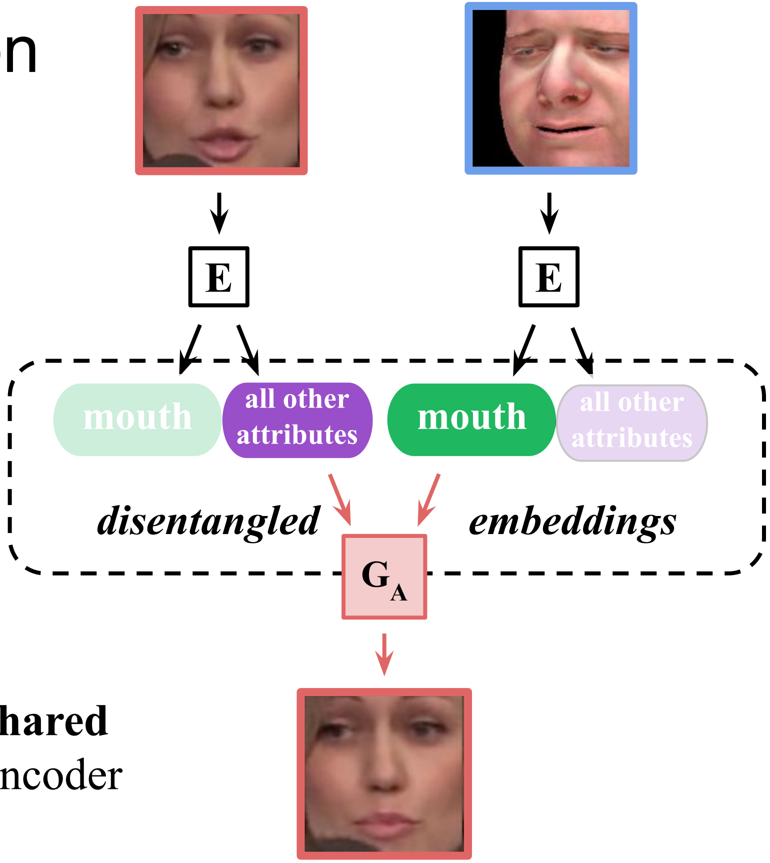
Example Application 3:
Cross-domain attribute manipulation

We trained a **disentangled autoencoder**: we **split** the encoded vector into **two parts** and **force** one part to represent the attribute we manipulate (mouth) and other attributes (hair, mic, …).

How?





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Example Application 3:
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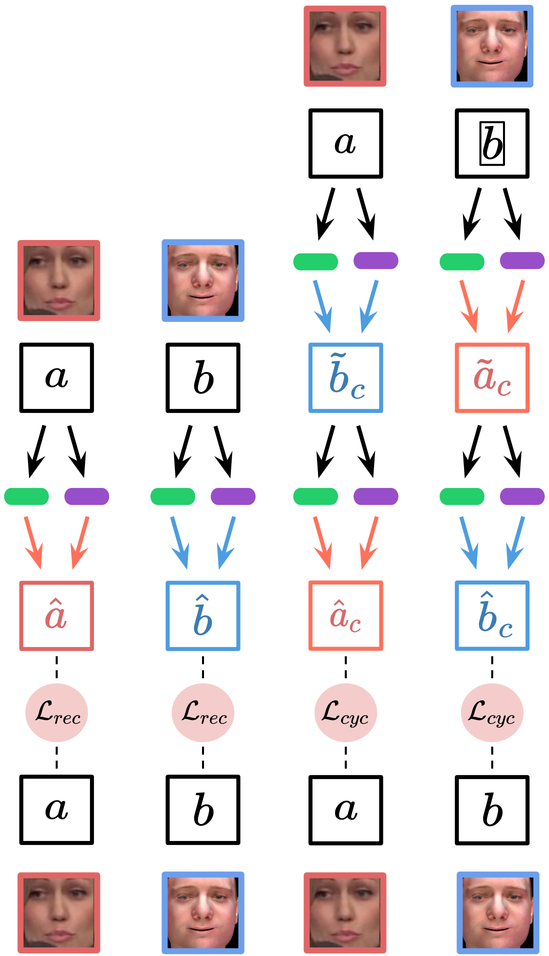
We combined **autoencoder** and **cycle losses** on both domains ...



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Example Application 3:
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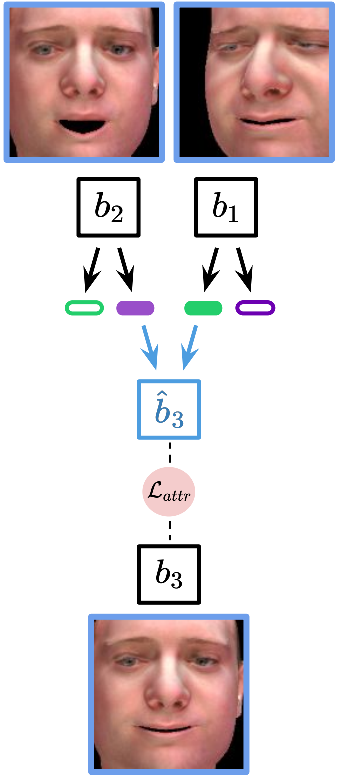
.. with **supervised losses** on synthetic data ...



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Example Application 3:
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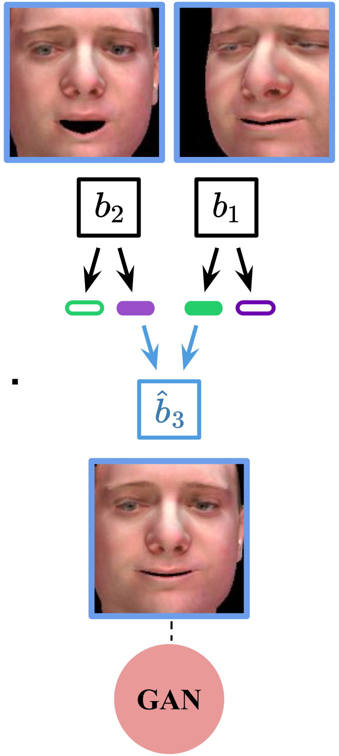
... with **GAN losses** ...



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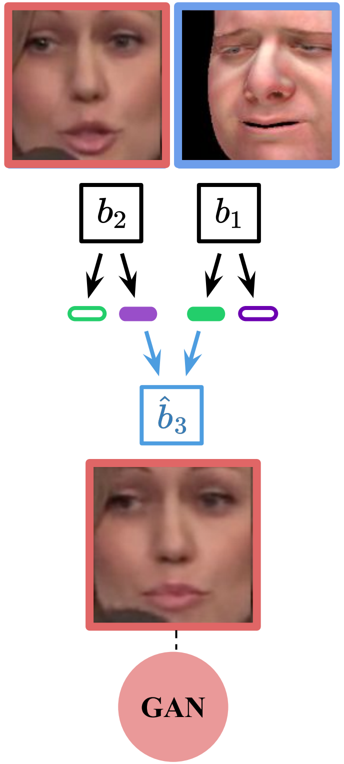

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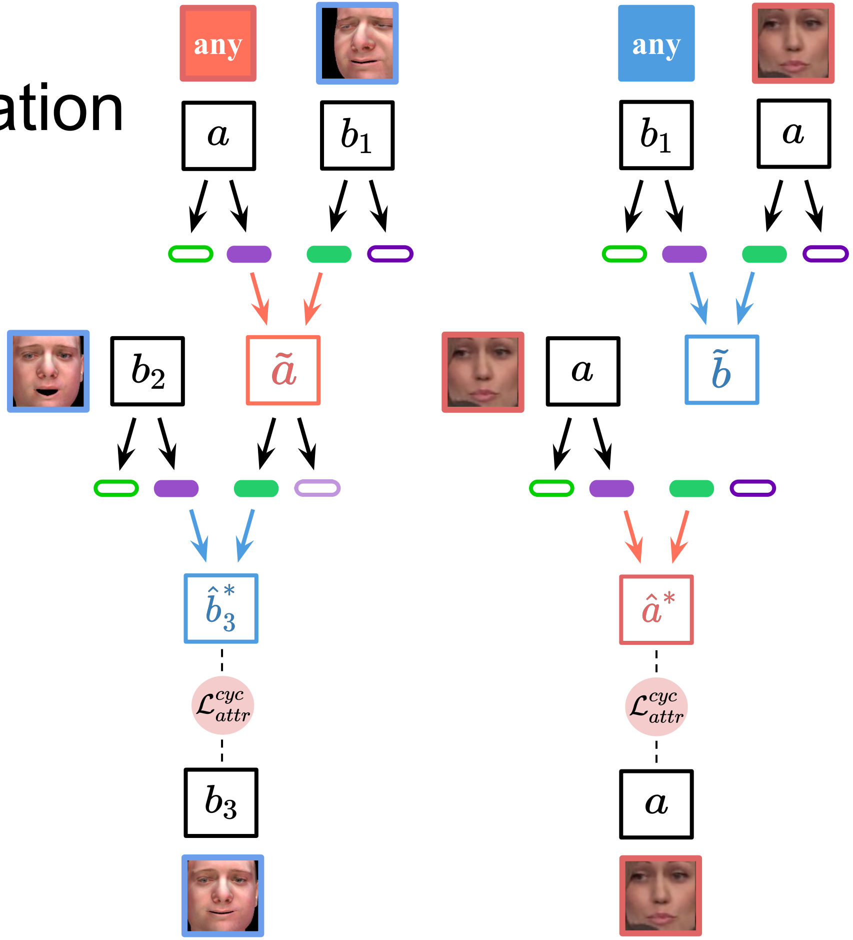
... and **compositional constraint losses** to ensure that all components are used.



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Example Application 3:
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Takeaway:

adversarial losses enable “forcing” the model to store
information necessary for reconstructing
specific “aspects” of the input image
at specific dimensions of the latent code

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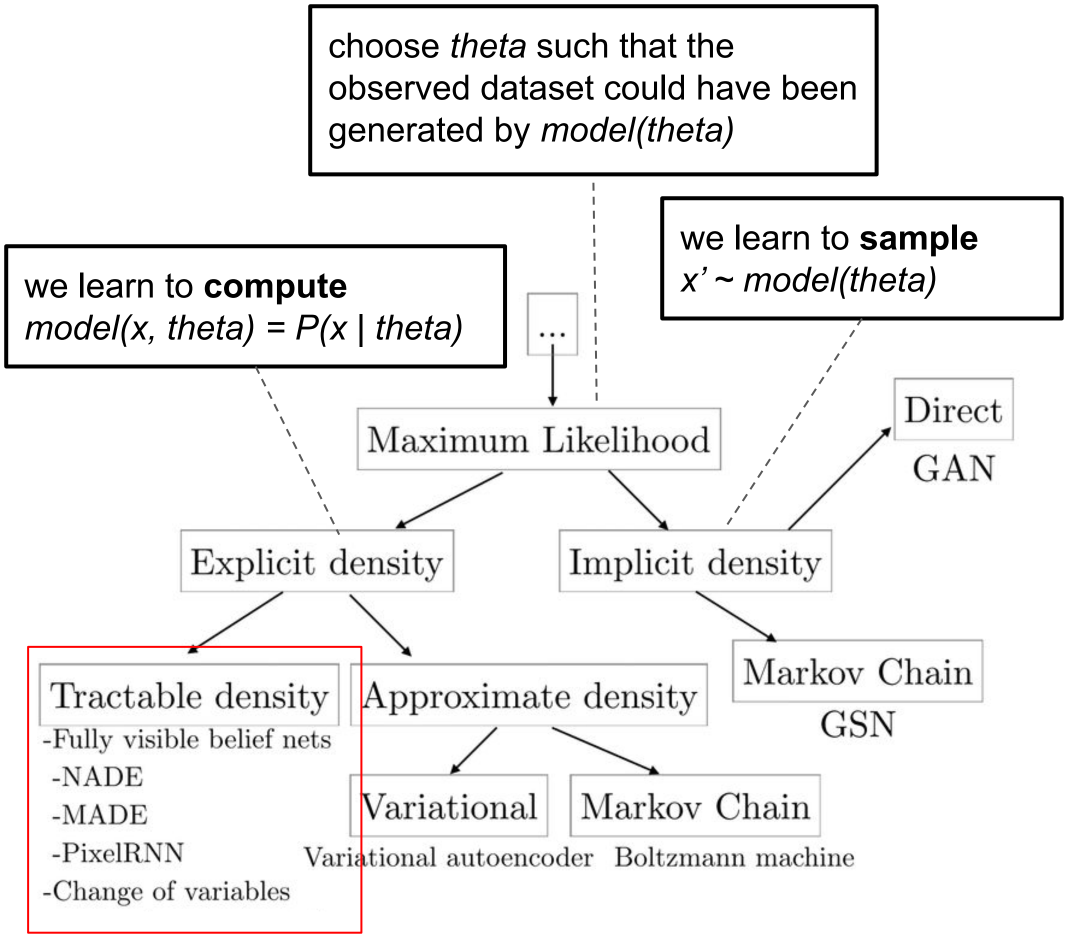
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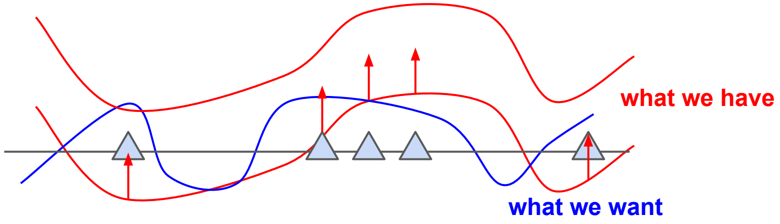
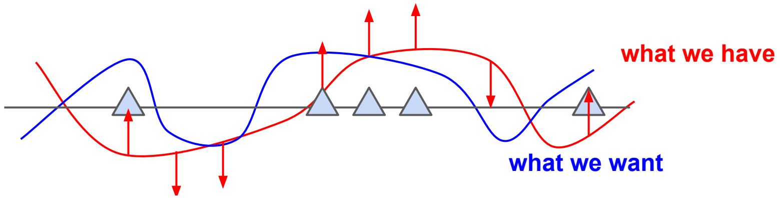
How to train a data model from positive samples only?



If we trained a neural network f(x; θ) to have high values at our training points x_i, it could just shift everything upwards.



We could train a GAN to generate “negative” samples, but the whole procedure becomes fragile.

We could use a model with a “fixed budget”, i.e. an autoencoder (# points it can “remember”) or a density models (integrates to one).

Why train a model from positive samples only?

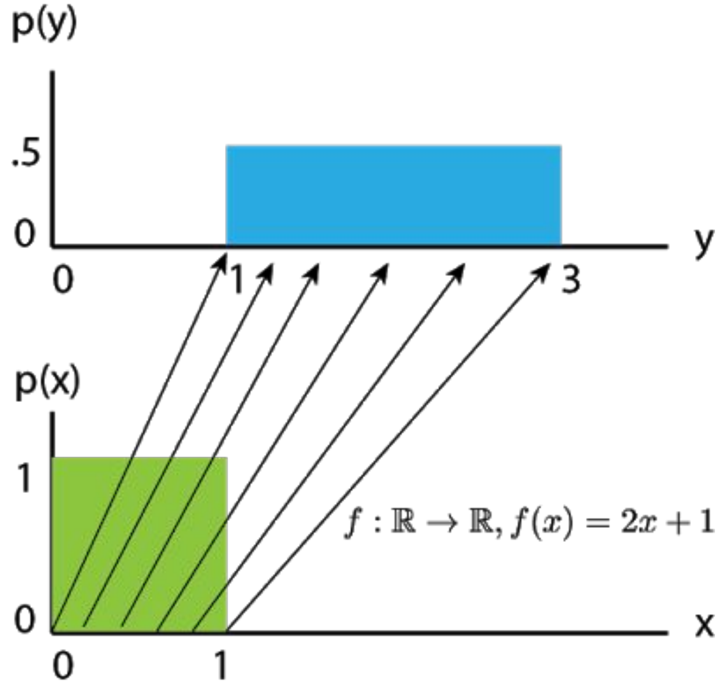
1. **Adversarial Robustness:** If the input X is not from the training distribution P(X), refuse classification
2. **Detecting Data Shift:** if P(X) shifted over time, retrain the model
3. **Outlier Detection:** detect abnormalities in observed data
4. **“Learned” data priors:** improved image synthesis or structure in segmentation maps

Background: change of variable formula

U[1, 3] **P(T(0.5)) =**
= P(2) = 0.5

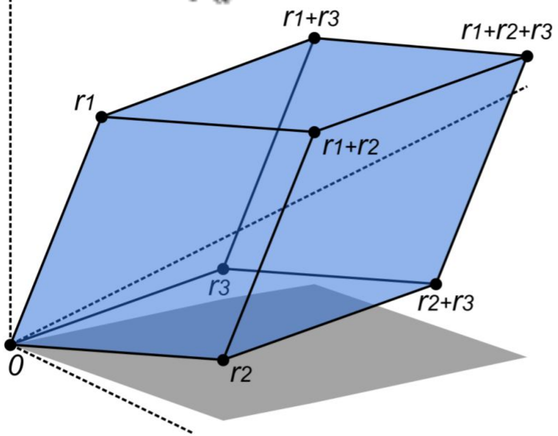
T(x) = 2x + 1

U[0, 1] **P(0.5) = 1**

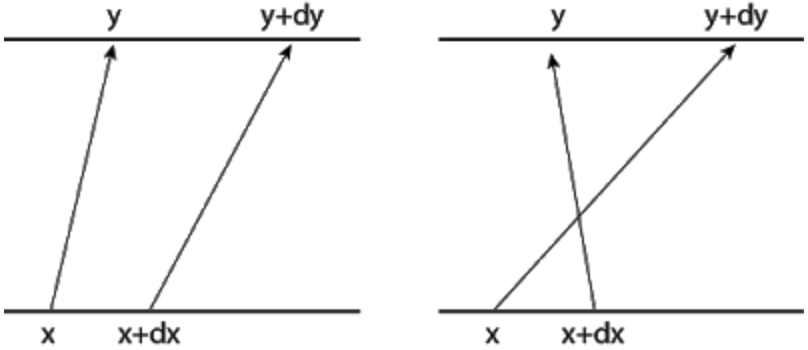


Background: change of variable formula

$$\int_{\varphi(a)}^{\varphi(b)} f(u)\,du = \int_a^b f(\varphi(x))\varphi'(x)\,dx.$$



$$\frac{dy}{dx} > 0 \qquad \frac{dy}{dx} < 0$$



p(x) dx = p(y) dy

p(y) = p(x) **det | (dT^{-1}(y)/dy) |**

log p(y) = log p(x) + log det | (dT^{-1}(y)/dy) |

Background: change of variable formula

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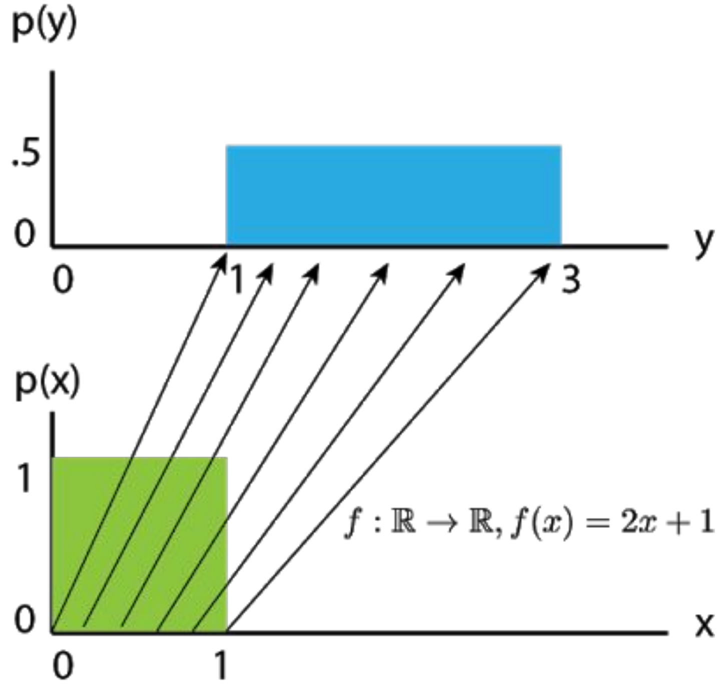
T(x) = 2x + 1
$T^{-1}(y) = y/2 - ½$
$dT^{-1}(y)/dy = ½$

U[0, 1] **P(0.5) = 1**

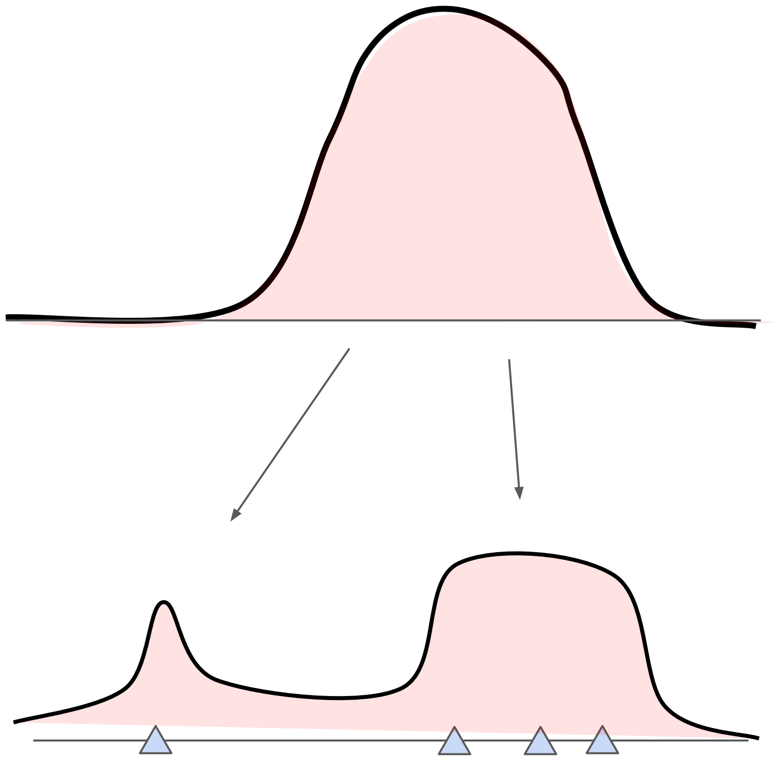
$p_Y(y) = p_X(T^{-1}(y))$ * **$\det | (dT^{-1}(y)/dy) |$**

$p_Y(y) = I[0 < (y/2 - ½) < 1] * ½$
$= I[1 < y < 3] * ½$



Normalizing flows for density estimation

like shuffling a sand castle - we move sand around to increase the amount of send near data points, but the total amount of the sand stays constant



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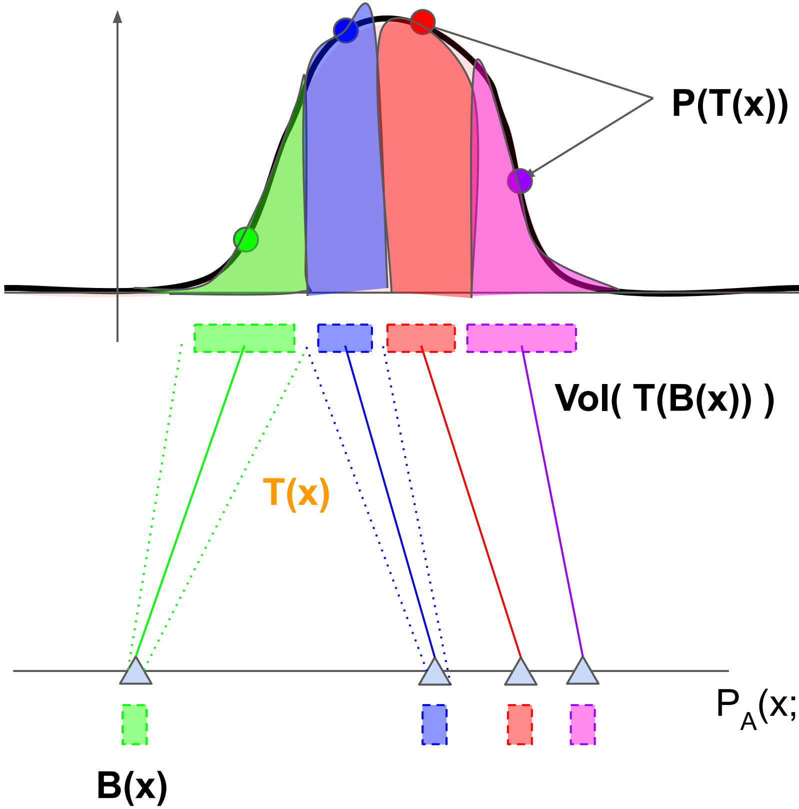
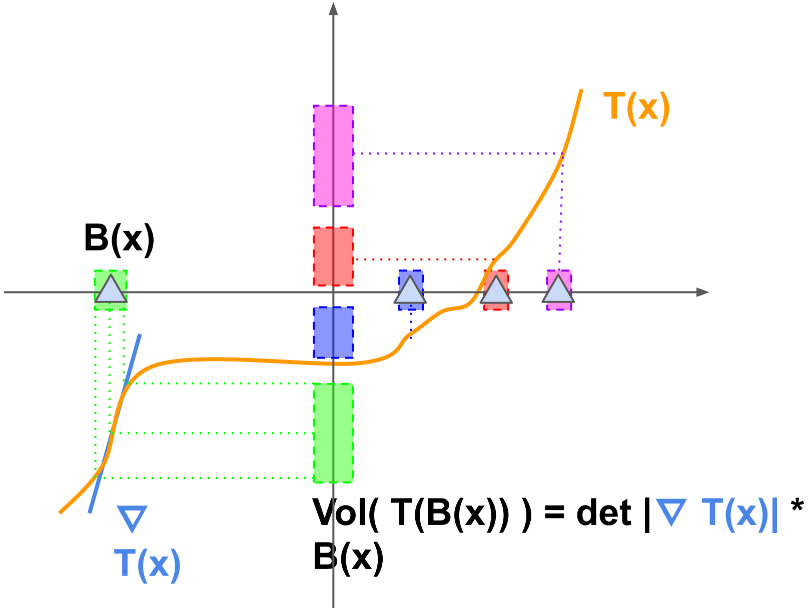
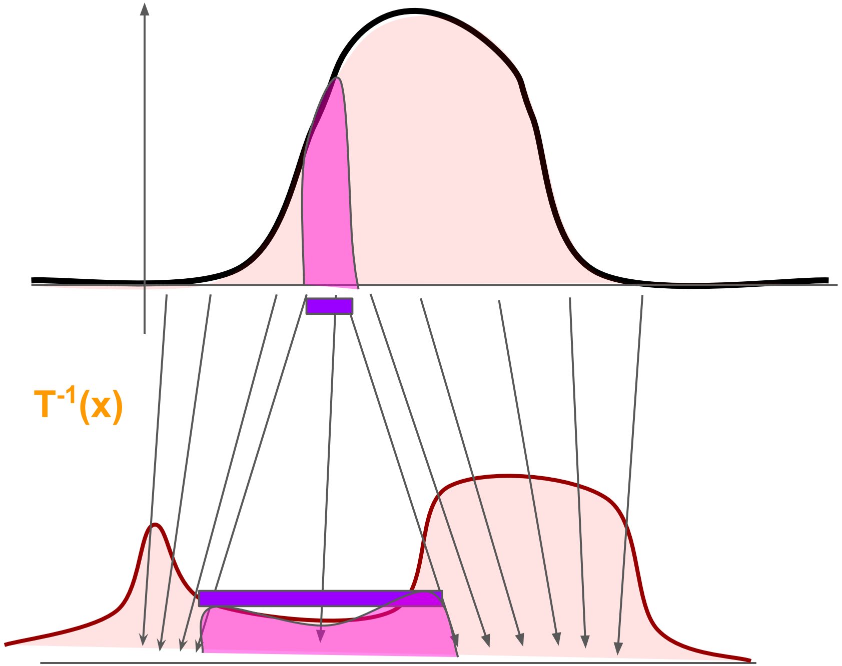


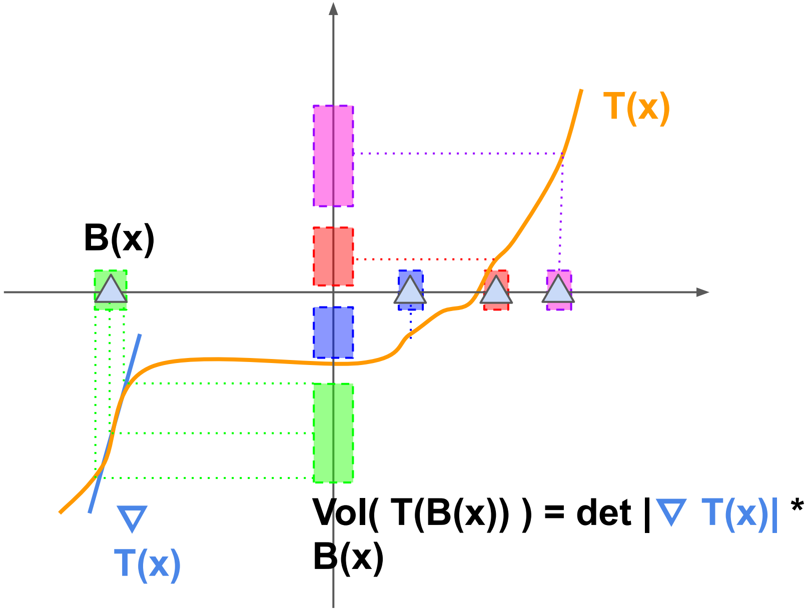


$P_A(x; T) = P(T(x)) * \det | \nabla T(x) | * \mathrm{Vol}(B(x))$

let’s solve the problem “backwards”

Normalizing flows for density estimation





$P_A(x; F) = P(T(x)) * \det | \nabla T(x) | * Vol(T(x))$

Low probability areas are “stretches”

In order to define a normalizing flow model we need

1. A **one-to-one** mapping $F(x,\boldsymbol{\theta})$: $\mathbf{R}^n \rightarrow \mathbf{R}^n$
2. $F^{-1}(x,\boldsymbol{\theta})$
3. $\det[\text{Jac } F(x,\boldsymbol{\theta})]$

$$\mathbf{J} = \begin{bmatrix} \dfrac{\partial \mathbf{f}}{\partial x_1} & \cdots & \dfrac{\partial \mathbf{f}}{\partial x_n} \end{bmatrix} = \begin{bmatrix} \dfrac{\partial f_1}{\partial x_1} & \cdots & \dfrac{\partial f_1}{\partial x_n} \\ \vdots & \ddots & \vdots \\ \dfrac{\partial f_m}{\partial x_1} & \cdots & \dfrac{\partial f_m}{\partial x_n} \end{bmatrix}.$$

Planar Flow

$$f(\mathbf{z}) = \mathbf{z} + \mathbf{u}h(\mathbf{w}^T\mathbf{z} + b), \tag{4}$$

with $\mathbf{u}, \mathbf{w} \in \mathbb{R}^d$ and $b \in \mathbb{R}$ and h an element-wise non-linearity. Let $\psi(\mathbf{z}) = h'(\mathbf{w}^T\mathbf{z} + b)\mathbf{w}$. The determinant can be easily computed as

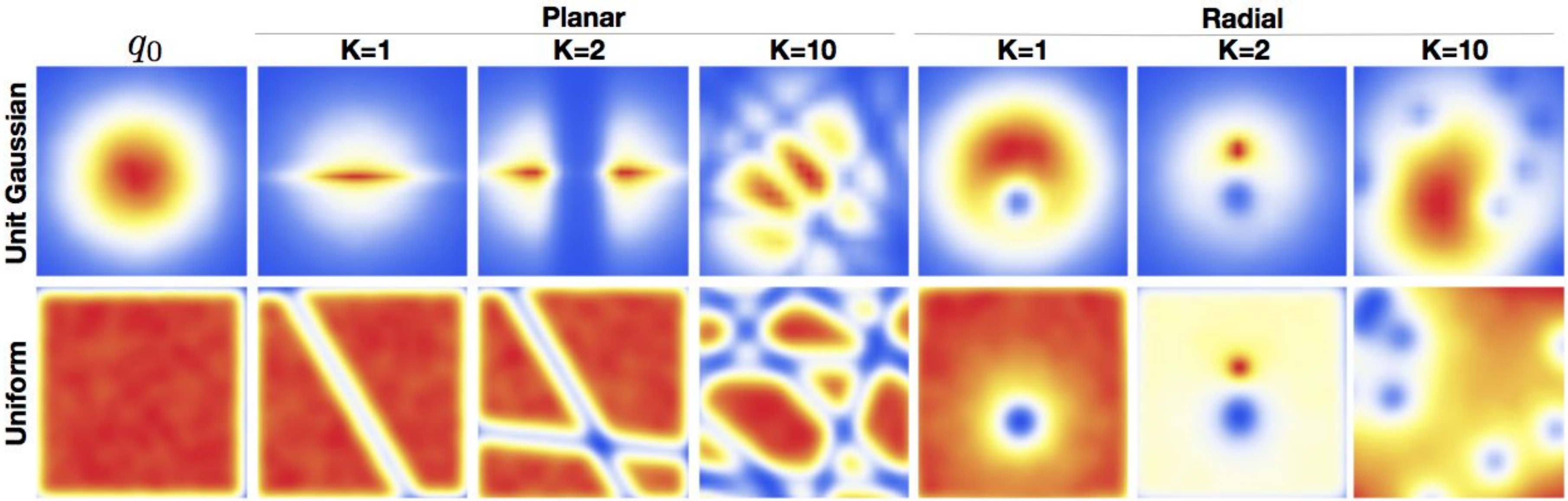
$$\left|\det \frac{\partial f}{\partial \mathbf{z}}\right| = \left|1 + \mathbf{u}^T\psi(\mathbf{z})\right|. \tag{5}$$

We can think of it as slicing the $\mathbf{z}$-space with straight lines (or hyperplanes), where each line contracts or expands the space around it, see figure 1.

Radial Flow

$$f(\mathbf{z}) = \mathbf{z} + \beta h(\alpha, r)(\mathbf{z} - \mathbf{z}_0), \tag{6}$$

with $r = \|\mathbf{z} - \mathbf{z}_0\|_2$, $h(\alpha, r) = \frac{1}{\alpha + r}$ and parameters $\mathbf{z}_0 \in \mathbb{R}^d, \alpha \in \mathbb{R}_+$ and $\beta \in \mathbb{R}$.



$$\mathbf{z}_K = f_K \circ \cdots \circ f_1(\mathbf{z}_0), \quad \mathbf{z}_0 \sim q_0(\mathbf{z}_0),$$

$$\mathbf{z}_K \sim q_K(\mathbf{z}_K) = q_0(\mathbf{z}_0) \prod_{k=1}^{K} \left| \det \frac{\partial f_k}{\partial \mathbf{z}_{k-1}} \right|^{-1}.$$

to learn more complex distributions, apply multiple flows in a row

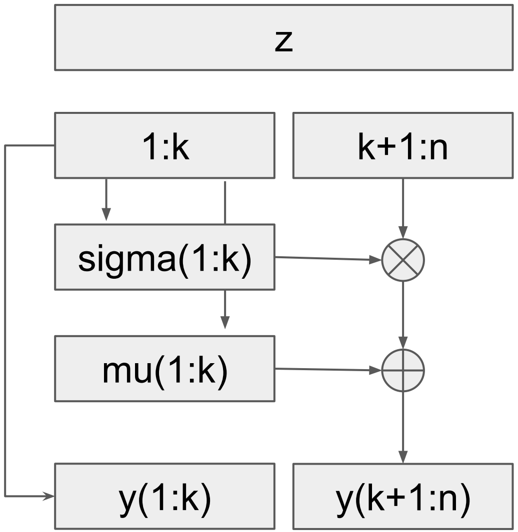
Real Non-Volume Preserving Flows (R-NVP)

$$\mathbf{y}_{1:k} = \mathbf{z}_{1:k},$$
$$\mathbf{y}_{k+1:d} = \mathbf{z}_{k+1:d} \circ \sigma(\mathbf{z}_{1:k}) + \mu(\mathbf{z}_{1:k}).$$

$$\begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \cdots & \frac{\partial f_1}{\partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial f_m}{\partial x_1} & \cdots & \frac{\partial f_m}{\partial x_n} \end{bmatrix}$$

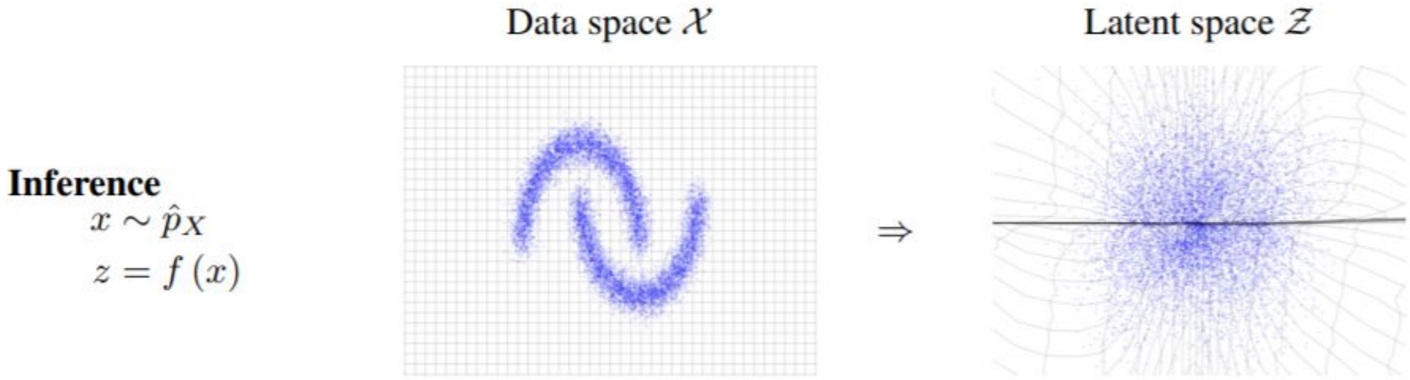
$$\det \frac{\partial \mathbf{y}}{\partial \mathbf{z}} = \prod_{i=1}^{d-k} \sigma_i(\mathbf{z}_{1:k}).$$

“affine coupling”



“Density estimation using Real NVP” by Laurent Dinh, Jascha Sohl-Dickstein, Samy Bengio

Real Non-Volume Preserving Flows (R-NVP)



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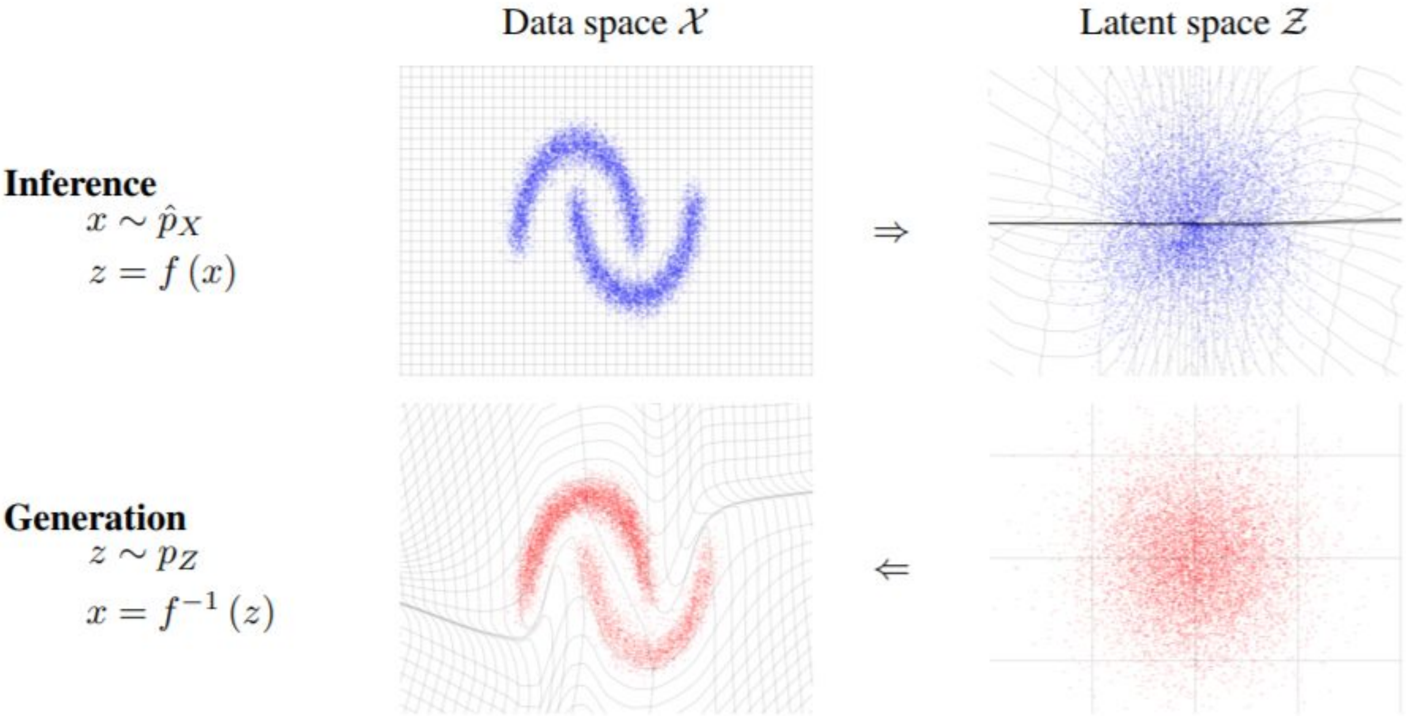
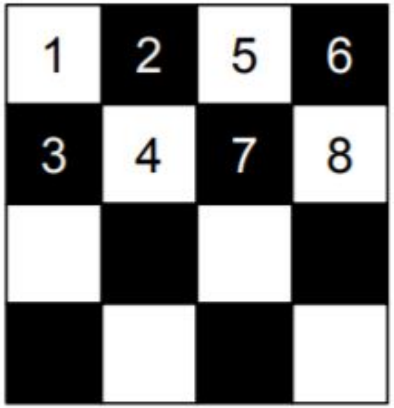
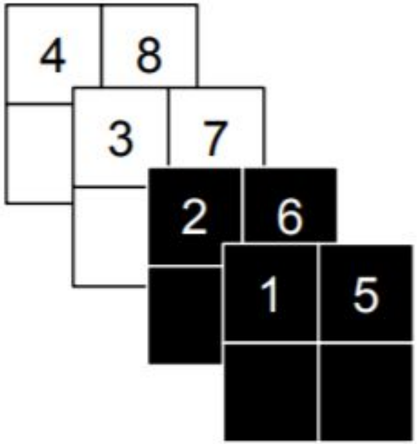


Real Non-Volume Preserving Flows (R-NVP)

checkerboard swap

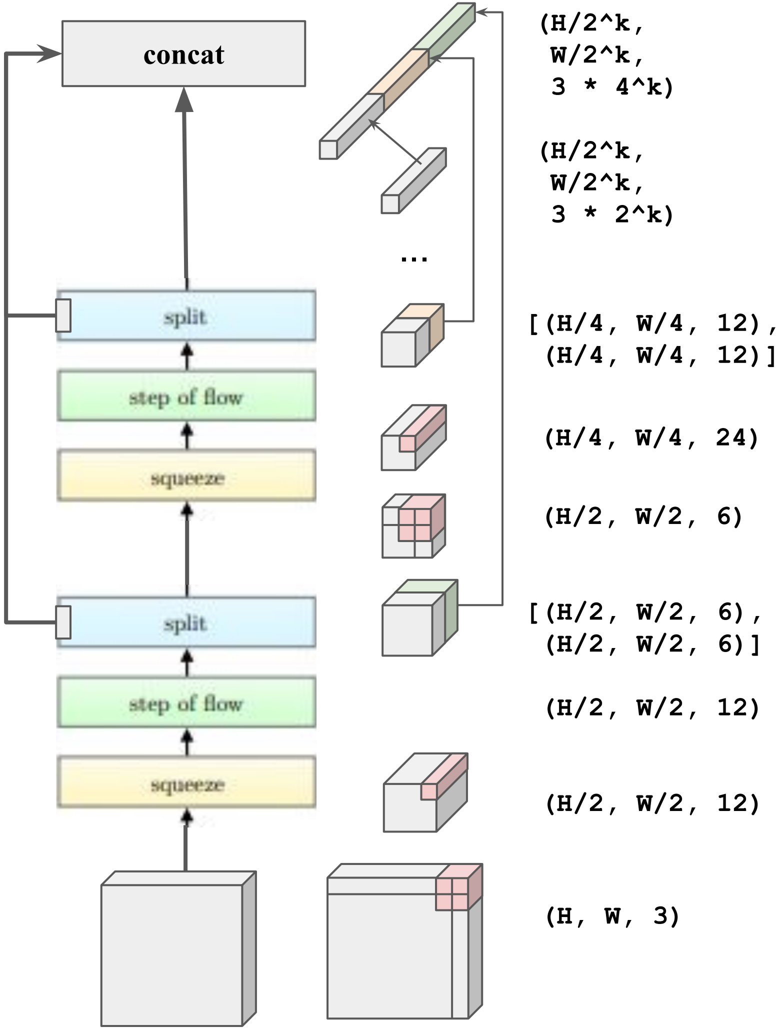


“squeeze”



Real Non-Volume Preserving Flows (R-NVP)

Glow: Generative Flow with Invertible 1x1 Convolutions



= very deep RealNVP
+ invertible 1x1 conv instead of swap
+ multiscale features

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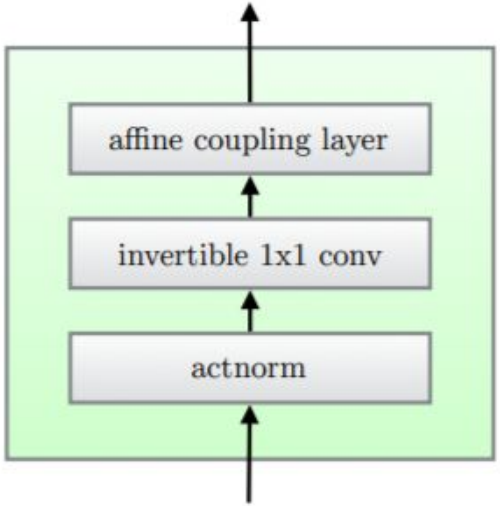

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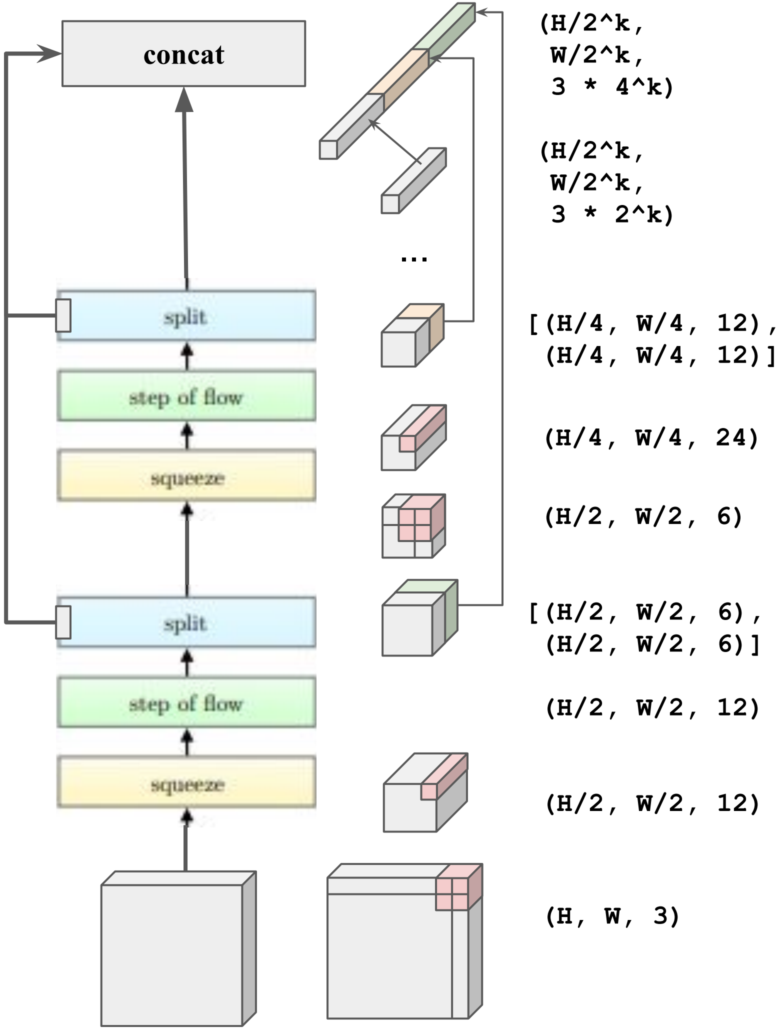
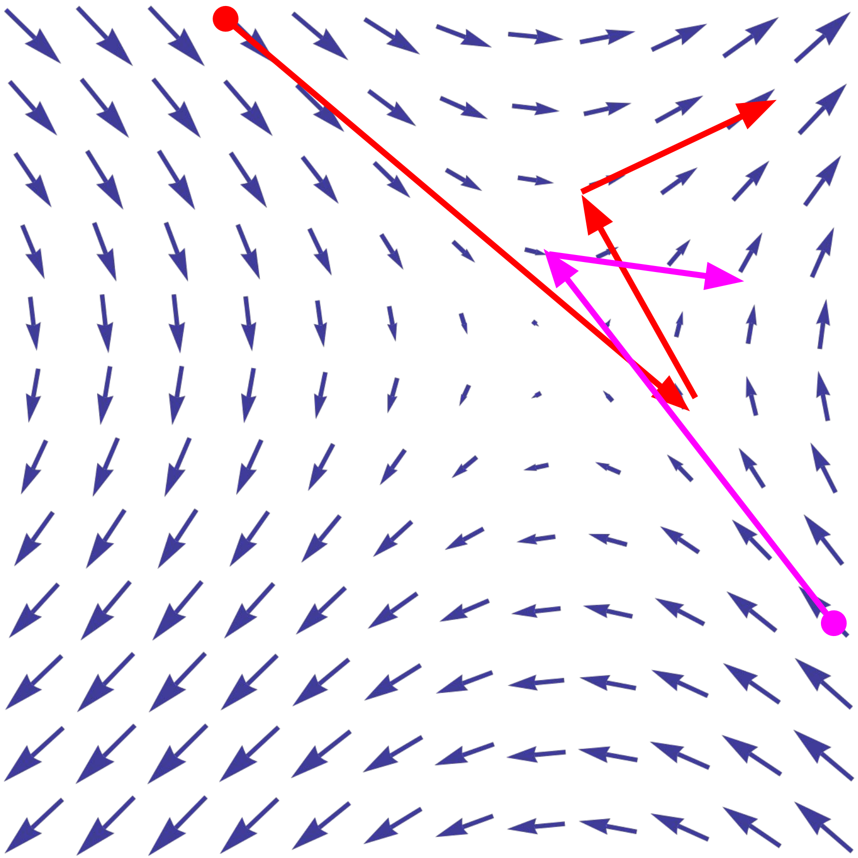


Neural ODE and FFJORD

$x(t_0) = x_0$
$x'(t) = \mathbf{f}(x(t))$
$x(t_1) = ?$

What if we use an **explicit method** with **fixed** step size?



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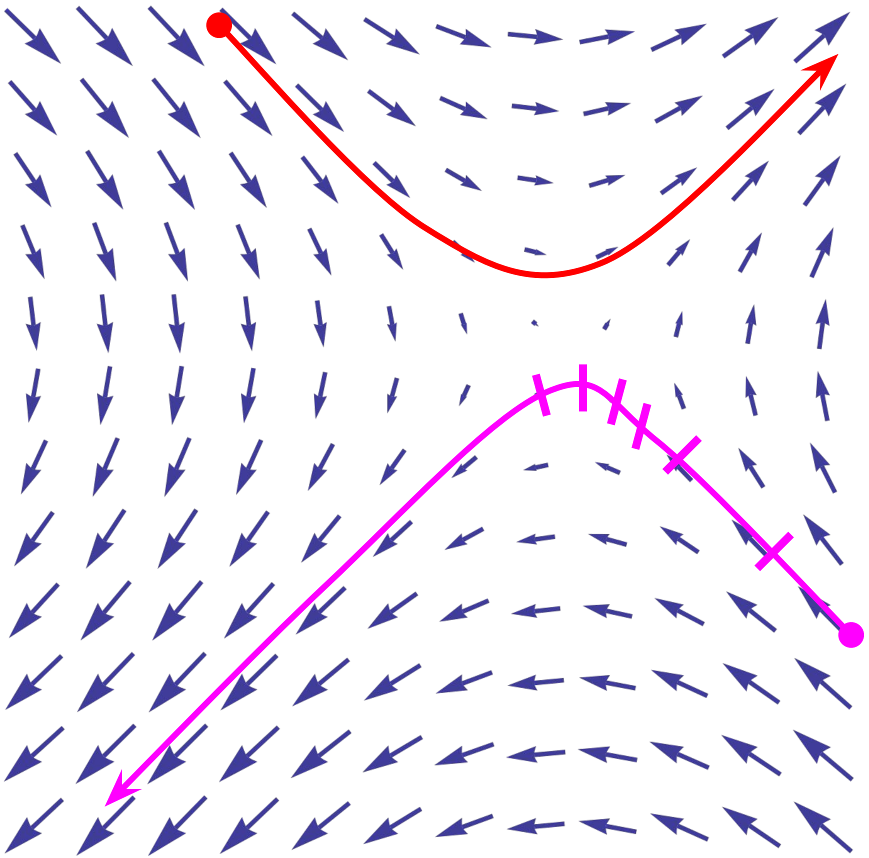
If we use a "proper solver", we get adaptive step size.



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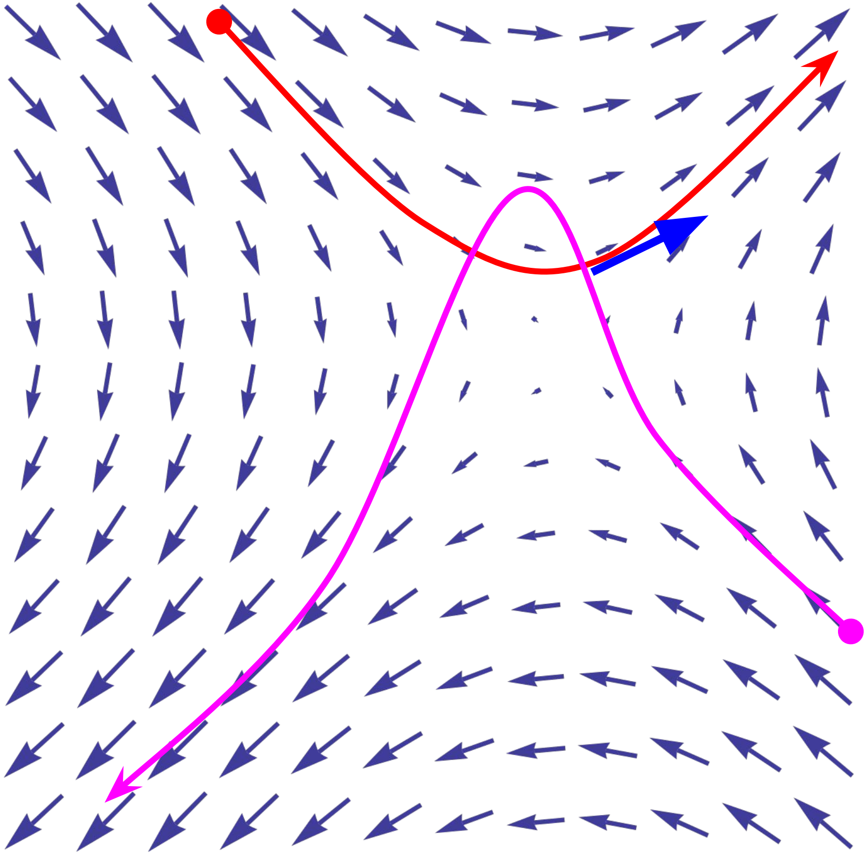
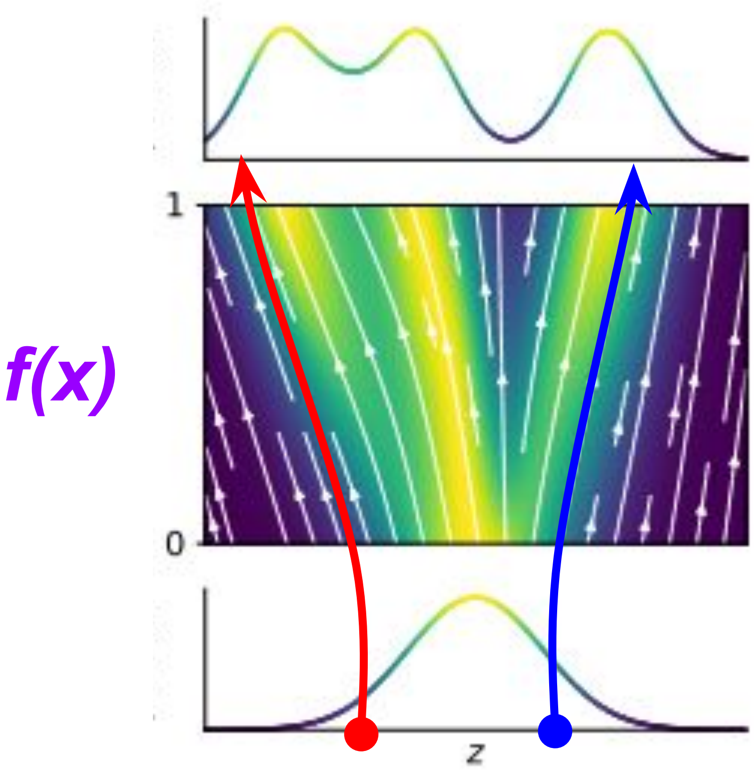


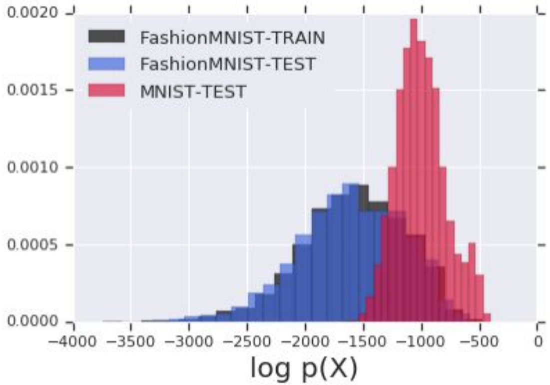
impossible!

Neural ODE and FFJORD

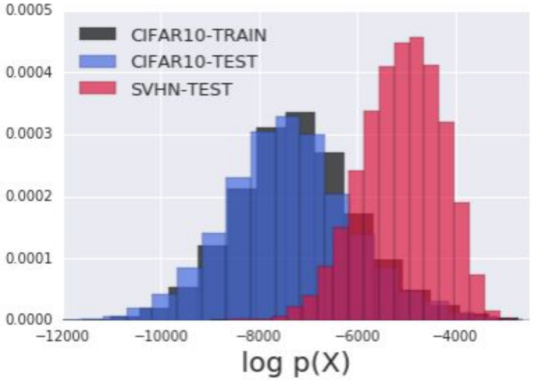


FFJORD: Free-form Continuous Dynamics for Scalable Reversible Generative Models

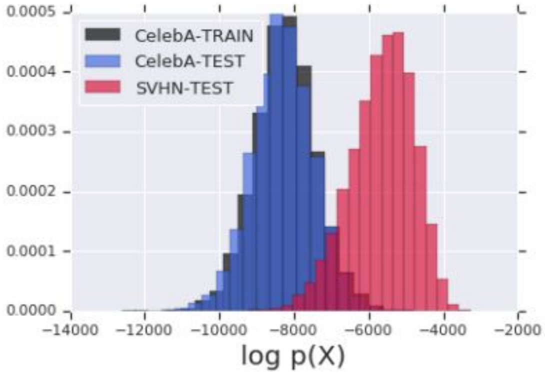
“Do Deep Generative Models Know What They Don't Know?”, ICLR’19



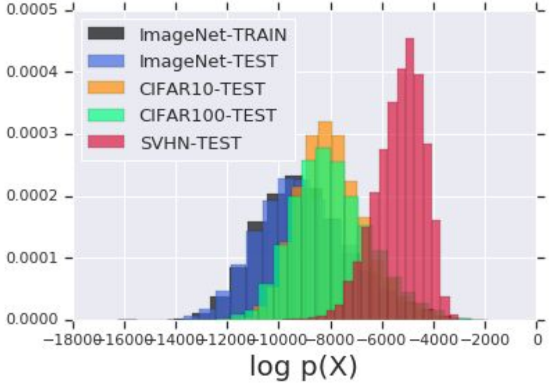
a) Train on FashionMNIST, Test on MNIST



(b) Train on CIFAR-10, Test on SVHN



(c) Train on CelebA, Test on SVHN



(d) Train on ImageNet,
Test on CIFAR-10 / CIFAR-100 / SVHN

If model $P_A(x)$ is **trained** on A then for many datasets B

$P_A(\mathbf{B}) > P_A(\mathbf{A})$

which is quite counter-intuitive …

and we never see anything like B if we sample from P(A) ..

High likelihood of X does not mean that X is likely!

$$A = \{y \in \mathbb{R}^{100} \mid ||y|| \leq \varepsilon\}$$

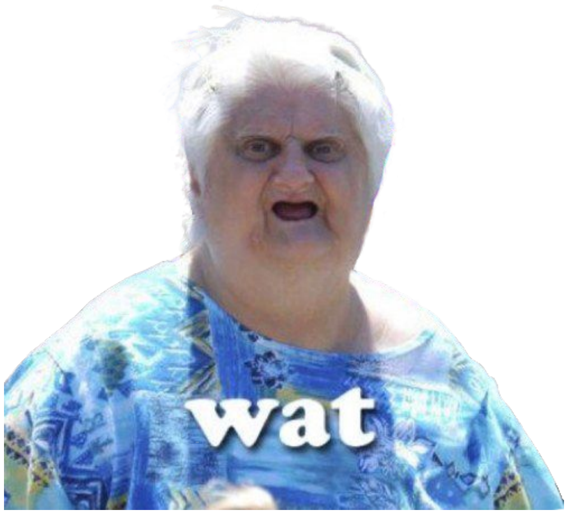
$$P(A) = \int_A \mathcal{N}_{100}(x; 0, I)dx$$

- the **probability** of point being in set A is **low**

$$B = \{x_i \in \mathbb{R}^{100} \mid ||x|| \leq \varepsilon\}_{i=0}^{N}$$

$$\mathcal{L}(B) = \frac{1}{N}\sum_{x_i \in B} \log \mathcal{N}_{100}(x; 0, I)$$

- but the mean **likelihood** of points from this set is **high**



Final takeaways

1. GANs can help to learn and use the structure of the output domain
2. Normalizing Flows enable density estimation in higher dimensions