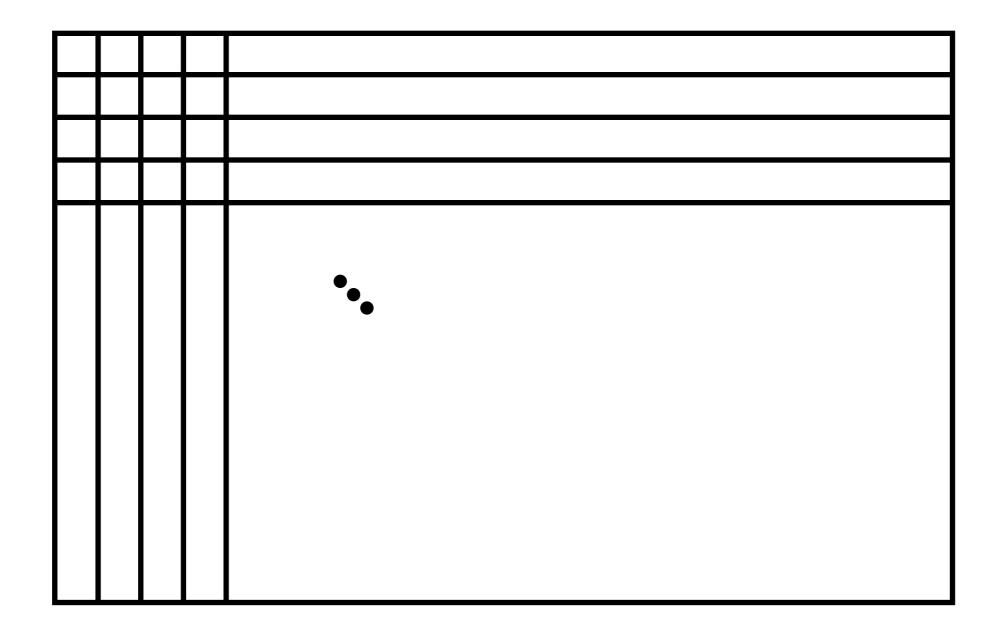
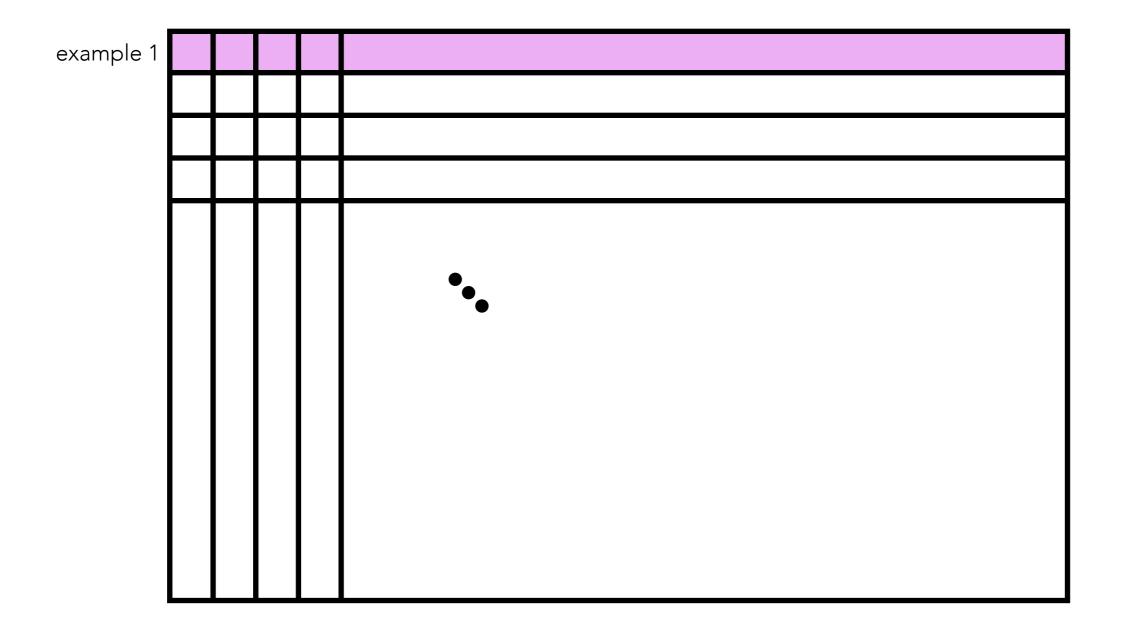
DEEP LEARNING

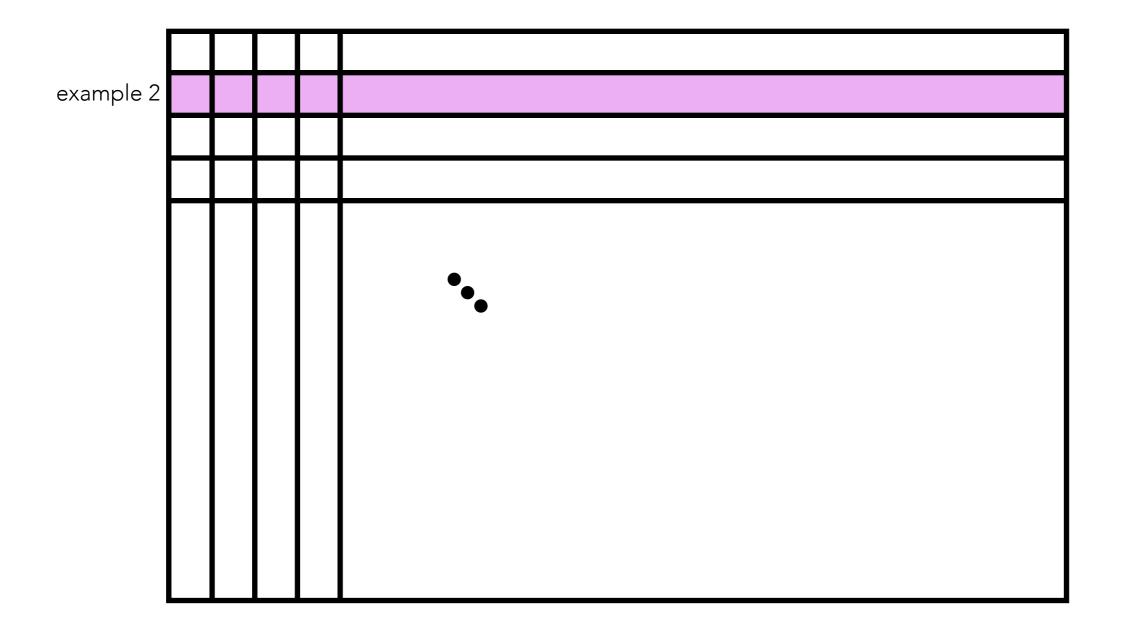
PART THREE - DEEP GENERATIVE MODELS

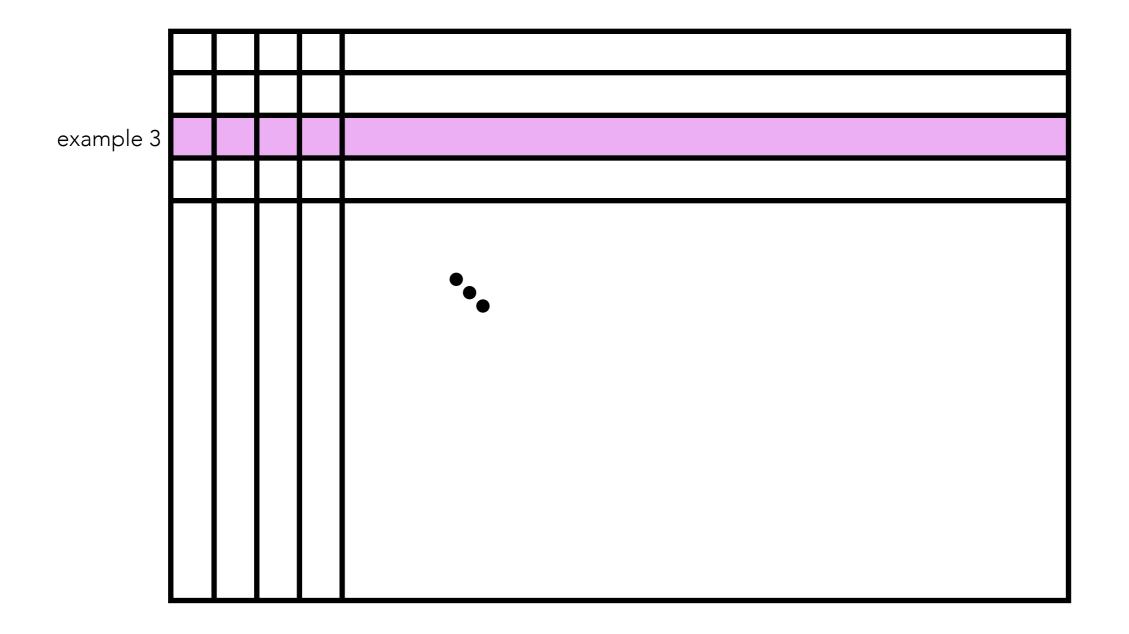
CS/CNS/EE 155 - MACHINE LEARNING & DATA MINING - LECTURE 17

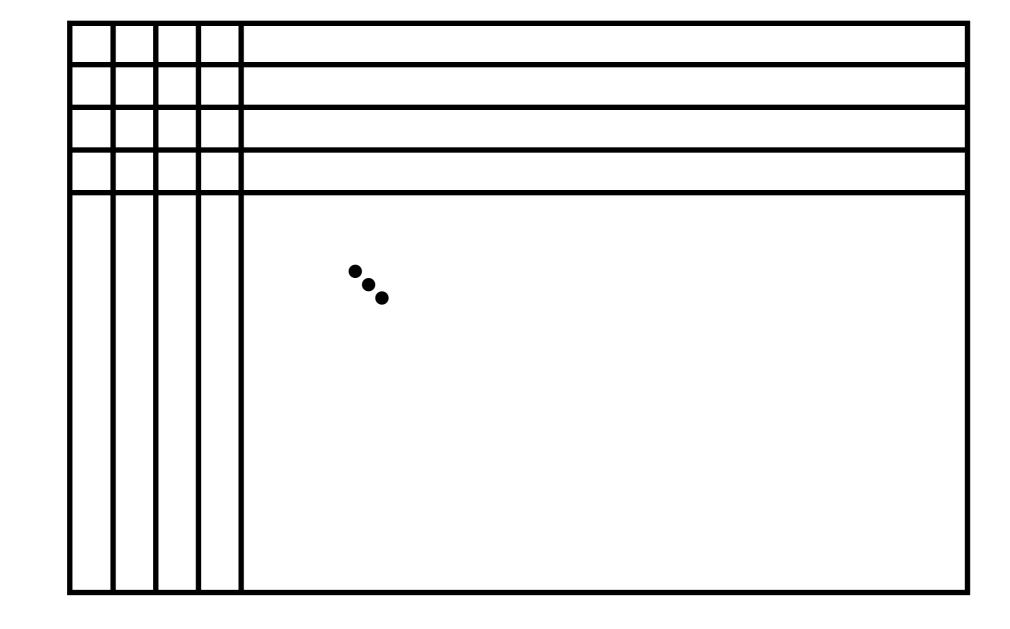
GENERATIVE MODELS

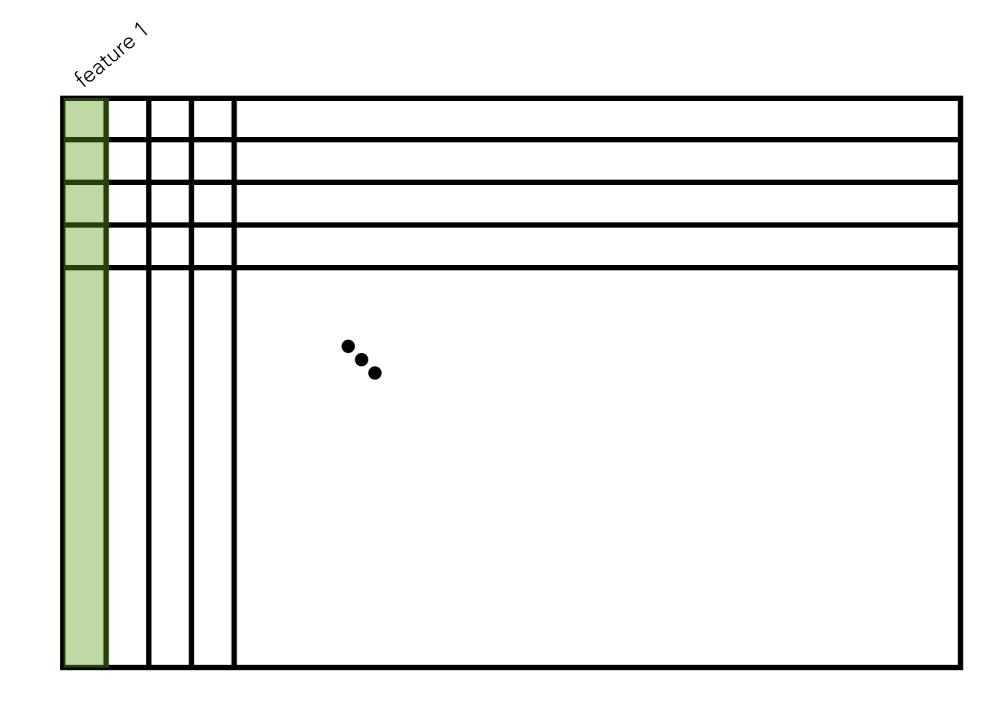


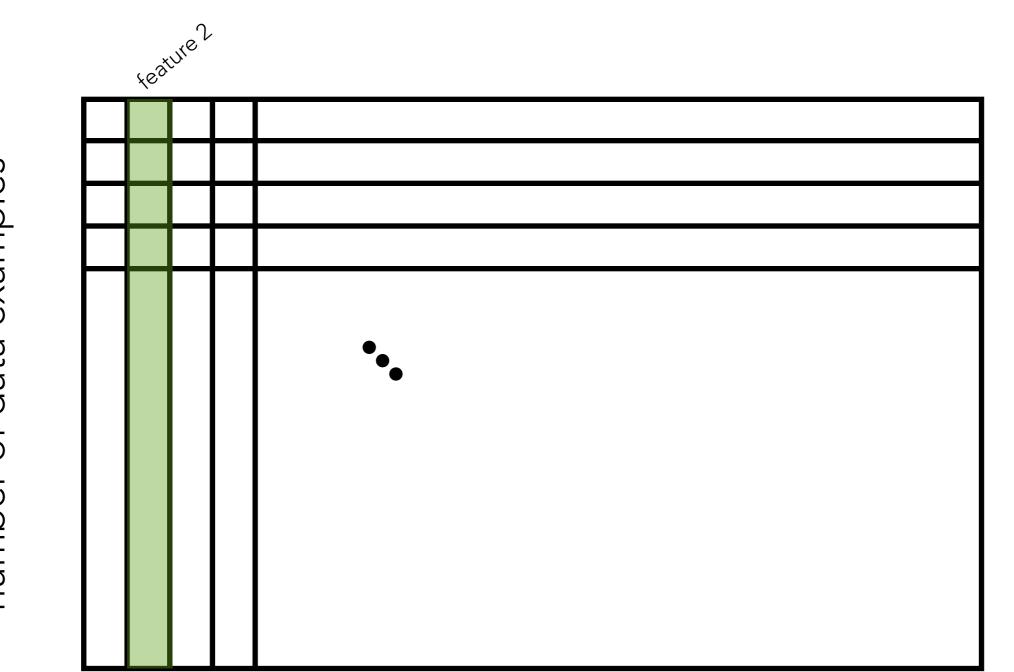


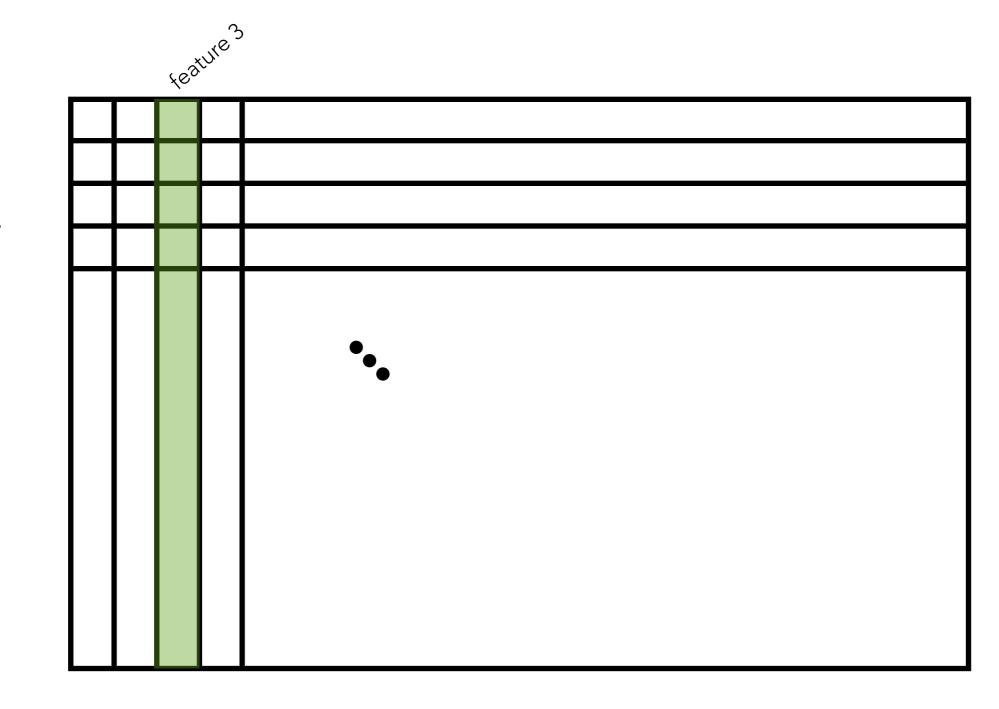




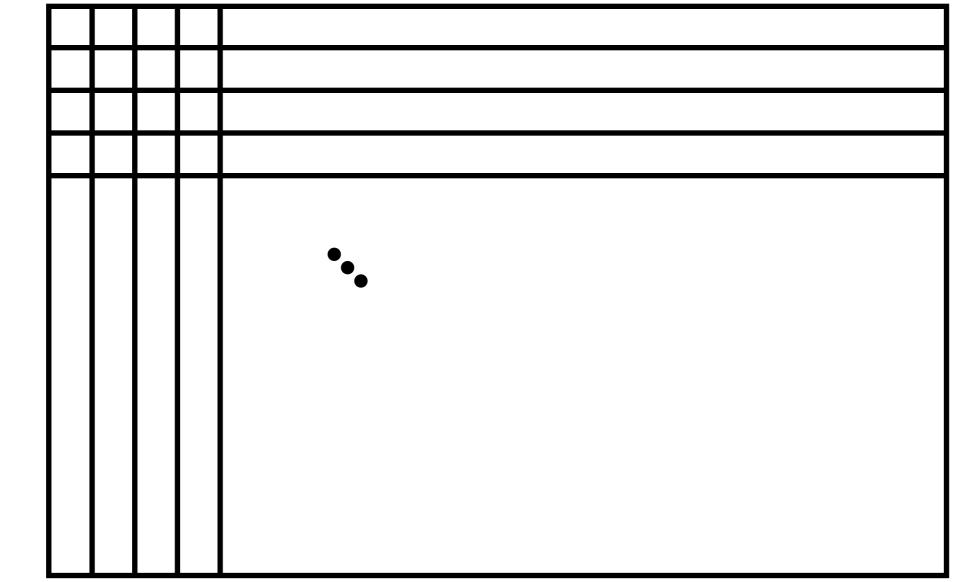






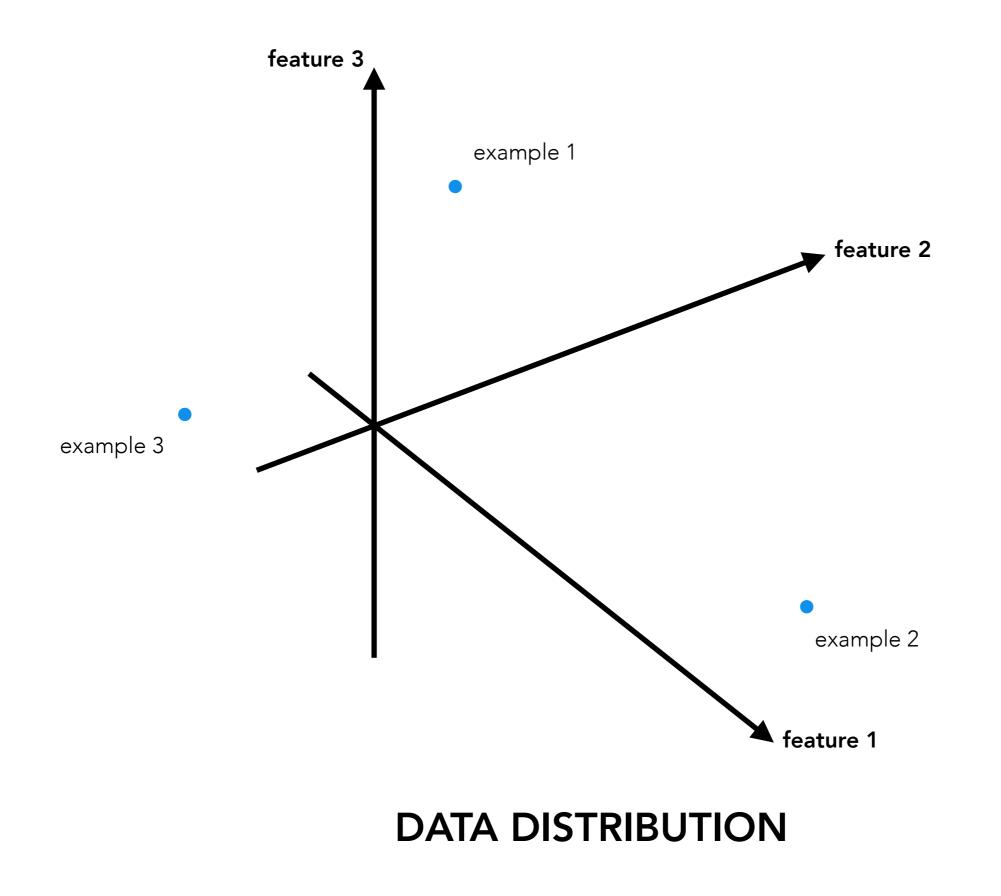


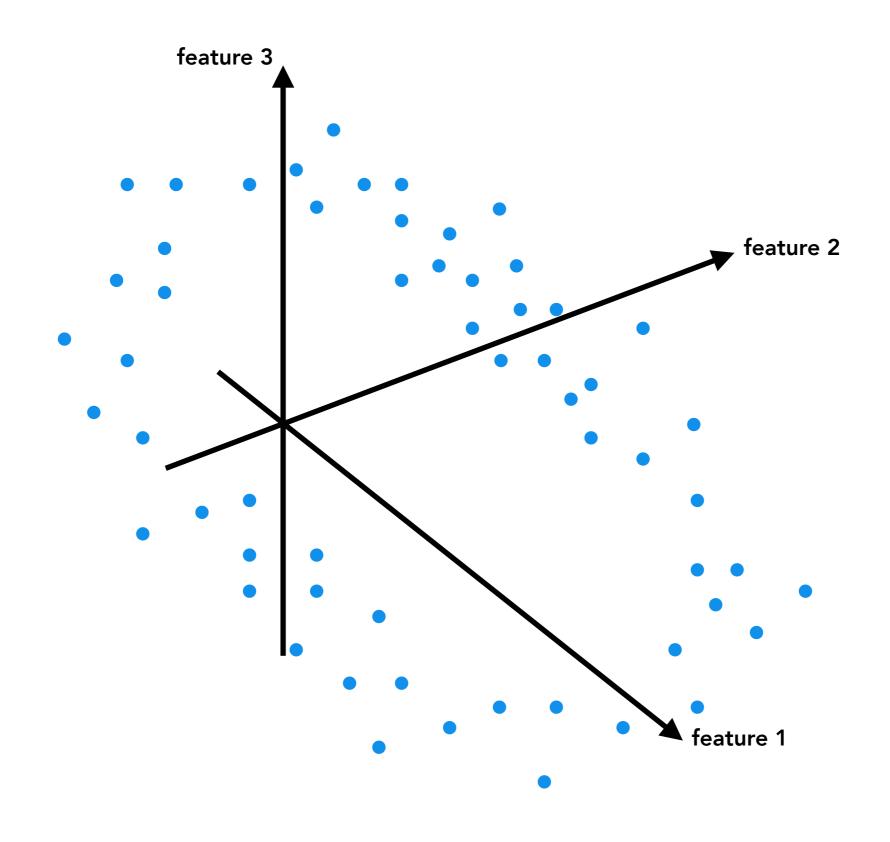
number of features



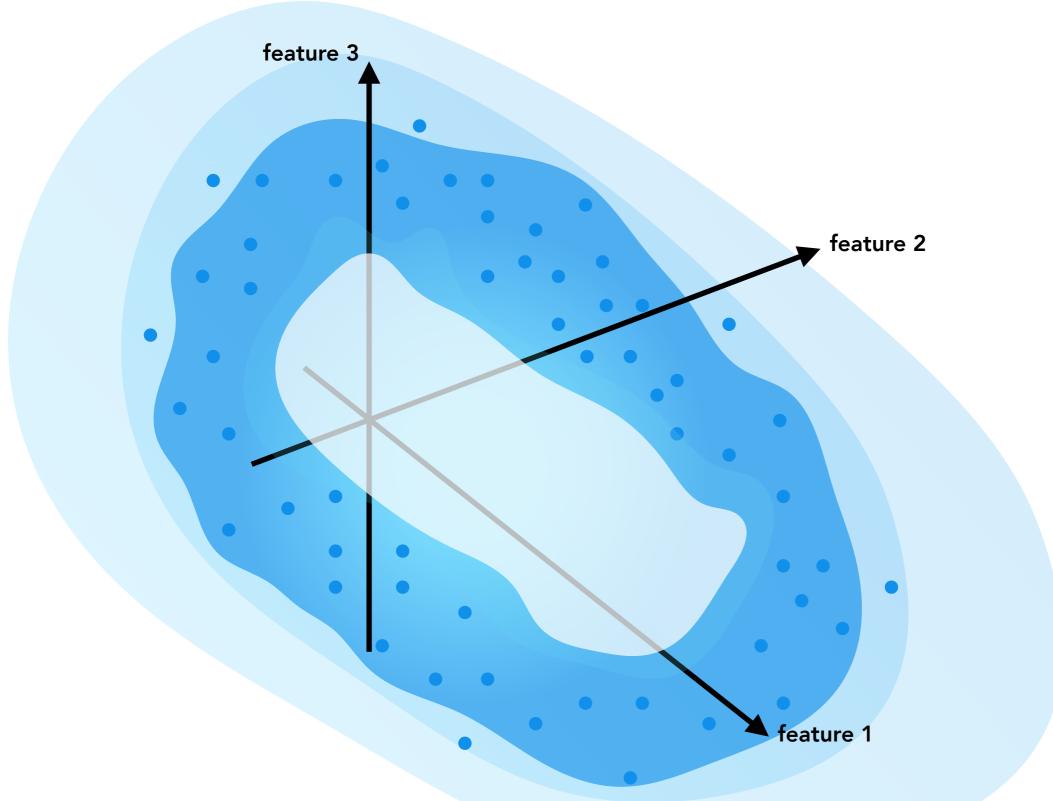
DATA

number of data examples





DATA DISTRIBUTION



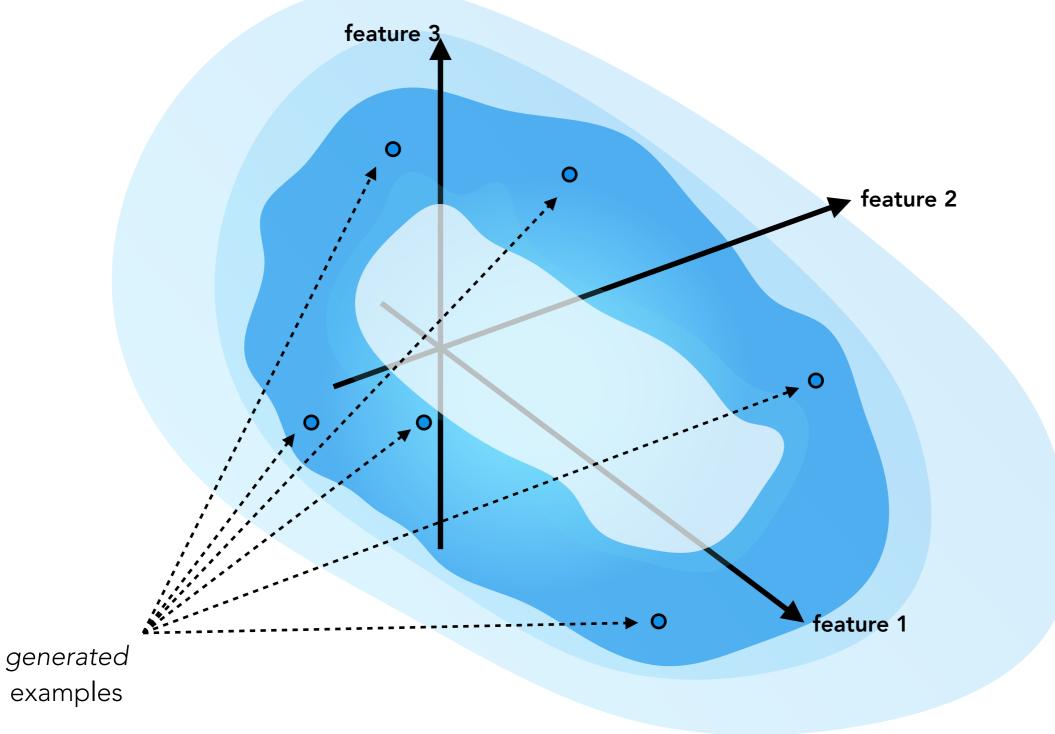
DENSITY ESTIMATION

estimating the density of the empirically observed data distribution

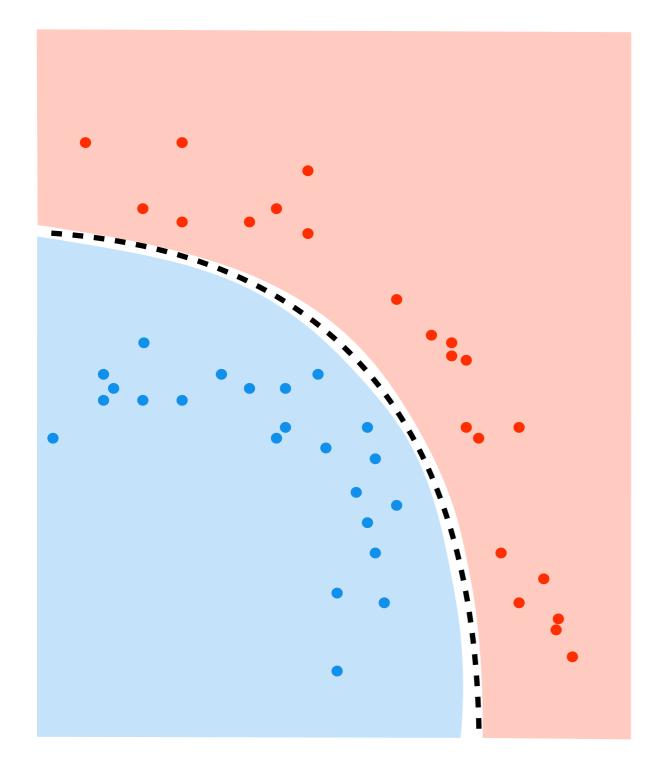
GENERATIVE MODEL

a model of the density of the data distribution

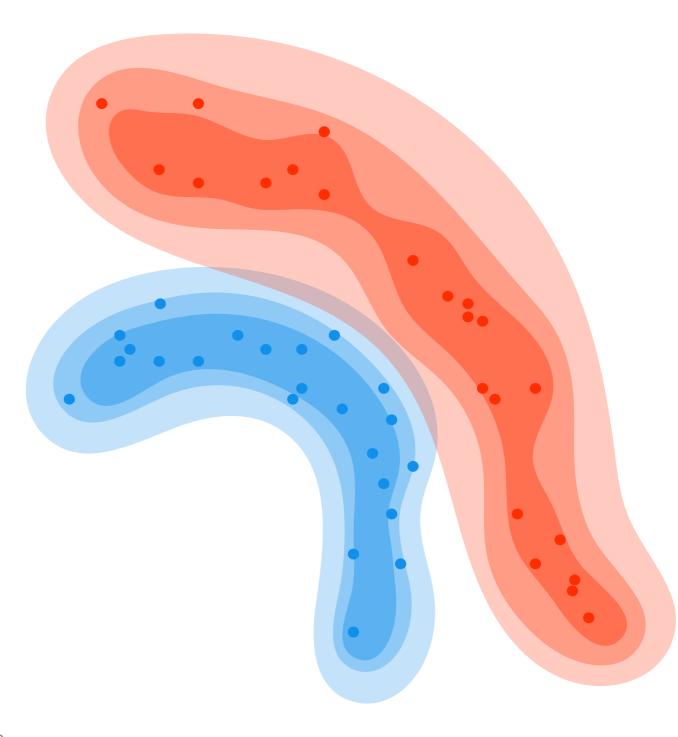
by modeling the data distribution, generative models are able to **generate** new data examples



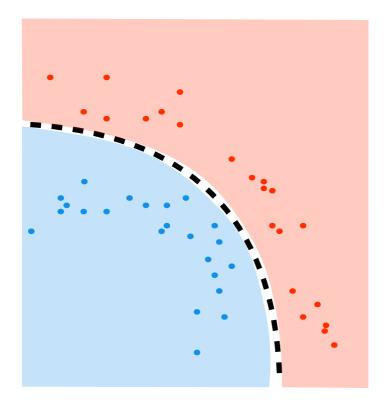
discriminative model

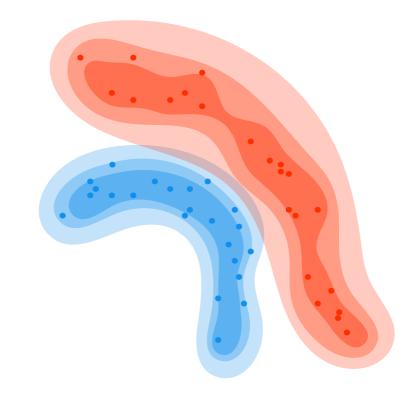


generative model



discriminative models vs. generative models





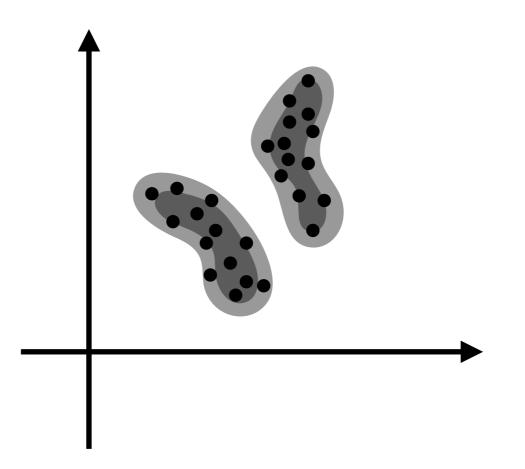
can both be trained using supervised learning

generative models are often easier to train with unsupervised methods

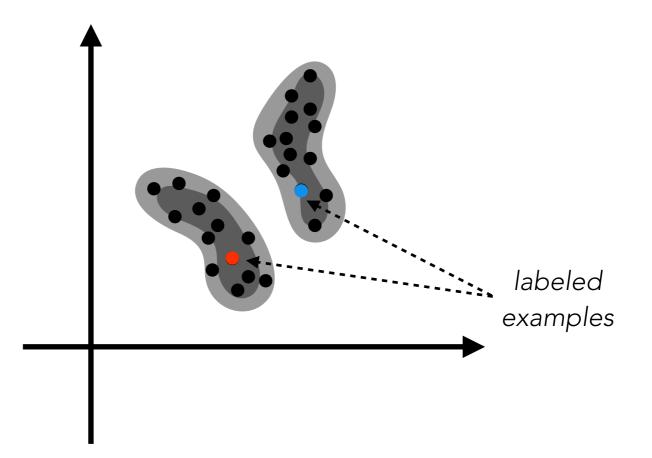
generative models typically require more modeling assumptions

straightforward to quantify uncertainty with generative models

one of the main benefits of generative modeling is the ability to automatically extract structure from data

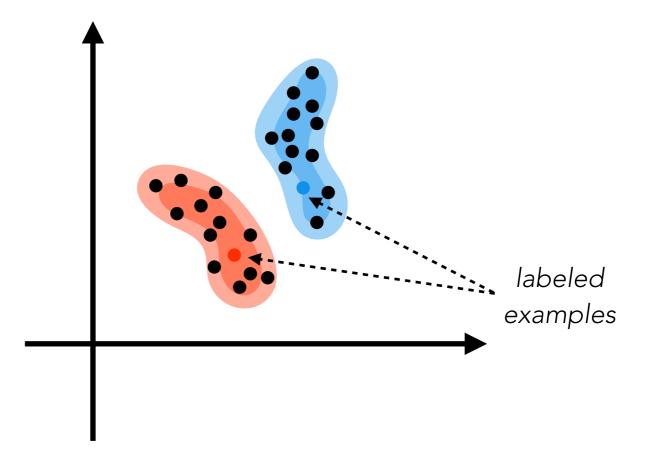


reducing the effective dimensionality of the data can make it easier to learn and generalize on new tasks one of the main benefits of generative modeling is the ability to automatically extract structure from data

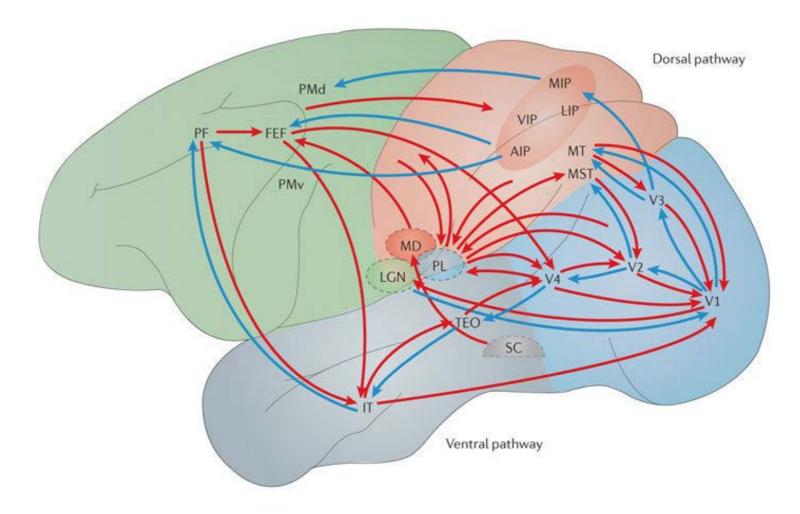


reducing the effective dimensionality of the data can make it easier to learn and generalize on new tasks

one of the main benefits of generative modeling is the ability to automatically extract structure from data



reducing the effective dimensionality of the data can make it easier to learn and generalize on new tasks any model that has an output in the data space can be considered a generative model



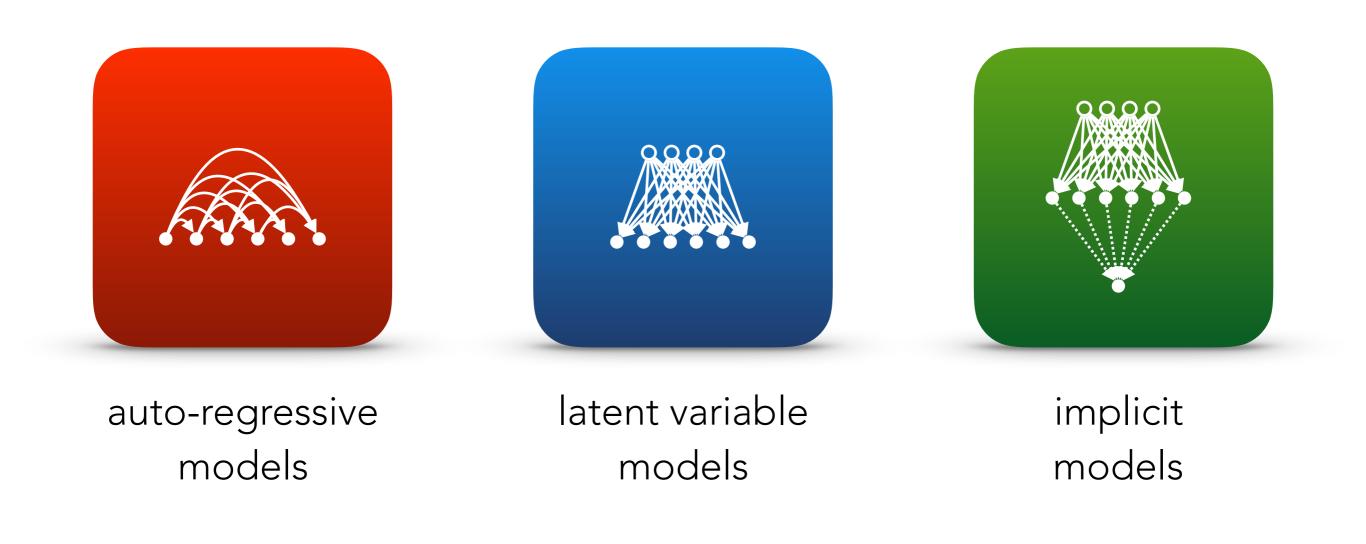
Nature Reviews | Neuroscience

nervous systems appear to use this mechanism in part prediction of sensory input using "top-down" pathways

deep generative model

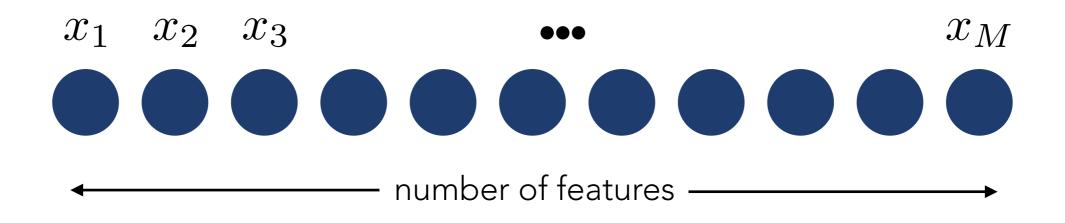
a generative model that uses deep neural networks to model the data distribution

FAMILIES OF (DEEP) GENERATIVE MODELS



AUTO-REGRESSIVE MODELS

a data example



$$p(\mathbf{x}) = p(x_1, x_2, \dots, x_M)$$

$$x_1 \quad x_2 \quad x_3 \qquad \cdots \qquad x_M$$

$$(\mathbf{x}) = p(x_1, x_2, \dots, x_M)$$

use <u>chain rule of probability</u> to split the joint distribution into a product of conditional distributions

definition of conditional probability

$$p(a|b) = \frac{p(a,b)}{p(b)} \longrightarrow p(a,b) = p(a|b)p(b)$$

recursively apply to $p(x_1, x_2, \ldots, x_M)$

$$p(x_1, x_2, \dots, x_M) = p(x_1 | x_2, \dots, x_M) p(x_2, \dots, x_M)$$

••••

 $p(x_1, x_2, \dots, x_M) = p(x_1 | x_2, \dots, x_M) p(x_2 | x_3, \dots, x_M) \dots p(x_{M-1} | x_M) p(x_M)$

note: conditioning order is arbitrary

$$p(x_1, \dots, x_M) = \prod_{j=1}^M p(x_j | x_1, \dots, x_{j-1})$$



learn to *auto-regress* to the missing values

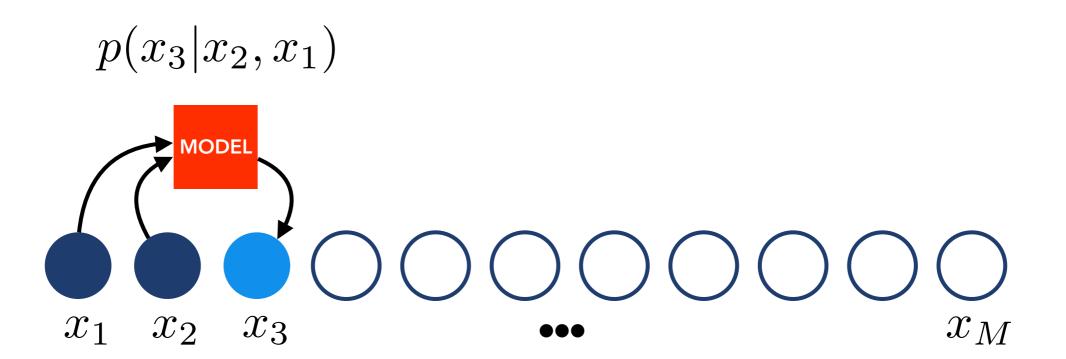
 $p(x_1)$

$\sum_{x_1} \sum_{x_2} \sum_{x_3} OOOOOOOOOOx_{x_M}$

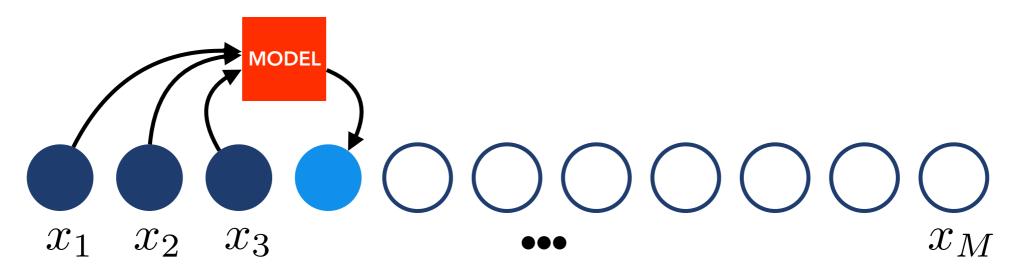
learn to *auto-regress* to the missing values

 $p(x_2|x_1)$ MODEL x_1 x_2 x_3

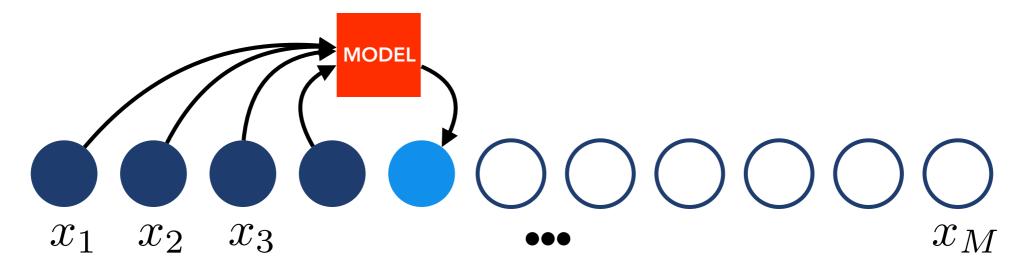
 x_M

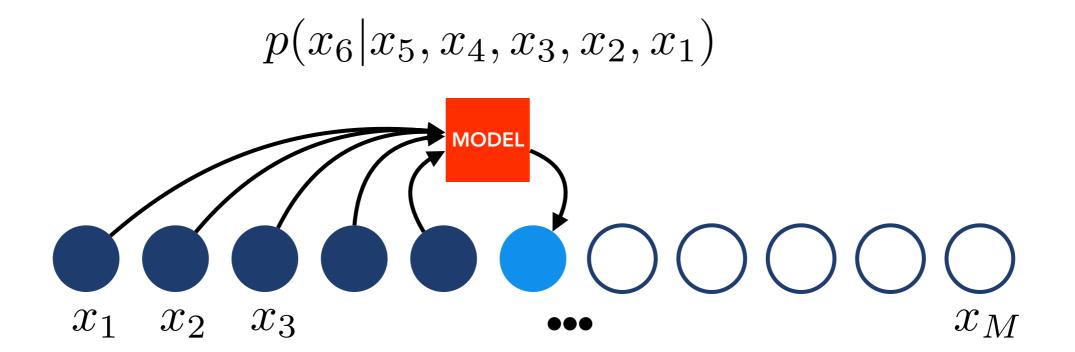


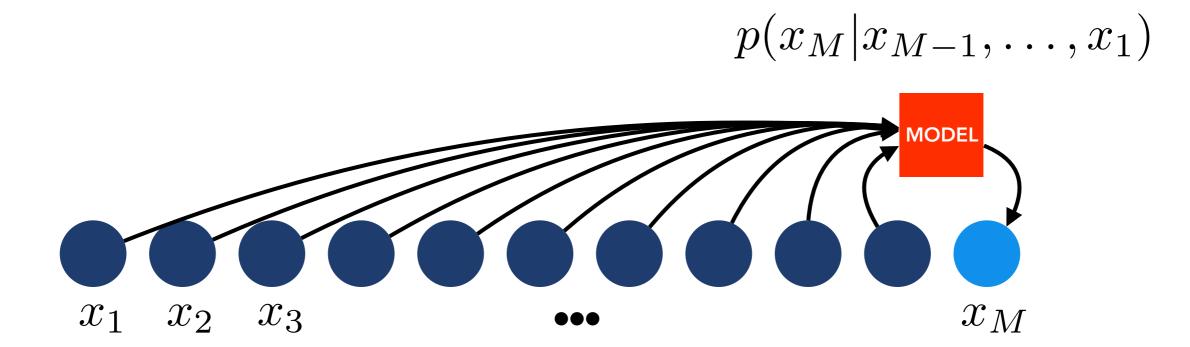
 $p(x_4|x_3, x_2, x_1)$



 $p(x_5|x_4, x_3, x_2, x_1)$







maximum likelihood

to fit the model to the empirical data distribution, maximize the *likelihood* of the true data examples

likelihood:
$$p(\mathbf{x}) = \prod_{j=1}^{M} p(x_j | \mathbf{x}_{< j})$$

auto-regressive conditionals

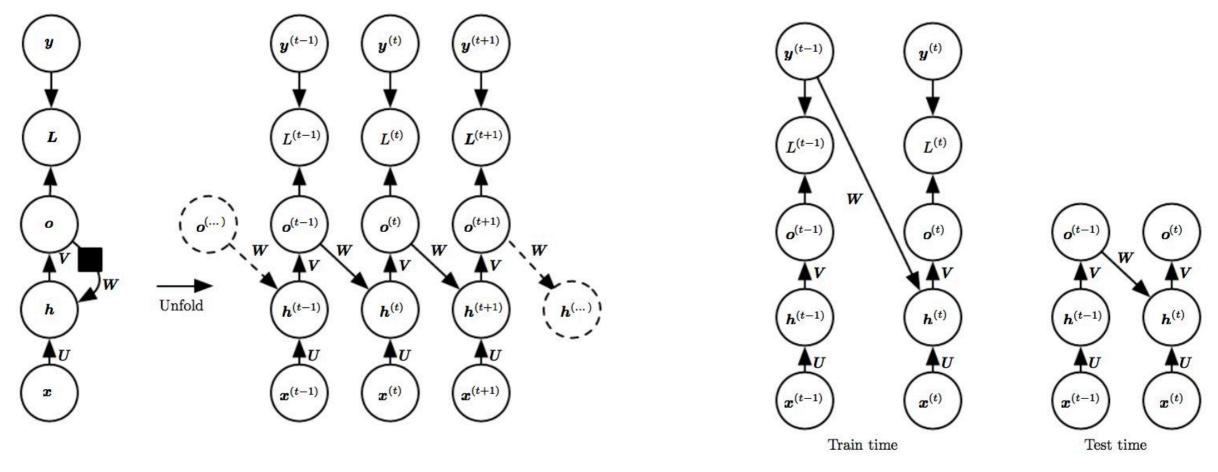
optimize the parameters to assign high (log) probability to the true data examples

learning:
$$\theta^* = \operatorname{argmax}_{\theta} \log p(\mathbf{x})$$

logarithm for numerical stability

models

can parameterize conditional distributions using a recurrent neural network



unrolling auto-regressive generation from an RNN

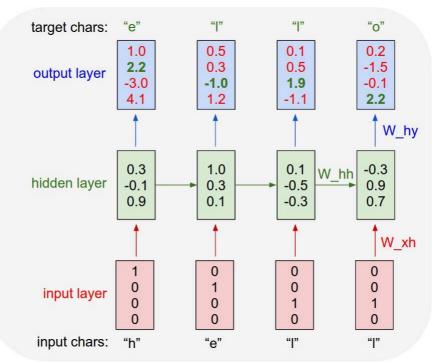
"teacher forcing"

Deep Learning, Goodfellow et al., 2016

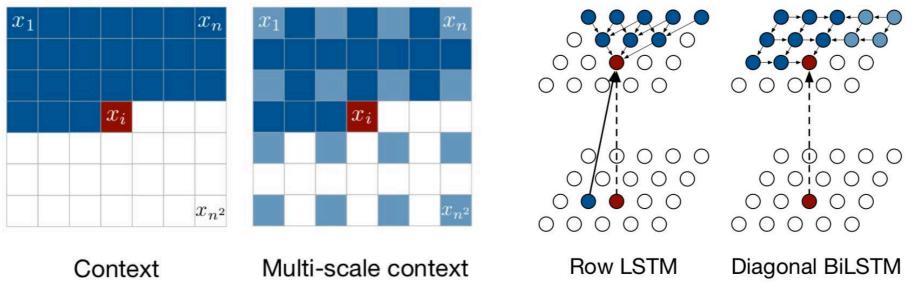
(chapter 10)

models

can parameterize conditional distributions using a recurrent neural network



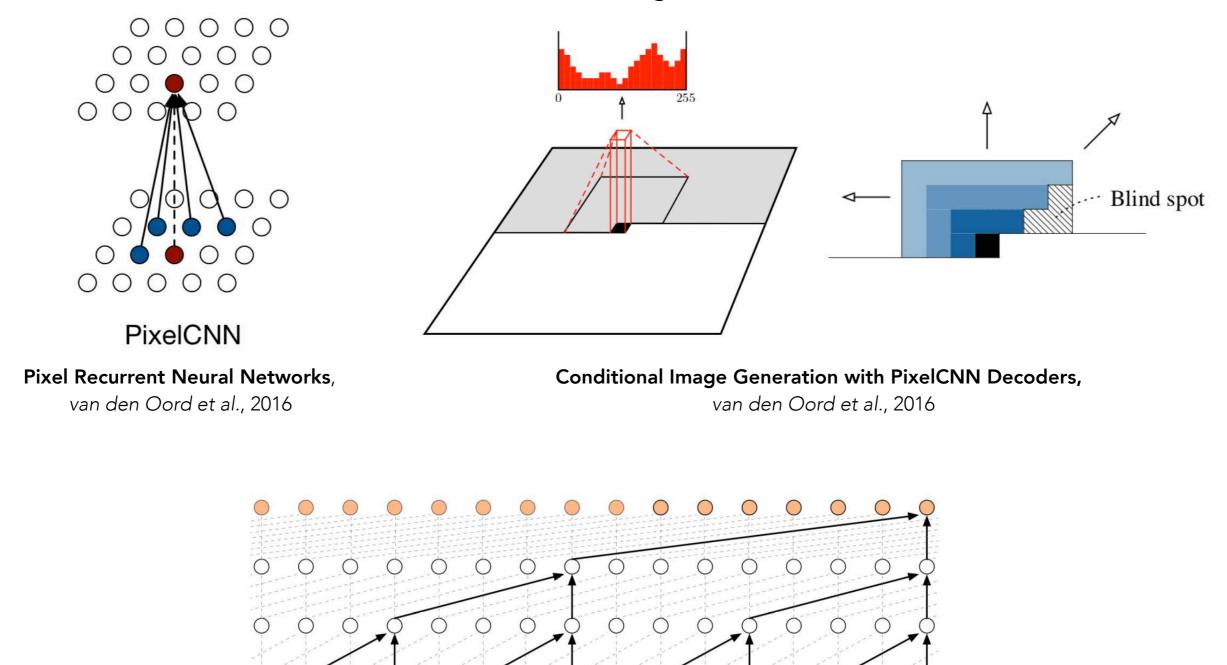
The Unreasonable Effectiveness of Recurrent Neural Networks, Karpathy, 2015



Pixel Recurrent Neural Networks, van den Oord et al., 2016

models

can also condition on a local window using **convolutional neural networks**



WaveNet: A Generative Model for Raw Audio, van den Oord et al., 2016

()

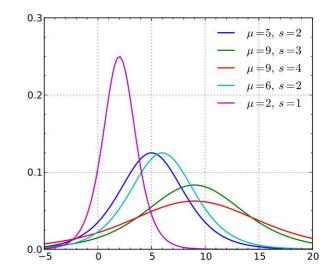
output distributions

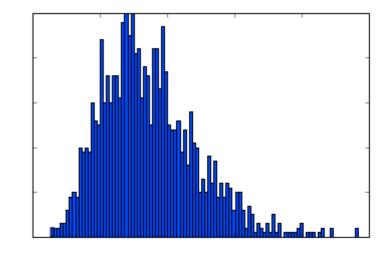
need to choose a form for the conditional **output distribution**, i.e. how do we express $p(x_j|x_1, ..., x_{j-1})$?

model the data as **categorical** variables

model the data as **continuous** variables

→ Gaussian, logistic, etc. output





example applications

text



occluded completions original Image: Sector Sec

images

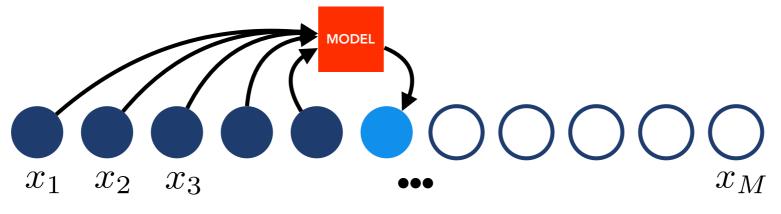
Pixel Recurrent Neural Networks, van den Oord et al., 2016

speech 1 Second

WaveNet: A Generative Model for Raw Audio, van den Oord et al., 2016

recap: auto-regressive models

 $p(x_6|x_5, x_4, x_3, x_2, x_1)$



model conditional distributions to auto-regress to missing values

<u>Pros</u>

tractable and straightforward to evaluate the (log) likelihood

great at capturing details

superior quantitative performance

<u>Cons</u>

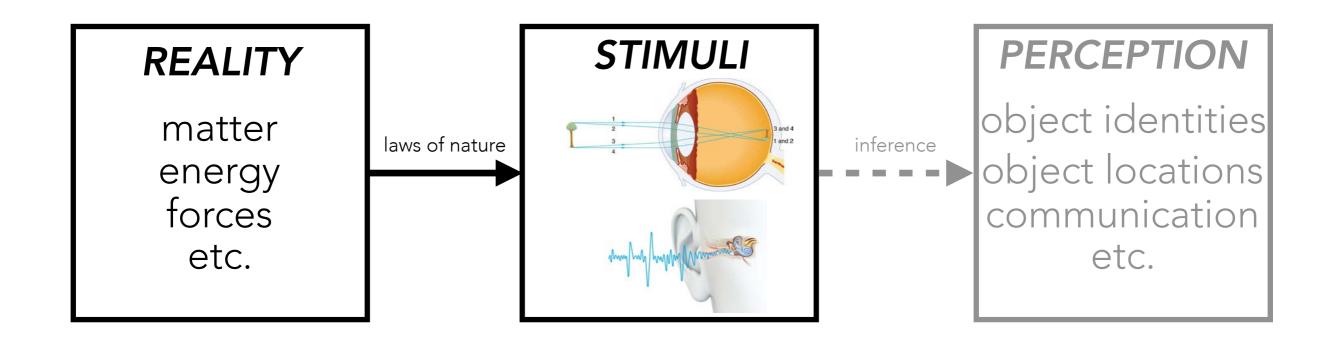
difficult to capture "high-level" global structure

> need to impose conditioning order

sequential sampling is computationally expensive

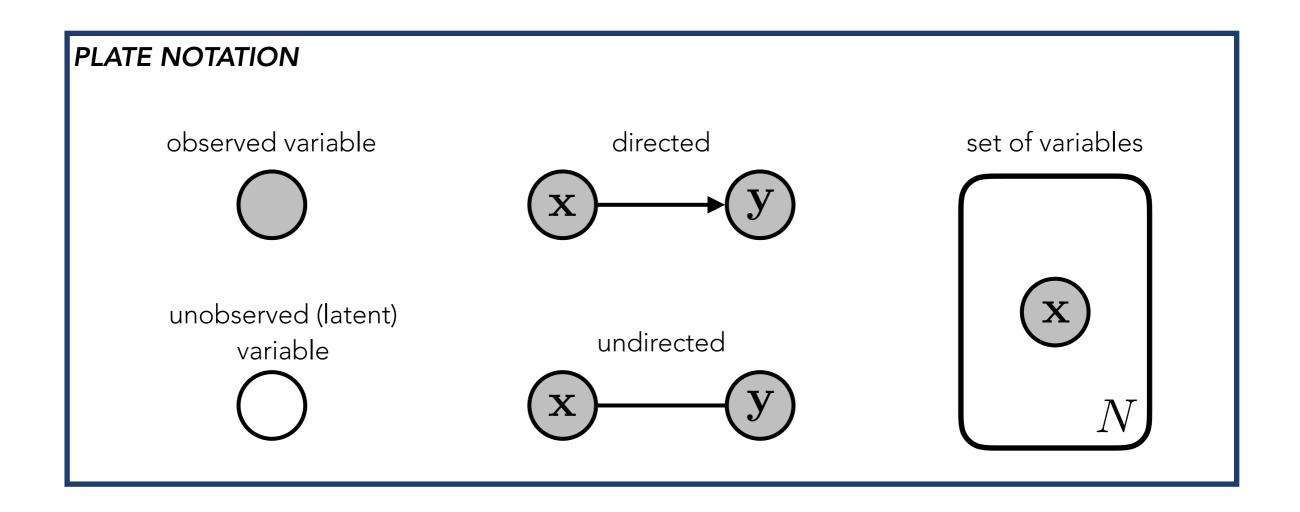
EXPLICIT LATENT VARIABLE MODELS

reality **generates** sensory stimuli from underlying latent phenomena



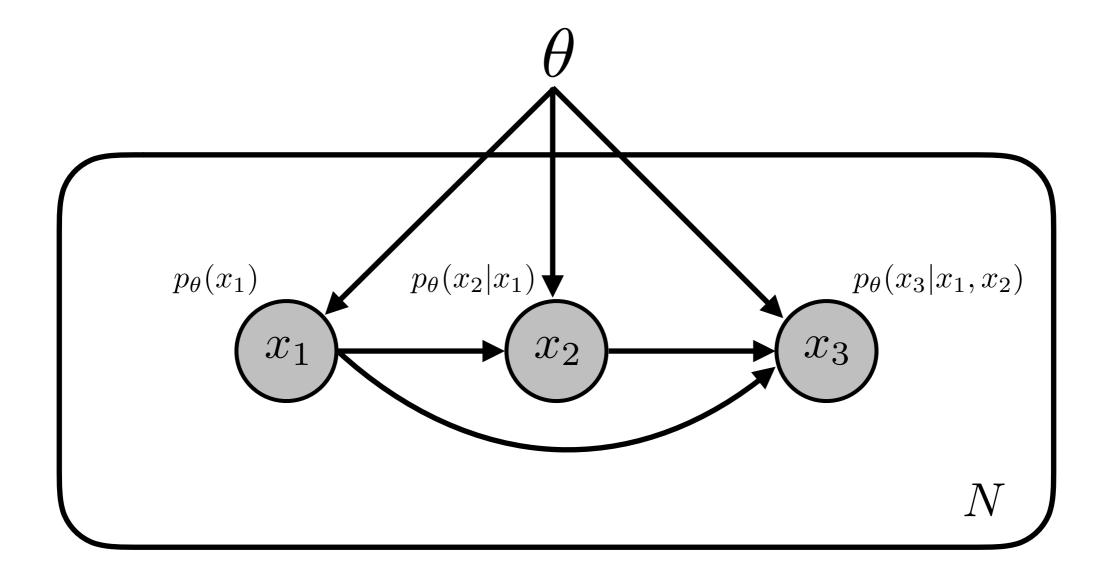
can use *latent variables* to help model these phenomena

probabilistic graphical models provide a framework for modeling relationships between random variables

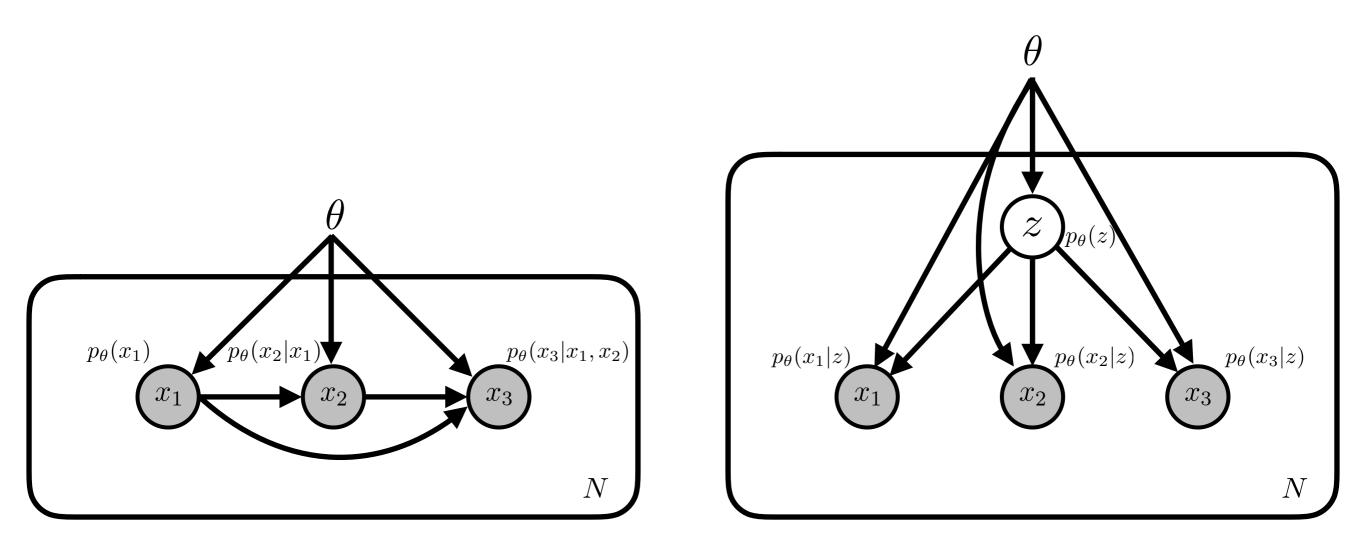


review exercise:

represent an auto-regressive model of 3 random variables with plate notation



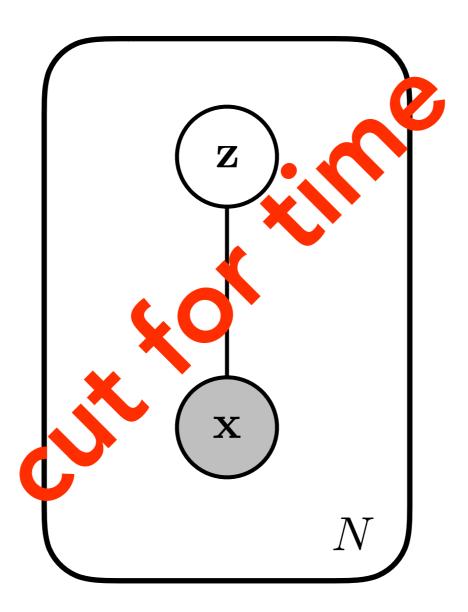
comparing auto-regressive models and latent variable models

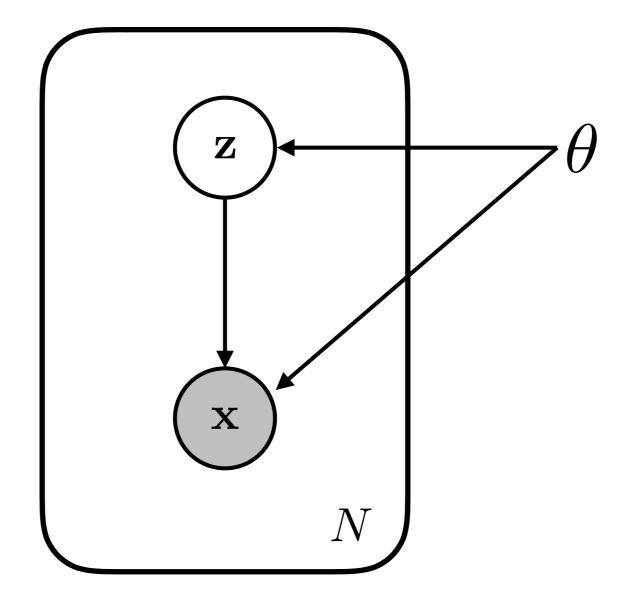


auto-regressive model

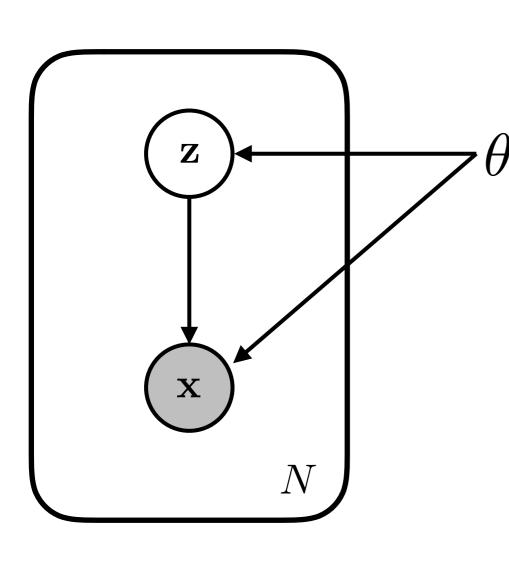
latent variable model

restricted Boltzmann machine



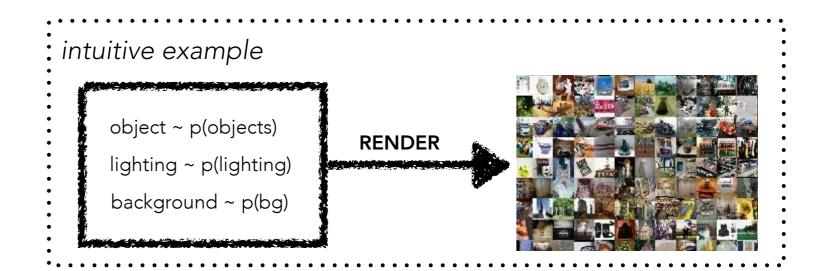


Generation

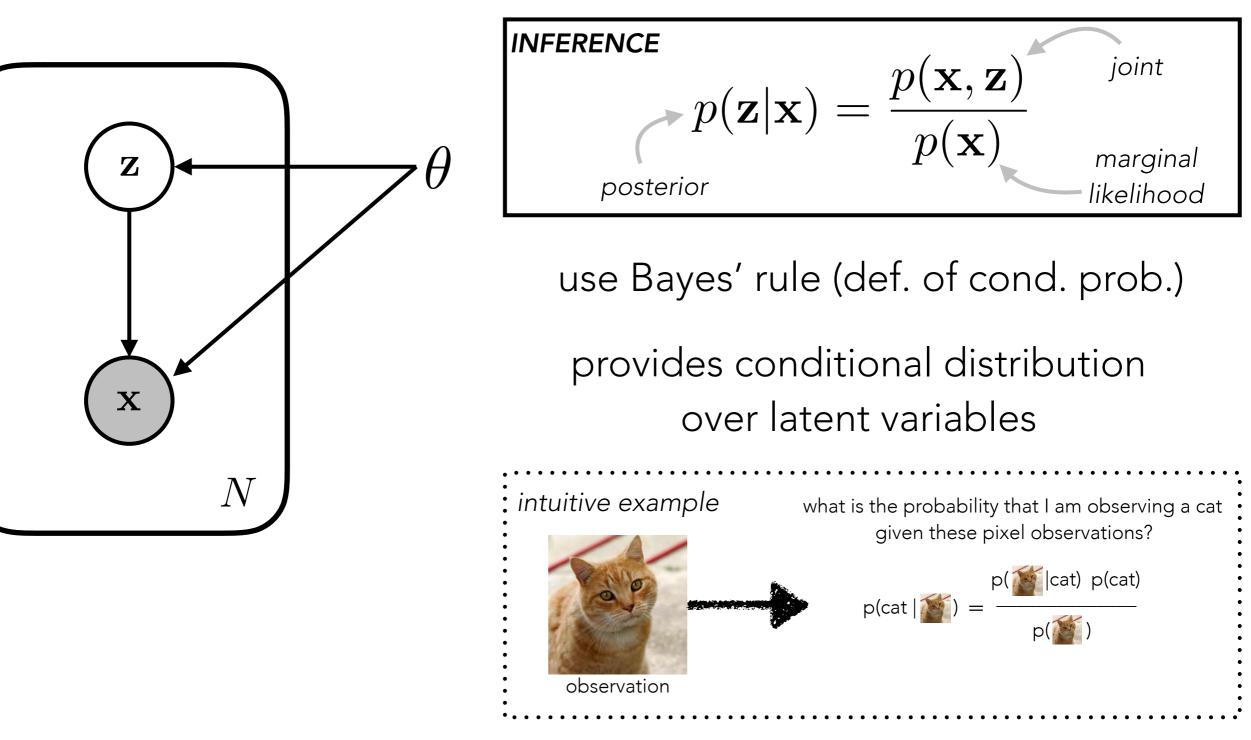


GENERATIVE MODEL $p(\mathbf{x}, \mathbf{z}) = p(\mathbf{x} | \mathbf{z}) p(\mathbf{z})$ prior joint conditional likelihood

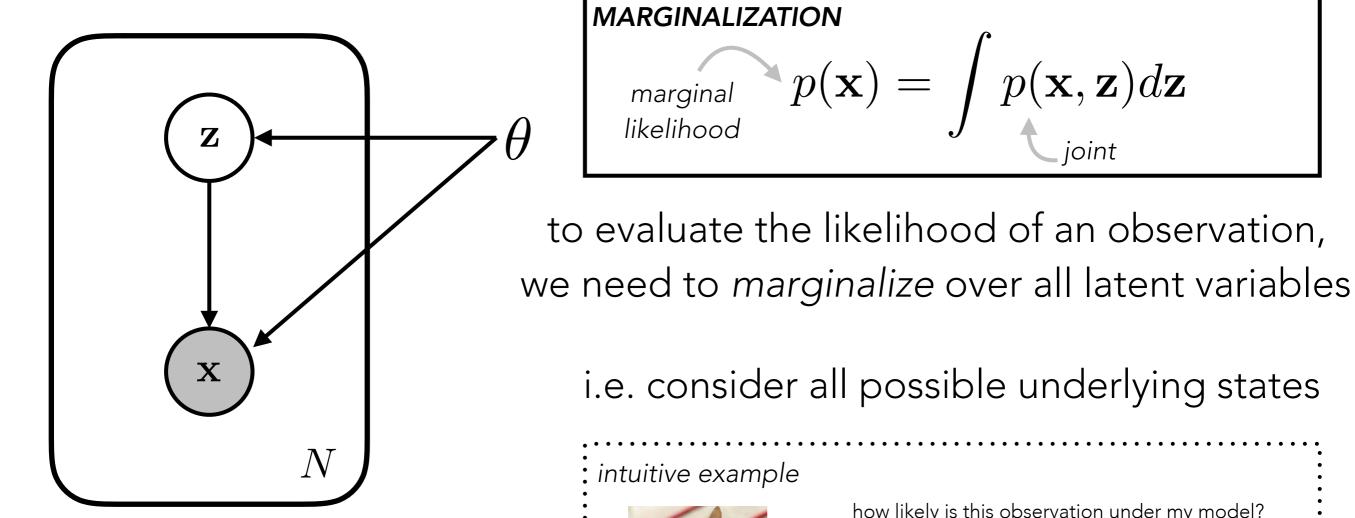
1. sample z from p(z)2. use z samples to sample x from p(x|z)



Posterior Inference



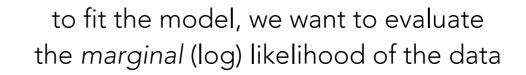
Model Evaluation





how likely is this observation under my model? (what is the probability of observing this?)

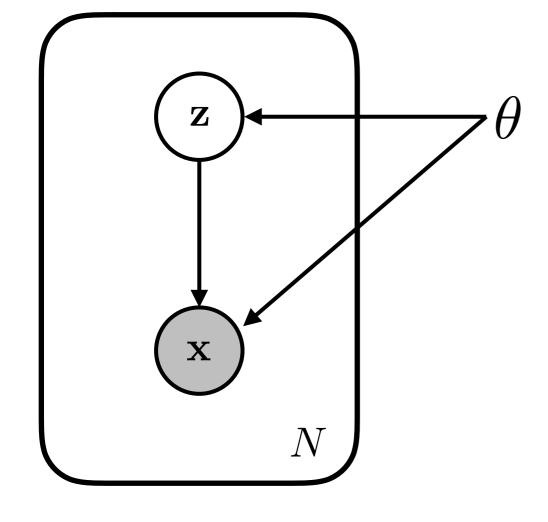
for all objects, lighting, backgrounds, etc.: how plausible is this example?



$$\theta^* = \operatorname{argmax}_{\theta} \log p(\mathbf{x})$$

however, this is generally *intractable*, due to the integration over latent variables

$$p(\mathbf{x}) = \int p(\mathbf{x}, \mathbf{z}) d\mathbf{z}$$
integration in
high-dimensions

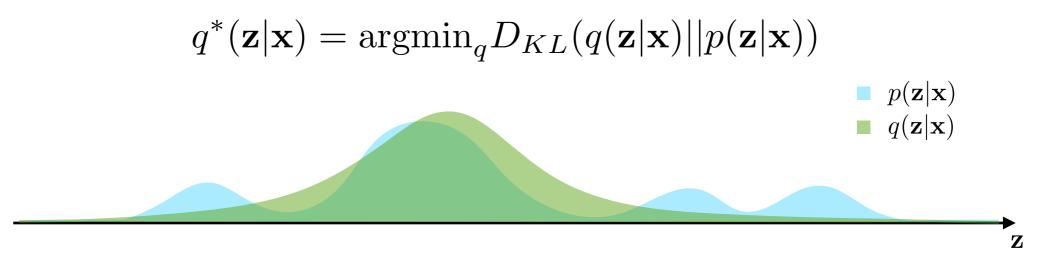


variational inference

<u>main idea</u>

instead of optimizing the (log) likelihood, optimize a lower bound on it

introduce an *approximate posterior*, then minimize KL-divergence to the true posterior



evaluating KL-divergence involves evaluating $p(\mathbf{z}|\mathbf{x})$, instead maximize \mathcal{L} :

$$q^*(\mathbf{z}|\mathbf{x}) = \operatorname{argmax}_q \mathcal{L}$$

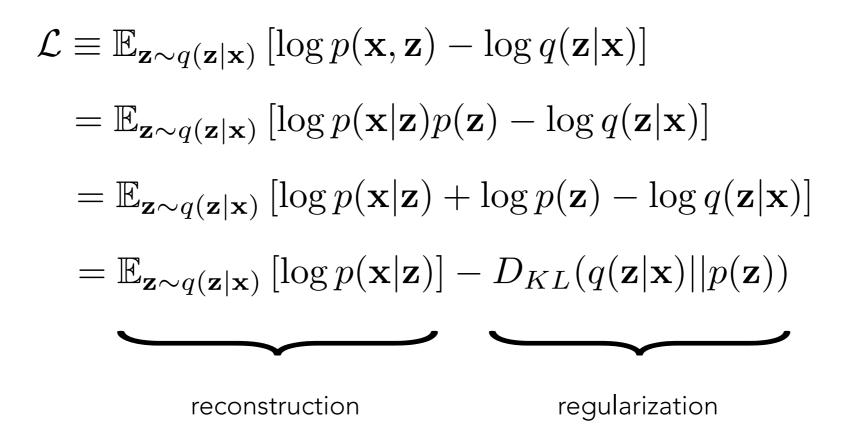
where \mathcal{L} is the evidence lower bound (ELBO), defined as $\mathcal{L} \equiv \mathbb{E}_{\mathbf{z} \sim q(\mathbf{z}|\mathbf{x})} \left[\log p(\mathbf{x}, \mathbf{z}) - \log q(\mathbf{z}|\mathbf{x})\right]$

 \mathcal{L} provides a lower bound on $\log p(\mathbf{x})$, so we can use \mathcal{L} to (approximately) fit the model \widetilde{o}^*

$$\theta^* = \operatorname{argmax}_{\theta} \mathcal{L}$$

interpreting the ELBO

we can write the ELBO as



 $q(\mathbf{z}|\mathbf{x})$ is optimized to represent the data while staying close to the prior

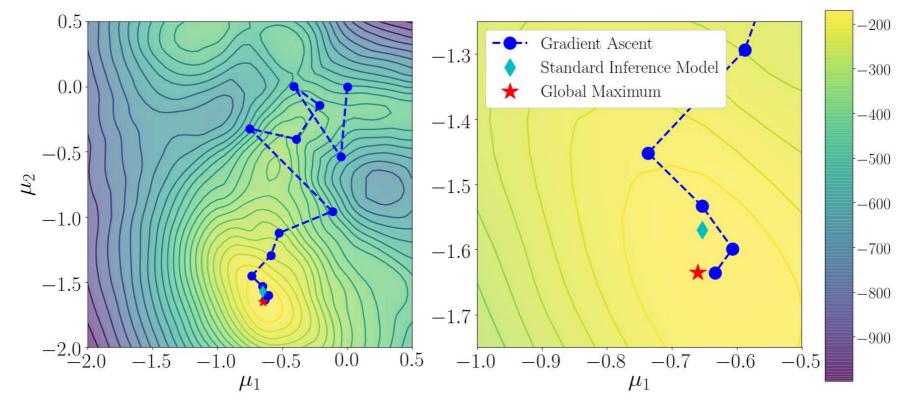
many connections to compression, information theory

resembles the "auto-encoding" framework

variational *inference* involves <u>optimizing</u> the approximate posterior for each data example

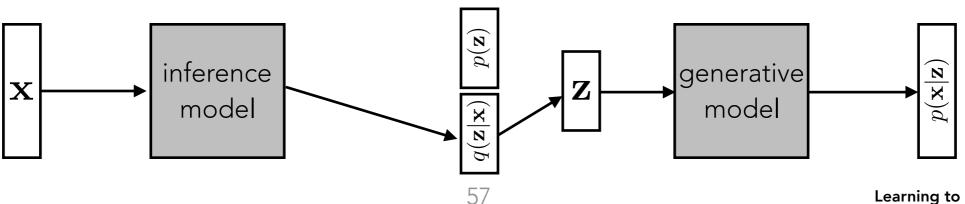
$$q^*(\mathbf{z}|\mathbf{x}) = \operatorname{argmax}_q \mathcal{L}$$

can be solved using gradient ascent and (stochastic) backpropagation / REINFORCE, but can be computationally expensive

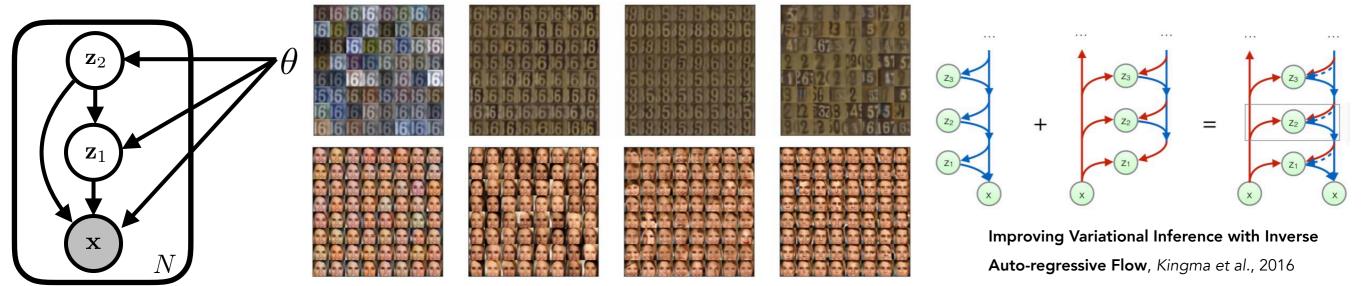


can instead *amortize* inference over data examples by learning a separate **inference model** to output approximate posterior estimates

"variational auto-encoder"

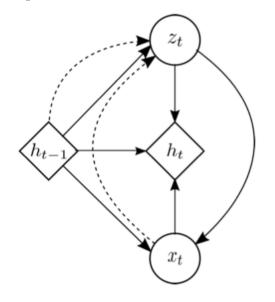


hierarchical latent variable models



Learning Hierarchical Features from Generative Models, Zhao et al., 2017

sequential latent variable models



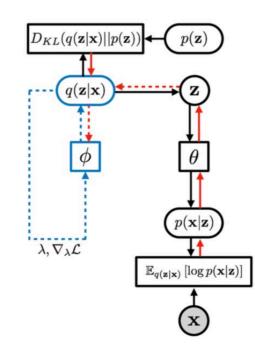


A Recurrent Latent Variable Model for Sequential Data, Chung et al., 2015

\mathbf{u}_{t} \mathbf{z}_{t} \mathbf{z}_{t+1} \mathbf{v}_{t} \mathbf{w}_{t} \mathbf{x}_{t+1}

Deep Variational Bayes Filters: Unsupervised Learning of State Space Models from Raw Data, Karl et al., 2016

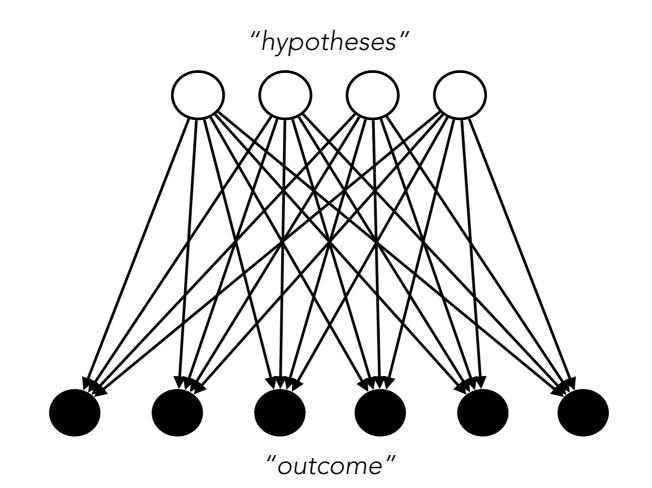
iterative inference models



Learning to Infer, Marino et al., 2017

58

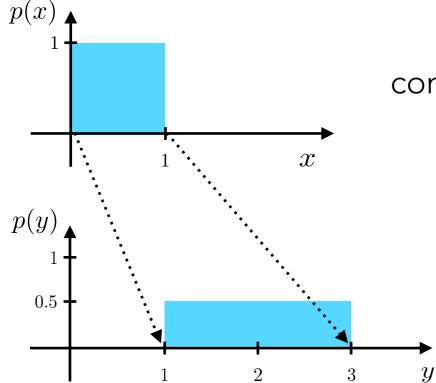
introducing latent variables to a generative model generally makes evaluating the (log) likelihood intractable



need to consider all possible "hypotheses" to evaluate (marginal) likelihood of the "outcome"

change of variables

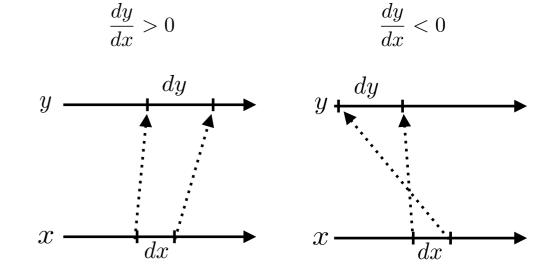
under certain conditions, we can use the <u>change of variables</u> formula to exactly evaluate the log likelihood



consider a variable in one dimension: $x \sim \text{Uniform}(0, 1)$

then let y be an affine transformation of x , e.g. y=2x+1.





Normalizing Flows Tutorial, Eric Jang, 2018

change of variables

in higher dimensions, conservation of probability mass generalizes to

CHANGE OF VARIABLES FORMULA

$$p(\mathbf{y}) = p(\mathbf{x}) \left| \det \frac{d\mathbf{x}}{d\mathbf{y}} \right| = p(\mathbf{x}) \left| \det \mathbf{J}^{-1} \right|$$

where **J** is the Jacobian matrix of the transformation, $\mathbf{J} = \frac{d\mathbf{y}}{d\mathbf{x}}$

 $\left|\det \mathbf{J}^{-1} \right|$ expresses the local distortion in volume from the linear transformation

"law of the unconscious statistician" (LOTUS)

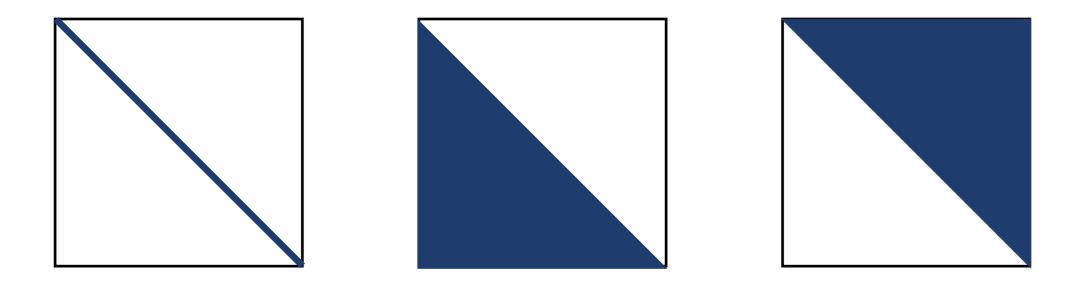
can evaluate the probability from one variable's distribution by evaluating the probability of a transformed variable and the volume transformation

for certain classes of transformations, this is *tractable* to evaluate

change of variables

to use the change of variables formula, we need to evaluate $\left|\det \mathbf{J}^{-1}\right|$

for an arbitrary $N \times N$ Jacobian matrix, this is worst case $O(N^3)$

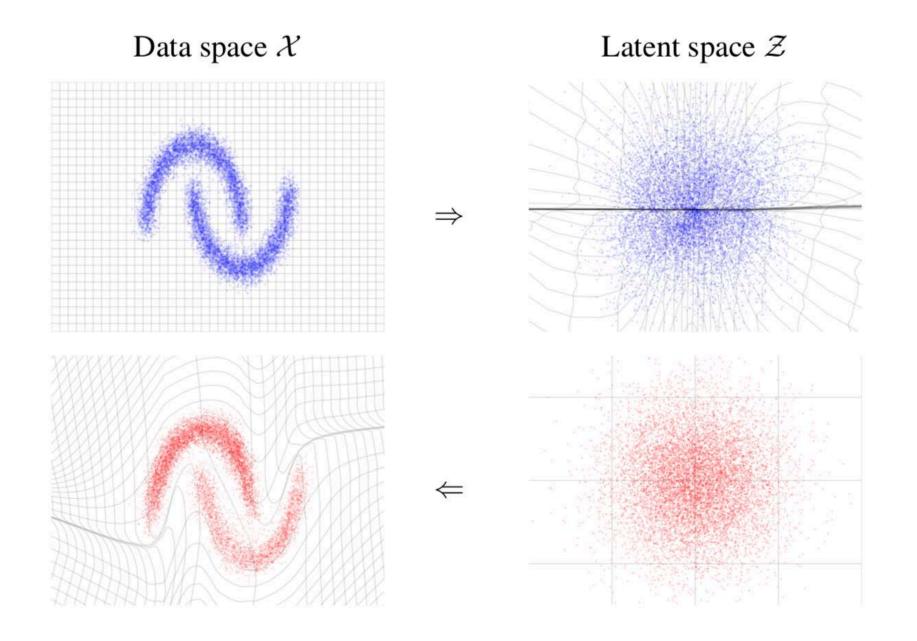


restricting the transformations to those with diagonal or triangular inverse Jacobians allows us to compute $|\det \mathbf{J}^{-1}|$ in O(N).

product of diagonal entries

change of variables

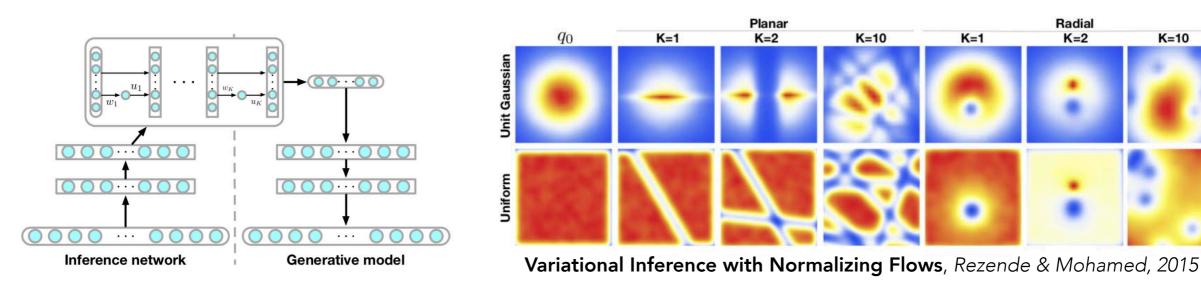
can transform the data into a space that is easier to model



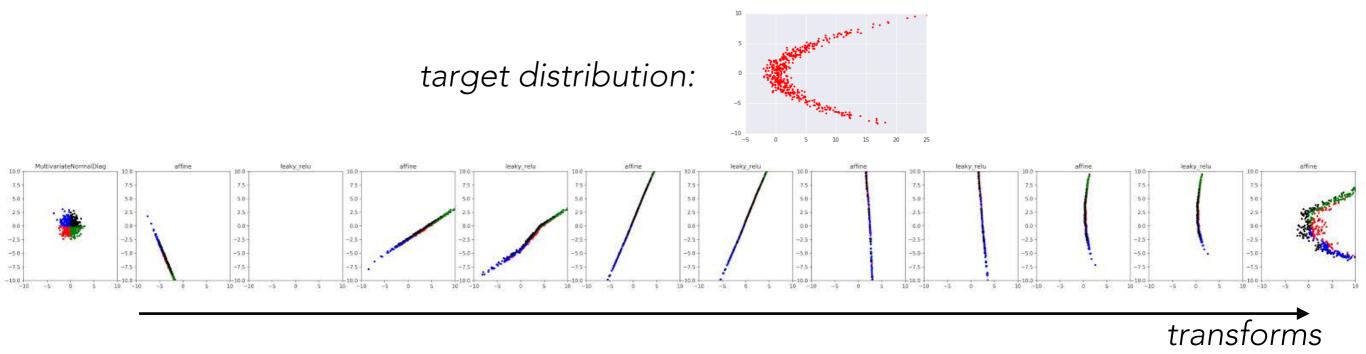
Density Estimation Using Real NVP, Dinh et al., 2016

change of variables for variational inference: **normalizing flows** use more complex approximate posterior, but evaluate a simpler distribution

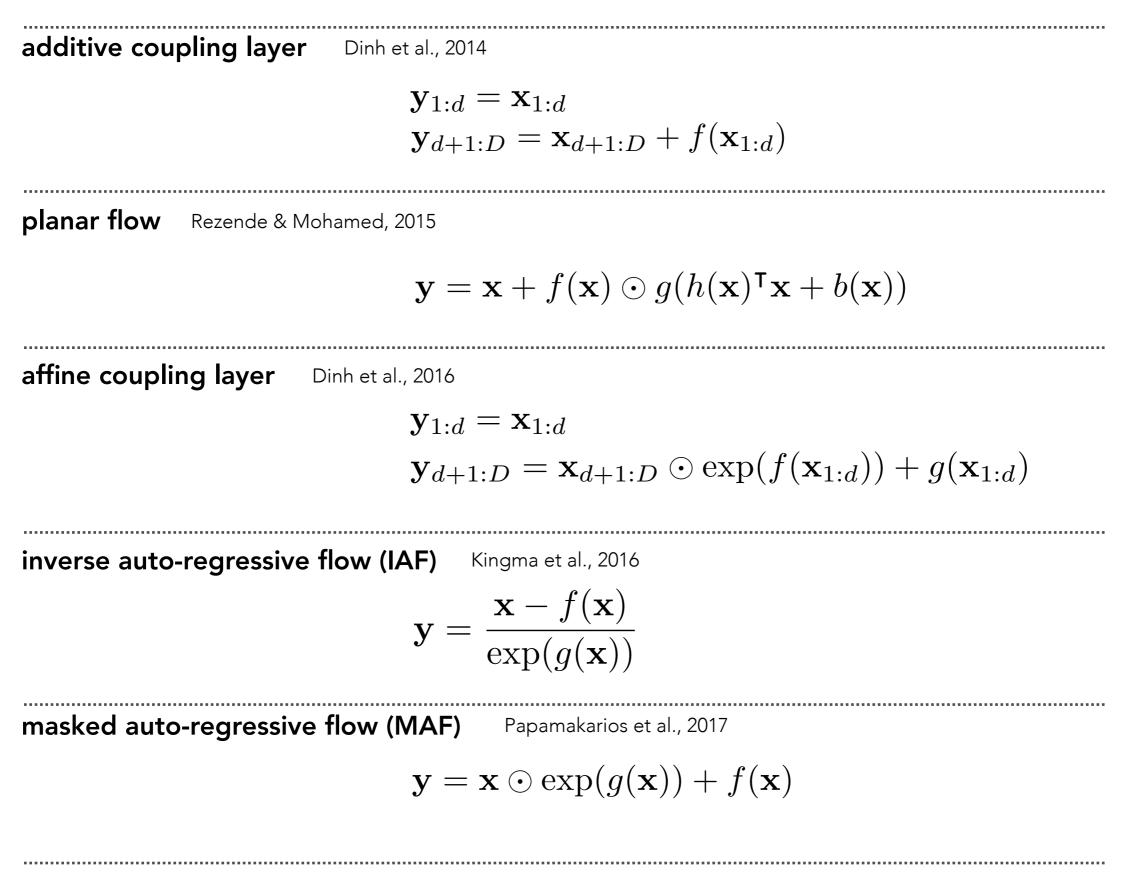
transform $q(\mathbf{z}|\mathbf{x})$



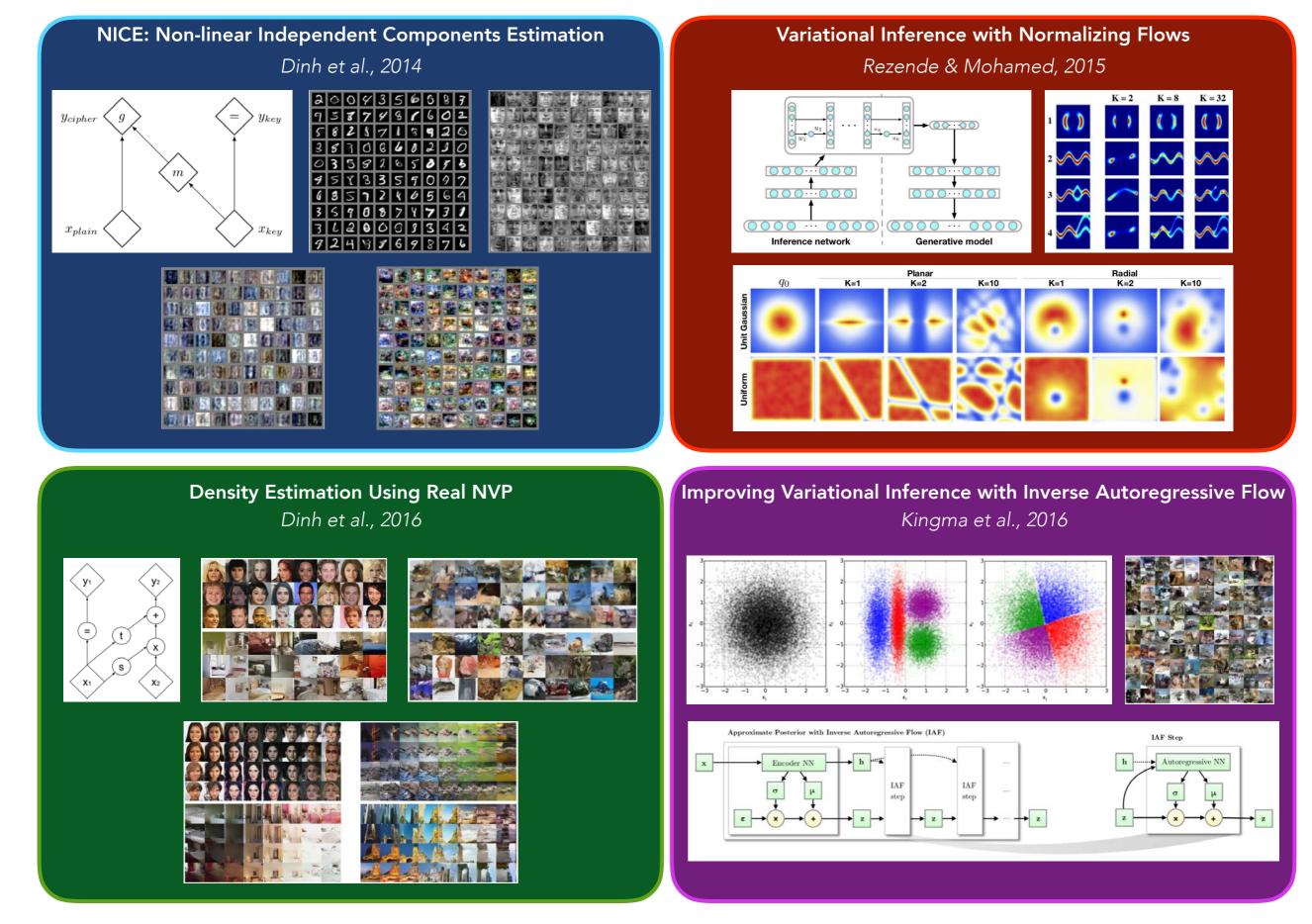
chain together multiple transforms to get more expressive model



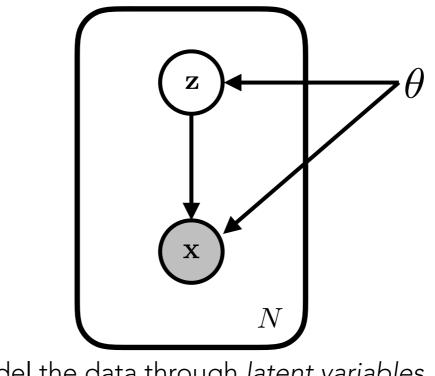
transforms



recent work



recap: explicit latent variable models



model the data through latent variables

Pros

can capture abstract variables, good for semi supervised learning

relatively fast sampling / training

theoretical foundations from info. theory

Cons

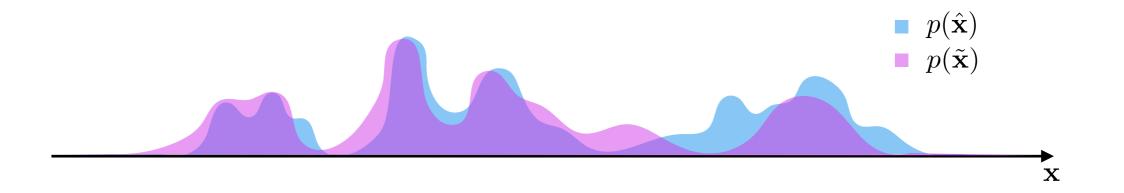
likelihood evaluation / inference often intractable

requires additional assumptions on latent variables

difficult to capture details

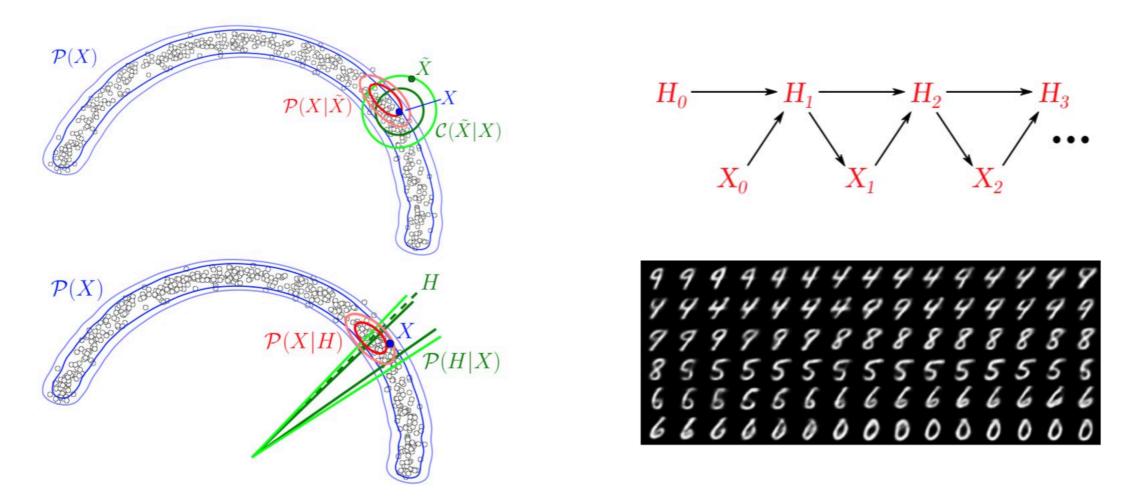
IMPLICIT LATENT VARIABLE MODELS

instead of using an *explicit* probability density, learn a model that defines an *implicit density*



specify a stochastic procedure for generating the data that does not require an explicit likelihood evaluation

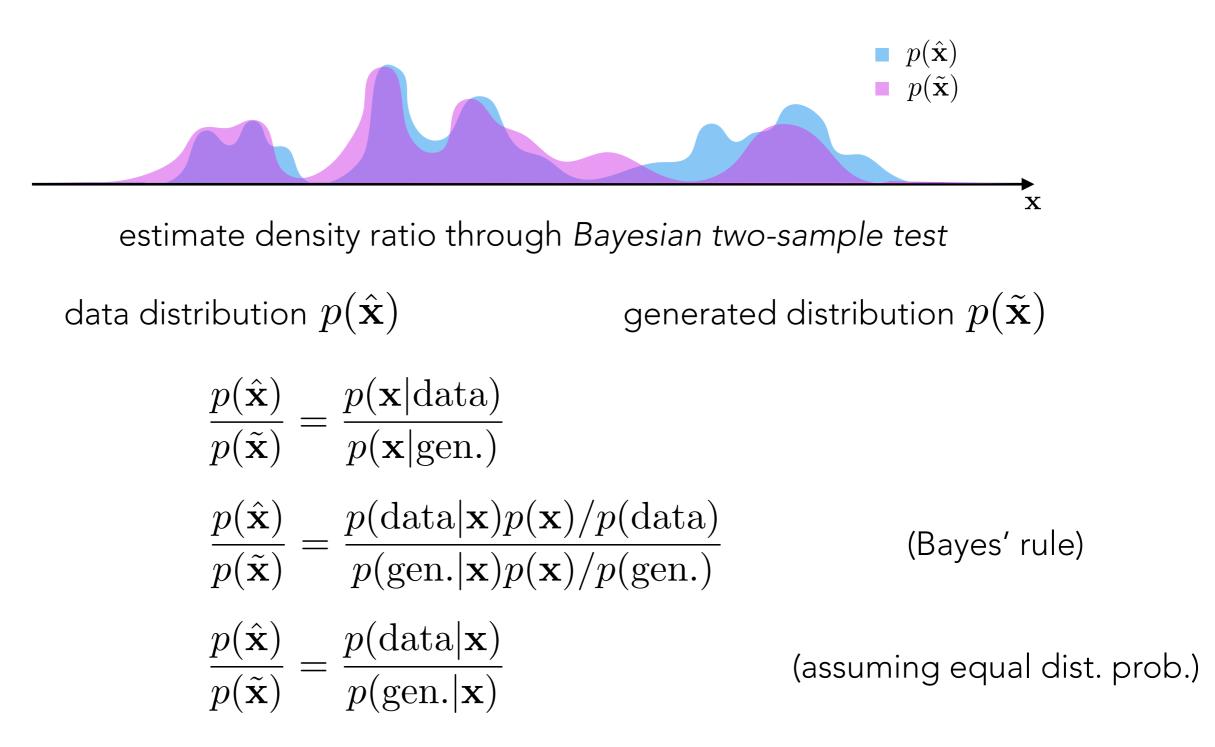
Generative Stochastic Networks (GSNs)



Deep Generative Stochastic Networks Trainable by Backprop, Bengio et al., 2013

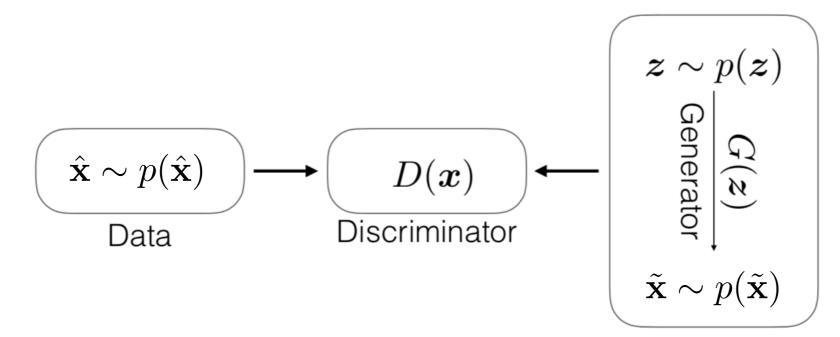
train an auto-encoder to learn Monte Carlo sampling transitions

the generative distribution is *implicitly* defined by this transition



density estimation becomes a sample discrimination task

Generative Adversarial Networks (GANs)



learn the discriminator:

$$p(\text{data}|\mathbf{x}) = D(\mathbf{x})$$
 $p(\text{gen.}|\mathbf{x}) = 1 - D(\mathbf{x})$

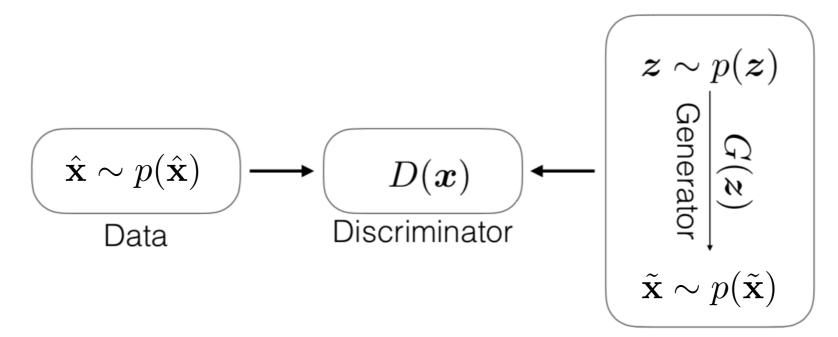
Bernoulli outcome: $y \in \{ data, gen. \}$

$$\log p(y|\mathbf{x}) = \log D(\hat{\mathbf{x}}) + \log(1 - D(\tilde{\mathbf{x}}))$$

two-sample criterion:

$$\min_{G} \max_{D} \mathbb{E}_{p(\hat{\mathbf{x}})} \left[\log D(\hat{\mathbf{x}}) \right] + \mathbb{E}_{p(\tilde{\mathbf{x}})} \left[\log(1 - D(\tilde{\mathbf{x}})) \right]$$

Generative Adversarial Networks (GANs)



two-sample criterion:

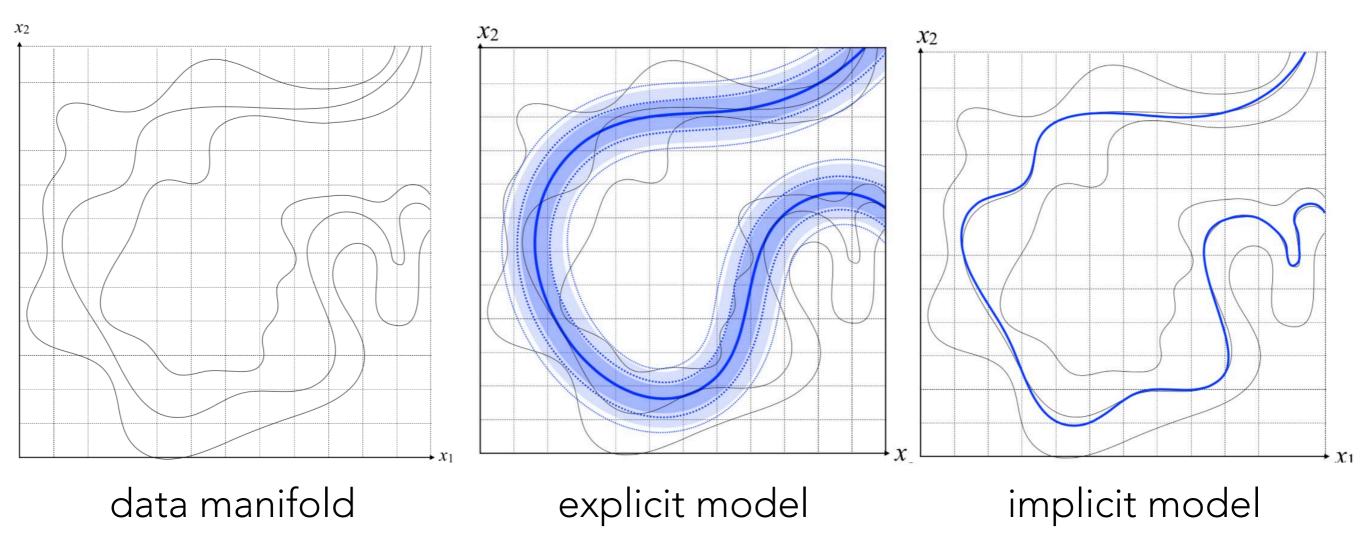
$$\min_{G} \max_{D} \mathbb{E}_{p(\hat{\mathbf{x}})} \left[\log D(\hat{\mathbf{x}}) \right] + \mathbb{E}_{p(\tilde{\mathbf{x}})} \left[\log(1 - D(\tilde{\mathbf{x}})) \right]$$

in practice:

$$\max_{D} \mathbb{E}_{p(\hat{\mathbf{x}})} \left[\log D(\hat{\mathbf{x}}) \right] + \mathbb{E}_{p(\tilde{\mathbf{x}})} \left[\log(1 - D(\tilde{\mathbf{x}})) \right]$$
$$\max_{G} \mathbb{E}_{p(\tilde{\mathbf{x}})} \left[\log D(\tilde{\mathbf{x}}) \right]$$

Goodfellow, 2016 Generative Adversarial Networks, Goodfellow et al., 2014

interpretation



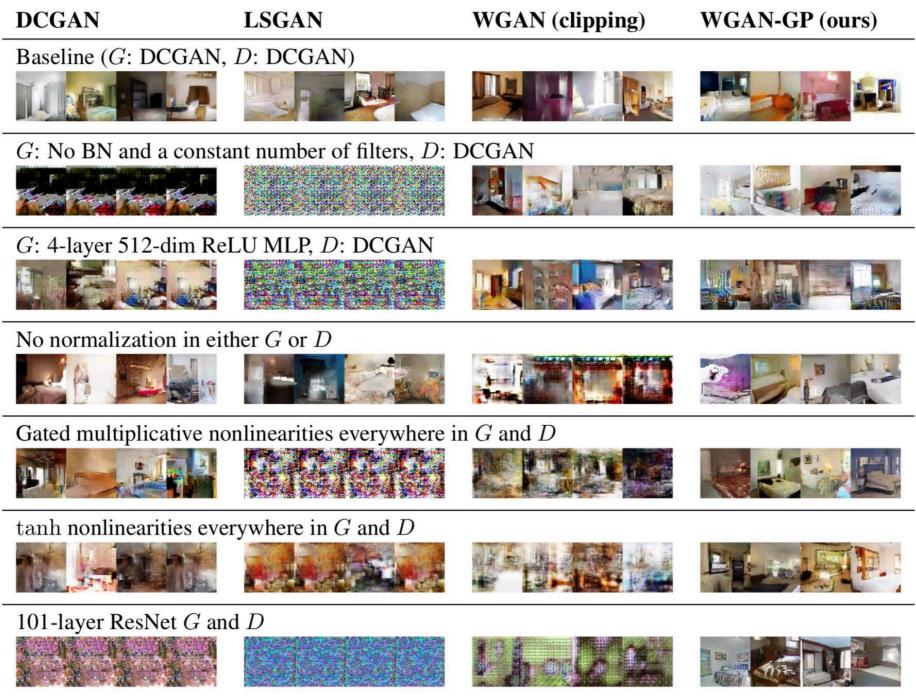
explicit models tend to cover the entire data manifold, but are constrained

implicit models tend to capture part of the data manifold, but can neglect other parts

→ "mode collapse"

Generative Adversarial Networks (GANs)

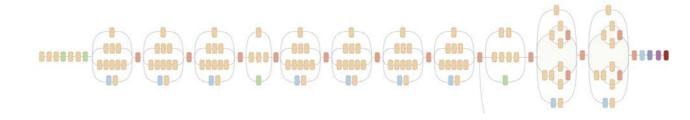
GANs can be difficult to optimize



Improved Training of Wasserstein GANs, Gulrajani et al., 2017

evaluation

without an explicit likelihood, it is difficult to quantify the performance



use a pre-trained Inception v3 model to quantify class and distribution entropy

$$\mathrm{IS}(G) = \exp\left(\mathbb{E}_{p(\tilde{\mathbf{x}})} D_{KL}(p(y|\tilde{\mathbf{x}})||p(y))\right)$$

 $p(y|\tilde{\mathbf{x}})$ is the class distribution for a given image

inception score

should be highly peaked (low entropy)

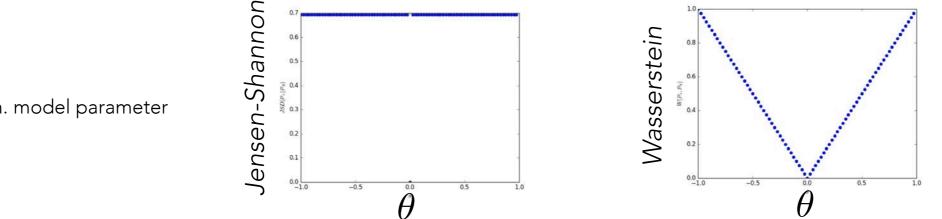
$$p(y) = \int p(y|\tilde{\mathbf{x}}) d\tilde{\mathbf{x}}$$
 is the marginal class distribution
want this to be uniform (high entropy)

extensions: Wasserstein GAN

under an "ideal" discriminator, the generator minimizes the Jensen-Shannon divergence

$$D_{JS}(p(\hat{\mathbf{x}})||p(\tilde{\mathbf{x}})) = \frac{1}{2}D_{KL}(p(\hat{\mathbf{x}})||\frac{1}{2}(p(\hat{\mathbf{x}}) + p(\tilde{\mathbf{x}}))) + \frac{1}{2}D_{KL}(p(\tilde{\mathbf{x}})||\frac{1}{2}(p(\hat{\mathbf{x}}) + p(\tilde{\mathbf{x}})))$$

however, this metric can be **<u>discontinuous</u>**, making it difficult to train



is a gen. model parameter

can instead use the Wasserstein (Earth Mover's) distance (which is continuous and diff. almost everywhere):

$$W(p(\hat{\mathbf{x}}), p(\tilde{\mathbf{x}})) = \inf_{\gamma \in \Pi(p(\hat{\mathbf{x}}), p(\tilde{\mathbf{x}}))} \mathbb{E}_{(\hat{\mathbf{x}}, \tilde{\mathbf{x}}) \sim \gamma} \left[||\hat{\mathbf{x}} - \tilde{\mathbf{x}}|| \right]$$

think of it as the "minimum cost of transporting points between two distributions"

intractable to actually evaluate Wasserstein distance, but by constraining the discriminator, can evaluate

$$\min_{G} \max_{D \in \mathcal{D}} \mathbb{E}_{p(\hat{\mathbf{x}})} \left[D(\hat{\mathbf{x}}) \right] - \mathbb{E}_{p(\tilde{\mathbf{x}})} \left[D(\tilde{\mathbf{x}}) \right]$$

 ${\cal D}$ is the set of Lipschitz functions, which can be enforced through weight clipping or gradient penalty.

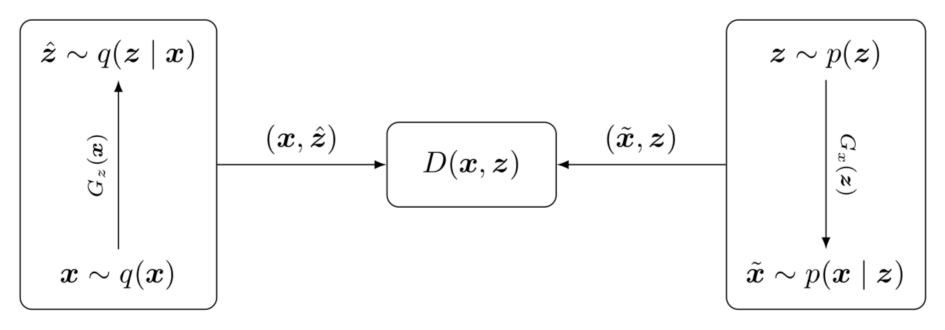
Wasserstein GANs, Arjovsky et al., 2017

Improved Training of Wasserstein GANs, Gulrajani et al., 2017

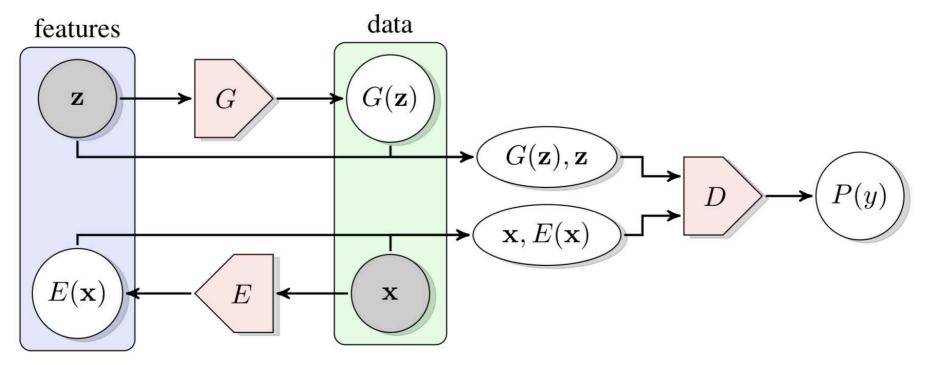
77

extensions: inference

can we also learn to **infer a latent representation**?



Adversarially Learned Inference, Dumoulin et al., 2017



Adversarial Feature Learning, Donahue et al., 2017

applications

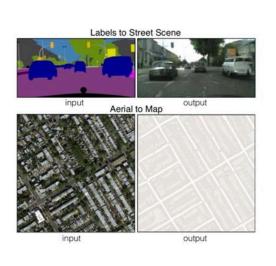
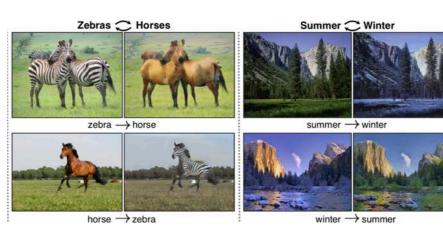
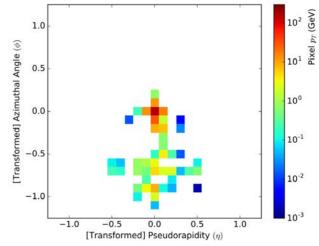


image to image translation



Unpaired Image-to-Image Translation using Cycle-Consistent Adversarial Networks, *Zhu et al.*, 2017

experimental simulation

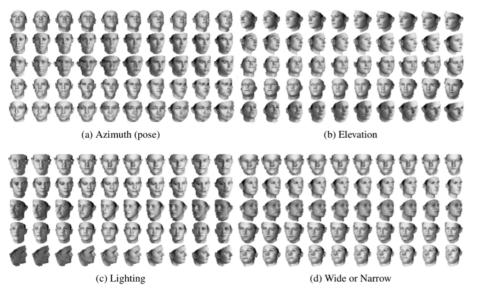


Learning Particle Physics by Example, de Oliveira et al., 2017

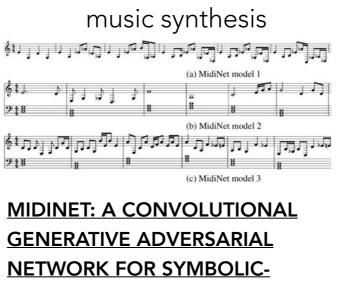
Adversarial Networks, Isola et al., 2016

Image-to-Image Translation with Conditional

interpretable representations



InfoGAN: Interpretable Representation Learning by Information Maximizing Generative Adversarial Nets, Chen et al., 2016



DOMAIN MUSIC GENERATION,

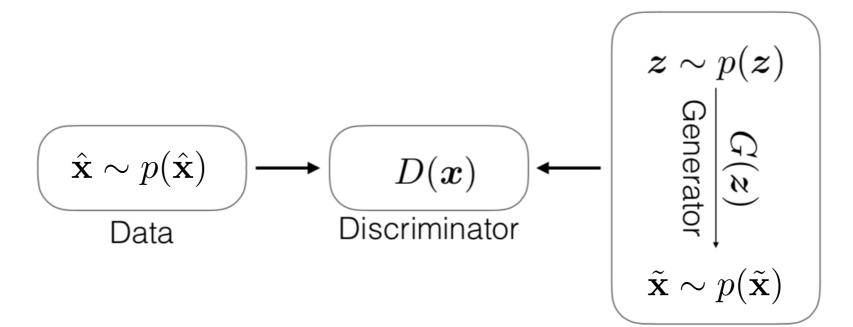
Yang et al., 2017

text to image synthesis

	This bird is red and brown in color, with a stubby beak	The bird is short and stubby with yellow on its body	A bird with a medium orange bill white body gray wings and webbed feet	This small black bird has a short, slightly curved bill and long legs	A small bird with varying shades of brown with white under the eyes	A small yellow bird with a black crown and a short black pointed beak	This small bird has a white breast, light grey head, and black wings and tail
7		-31	-	8			1

StackGAN: Text to Photo-realistic Image Synthesis with Stacked Generative Adversarial Networks, *Zhang et al.*, 2016

recap: implicit latent variable models



Pros

able to learn flexible models

requires fewer modeling assumptions

capable of learning latent representation

Cons

difficult to evaluate

sensitive, difficult to optimize

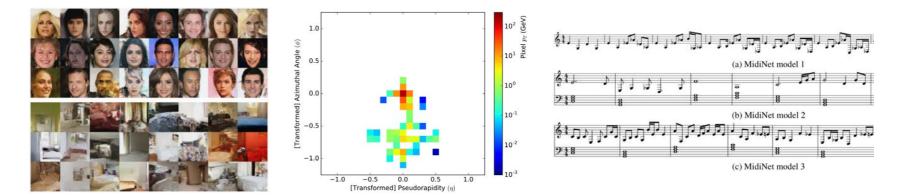
can be difficult to incorporate model assumptions

DISCUSSION

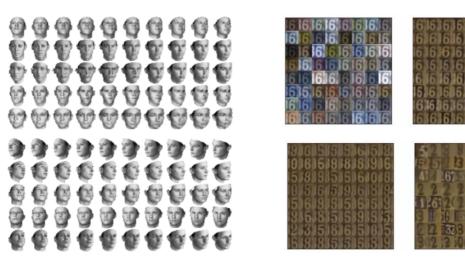
generative models: what are they good for?

generative models model the data distribution

1. can generate and simulate data



2. can extract structure from data



generative models: what's next?

applying generative models to new forms of data







incorporating generative models into *complementary* learning systems

