ECE598: Generative AI Models

March 7, 2022

1 Lecture 2-3: Normalizing Flows

1.1 Generating a random variable with specified distribution

- Want to generate sample from random variable (RV) with given cumulative distribution function (CDF)
- Have access to realization of $U(0,1)$

① Apply F_x to X
Let $Y = F_x(x)$. Since F_x is non-decreasing from 0 to 1, there is a value C_v such that $F_x(C_v) = V$
$\Rightarrow Pr[F_x(x) \leq V] = Pr[x \leq C_v] = F_x(C_v) = V$
So $F_x(x)$ is $U(0,1)$.
② Go backwards
Apply $F_x^{-1}(.)$ to uniform RV $U(0,1)$, call u
Should replace cv with cdf F_x
$F^{-1}(u) = min\{c : F(c) \geq u\}$
For real C_0 and U_0, with $0 < U_0 < 1$
$F^{-1}(U_0) \leq C_0$, iff $U_0 \leq F(C_0)$.
If $X = F^{-1}(V)$, then $F_x(c) = Pr[F^{\lfloor} - 1](V) \leq C] = Pr[V \leq F(c)] = F(c)$
In ML, $g(.) = F^{-1}(.)$ is called a generator. In Statistics, it's called simulation.

$U(0,1) \xrightarrow{g} N(0,1)$, Box-Muller transform
Suppose u_1, u_2 are $iid \sim U(0,1)$, Let
$Z_0 = \sqrt{-2lnu_1}cos(2\pi u_2) = Rcos(\Theta)$
$Z_1 = \sqrt{-1lnu_1}sin(2\pi u_2) = Rsin(\Theta)$, where $R^2 = -2lnu_1, \Theta = 2\pi u_2$ in polar coordinates.
Then $Z_1 \perp Z_2$, both $\sim N(0,1)$

For discrete distributions
Gambel-Max generator:
If $Z \sim U(0,1)$, then $g(Z) \sim P$
If $g(Z) = \underset{x}{argmax}(log\ P(x) - log\ log(1/Z))$

Transformation of joint pdfs (**linear mapping**).

Suppose we have joint pdf $f_{xy}(u,v)$ of $RV(x,y)$, vector form $f_{xy}(\begin{bmatrix} u \\ v \end{bmatrix})$

Have 2 new rv (W,Z), linear function of (X,Y), find $f_{W,Z}$

eg. $\begin{bmatrix} W \\ Z \end{bmatrix} = A\begin{bmatrix} X, Y \end{bmatrix}$, where $A = \begin{bmatrix} a & b \\ c & d \end{bmatrix}$, $det(A) = ad - bc$.

If $det(A) \neq 0$, A has inverse $A^{-1} = \frac{1}{det(A)}\begin{bmatrix} d & -b \\ -c & a \end{bmatrix}$

Theorem : Suppose $\begin{bmatrix} W \\ Z \end{bmatrix} = A \begin{bmatrix} X \\ y \end{bmatrix}$, where $\begin{bmatrix} X \\ Y \end{bmatrix} \sim f_{xy}$, $det(A) \neq 0$, then $\begin{bmatrix} W \\ Z \end{bmatrix}$ has joint pdf $f_{W,Z}(\begin{bmatrix} \alpha \\ \beta \end{bmatrix}) = \frac{1}{|det(A)|} f_{xy}(A^{-1}(\begin{bmatrix} \alpha \\ \beta \end{bmatrix}))$

Non-linear: $\begin{bmatrix} W \\ Z \end{bmatrix} = g(\begin{bmatrix} X \\ Y \end{bmatrix})$
Recall Jacobian of g,
$J = J(u,v) = \begin{bmatrix} \frac{\partial\, g_1(u,v)}{\partial\, u} & \frac{\partial\, g_1(u,v)}{\partial\, v} \\ \frac{\partial\, g_2(u,v)}{\partial\, u} & \frac{\partial\, g_2(u,v)}{\partial\, v} \end{bmatrix}$, where g_1, g_2 are coordinates of g.

Theorem : Suppose $\begin{bmatrix} W \\ Z \end{bmatrix} = g(\begin{bmatrix} X \\ Y \end{bmatrix})$, where $\begin{bmatrix} X \\ Y \end{bmatrix}$ has pdf f_{xy} and g is a one-to-one mapping from support of f_{xy} to $\mathbb{R}^2$.
Suppose J of g exists, is continuous and has a non-zero determinant everywhere
$f_{WZ}(\begin{bmatrix} \alpha \\ \beta \end{bmatrix}) = \frac{1}{|det(J)|} f_{xy}(g^{-1} \begin{bmatrix} \alpha \\ \beta \end{bmatrix})$ for (α, β) in support of f_{WZ}. If g is many to one, just sum over pieces.
Other approach to sample from distributions:

- rejection sampling
- Markov chain Monte Carlo (MCMC)

If we just have iid samples from P, estimate $\hat{P}$ from P using samples, then generate using $\hat{P}$.
To estimate arbitrary pmf from samples, just use empirical counts. This is actually the maximum likelihood estimate (MLE)
$\hat{P} \to P, \#samples \to \infty$
Laplacian smoothing $\Rightarrow$ assign small probability to all possible outcomes.
Continuous setting
$\to$ Parametric density estimation, eg. mean/variance of Gaussian.
$\to$ Non-parametric density estimation, eg. kernel density estimation.
Want to sample from $\hat{P}$, not evalutate $\hat{P}(X)$ at various values. In generative models, we use $\hat{P}$ implicitly, and it's difficult ot backing out $\hat{P}(X)$.

1.2 Normalizing Flows

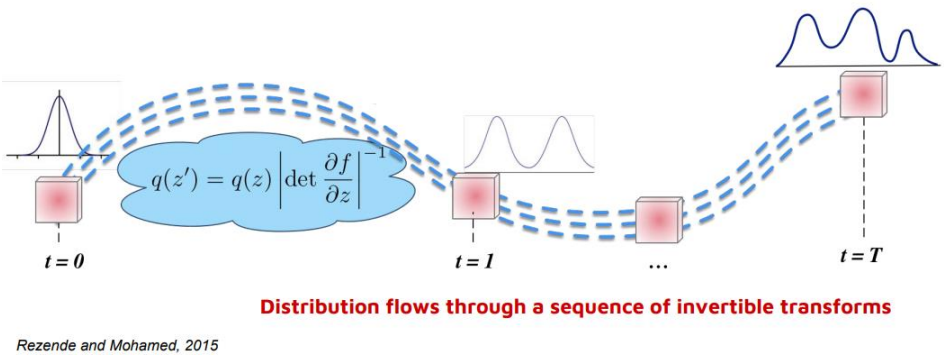


Figure 1: Normalizing Flows. See: https://www.shakirm.com/slides/DeepGenModelsTutorial.pdf

Construct a normalizing flow $\Rightarrow$ a sequence of invertible transformations that convert simple distribution to complex one.
Invertible smooth mapping: $f : \mathbb{R}^d \to \mathbb{R}^d$ with $f^{-1} = g$
$g \cdot f(x) = X$ if we use this to transform rv X with distribution q. $\tilde{X} = f(x)$ have distribution.
(*) $q(\tilde{x}) = q(x)|det\frac{\partial\ f^{-1}}{\partial\ x}| = q(x)|det\frac{\partial\ f}{\partial\ x}|^{-1}$
Successively apply (*) when each map is simple.
$X_k = f_k \circ f_{k-1}\circ, ..., \circ f_2 \circ f_1(X_0)$
So $ln(q_k(x_k)) = lnq_0(x_0) - \sum_{k=1}^{K} ln|det\frac{\partial\ f_k}{\partial\ x_{k-1}}|$

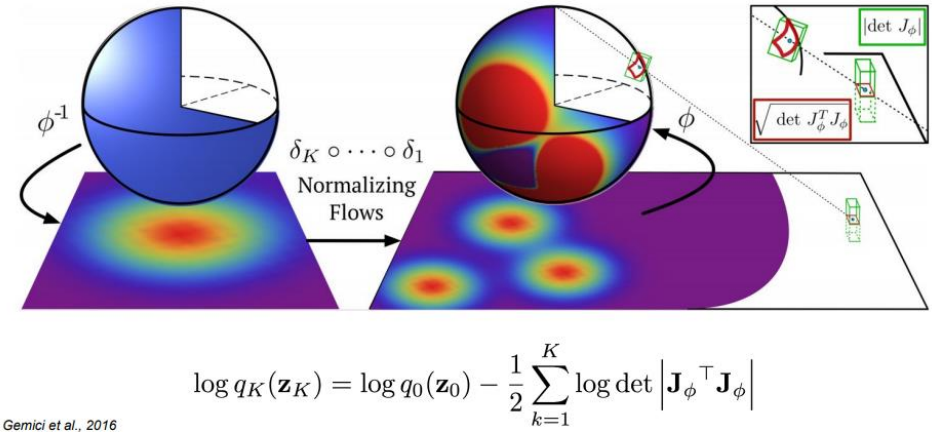


Figure 2: https://www.shakirm.com/slides/DeepGenModelsTutorial.pdf

- The path traversed by rv $X_k = f_k(x_{k-1})$ is flow. Path successive distribution q_k is normalizing flow. Want inverse and Jacobian to be simple but don't want to lose expressibility.
- Use sequence of invertible transformations until desired complexity.
- Equality is by applying chain rule.

Generative models from learning from data iid samples from P. Try to get estimate $\hat{P}$, then use it to generate new sample, rather than evaluate $\hat{P}(x)$. Often have generative model where $\hat{P}$ is implicit rather than explicit. Backing out $\hat{P}(x)$ is hard.
Suppose $\hat{P}$ is defined implicitly as probability integral transform of density q by $g : \xi \to X$, so for event A:
$Pr[A] = Pr[g^{-1}[A]] = \int_{g^{-1}A} q(Z)dZ = \int_A q(g^{-1}(X))|\nabla_X g^{-1}(X)|dX$,
where $\hat{P}(X) = q(g^{-1}(X))|\nabla_X g^{-1}(X)|$ and when inverse and Jacobian are easy to compute, converting generator to density estimator easily.

LOTUS property: Law of unconscious statistician.
$\mathbb{E}[g(x)] = \sum_k g(x_k)P_x(x_k)$
The expectation wrt transformed density q_k can be computed without explicitly knowing q_k. Any $\mathbb{E}_{q_k}(h(x))$ can be written under q_k without the need to compute the largest Jacobian term after $h(x)$.
$\mathbb{E}_{q_k}[h(x)] = \mathbb{E}_{q_0}[h(f_k \circ f_{k-1\circ...\circ f_1(x_0)})]$ when $h(x)$ doesn't depend on q_k.

In discrete setting, change of variable formula is easier.
Let x be discrete rv, $Y = f(x)$. The induced pmf of g is sum over inverse (???) of f:
$P[Y = y] = \sum_{x:f^{-1}(y)} Pr[X = x]$ where $f^{-1}(y)$ is set of all elements to $f(x) = y$.
f is invertible, then $P[Y = y] = P(X = f^{-1}(y))$

Infinitesimal flows: let the number of transformation $k \to \infty$. Describe how the initial density $q_0(x)$ evolves over time using PDE:
$\frac{\partial}{\partial t} q_t(x) = J_t[q_t(x)]$, J_t is continuous time (???) dynamics.

1.3 Glow

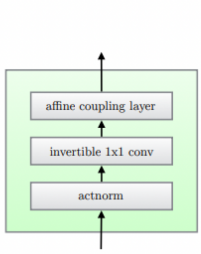
Let X be high-dimensional rv with unknown time distribution $X \sim P(X)$. Collect iid dataset D of size M and model class $P_\theta(X)$ with parameter θ. Consider maximum likelihood, so minimize objective $\mathcal{L}(D) = \frac{1}{N}\sum_{i=1}^{N} - logP_\theta(X^{(i)})$.
For continuous data,
$\mathcal{L}(D) \approx \frac{1}{N}\sum_{i=1}^{N} - logP_\theta(\bar{x}^i) + C$, where $\bar{x}^{(i)} = x^{(i)} + u$ with $u \sim U(0, a)$, $C = Mlog\ a$, where a is the quantization level. M is dimension. Optimize using eg. stochastic gradient descent.
In flow-based generation, $Z \sim P_\theta(Z)$ where Z is latent variable and $P_Z(Z)$ is simple density $X = g_\theta(Z)$ where $g_k(.)$ is invertible so $Z = f_\theta(x) = g_\theta^{-1}(x)$.
$f = f_1 \cdot f_2 \cdot ... \cdot f_k$
$H_0 = x \overset{f_1}{\longleftrightarrow} H_1 \overset{f_2}{\longleftrightarrow} H2... \overset{f_k}{\longleftrightarrow} Z = H_k$
$$logP_\theta(x) = logP_\theta(Z) + \sum_{k=1}^{K} log|det(\frac{\partial\ H_k}{\partial\ H_{k-1}})|.$$
Easy to get Jacobian where $det(\frac{\partial\ H_k}{\partial\ H_{k-1}})$ is lower triangular. $log|det(\frac{\partial\ H_k}{\partial\ H_{k-1}})| = \sum(log|diag(\frac{\partial\ H_k}{\partial\ H_{k-1}})|)$

GLOW architecture

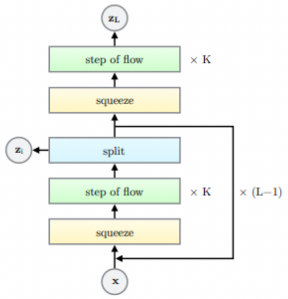
affine coupling layer basically learns a nonlinear independent components representation with easy inverse and easy log det Jacobian, since disentangling is a good representation

invertible convolution is generalization of learned rotation

activation normalization (actnorm) learns affine transformation of activations using a scale and bias parameter per channel



(a) One step of our flow.



(b) Multi-scale architecture (Dinh et al., 2016).

2 Lecture 4-6: Autoencoder

An autoencoder is a neural network trained to attempt to copy its input to its output. Internally, it has hidden layer h that describes a code or latent space used to represent the input.
$\underset{input}{\mathbb{X}} \overset{f}{\underset{encoder}{\longrightarrow}} \underset{code}{\mathbb{H}} \overset{g}{\underset{decoder}{\longrightarrow}} \underset{reconstruction}{\mathbb{R}}$
Tries to set $g(f(x)) = x$ but are designed to be unable to learn to copy perfectly.

- restricted to prevent exact copying
- model forced to prioritize which aspects of the input should be copied, so often learns most useful properties of data

Not just deterministic functions f, g, but also stochastic mappings
$P_{encoder}(h|x)$ and $P_{decoder}(x|h)$.

2.1 undercomplete autoencoders

Constrain h to have smaller dimension than x, to force to have preserved most salient properties.
Reminiscent of data compression and very much a form of approximation theory.
Learning process is minimizing loss function
$L(x, g(f(x)))$ where L is loss function penalizing $g(f(x))$ for lack of fidelity with x.
When $g(\cdot)$ fixed to be linear and L is mean-square error, an undercomplete autoencoder recovers principle components analysis (PCA), the Karhunen-Loeve transform.
Why? When allowing nonliear (f,g), get generalization of PCA.
One can also generalize, e.g. with sparsity autoencoder.
$L(x, g(f(x))) + \Omega(h)$, where $\Omega(\cdot)$ is sparsity penalty on latent space h in addition to data fidelity term. Hopefully, this forces learning of relevant things.

2.2 Denoising autoencoders

minimize $L(x, g(f(\hat{x})))$ in stead of $L(x, g(f(x)))$, where $\hat{x}$ is noisy version of x.
DAE have to undo the noise corruption rather than simply copying, so again fry to get most informative elements.

2.3 Contractive autoencoders

Different kind of regularization, to force a function that doesn't change much when x changes a little.
$L(x, g(f(x))) + \Omega(h, x)$ where $\Omega(h, x) = \lambda \sum_i \|\nabla_x h_i\|^2$
or $\Omega(h) = \lambda \| \frac{\partial\, f(x)}{\partial\, x} \|_F^2$ where penalty is squared Frobenius norm (sum of squared elements) of Jacobian matrix of partial derivatives associated with encoder function.

2.4 AE with NN

AE used for dimensionality reduction, etc, but what about generation?
$\textcircled{x} \xrightarrow{P_{encoder}(h|x)} \textcircled{h} \xrightarrow{P_{decoder}(x|h)} \textcircled{r}$
Stochastic encoder/decoder. Note that $P_{encoder}$, $P_{decoder}$ don;t have to correspond to same valid joint distribution. $P_{model}(x, h)$ in fact usually don't.

Back up to graphical models before getting to variational autoencoders (VAEs).
Consider conditional model $P_\theta(y|x)$ that approximates underlying conditional distribution $P^*(y|x)$, a distribution over variable y conditioned on input x.
Want to learn $P_\theta(y|x) \approx p^*(y|x)$
→ Graphical models have an interesting calculus, e.g. Forney style graphs ⇔ block diagrams.
Parameterizing conditional distributions with neural networks
Differentiable feedforward neural networks are a flexible computationally-scalable kind of function approximator (universal approximation theorem).
Learning models with neural networks with many hidden layers is deep learning. Notably NNs can be used to approximate pdfs and pmfs.
→ probability models based on neural networks are computationally scalable since they allow stochastic gradient-based optimizer and scaling to large models, large datasets.
→ think of them as an operator $NN(\cdot)$

e.g. neural net can parameterize categorical distribution $P_\theta(y|x)$ over a class label y, conditioned on image x as $P = NN(x), P_\theta(y|x) = categorical(y; P)$

Consider directed graphical models that have latent variables. $\rightarrow$ latent variables are part of model but not observed directly and not part of dataset denote by Z.
$\rightarrow$ Joint distribution $P_\theta(x, Z)$ considers observed variables and latent variables Z.
A deep latent variable model (DLVM) denotes a latent variable model $P_\theta(x, Z)$ whose distributional properties parameterized by neural networks. Also conditional $P_\theta(x, Z|y)$.
Even when each factor (prior or conditional distribution) is relatively simple, marginal $P_\theta(x)$ can be very complex.
A main difficulty of maximum likelihood learning in DLVMs is that marginal probability of data under model is typically intractable since $P_\theta(x) = \int P_\theta(x, Z)dZ$ may not have analytical solution or efficient estimator.
Due to intractability, we cannot differentiate w.r.t its parameters and optimize, as we can with fully observed models (Main difficulty is posterior $P_\theta(Z|x)$). There are approximate inference techniques but ofter computationally intense.
The framework of VAE provides a computationally efficient way of optimizing DLVMs jointly with corresponding inference model using stochastic gradient descent (SGD).
To turn DLVM's intractable learning problem into tractable problem, introduce a parametric inference model $q_\phi(Z|x)$ which is an encoder (recognition model). ϕ are parameters of inference model, called variational parameters.
Optimize variance parameters ϕ such that $q_\phi = p_\theta(Z|x)$

2.5 VAE

Encoder has a directed graphical model, can be factorized:
$q_\phi = q_\phi(Z_1, ..., Z_n|x) = \prod_{i=1}^{M} q_\phi(Z_i|P_a(Z_i), x)$ where $P_a(Z_i)$ is set of parent of Z_i in directed graph.
Once we have factorization $q_\phi(Z|x)$ can be parameterized using NN where ϕ is weights, bias of NN.

The optimization objective of VAE is evidence lower bound (ELBO). For any choice of $q_\phi(Z|x)$ including choice of ϕ

$$
\begin{aligned}
logp_\theta(x) &= \mathbb{E}_{q_\phi(Z|x)}[logp_\theta(x)] \\
&= \mathbb{E}_{q_\phi(Z|x)}[log\frac{p_\theta(x, Z)}{p_\theta(Z|x)}] \\
&= \mathbb{E}_{q_\phi(Z|x)}[log\frac{p_\theta(x, Z)q_\phi(Z|x)}{p_\theta(Z|x)q_\phi(Z|x)}] \\
&= \mathbb{E}_{q_\phi(Z|x)}[log\frac{p_\theta(x, Z)}{q_\phi(Z|x)}] + \mathbb{E}_{q_\phi(Z|x)}[log\frac{q_\phi(Z|x)}{p_\theta(Z|x)}] \\
&= \mathcal{L}_{\theta,\phi}(x) + D_{KL}(q_\phi(Z|x)||p_\theta(Z|x)) \\
&\Rightarrow [ELBO]
\end{aligned}
\tag{1}
$$

where D_{KL} is non-negative, so $\mathcal{L}_{\theta,\phi} = \mathbb{E}_{q_\phi(Z|x)}[logp_\theta(x, Z) - log(q_\phi(Z|x))]$
$= logp_\theta(x) - D_{KL}(q_\phi(Z|x)||p_\theta(Z|x))$
So $\mathcal{L}_{\theta,\phi} \leq logp_\theta(x) \Rightarrow$ lower bound of log-likelihood.
KL divergence two solutions:

- divergence of approximate posterior from true posterior (???).
- gap between ELBO and $logp_\theta(x)$

Better approximation → higher bound.

Maximizing ELBO will optimize:
1. approximately maximize $p_\theta(x)$, so generative model is better
2. minimize KL divergence of approximation $q_\phi(Z|x)$ from $p_\theta(Z|x)$ so $q_\phi(Z|x)$ become better.
Jointly optimize ϕ and θ using SGD
Reparameterization trick
For continuous latent variables and a differentiable en/decoder, ELBO can be differentiated w.r.t both ϕ and θ if we reparameterize.
First, express rv $Z \sim q_\phi(Z|x)$ as differentiable/invertible transformation of another rv ε.
Given ϕ, x, $Z = g(Z, \phi, x)$, ε independent of x and ϕ.
$\mathbb{E}_{q_\phi(Z|x)}[f(Z)] = \nabla_\phi \mathbb{E}_{p(\varepsilon)}[f(Z)]$
And since expectation and gradient commute by linearity:
$\nabla_\phi \mathbb{E}_{q_\phi(Z|x)}[f(Z)] = \nabla \mathbb{E}_{p(\varepsilon)}[f(Z)] = \mathbb{E}_{p(\varepsilon)}[\nabla_\phi f(Z)] \approx \nabla_\phi f(Z)$
where we can estimate by Monte Carlo:
$\mathcal{L}_{\phi,\theta}(x) = \mathbb{E}_{q_\phi(Z|x)}[logp_\theta(x, Z) - logq_\phi(Z|x)] = \mathbb{E}_{p(\varepsilon)}[logp_\theta(x, Z) - logq_\phi(Z|x)]$, where $Z = g(\varepsilon, \phi, x)$.
So we can get single Monte Carlo estimate $\hat{\mathcal{L}}_\theta p(x)$ of individual ELBO.

VAE problems: Approximate inference distribution is often different from true posterior (from ELBO object).
Can modify ELBO objective itself to balance correct inference and fitting training data?
Assign some weight to balance the two parts? Introduce a mutual information term? $I_{q(x,Z)}$:

$\mathcal{L}_{InfoVAE} = -\lambda DL(q_\phi(Z)||p_\theta(Z)) - \mathbb{E}_{q(Z)}[D_{KL}(q_\phi(x|Z))||p_\theta(x|Z)] + \alpha I(x, Z)$
$= \mathbb{E}_{q_\phi(x,Z)}[logp_\theta(x|Z) - log\frac{q_\phi(Z)^{\lambda+\alpha-1}p_\theta(x)}{p(Z)^\lambda q_\phi(Z|x)^{\alpha-1}}]$
$= \mathbb{E}_{p_\theta(x)}\mathbb{E}_{q_\phi(Z|x)}[logp_\theta(x|Z)] - (1-\alpha)\mathbb{E}_{p_\theta} D_{KL}(q_\phi(Z|x)||p(Z)) - (\alpha+\lambda-1)D_{KL}(q_\phi(Z)||p(Z)) - \mathbb{E}_{p_\theta}(logp_\theta(x))$
Variational Autoencoders Map input to a distribution rather vector.
P_θ with parameters θ, relationship between the input x and latent encoding Z.
Prior $p_\theta(Z)$, likelihood $p_\theta(x|Z)$, posterior $p_\theta(Z|x)$.
If we know actual θ^* to generate:
1. a sample $Z^{(c)} \sim p_{\theta^*}(Z)$
2. generate value $x^{(c)}$, $p_{\theta^*}(x|Z = Z^{(i)})$, $\theta^* = \underset{\theta}{argmax} \prod_{i=1}^n p_\theta(x^{(i)})$

For computation, we approximate p_θ by $q_\phi(Z|x)$. Conditional probability $p_\theta(x|Z)$ is generative model. Approximate function $q_\phi(Z|x)$ is probalistic encoder. $q_\phi(Z|x)$ should be close to $p_\theta(Z|x)$, so minimize $D_{KL}(q_\phi(Z|x)||p_\theta(Z|x))$

Use more of latent code to encourage less blurring. Disentangle latent representation:
①. Allow some Lagrangian weight between 2 ELBO terms.
②. introduce a mutual information term.
Vector quantized VAE(VQ-VAE) Constrain latent space to discrete.
Introduction to quantization:
Consider iid sequence of analog rv $v_1, v_2 \sim P_U(u)$ quantizer maps this sequence into a sequence of discrete rv $v_1, v_2, ...$ If restrict to alphabet of size M, then v_M can't represent V_M perfectly on general, larger M implies less distortion.
$V_m \longrightarrow \boxed{\text{encoder}} \overset{I \leftarrow \{1,...,M\}}{\longrightarrow} \boxed{\text{decoder}} \longrightarrow V_m$
Mean-squared distortion is $\mathbb{E}[(u - v)^2]$

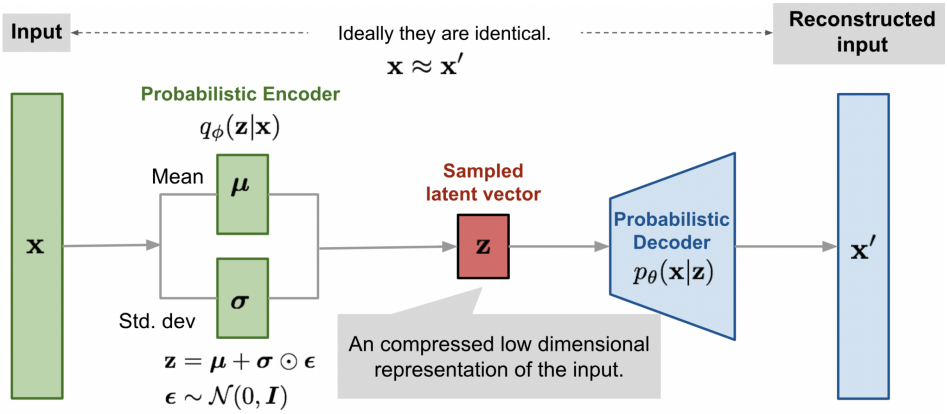
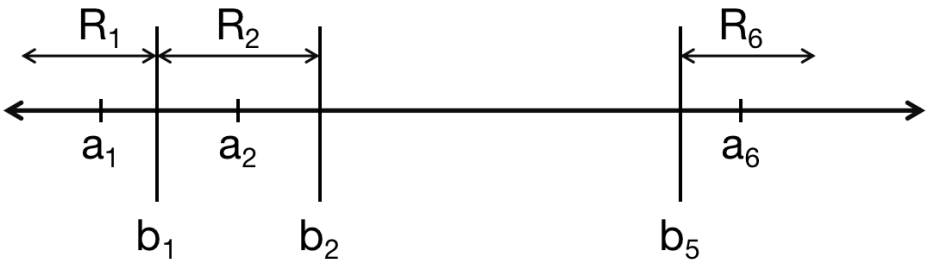


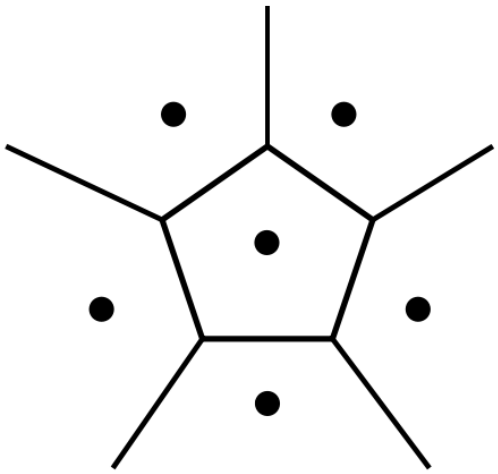
Illustration of variational autoencoder model with the multivariate Gaussian assumption.



- Given representation points $\{a_j\}$, how should intervals $\{R_j\}$ chosen?
  Nearest neighbor condition, $b_j = \dfrac{a_j + a_{j+1}}{2}$
- Given intervals $\{R_j\}$, how should representation points $\{a_j\}$ be chosen?
  $a_j = \mathbb{E}[V|V \in R_j]$

Lloyd-Max algorithm:
Given M, $f_u(U)$;
①. Choose arbitrary initial set of M representation points, $a_1 > a_2 < ... < a_M$
②. for each j, $b_j = \dfrac{a_j + a_{j+1}}{2}$
③. for each j, set $a_j = \mathbb{E}[V|V \in [b_{j-1}, b_j]]$
④. Repeat ①,② until MSE doesn't change.

Vector quantization Quantize n rv together. Region R_j must be set of points that are closest to (a_j, a_j), then to any other representation points.
Varanoi regions:
Convex polygonal regions; boundaries are perpendicular; bisectors between neighboring parts.
VQ advantages:
1. space filling; 2. shape; 3. memory
VQ-VAE encoder which parameterize approximate posterior $q(Z|x)$ decode $p(x|Z)$ prior $p(Z)$.
Define latent embedding space as subset of R^D with k representation points, $e_i \in \mathbb{R}^D, i = 1, ..., k$.
The encoder output $Z(x) = Z_e$ goes through nearest neighbor. Look up to match one of the k embedding vectors and then this input to decoder $D(.)$.
$Z_q(x) = quantize(E(x)) \cdot e_k$, where $k = argmin\|E(x) - e_i\|_2$. For training, since argmin not differentiable in discrete case, gradient of loss function $\nabla_Z L$ from discrete input Z_q copy to encoder output.
Consider 3 terms in loss:
1. Reconstruction loss, which optimizes encoder/decoder
2. Due to copying from Z_e to Z_q, need something to form VQ
3. Ensure encoder commits to a representation



Let $sg(.)$ be stop gradient, defined as identity of forward computation and has D partial derivatives:
$L = \underset{reconstruction\ loss}{\|x - D(e_k)\|_2^2} + \underset{VQ\ loss}{\|sg[E(x) - e_k]\|_2^2} + \beta \underset{constraint\ loss}{\|E(x) - sg(e_k)\|_2^2}$
Let piece is learn a prior in latent space $P(Z)$, so we can sample from it to do generalization via decoders.

3 Lecture 7-9: generative adversarial networks (GANs)

One weakness of VAE is the variational bounds has a gap such that the model will not be consistent.
GAN approach differently circumvents needs for variational bound $\Rightarrow$ NN models within GAN are universal approximators, and this enables a proof of asymptotic consistency in getting true objective distributions.
Training requires finding Nash equilibrium of a game, which is in general more difficult than optimizing an objective function.
Generator creates sampler that are intended to come from same distribution as training data
Discriminator examines samples to determine whether real or fake (supervised learning for binary classification).
In graphical model form of GAN, there will be observed variable X and latent variable Z. The players in game are represented by 2 functions, that one differentiable w.r.t their inputs and their parameters.
Discriminator is function D that takes x as input has parameters $\Theta^{(D)}$; generator is function that takes Z as input with parameters $\Theta^{(G)}$. Both players have cost functions that are defined in terms of both player's parameters.
Discriminator wants to minimize $J^{(D)}(\Theta^{(D)}, \Theta^{(G)})$, only controls $\Theta^{(D)}$. Generator wants to minimize $J^{(G)}(\Theta^{(D)}, \Theta^{(G)})$, only controls $\Theta^{(G)}$. Each player's cost depends on other player parameters $\Rightarrow$ Game, rather than optimization.

3.1 Nash Equilibrium

a tuple $(\Theta^{(D)}, \Theta^{(G)})$ is local minimum of $J^{(D)}$ w.r.t. $\Theta^{(D)}$ and is local minimum $J^{(G)}$ w.r.t $\Theta^{(G)}$.
Normal form games: An N-player normal form game consists of:
1. finite set of N players
2. strategy spaces for players, $S_1, S_2, ..., S_N$
3. payoff function for players, $U_1 : S_1 \times S_2 \times ... \times S_N \to \mathbb{R}$

A natural representation of a two-player game is using a bi-matrix colum strategy.

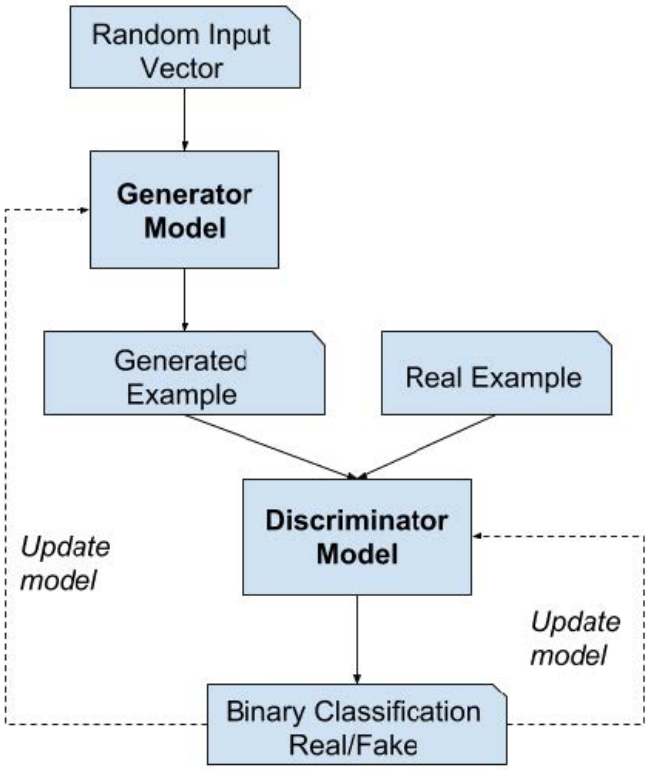


Figure 3: GAN architecture

	column strategy
row strategy	$\begin{bmatrix} (u_1(r_1,c_1),u_2(r_1,c_1)) & (u_1(r_1,c_2),u_2(r_1,c_2)) & \dots \\ (u_1(r_2,c_1),u_2(r_2,c_1)) & \dots & \dots \\ \dots & \dots & (u_1(r_m,c_n),u_2(r_m,c_n)) \end{bmatrix}$

where $s_1 = \{r_i, i = 1, 2, ..m\}$, $s_2 = \{c_j, j = 1, ..., n\}$
Proofs of existence of Nash equilibrium come from fixed point theorems like Bronwer, Kakutari, etc.
Training process consists of simultaneous SGD $\Rightarrow$ in each time step, two datasets sampled:
①. subset of x, training data
②. set of z values drawn from current models prior over latent variables.
Two simultaneous gradient steps:
One updates $\Theta^{(D)}$ to reduce $J^{(D)}$
One updates $\Theta^{(G)}$ to reduce $J^{(G)}$
Cost function for discriminator for binary classification.
$J^{(D)}(\Theta^{(D)}, \Theta^{(G)}) = -\frac{1}{2}\mathbb{E}_{x\sim P_{data}(x)} log D(x) - \frac{1}{2}\mathbb{E}_Z log(1 - D(G(Z)))$
Cross entropy cost to minimize to train standard binary classification. with a sigmoid output.
By training discriminator, we can also estimate $\frac{P_{data}(x)}{P_{model}(x)}$. Estimating this ratio allows computing various divergences. Rather than lower bounds like ELBO, GAN approximation based on using supervised learning to estimate ratio of two densities.

What's cost function for generator?
Simplest approach is to require game to be zero sum, so sum of costs of all players is 0. $J^{(G)} = -J^{(D)}$.
So entire game can be summarized by value function specifying the discriminator's payoff:
$V(\Theta^{(D)}, \Theta^{(G)}) = -J^{(D)}(\Theta^{(D)}, \Theta^{(G)})$
Since zero sum games yield minmax characterization:
$\Theta^{(G)^*} = \underset{\Theta^{(G)}}{argmin}\ \underset{\Theta^{(D)}}{max} V(\Theta^{(D)}, \Theta^{(G)})$, where $\Theta^{(G)^*}$ corresponding to minimizing Jenson-Shanon (JS) divergence between data and model distribution.

An alternative heuristic that seems to work better in practice ⇒ still use cross entropy minimization for generator, but instead of flipping sign on discriminator, we flip the target used to construct cross entropy.

$J^{(G)} = -\frac{1}{2}\mathbb{E}_Z log D(G(Z))$.

So generator maximizing the log-probability of discriminator being mistaken rather than minimizing log probability of discriminator being correct.

Maximum likelihood

MLE is minimizing KL divergence.

$\Theta^* = \underset{\theta}{argmin} D_{KL}(P_{data}(x)||P_{model}(x,\theta))$

If discriminator optimal, then we can minimize to obtain MLE when

$J^{(G)} = -\frac{1}{2}\mathbb{E}_Z\ exp(\sigma^{-1}(D(G(Z))))$, where σ is logistic sigmoid.

minmax ⇔ JS & MLE ⇔ KL

Goals of discriminator is to minimize:

$J^{(D)}(\Theta^{(D)}, \Theta^{(G)}) = -\frac{1}{2}\mathbb{E}_{x\sim P_{data}(x)} log D(x) - -\frac{1}{2}\mathbb{E}_Z log(1 - D(x))$ w.r.t $\Theta^{(D)}$

Value for $D(x)$ is specified for each value x to minimize $J^{(D)}$ w.r.t D. Write functional derivatives for a given x, set it zero: $\frac{\partial\ J^{(D)}}{\partial\ D(x)} = 0$. Solving will yield $D^*(x) = \frac{P_{data}(x)}{P_{data}(x) + P_{model}(x)}$

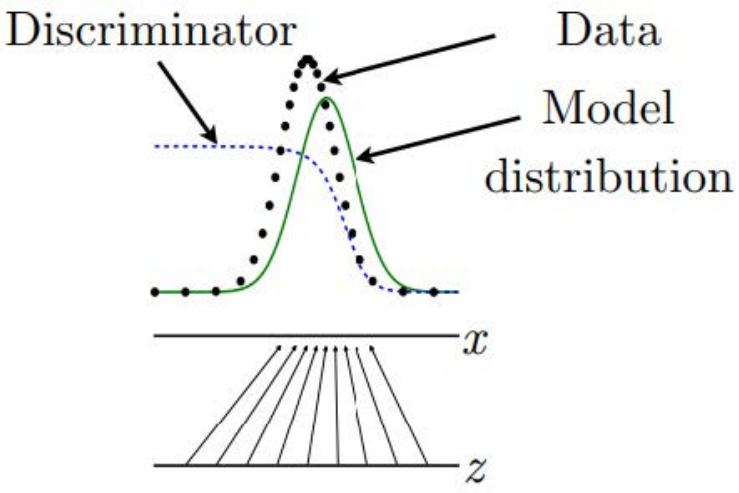


Figure 35: An illustration of how the discriminator estimates a ratio of densities. In this example, we assume that both z and x are one dimensional for simplicity. The mapping from z to x (shown by the black arrows) is non-uniform so that $p_{\text{model}}(x)$ (shown by the green curve) is greater in places where z values are brought together more densely. The discriminator (dashed blue line) estimates the ratio between the data density (black dots) and the sum of the data and model densities. Wherever the output of the discriminator is large, the model density is too low, and wherever the output of the discriminator is small, the model density is too high. The generator can learn to produce a better model density by following the discriminator uphill; each $G(z)$ value should move slightly in the direction that increases $D(G(z))$. Figure reproduced from Goodfellow *et al.* (2014b).

MLE:

$\frac{\partial\ J^{(G)}}{\partial\ G} = \mathbb{E}_{x\sim p_g} f(x) \frac{\partial\ log(P_g(x))}{\partial\ G}$, where we assumes:

1. $P_g(x) \geq 0$ everywhere, so $P_{g(x)} = exp(log(P_g(x)))$
2. function derivative is continuous, so we can interchange derivative integral (Leibniz rule)

So we see derivatives of $J^{(G)}$ are close to what we want, just expectation is w.r.t samples from ¶$_g$ rather that P_{data}, so pick $f(x) = \dfrac{P_{data}(x)}{P_g(x)}$ by importance sampling trick.

GAN is zero sum mimax game with ① discriminator ② generator. Most people think GAN successful if:

1. generator reliably generates data that fools discriminator
2. creates sample that are as diverse as distribution of real world

2.1. Desiderata

Before delving into the explanation of evaluation measures, first I list a number of desired properties that an efficient GAN evaluation measure should fulfill. These properties can serve as meta measures to evaluate and compare the GAN evaluation measures. Here, I emphasize on the qualitative aspects of these measures. As will be discussed in Section 3, some recent works have attempted to compare the meta measures quantitatively (*e.g.* computational complexity of a measure). An efficient GAN evaluation measure should:

1. favor models that generate high fidelity samples (*i.e.* ability to distinguish generated samples from real ones; discriminability),
2. favor models that generate diverse samples (and thus is sensitive to over-fitting, mode collapse and mode drop, and can undermine trivial models such as the memory GAN),
3. favor models with disentangled latent spaces as well as space continuity (*a.k.a* controllable sampling),
4. have well-defined bounds (lower, upper, and chance),
5. be sensitive to image distortions and transformations. GANs are often applied to image datasets where certain transformations to the input do not change semantic meanings. Thus, an ideal measure should be invariant to such transformations. For instance, score of a generator trained on CelebA face dataset should not change much if its generated faces are shifted by a few pixels or rotated by a small angle.
6. agree with human perceptual judgments and human rankings of models, and
7. have low sample and computational complexity.

In what follows, GAN measures will be discussed and assessed with respect to the above desiderata, and a summary will be presented eventually in Section 3. See Table 2.

	Measure	Description
Quantitative	1. Average Log-likelihood [18, 22]	• Log likelihood of explaining realworld held out/test data using a density estimated from the generated data (*e.g.* using KDE or Parzen window estimation). $L = \frac{1}{N}\sum_i \log P_{model}(\mathbf{x}_i)$
	2. Coverage Metric [33]	• The probability mass of the true data "covered" by the model distribution $C := P_{data}(dP_{model} > t)$ with t such that $P_{model}(dP_{model} > t) = 0.95$
	3. Inception Score (IS) [3]	• KLD between conditional and marginal label distributions over generated data. $\exp\left(\mathbb{E}_{\mathbf{x}}\left[\mathbb{KL}\left(p\left(\mathrm{y} \mid \mathbf{x}\right) \parallel p\left(\mathrm{y}\right)\right)\right]\right)$
	4. Modified Inception Score (m-IS) [34]	• Encourages diversity within images sampled from a particular category. $\exp(\mathbb{E}_{\mathbf{x}_i}[\mathbb{E}_{\mathbf{x}_j}[(\mathbb{KL}(P(y\|\mathbf{x}_i)\|P(y\|\mathbf{x}_j))]])$
	5. Mode Score (MS) [35]	• Similar to IS but also takes into account the prior distribution of the labels over real data. $\exp\left(\mathbb{E}_{\mathbf{x}}\left[\mathbb{KL}\left(p\left(y \mid \mathbf{x}\right) \parallel p\left(y^{train}\right)\right)\right] - \mathbb{KL}\left(p\left(y\right) \parallel p\left(y^{train}\right)\right)\right)$
	6. AM Score [36]	• Takes into account the KLD between distributions of training labels vs. predicted labels, as well as the entropy of predictions. $\mathbb{KL}(p(y^{\text{train}}) \parallel p(y)) + \mathbb{E}_{\mathbf{x}}\left[H(y\|\mathbf{x})\right]$
	7. Fréchet Inception Distance (FID) [37]	• Wasserstein-2 distance between multi-variate Gaussians fitted to data embedded into a feature space $FID(r, g) = \|\mu_r - \mu_g\|_2^2 + Tr(\Sigma_r + \Sigma_g - 2(\Sigma_r\Sigma_g)^{\frac{1}{2}})$
	8. Maximum Mean Discrepancy (MMD) [38]	• Measures the dissimilarity between two probability distributions P_r and P_g using samples drawn independently from each distribution. $M_k(P_r, P_g) = \mathbb{E}_{\mathbf{x},\mathbf{x}'\sim P_r}[k(\mathbf{x},\mathbf{x}')] - 2\mathbb{E}_{\mathbf{x}\sim P_r,\mathbf{y}\sim P_g}[k(\mathbf{x},\mathbf{y})] + \mathbb{E}_{\mathbf{y},\mathbf{y}'\sim P_g}[k(\mathbf{y},\mathbf{y}')]$
	9. The Wasserstein Critic [39]	• The critic (*e.g.* an NN) is trained to produce high values at real samples and low values at generated samples $W(\mathbf{x}_{test}, \mathbf{x}_g) = \frac{1}{N}\sum_{i=1}^{N} f(\mathbf{x}_{test}[i]) - \frac{1}{N}\sum_{i=1}^{N} f(\mathbf{x}_g[i])$
	10. Birthday Paradox Test [27]	• Measures the support size of a discrete (continuous) distribution by counting the duplicates (near duplicates)
	11. Classifier Two Sample Test (C2ST) [40]	• Answers whether two samples are drawn from the same distribution (*e.g.* by training a binary classifier)
	12. Classification Performance [1, 15]	• An indirect technique for evaluating the quality of unsupervised representations (*e.g.* feature extraction; FCN score). See also the GAN Quality Index (GQI) [41].
	13. Boundary Distortion [42]	• Measures diversity of generated samples and covariate shift using classification methods.
	14. Number of Statistically-Different Bins (NDB) [43]	• Given two sets of samples from the same distribution, the number of samples that fall into a given bin should be the same up to sampling noise
	15. Image Retrieval Performance [44]	• Measures the distributions of distances to the nearest neighbors of some query images (*i.e.* diversity)
	16. Generative Adversarial Metric (GAM) [31]	• Compares two GANs by having them engaged in a battle against each other by swapping discriminators or generators. $p(\mathbf{x}\|y=1; M_1)/p(\mathbf{x}\|y=1; M_2) = (p(y=1\|\mathbf{x}; D_1)p(\mathbf{x}; G_2))/(p(y=1\|\mathbf{x}; D_2)p(\mathbf{x}; G_1))$
	17. Tournament Win Rate and Skill Rating [45]	• Implements a tournament in which a player is either a discriminator that attempts to distinguish between real and fake data or a generator that attempts to fool the discriminators into accepting fake data as real.
	18. Normalized Relative Discriminative Score (NRDS) [32]	• Compares n GANs based on the idea that if the generated samples are closer to real ones, more epochs would be needed to distinguish them from real samples.
	19. Adversarial Accuracy and Divergence [46]	• Adversarial Accuracy. Computes the classification accuracies achieved by the two classifiers, one trained on real data and another on generated data, on a labeled validation set to approximate $P_g(y\|\mathbf{x})$ and $P_r(y\|\mathbf{x})$. Adversarial Divergence: Computes $\mathbb{KL}(P_g(y\|\mathbf{x}), P_r(y\|\mathbf{x}))$
	20. Geometry Score [47]	• Compares geometrical properties of the underlying data manifold between real and generated data.
	21. Reconstruction Error [48]	• Measures the reconstruction error (*e.g.* L_2 norm) between a test image and its closest generated image by optimizing for z (*i.e.* $min_{\mathbf{z}}\|G(\mathbf{z}) - \mathbf{x}^{(test)}\|^2$)
	22. Image Quality Measures [49, 50, 51]	• Evaluates the quality of generated images using measures such as SSIM, PSNR, and sharpness difference
	23. Low-level Image Statistics [52, 53]	• Evaluates how similar low-level statistics of generated images are to those of natural scenes in terms of mean power spectrum, distribution of random filter responses, contrast distribution, etc.
	24. Precision, Recall and F-score [23]	• These measures are used to quantify the degree of overfitting in GANs often over toy datasets

Model collapse

Fail to achieve ② by achieving ① through a concentrated distribution. Model collapse may arise because maxmin solution of GAN game is different from minmax solution.
When we find model $G^* = \min_G \max_D V(G, D)$, G^* will draw sample from the full distribution when we exchange order to have maxmin $G^* = \max_D \min_G V(G, D)$. Min of G is inner loop of optimization. The generator asked to map every Z value to the single output x that the discriminator believes is most to be real rather than fake.
Simultaneous gradient descent doesn't clearly privilege minmax over maxmin.
Unrolling: updating generator's loss function to backpropagate through k steps of gradient updates for discriminator. Let generator see k steps into future to encourage more diverse samples.
Parking: modify discriminator to make decisions on several samples of same class, either real or fake. Seeing multiple identical cases is give a way (???) for fake.

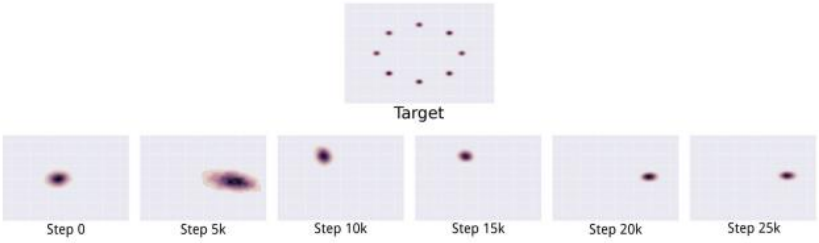


Figure 22: An illustration of the mode collapse problem on a two-dimensional toy dataset. In the top row, we see the target distribution p_{data} that the model should learn. It is a mixture of Gaussians in a two-dimensional space. In the lower row, we see a series of different distributions learned over time as the GAN is trained. Rather than converging to a distribution containing all of the modes in the training set, the generator only ever produces a single mode at a time, cycling between different modes as the discriminator learns to reject each one. Images from Metz *et al.* (2016).

3.2 Wasserstein Loss

Formulate loss functions to more directly represent minimizing distance between two probability distributions.
⇒ Make a winning turn in the game correlate with actually reducing distance between P_g and P_{data} rather than just fooling discriminator.
Recall JS divergence, $JS(P||Q) = \frac{1}{2}D_{KL}(P||M) + \frac{1}{2}D_{KL}(M||Q)$, where $M = (P+Q)/2$ was implicit objective in original GAN.
Now consider Wasserstein distance instead (optimal transportation theory):
$W(P, Q) = \inf_{\delta \in \Pi(P,Q)} \mathbb{E}_{(x,y)\sim\delta}[\|x - y\|]$, where $\Pi(P, Q)$ is a set of all joint distribution with marginal P, Q, $\delta(x, y)$ is amount of mass that must be moved from x to y to convert P to Q.
Wasserstein distance is the cost of optimal transport map
⇒ continuous almost differentiable everywhere
⇒ JSD locally saturates as discriminator gets better, so gradients become zero and vanish.

Hard to handel inf, we can use Kantorovich-Rubirstein duality.
$W(P, Q) = \sup_{\|f\|_L \leq 1} \mathbb{E}_{x\sim P}[f(x)] - \mathbb{E}_{x\sim Q}[f(x)]$, where sup is over all 1-Lipshitz continuous functions.
K-Lipshitz continuity: given metric spaces $(x, dx), (y, dy)$, map $f : x \to y$ is k-Lipshitz if $dy(f(x_1), f(x_2)) \leq kdx(x_1, x_2)$ for all $(x_1, x_2) \in X$

Proof of K-R duality
Introduce Lagrangian multipliers $f, g : \lambda \to R$ (bounded measurable):

$$\mathcal{L}(\delta, f, g) = \int_{X\to x} \|x-y\|^2 \delta(x,y)dydx - \int_X (P(x) - \int \delta(x,y)dy)f(x)dx - \int_x (q(y) - \int (x,y)dx)g(y)dy$$
$$\mathcal{L}(\delta, f, g) = \mathbb{E}_{x\sim P}[f(x)] + \mathbb{E}_{y\sim q}[g(y)] + \int_{X\to x} (\|x-y\|_2 - f(x) - g(y))\delta(x,y)dydx$$
$$W(P, P_g) = \inf_{\delta} \sup_{f,g} L(\delta, f, g) = \sup_{f,g} \inf_{\delta} L(\delta, f, g) \tag{2}$$

Note if $\|x-y\|_2 < f(x) + g(y)$ for some $x, y \in X$, then we can concentrate mass of δ at (x, y) and sent $\mathcal{L}(\delta, f, g) \to -\infty$, so for all x, y, we must have $f(x) + g(y) \le \|x-y\|_2$
Best we can do is minimize δ over $\delta = 0$
$\sup_{f,g} \inf_{\delta} \mathcal{L}(\delta, f, g) = \sup_{f,g, f(x)+g(y)\le\|x-y\|_2} [\mathbb{E}_{x\sim p}[f(x)] + \mathbb{E}_{y\sim q}[g(y)]] = W(p, q)$
Observe that optimizing over class of 1-Lipshitz function is lower bound on Wasserstein.
If h is 1-Lipshitz,
$\mathbb{E}_{x\sim p}[h(x)] - \mathbb{E}_{y\sim q}[h(y)] = \int_{X\sim x}(h(x) - h(y))\delta(x,y)dxdy$
$\le \int_{X\sim x} \|x-y\|_2 \delta(x,y)dxdy$
$\le W(p, q)$
$\Rightarrow \sup_{\|h\|_L \le 1} [\mathbb{E}_{x\sim p}[h(x) - \mathbb{E}_{y\sim q}[h(y)]]] \le W(p, q)$. Wants to show this holds with equality.
Consider a function $\mathcal{K}$ defined as:
$\mathcal{K} : x \to \inf_u [\|x-u\|_2 - g(u)]$, since g is bounded, inf is finite, and $\mathcal{K}$ is well-defined.
Claim: $\mathcal{K}$ is 1-Lipshitz
Proof: given $x, y \in X$. For any $u \in X$, by triangular inequality:
$\mathcal{K}(x) \le \|x-u\|_2 - g(y) \le \|x-y\|_2 + \|y-u\|_2 - g(u)$
This holds for any u, $\mathcal{K}(x) \le \|x-y\|_2 + \inf_u [\|x-u\|_2 - g(u)] = \|x-y\|_2 + \mathcal{K}(y)$
$\mathcal{K}(x) - \mathcal{K}(y) \le \|x-y\|_2$, exchange x,y
$|\|\mathcal{K}(x) - \mathcal{K}(y)\|_2| \le \|x-y\|_2$. It's 1-Lipshitz.
For any f, g that satisfy $f(x) + g(y) \le \|x-y\|_2$,
$f(x) \le \mathcal{K}(x) \le \|x-x\|_2 - g(x) = -g(x)$
Plugin in: $\mathbb{E}_{x\sim p} + \mathbb{E}_{y\sim q}[g(y)] \le \mathbb{E}_{x\sim p}[\mathcal{K}(x)] - \mathbb{E}_{y\sim q}[\mathcal{K}(y)]$
We conclude
$W(p, q) = \sup_{f,g, f(x)+g(y)\le\|x-y\|_2} [\mathbb{E}_{x\sim p}[f(x)] + \mathbb{E}_{f\sim q}[g(y)]] \le \sup_{\|w\|_2\le 1} [\mathbb{E}_{x\sim p}[h(x)] - \mathbb{E}_{y\sim q}[h(y)]] \le W(p, q)$
End of proof.

Objective of generator $\Rightarrow$ minimize Wasserstein distance rather than fooling discriminator.

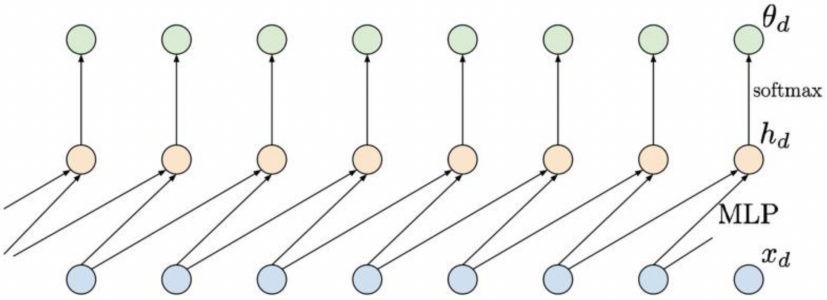
3.3 f-GAN

Have different f-divergences as their objective.
Let P, Q be defined over the same space $P << Q$ (P is absolutely continuous w.r.t Q), then for a convex function $f : f(1) = 0$, f-divergence of P from Q:
$D_f(P||Q) = \int f(\frac{dP}{dQ})dQ.$
When both absolutely continuous w.r.t a common reference measure (Lebesgue measure).
$D_f(P||Q) = \int f(\frac{p(x)}{q(x)})q(x)dx$
1. if $f(t) = t\log t \Rightarrow$ KL divergence.
2. if $f(t) = \frac{1}{2}[(t+1)\log \frac{2}{t+1} + t\log t] \Rightarrow$ JS.
We can put in f-divergence as objective to define f-GAN. Match distribution as design idea, "density approximation".

Reformulation of GANs in robust statistics framework
Picking a generator $g(.)$ for $\mathcal{Y}$, minimize loss $\mathcal{L}(P_{g(Z)}, P_x)$ over all $g \in \mathcal{Y}$
$\mathcal{L}(P_{g(Z)}, P_x)$ to be small. If $\mathcal{L}$ and $\mathcal{Y}$ don't get right kind of small, try something else.
How to have P_x to be a slight perturbation of $g \in \mathcal{Y}$ under $\mathcal{L}$ that make sense?

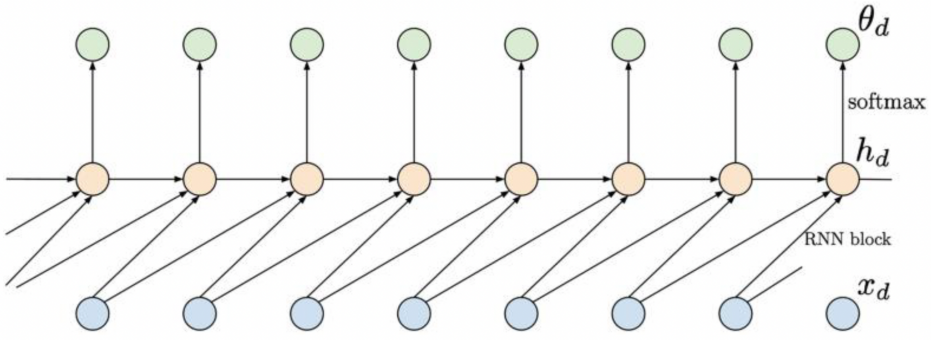
4 Lecture 10-11: Auto regressive model

$P(x, y) = P(x|y)P(y) = P(y|x)P(x)$, $P(x) = \sum_y P(x, y)$
Broadly, we want to model some $P(x)$. We hypothesize some factored form.
First, we generally write $P(x)$ for $x \in X^D$. e.g. $X = \{a, b, ..., z\}$ or $x = \{1, 2, ..., 256\}$.
$P(x) = P(x_0) \prod_{d=2}^{D} P(x_d|x_{<d})$, $x_{<d} = \{x_1, ..., x_{d-1}\}$. e.g. $P(x)$ for $D = 3$, $P(x_1)P(x_2|x_1)P(x_3|x_1, x_2)$.
This is too computation heavy.
To help, we consider auto regressive models:
1. finite memory; 2. approximation; 3. shared parameters (NN)
Finite memory:
$P(x_1)P(x_2|x_1) \prod_{d=3}^{D} P(x_d|x_{d-1}, x_{d-2})$, then also use a small multilayer perceptron to model the parameters. Single shared MLP to prevent the probability for x_d.



An example of applying a shared MLP depending on two last inputs. Inputs are denoted by blue nodes (bottom), intermediate representations are denoted by orange nodes (middle), and output probabilities are denoted by green nodes (top). Notice that a probability θ_d is not dependent on x_d

Long range memory:
Recurrent neural network. Make conditional distribution of form $P(x_d|x_{<d}) = P(x_d|RNN(x_{d-1}, h_{d-1}))$ where $h_d = RNN(x_{d-1}, h_{d-1})$ and h_d is hidden content that act as memory to capture long-range content.



An example of applying an RNN depending on two last inputs. Inputs are denoted by blue nodes (bottom), intermediate representations are denoted by orange nodes (middle), and output probabilities are denoted by green nodes (top). Notice that compared to the approach with a shared MLP, there is an additional dependency between intermediate nodes h_d

issue:
They are sequential, slow in training/inference. Numerical issues in training them.

Conditional neural network: can be used to model long-range dependencies rather than RNN. Advantages:
1. kernels are shared (efficient parameterization)
2. processing in parallel (speedy computation)
3. stacking more layers allows effective kernel size to grow with network depth.

Discrete time random process:
One view of auto-regressive models is that they are predictors connect back to classic work in random process.
$x[n]$ is a sequence of random variables, defined for indices $n = -\infty, ..., 0, 1, 2, ...,$
$\Omega \to x[n]$, $\Gamma(z) = \dfrac{1}{L(z)}$
A discrete-time system is minimum phase if its system $L(z)$ and its inverse $\Gamma(z)$ are analytic in the exterior of unit disk $|z| > 1$.
A real wide-sense stationary digital process is regular if it's power spectrum:
$\{S(z) = \sum_{m=-\infty}^{\infty} R[m]z^{-m}\}$, where $R[m]$ is autocorrelation and this is Z transform.

Can be written as a product: $S(z) = L(z)L(\frac{1}{z})$. Denote by $l(n)$ and $\gamma[n]$, the delta response of $L(z)$ and $\Gamma(z)$.

Whiken process:
We can conclude that a regular process $x[n]$ is linearly equivalent with a whik-noise process $i[n]$:
$i[n] = \sum_{k=0}^{\infty} \gamma[k]x[n-k]$, where $R_{L1} = \delta[m]$
$x[n] = \sum_{k=0}^{\infty} l[k]i[n-k]$, where $\mathbb{E}[x^2[n]] = \sum_{k=0}^{\infty} l^2[k] < \infty$
$x[n] \longrightarrow \boxed{\Gamma(z)} \xrightarrow{i[n]} \boxed{L(z)} \longrightarrow x[n]$
The process $i[n]$ is the innovation sequence of $x[n]$, and $L(z)$ is its innovations filter. The whikening filter of $x[n]$ is $\Gamma(z) = \dfrac{1}{L(z)}$. H can be shown that the power spectrum $S(z)$ of a process $x[n]$ can be factored as $S(z) = L(z)L(\frac{1}{z})$ if it satisfies Paley-Wipper condition (P-W condition).

P-W condition:
$\int_{-\pi}^{\pi} |logS(w)dw| < \infty$. If power spectrum $S(w)$ is integrable function, the P-W condition reduces to
$\dfrac{1}{2\pi}\int_{-\pi}^{\pi} lnS(w)dw > -\infty$

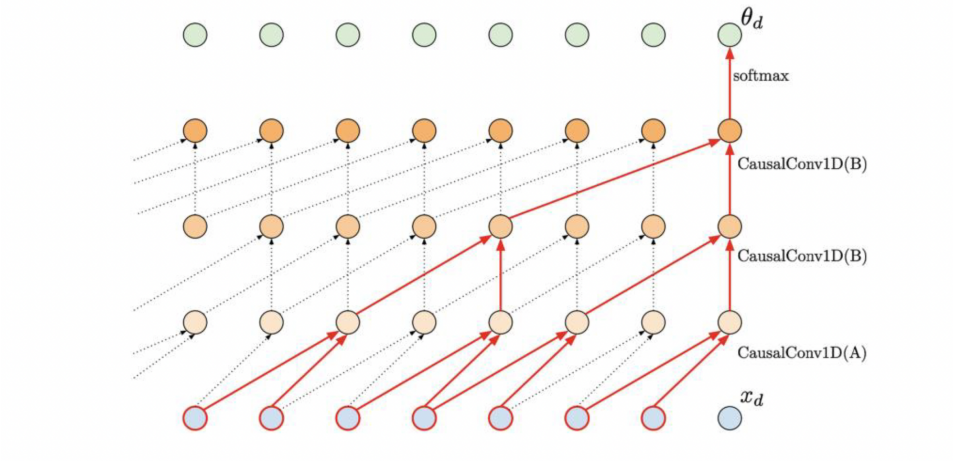
Auto-regressive
The process $x[n]$ is called autoregressive (AR) if $\mathcal{L}(z) = \dfrac{b_0}{1 + a_1 z^{-1} + ... + a_n z^{-n}}$ and so process $x[n]$ satisfies recursion
$x[n] + a_1 x[n-1] + ... + a_N x[n-N] = b_0 i[n]$ where $i[n]$ is whik-noise process.
The past $x[n-N]$ of $x[n]$ only depends on the past of $i[n]$ where $\mathbb{E}[i^2[n]] = 1$
Estimation/prediction of AR processes:
Suppose $s[n]$ is an AR process of order M with autocorrelation $R[m]$. $\bar{S}[m]$ is some other general process with autocorrelation $\bar{R}[m]$, s.t. $\bar{R}[m] = R[m]$ for $|m| < M$. The predictor (MSE optimizing)

for these two process of order M util be identical, because they depend only on $R[m]$ for $|m| < M$. Consider a class C_M of processes with identical autocorrelation for $|m| < M$, each $R[m]$ is an extrapolation of given data, and it can be shown the extrapolating sequence, obtained using maximum entropy, method is autocorrelation of an AR process of order M.
So maximum entropy extrapolation is autocorrelation of $S[n] \leftarrow C_m$ where optimized predictor maximize the minimum MSE.
Max entropy $\Leftrightarrow$ MMSE prediction

Deep generative AR models
Think of x the thing we are modeling as categorical
$x = \{1, ..., 256\}^{256 \times 256}$
We model $P(x)$ using the casual convolution-type architecture with many layers. Each conditional as follows:
$P(x_d|x_{<d}) = categorical(x_d|\theta_d(x_{<d})) = \prod_{l=1}^{L}(\theta_{d,l})^{x_d=l}$, where $[a = b]$ is Iverson bracket notation:

$$\begin{cases} [a = b] = 1 & if\ a = b \\ [a = b] = 0 & if\ a \neq b \end{cases}$$

and $\theta_d(x < d)$ is the output of the casual convolution layer with softmax in last layer, so $\sum_{l=1}^{L}\theta_{d,l} = 1$



An example of applying causal convolutions. The kernel size is 2, but by applying dilation in higher layers, a much larger input could be processed (red edges), thus, a larger memory is utilized. Notice that the first layers must be option A to ensure proper processing

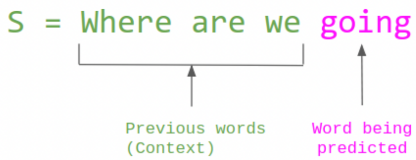
What should be training objective?
we can maximize log-likelihood $ln\ P(D)$ where D is iid dataset of $\{x_1, ..., x_N\}$. So

$$
\begin{aligned}
max\ lnP(D) &= ln \prod_n P(x_n) \\
&= \sum_n P(x_n) \\
&= \sum_n ln \prod_d P(x_{n,d}|x_{n,<d}) \\
&= \sum_n \sum_d^l nP(x_{n,d}|x_{n,<d}) \\
&= \sum_n (\sum_d ln\ Categorical(x_d|\theta_d(x_{<d}))) \\
&= \sum_n \sum_d (\sum_{l=1}^L [x_d = l] ln \theta_d(x_{<d}))
\end{aligned}
$$

5 Lecture 12-13: Transformers

Language model:

$$
\begin{aligned}
P_{(w_1,w_2,\ldots,w_n)} &= p(w_1)p(w_2|w_1)p(w_3|w_1,w_2)...p(w_n|w_1,w_2,..,w_{n-1}) \\
&= \prod_{i=1}^n p(w_i|w_1,...,w_{i-1})
\end{aligned}
$$



P(S) = P(Where) x P(are | Where) x P(we | Where are) x P(going | Where are we)

5.1 Attention mechanism

Deconstructing BERT: Distilling 6 Patterns from 100 Million Parameters
Attention in seq-to-seq models: Visualizing A Neural Machine Translation Model (Mechanics of Seq2seq Models With Attention)
Attention in transformers: The Illustrated Transformer
Transformer as universal computation engine: Pretrained Transformer as Universal Computation Engines
Transformer blocks:

2 Transformer networks

A Transformer block is a sequence-to-sequence function mapping $\mathbb{R}^{d\times n}$ to $\mathbb{R}^{d\times n}$. It consists of two layers: a self-attention layer and a token-wise feed-forward layer, with both layers having a skip connection. More concretely, for an input $\boldsymbol{X} \in \mathbb{R}^{d\times n}$ consisting of d-dimensional embeddings of n tokens, a Transformer block with *multiplicative* or *dot-product* attention [Luong et al., 2015] consists of the following two layers[1]:

$$\mathrm{Attn}(\boldsymbol{X}) = \boldsymbol{X} + \sum_{i=1}^{h} \boldsymbol{W}_O^i \boldsymbol{W}_V^i \boldsymbol{X} \cdot \sigma[(\boldsymbol{W}_K^i \boldsymbol{X})^T \boldsymbol{W}_Q^i \boldsymbol{X}], \tag{1}$$

$$\mathrm{FF}(\boldsymbol{X}) = \mathrm{Attn}(\boldsymbol{X}) + \boldsymbol{W}_2 \cdot \mathrm{ReLU}(\boldsymbol{W}_1 \cdot \mathrm{Attn}(\boldsymbol{X}) + \boldsymbol{b}_1 \boldsymbol{1}_n^T) + \boldsymbol{b}_2 \boldsymbol{1}_n^T, \tag{2}$$

where $\boldsymbol{W}_O^i \in \mathbb{R}^{d\times m}$, $\boldsymbol{W}_V^i, \boldsymbol{W}_K^i, \boldsymbol{W}_Q^i \in \mathbb{R}^{m\times d}$, $\boldsymbol{W}_2 \in \mathbb{R}^{d\times r}$, $\boldsymbol{W}_1 \in \mathbb{R}^{r\times d}$, $\boldsymbol{b}_2 \in \mathbb{R}^d$, $\boldsymbol{b}_1 \in \mathbb{R}^r$, and $\mathrm{FF}(\boldsymbol{X})$ is the output of the Transformer block. The number of heads h and the head size m are two main parameters of the attention layer; and r denotes the hidden layer size of the feed-forward layer.

Transformer net:

We define the Transformer networks as the composition of Transformer blocks. The family of the sequence-to-sequence functions corresponding to the Transformers can be defined as:

$$\mathcal{T}^{h,m,r} := \{g : \mathbb{R}^{d\times n} \to \mathbb{R}^{d\times n} \mid g \text{ is a composition of Transformer blocks } t^{h,m,r}\text{'s}\}. \tag{3}$$

where $t^{h,m,r} : \mathbb{R}^{d\times n} \to \mathbb{R}^{d\times n}$ denotes a Transformer block defined by an attention layer with h heads of size m each, and a feed-forward layer with r hidden nodes.

We say that a function $f : \mathbb{R}^{d\times n} \to \mathbb{R}^{d\times n}$ is *permutation equivariant* if for any permutation matrix $\boldsymbol{P}$, we have $f(\boldsymbol{X}\boldsymbol{P}) = f(\boldsymbol{X})\boldsymbol{P}$; i.e., if we permute the columns of $\boldsymbol{X}$, then the columns of $f(\boldsymbol{X})$ are permuted in the same way. A Transformer block is permutation equivariant, which we formally prove in Section B. This consequently establishes the permutation equivariance of the class $\mathcal{T}^{h,m,r}$.

Claim 1. *A Transformer block $t^{h,m,r}$ defines a permutation equivariant map from $\mathbb{R}^{d\times n}$ to $\mathbb{R}^{d\times n}$.*

3 Transformers are universal approximators of seq-to-seq functions

In this section, we present our results showing that the Transformer networks are universal approximators of sequence-to-sequence functions. Let us start by defining the target function class $\mathcal{F}_{\mathrm{PE}}$, which consists of all continuous permutation equivariant functions with compact support that map $\mathbb{R}^{d\times n}$ to $\mathbb{R}^{d\times n}$. Here, continuity is defined with respect to any entry-wise ℓ^p norm, $1 \le p < \infty$. Given two functions $f_1, f_2 : \mathbb{R}^{d\times n} \to \mathbb{R}^{d\times n}$, for $1 \le p < \infty$, we define a distance between them as

$$\mathsf{d}_p(f_1, f_2) := \Big(\int \|f_1(\boldsymbol{X}) - f_2(\boldsymbol{X})\|_p^p \, d\boldsymbol{X} \Big)^{1/p}.$$

The following result shows that a Transformer network with a constant number of heads h, head size m, and hidden layer of size r can approximate any function in $\mathcal{F}_{\mathrm{PE}}$.

Theorem 2. *Let $1 \le p < \infty$ and $\epsilon > 0$, then for any given $f \in \mathcal{F}_{\mathrm{PE}}$, there exists a Transformer network $g \in \mathcal{T}^{2,1,4}$, such that $\mathsf{d}_p(f, g) \le \epsilon$.*

3.1 Transformers with trainable positional encodings

In order to endow the Transformer networks with the ability to capture the information about the position of tokens in the input sequence, it is a common practice to add positional encodings $\boldsymbol{E} \in \mathbb{R}^{d\times n}$ to the input sequence before feeding it to the Transformer network [Vaswani et al., 2017, Devlin et al., 2018]. Consider the functions represented by Transformers with positional encodings:

$$\mathcal{T}_{\mathrm{P}}^{h,m,r} := \{g_{\mathrm{P}}(\boldsymbol{X}) = g(\boldsymbol{X} + \boldsymbol{E}) \mid g \in \mathcal{T}^{h,m,r} \text{ and } \boldsymbol{E} \in \mathbb{R}^{d\times n}\}. \tag{4}$$

Here we show that if $\boldsymbol{E}$ is trainable, these positional encodings are sufficient to remove the permutation equivariance restriction of the Transformers. Towards this, we define $\mathcal{F}_{\mathrm{CD}}$ to be the set of all continuous functions that map a compact domain in $\mathbb{R}^{d\times n}$ to $\mathbb{R}^{d\times n}$. Note that $\mathcal{F}_{\mathrm{CD}}$ does not have the restriction of permutation equivariance as in $\mathcal{F}_{\mathrm{PE}}$, but any $f \in \mathcal{F}_{\mathrm{CD}}$ is defined on a compact domain instead of the whole $\mathbb{R}^{d\times n}$. The following result states that, equipped with the trainable positional encodings, Transformers can approximate any sequence-to-sequence function in $\mathcal{F}_{\mathrm{CD}}$.

Theorem 3. *Let $1 \le p < \infty$ and $\epsilon > 0$, then for any given $f \in \mathcal{F}_{\mathrm{CD}}$, there exists a Transformer network $g \in \mathcal{T}_{\mathrm{P}}^{2,1,4}$ such that we have $\mathsf{d}_p(f, g) \le \epsilon$.*

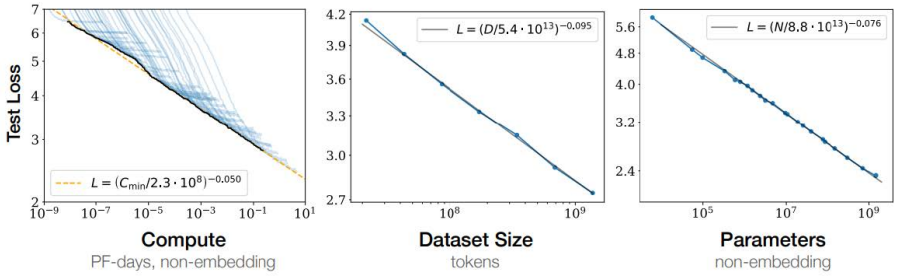
5.2 Allometric scaling

In neurobiology, one can look at allometric scaling relationships:

- across different species with similar brain architectures [evolution],

- scaling relationships for different individuals of same species [growth],
- properties of the brain within the same individual [structure]

The relationship between the two measured quantities is usually expressed as a power law equation: $y = kx^{\alpha}$, where α is the scaling exponent of the law.
How should we interpret superlinear ($\alpha > 1$)) or sublinear ($\alpha < 1$) scaling?
Scaling law for transformers:
Model performance depends most strongly on scale, which consists of three factors: the number of model parameters N (excluding embeddings), the size of the dataset D, and the amount of compute C used for training. Within reasonable limits, performance depends very weakly on other architectural hyperparameters such as depth vs. width.
Performance has a power law relationship with each of the three scale factors N, D, C when not bottlenecked by the other two, with trends spanning more than six orders of magnitude



Universality of overfitting : Performance improves predictably as long as we scale up N and D in tandem, but enters a regime of diminishing returns if either N or D is held fixed while the other increases. The performance penalty depends predictably on the ratio $N^0.74/D$, meaning that every time we increase the model size 8x, we only need to increase the data by roughly 5x to avoid a penalty.
Universality of training : Training curves follow predictable power laws whose parameters are roughly independent of the model size. By extrapolating the early part of a training curve, we can roughly predict the loss that would be achieved if we trained for much longer.
Transfer improves with test performance : When we evaluate models on text with a different distribution than they were trained on, the results are strongly correlated to those on the training validation set with a roughly constant offset in the loss in other words, transfer to a different distribution incurs a constant penalty but otherwise improves roughly in line with performance on the training set.
Sample efficiency : Large models are more sample efficient than small models, reaching the same level of performance with fewer optimization steps and using fewer data points.
Convergence is inefficient : When working within a fixed compute budget C but without any other restrictions on the model size N or available data D, we attain optimal performance by training very large models and stopping significantly short of convergence. Maximally compute efficient training would therefore be far more sample efficient than one might expect based on training small models to convergence, with data requirements growing very slowly as $D \sim C^{0.27}$ with training compute.