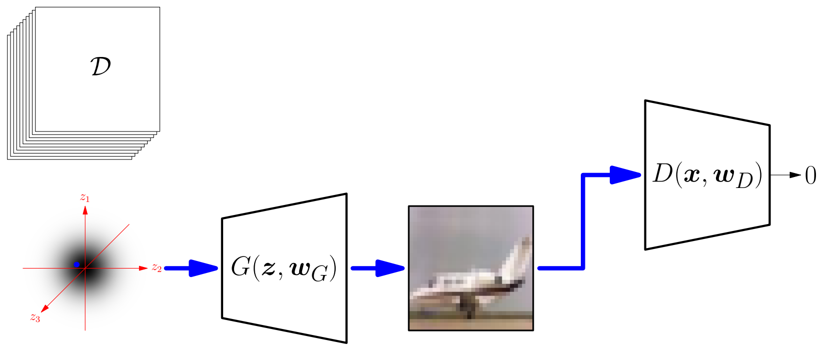
Advanced Machine Learning

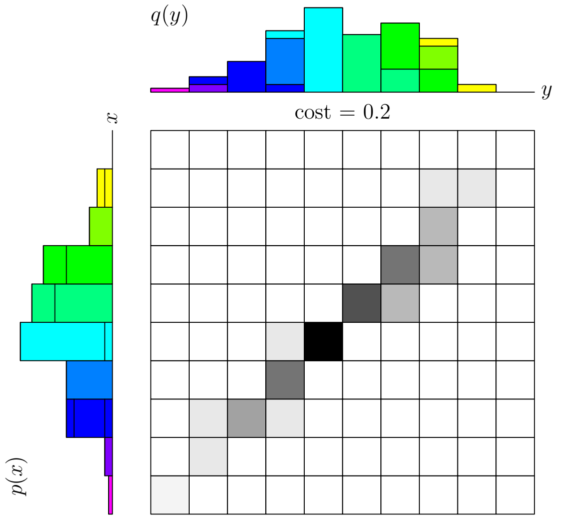
Wasserstein GANs



$\mathcal{D}$
z_1
z_2
z_3
$G(\boldsymbol{z}, \boldsymbol{w}_G)$
$D(\boldsymbol{x}, \boldsymbol{w}_D)$
0

GANs, Wasserstein distance, Duality, WGANs

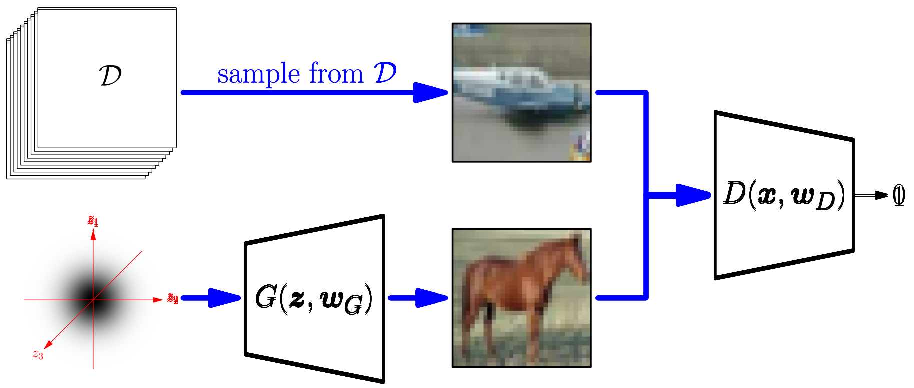
Outline



Generative Adversarial Networks

- One of the applications of Deep Learning that has most excited the public are **Generative Adversarial Networks** or GANs
- Their aim is to generate new random samples from the same distribution as some training set, $\mathcal{D}$
- Their number of real world applications are questionable
- But nobody cares because they are cool!
- *Out of date warning:* someone invented diffusion models

How GANs Work



$\mathcal{D}$
sample from $\mathcal{D}$
z_1
z_2
z_3
$G(\boldsymbol{z}, \boldsymbol{w}_G)$
$D(\boldsymbol{x}, \boldsymbol{w}_D)$
0
1

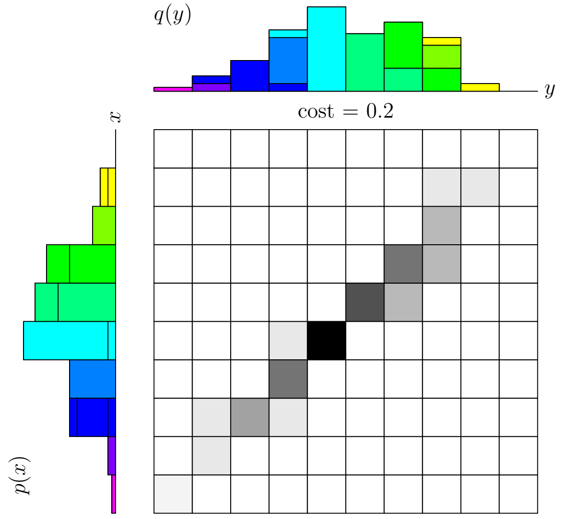
Training GANs

- The loss of the generator depends on its ability to trick the discriminator
- The loss of the discriminator depends on its ability not to be tricked
- We try to train the two networks simultaneously
- We hope that over time the generator produces better and better fakes

Problems of GANs

- GANs are notoriously difficult to train
- The generator and discriminator training can decouple
- Often the discriminator becomes too good at correctly identifying the generated images
- Then there can be little gradient information to help the generator as every small change in parameters doesn't significantly change the discriminator decision
- To try to solve this problem we first make a seemly unconnected diversion

Outline



Measuring Distances Between Distributions

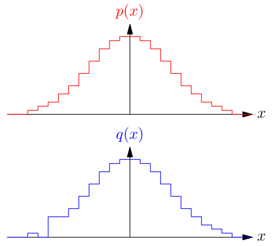
- In many machine learning tasks we want to minimise the distance between two probability distributions
- This requires that we can measure distances between probability distributions
- One prominent measure is the Kullback-Leibler or KL divergence

$$\mathrm{KL}(p\|q) = \int p(\boldsymbol{x}) \log\left(\frac{p(\boldsymbol{x})}{q(\boldsymbol{y})}\right) \mathrm{d}\boldsymbol{x}$$

- This is very commonly used in ML (e.g. VAEs, Variational Approximation)

Trouble with KL

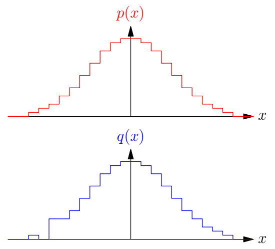
- KL-divergences are non-negative quantities that are minimised when the two probability distributions are the same
- They are not distances (they aren't symmetric and they don't satisfy the triangular inequality)
- We don't really care about this, but what we do care about is that if $q(\boldsymbol{x}) = 0$ when $p(\boldsymbol{x}) \neq 0$ then $\log\left(\frac{p(\boldsymbol{x})}{q(\boldsymbol{y})}\right)$ diverges



- We can therefore have distributes that seem very similar but their KL-divergence is huge (or infinite)

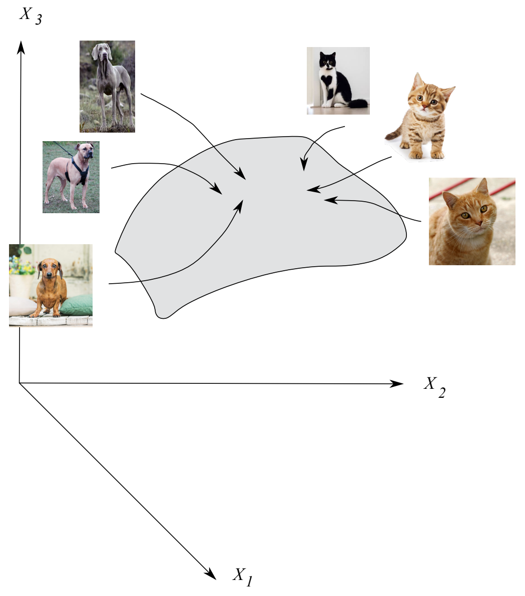
Wasserstein Distance

- A more benign measure of the differences between two probability functions is the **Wasserstein** or **Earth Moving** distance
- This is a true distance, but more importantly for us it measure distance in a very natural way so that distributions that are close has a small Wasserstein distance



- Although this seems contrived if our probability distribution represents the probability of a 128×128 matrix of real valued triples represents an image of dog, then it is easy to imagine that the Wasserstein distance may be more benign than the KL-divergence

High Probability Manifold



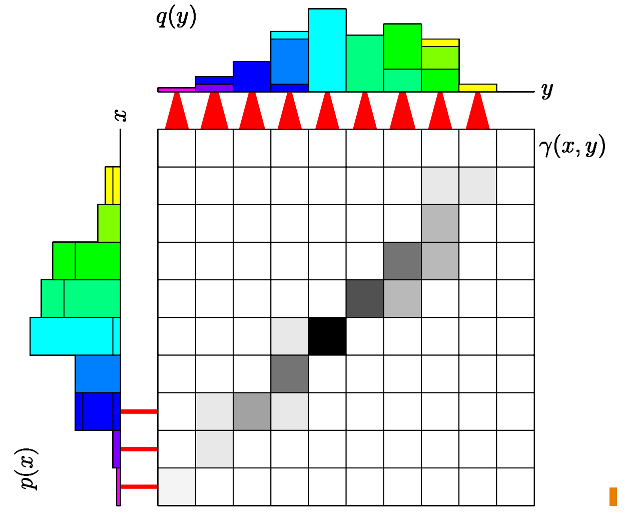
Transportion Policy

- But how do we formalise the Wasserstein distance?
- A good place to start is to define a transportation policy $\gamma(\boldsymbol{x},\boldsymbol{y})$ with

$$\int \gamma(\boldsymbol{x},\boldsymbol{y})\mathrm{d}\boldsymbol{y} = p(\boldsymbol{x}) \qquad \int \gamma(\boldsymbol{x},\boldsymbol{y})\mathrm{d}\boldsymbol{x} = q(\boldsymbol{y})$$

- This looks like a joint probability distribution, but we interpret $\gamma(\boldsymbol{x},\boldsymbol{y})$ as the amount of probability mass/density that we transfer from $p(\boldsymbol{x})$ to $q(\boldsymbol{y})$

Transportation Policy



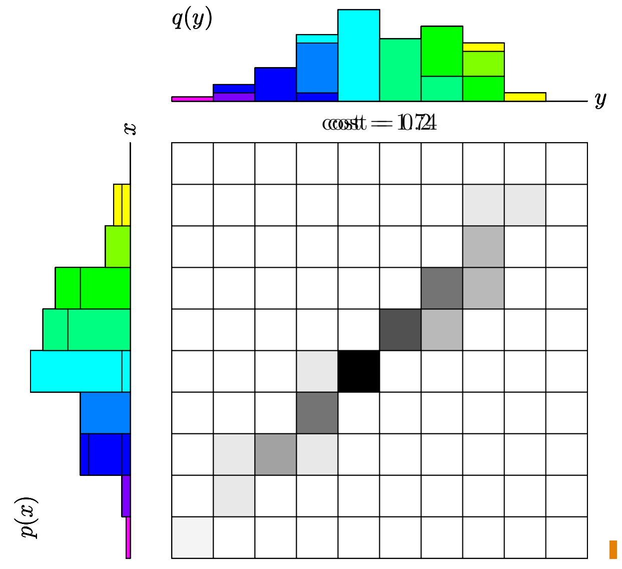
The Cost of Transport

- We want to choose the transportation policy that minimises the amount of probability mass we need to move
- Let $d(\boldsymbol{x}, \boldsymbol{y}) = \|\boldsymbol{x} - \boldsymbol{y}\|$ be a distance measure then the cost of a transportation policy is

$$C(\gamma) = \int\int d(\boldsymbol{x}, \boldsymbol{y}) \gamma(\boldsymbol{x}, \boldsymbol{y}) \mathrm{d}\boldsymbol{x} \mathrm{d}\boldsymbol{y} = \mathbb{E}_\gamma[d(\boldsymbol{x}, \boldsymbol{y})]$$

  where we interpret $\gamma(\boldsymbol{x}, \boldsymbol{y})$ as a probability distribution
- Usually we take $d(\boldsymbol{x}, \boldsymbol{y})$ to be the Euclidean distance, but we can choose any distance

Transportation Cost



The Wasserstein Distance

- The Wasserstein distance $W(p, q)$ between two probability distributions is defined as

$$W(p, q) = \min_{\gamma \in \Lambda(p,q)} \mathbb{E}_\gamma[d(\boldsymbol{x}, \boldsymbol{y})]$$

- Where $\Lambda(p, q)$ is the set of joint distributions $\gamma(\boldsymbol{x}, \boldsymbol{y})$ such that

$$\int \gamma(\boldsymbol{x}, \boldsymbol{y}) \mathrm{d}\boldsymbol{y} = p(\boldsymbol{x}) \qquad \int \gamma(\boldsymbol{x}, \boldsymbol{y}) \mathrm{d}\boldsymbol{x} = q(\boldsymbol{y})$$

Computing the Wasserstein Distance

- To compute the Wasserstein distance we have to solve a minimisation task!
- This looks nasty, but it is a (continuous) linear programmming problem
- Suppose p and q were discrete distribution (i.e. $\boldsymbol{x}$ and $\boldsymbol{y}$ only take discrete points)
- Then we could treat each value of $\gamma(\boldsymbol{x},\boldsymbol{y})$ as an element of a vector $\boldsymbol{\gamma}$ and each value of $d(\boldsymbol{x},\boldsymbol{y})$ as an element of a vector $\boldsymbol{D}$
- Our objective is to choose $\boldsymbol{\gamma}$ to minimise $\boldsymbol{D}^{\mathsf{T}}\boldsymbol{\gamma}$

Constraints

$$\sum_j \gamma(\boldsymbol{x}_i,\boldsymbol{y}_j) = p(\boldsymbol{x}_i) \qquad\qquad \sum_i \gamma(\boldsymbol{x}_i,\boldsymbol{y}_j) = q(\boldsymbol{y}_j)$$

$$\mathbf{A}\,\boldsymbol{\gamma} = \boldsymbol{P}$$

$$\left(\begin{array}{cccc:cccc:c:cccc}
1 & 1 & \cdots & 1 & 0 & 0 & \cdots & 0 & \cdots\cdots & 0 & 0 & \cdots & 0\\
0 & 0 & \cdots & 0 & 1 & 1 & \cdots & 1 & \cdots\cdots & 0 & 0 & \cdots & 0\\
\vdots & \vdots & \cdots & \vdots & \vdots & \vdots & \cdots & \vdots & \vdots\ \vdots \cdots \vdots & \vdots & \vdots & \cdots & \vdots\\
0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 & \cdots\cdots & 1 & 1 & \cdots & 1\\
\hdashline
1 & 0 & \cdots & 0 & 1 & 0 & \cdots & 0 & \cdots\cdots & 1 & 0 & \cdots & 0\\
0 & 1 & \cdots & 0 & 0 & 1 & \cdots & 0 & \cdots\cdots & 0 & 1 & \cdots & 0\\
\vdots & \vdots & \cdots & \vdots & \vdots & \vdots & \cdots & \vdots & \vdots\ \vdots \cdots \vdots & \vdots & \vdots & \cdots & \vdots\\
0 & 0 & \cdots & 1 & 0 & 0 & \cdots & 1 & \cdots\cdots & 0 & 0 & \cdots & 1
\end{array}\right)
\left(\begin{array}{c}
\gamma(x_1,\, y_1)\\ \gamma(x_2,\, y_1)\\ \vdots\\ \gamma(x_n,\, y_1)\\ \hdashline
\gamma(x_1,\, y_2)\\ \gamma(x_2,\, y_2)\\ \vdots\\ \gamma(x_n,\, y_2)\\ \hdashline
\vdots\\ \vdots\\ \vdots\\ \hdashline
\gamma(x_1,\, y_n)\\ \gamma(x_2,\, y_n)\\ \vdots\\ \gamma(x_n,\, y_n)
\end{array}\right)
=
\left(\begin{array}{c}
q(y_1)\\ q(y_2)\\ \vdots\\ q(y_n)\\ \hdashline
p(x_1)\\ p(x_2)\\ \vdots\\ p(x_n)
\end{array}\right)$$

Lagrange Formulation

- For discrete distributions

$$\min_{\boldsymbol{\gamma}} \boldsymbol{D}^{\mathsf{T}}\gamma$$

$$\text{subject to} \quad \mathbf{A}\boldsymbol{\gamma} = \boldsymbol{P}, \quad \boldsymbol{\gamma} \geq 0$$

- Writing the Lagrangian

$$\mathcal{L}(\boldsymbol{\gamma},\boldsymbol{\alpha}) = \boldsymbol{D}^{\mathsf{T}}\boldsymbol{\gamma} - \boldsymbol{\alpha}^{\mathsf{T}}\left(\mathbf{A}^{\mathsf{T}}\boldsymbol{\gamma} - \boldsymbol{P}\right)$$

where $\boldsymbol{\alpha}$ is a vector of Lagrange multipliers

- The solution to the discrete optimisation problem is given by

$$\min_{\boldsymbol{\gamma}} \max_{\boldsymbol{\alpha}} \mathcal{L}(\boldsymbol{\gamma},\boldsymbol{\alpha})$$

Dual Form

- We can rearrang

$$\begin{aligned}
\mathcal{L}(\boldsymbol{\gamma},\boldsymbol{\alpha}) &= \boldsymbol{D}^{\mathsf{T}}\boldsymbol{\gamma} - \boldsymbol{\alpha}^{\mathsf{T}}(\mathbf{A}\boldsymbol{\gamma} - \boldsymbol{P})\\
&= \boldsymbol{P}^{\mathsf{T}}\boldsymbol{\alpha} - \boldsymbol{\gamma}^{\mathsf{T}}\left(\mathbf{A}^{\mathsf{T}}\boldsymbol{\alpha} - \boldsymbol{D}\right)
\end{aligned}$$

- We note that $\boldsymbol{\gamma} \geq 0$ so the dual problem is to find a vector $\boldsymbol{\alpha}$ that maximises $\boldsymbol{P}^{\mathsf{T}}\boldsymbol{\alpha}$ subject to the constraints $\mathbf{A}^{\mathsf{T}}\boldsymbol{\alpha} \leq \boldsymbol{D}$
- Although the vector form allows us to make connections with our earlier discussion of linear programming, it is a little difficult to interpret

Explicit Form

- We can write a Lagrangian for the original problem

$$\mathcal{L} = \sum_{i,j} d(\boldsymbol{x}_i,\boldsymbol{y}_i)\gamma(\boldsymbol{x}_i,\boldsymbol{y}_j) - \sum_i \alpha(\boldsymbol{x}_i)\left(\sum_j \gamma(\boldsymbol{x}_i,\boldsymbol{y}_j) - p(\boldsymbol{x}_i)\right) - \sum_j \beta(\boldsymbol{y}_j)\left(\sum_i \gamma(\boldsymbol{x}_i,\boldsymbol{y}_j) - q(\boldsymbol{y}_j)\right)$$

  subject to $\gamma(\boldsymbol{x}_i,\boldsymbol{y}_j) \geq 0$ where $\alpha(\boldsymbol{x}_i)$ and $\beta(\boldsymbol{y}_j)$ are Lagrange multipliers (they are components of $\boldsymbol{\alpha}$)

- Rearranging

$$\mathcal{L} = \sum_i \alpha(\boldsymbol{x}_i)p(\boldsymbol{x}_i) + \sum_j \beta(\boldsymbol{y}_j)q(\boldsymbol{y}_j) - \sum_{i,j} \gamma(\boldsymbol{x}_i,\boldsymbol{y}_j)\big(\alpha(\boldsymbol{x}_i) + \beta(\boldsymbol{y}_j) - d(\boldsymbol{x}_i,\boldsymbol{y}_i)\big)$$

- This is eqivalent to maximising $\sum_i \alpha(\boldsymbol{x}_i)p(\boldsymbol{x}_i) + \sum_j \beta(\boldsymbol{y}_j)q(\boldsymbol{y}_j)$, subject to

$$\forall i,j \quad \alpha(\boldsymbol{x}_i) + \beta(\boldsymbol{y}_j) \leq d(\boldsymbol{x}_i,\boldsymbol{y}_j)$$

Continuous Form

- We can write a Lagrangian for the continuous problem

$$\mathcal{L} = \iint d(\boldsymbol{x},\boldsymbol{y})\gamma(\boldsymbol{x},\boldsymbol{y})\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{y} - \int \alpha(\boldsymbol{x})\left(\int \gamma(\boldsymbol{x},\boldsymbol{y})\,\mathrm{d}\boldsymbol{y} - p(\boldsymbol{x})\right)\mathrm{d}\boldsymbol{x} - \int \beta(\boldsymbol{y})\left(\int \gamma(\boldsymbol{x},\boldsymbol{y})\,\mathrm{d}\boldsymbol{x} - q(\boldsymbol{y})\right)\mathrm{d}\boldsymbol{y}$$

  subject to $\gamma(\boldsymbol{x},\boldsymbol{y}) \geq 0$ where $\alpha(\boldsymbol{x})$ and $\beta(\boldsymbol{y})$ are Lagrange multiplier functions

- Rearranging

$$\mathcal{L} = \int \alpha(\boldsymbol{x})p(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} + \int \beta(\boldsymbol{y})q(\boldsymbol{y})\,\mathrm{d}\boldsymbol{y} - \iint \gamma(\boldsymbol{x},\boldsymbol{y})\big(\alpha(\boldsymbol{x}) + \beta(\boldsymbol{y}) - d(\boldsymbol{x},\boldsymbol{y})\big)\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{y}$$

- This is eqivalent to maximising $\int \alpha(\boldsymbol{x})p(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} + \int \beta(\boldsymbol{y})q(\boldsymbol{y})\,\mathrm{d}\boldsymbol{y}$, subject to

$$\alpha(\boldsymbol{x}) + \beta(\boldsymbol{y}) \leq d(\boldsymbol{x},\boldsymbol{y})$$

Dual Form Constraint

- We note that $\alpha(\boldsymbol{x}) + \beta(\boldsymbol{y}) \leq d(\boldsymbol{x},\boldsymbol{y})$ for all $\boldsymbol{x}$ and $\boldsymbol{y}$
- This has to be true when $\boldsymbol{x} = \boldsymbol{y}$ so that

$$\alpha(\boldsymbol{x}) + \beta(\boldsymbol{x}) \leq d(\boldsymbol{x},\boldsymbol{x}) = 0$$

- So $\beta(\boldsymbol{x}) = -\alpha(\boldsymbol{x}) - \epsilon(\boldsymbol{x})$ where $\epsilon(\boldsymbol{x}) \geq 0$
- But want to maximise

$$\int \alpha(\boldsymbol{x})p(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} + \int \beta(\boldsymbol{y})q(\boldsymbol{y})\,\mathrm{d}\boldsymbol{y} = \int \alpha(\boldsymbol{x})\big(p(\boldsymbol{x}) - q(\boldsymbol{x})\big)\,\mathrm{d}\boldsymbol{x} - \int q(\boldsymbol{x})\epsilon(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x}$$

- This is maximised when $\epsilon(\boldsymbol{x}) = 0$ i.e. $\beta(\boldsymbol{x}) = -\alpha(\boldsymbol{x})$

Dual Form

- Thus the dual problem is to find a function $\alpha(\boldsymbol{x})$—or a vector of functions $(\alpha(\boldsymbol{x}_i)|i)$—that maximises

$$\int \alpha(\boldsymbol{x})\big(p(\boldsymbol{x}) - q(\boldsymbol{x})\big)\,\mathrm{d}\boldsymbol{x}$$

- Subject to the constraint

$$\alpha(\boldsymbol{x}) - \alpha(\boldsymbol{y}) \leq d(\boldsymbol{x},\boldsymbol{y}) = \|\boldsymbol{x} - \boldsymbol{y}\|$$

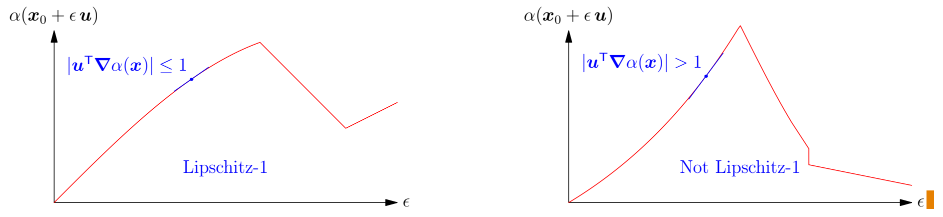
- This is a continuity constraint on the Lagrange multiplier function $\alpha(\boldsymbol{x})$ known as Lipschitz-1

Lipschitz-1 Functions

- We note for a Lipschitz-1 function and any unit vector $\boldsymbol{u}$

$$\boldsymbol{u}^{\mathsf{T}}\boldsymbol{\nabla}\alpha(\boldsymbol{x}) = \lim_{\epsilon\to 0}\frac{\alpha(\boldsymbol{x}) - \alpha(\boldsymbol{x}+\epsilon\boldsymbol{u})}{\epsilon} \leq \frac{\epsilon}{\epsilon} = 1$$

- That is, at every point the gradient in all directions must be less than 1 (since the gradient defines the direction of greatest increase it is both necessary and sufficient for $\|\boldsymbol{\nabla}\alpha(\boldsymbol{x})\| \leq 1$ everywhere)



Calculating the Wasserstein Distance

- To recall the big picture we want to compute the Wasserstein distance

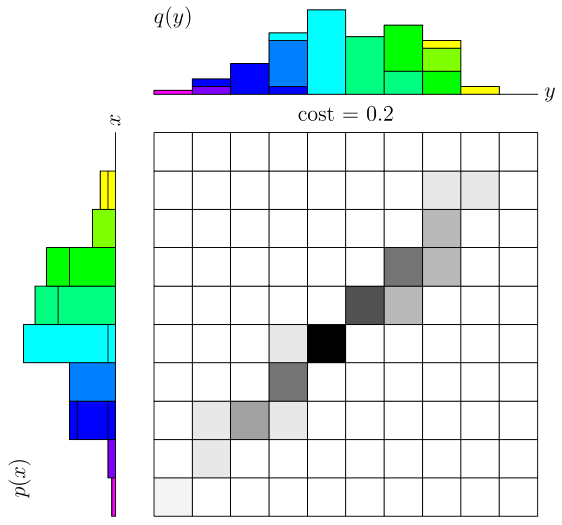
$$W(p,q) = \min_{\gamma\in\Lambda(p,q)} \mathbb{E}_{\gamma}[d(\boldsymbol{x},\boldsymbol{y})]$$

- For high dimensional objects $\gamma(\boldsymbol{x},\boldsymbol{y})$ would be a huge object to approximate
- Instead we can compute the Wasserstein distance in the dual formulation

$$W(p,q) = \max_{\alpha(\boldsymbol{x})}\int \alpha(\boldsymbol{x})\,(p(\boldsymbol{x}) - q(\boldsymbol{x}))\,\mathrm{d}\boldsymbol{x} = \max_{\alpha}\mathbb{E}_p[\alpha(\boldsymbol{X})] - \mathbb{E}_q[\alpha(\boldsymbol{X})]$$

subject to the constraint that $\alpha(\boldsymbol{x})$ is a Lipschitz-1 function

Outline



Back to GANs

- What has this got do with GANs?
- Suppose we want to minimise the distance between the distribution $p(\boldsymbol{x})$ of real images (of which $\mathcal{D}$ are samples) and the distribution $q(\boldsymbol{x})$ of images drawn from a generator
- We can use a normal GAN generator, $G(\boldsymbol{z},\boldsymbol{w}_G)$, that generates an image when given a random variable $\boldsymbol{z} \sim \mathcal{N}(\boldsymbol{0},\mathbf{I})$
- To do this we choose the weights, $\boldsymbol{w}_G$ of the generator to minimise

$$W(p,q) = \max_{\alpha(\boldsymbol{x})}(\mathbb{E}_{\boldsymbol{x}\sim p}[\alpha(\boldsymbol{x})] - \mathbb{E}_{\boldsymbol{x}\sim q}[\alpha(\boldsymbol{x})])$$

Estimating Expectations

- Although we can't compute $\mathbb{E}_p[\alpha(\boldsymbol{x})]$ and $\mathbb{E}_q[\alpha(\boldsymbol{x})]$ exactly, we can estimate them from samples

$$\mathbb{E}_p[\alpha(\boldsymbol{x})] \approx \frac{1}{|\mathcal{B}|}\sum_{\boldsymbol{x}\in\mathcal{B}}\alpha(\boldsymbol{x}), \qquad \mathbb{E}_q[\alpha(\boldsymbol{x})] \approx \frac{1}{n}\sum_{i=1}^{n}\alpha(G(\boldsymbol{z}_i,\boldsymbol{w}_G))$$

- where $\mathcal{B} \subset \mathcal{D}$ is a minibatch of true images and $\boldsymbol{z}_i \sim \mathcal{N}(\boldsymbol{0},\mathbf{I})$
- From this we can choose $\boldsymbol{w}_G$ to minimise

$$C = \frac{1}{|\mathcal{B}|}\sum_{\boldsymbol{x}\in\mathcal{B}}\alpha(\boldsymbol{x}) - \frac{1}{n}\sum_{i=1}^{n}\alpha(G(\boldsymbol{z}_i,\boldsymbol{w}_G))$$

The Critic

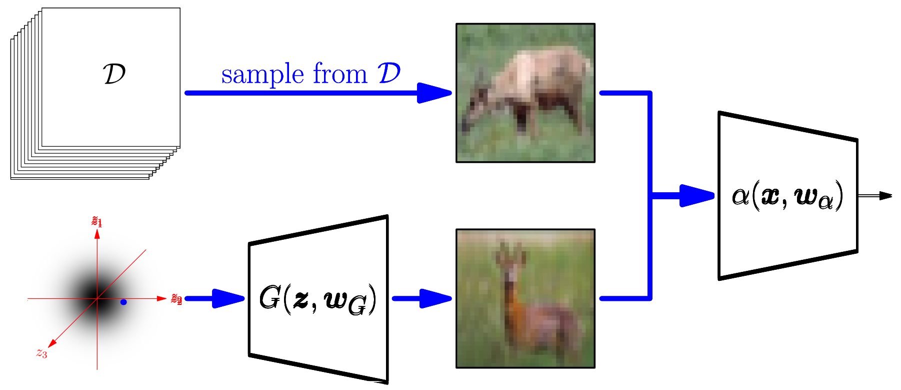
- For this quantity to approximate the Wasserstein distance we need to find a function $\alpha(\boldsymbol{x},\boldsymbol{w}_\alpha)$ that maximises C
- To do this we learn a second network, the critic or discriminator whose job it is to maximise

$$C = \frac{1}{|\mathcal{B}|}\sum_{\boldsymbol{x}\in\mathcal{B}}\alpha(\boldsymbol{x},\boldsymbol{w}_\alpha) - \frac{1}{n}\sum_{i=1}^{n}\alpha(G(\boldsymbol{z}_i,\boldsymbol{w}_G),\boldsymbol{w}_\alpha)$$

- The network $\alpha(\boldsymbol{x},\boldsymbol{w}_\alpha)$ should be Lipschitz-1 (which we usually botched by, for example, by setting the spectral norm of the convolutional weight matrix to 1)

Wasserstein GANs

$$\max_{\boldsymbol{w}_\alpha}\min_{\boldsymbol{w}_G} \frac{1}{|\mathcal{B}|}\sum_{\boldsymbol{x}\in\mathcal{B}}\alpha(\boldsymbol{x},\boldsymbol{w}_\alpha) - \frac{1}{n}\sum_{i=1}^{n}\alpha(G(\boldsymbol{z}_i,\boldsymbol{w}_G),\boldsymbol{w}_\alpha)$$


$\mathcal{D}$
sample from $\mathcal{D}$
$\alpha(\boldsymbol{x},\boldsymbol{w}_\alpha)$
z_1
z_2
z_3
$G(\boldsymbol{z},\boldsymbol{w}_G)$

Lesson

- Wasserstein GANs are, at least for me, one of the most elegant pieces of theory in recent years
- By trying to minimise the Wasserstein distance between the distribution of a generator and a true distribution we arrive at optimising two adversarial networks just like a GAN
- This uses a rather beautiful dual formulation
- It is claimed that W-GANs solve many of the problems of traditional GANs