

Deep Learning

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Credit for slides: Sanjeev Arora; Yoshua Bengio; Yann LeCun; Nando de Freitas; Pascal Germain; Léon Gatys; Weidi Xie; Max Welling; Victor Berger; Kevin Frans; Lars Mescheder et al.; Mehdi Sajjadi et al.

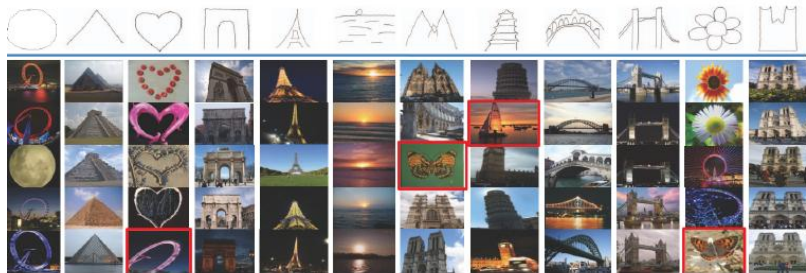


Siamese Networks

Variational Auto-Encoders

Generative Adversarial Networks

Siamese Networks



Classes or similarities ?

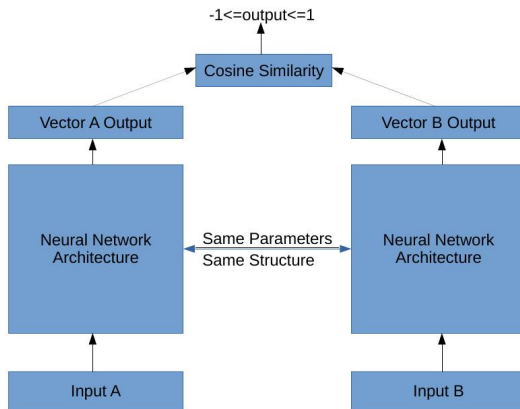
Siamese Networks

Bromley et al. 93

Principle

- ▶ Neural Networks can be used to define a latent representation
- ▶ Siamese: optimize the related metrics

Schema



Siamese Networks, 2

Data

$$\mathcal{E} = \{x_i \in \mathbb{R}^d, i \in [[1, n]]\}; \mathcal{S} = \{(x_{i_\ell}, x_{j_\ell}, c_\ell) \text{ s.t. } c_\ell \in \{-1, 1\}, \ell \in [[1, L]]\}$$

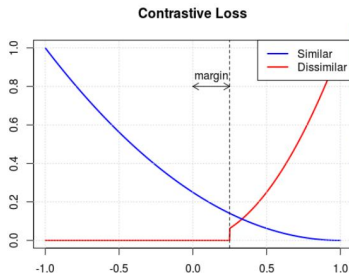
Experimental setting

- ▶ Often: few similar pairs; by default, pairs are dissimilar
- ▶ Subsample dissimilar pairs (optimal ratio between 2/1 ou 10/1)
- ▶ Possible to use domain knowledge in selection of dissimilar pairs

Loss

Given similar and dissimilar pairs (E_+ and E_-)

$$\mathcal{L} = \sum_{(i,j) \in E_+} L_+(i,j) + \sum_{(k,\ell) \in E_-} L_-(k,\ell)$$



$$L_+ = \frac{1}{4} \cdot (1 - \cosine(x_1, x_2))^2$$

$$L_- = \begin{cases} \cosine(x_1, x_2)^2, & \text{if } x \geq \text{margin} \\ 0, & \text{otherwise} \end{cases}$$





Applications

- ▶ Signature recognition
- ▶ Image recognition, search
- ▶ Article, Title
- ▶ Filter out typos
- ▶ Recommendation systems, collaborative filtering

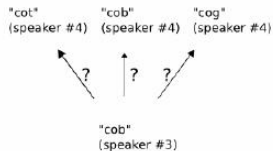
Siamese Networks for one-shot image recognition

Koch, Zemel, Salakhutdinov 15

Training similarity

	same	"cow" (speaker #1)	"cow" (speaker #2)	same
	different	"cow" (speaker #1)	"cat" (speaker #2)	different
	same	"can" (speaker #1)	"can" (speaker #2)	same
	different	"can" (speaker #1)	"cab" (speaker #2)	different

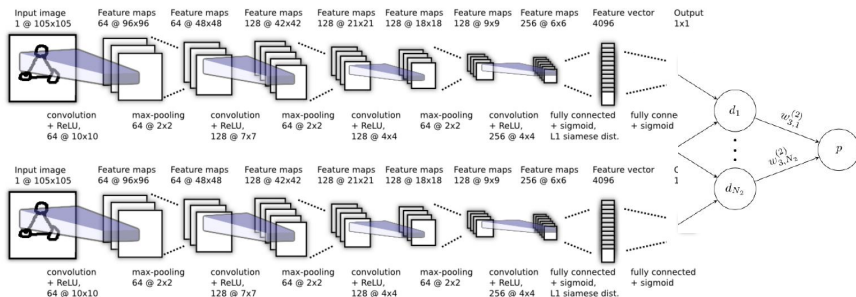
One-shot setting



Ingredients

Koch et al. 15

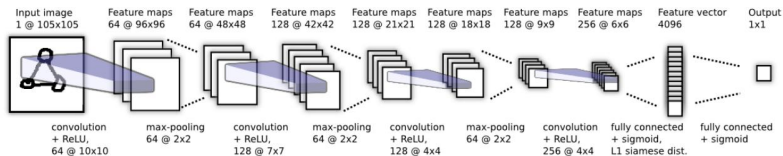
Architecture



Ingredients, 2

Koch et al. 15

Architecture



Distance

$$d(x, x') = \sigma \left(\sum_k \alpha_k |z_k(x) - z_k(x')| \right)$$

Loss

Given a batch $((x_i, x'_i), y_i)$ with $y_i = 1$ iff x_i and x'_i are similar

$$\mathcal{L}(w) = \sum_i y_i \log d(x_i, x'_i) + (1 - y_i) \log (1 - d(x_i, x'_i)) + \lambda \|w\|^2$$

Omniglot



Results

Method	Test
Humans	95.5
Hierarchical Bayesian Program Learning	95.2
Affine model	81.8
Hierarchical Deep	65.2
Deep Boltzmann Machine	62.0
Simple Stroke	35.2
1-Nearest Neighbor	21.7
Siamese Neural Net	58.3
Convolutional Siamese Net	92.0

Siamese Networks

PROS

- ▶ Learn metrics, invariance operators
- ▶ Generalization beyond train data

CONS

- ▶ More computationally intensive
- ▶ More hyperparameters and fine-tuning, more training

Siamese Networks

Variational Auto-Encoders

Generative Adversarial Networks

Beyond AE

- ▶ A compressed (latent) representation

$$x \in \mathbb{R}^D \mapsto z = \text{Enc}(x) \in \mathbb{R}^d \mapsto \text{Dec}(z) \in \mathbb{R}^D \approx x$$

- ▶ Distance in latent space is meaningful $d(\text{Enc}(x), \text{Enc}(x'))$ reflects $d(x, x')$
- ▶ But $\forall z \in \mathbb{R}^d$: is $\text{Dec}(z) \in \mathbb{R}^D$ meaningful ?

Beyond AE

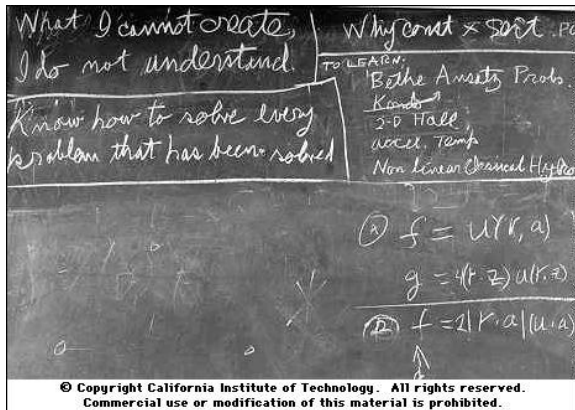
- ▶ A compressed (latent) representation

$$x \in \mathbb{R}^D \mapsto z = \text{Enc}(x) \in \mathbb{R}^d \mapsto \text{Dec}(z) \in \mathbb{R}^D \approx x$$

- ▶ Distance in latent space is meaningful $d(\text{Enc}(x), \text{Enc}(x'))$ reflects $d(x, x')$
- ▶ But $\forall z \in \mathbb{R}^d$: is $\text{Dec}(z) \in \mathbb{R}^D$ meaningful?

“What I cannot create I do not understand”

Feynman 88

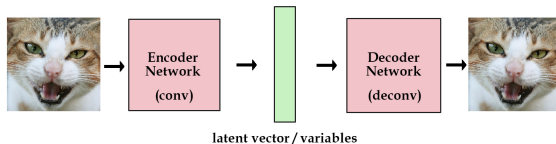


Variational Auto-Encoders

Kingma Welling 14, Salimans Kingma Welling 15

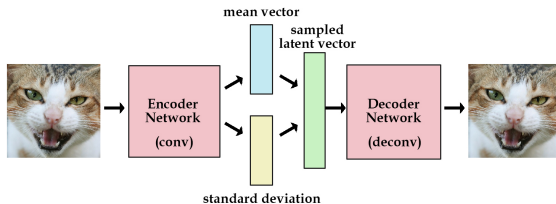
What we have:

- Enc a memorization of the data s.t. exists $Dec \approx Enc^{-1}$



What we want:

- $z \sim \mathcal{P}$ s.t. $Dec(z) \sim \mathcal{D}_{data}$



Distribution estimation

Data

$$\mathcal{E} = \{x_1, \dots, x_n, x_i \in \mathcal{X}\}$$

Goal

- Find a probability distribution that models the data

$$p_\theta : \mathcal{X} \mapsto [0, 1] \quad \text{s.t.} \quad \theta = \arg \max \prod_i p_\theta(x_i)$$

≡ **maximize the log likelihood of data**

$$\arg \max \prod_i p_\theta(x_i) = \arg \max \sum_i \log(p_\theta(x_i))$$

Gaussian case

$$\theta = (\mu, \sigma) \quad p_\theta(x) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{1}{2\sigma^2}(x - \mu)^2\right)$$

Akin Graphical models

Find hidden variables z s.t.

$$z \mapsto \mathbf{x} \text{ s.t. } \text{good } p(\mathbf{x}|z)$$

Bayes relation

$$p(\mathbf{x}, z) = p(z|\mathbf{x}) \cdot p(\mathbf{x}) = p(\mathbf{x}|z) \cdot p(z)$$

Hence

$$p(z|\mathbf{x}) = p(\mathbf{x}|z) \cdot p(z) / \int p(\mathbf{x}|z) \cdot p(z) dz$$

Problem:

denominator computationally intractable...

State of art

- ▶ Monte-Carlo estimation
- ▶ Variational Inference
choose z well-behaved, and make $q(z)$ “close” to $p(z|\mathbf{x})$.

Variational Inference

- ▶ Approximate $p(\mathbf{z}|\mathbf{x})$ by $q(\mathbf{z})$
- ▶ Minimize distance between both, using Kullback-Leibler divergence

Reminder

- ▶ information $(\mathbf{x}) = -\log(p(\mathbf{x}))$
- ▶ entropy $(\mathbf{x}_1, \dots, \mathbf{x}_k) = -\sum_i p(\mathbf{x}_i) \log(p(\mathbf{x}_i))$
- ▶ Kullback-Leibler divergence between distribution q and p

$$KL(q||p) = \sum_{\mathbf{x}} q(\mathbf{x}) \log \frac{q(\mathbf{x})}{p(\mathbf{x})}$$

Beware: not symmetrical, hence not a distance; plus numerical issues when supports are different

Variational inference

$$\text{Minimize } KL(q(\mathbf{z})||p(\mathbf{z}|\mathbf{x})) = \int q(\mathbf{z}) \log \frac{q(\mathbf{z})}{p(\mathbf{z}|\mathbf{x})} d\mathbf{z}$$

Evidence Lower Bound (ELBO)

$$KL(q(\mathbf{z})||p(\mathbf{z}|\mathbf{x})) = \int q(\mathbf{z}) \log \frac{q(\mathbf{z})}{p(\mathbf{z}|\mathbf{x})} d\mathbf{z}$$

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use $p(\mathbf{z}|\mathbf{x}) = p(\mathbf{z}, \mathbf{x})/p(\mathbf{x})$

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$$KL(q(z)||p(z|x)) = \int q(z) \log \frac{q(z)}{p(z|x)} dz$$

use $p(z|x) = p(z, x)/p(x)$

$$KL(q(z)||p(z|x)) = \int q(z) \log \frac{q(z)p(x)}{p(z, x)} dz$$

$$KL(q(z)||p(z|x)) = \int q(z) \log \frac{q(z)}{p(z, x)} dz + \int q(z) \log(p(x)) dz$$

as $\int q(z) dz = 1$

$$KL(q(z)||p(z|x)) = \int q(z) \log \frac{q(z)}{p(z, x)} dz + \log(p(x))$$

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$$KL(q(z)||p(z|x)) = \int q(z) \log \frac{q(z)}{p(z, x)} dz + \log(p(x))$$

recover $KL(q(z)||p(z, x))$

$$KL(q(z)||p(z|x)) = - \int q(z) \log \frac{p(z, x)}{q(z)} dz + \log(p(x))$$

Evidence Lower Bound, 2

Define

$$L(q(\mathbf{z})) = \int q(\mathbf{z}) \log \frac{p(\mathbf{z}, \mathbf{x})}{q(\mathbf{z})} d\mathbf{z}$$

Last slide:

$$KL(q(\mathbf{z})||p(\mathbf{z}|\mathbf{x})) = \log(p(\mathbf{x})) - L(q(\mathbf{z}))$$

Hence

Minimize Kullback-Leibler divergence \equiv Maximize $\mathbf{L}(\mathbf{q}(\mathbf{z}))$

Evidence Lower Bound, 3

More formula massaging

$$L(q(z)) = \int q(z) \log \frac{p(z, \mathbf{x})}{q(z)} dz$$

Evidence Lower Bound, 3

More formula massaging

$$L(q(z)) = \int q(z) \log \frac{p(z, \mathbf{x})}{q(z)} dz$$

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$$L(q(z)) = \int q(z) \log \frac{p(z|\mathbf{x})}{q(z)} dz + \int q(z) \log(p(\mathbf{x})) dz$$

$$L(q(z)) = -KL(q(z)||p(z|\mathbf{x})) + \mathbb{E}_q[\log(p(\mathbf{x}))]$$

Finally

$$\text{Maximize } \mathbb{E}_q[\log(p(\mathbf{x}))] - KL(q(z)||p(z|\mathbf{x}))$$

make $p(\mathbf{x})$ great under q

while minimizing the KL divergence between the two

akin data fitting
akin regularization

Where neural nets come in

Searching p and q

- ▶ We want $p(\mathbf{x}|\mathbf{z})$, we search $p(\mathbf{z}|\mathbf{x})$
- ▶ Let $p(\mathbf{z}|\mathbf{x})$ be defined as a neural net (encoder)
- ▶ We want it to be close to a well-behaved (**Gaussian**) distribution $q(\mathbf{z})$

$$\text{Minimize } KL(q(\mathbf{z})||p(\mathbf{z}|\mathbf{x}))$$

- ▶ And from \mathbf{z} we generate a distribution $p(\mathbf{x}|\mathbf{z})$ (defined as a neural net, “decoder”)
- ▶ such that $p(\mathbf{x}|\mathbf{z})$ gives a high probability mass to our data (next slide)

$$\text{Maximize } \mathbb{E}_q[\log(p(\mathbf{x}))]$$

Good news

All these criteria are differentiable !

can be used to train the neural net.

The loss of the variational decoder

Continuous case

- ▶ $\mathbf{x} \mapsto \mathbf{z}$; Gaussian case, $\mathbf{z} \sim p(\mathbf{z}|\mathbf{x})$
- ▶ Now \mathbf{z} is given as input to the decoder, generates $\hat{\mathbf{x}}$ (deterministic)
- ▶ $p(\mathbf{x}|\hat{\mathbf{x}}) = F(\exp\{-\|\mathbf{x} - \hat{\mathbf{x}}\|^2\})$
- ▶ ... back to the L_2 loss

Binary case

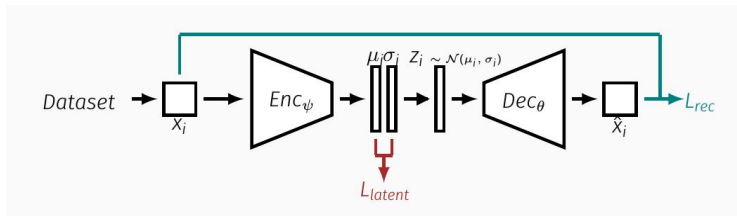
- ▶ Exercise: back to the cross-entropy loss

Variational auto-encoders

Kingma et al. 13

Position

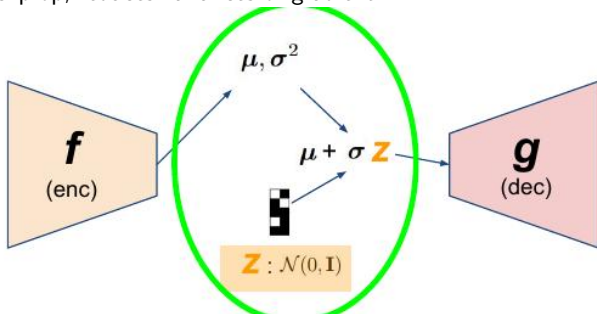
- ▶ Like an auto-encoder (data fitting term) with a regularizer, the KL divergence between the distribution of the hidden variables \mathbf{z} and the target distribution.
- ▶ Say the hidden variable follows a Gaussian distribution: $\mathbf{z} \sim \mathcal{N}(\mu, \Sigma)$
- ▶ Therefore, the encoder must compute the parameters μ and Σ



The reparameterization trick

Principle

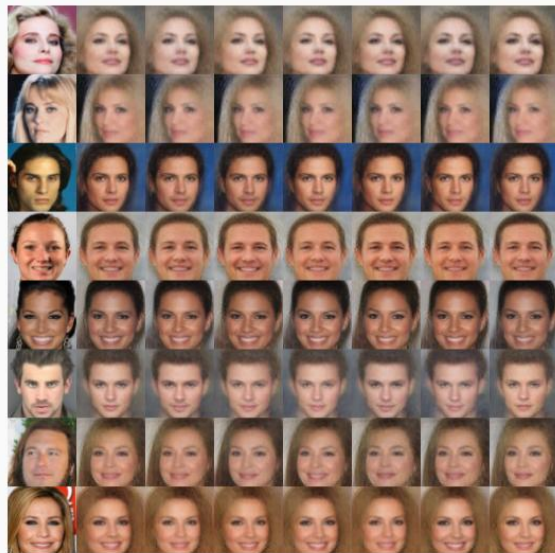
- ▶ Hidden layer: parameters of a distribution $\mathcal{N}(\mu, \sigma^2)$
- ▶ Distribution used to generate values $z = \mu + \sigma \times \mathcal{N}(0, 1)$
- ▶ Enables backprop; reduces variances of gradient



Examples



Examples



Also: <https://www.youtube.com/watch?v=XNZIN7Jh3Sg>

Discussion

PROS

- ▶ A trainable generative model

CONS

- ▶ The generative model has a Gaussian distribution at its core: blurry

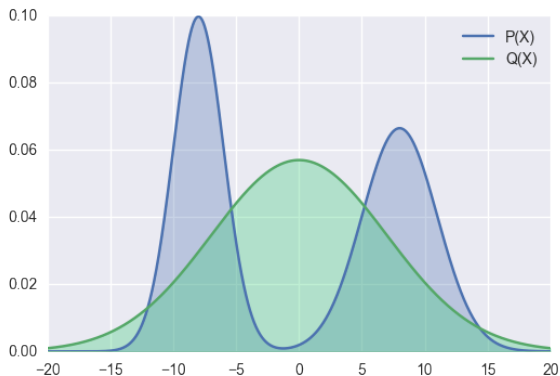
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Siamese Networks

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Generative Adversarial Networks

Generative Adversarial Networks

Goodfellow et al., 14

Goal: Find a generative model

- ▶ Classical: learn a distribution hard
- ▶ Idea: replace a distribution evaluation by a 2-sample test

Principle

- ▶ Find a good generative model, s.t. generated samples **cannot be discriminated** from real samples

(not easy)

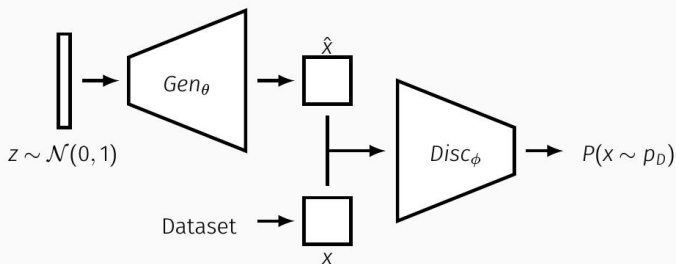
Principle

Goodfellow, 2017

Elements

- ▶ True samples \mathbf{x} (**real**)
- ▶ A generator G (variational auto-encoder):
generates from \mathbf{z} (**reconstructed**) or from scratch (fake)
- ▶ A discriminator D : discriminates *fake* from others (**real** and **reconstructed**)

- Generator $G_\theta : \mathcal{Z} \rightarrow \mathcal{D}$
- Discriminator $D_\phi : \mathcal{D} \rightarrow [0, 1]$



Principle, 2

Goodfellow, 2017

Mechanism

- ▶ Alternate minimization
- ▶ Optimize D to tell fake from rest
- ▶ Optimize G to deceive D

Turing test

$$\text{Min}_G \text{Max}_D \mathbb{E}_{\mathbf{x} \in \text{data}} [\log(D(\mathbf{x}))] + \mathbb{E}_{z \sim p_x(z)} [\log(1 - D(z))]$$

Caveat

- ▶ The above loss has a vanishing gradient problem because of the terms in $\log(1 - D(z))$.
- ▶ We can replace it with $-\log((1 - D(z))/D(z))$, which has the same fixed point (the true distribution) but doesn't saturate.

GAN vs VAE

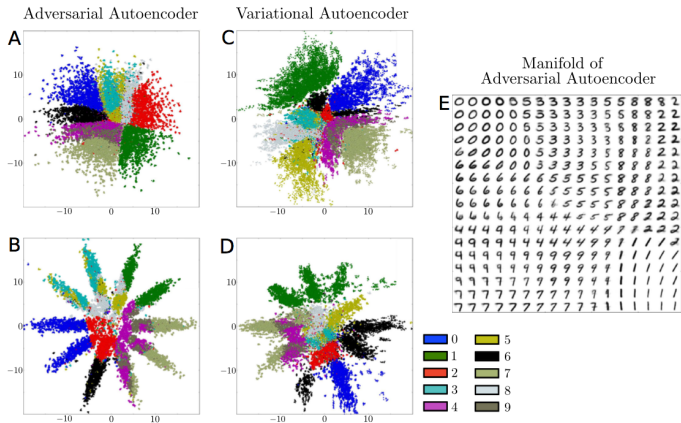
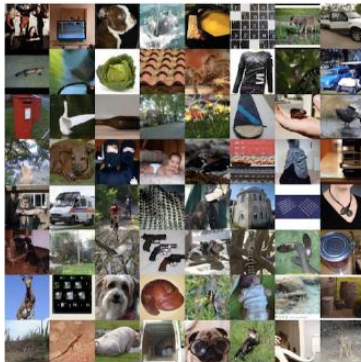


Figure 2: Comparison of adversarial and variational autoencoder on MNIST. The hidden code z of the *hold-out* images for an adversarial autoencoder fit to (a) a 2-D Gaussian and (b) a mixture of 10 2-D Gaussians. Each color represents the associated label. Same for variational autoencoder with (c) a 2-D gaussian and (d) a mixture of 10 2-D Gaussians. (e) Images generated by uniformly sampling the Gaussian percentiles along each hidden code dimension z in the 2-D Gaussian adversarial autoencoder.

Generative adversarial networks

Goodfellow, 2017



Generative adversarial networks, 2

Goodfellow, 2017

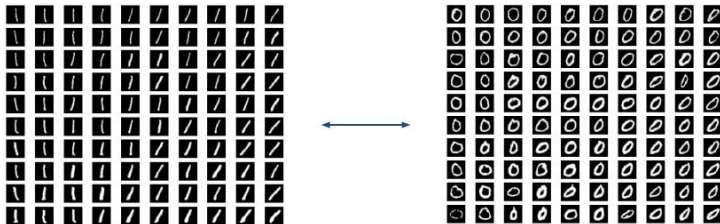


Limitations

Training instable

co-evolution of Generator / Discriminator

Mode collapse



Limitations, 2

Generating monsters



(Goodfellow 2016)

Towards Principled Methods for Training Generative Adversarial Networks

Arjovsky, Bottou 17

Why minimizing KL fails

$$\text{Minimizing } KL(P_{real} || P_{gen}) = \int P_{real} \log \frac{P_{real}}{P_{gen}}$$

- ▶ For P_{real} high and P_{gen} low (mode dropping), high cost
- ▶ For P_{real} low and P_{gen} high (gen. monsters), no cost

The GAN solution: minimizing

$$\mathbb{E}_{x \sim P_r} [\log D(x)] + \mathbb{E}_{x \sim P_g} [\log 1 - D(x)]$$

with

$$D^*(x) = \frac{P_r(x)}{P_r(x) + P_g(x)}$$

i.e., up to a constant, GAN minimizes

$$JS(P_{real}, P_{gen}) = \frac{1}{2} (KL(P_{real} || M) + KL(P_{gen} || M))$$

with $M = \frac{1}{2}(P_{real} + P_{gen})$

Towards Principled Methods for Training Generative Adversarial Networks, 2

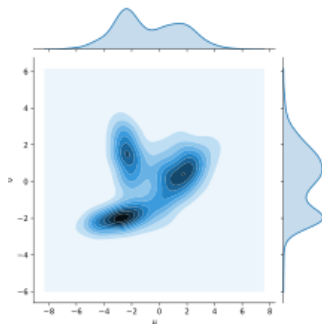
Arjovsky, Bottou 17

Unfortunately

If P_r and P_g lie on non-aligned manifolds, exists a perfect discriminator; this is the end of optimization !

Proposed alternative: use Wasserstein distance

$$\min_G \max_D \mathbb{E}_{x \sim P_g} [D(x)] - \mathbb{E}_{x \sim P_r} [D(x)] = \min_G W(P_r, P_g)$$



Does not solve all issues !

Pb of vanishing/exploding gradients in WGAN, addressed through weight clipping
careful tuning needed

New Regularizations

Improved Training of Wasserstein GANs

Gulrajani, Ahmed, Arjovsky, Dumoulin, Courville 17

Stabilizing Training of Generative Adversarial Networks through Regularization

Roth, Lucchi, Nowozin, Hofmann, 17

Which Training Methods for GANs do actually Converge?

Mescheder, Geiger and Nowozin, 18

Simple experiments, simple theorems are the building blocks that help us understand more complicated systems. Ali Rahimi - Test of Time Award speech, NIPS 2017

Which Training Methods for GANs do actually Converge? 2

Mescheder, Geiger and Nowozin, 18

Toy example

$$P_r = \delta_0 \quad P_g = \delta_\theta$$

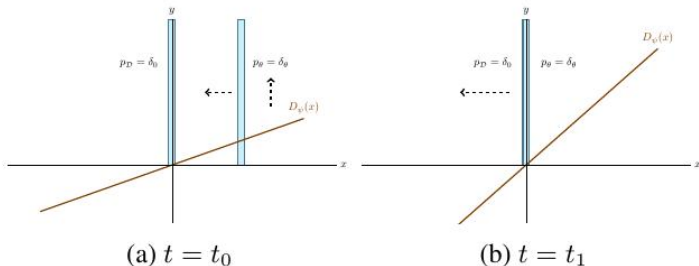
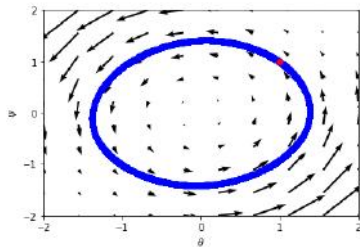


Figure 1. Visualization of the counterexample showing that in the general case, gradient descent GAN optimization is not convergent: (a) In the beginning, the discriminator pushes the generator towards the true data distribution and the discriminator's slope increases. (b) When the generator reaches the target distribution, the slope of the discriminator is largest, pushing the generator away from the target distribution. This results in oscillatory training dynamics that never converge.

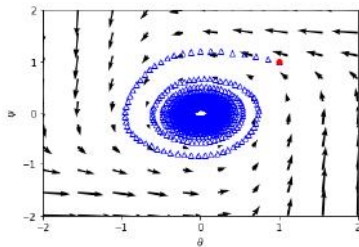
Which Training Methods for GANs do actually Converge? 2

Mescheder, Geiger and Nowozin, 18

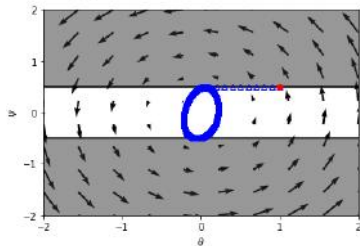
Lesson learned: cyclic behavior for GAN and WGAN



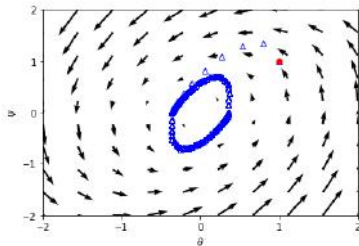
(a) Standard GAN



(b) Non-saturating GAN



(c) WGAN ($n_d = 5$)



(d) WGAN-GP ($n_d = 5$)

State-of-the-art Generative Adversarial Networks

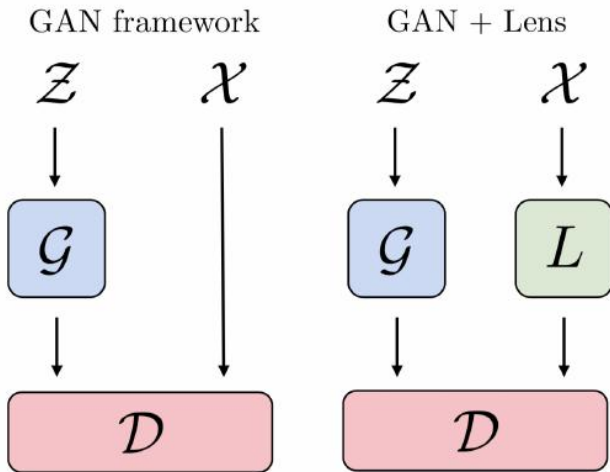
Mescheder, Geiger and Nowozin, 2018



Tempered Adversarial Networks

Sajjadi, Parascandolo, Mehrjou, Scholkopf 18

Principle: Life too easy for the discriminator !



Tempered Adversarial Networks

Sajjadi, Parascandolo, Mehrjou, Scholkopf 18

Principle: An adversary to the adversary

- \Rightarrow Provide $L(X)$ instead, with L aimed at: i) deceiving the discriminator; ii) staying close from original images

$$\min_G \max_D \mathbb{E}_{x \sim P_r} [\log D(x)] + \mathbb{E}_{x \sim P_g} [\log(1D(x))]$$

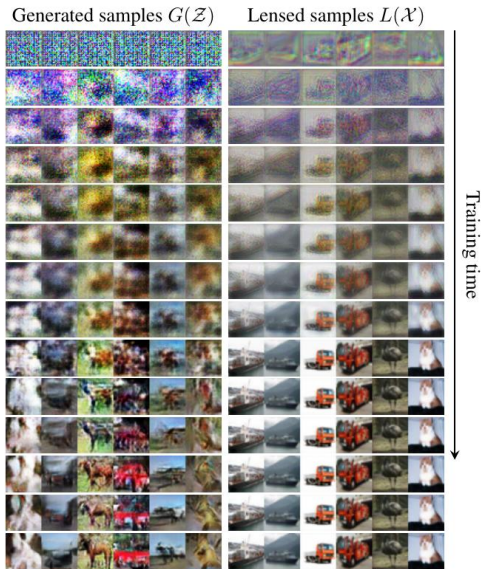
with D trained from $\{(L(x), 1)\} \cup \{G(z), 0\}$ and Lens L optimized

$$L^* = \arg \min -\lambda \mathcal{L}(D) + \sum_i \|L(x_i) - x_i\|^2$$

and $\lambda \rightarrow 0$.

Tempered Adversarial Networks, 2

Sajjadi, Parascandolo, Mehrjou, Scholkopf 18



Partial conclusions

- ▶ Deep revolution: Learning representations
- ▶ Adversarial revolution: a Turing test for machines
- ▶ Where is the limitation ?
 - VAE: great but blurry
 - GAN: great but mode dropping
 - the loss function needs more work.

References (tbc)

see: github.com/artix41/awesome-transfer-learning

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