

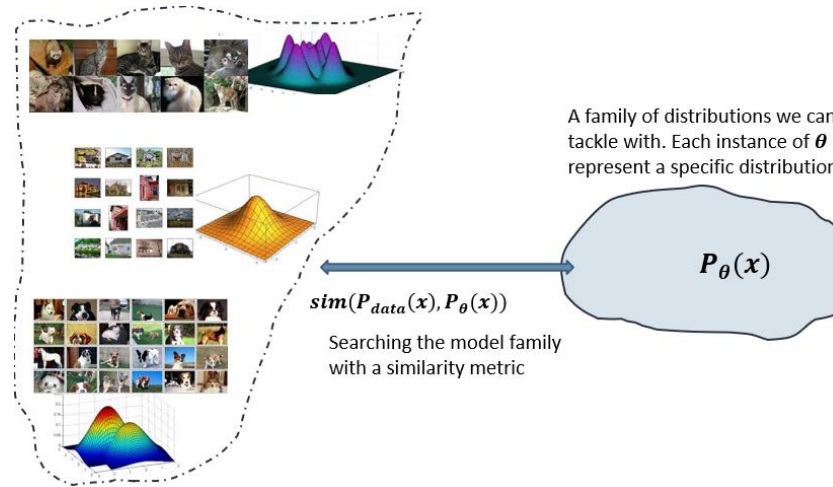


# Generative adversarial networks

22-808: Generative models  
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# Recap



- ▶ We need a framework to interact with distributions for statistical generative models.
  - ▶ Probabilistic generative models
  - ▶ Deep generative models
    - ▶ Autoregressive models  $p_{\theta}(\mathbf{x}) = \prod_{i=1}^n p_{\theta}(x_i | \mathbf{x}_{<i})$
    - ▶ Variational Autoencoders  $p_{\theta}(\mathbf{x}) = \int p_{\theta}(\mathbf{x}, \mathbf{z}) d\mathbf{z}$
    - ▶ **Generative adversarial networks**
  - ▶ Both AR and VAE model families attempted to minimize the KL divergence between model family and data distribution, or equivalently attempt to maximize the likelihood.
  - ▶ In GAN we are going to use an alternative choice for the similarity measure between model distribution and data distribution.

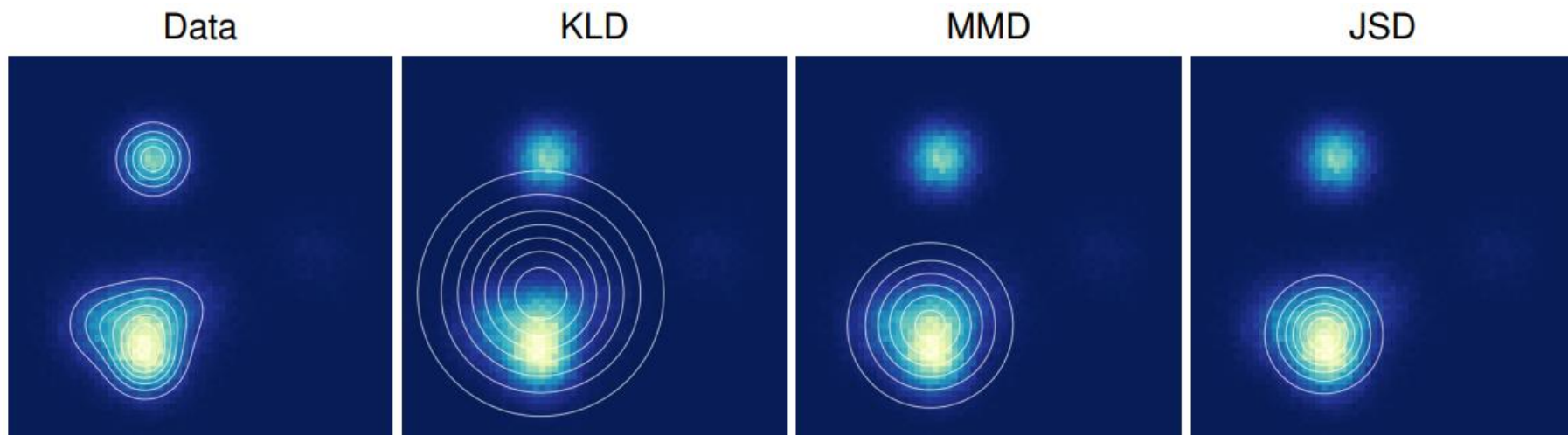
# Maximizing the likelihood

$$\hat{\theta} = \operatorname{argmax}_{\theta} \sum_{i=1}^M \log p_{\theta}(\mathbf{x}_i), \quad \mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_M \sim p_{\text{data}}(\mathbf{x})$$

- ▶ Optimal statistical efficiency
  - ▶ Assume sufficient model capacity, such that there exists a unique  $\theta^*$  that satisfy  $p_{\theta^*} = p_{\text{data}}$ .
  - ▶ The convergence of  $\hat{\theta}$  to  $\theta^*$  when  $M \rightarrow \infty$ , is the fastest among all statistical methods when using maximum likelihood training.

# Maximizing the likelihood

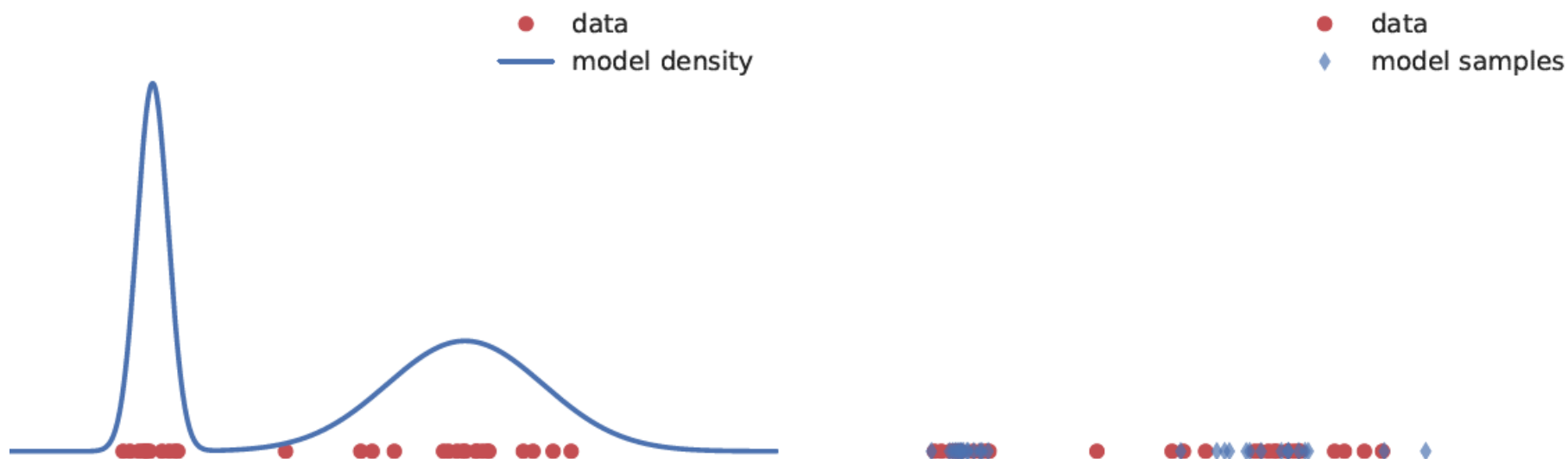
- ▶ For imperfect models, achieving high log-likelihoods might not always imply good sample quality.



An isotropic Gaussian distribution was fit to data drawn from a mixture of Gaussians by either minimizing KL divergence (KLD), maximum mean discrepancy (MMD), or Jensen-Shannon divergence (JSD). The different fits demonstrate different tradeoffs made by the three measures of distance between distributions.

# Implicit generative models

- ▶ Kind of probabilistic generative models without an explicit likelihood function
- ▶ We use a likelihood-free approach to train these models
  - ▶ Training by comparing samples



Explicit models vs. implicit models

# Learning by comparing samples

- ▶ We should define a distance(similarity) measure between two distributions that:
  - ▶ Provides guarantees about learning the data distribution.

$$\operatorname{argmin}_{p_{\theta}} D(p_{data}, p_{\theta}) = p_{data}$$

- ▶ Can be evaluated only using samples from the data and model distribution.
  - ▶ Are computationally cheap to evaluate.
- ▶ Many distributional distances and divergences fail to satisfy the later two requirements

# Learning by comparing samples

- ▶ The main approach to overcome these challenges is to approximate the desired quantity through optimization by introducing a comparison model, often called a **discriminator** or a **critic**  $D$ , such that:

$$\mathcal{D}(p^*, q) = \operatorname{argmax}_D \mathcal{F}(D, p^*, q)$$

- ▶ where  $\mathcal{F}$  is a functional that can be estimated using only samples from  $p^*(p_{data})$  and  $q$ . One way is that it depends on distributions only in expectations.
  - ▶ Therefore, it can be estimated using Monte Carlo estimation.

# Learning by comparing samples

- ▶ As we usually use parametric functions (ex. Neural networks) for both the model and discriminator.
- ▶ Therefore, by the following optimization we estimate the distance measure  $\mathcal{D}(p^*, q_\theta)$

$$\operatorname{argmax}_{\phi} \mathcal{F}(D_{\phi}, p^*, q_{\theta})$$

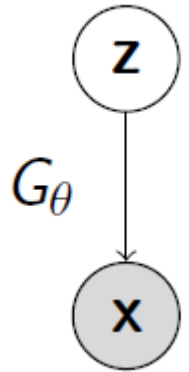
- ▶ Then, instead of optimizing the exact objective  $\mathcal{D}(p^*, q_\theta)$  we use the tractable approximation provided through the optimal  $D_{\phi}$ .



# Generative adversarial networks

## (Goodfellow GAN)

- ▶ A finite number of samples from the desired real distribution is available:  $x_1, x_2, \dots, x_n$
- ▶ Like VAEs, we consider a latent variable model for the model generation process and attempt to learn  $G_\theta$ . However, here we learn this function by Comparing samples.



# The Goodfellow GAN

## The probabilistic classification view

- ▶ Assuming  $D(x)$  as a binary classifier which predicts whether a given point  $x$  was sampled from the real distribution or it is a fake sample from the generator  $G_\theta$ .

- ▶ A cross entropy loss to train this classifier:

$$E_{\mathbf{x} \sim p_{\text{data}}} [\log D_\phi(\mathbf{x})] + E_{\mathbf{x} \sim p_\theta} [\log(1 - D_\phi(\mathbf{x}))]$$

- ▶ We can see that the optimal discriminator for a fixed generator  $G_\theta$  is:

$$\frac{p(x)}{p(x) + p_\theta(x)}$$

# The Goodfellow GAN

## The objective function

- By substitution the optimal discriminator into the cross-entropy loss, we have:

$$\begin{aligned} V^*(q_\theta, p^*) &= \frac{1}{2} \mathbb{E}_{p^*(\mathbf{x})} \left[ \log \frac{p^*(\mathbf{x})}{p^*(\mathbf{x}) + q_\theta(\mathbf{x})} \right] + \frac{1}{2} \mathbb{E}_{q_\theta(\mathbf{x})} \left[ \log \left( 1 - \frac{p^*(\mathbf{x})}{p^*(\mathbf{x}) + q_\theta(\mathbf{x})} \right) \right] \\ &= \frac{1}{2} \mathbb{E}_{p^*(\mathbf{x})} \left[ \log \frac{p^*(\mathbf{x})}{\frac{p^*(\mathbf{x}) + q_\theta(\mathbf{x})}{2}} \right] + \frac{1}{2} \mathbb{E}_{q_\theta(\mathbf{x})} \left[ \log \left( \frac{q_\theta(\mathbf{x})}{\frac{p^*(\mathbf{x}) + q_\theta(\mathbf{x})}{2}} \right) \right] - \log 2 \\ &= \frac{1}{2} D_{\text{KL}} \left( p^* \parallel \frac{p^* + q_\theta}{2} \right) + \frac{1}{2} D_{\text{KL}} \left( q_\theta \parallel \frac{p^* + q_\theta}{2} \right) - \log 2 \\ &= JSD(p^*, q_\theta) - \log 2 \end{aligned}$$

where JSD is the Jensen-Shannon divergence.

# The Goodfellow GAN

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- ▶ This establishes a connection between optimal binary classification and distributional divergences.
- ▶ By using binary classification, we were able to compute the distributional divergence using only samples, which is the important property needed for learning implicit generative models
- ▶ We have turned an intractable estimation problem (how to estimate the JSD divergence) into an optimization problem (how to learn a classifier) which can be used to approximate that divergence.

# The Goodfellow GAN

- ▶ With optimal discriminator, we attempt to find the generative model  $G_\theta$  that minimizes the JSD divergence.

$$\begin{aligned}\min_{\theta} JSD(p^*, q_\theta) &= \min_{\theta} V^*(q_\theta, p^*) + \log 2 \\ &= \min_{\theta} \frac{1}{2} \mathbb{E}_{p^*(\mathbf{x})} \log D^*(\mathbf{x}) + \frac{1}{2} \mathbb{E}_{q_\theta(\mathbf{x})} \log(1 - D^*(\mathbf{x})) + \log 2\end{aligned}$$

# Training procedure of GAN

Sample minibatch of  $m$  training points  $\mathbf{x}^{(1)}, \mathbf{x}^{(2)}, \dots, \mathbf{x}^{(m)}$  from  $\mathcal{D}$

Sample minibatch of  $m$  noise vectors  $\mathbf{z}^{(1)}, \mathbf{z}^{(2)}, \dots, \mathbf{z}^{(m)}$  from  $p_z$

Update the discriminator parameters  $\phi$  by stochastic gradient **ascent**

$$\nabla_{\phi} V(G_{\theta}, D_{\phi}) = \frac{1}{m} \nabla_{\phi} \sum_{i=1}^m [\log D_{\phi}(\mathbf{x}^{(i)}) + \log(1 - D_{\phi}(G_{\theta}(\mathbf{z}^{(i)})))]$$

Update the generator parameters  $\theta$  by stochastic gradient **descent**

$$\nabla_{\theta} V(G_{\theta}, D_{\phi}) = \frac{1}{m} \nabla_{\theta} \sum_{i=1}^m \log(1 - D_{\phi}(G_{\theta}(\mathbf{z}^{(i)})))$$

Repeat for fixed number of epochs

Active

# Training convergence

- ▶ If G and D have enough capacity, and at each step of training procedure, the discriminator is allowed to reach its optimum for a specific  $G_\theta$ , and then  $p_\theta$  is updated so as to improve

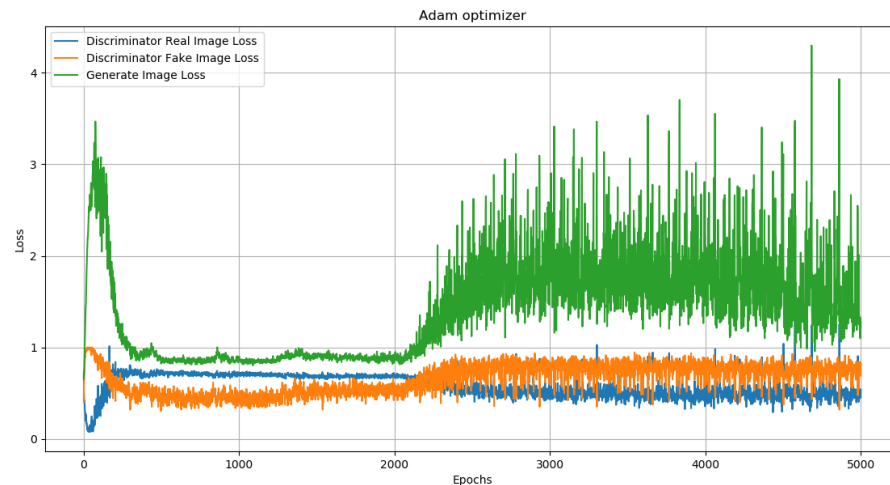
$$\mathbb{E}_{\mathbf{x} \sim p_{data}} [\log D_G^*(\mathbf{x})] + \mathbb{E}_{\mathbf{x} \sim p_g} [\log(1 - D_G^*(\mathbf{x}))]$$

then  $p_\theta$  converges to  $p_{data}$ .

- ▶ Unrealistic assumptions ☹️

# Training convergence

- ▶ However, we do not have access to the optimal discriminator and only we can approximate it with a parametrized function: neural network  $D_\phi$
- ▶ No guarantee for convergence
- ▶ In practice, the generator and discriminator loss keeps oscillating during GAN training



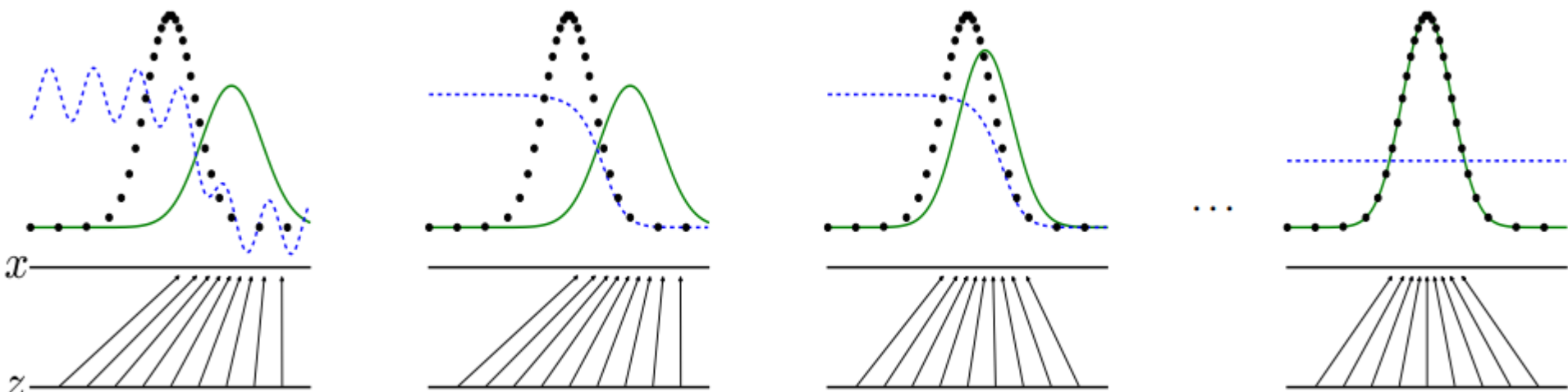


# The min-max game

## ► The minmax game

$$\min_{\theta} \max_{\phi} V(G_{\theta}, D_{\phi}) = E_{\mathbf{x} \sim p_{\text{data}}} [\log D_{\phi}(\mathbf{x})] + E_{\mathbf{z} \sim p(\mathbf{z})} [\log(1 - D_{\phi}(G_{\theta}(\mathbf{z})))]$$

- It is a game not an optimization problem
- It should reach to a Nash equilibria



# Example

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- ▶ Which one is real?



# *F-divergence*

- ▶ Let  $f: \mathbb{R} \rightarrow \mathbb{R}$  be a convex lower-semicontinuous function, such that  $f(1) = 0$ . We define the *f-divergence* between two distributions with densities  $p$  and  $q$  by:

$$D_f(p \parallel q) \equiv \int_{\mathcal{X}} q(x) f\left(\frac{p(x)}{q(x)}\right) dx.$$

- ▶ What's interesting about *f-divergence* is that we can construct a variational representation for it.
  - ▶ Alternating the integral to an optimization

# Fenchel duality

- ▶ The idea is to use the convex conjugate of the function  $f$ , which is defined as follows:

$$f^*(t) \equiv \sup_x \{tx - f(x)\}.$$

- ▶ Fenchel duality: repeat application of the conjugate operation to convex lower-semicontinuous function  $f$  yields  $f^{**} = f$ . Therefore, we have:

$$f(x) = \sup_t \{tx - f^*(t)\}.$$

# Variational representation of $F$ -divergence

- ▶ Using Fenchel duality, we obtain the variational representation of the  $f$ -divergence.

$$\begin{aligned} D_f(p \parallel q) &= \int_{\mathcal{X}} q(x) \sup_t \left[ t \frac{p(x)}{q(x)} - f^*(t) \right] dx \\ &= \int_{\mathcal{X}} \sup_t [tp(x) - f^*(t)q(x)] dx \\ &= \sup_{T: \mathcal{X} \rightarrow \mathbb{R}} \int_{\mathcal{X}} (T(x)p(x) - f^*(T(x))q(x)) dx \\ &= \sup_{T: \mathcal{X} \rightarrow \mathbb{R}} \left[ \mathbb{E}_{x \sim p} T(x) - \mathbb{E}_{x \sim q} f^*(T(x)) \right]. \end{aligned}$$

# F-GAN

- ▶ The dual form can be approximated using Monte Carlo estimation.
- ▶ Assuming a parametric family of functions  $T\varphi$  (ex. a neural network) and the generator function  $g_\theta$ , and a valid f-divergence, the F-GAN objective is,

$$\begin{aligned}\theta_f &= \arg \min_{\theta} \sup_{\varphi} \left[ \mathbb{E}_{x \sim p} T_{\varphi}(x) - \mathbb{E}_{x \sim p_{\theta}} f^*(T_{\varphi}(x)) \right] \\ &= \arg \min_{\theta} \sup_{\varphi} \left[ \mathbb{E}_{x \sim p} T_{\varphi}(x) - \mathbb{E}_{z \sim q} f^*(T_{\varphi}(g_{\theta}(z))) \right].\end{aligned}$$

- ▶ Generator  $g_\theta$  tries to minimize the divergence estimate and discriminator  $T\varphi$  tries to tighten the lower bound

# *F-divergence*

distance or divergence	corresponding $g(t)$ ( $t = \frac{p_i(x)}{p_j(x)}$ )
Bhattacharyya distance <sup>1</sup>	$\sqrt{t}$
KL-divergence	$t \log(t)$
Symmetric KL-divergence	$t \log(t) - \log(t)$
Hellinger distance	$(\sqrt{t} - 1)^2$
Total variation	$ t - 1 $
Pearson divergence	$(t - 1)^2$
Jensen-Shannon divergence	$\frac{1}{2} (t \log \frac{2t}{t+1} + \log \frac{2}{t+1})$

# The Goodfellow GAN as F-GAN

- ▶ The Goodfellow GAN is an instances of the  $f$ -GAN.
- ▶ Modified version of the Jensen-Shannon

$$2\text{JSD}(p, q) - \log(4) = D_{\text{KL}} \left( p \left\| \frac{p+q}{2} \right. \right) + D_{\text{KL}} \left( p_g \left\| \frac{p+q}{2} \right. \right) - \log(4).$$

- ▶ The  $f$ -divergence:

$$f(x) = x \log x - (x+1) \log(x+1)$$

$$f^*(t) = -\log(1 - e^t).$$

$$T_\varphi(x) = \log(d_\varphi(x))$$

- ▶ We can obtain the Goodfellow GAN :

$$_{24} \theta_f = \arg \min_{\theta} \sup_{\varphi} \left[ \mathbb{E}_{x \sim p} \log d_\varphi(x) + \mathbb{E}_{z \sim q} \log(1 - d_\varphi(g_\theta(z))) \right]$$