Generative Adversarial Networks (GANs)

Ian Goodfellow, OpenAI Research Scientist

NIPS 2016 tutorial

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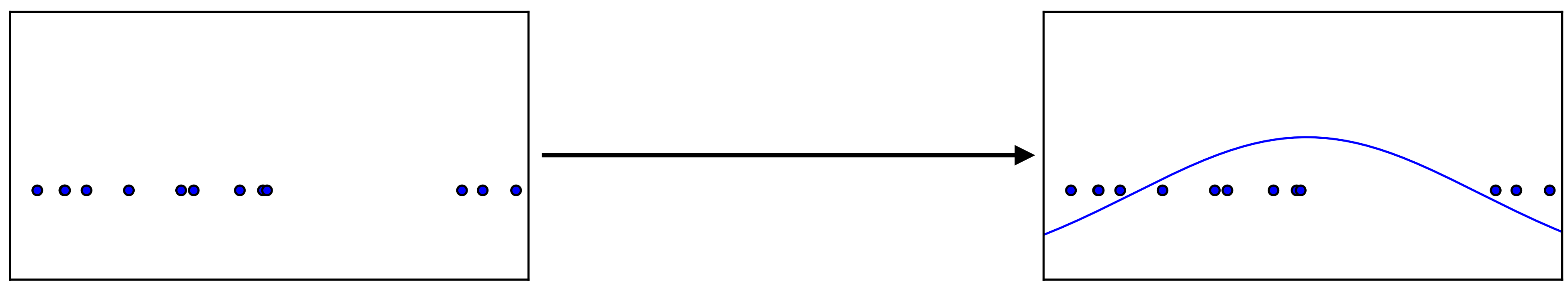
OpenAI

Generative Modeling

- Density estimation



- Sample generation

Training examples Model samples

(Goodfellow 2016)

Roadmap

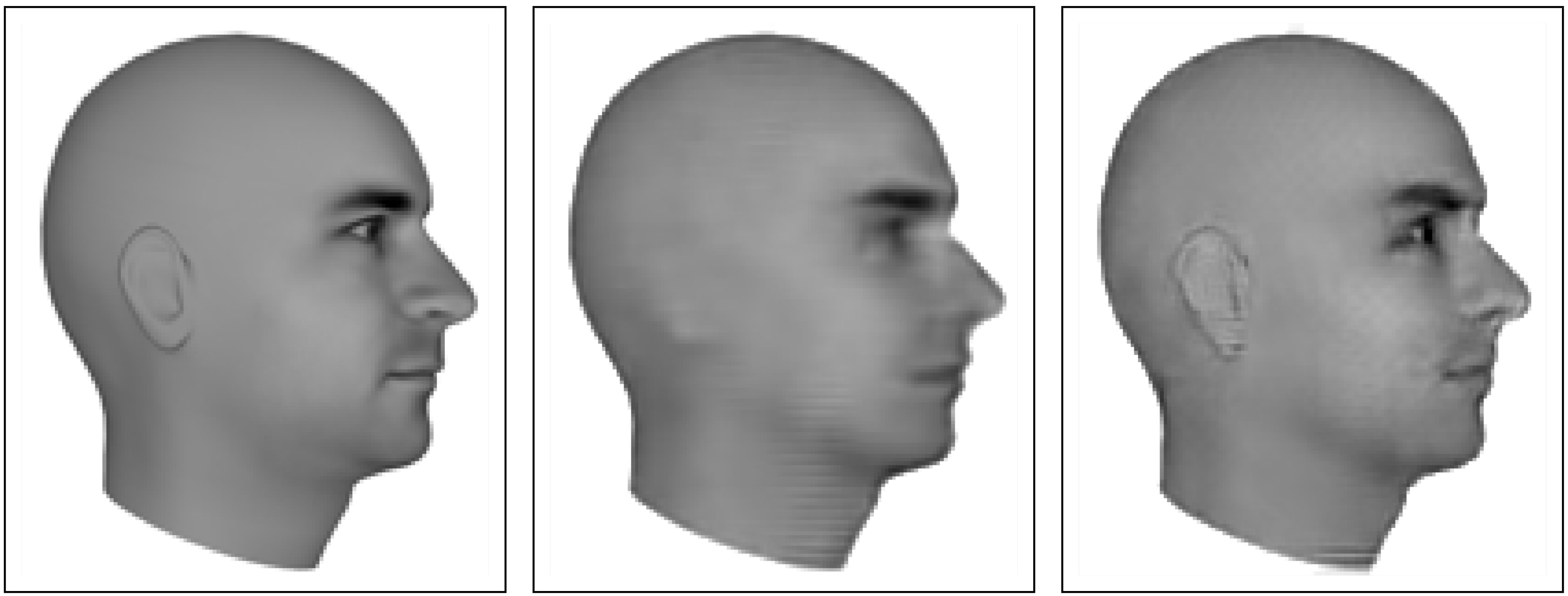
- Why study generative modeling?
- How do generative models work? How do GANs compare to others?
- How do GANs work?
- Tips and tricks
- Research frontiers
- Combining GANs with other methods

Why study generative models?

- Excellent test of our ability to use high-dimensional, complicated probability distributions
- Simulate possible futures for planning or simulated RL
- Missing data
  - Semi-supervised learning
- Multi-modal outputs
- Realistic generation tasks

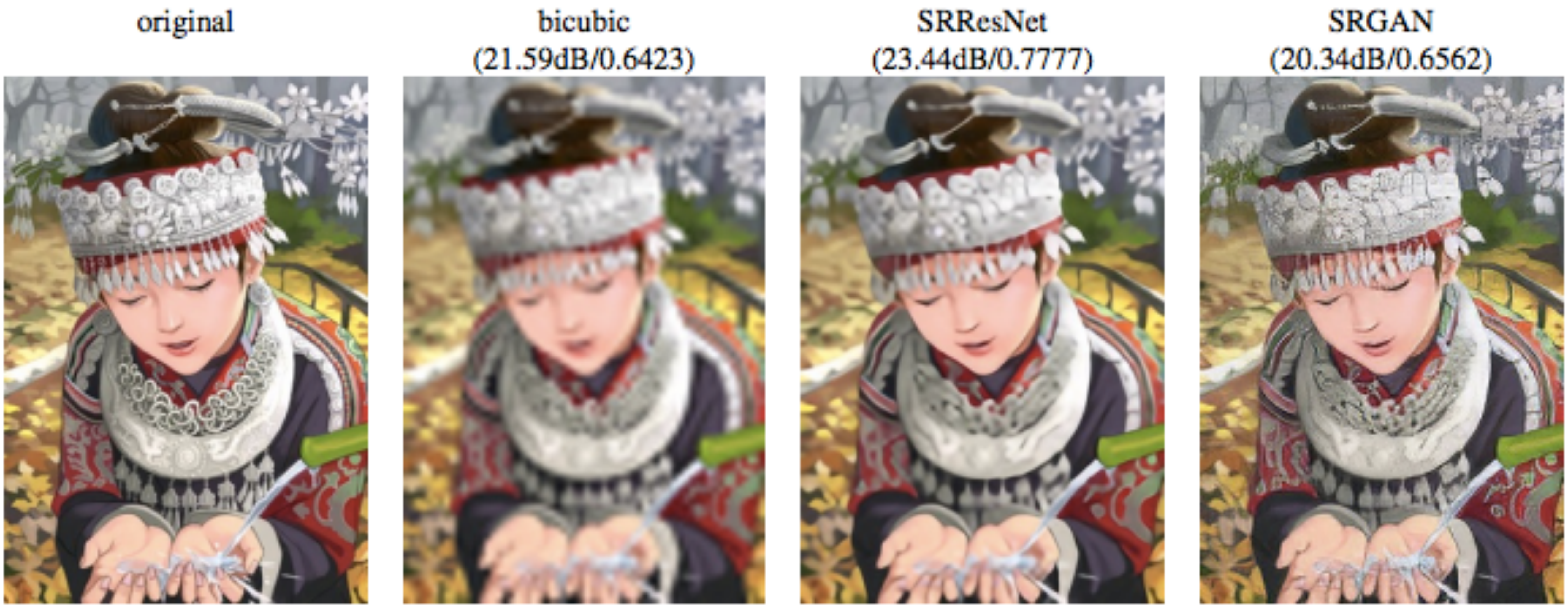
Next Video Frame Prediction

Ground Truth MSE Adversarial



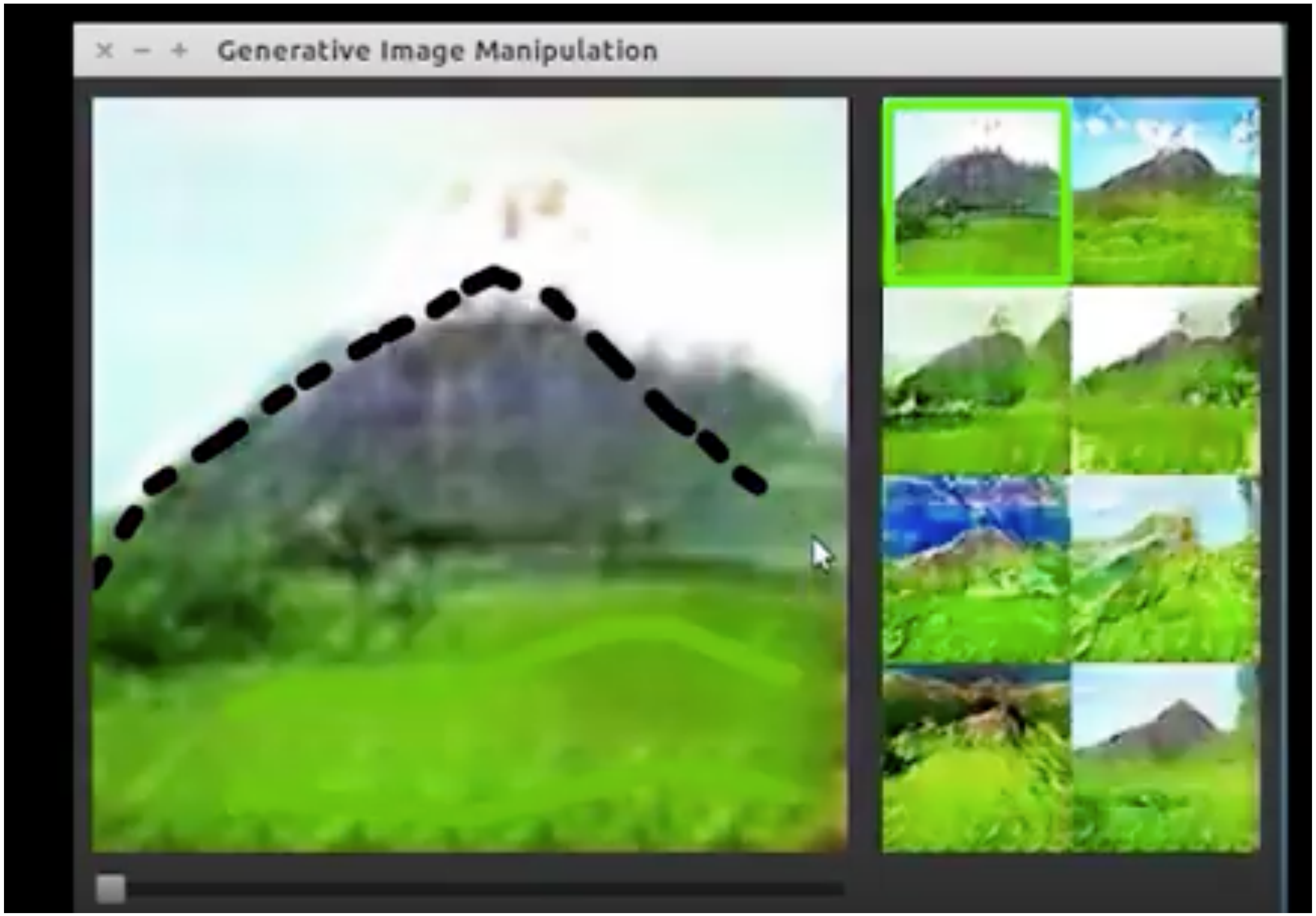
(Lotter et al 2016)

Single Image Super-Resolution



(Ledig et al 2016)

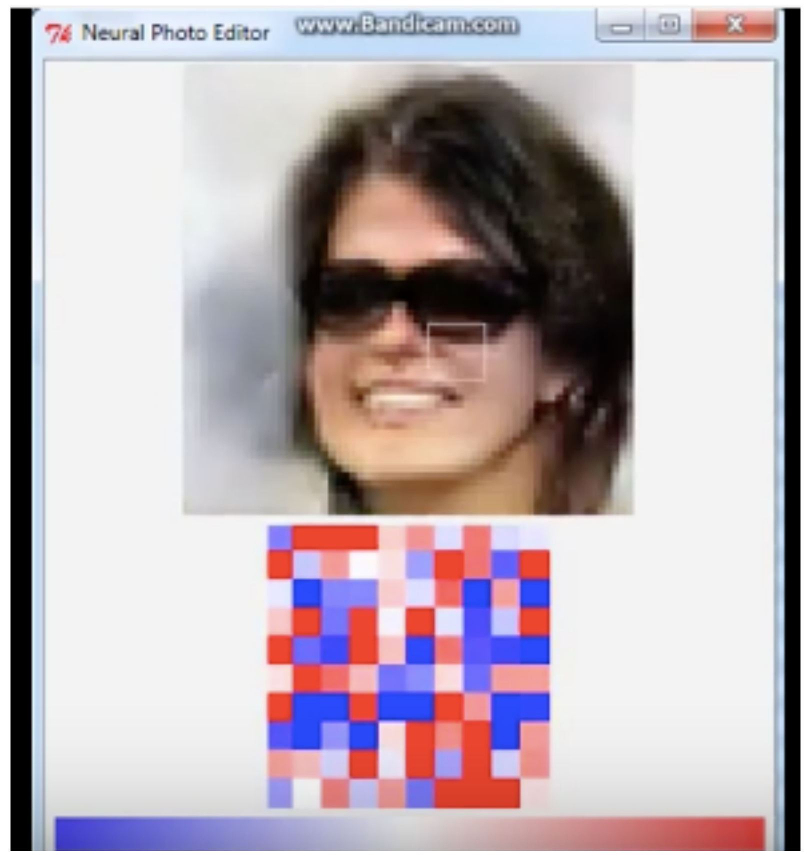
iGAN



youtube

(Zhu et al 2016)

Introspective Adversarial Networks



youtube

(Brock et al 2016)

Image to Image Translation

(Isola et al 2016)

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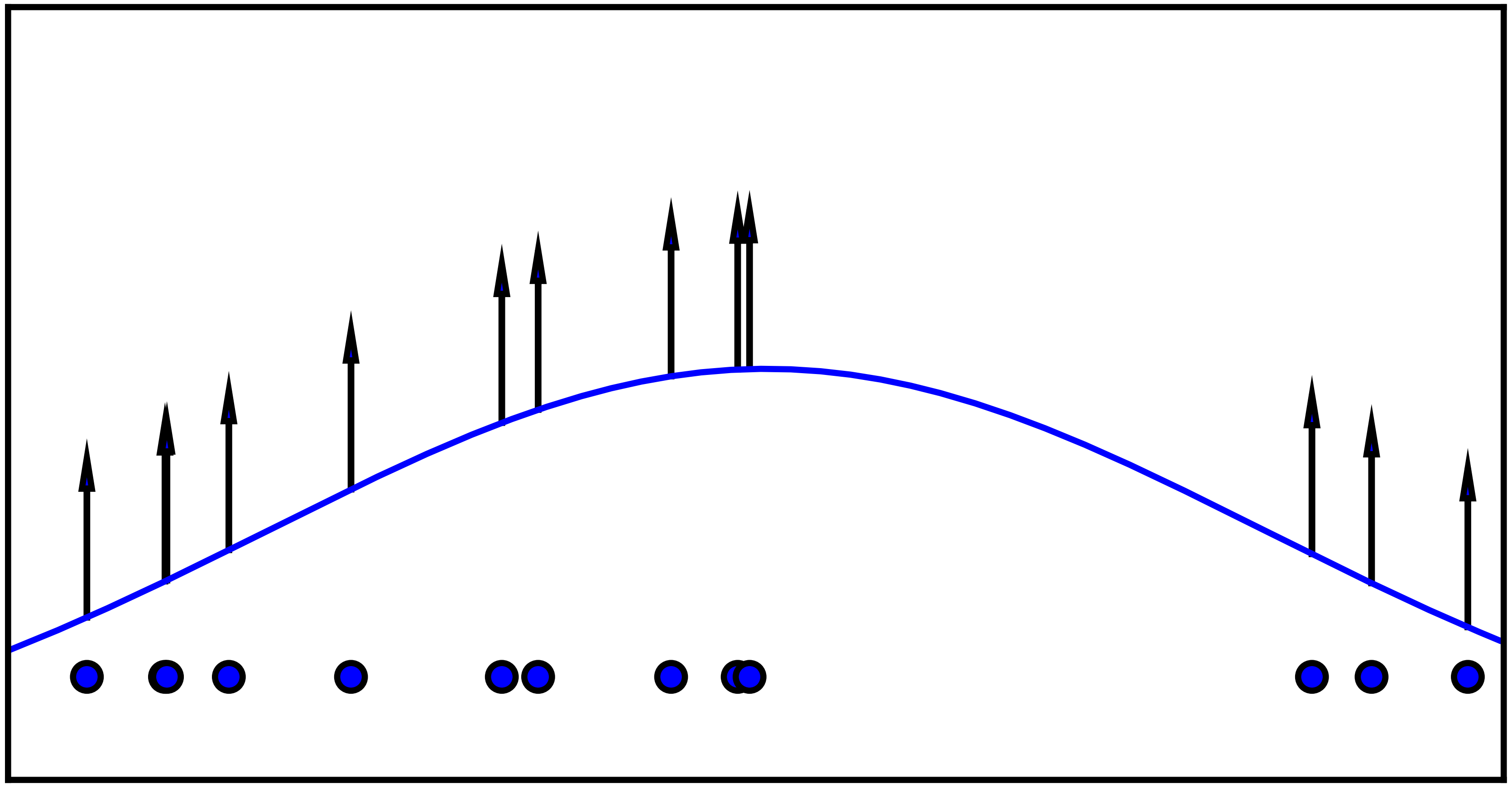
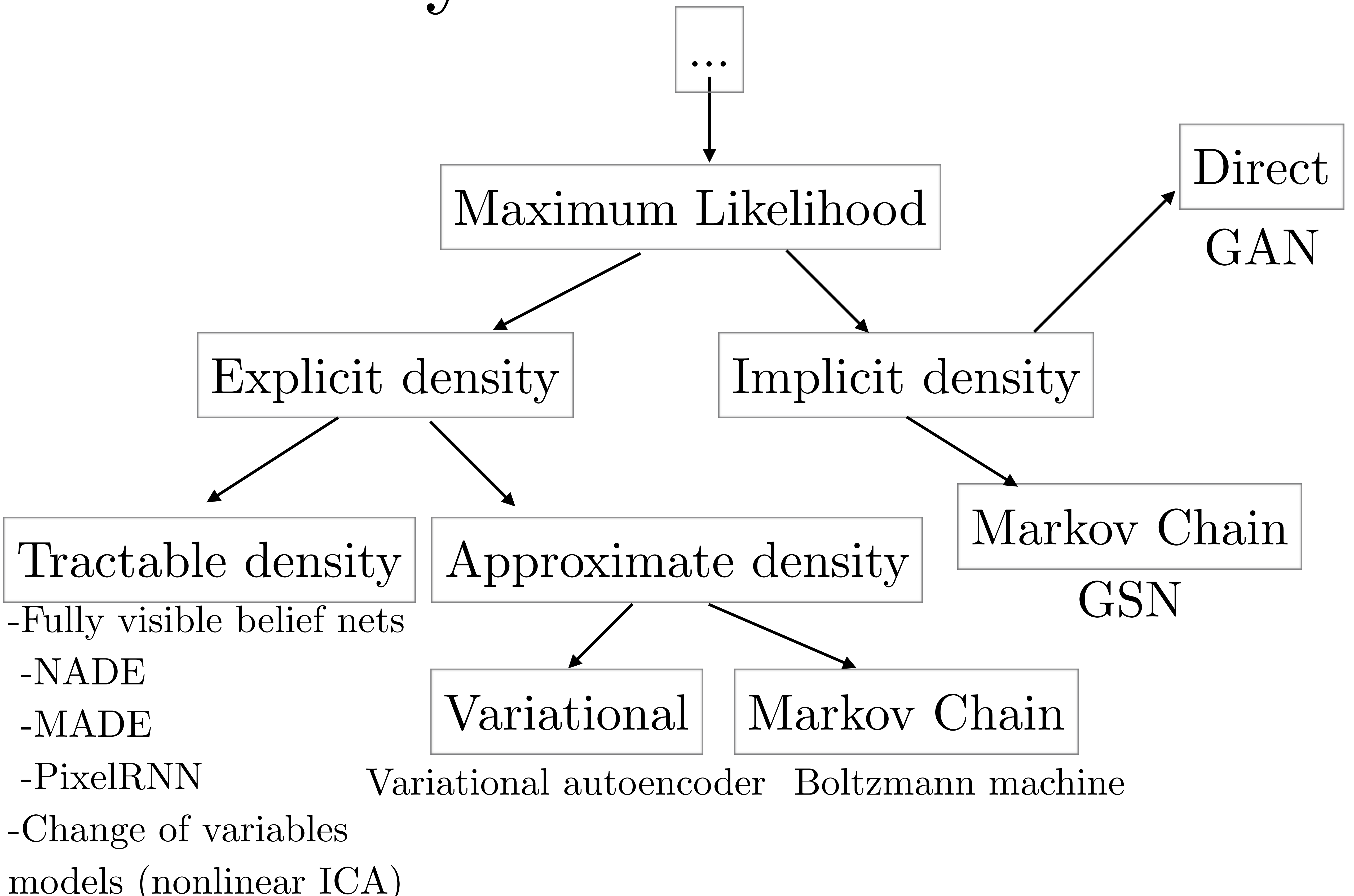
Maximum Likelihood



$$\boldsymbol{\theta}^* = \arg\max_{\boldsymbol{\theta}} \mathbb{E}_{x \sim p_{\text{data}}} \log p_{\text{model}}(\boldsymbol{x} \mid \boldsymbol{\theta})$$

(Goodfellow 2016)

Taxonomy of Generative Models



(Goodfellow 2016)

Fully Visible Belief Nets

- Explicit formula based on chain rule: (Frey et al, 1996)

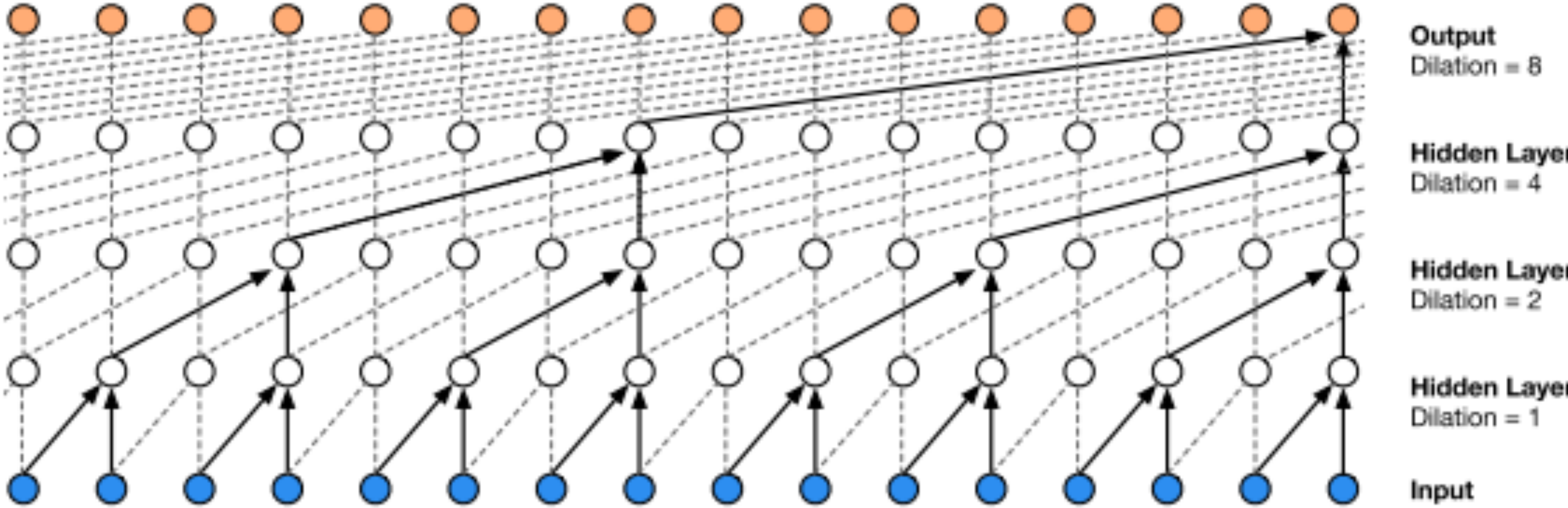
$$p_{\text{model}}(\boldsymbol{x}) = p_{\text{model}}(x_1) \prod_{i=2}^{n} p_{\text{model}}(x_i \mid x_1, \ldots, x_{i-1})$$

- Disadvantages:
  - O(n) sample generation cost
  - Generation not controlled by a latent code

PixelCNN elephants
(van den Ord et al 2016)

(Goodfellow 2016)

WaveNet



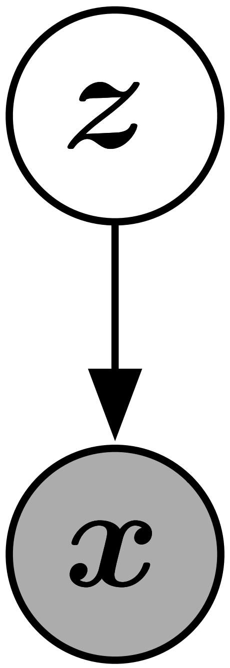
Amazing quality
Sample generation slow

Two minutes to synthesize one second of audio

(Goodfellow 2016)

Variational Autoencoder

(Kingma and Welling 2013, Rezende et al 2014)



$$\log p(\boldsymbol{x}) \geq \log p(\boldsymbol{x}) - D_{\mathrm{KL}}\left(q(\boldsymbol{z}) \| p(\boldsymbol{z} \mid \boldsymbol{x})\right)$$
$$= \mathbb{E}_{\boldsymbol{z} \sim q} \log p(\boldsymbol{x}, \boldsymbol{z}) + H(q)$$

CIFAR-10 samples
(Kingma et al 2016)

Disadvantages:
-Not asymptotically consistent unless q is perfect
-Samples tend to have lower quality

GANs

- Use a latent code
- Asymptotically consistent (unlike variational methods)
- No Markov chains needed
- Often regarded as producing the best samples
    - No good way to quantify this

(Goodfellow 2016)

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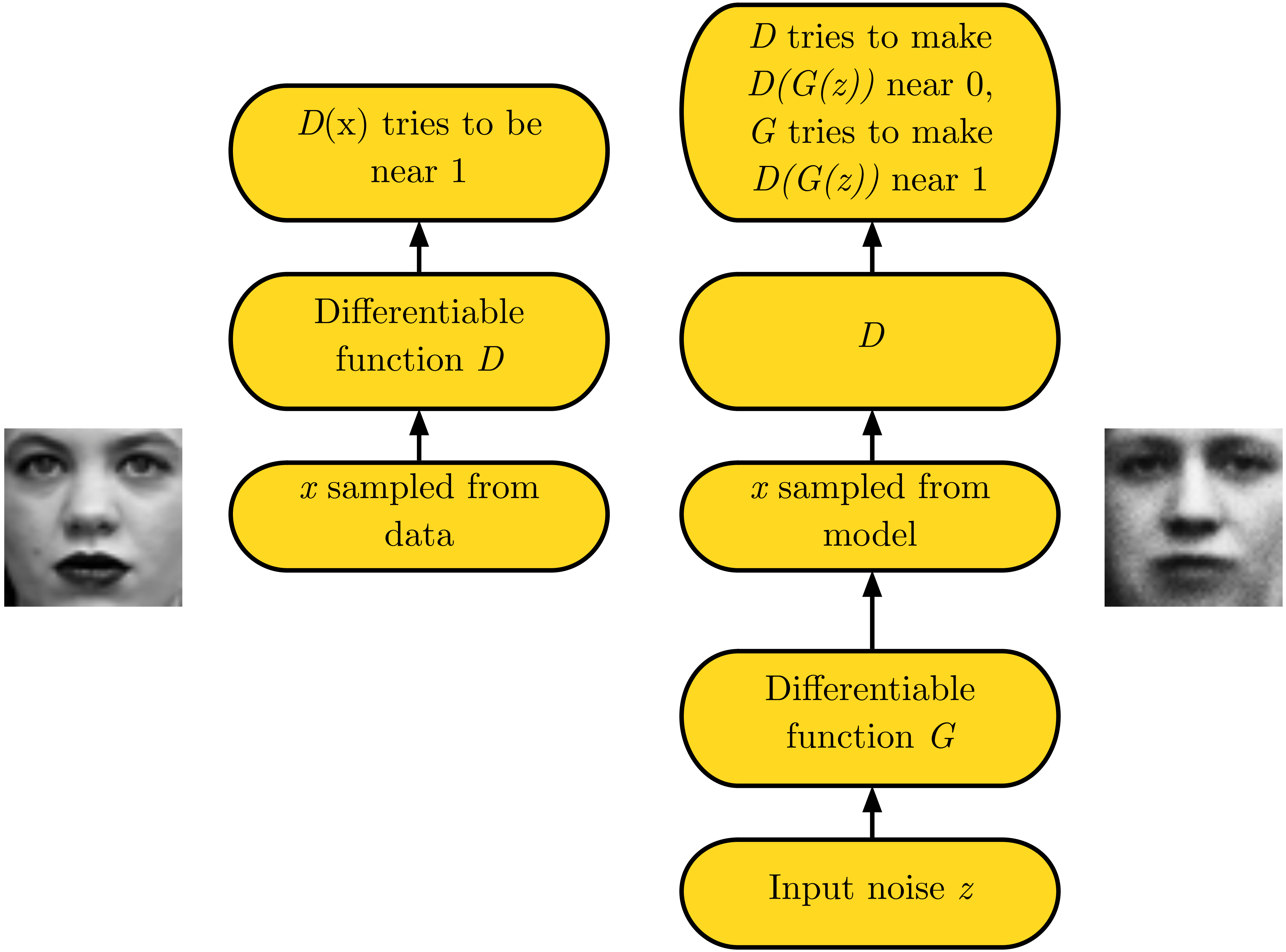
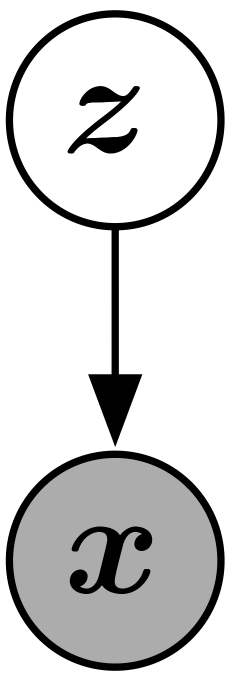
Adversarial Nets Framework



(Goodfellow 2016)

Generator Network

$$\boldsymbol{x} = G(\boldsymbol{z}; \boldsymbol{\theta}^{(G)})$$



-Must be differentiable

- No invertibility requirement
- Trainable for any size of z
- Some guarantees require z to have higher dimension than x
- Can make x conditionally Gaussian given z but need not do so

(Goodfellow 2016)

Training Procedure

- Use SGD-like algorithm of choice (Adam) on two minibatches simultaneously:
  - A minibatch of training examples
  - A minibatch of generated samples
- Optional: run k steps of one player for every step of the other player.

Minimax Game

$$J^{(D)} = -\frac{1}{2}\mathbb{E}_{\boldsymbol{x}\sim p_{\text{data}}} \log D(\boldsymbol{x}) - \frac{1}{2}\mathbb{E}_{\boldsymbol{z}} \log\left(1 - D\left(G(\boldsymbol{z})\right)\right)$$

$$J^{(G)} = -J^{(D)}$$

-Equilibrium is a saddle point of the discriminator loss

-Resembles Jensen-Shannon divergence

-Generator minimizes the log-probability of the discriminator being correct

(Goodfellow 2016)

Exercise 1

$$J^{(D)} = -\frac{1}{2}\mathbb{E}_{\boldsymbol{x}\sim p_{\text{data}}} \log D(\boldsymbol{x}) - \frac{1}{2}\mathbb{E}_{\boldsymbol{z}} \log\left(1 - D\left(G(\boldsymbol{z})\right)\right)$$
$$J^{(G)} = -J^{(D)}$$

- What is the solution to $D(x)$ in terms of p_{data} and $p_{\text{generator}}$?
- What assumptions are needed to obtain this solution?

(Goodfellow 2016)

Solution

- Assume both densities are nonzero everywhere
  - If not, some input values x are never trained, so some values of $D(x)$ have undetermined behavior.
- Solve for where the functional derivatives are zero:

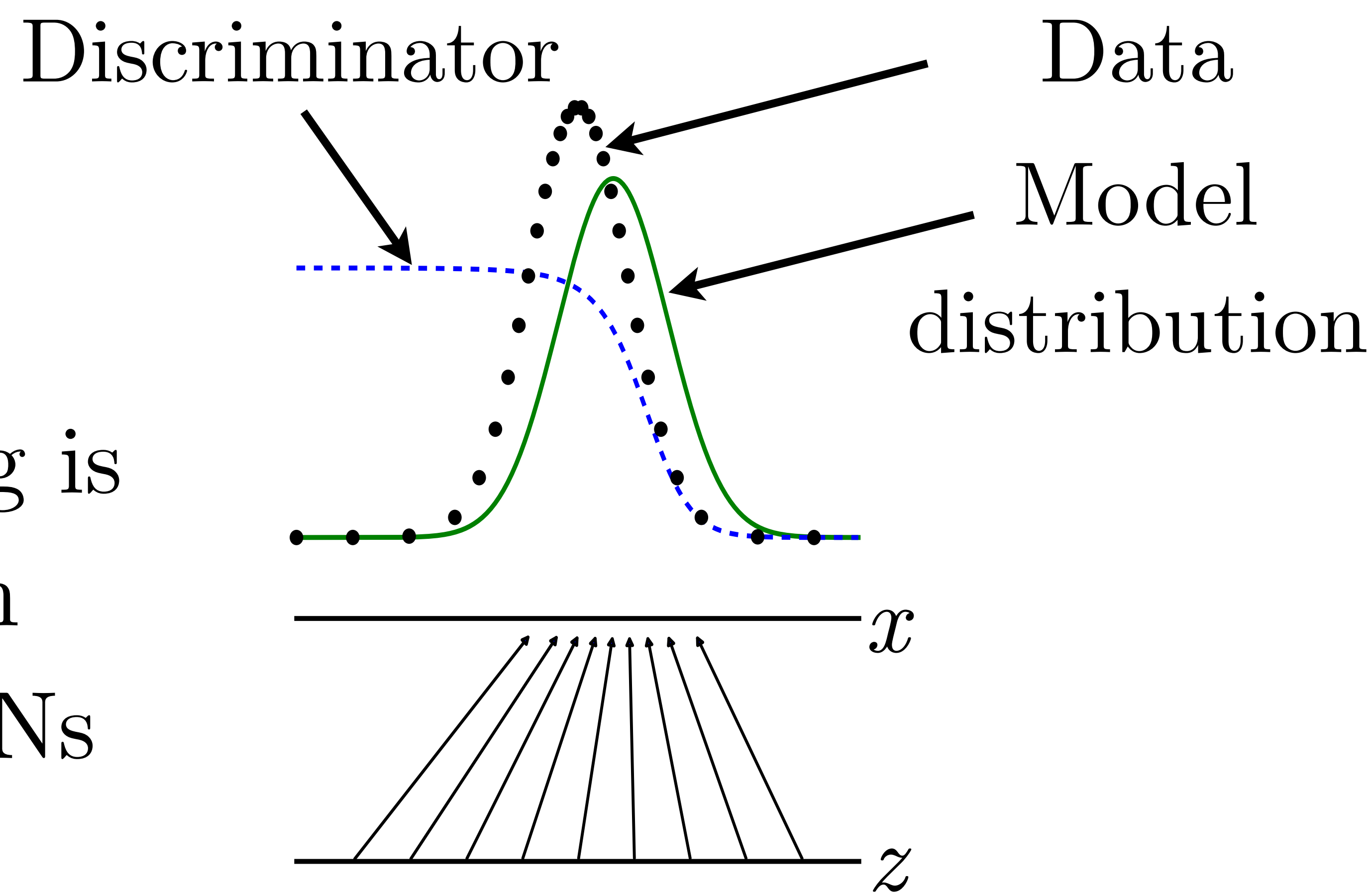
$$\frac{\delta}{\delta D(\boldsymbol{x})} J^{(D)} = 0$$

(Goodfellow 2016)

Discriminator Strategy

Optimal $D(\boldsymbol{x})$ for any $p_{\text{data}}(\boldsymbol{x})$ and $p_{\text{model}}(\boldsymbol{x})$ is always

$$D(x) = \frac{p_{\text{data}}(x)}{p_{\text{data}}(x) + p_{\text{model}}(x)}$$



Estimating this ratio using supervised learning is the key approximation mechanism used by GANs

(Goodfellow 2016)

Non-Saturating Game

$$J^{(D)} = -\frac{1}{2}\mathbb{E}_{\boldsymbol{x}\sim p_{\text{data}}} \log D(\boldsymbol{x}) - \frac{1}{2}\mathbb{E}_{\boldsymbol{z}} \log\left(1 - D\left(G(\boldsymbol{z})\right)\right)$$

$$J^{(G)} = -\frac{1}{2}\mathbb{E}_{\boldsymbol{z}} \log D\left(G(\boldsymbol{z})\right)$$

-Equilibrium no longer describable with a single loss

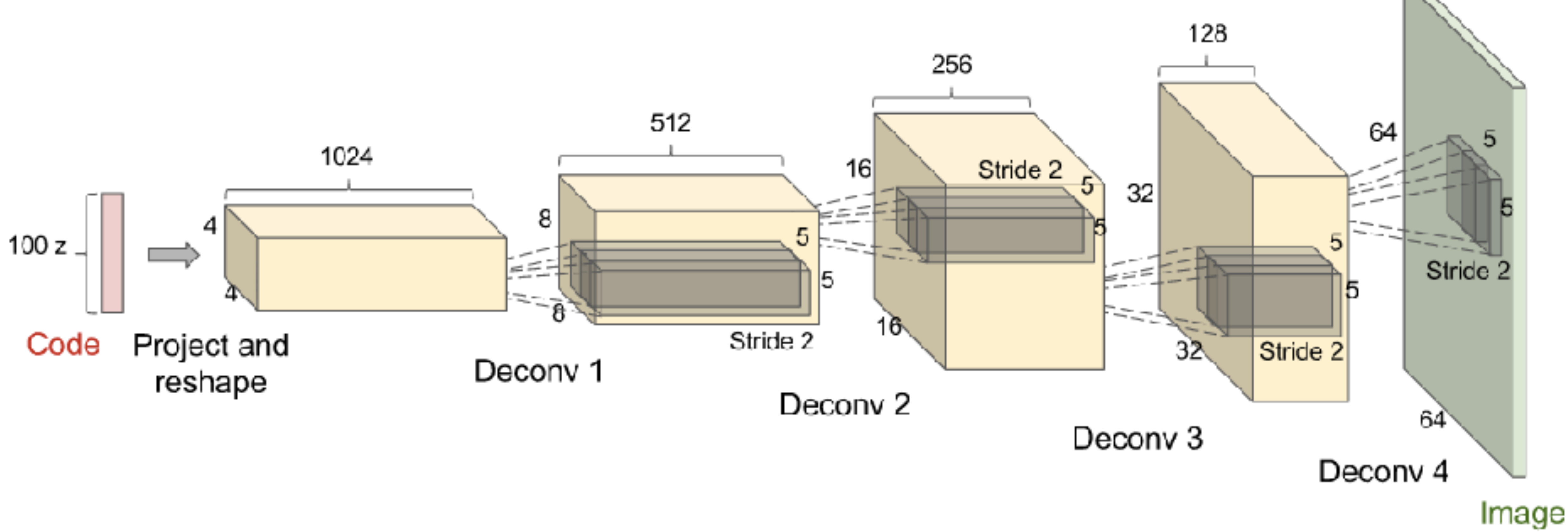
-Generator maximizes the log-probability of the discriminator being mistaken

-Heuristically motivated; generator can still learn even when discriminator successfully rejects all generator samples

(Goodfellow 2016)

DCGAN Architecture

Most "deconvs" are batch normalized

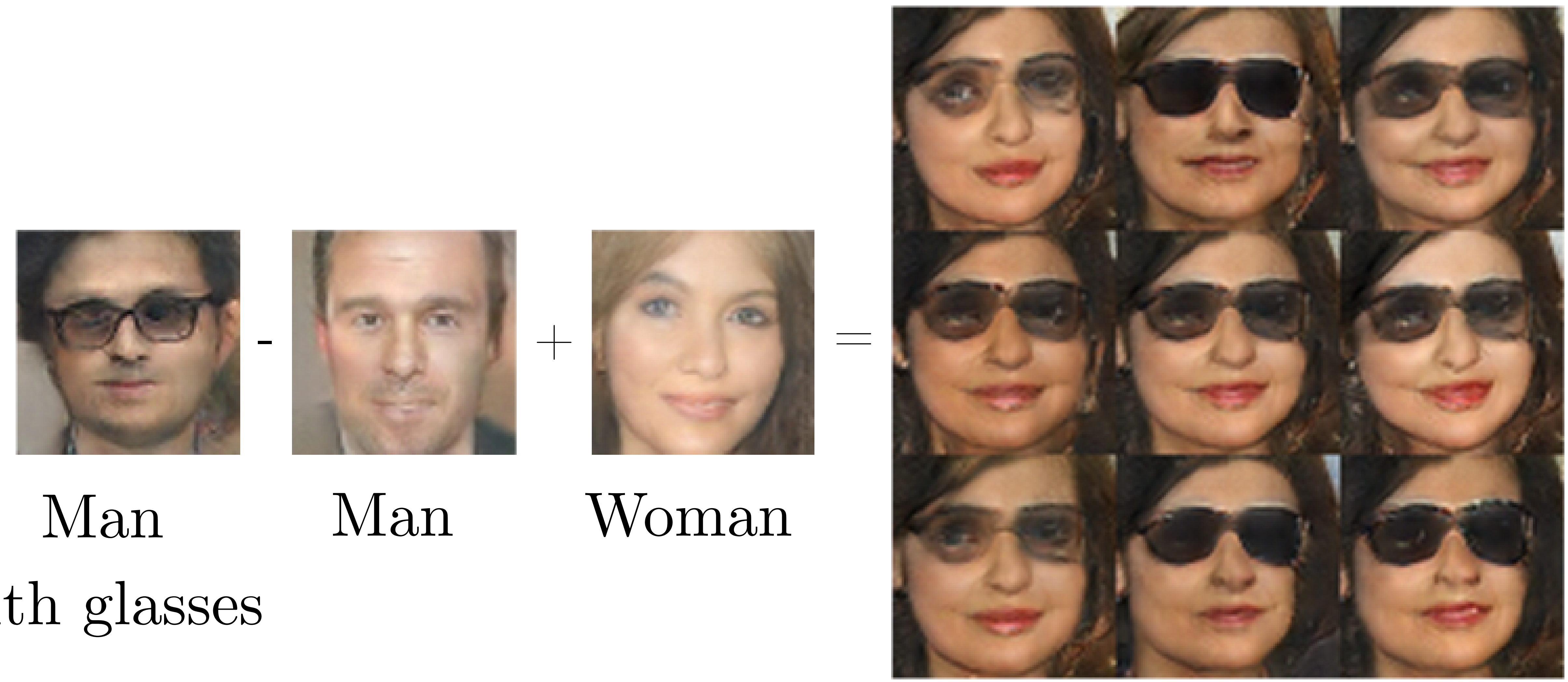


(Radford et al 2015)

DCGANs for LSUN Bedrooms

(Radford et al 2015)

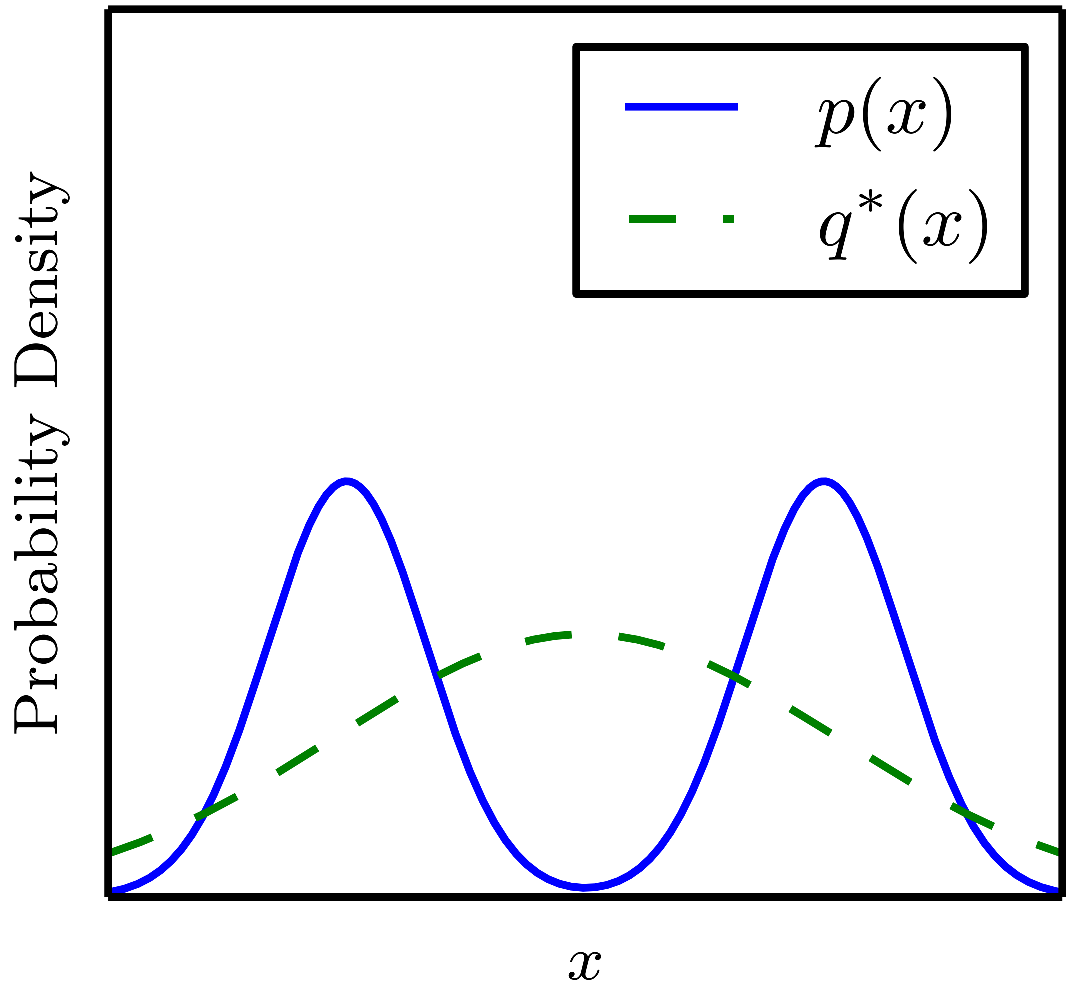
Vector Space Arithmetic



(Radford et al, 2015)

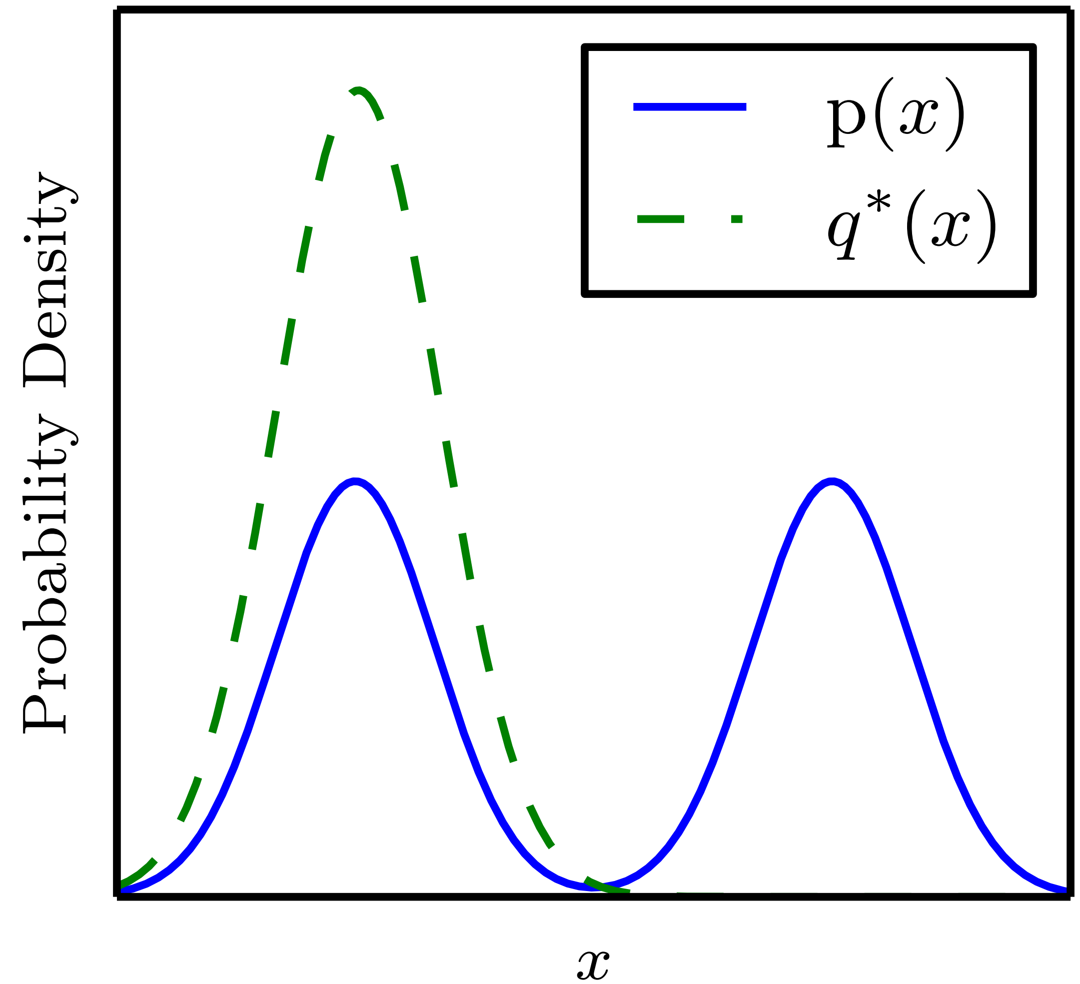
Is the divergence important?

$q^* = \text{argmin}_q D_{\text{KL}}(p\|q)$



Maximum likelihood

$q^* = \text{argmin}_q D_{\text{KL}}(q\|p)$



Reverse KL

(Goodfellow et al 2016)

Modifying GANs to do Maximum Likelihood

$$J^{(D)} = -\frac{1}{2}\mathbb{E}_{\boldsymbol{x}\sim p_{\text{data}}} \log D(\boldsymbol{x}) - \frac{1}{2}\mathbb{E}_{\boldsymbol{z}} \log\left(1 - D\left(G(\boldsymbol{z})\right)\right)$$

$$J^{(G)} = -\frac{1}{2}\mathbb{E}_{\boldsymbol{z}} \exp\left(\sigma^{-1}\left(D\left(G(\boldsymbol{z})\right)\right)\right)$$

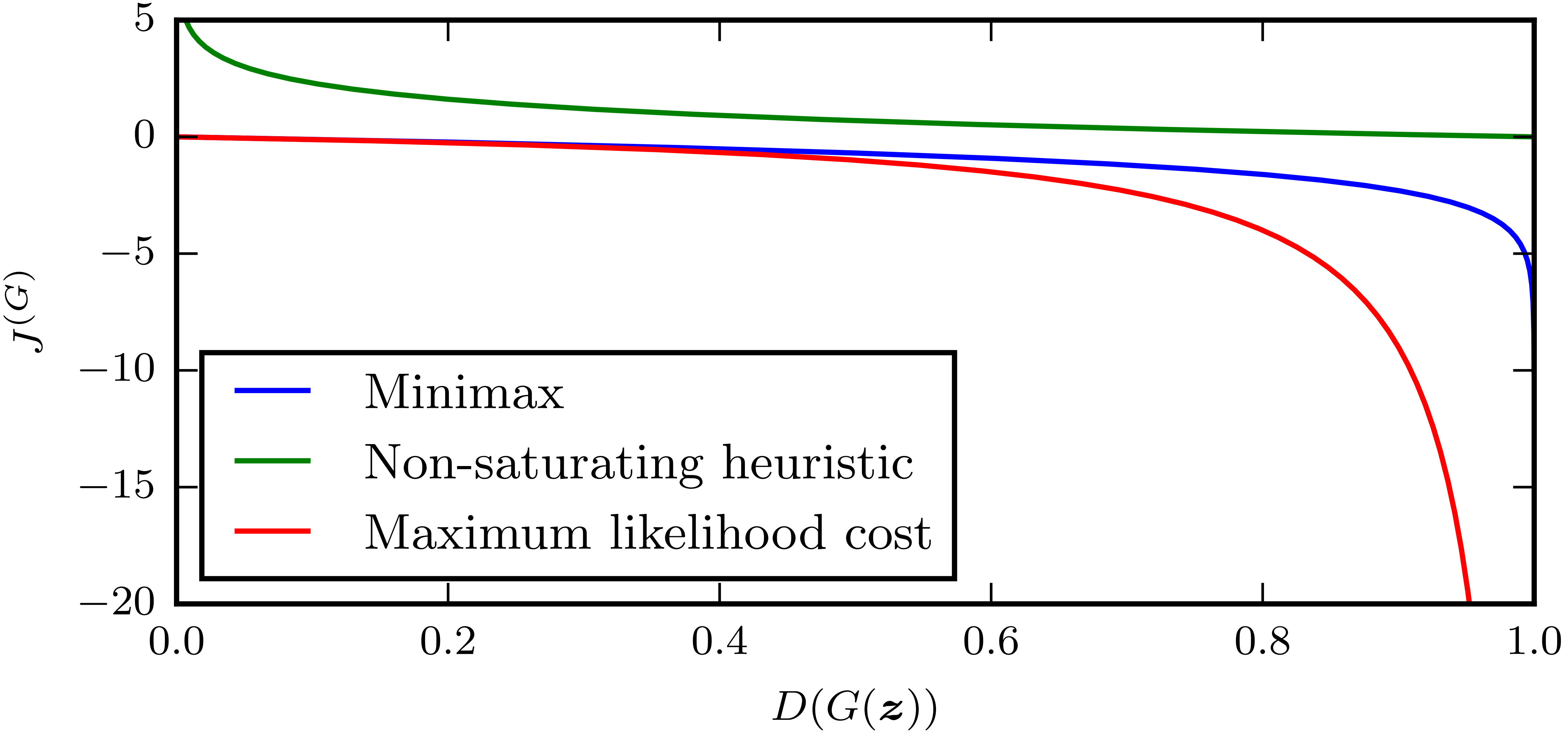
When discriminator is optimal, the generator gradient matches that of maximum likelihood

("On Distinguishability Criteria for Estimating Generative Models", Goodfellow 2014, pg 5)

Reducing GANs to RL

- Generator makes a sample
- Discriminator evaluates a sample
- Generator's cost (negative reward) is a function of $D(G(z))$
- Note that generator's cost does not include the data, x
- Generator's cost is always monotonically decreasing in $D(G(z))$
- Different divergences change the location of the cost's fastest decrease

Comparison of Generator Losses



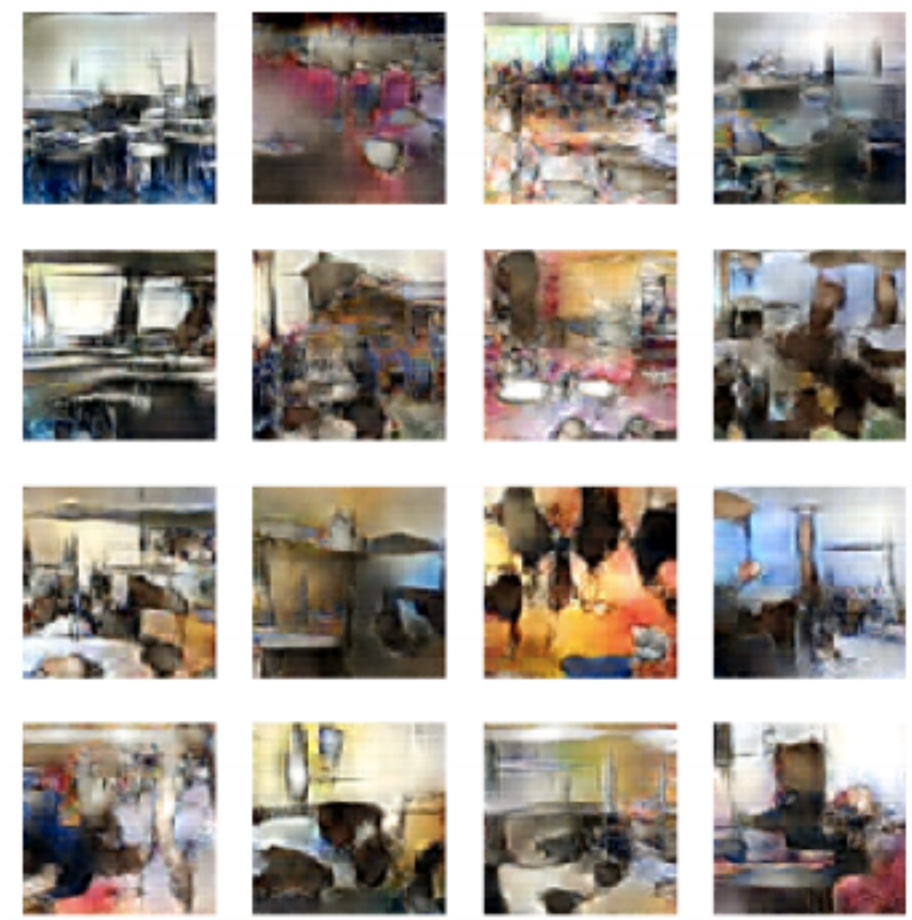
(Goodfellow 2014)

Loss does not seem to explain why GAN samples are sharp

KL

Reverse KL

(Nowozin et al 2016)



KL samples from LSUN

Takeaway: the approximation strategy matters more than the loss

(Goodfellow 2016)

Comparison to NCE, MLE

$$V(G, D) = \mathbb{E}_{p_{\text{data}}} \log D(\boldsymbol{x}) + \mathbb{E}_{p_{\text{generator}}} \left(\log\left(1 - D(\boldsymbol{x})\right)\right)$$

	NCE (Gutmann and Hyvärinen 2010)	MLE	GAN
D	$D(x) = \frac{p_{\text{model}}(\boldsymbol{x})}{p_{\text{model}}(\boldsymbol{x}) + p_{\text{generator}}(\boldsymbol{x})}$		Neural network
Goal	Learn p_{model}		Learn $p_{\text{generator}}$
G update rule	None (G is fixed)	Copy p_{model} parameters	Gradient descent on V
D update rule	Gradient ascent on V		

("On Distinguishability Criteria...", Goodfellow 2014)

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Labels improve subjective sample quality

- Learning a conditional model $p(y|x)$ often gives much better samples from all classes than learning $p(x)$ does (Denton et al 2015)

- Even just learning $p(x,y)$ makes samples from $p(x)$ look much better to a human observer (Salimans et al 2016)

- Note: this defines three categories of models (no labels, trained with labels, generating condition on labels) that should not be compared directly to each other

One-sided label smoothing

- Default discriminator cost:

```
cross_entropy(1., discriminator(data))
+ cross_entropy(0., discriminator(samples))
```

- One-sided label smoothed cost (Salimans et al 2016):

```
cross_entropy(.9, discriminator(data))
+ cross_entropy(0., discriminator(samples))
```

(Goodfellow 2016)

Do not smooth negative labels

```
cross_entropy(1.-alpha, discriminator(data))
+ cross_entropy(beta, discriminator(samples))
```

Reinforces current generator behavior

$$D(\boldsymbol{x}) = \frac{(1-\alpha)p_{\text{data}}(\boldsymbol{x}) + \beta p_{\text{model}}(\boldsymbol{x})}{p_{\text{data}}(\boldsymbol{x}) + p_{\text{model}}(\boldsymbol{x})}$$

Benefits of label smoothing

- Good regularizer (Szegedy et al 2015)
- Does not reduce classification accuracy, only confidence
- Benefits specific to GANs:
  - Prevents discriminator from giving very large gradient signal to generator
  - Prevents extrapolating to encourage extreme samples

Batch Norm

- Given inputs $X=\{x^{(1)}, x^{(2)}, .., x^{(m)}\}$
- Compute mean and standard deviation of features of X
- Normalize features (subtract mean, divide by standard deviation)
- Normalization operation is part of the graph
  - Backpropagation computes the gradient through the normalization
  - This avoids wasting time repeatedly learning to undo the normalization

(Goodfellow 2016)

Batch norm in G can cause strong intra-batch correlation

(Goodfellow 2016)

Reference Batch Norm

- Fix a *reference batch* $R=\{r^{(1)}, r^{(2)}, .., r^{(m)}\}$
- Given new inputs $X=\{x^{(1)}, x^{(2)}, .., x^{(m)}\}$
- Compute mean and standard deviation of features of R
  - Note that though R does not change, the feature values change when the parameters change
- Normalize the features of X using the mean and standard deviation from R
- Every $x^{(i)}$ is always treated the same, regardless of which other examples appear in the minibatch

Virtual Batch Norm

- Reference batch norm can overfit to the reference batch. A partial solution is *virtual batch norm*
- Fix a *reference batch* $R=\{r^{(1)}, r^{(2)}, .., r^{(m)}\}$
- Given new inputs $X=\{x^{(1)}, x^{(2)}, .., x^{(m)}\}$
- For each $x^{(i)}$ in X:
    - Construct a *virtual batch* V containing both $x^{(i)}$ and all of R
    - Compute mean and standard deviation of features of V
    - Normalize the features of $x^{(i)}$ using the mean and standard deviation from V

(Goodfellow 2016)

Balancing G and D

- Usually the discriminator “wins”
- This is a good thing—the theoretical justifications are based on assuming D is perfect
- Usually D is bigger and deeper than G
- Sometimes run D more often than G. Mixed results.
- Do not try to limit D to avoid making it “too smart”
  - Use non-saturating cost
  - Use label smoothing

(Goodfellow 2016)

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Non-convergence

- Optimization algorithms often approach a saddle point or local minimum rather than a global minimum

- Game solving algorithms may not approach an equilibrium at all

Exercise 2

- For scalar x and y, consider the value function:

$$V(x, y) = xy$$

- Does this game have an equilibrium? Where is it?

- Consider the learning dynamics of simultaneous gradient descent with infinitesimal learning rate (continuous time). Solve for the trajectory followed by these dynamics.

$$\frac{\partial x}{\partial t} = -\frac{\partial}{\partial x} V(x(t), y(t))$$

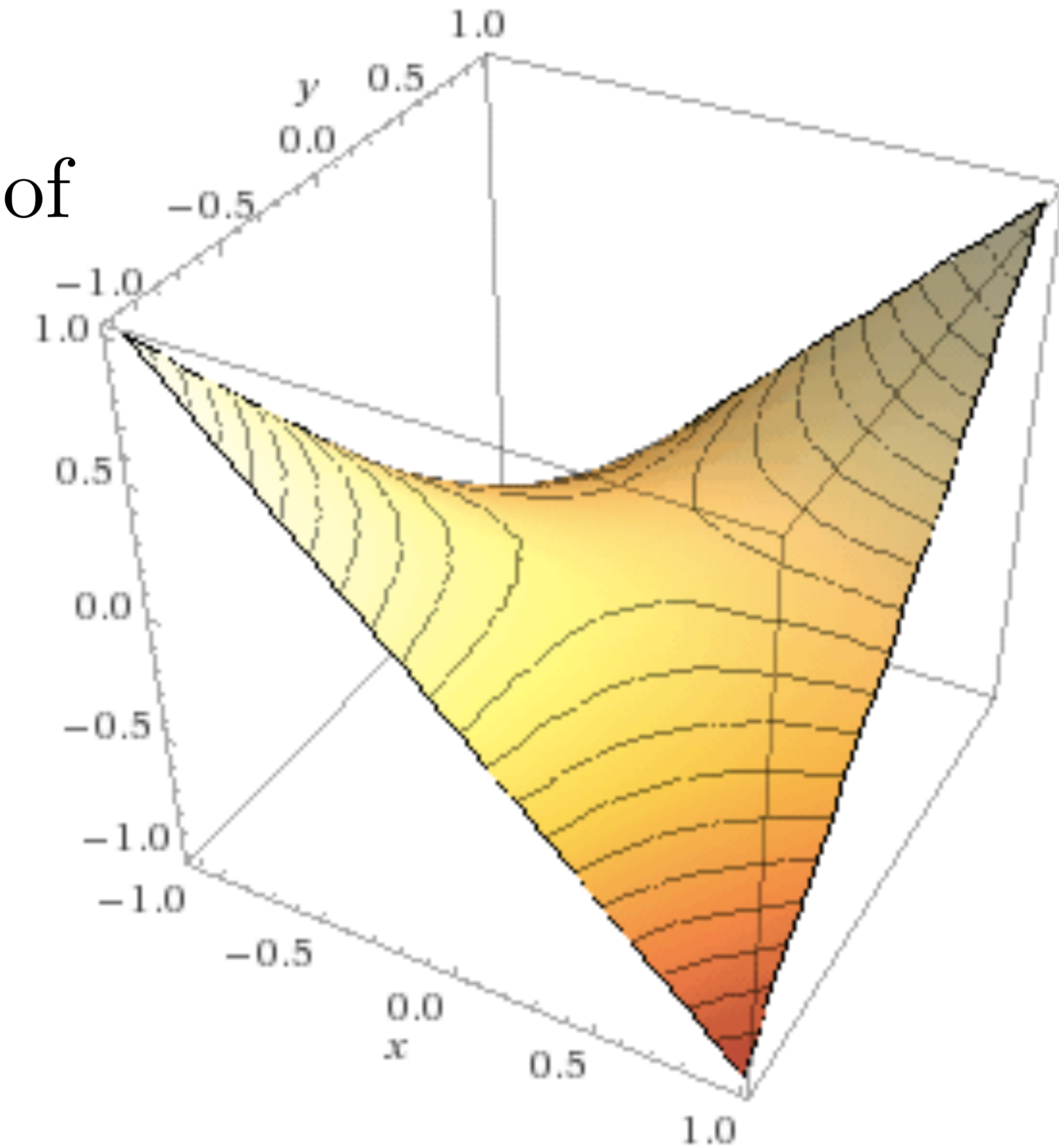
$$\frac{\partial y}{\partial t} = \frac{\partial}{\partial y} V(x(t), y(t))$$

(Goodfellow 2016)

Solution

This is the canonical example of a saddle point.

There is an equilibrium, at $x = 0$, $y = 0$.



(Goodfellow 2016)

Solution

- The gradient dynamics are:

$$\frac{\partial x}{\partial t} = -y(t)$$
$$\frac{\partial y}{\partial t} = x(t)$$

- Differentiating the second equation, we obtain:

$$\frac{\partial^2 y}{\partial t^2} = \frac{\partial x}{\partial t} = -y(t)$$

- We recognize that *y(t)* must be a sinusoid

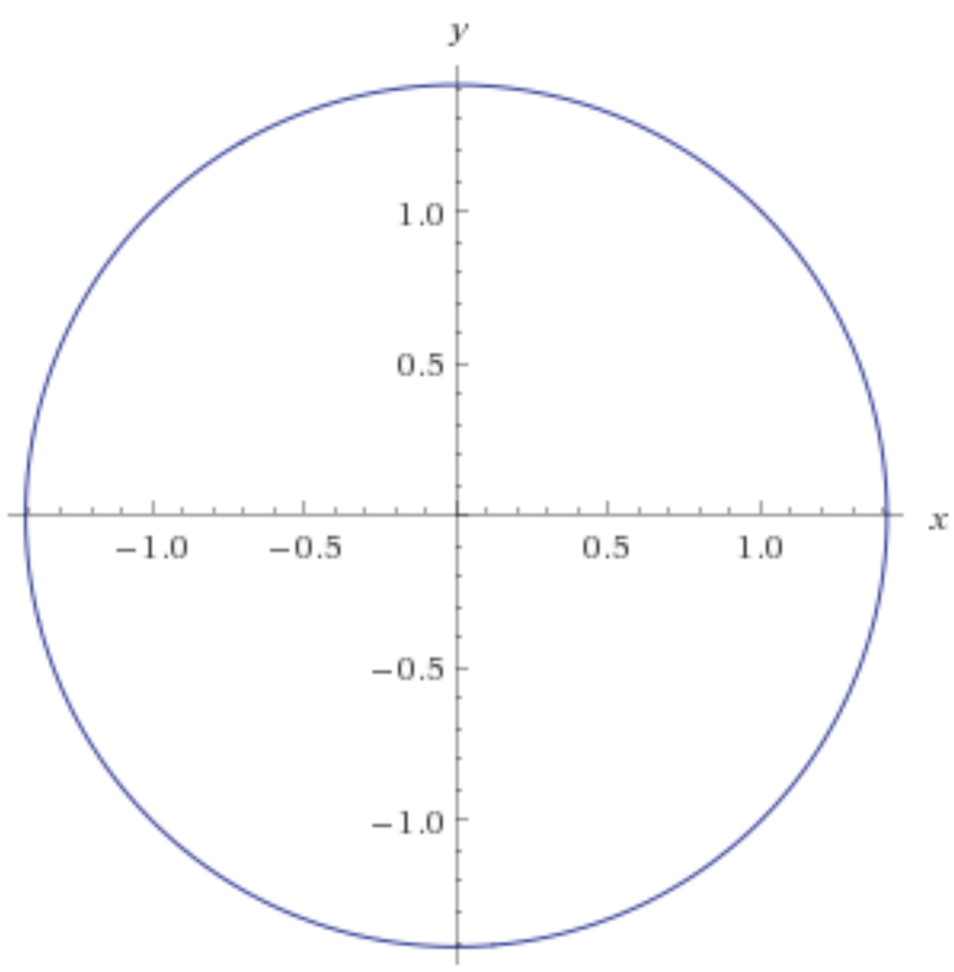
(Goodfellow 2016)

Solution

- The dynamics are a circular orbit:

$$x(t) = x(0)\cos(t) - y(0)\sin(t)$$
$$y(t) = x(0)\sin(t) + y(0)\cos(t)$$

Discrete time gradient descent can spiral outward for large step sizes



(Goodfellow 2016)

Non-convergence in GANs

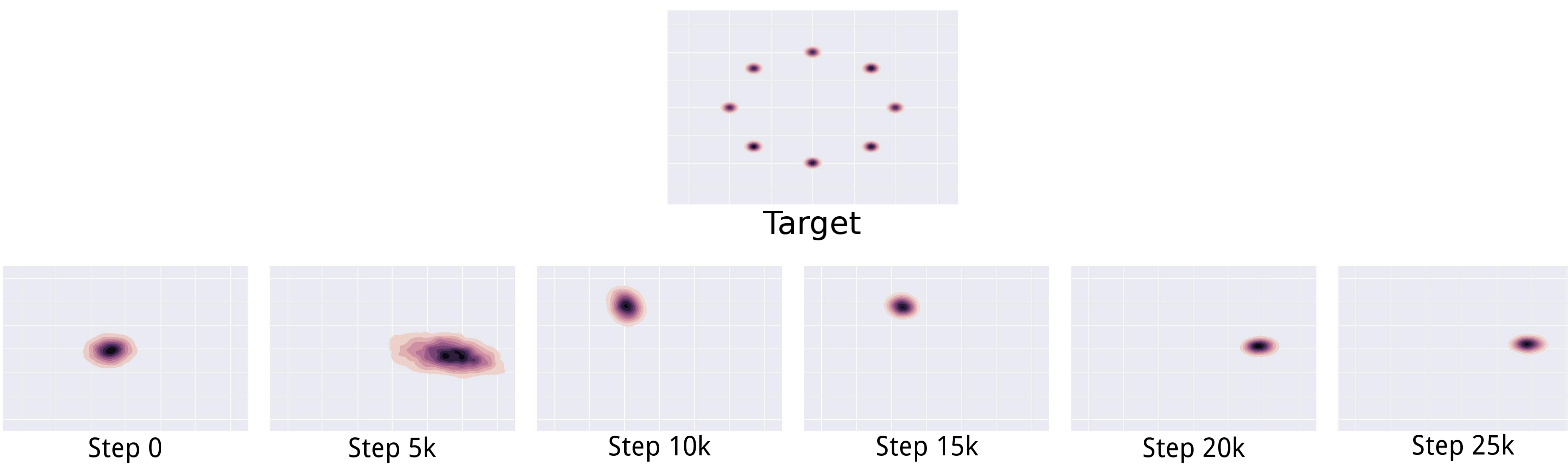
- Exploiting convexity in function space, GAN training is theoretically guaranteed to converge if we can modify the density functions directly, but:
    - Instead, we modify G (sample generation function) and D (density ratio), not densities
    - We represent G and D as highly non-convex parametric functions
- "Oscillation": can train for a very long time, generating very many different categories of samples, without clearly generating better samples
- Mode collapse: most severe form of non-convergence

(Goodfellow 2016)

Mode Collapse

$$\min_G \max_D V(G, D) \neq \max_D \min_G V(G, D)$$

- D in inner loop: convergence to correct distribution
- G in inner loop: place all mass on most likely point

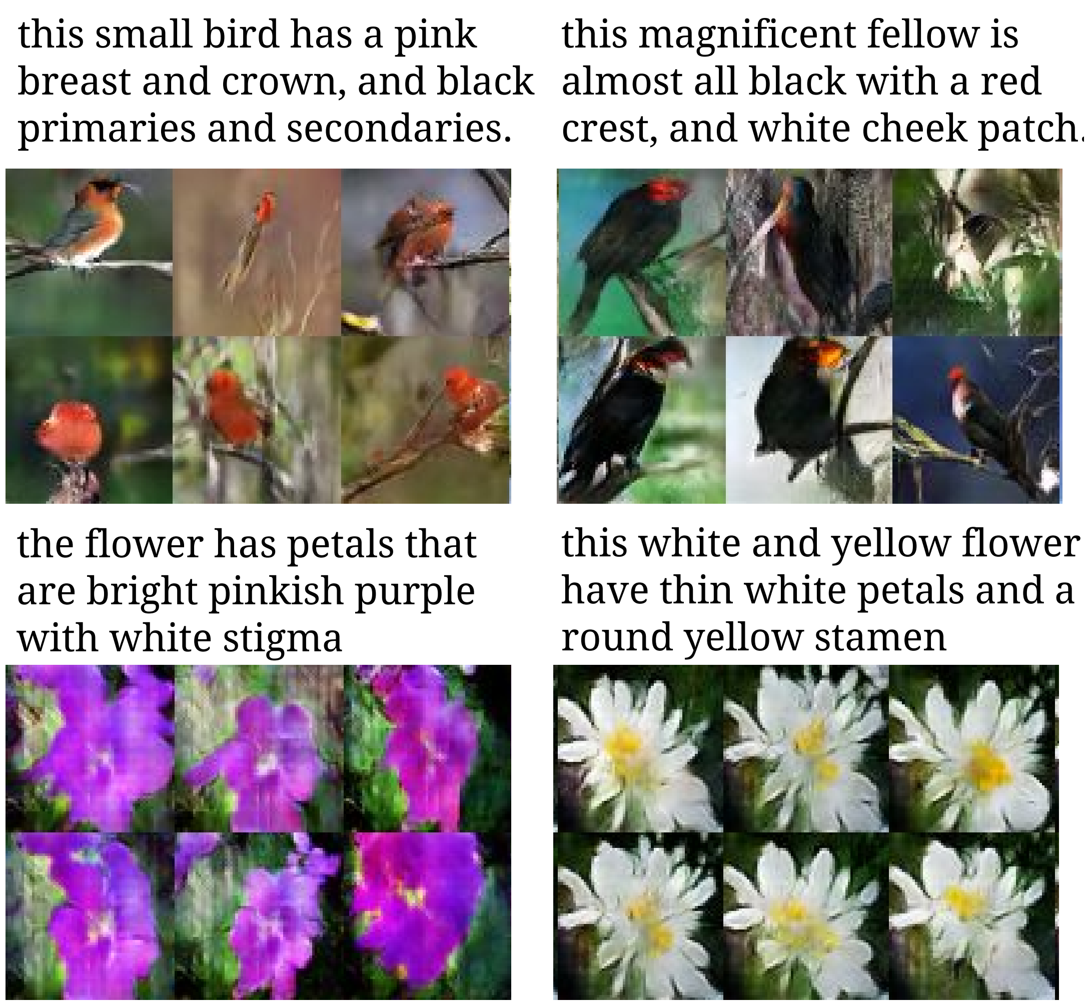


(Metz et al 2016)

Reverse KL loss does not explain mode collapse

- Other GAN losses also yield mode collapse
- Reverse KL loss prefers to fit as many modes as the model can represent and no more; it does not prefer fewer modes in general
- GANs often seem to collapse to far fewer modes than the model can represent

Mode collapse causes low output diversity



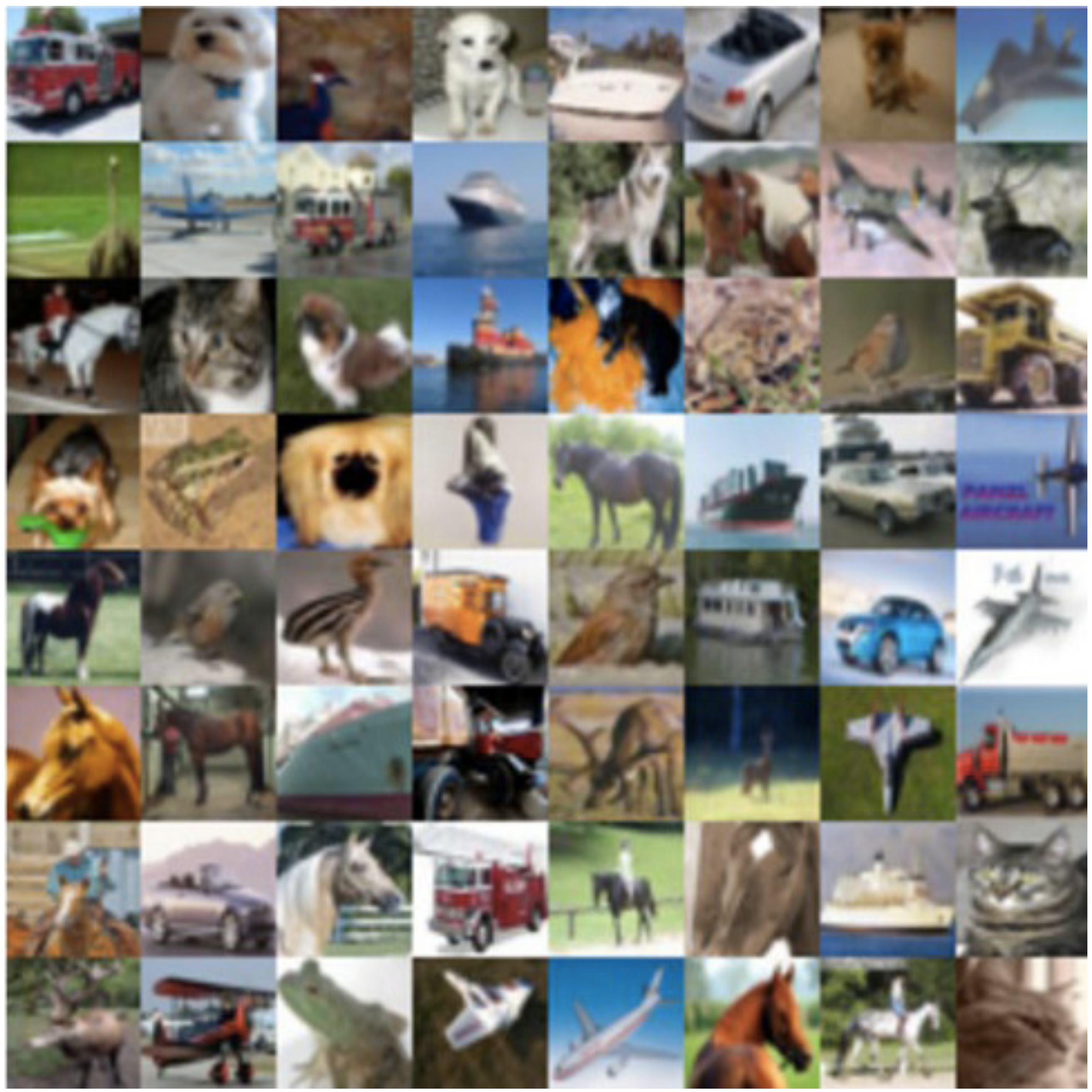
(Reed et al 2016)

(Reed et al, submitted to ICLR 2017)

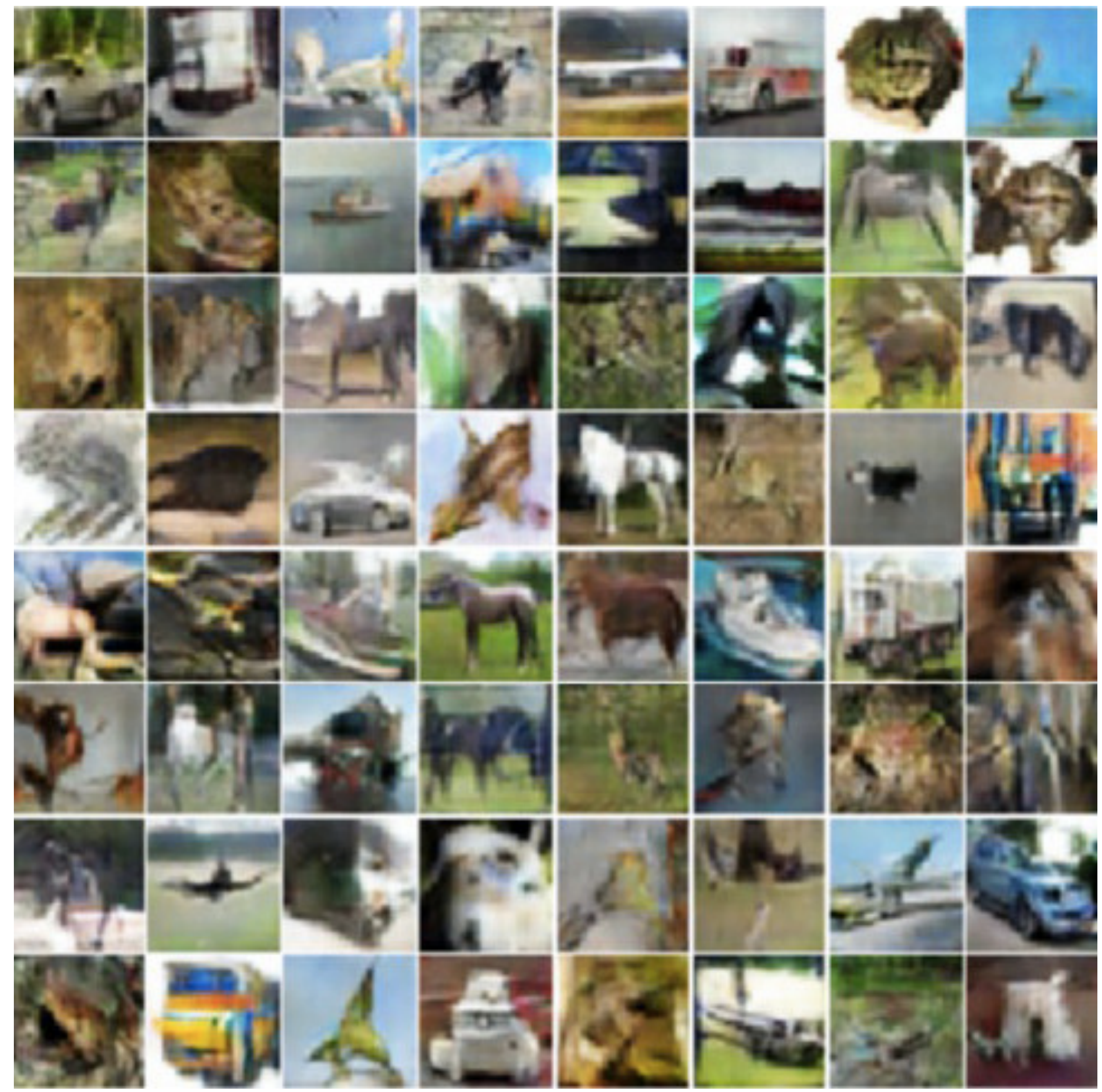
Minibatch Features

- Add minibatch features that classify each example by comparing it to other members of the minibatch (Salimans et al 2016)
- Nearest-neighbor style features detect if a minibatch contains samples that are too similar to each other

Minibatch GAN on CIFAR



Training Data

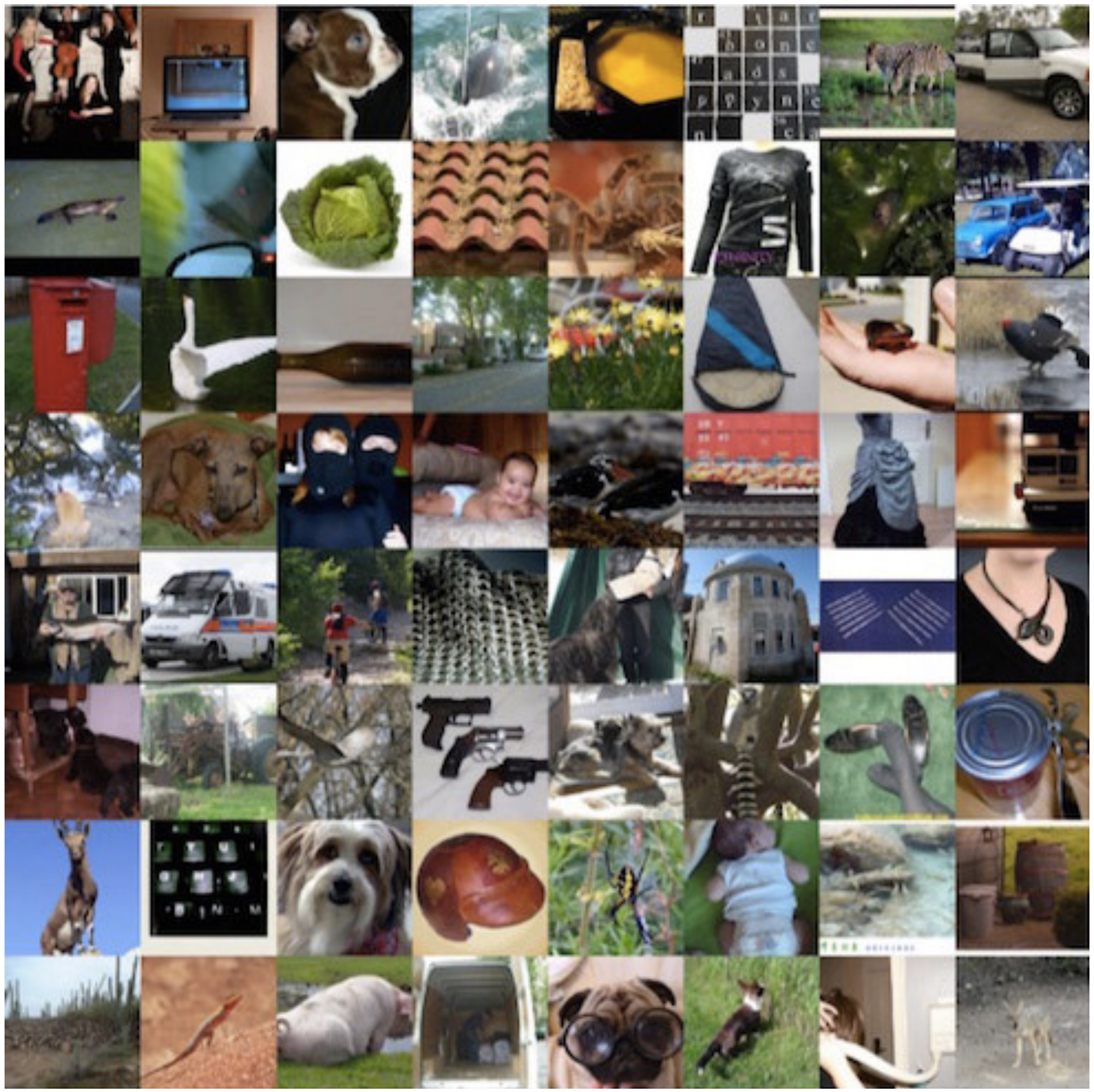


Samples

(Salimans et al 2016)

(Goodfellow 2016)

Minibatch GAN on ImageNet

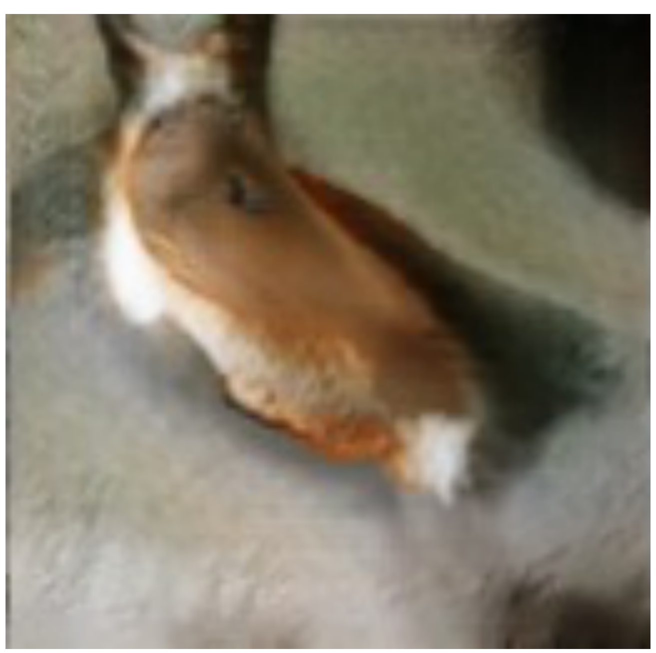


(Salimans et al 2016)

Cherry-Picked Results







(Goodfellow 2016)

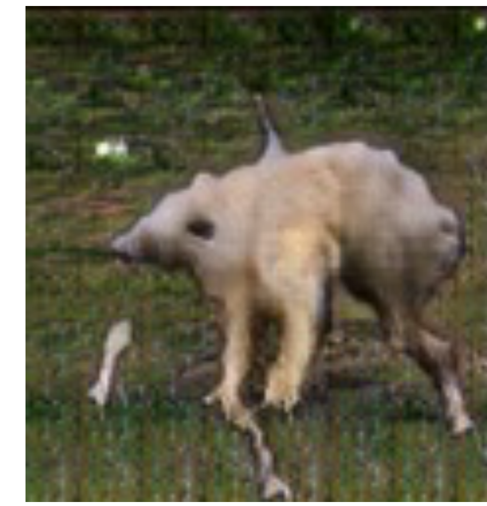
Problems with Counting

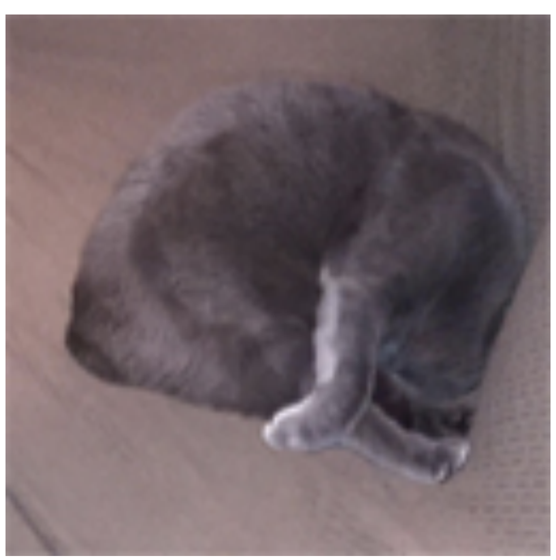


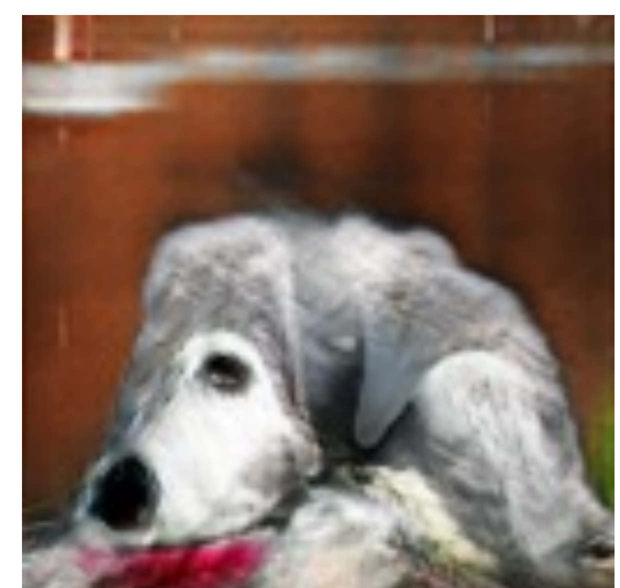



(Goodfellow 2016)

Problems with Perspective

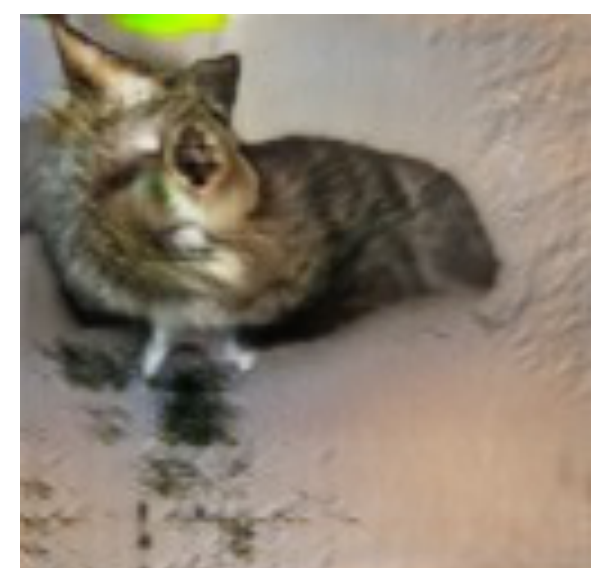






(Goodfellow 2016)

Problems with Global Structure



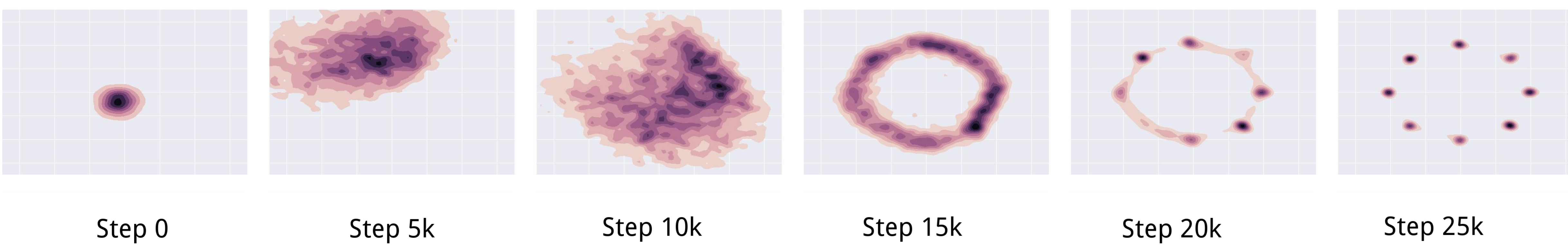
(Goodfellow 2016)

This one is real

(Goodfellow 2016)

Unrolled GANs

- Backprop through k updates of the discriminator to prevent mode collapse:



(Metz et al 2016)

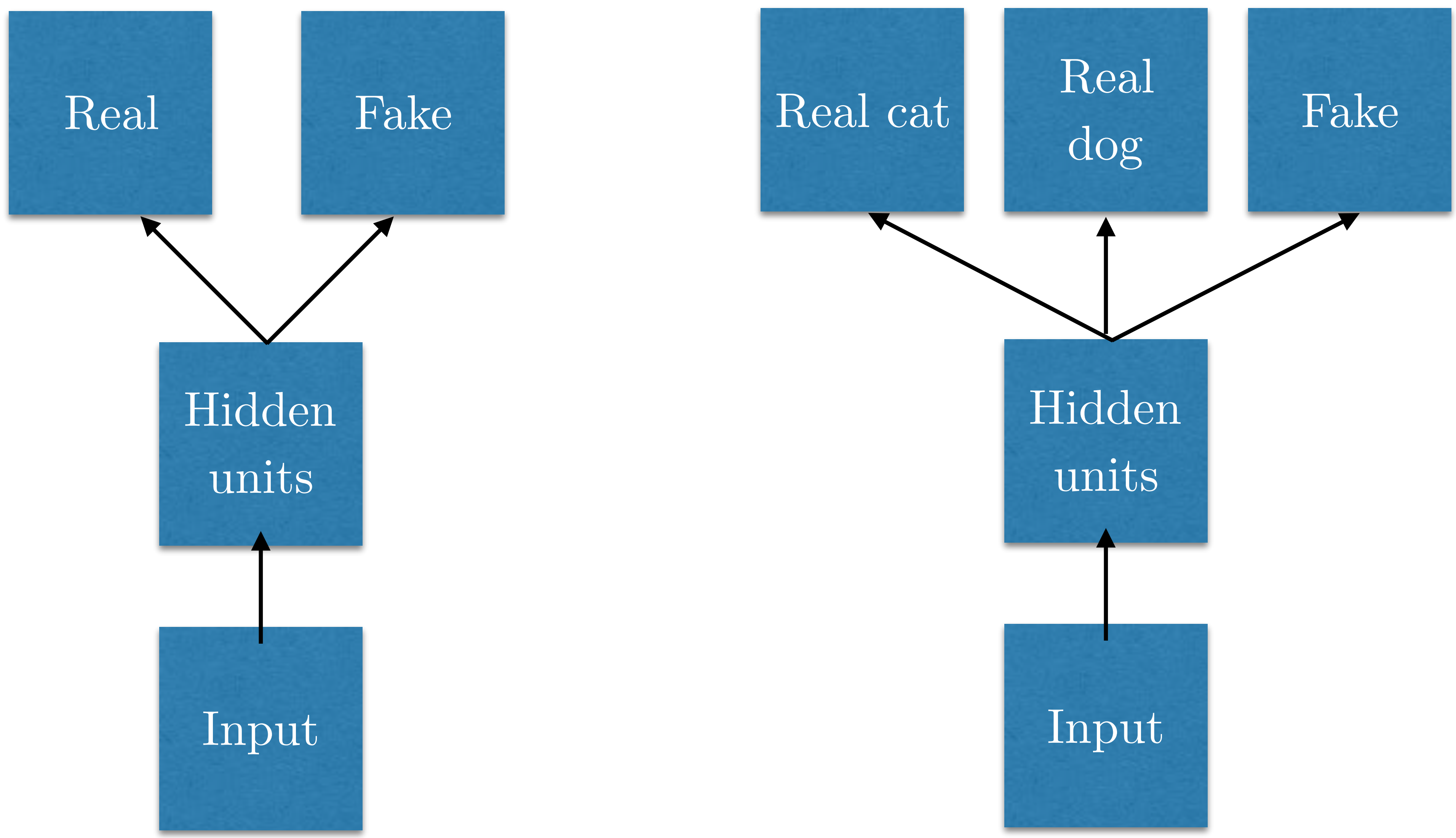
Evaluation

- There is not any single compelling way to evaluate a generative model
  - Models with good likelihood can produce bad samples
  - Models with good samples can have bad likelihood
  - There is not a good way to quantify how good samples are
- For GANs, it is also hard to even estimate the likelihood
- See "A note on the evaluation of generative models," Theis et al 2015, for a good overview

Discrete outputs

- G must be differentiable
- Cannot be differentiable if output is discrete
- Possible workarounds:
  - REINFORCE (Williams 1992)
  - Concrete distribution (Maddison et al 2016) or Gumbel-softmax (Jang et al 2016)
  - Learn distribution over continuous embeddings, decode to discrete

Supervised Discriminator



(Odena 2016, Salimans et al 2016)

Semi-Supervised Classification

MNIST (Permutation Invariant)

Model	Number of incorrectly predicted test examples for a given number of labeled samples			
	20	50	100	200
DGN [21]			333 ± 14	
Virtual Adversarial [22]			212	
CatGAN [14]			191 ± 10	
Skip Deep Generative Model [23]			132 ± 7	
Ladder network [24]			106 ± 37	
Auxiliary Deep Generative Model [23]			96 ± 2	
Our model	1677 ± 452	221 ± 136	93 ± 6.5	90 ± 4.2
Ensemble of 10 of our models	1134 ± 445	142 ± 96	86 ± 5.6	81 ± 4.3

(Salimans et al 2016)

Semi-Supervised Classification

CIFAR-10

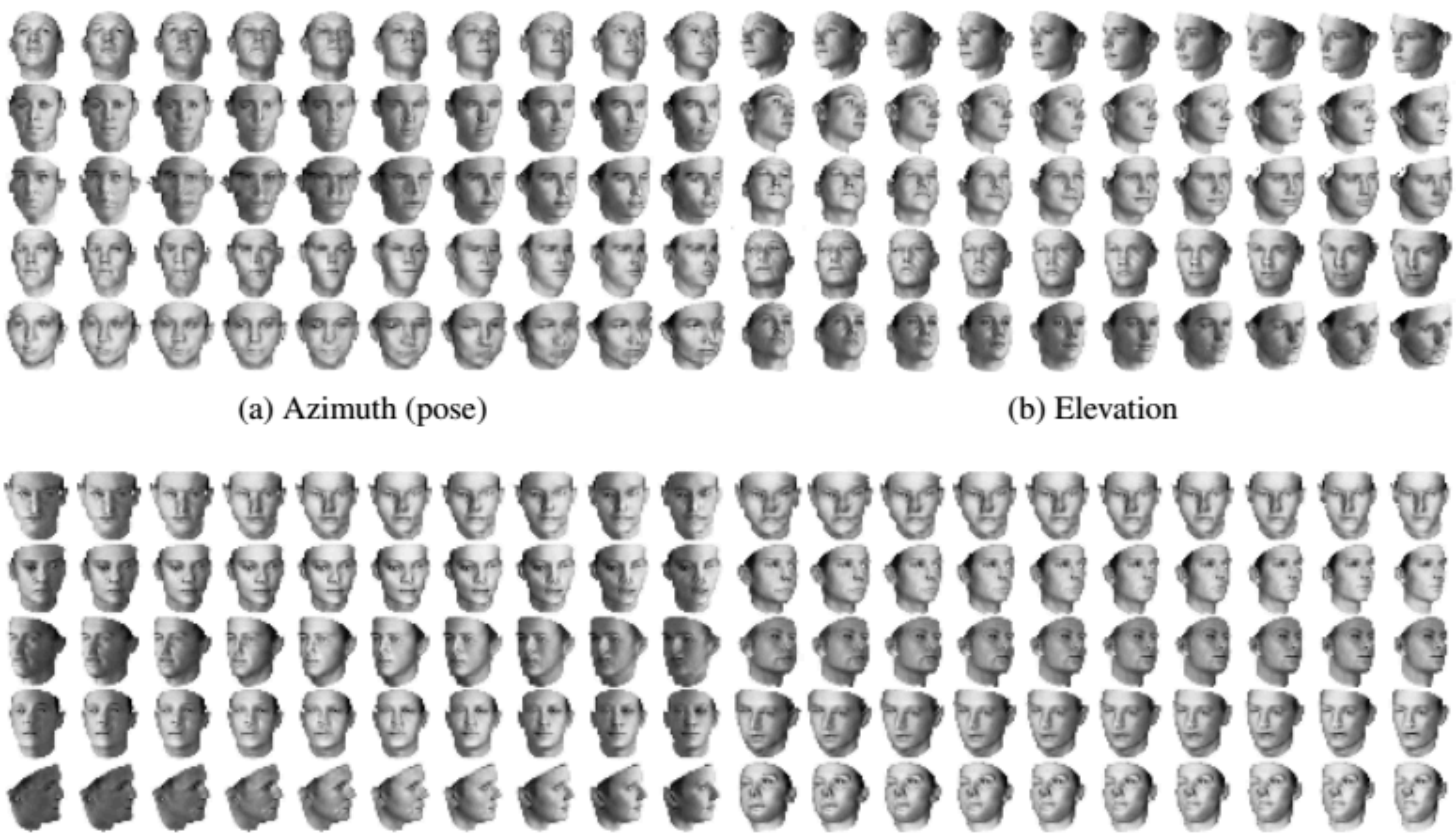
Model	Test error rate for a given number of labeled samples			
	1000	2000	4000	8000
Ladder network [24]			20.40 ± 0.47	
CatGAN [14]			19.58 ± 0.46	
Our model	21.83 ± 2.01	19.61 ± 2.09	18.63 ± 2.32	17.72 ± 1.82
Ensemble of 10 of our models	19.22 ± 0.54	17.25 ± 0.66	15.59 ± 0.47	14.87 ± 0.89

SVHN

Model	Percentage of incorrectly predicted test examples for a given number of labeled samples		
	500	1000	2000
DGN [21]		36.02 ± 0.10	
Virtual Adversarial [22]		24.63	
Auxiliary Deep Generative Model [23]		22.86	
Skip Deep Generative Model [23]		16.61 ± 0.24	
Our model	18.44 ± 4.8	8.11 ± 1.3	6.16 ± 0.58
Ensemble of 10 of our models		5.88 ± 1.0	

(Salimans et al 2016)

Learning interpretable latent codes / controlling the generation process



(a) Azimuth (pose) (b) Elevation

(c) Lighting (d) Wide or Narrow

InfoGAN (Chen et al 2016)

RL connections

- GANs interpreted as actor-critic (Pfau and Vinyals 2016)
- GANs as inverse reinforcement learning (Finn et al 2016)
- GANs for imitation learning (Ho and Ermon 2016)

Finding equilibria in games

- Simultaneous SGD on two players costs may not converge to a Nash equilibrium
- In finite spaces, fictitious play provides a better algorithm
- What to do in continuous spaces?
    - Unrolling is an expensive solution; is there a cheap one?

(Goodfellow 2016)

Other Games in AI

- Board games (checkers, chess, Go, etc.)
- Robust optimization / robust control
    - for security/safety, e.g. resisting adversarial examples
- Domain-adversarial learning for domain adaptation
- Adversarial privacy
- Guided cost learning
- ...

Exercise 3

- In this exercise, we will derive the maximum likelihood cost for GANs.

- We want to solve for $f(x)$, a cost function to be applied to every sample from the generator:

$$J^{(G)} = \mathbb{E}_{\boldsymbol{x} \sim p_g} f(\boldsymbol{x})$$

- Show the following:

$$\frac{\partial}{\partial \theta} J^{(G)} = \mathbb{E}_{x \sim p_g} f(x) \frac{\partial}{\partial \theta} \log p_g(x)$$

- What should $f(x)$ be?

(Goodfellow 2016)

Solution

- To show that $\frac{\partial}{\partial \theta} J^{(G)} = \mathbb{E}_{x \sim p_g} f(x) \frac{\partial}{\partial \theta} \log p_g(x)$
  - Expand the expectation to an integral

$$\frac{\partial}{\partial \theta} \mathbb{E}_{\boldsymbol{x} \sim p_g} f(\boldsymbol{x}) = \frac{\partial}{\partial \theta} \int p_g(\boldsymbol{x}) f(\boldsymbol{x}) d\boldsymbol{x}$$

  - Assume that Leibniz's rule may be used

$$\int f(\boldsymbol{x}) \frac{\partial}{\partial \theta} p_g(\boldsymbol{x}) d\boldsymbol{x}$$

  - Use the identity

$$\frac{\partial}{\partial \theta} p_g(\boldsymbol{x}) = p_g(\boldsymbol{x}) \frac{\partial}{\partial \theta} \log p_g(\boldsymbol{x})$$

(Goodfellow 2016)

Solution

- We now know $\frac{\partial}{\partial\theta} J^{(G)} = \mathbb{E}_{x\sim p_g} f(x) \frac{\partial}{\partial\theta} \log p_g(x)$
- The KL gradient is $-\mathbb{E}_{\boldsymbol{x}\sim p_{\text{data}}} \frac{\partial}{\partial\theta} \log p_g(\boldsymbol{x})$
- We can do an importance sampling trick

$$f(\boldsymbol{x}) = -\frac{p_{\text{data}}(\boldsymbol{x})}{p_g(\boldsymbol{x})}$$

- Note that we must *copy* the density p_g or the derivatives will double-count

(Goodfellow 2016)

Solution

- We want $f(\boldsymbol{x}) = -\frac{p_{\text{data}}(\boldsymbol{x})}{p_g(\boldsymbol{x})}$
- We know that $D(\boldsymbol{x}) = \sigma(a(\boldsymbol{x})) = \frac{p_{\text{data}}(\boldsymbol{x})}{p_{\text{data}}(\boldsymbol{x}) + p_g(\boldsymbol{x})}$
- By algebra $f(x) = -\exp(a(\boldsymbol{x}))$

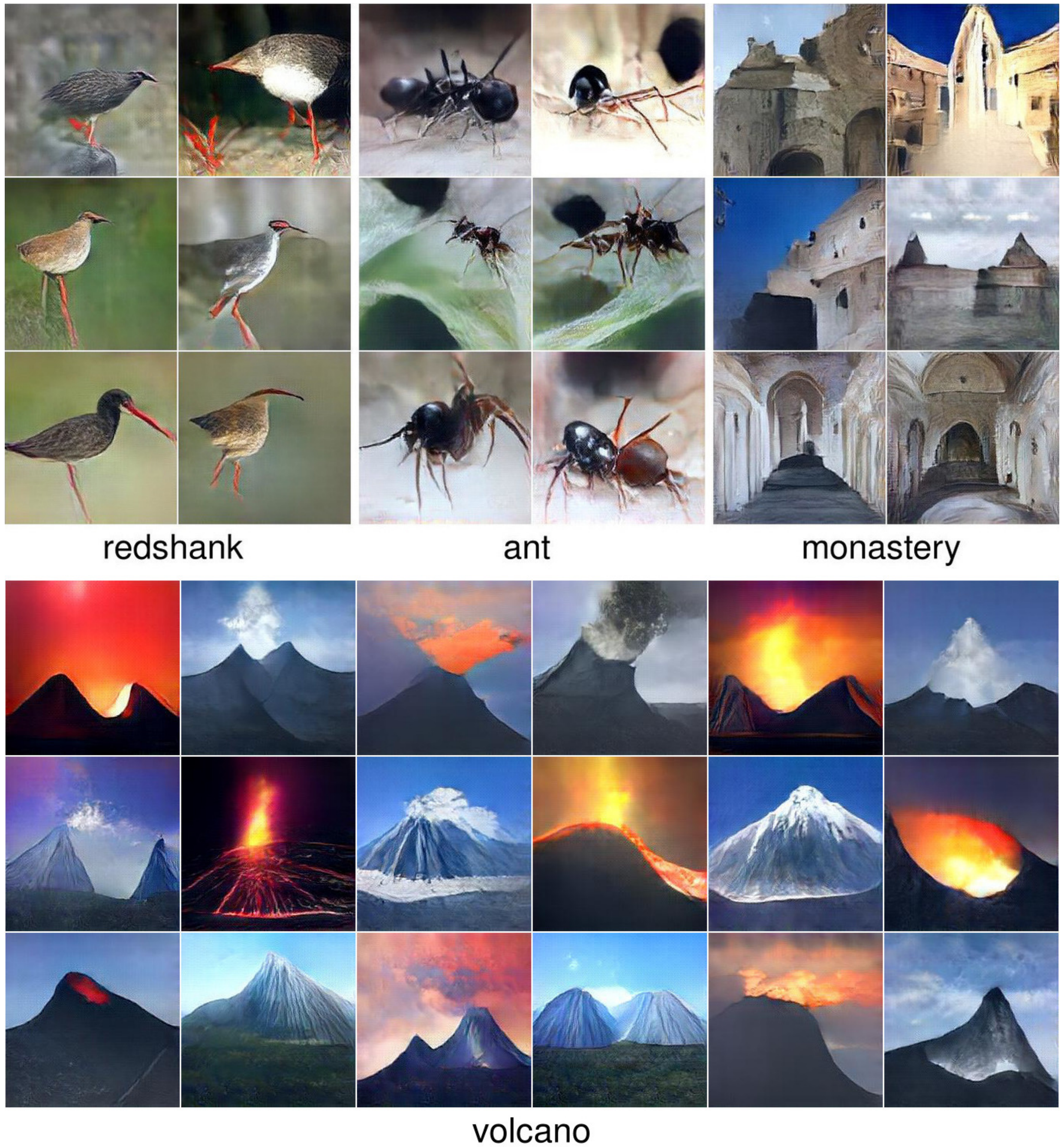
Roadmap

- Why study generative modeling?
- How do generative models work? How do GANs compare to others?
- How do GANs work?
- Tips and tricks
- <u>Combining GANs with other methods</u>

Plug and Play Generative Models

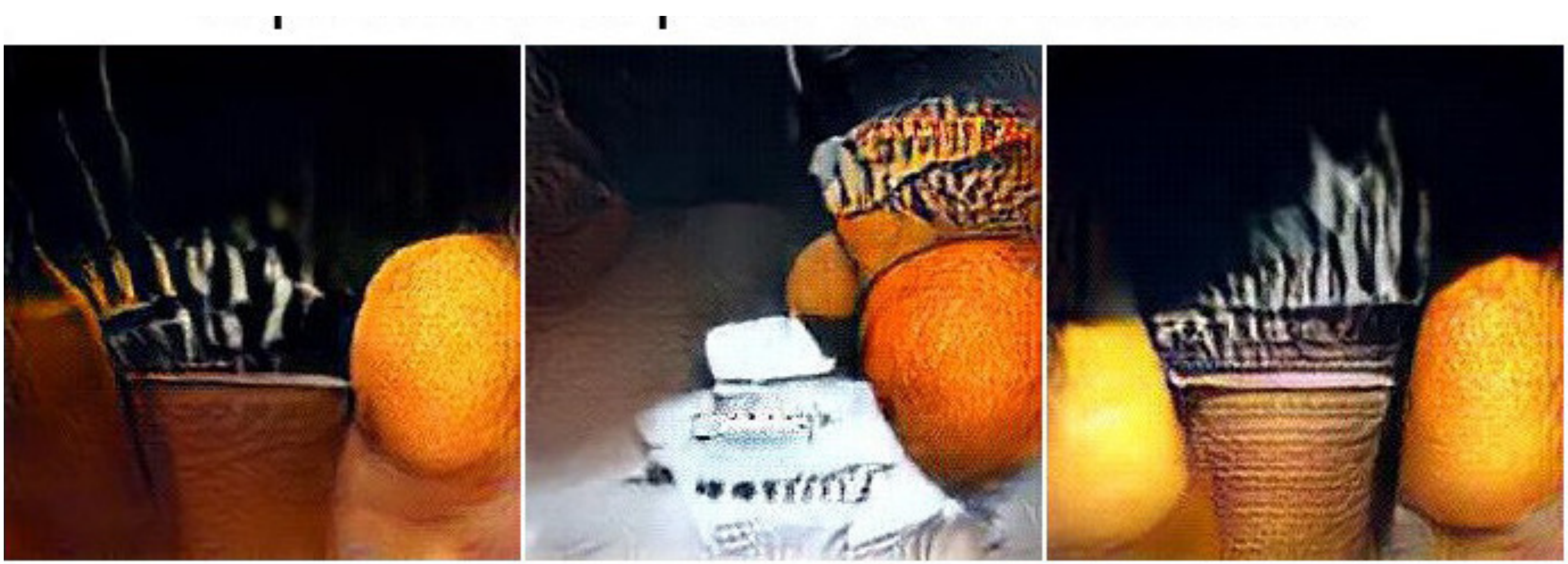
- New state of the art generative model (Nguyen et al 2016) released days before NIPS
- Generates 227x227 realistic images from all ImageNet classes
- Combines adversarial training, moment matching, denoising autoencoders, and Langevin sampling

PPGN Samples



(Nguyen et al 2016)

PPGN for caption to image



oranges on a table next to a liquor bottle

(Nguyen et al 2016)

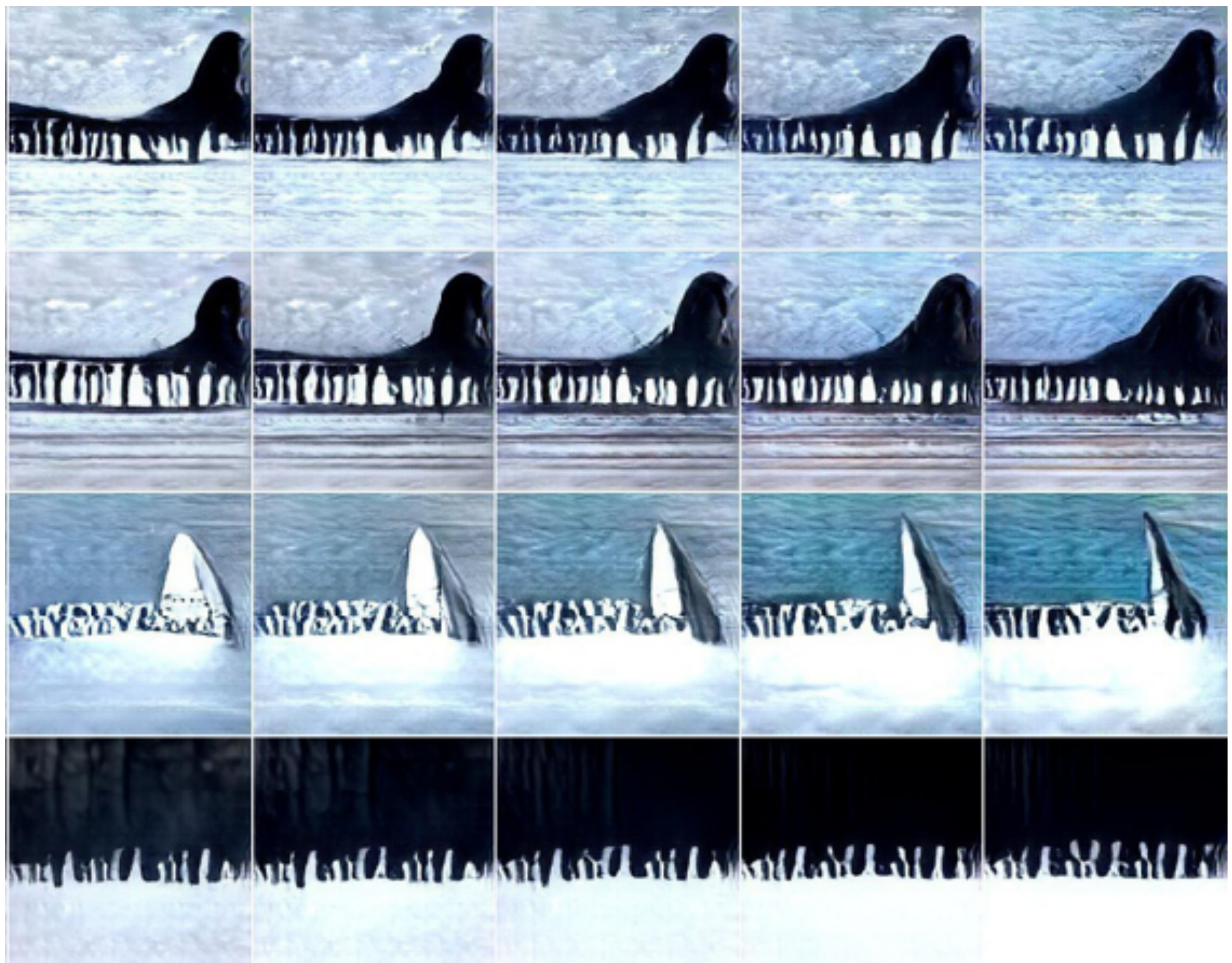
Basic idea

- Langevin sampling repeatedly adds noise and gradient of log $p(x,y)$ to generate samples (Markov chain)

- Denoising autoencoders estimate the required gradient

- Use a special denoising autoencoder that has been trained with multiple losses, including a GAN loss, to obtain best results

Sampling without class gradient



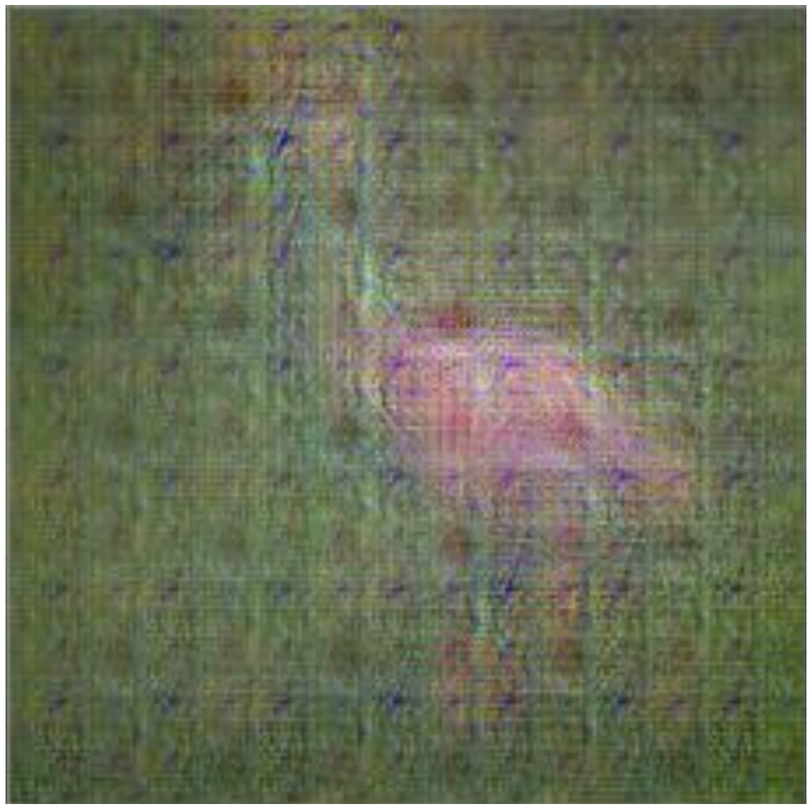
epsilon1 = 0, epsilon2 = 1e-5

(Nguyen et al 2016)

GAN loss is a key ingredient

Raw data

Reconstruction by PPGN



Reconstruction by PPGN without GAN

Images from Nguyen et al 2016

First observed by Dosovitskiy et al 2016

Conclusion

- GANs are generative models that use supervised learning to approximate an intractable cost function
- GANs can simulate many cost functions, including the one used for maximum likelihood
- Finding Nash equilibria in high-dimensional, continuous, non-convex games is an important open research problem
- GANs are a key ingredient of PPGNs, which are able to generate compelling high resolution samples from diverse image classes