Inference and Representation
Lecture 11

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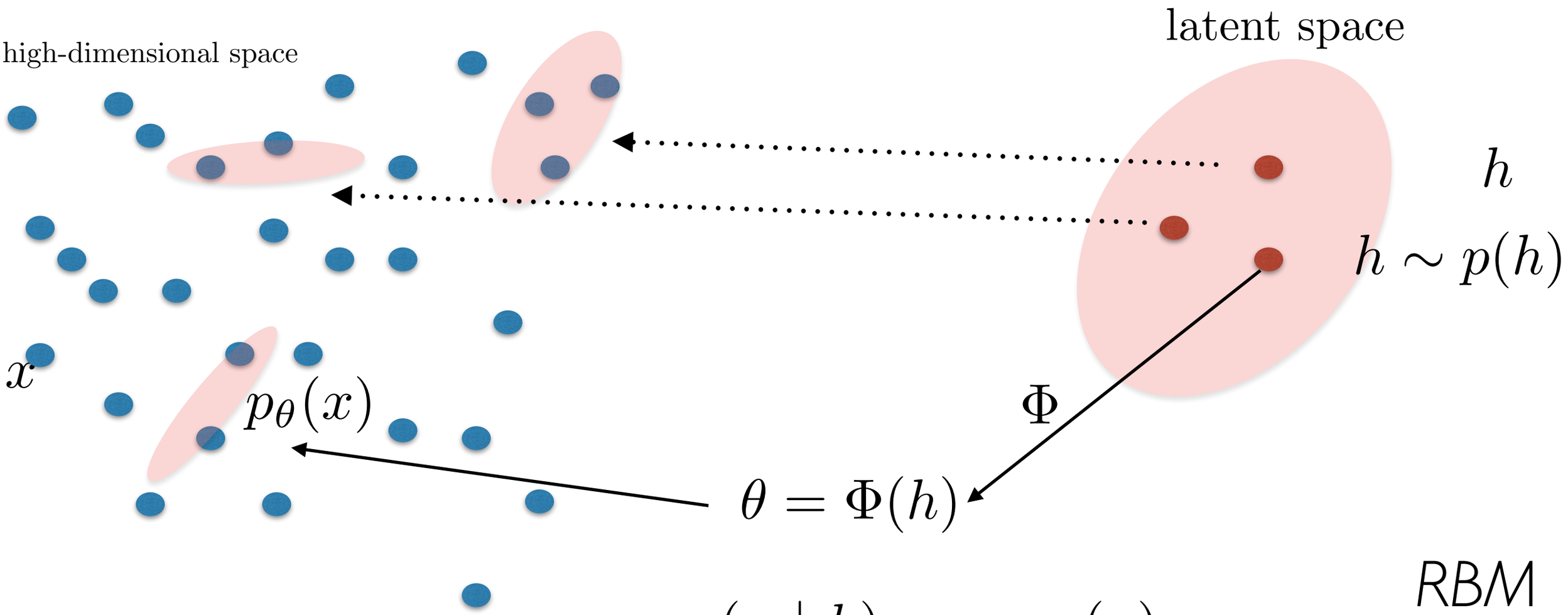
Latent Graphical Models

- Latent Graphical Models or *Mixtures*.



$$p(x \mid h) = p_{\Phi(h)}(x)$$

$$p(x) = \int p(x, h) dh = \int p(x \mid h) p(h) dh$$

RBM
DBN
DBM
VAE
...

Model: additive combination of simple parametric models

Objectives lectures 11 and 12

- Variational Flows
- Generative Adversarial Networks
- Autoregressive Models
- Open Research

Limitations of Mixture Models

- Inference is computationally expensive for large models.
- The modeling $p(x)$ is reduced to the task of modeling $p(x|z)$

- Q: How to account for image variability?
  - $p(x|z) = \mathcal{N}(\Phi(z), \Sigma(z))$ corresponds to a model of *additive variability*:

$$x = \Phi(z) + \epsilon \ , \ \epsilon \sim \mathcal{N}(0, \Sigma(z))$$

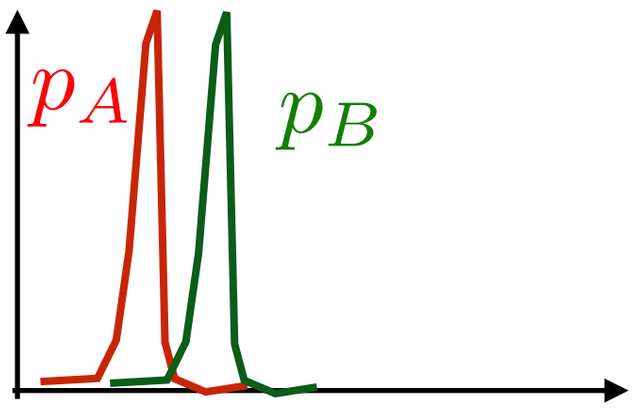
$$-\log p(x|z) \propto \|\Sigma(z)^{-1/2}(x - \Phi(z))\|^2$$

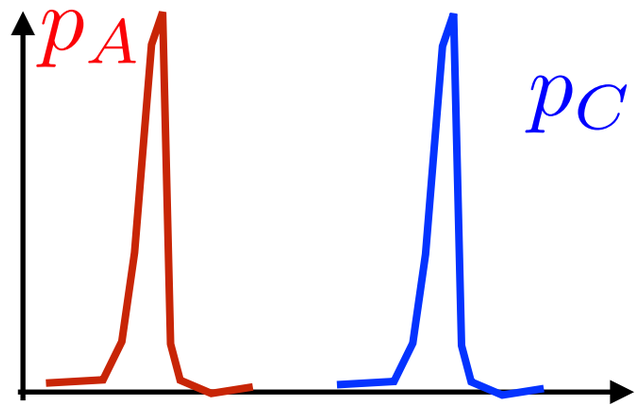
  - In particular, can we guarantee that $|p(x_\tau) - p(x)| \lesssim \|\tau\|$ with a mixture model?
  - Gaussian likelihoods suffer from regression to the mean.

LIMITATIONS OF LIKELIHOOD-BASED LEARNING

- Singular measures do not have density with respect to Lebesgue.
  - Need to add "artificial" noise to make ML work, e.g. $X \,|\, \{Z = z\} \sim \mathcal{N}(\mu_z, \Sigma_z)$

- Topology is too strong: geometry of input space does not play any role.



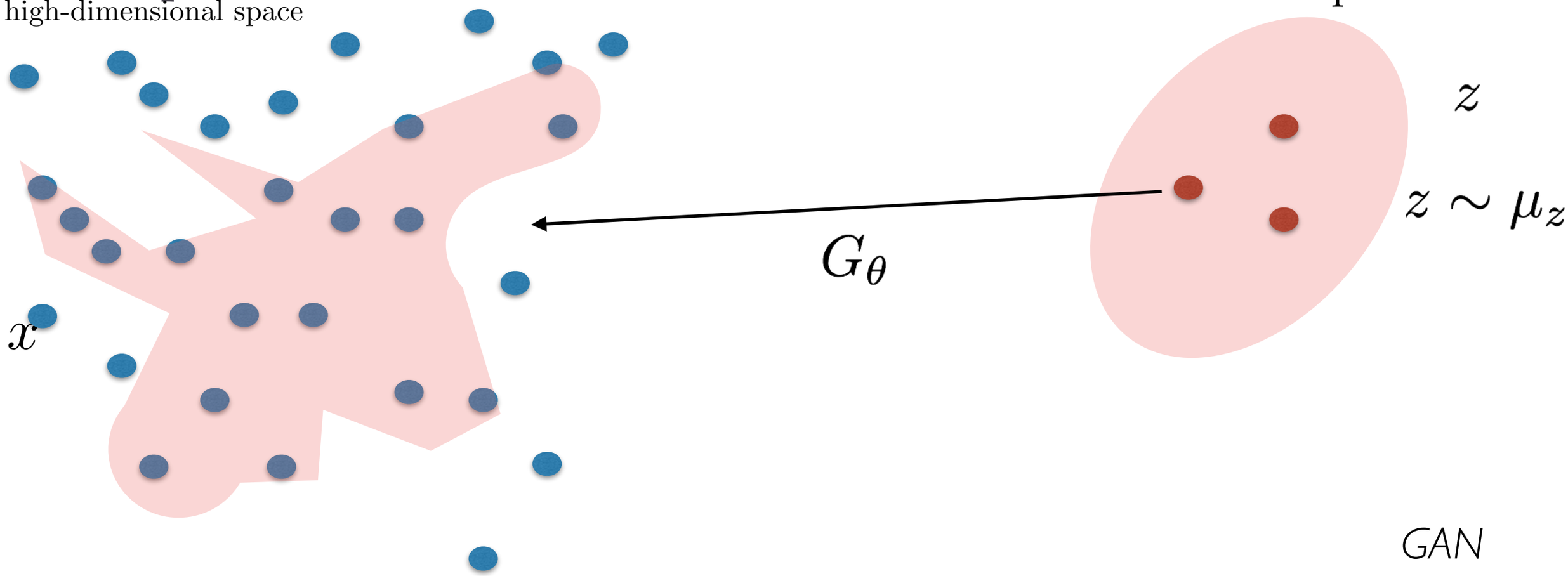


$$\mathrm{MSE}(p_A, p_B) \approx \mathrm{MSE}(p_A, p_C) = O(1)$$

- In particular, stable to deformations?

GENERATIVE MODELS OF COMPLEX DATA

➤ Implicit Models



GAN
NormFlow
…

Pushforward measure: $P_\theta := G_\theta \# \mu_z$

$$P_\theta(A) = \mu_z(G_\theta^{-1}(A))$$

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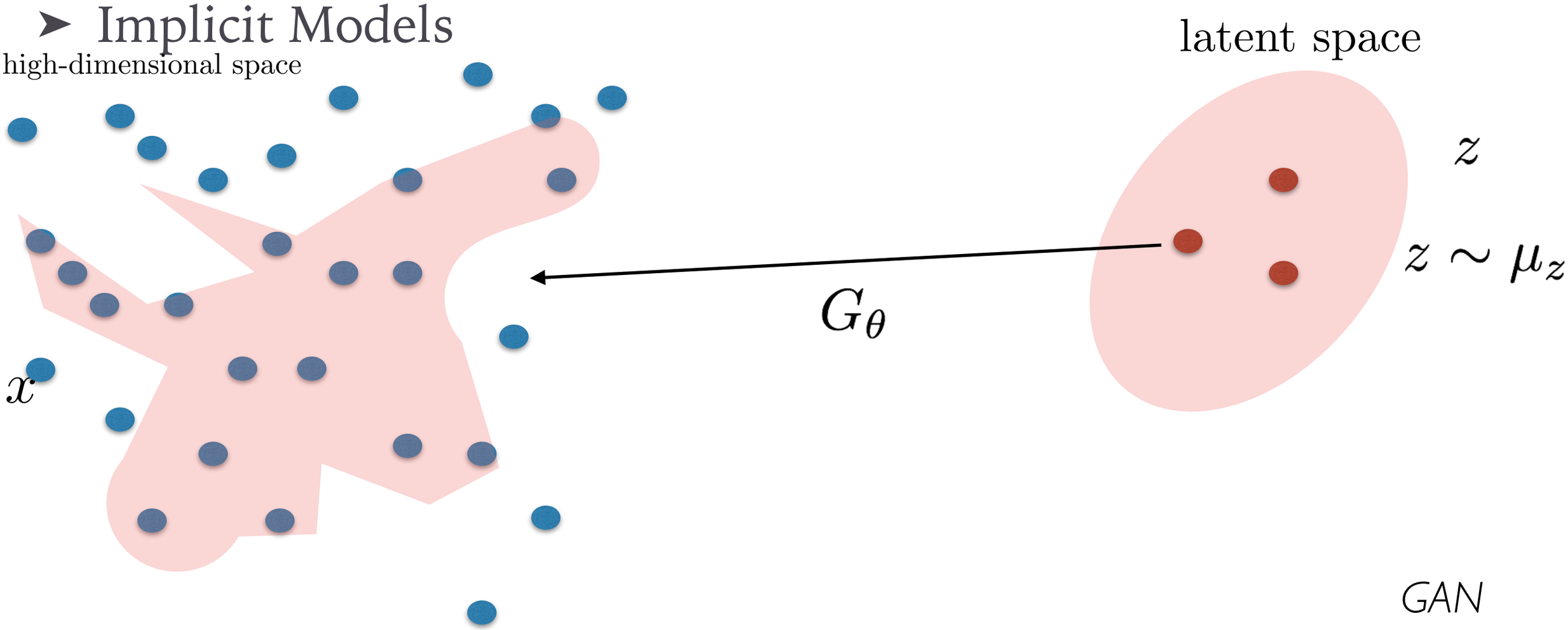

GAN
NormFlow
...

$p(x)$ defined implicitly with

$$\int f(x)p(x)d\mu(x) = \int f(G_\theta(z))d\mu_z(z) \;\forall\, f \text{ measurable}$$

MEASURE TRANSPORTS

- How to train the transport G_θ?

- We will see two methods:
  - Directly by optimizing data log-likelihood assuming measure admits a density [Normalizing Flows]
  - Using a Discriminative Model [Generative Adversarial Networks]
  - and weaker distances [Wasserstein GANs].

NORMALIZING FLOWS

➤ The density $q_K(z)$ obtained by transporting a base measure q_0 through a cascade of K diffeomorphisms $\Phi_1, \ldots, \Phi_K$ is

$$z_K = \Phi_K \circ \ldots \Phi_1(z_0) \ , \ \text{with } z_0 \sim q_0(z)$$

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- ➤ One can parametrize invertible flows and use them within Variational Inference to improve the variational approximation. [Rezende et al.'15]
- ➤ Also considered in ["NICE", Dinh et al'15].
- ➤ Special case: *Inverse Autoregressive Flows* (i.e. Jacobian triangular) explored in "Variational Inference with Inverse Autoregressive Flows", by [Kingma, Salimans & Welling, NIPS'16].

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- ➤ More recently: RealNVP [Dinh et al'16], Glow [Kingma et al.'18].

Diffusion and Non-equilibrium Thermodynamics

[Sohl-Dickstein et al.'15]

- We can also consider *infinitesimal* flows:

$$\frac{\partial q_t(z)}{\partial t} = \mathcal{F}(q_t(z)) \ , \ q_0(z) = p_0(z) \ .$$

$\mathcal{F}$ describes the dynamics.

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$\mathcal{F}$ describes the dynamics.

- For $\mathcal{F} = -\Delta$ we have Gaussian diffusion.
- It defines a Markov diffusion kernel that successively transforms data distribution $p_0(x)$ into a tractable distribution $\pi(x)$:

$$\pi(x) = \int T_\pi(x|x')\pi(x')dx'$$

$q(x^{(t+1)}|x^{(t)}) = T_\pi(x^{(t+1)}|x^{(t)}, \beta_t)$ $\qquad$ β_t: diffusion rate.

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$$p(x^{(0\ldots T)}) = p(x^{(T)}) \prod_{t \leq T} p(x^{(t-1)}|x^{(t)}) \ .$$

  - in the limit of infinitesimal diffusion, the forward and backward kernel have the same functional form (Gaussian).
  - The parameters of the model are $\{\mu(x^{(t)}, t), \Sigma(x^{(t)}, t)\}_{t \leq T}$
- The data likelihood admits lower bound that can be evaluated efficiently using annealed importance sampling.

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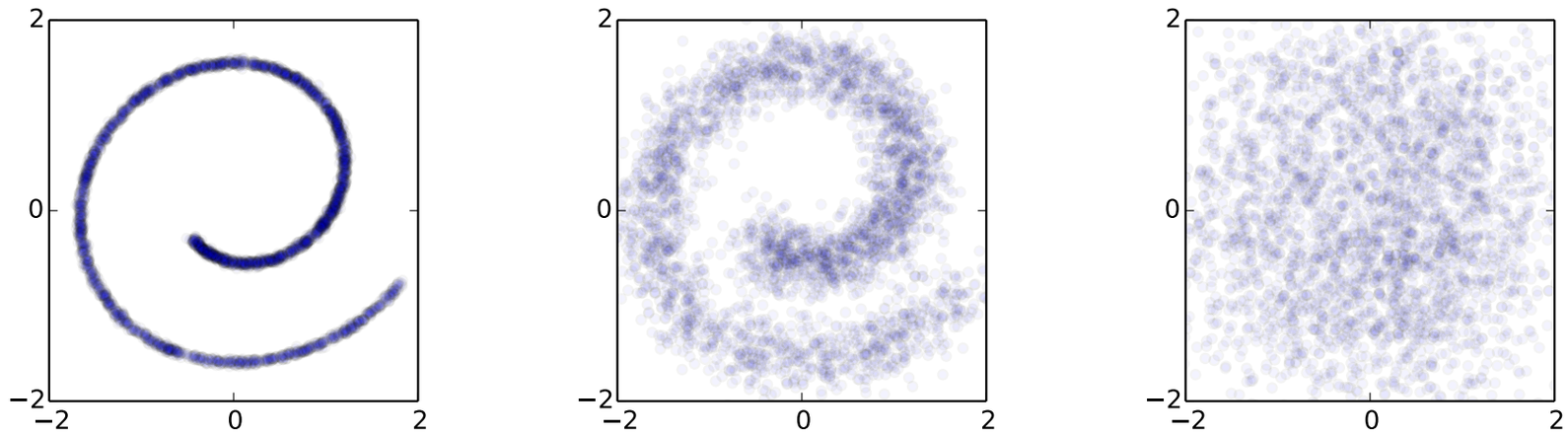
- Issue: cursed by the dimensionality.

Diffusion and Non-equilibrium Thermodynamics

[Sohl-Dickstein et al.'15]

$t = 0$ $\quad t = \frac{T}{2}$ $\quad t = T$

$q\left(\mathbf{x}^{(0 \cdots T)}\right)$



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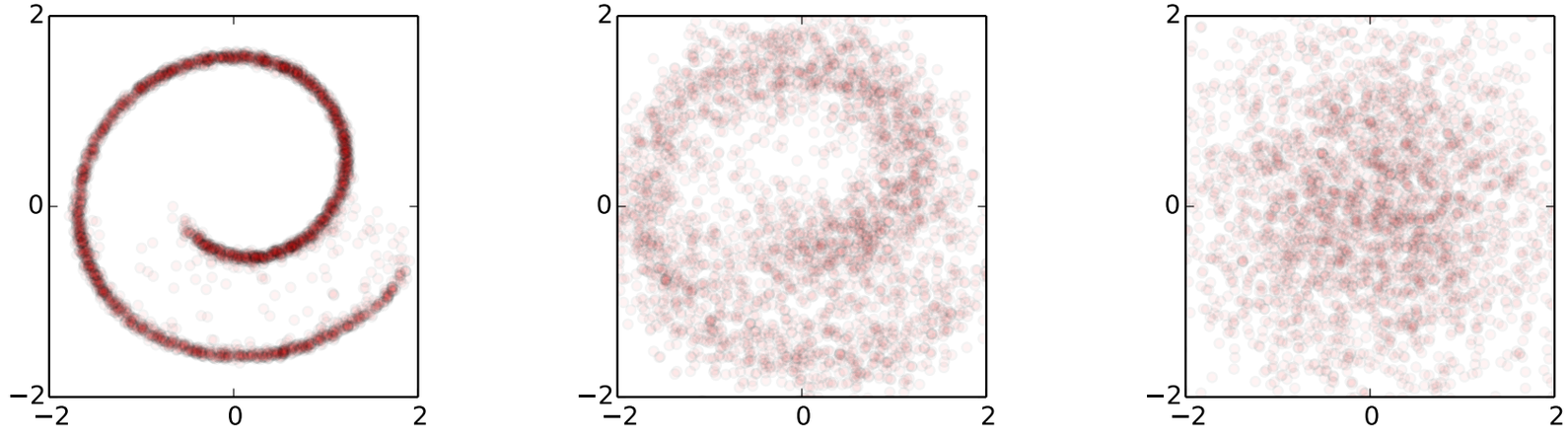
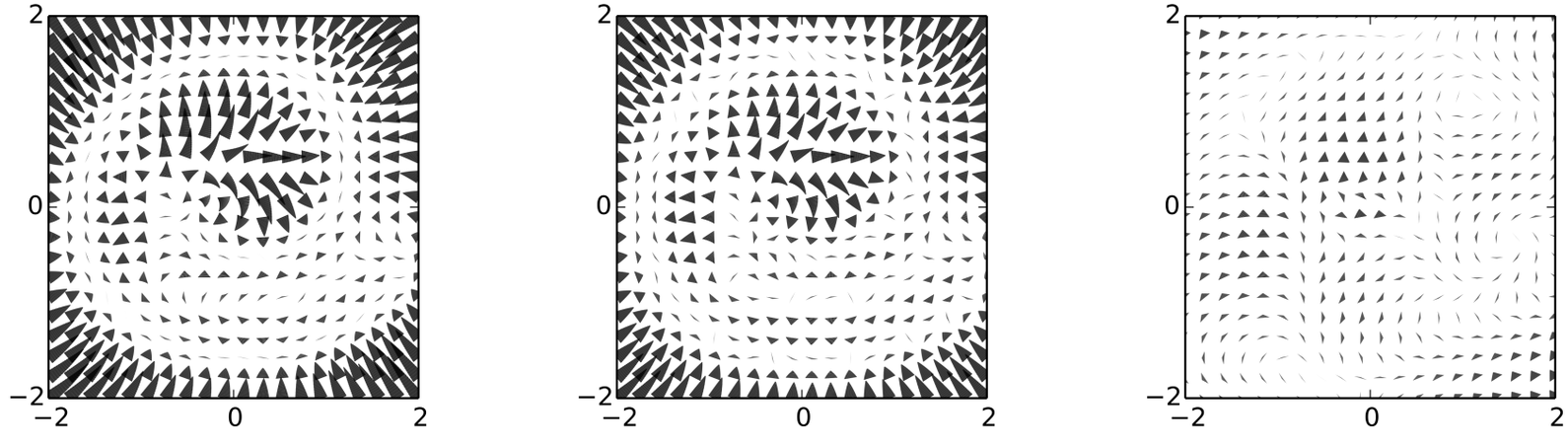


$\mathbf{f}_\mu\left(\mathbf{x}^{(t)}, t\right) - \mathbf{x}^{(t)}$



ADVERSARIAL TRAINING WITH IMPLICIT MODELS

- More generally, we consider criteria to compare distributions of the form

$$D(Q, P) = \sup_{(f_Q, f_P) \in \mathcal{S}} \mathbb{E}_Q[f_Q(X)] - \mathbb{E}_P[f_P(X)] \ .$$

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- Slight generalization of Integral Probability Metrics (IPMs).

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- When $P = P_\theta$, this leads to the saddle-point or *adversarial* learning objective:

$$\min_\theta \left\{ C(\theta) := \sup_{(f_Q, f_P) \in \mathcal{S}} \mathbb{E}_Q[f_Q(X)] - \mathbb{E}_{z \sim \mu}[f_P(G_\theta(z))] \right\} \ .$$

DIFFERENT PROBABILITY METRICS

- This adversarial framework includes many existing probability metrics:
- Integral Probability Metrics: $\mathcal{S} = \{(f, f); f, -f \in \mathcal{R}\}$
  - ex the Total Variation distance:

$$D_{TV}(Q, P) := \sup_A |P(A) - Q(A)| = \sup_{f \in C(\mathcal{X}, [-1,1])} \mathbb{E}_Q[f(X)] - \mathbb{E}_P[f(X)]$$

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- F-divergences: $D_f(Q, P) = \int f\left(\frac{q(x)}{p(x)}\right) p(x) d\mu(x)$
  - under appropriate regularity

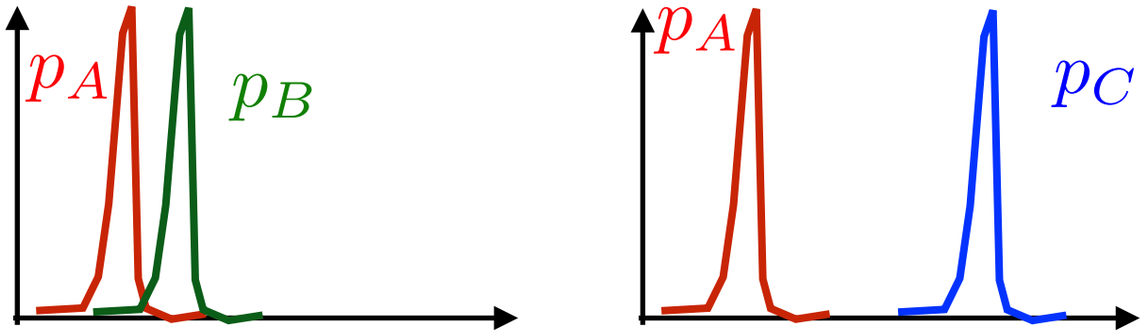
$$D_f(Q, P) = \sup_{|g| < \infty, g(\mathcal{X}) \subseteq \mathrm{dom}(f^*)} \mathbb{E}_Q[g(x)] - \mathbb{E}_P[f^*(g(x))] \ .$$

WASSERSTEIN DISTANCES

- For $p \geq 1$, the p-Wasserstein distance is

$$W_p(Q,P)^p := \inf_{\pi \in \Pi(Q,P)} \mathbb{E}_{(x,y)\sim\pi}[d(x,y)^p]$$

$\Pi(Q,P)$: measures on $\mathcal{X} \times \mathcal{X}$ with marginals Q and P.



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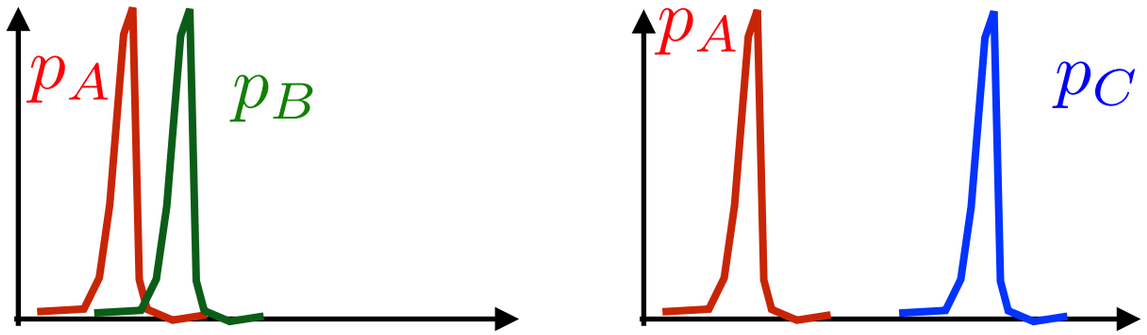

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- Variational form is given by Kantorovich duality:

$$W_p(Q,P)^p = \sup_{(f_Q, f_P) \in \mathcal{S}_c} \mathbb{E}_Q[f_Q(X)] - \mathbb{E}_P[f_P(X)]$$

  - p=1 simplifies to

$$W_1(Q,P) = \sup_{f \in \mathrm{Lip}_1} \mathbb{E}_Q[f(X)] - \mathbb{E}_P[f(X)]$$

ENERGY DISTANCES

- The (Euclidean) Energy Distance is defined as

$$\mathcal{E}(Q,P)^2 := 2\mathbb{E}_{X\sim Q,Y\sim P}[\|X-Y\|] - \mathbb{E}_{X\sim Q,X'\sim Q}[\|X-X'\|] - \mathbb{E}_{Y\sim P,Y'\sim P}[\|Y-Y'\|] \,.$$

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- Its generalization replaces euclidean distance by a generic symmetric function *d(x,y)*, leading to the *Maximum Mean Discrepancies* (MMD):

$$\mathcal{E}_d(Q,P) = \sup_{\|f\|_{\mathcal{H}}\leq 1} \mathbb{E}_P[f(X)] - \mathbb{E}_Q[f(X)] \ ,$$

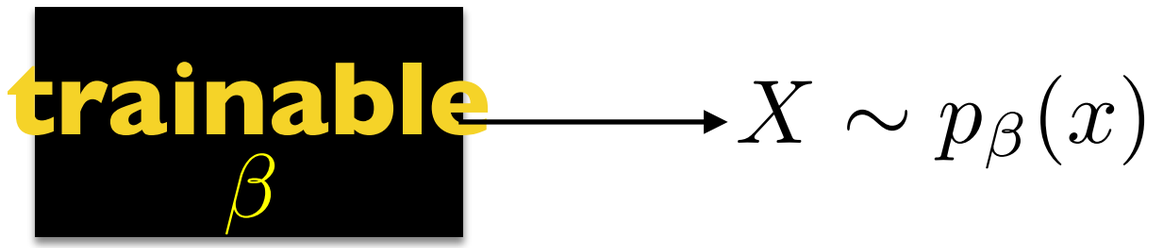
- $\mathcal{H}$ is a Reproducing Kernel Hilbert Space associated with the so-called *triangular gap* Kernel associated with *d*:

$$K_d(x,y) := \frac{1}{2}\left(d(x,x_0) + d(y,x_0) - d(x,y)\right) \ .$$

Generative Adversarial Networks

[Goodfellow et al., '14]

- Suppose we have a *trainable* black box generator:



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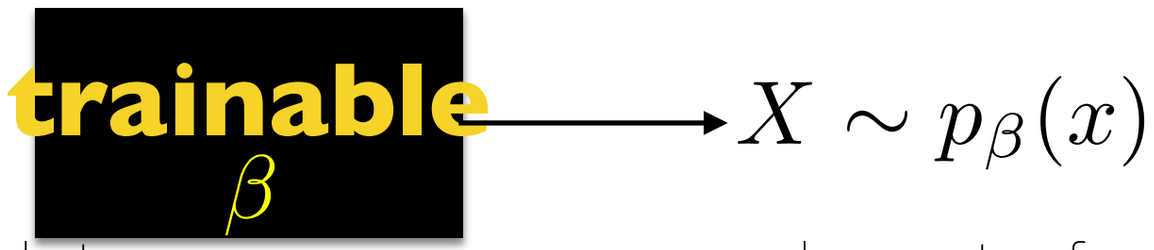
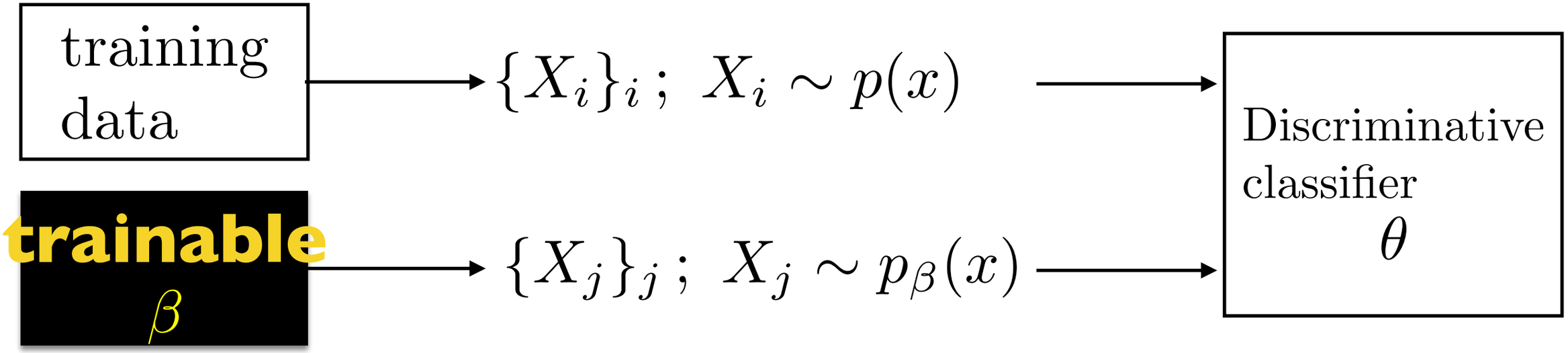


- Given observed data $\{X_i\}_i\,;\; X_i \sim p(x)$ how to force our generator to produce samples from $p(x)$?



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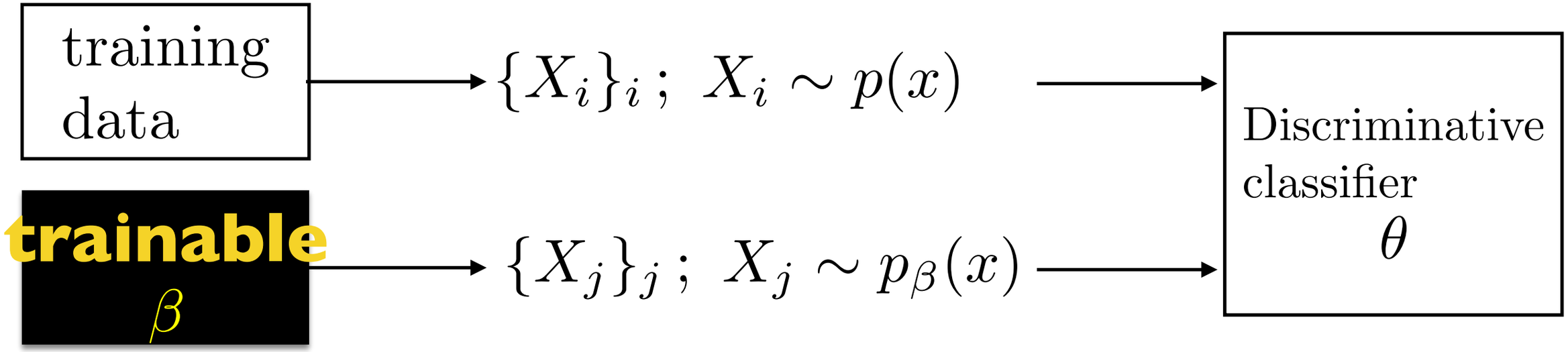
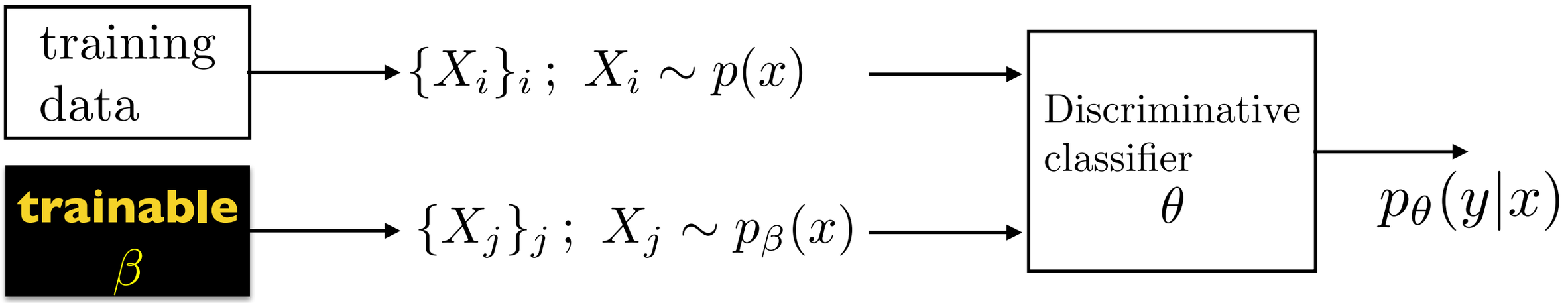


- The generator should make the classification task as hard as possible *for any discriminator.*

Generative Adversarial Networks

[Goodfellow et al., '14]

- Train generator and discriminator in a minimax setting:



$y = 1$: "real" samples
$y = 0$: "fake" samples

$$\min_{\beta} \max_{\theta} \left(\mathbb{E}_{x \sim p_{data}} \log p_\theta(y = 1|x) + \mathbb{E}_{x \sim p_\beta} \log p_\theta(y = 0|x) \right) \quad .$$

Generative Adversarial Networks

- Q: Do we have consistency? (in the limit of infinite capacity)

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For each x,

$$p_{data}(x) \log D(x) + p_\beta(x) \log(1 - D(x)) = (p_{data}(x) + p_\beta(x)) \left(\alpha \log \gamma + (1 - \alpha \log(1 - \gamma)\right) \ ,$$

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But

$$\alpha \log \gamma + (1 - \alpha) \log(1 - \gamma) = -H(\bar{\alpha}) - D_{KL}(\bar{\alpha}||p(y|x)) \leq -H(\bar{\alpha})$$

Generative Adversarial Networks

- It follows that

$$\min -H(\bar{\alpha}) \text{ is attained when } \alpha = 1/2, \text{ thus}$$

$$p_\beta(x) = p_{data}(x)$$

- In practice, however, we parametrize both generator and discriminator using neural networks.

- Optimize the cost using gradient descent
  - No guarantees of consistency
  - No guarantees of convergence (it is not gradient descent).

Generative Adversarial Training

- Challenge: it is unfeasible to optimize fully in the inner discriminator loop:

$$\min_{\beta} \max_{\theta} F(\beta, \theta)$$

$$F(\beta, \theta) = \left(\mathbb{E}_{x \sim p_{data}} \log p_\theta(y = 1|x) + \mathbb{E}_{x \sim p_\beta} \log p_\theta(y = 0|x) \right) .$$

$$\theta^*(\beta) = \arg\max_{\theta} F(\beta, \theta) \ . \qquad G(\beta) := F(\beta, \theta^*(\beta))$$

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- Indeed,

$$\theta^*(\beta) = \arg\max_{\theta} F(\beta, \theta) \ . \qquad G(\beta) := F(\beta, \theta^*(\beta))$$

$$\frac{\partial G(\beta)}{\partial \beta} = 0 \quad w.h.p.$$

- Numerical approach: alternate *k* steps of discriminator update with 1 step of generator update.
- Also, heuristic uses different false positive and false negative losses to improve numerical gradient computations.

LAPGAN

[Denton, Chintala et al.'15]

- Initial GAN models were hard to scale to large input domains.
- Laplacian Pyramid of Adversarial Networks significantly improved quality by generating independently at each scale.
- Laplacian Pyramids are invertible linear multi-scale decompositions:

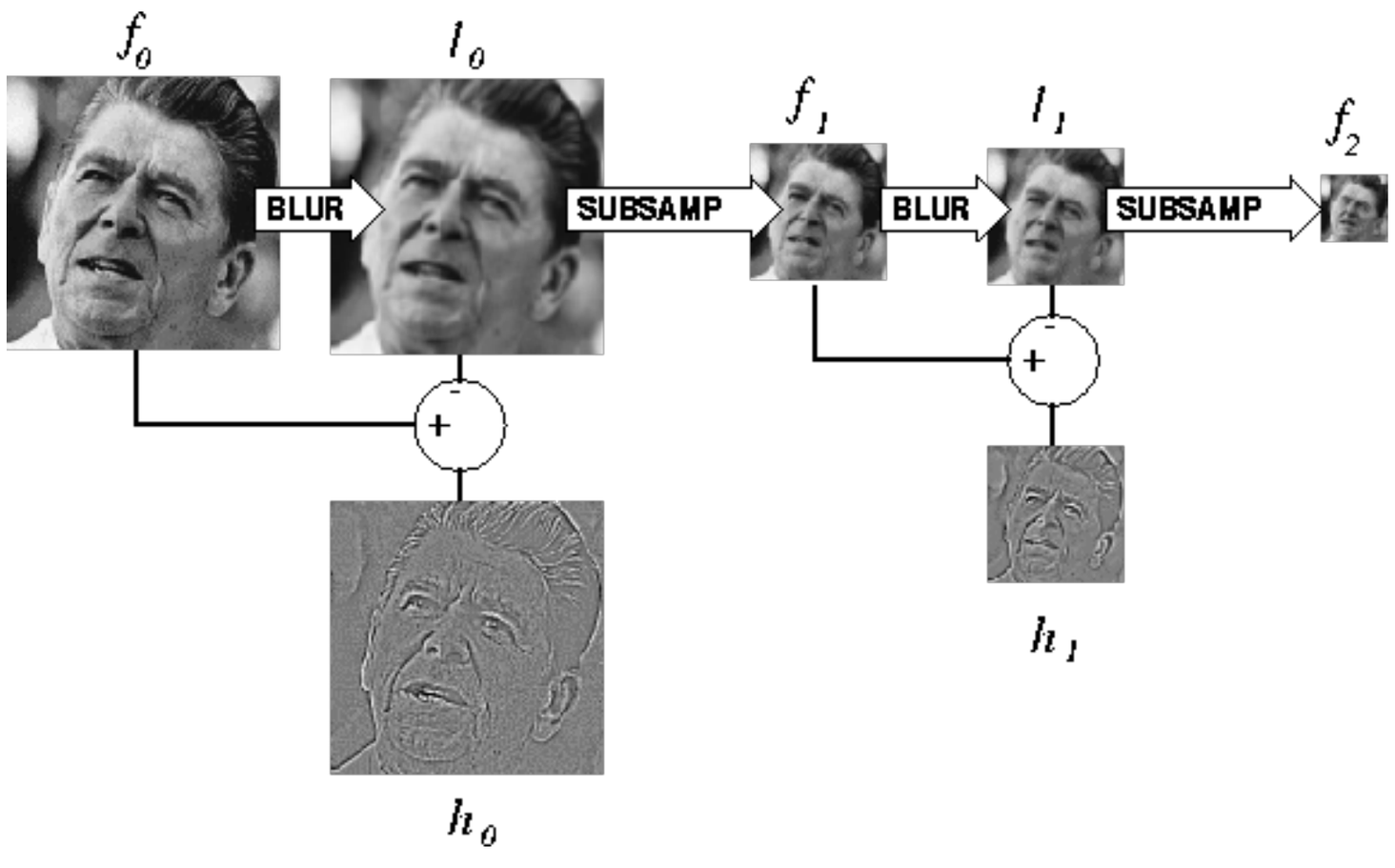
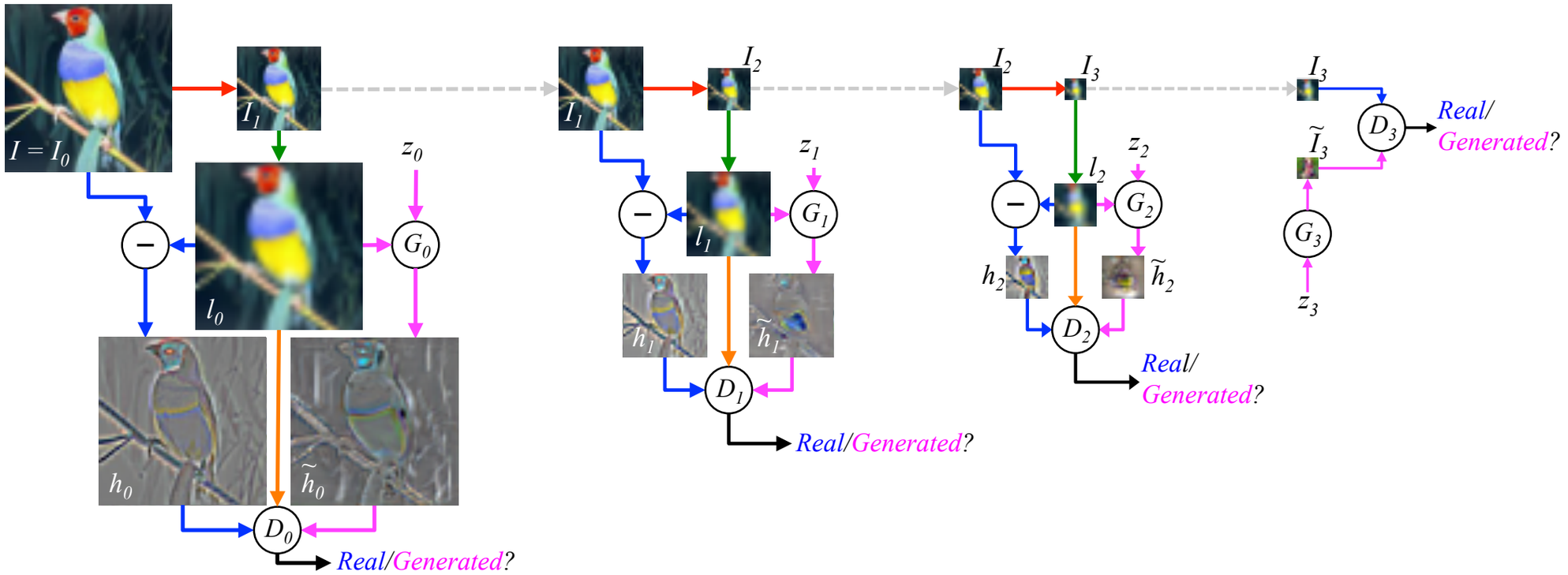


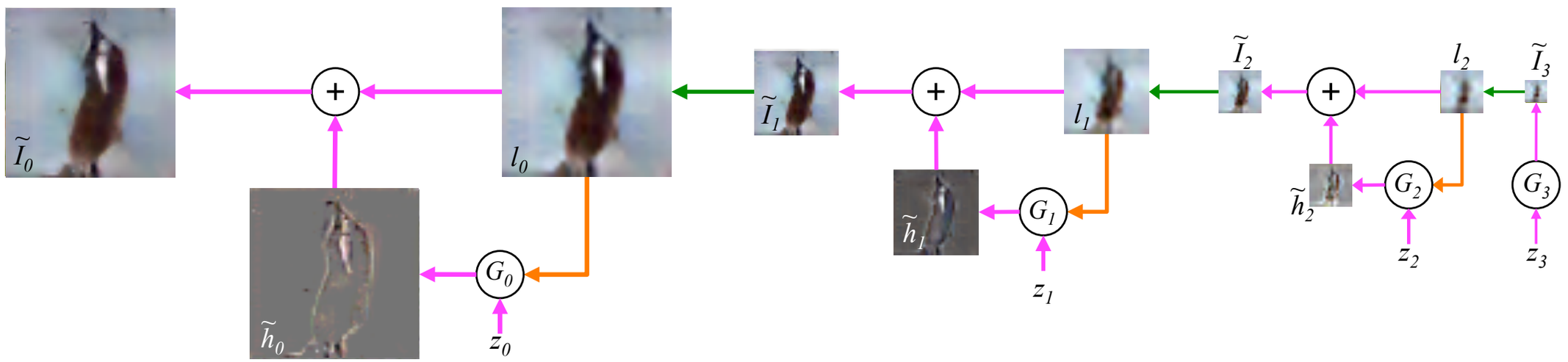
figure source: http://sepwww.stanford.edu

LAPGAN

- Training procedure:

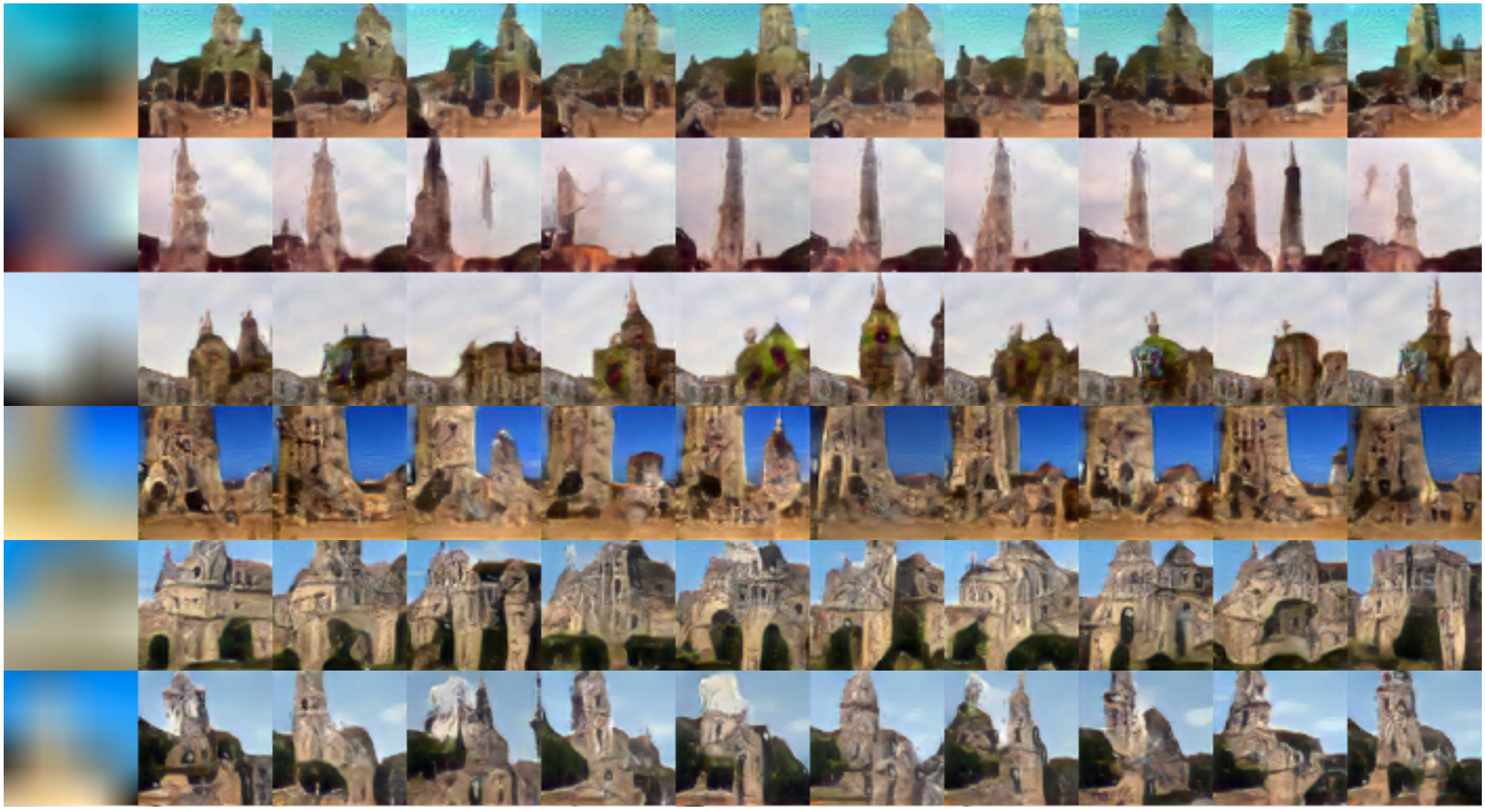


- Sampling procedure:



LAPGAN

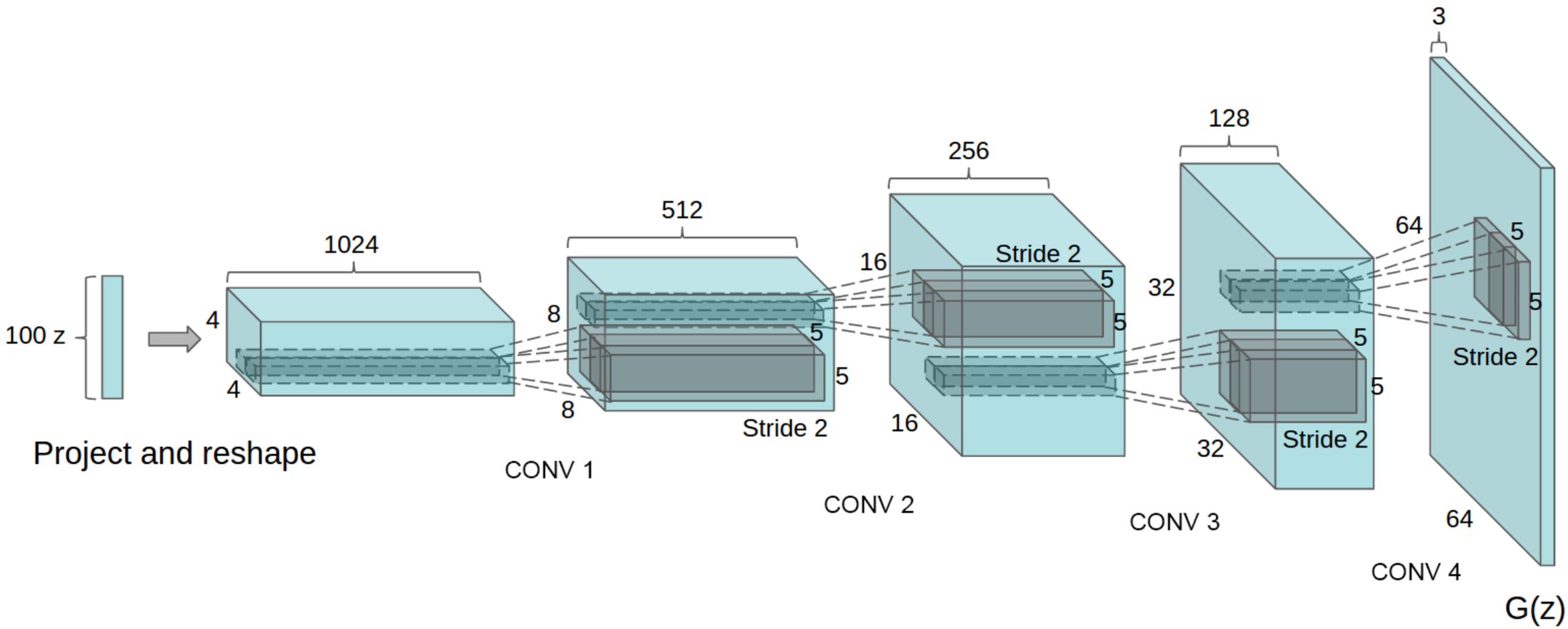
- Samples generated from the model:



DC-GAN

[Radford et al.'16]

- Improved multi-scale architecture and Batch-Normalization:



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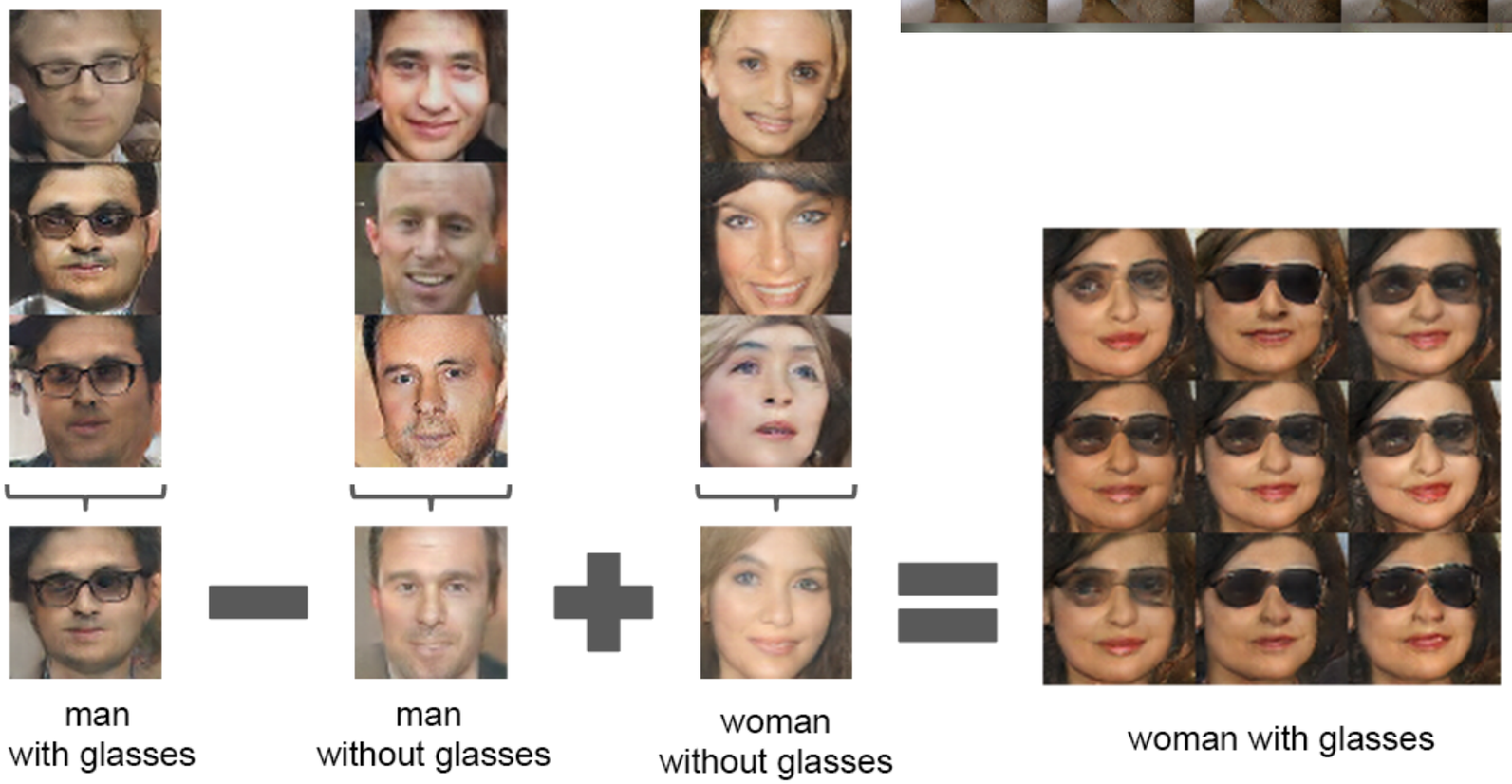

GANs and Optimal Transport

- So far, we have measured/trained density models using log-likelihood:

$$\textbf{Model : } p(x;\theta)$$
$$E(\theta) = \frac{1}{L}\sum_{l\leq L} \log p(x_l;\theta).$$

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- This requires ability to measure model likelihoods.
  - (or at least a good lower bound as in variational autoencoders).
- The underlying "distance" in the space of distributions is the Kullback-Liebler divergence

$$KL(p_r \,||\, p_m) = \int \log\left(\frac{p_r(x)}{p_m(x)}\right) p_r(x) d\mu(x) \;,$$

- Estimated from finite data sample with

$$\widehat{KL}(p_r \,||\, p_m) = \frac{1}{L}\sum_{l\leq L}\left(\frac{p_r(x_l)}{p_m(x_l;\theta)}\right) \propto -E(\theta) + C \;.$$

GANs and Optimal Transport

- Original GANs are associated with Jensen-Shannon divergence

$$JS(P||Q) = \frac{1}{2}\left(D_{KL}(P||1/2(P+Q)) + D_{KL}(Q||1/2(P+Q))\right).$$

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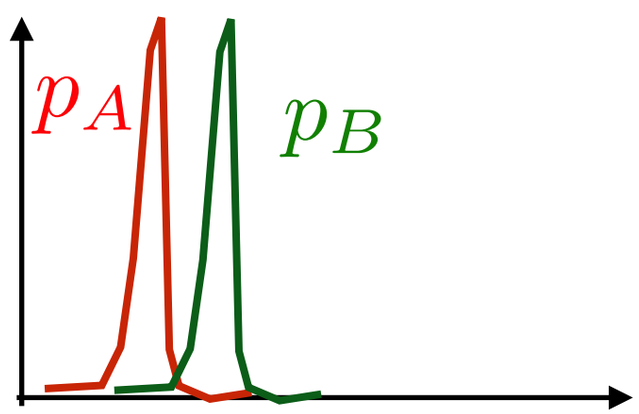
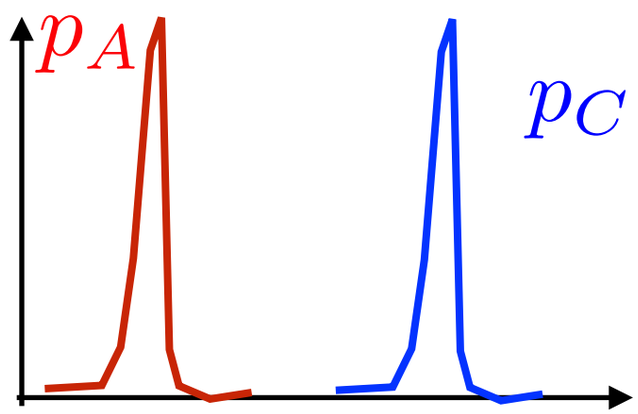
- Limitations:
  - Expression of densities not always available.
  - These metrics require the distributions to be absolutely continuous with respect to each other, e.g. by having densities wrt Lebesgue.
  - May be too 'strong' a distance for many applications:





$$JS(p_A, p_B) \approx JS(p_A, p_C) \approx 0 \ .$$

Earth-Mover Distance

- Alternatively, we can consider the Earth-Mover Distance (EMD)

$$W(P_r, P_m) = \inf_{\gamma \in \Pi(P_r, P_m)} \mathbb{E}_{(x,y)\sim\gamma}\{\|x - y\|\} \ ,$$

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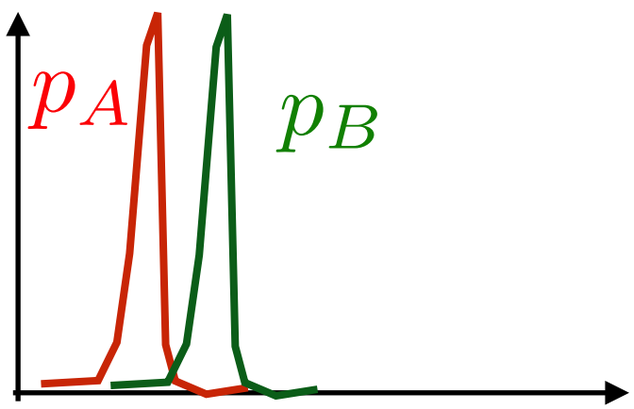
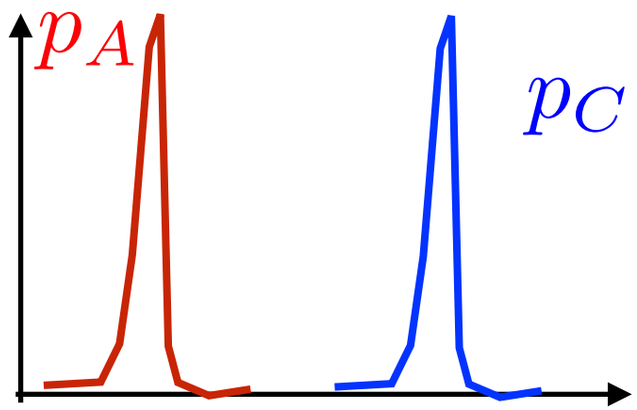
$\Pi(P_r, P_m)$: Set of joint distributions in (x, y) whose marginals are P_r, P_m.

  - Measures how much mass needs to be transported from P_r to P_m, measured with the Euclidean metric here (Wasserstein-1 distance).
  - It defines a "weaker" topology in the space of probability distributions:





$$W(p_A, p_B) \ll W(p_A, p_C)$$

Kantorovich Duality

- In general, computing such "couplings" is hard.
- However, in the Wasserstein-1 case, we have the following dual representation:

$$W(p_r, p_m) = \sup_{\mathrm{Lip}(f)\leq 1} \mathbb{E}_{x\sim p_r}\{f(x)\} - \mathbb{E}_{x\sim p_m}\{f(x)\} \ .$$

$$f : \mathcal{X} \to \mathbb{R} \text{ continuous,}$$

$\mathrm{Lip}(f)$: Lipschitz constant of f:

$$\forall\ x, x' \ , \ |f(x) - f(x')| \leq \mathrm{Lip}(f)\|x - x'\| \ .$$

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- Recall the discriminator loss of the "classic" GAN:

$$-\mathbb{E}_{x\sim p_r}\{\log D(x)\} + \mathbb{E}_{x\sim p_m}\{\log(1 - D(x))\}$$

Wasserstein GAN [Arjovsky et al]

- In practice, we approximate the supremum over Lipschitz functions with a class of functions parametrized by a neural network:

$$W(p_r, p_m) = \sup_{\theta \in \mathcal{K}} \mathbb{E}_{x \sim p_r}\{f_\theta(x)\} - \mathbb{E}_{x \sim p_m}\{f_\theta(x)\} \ .$$

- Lipschitz bounds are enforced in [Arjovsky et al.] by simply clipping the weights ($\theta \in \mathcal{K}$).
- Better control of Lipchitz regularity in, e.g. [Gulrajani et al].

➤ Other works train directly the primal objective using the *Sinkhorn algorithm* [Genevay et al.'17, Bellemare et al'17, Salimans et al'17].

LIMITATIONS OF GAN MODELING

- We are attempting to fit a distribution p_m to the "real" distribution p_r using a distance/divergence criteria ρ :

$$\inf_{\theta} \rho(p_r, p_m(\theta)) \ .$$

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- Triangle Inequality:

$$\rho(p_r, p_m(\theta)) \leq \rho(p_r, \hat{p}_{r,L}) + \rho(\hat{p}_{r,L}, p_m(\theta)) \ .$$

Statistical Error

Modeling Error

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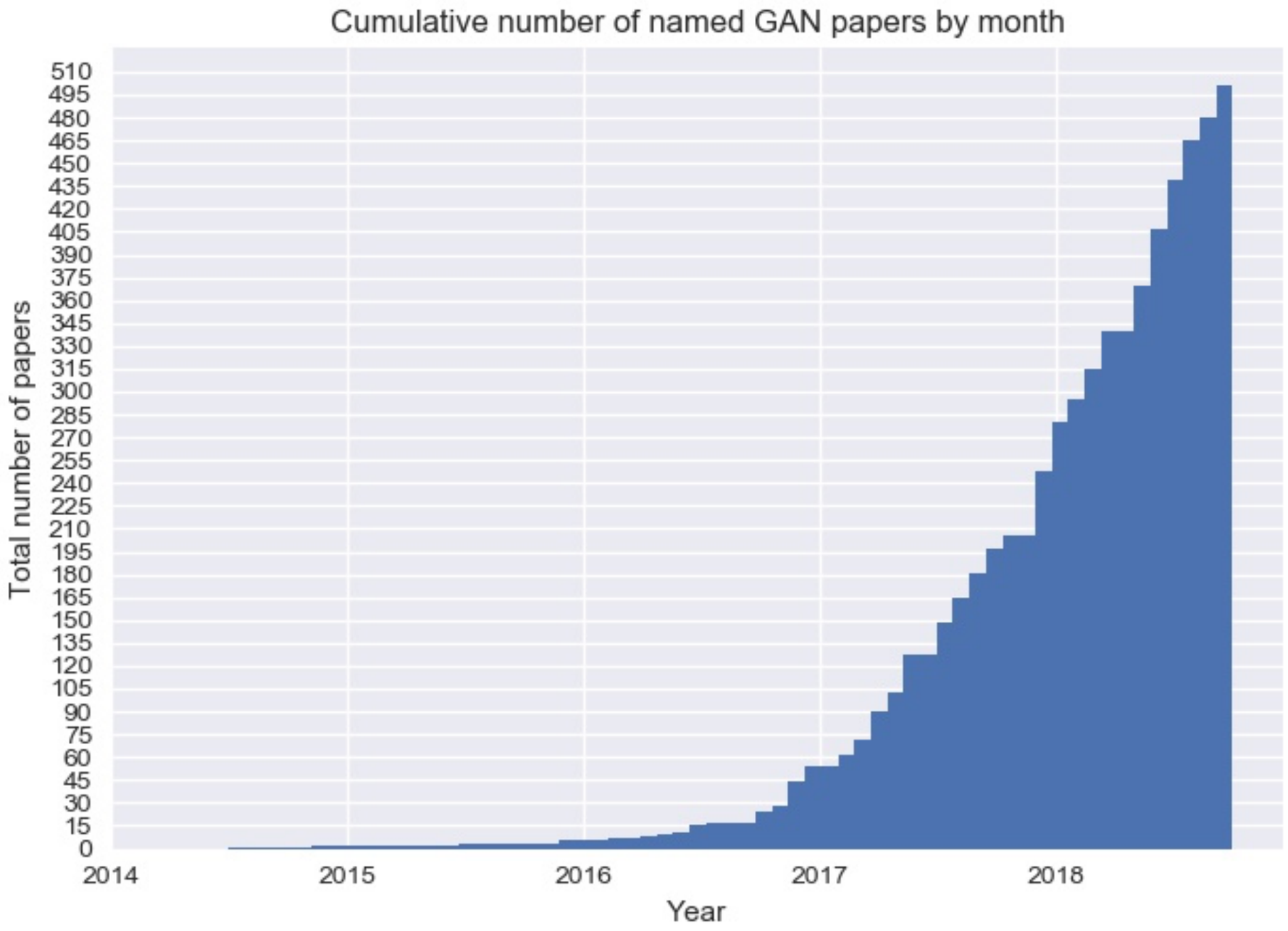
- Thus, we need to regularize the density estimation problem to avoid fitting the empirical measure instead of the underlying real distribution.

- In the case of Wasserstein distance, we have the curse of dimensionality: if input space is $\mathcal{X} = \mathbb{R}^d$ then,

$$\mathbb{E}\{\rho(p_r, \hat{p}_{r,L})\} \simeq L^{-\frac{1}{d}}$$

  - so we need a number of samples exponential in the dimension to make sampling error disappear.
  - Energy distances do not have this curse: $\mathbb{E}\{\rho(p_r, \hat{p}_{r,L})\} \simeq L^{-1/2}$
  - Open: why in practice W_1 is more efficient?

GANS ARE POPULAR!



source: https://github.com/hindupuravinash/the-gan-zoo

OPTIMAL TRANSPORT OVER GEOMETRIC DISTANCES

- So far, Wasserstein distances are defined over generic metric spaces.
- Consider now the setup where $\mathcal{X} = L^2(\Omega)$ (images)
- How to choose the base distance $d(x, y)$ so that the corresponding Wasserstein metric over is stable with respect to deformations?

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- Consider now the setup where $\mathcal{X} = L^2(\Omega)$ (images)
- How to choose the base distance $d(x, y)$ so that the corresponding Wasserstein metric over is stable with respect to deformations?
- Possible idea:

$$d(x, y) := \|\Phi(x) - \Phi(y)\|$$

Φ: Scattering or CNN representation

- Open: Study properties of induced W_Φ. Pseudodistance. When is it a distance?

SOME RECENT EXTENSIONS

- *Image-to-Image Translation with Conditional Adversarial Networks* [Isola et al., '16]

- CycleGAN [Zhu, Park, Isola, Efros]

- Progressive GAN [Karras et al]

- **OT with mixture models: Wasserstein Autoencoders** [Tolstikhin, Bousquet, Gelly, Schoelkopf,'17].

- **Large Scale Gan Training [anonymous,ICLR'19 subm]**

CONDITIONAL GANS

Labels to Street Scene

input

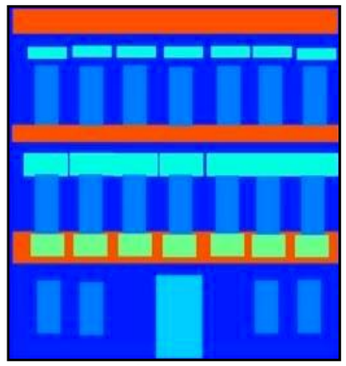
output

Aerial to Map

input

output

Labels to Facade



input

output

Day to Night

input

output

BW to Color

input

output

Edges to Photo

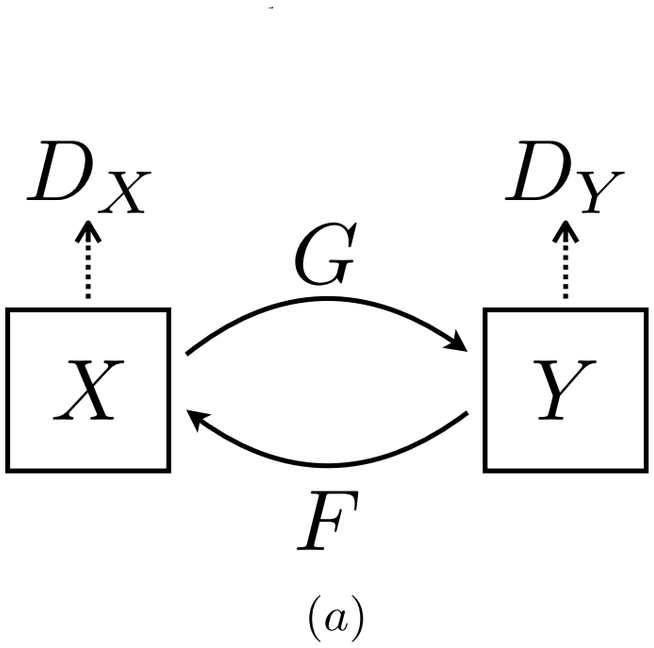
input

output

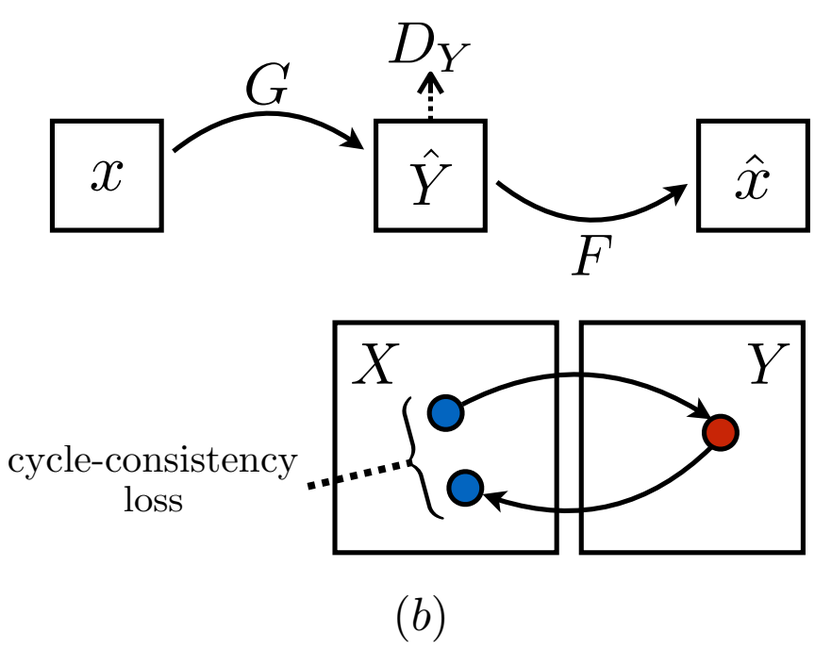
"Image-to-Image translation with Conditional Adversarial Networks", Isola et al,'16

CYCLE GAN [ZHU, PARK, ISOLA, EFROS]

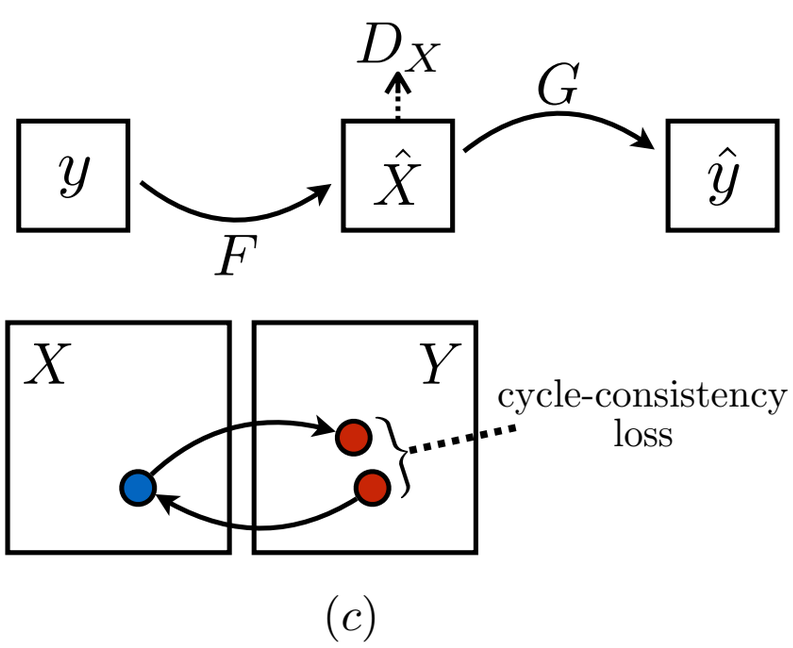
CYCLE GAN



(a)

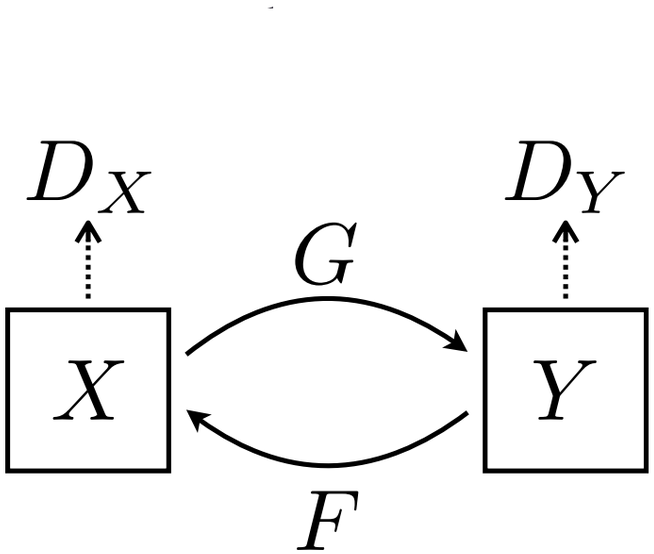


(b)



(c)

CYCLE GAN



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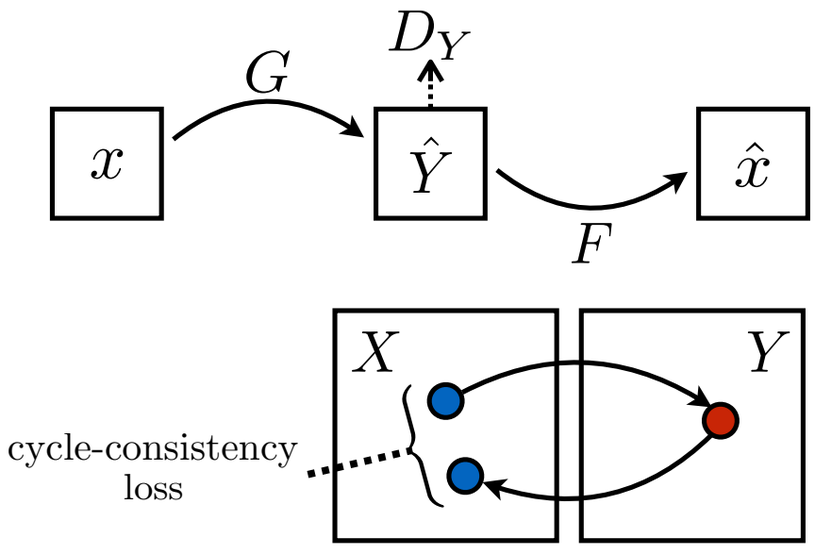
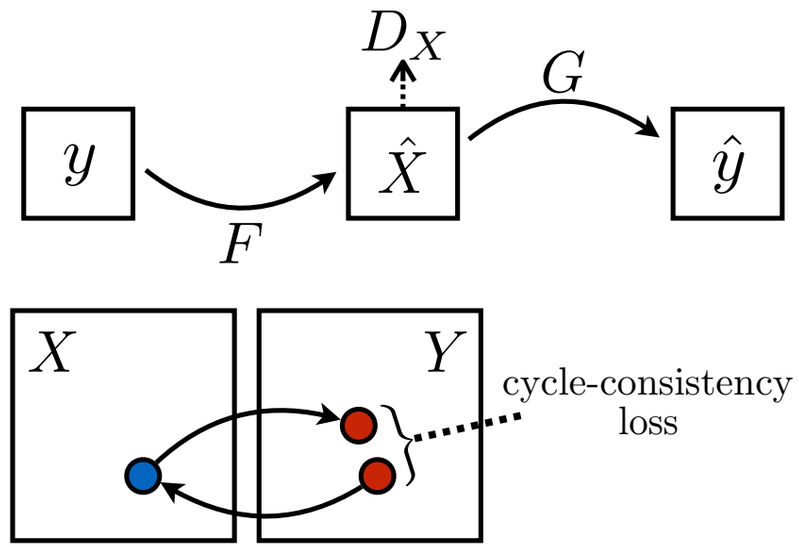


(b)



(c)

$$\mathcal{L}_{\text{GAN}}(G, D_Y, X, Y) = \mathbb{E}_{y \sim p_r(y)}\{\log D_Y(y)\} + \mathbb{E}_{x \sim p_r(x)}\{\log(1 - D_Y(G(x))\} \ .$$
$$\mathcal{L}_{\text{GAN}}(F, D_X, Y, X) = \mathbb{E}_{x \sim p_r(x)}\{\log D_X(x)\} + \mathbb{E}_{y \sim p_r(y)}\{\log(1 - D_X(F(y))\} \ .$$
$$\mathcal{L}_{\text{cyc}}(G, F) = \mathbb{E}_{x \sim p_r(x)}\{\|F(G(x)) - x\|\} + \mathbb{E}_{y \sim p_r(y)}\{\|G(F(y)) - y\|\} \ .$$

Full objective function:

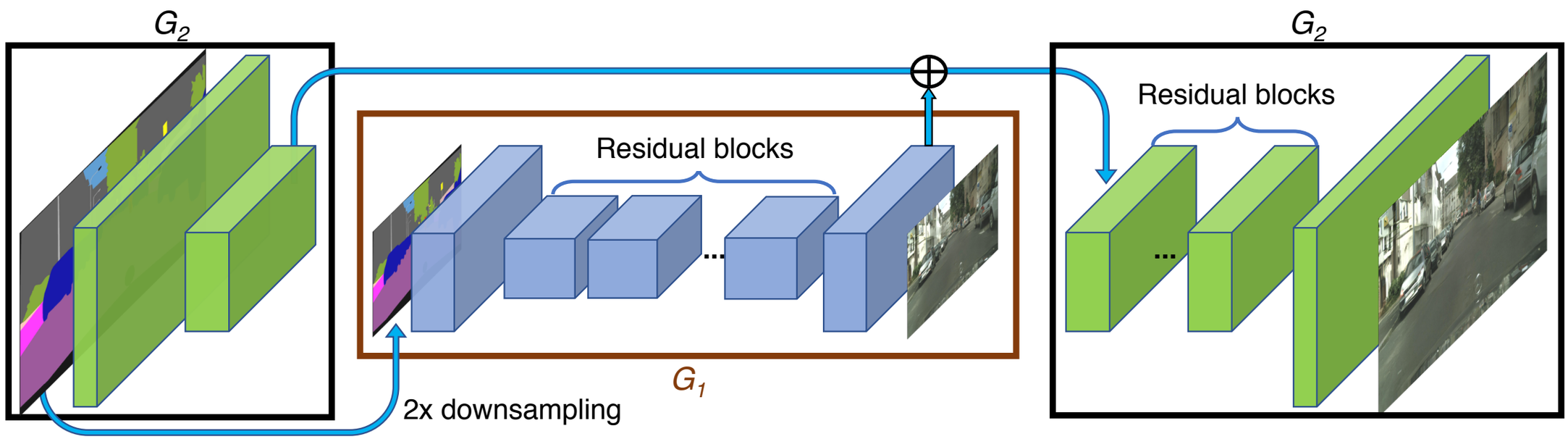
$$\mathcal{L}(G, F, D_X, D_Y) = \mathcal{L}_{\text{GAN}}(G, D_Y, X, Y) + \mathcal{L}_{\text{GAN}}(F, D_X, Y, X) + \lambda \mathcal{L}_{\text{cyc}}(G, F) \ .$$

PHOTO REALISTIC GAN [WANG ET AL]

➤Enhance the multiscale architecture with resolution-specific discriminators

$$\min_{G} \max_{D_1, D_2, D_3} \sum_{i=1}^{3} \mathcal{L}_{\mathrm{GAN}}(G, D_i) \ ,$$

➤Also includes a “feature-matching” term that stabilizes training.



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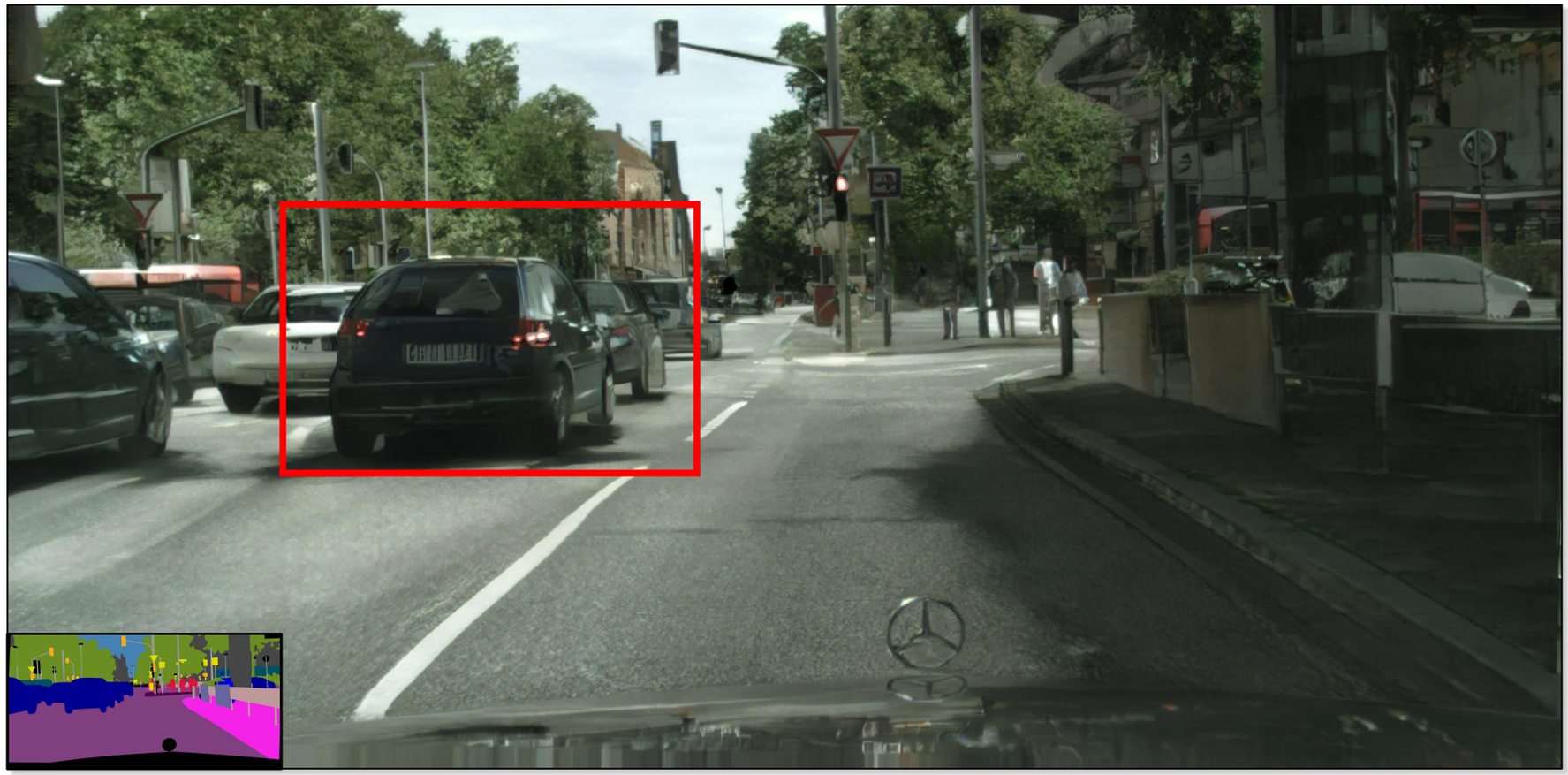


(a) Synthesized result

Cascaded refinement network [5]

Our result

(b) Application: Change label types

(c) Application: Edit object appearance

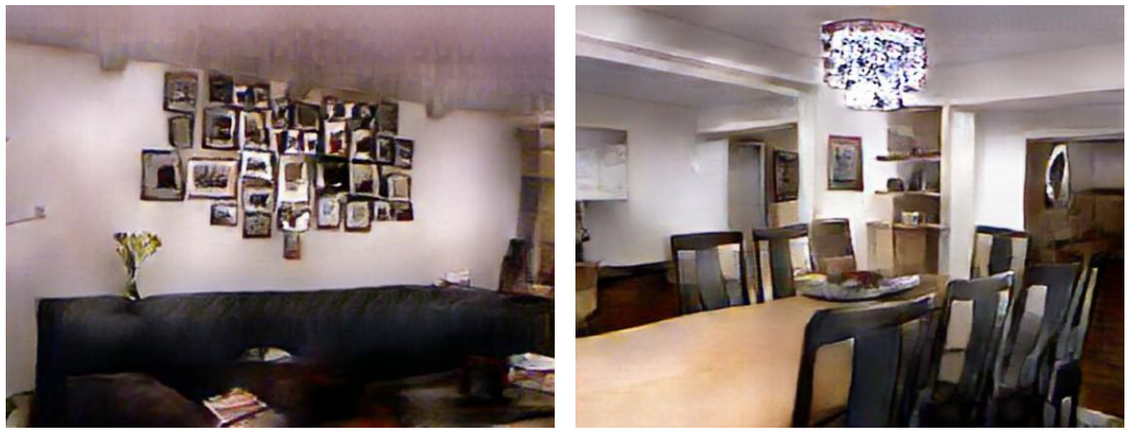
PHOTO-REALISTIC GAN

(a) Labels

(b) pix2pix

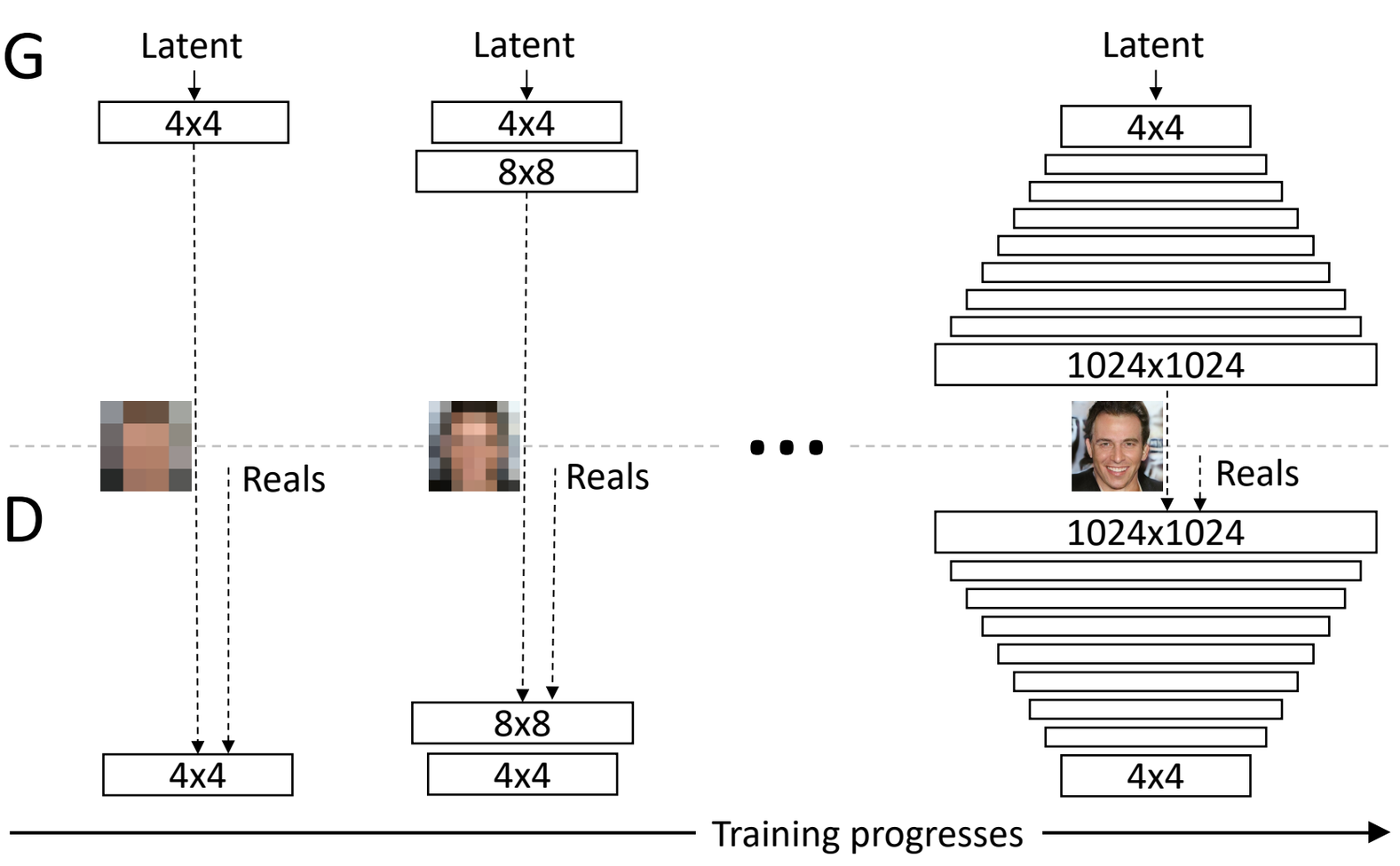
(c) CRN

(d) Ours



PROGRESSIVE GANS [KARRAS ET AL]

- Multiscale training: fine scales are included in the training progressively.



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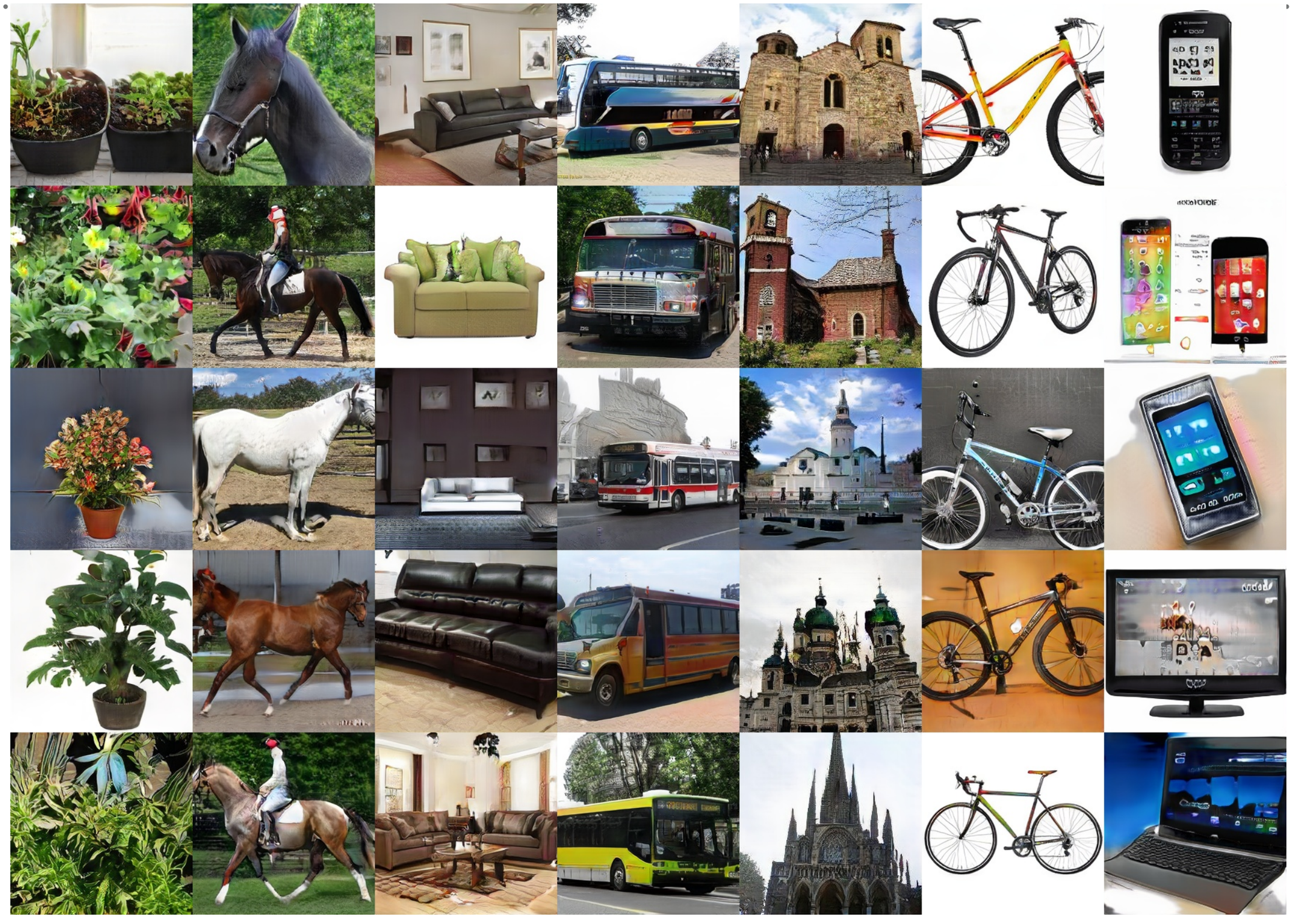

POTTEDPLANT HORSE SOFA BUS CHURCHOUTDOOR BICYCLE TVMONITOR

LARGE-SCALE GANS (2018)

LARGE SCALE GAN TRAINING FOR HIGH FIDELITY NATURAL IMAGE SYNTHESIS

Anonymous authors
Paper under double-blind review

Figure 1: Class-conditional samples generated by our model.

GENERATIVE LATENT OPTIMIZATION (GLO) [BOJANOWSKY, SZLAM ET AL'18]

- GAN image models show high-quality reconstructions.
- Is this due to the inductive bias from the deep convolutional architecture? or from the adversarial training protocol?

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- GAN image models show high-quality reconstructions.
- Is this due to the inductive bias from the deep convolutional architecture? or from the adversarial training protocol?
- The authors consider the following problem:

$$\min_{\theta \in \Theta} \frac{1}{N} \sum_{i \leq N} \min_{z_i \in \mathcal{Z}} \ell(x_i, G_\theta(z_i)) \ .$$

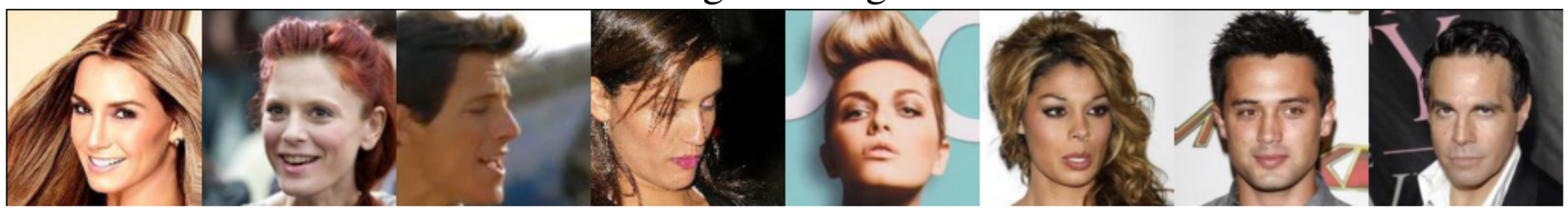
$G_\theta(z)$: DC-GAN architecture.

- Non-linear Dictionary learning.
- Latent space has simple uniform prior over hypercube.

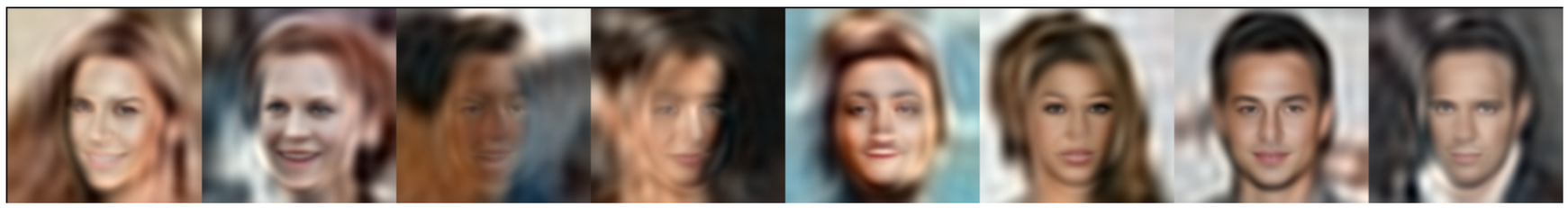
GENERATIVE LATENT OPTIMIZATION (GLO) [BOJANOWSKY, SZLAM ET AL'18]

- Some reconstruction results.

Original images

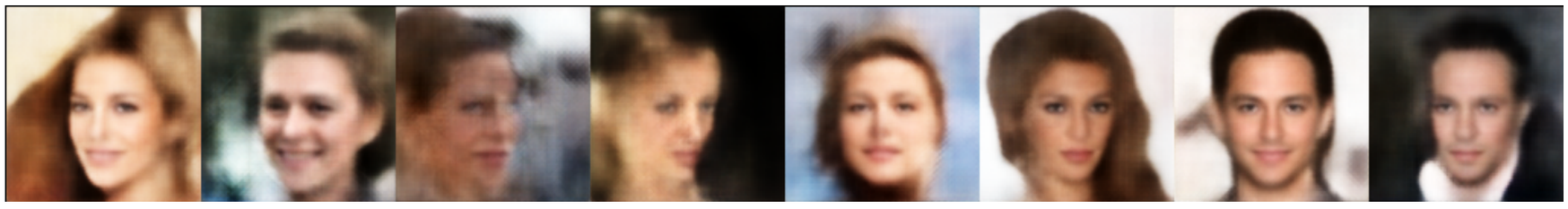


PCA

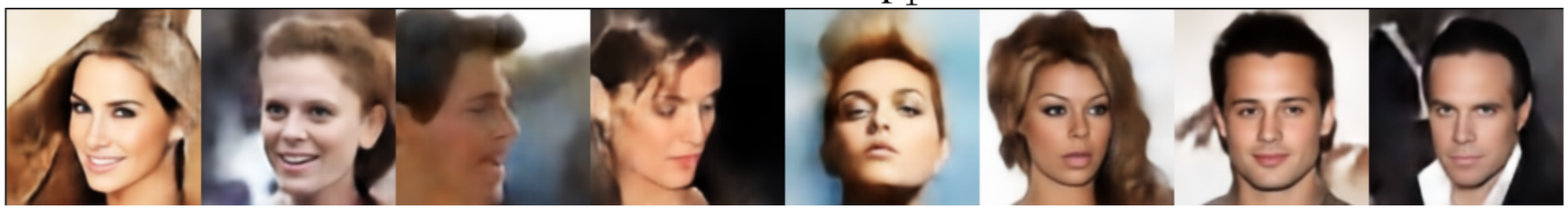


GAN with MSE

GLO with MSE



GLO with Lap_1



Autoregressive Models

- So far, we have seen models that attempt to estimate a density of the input domain $x \in \mathbb{R}^n$

$$p(x) = \int p(h)p(x|h)dh \ , \ p(x|h) = \exp(\langle \theta_h, \Phi(x) \rangle - A(\theta_h))$$

$$p(x) = p_0(\Phi(x)) \cdot |\det \nabla \Phi(x)|^{-1}$$

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- Chained Bayes Rule: for any ordering $(x_{\sigma(1)}, \ldots, x_{\sigma(n)})$ of the coordinates we have

$$p(x) = \prod_{i \leq n} p(x_{\sigma(i)} | x_{\sigma(1)} \ldots x_{\sigma(i-1)})$$

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- Q: In which situations is it better to use the factorized?

Autoregressive Models

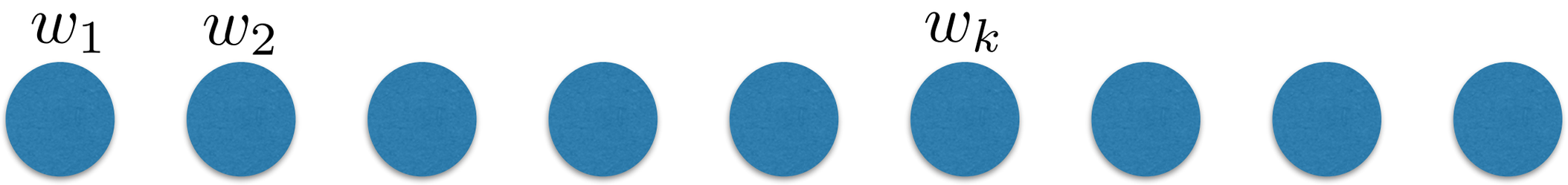
- Time Series
  - Speech, Music
  - Video
  - Language
  - Other time series (Weather, Finance, …)
- Spatially ordered data, Multi-Resolution data
  - Images

- Learning is thus reduced to the problem of conditional prediction.

$$p(x) \rightarrow \{p(x_i|x_{N(i)})\}_i$$

Word2vec [Mikolov et al.'13].

- Unsupervised learning "success story".



Word2vec [Mikolov et al.'13].

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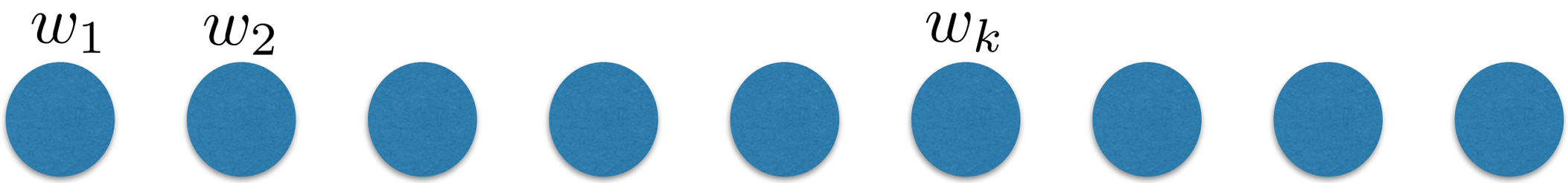
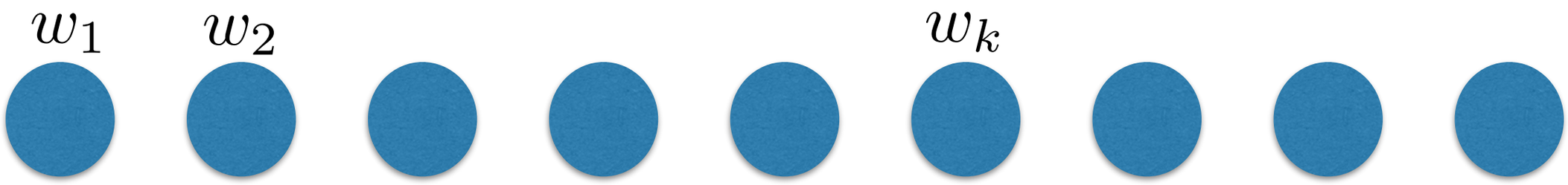


- Language creates a notion of similarity between words:

words w_1, w_2 are similar if they are "exchangeable"
i.e., they appear often within the same context.

Word2vec [Mikolov et al.'13].

- Unsupervised learning "success story".



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  words w_1, w_2 are similar if they are "exchangeable"
  i.e., they appear often within the same context.

- *Goal*: find a word representation $\Phi(w_i) \in \mathbb{R}^d$ that expresses this similarity as a dot product

$$\mathrm{sim}(w_i, w_j) \approx \langle \Phi(w_i), \Phi(w_j) \rangle \ .$$

Word2vec [Mikolov et al.'13].

- Main idea: Skip-gram with negative sampling.
- Construct a "training set"
  - *positive pairs* $\mathcal{D} = \{(w_k, c_k)\}_k$ of (words, contexts) appearing in a huge language corpus.
  - negative pairs $\mathcal{D}' = \{(w_{k'}, c_{k'})\}_{k'}$ of (words, contexts) not appearing in the corpus.

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- Model the probability of a pair (w, c) being positive as

$$p(D = 1|c, w) = \sigma(\langle v_w, v_c \rangle) \ , \ v_w, v_c \in \mathbb{R}^d$$

$$\sigma(x) = \frac{1}{1 + e^{-x}}$$

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- Training with Maximum Likelihood:

$$\sigma(x) = \frac{1}{1 + e^{-x}}$$

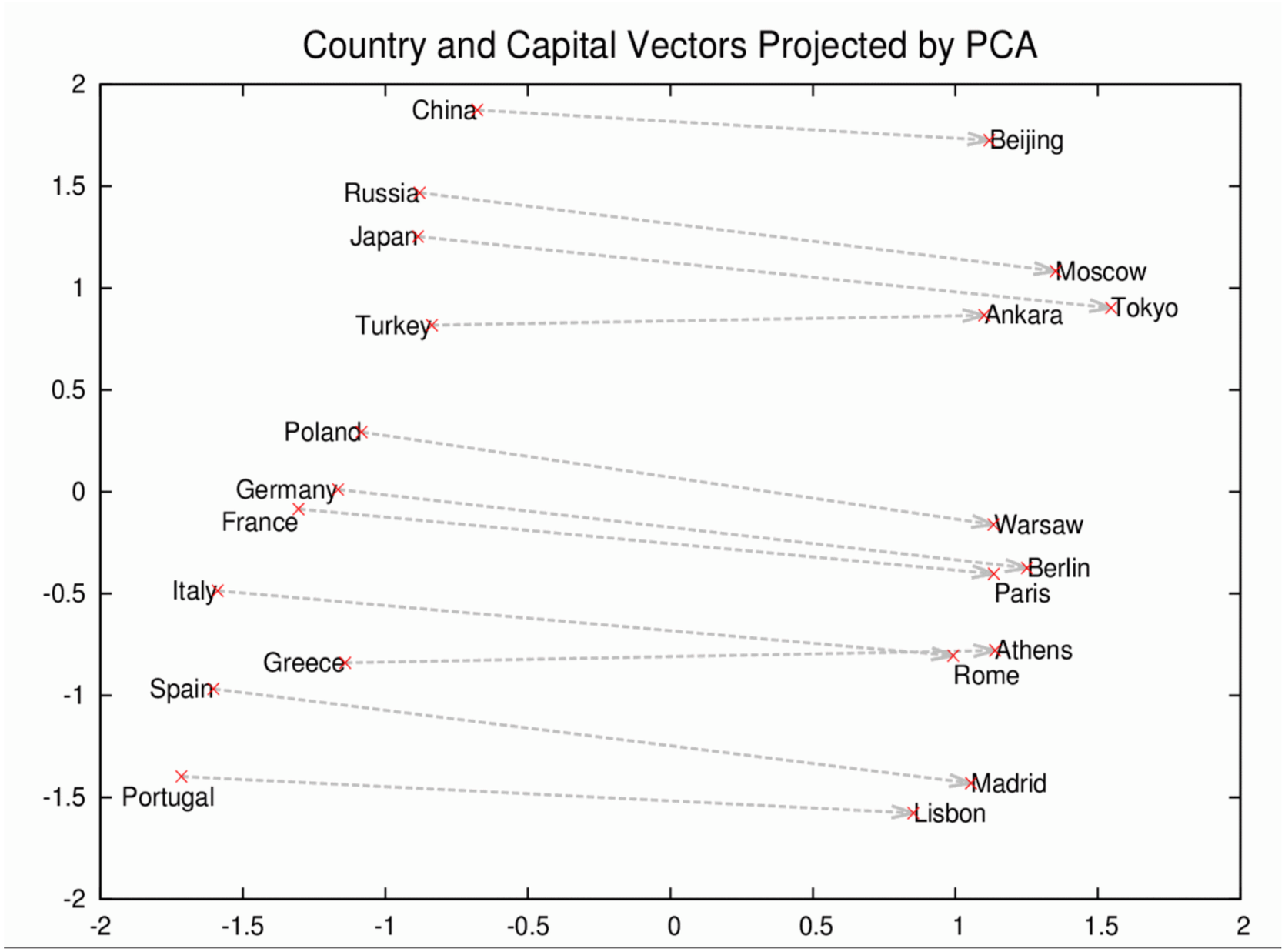
$$\arg\max_\theta \prod_{(w,c)\sim\mathcal{D}} p(D = 1|c, w, \theta) \prod_{(w,c)\sim\mathcal{D}'} p(D = 0|c, w, \theta)$$

$$\arg\max_\theta \sum_{(w,c)\sim\mathcal{D}} \log \sigma(\langle v_w, v_c \rangle) + \sum_{(w,c)\sim\mathcal{D}'} \log \sigma(-\langle v_w, v_c \rangle)$$

$\mathcal{D}$: positive contexts $\quad$ $\mathcal{D}'$: negative contexts

Word2vec [Mikolov et al.'13].

- Can be seen as an implicit matrix factorization using a mutual information criteria [Yoav & Goldberg,'14].
- Huge impact on Google's business bottom-line.



[google]

Video Prediction

- Rather than modeling the density of natural images

$$p(x) \ , \ x \in \mathbb{R}^d$$

we may be also interested in modeling the conditional distributions

$$p(x_{t+1}|x_1, \ldots, x_t)$$

where $(x_t)_t$ is temporally ordered data.

Video Prediction

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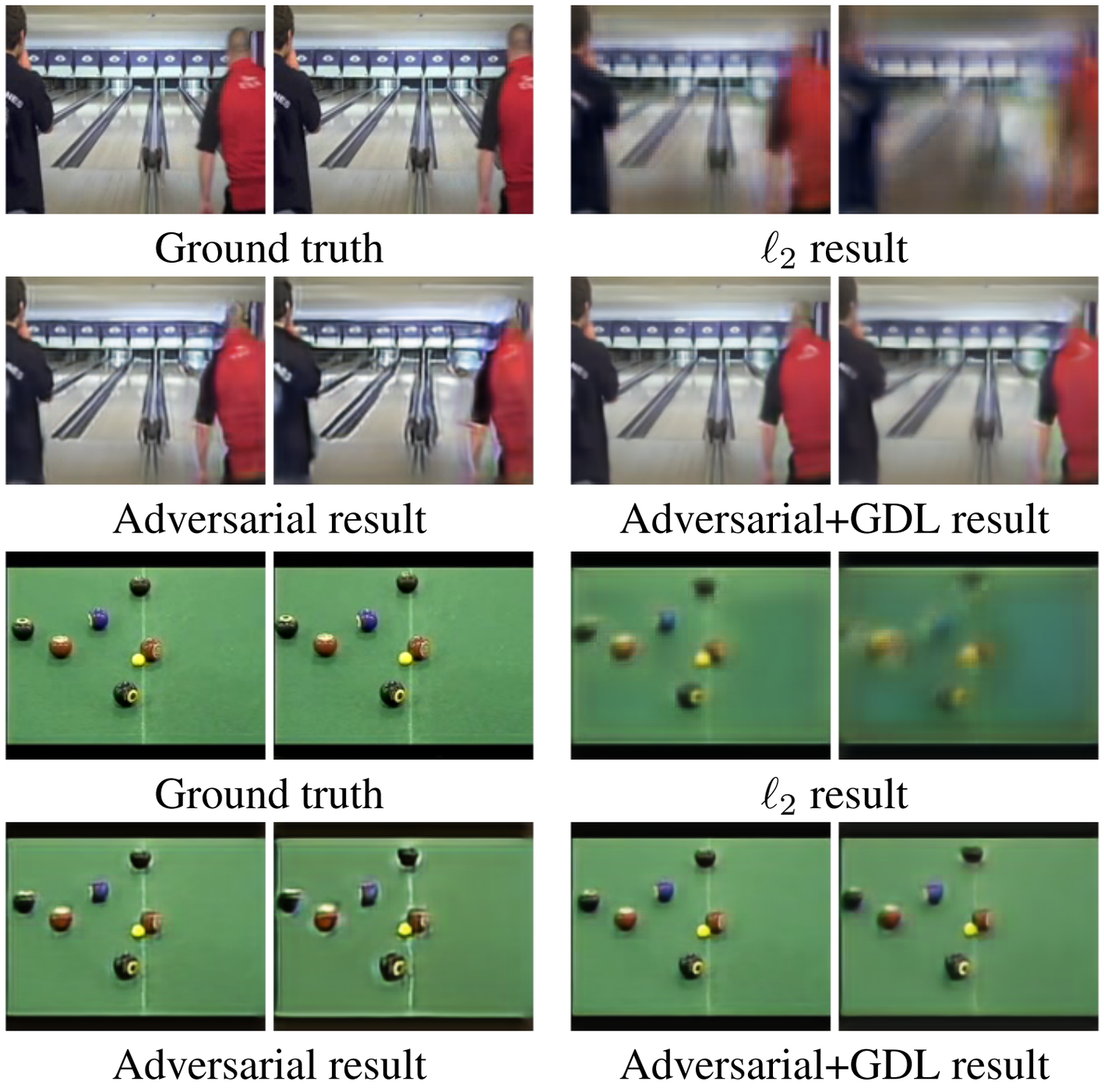
- Similarly, can we find a signal representation $\Phi(x_t)$ that is consistent with the "video language" metric? i.e.

$$\langle \Phi(x_t), \Phi(x_s) \rangle \approx h(|t-s|)$$

- This is the objective of Slow Feature Analysis [Sejnowski et al'02, Cadieu& Olshausen'10 and many others].

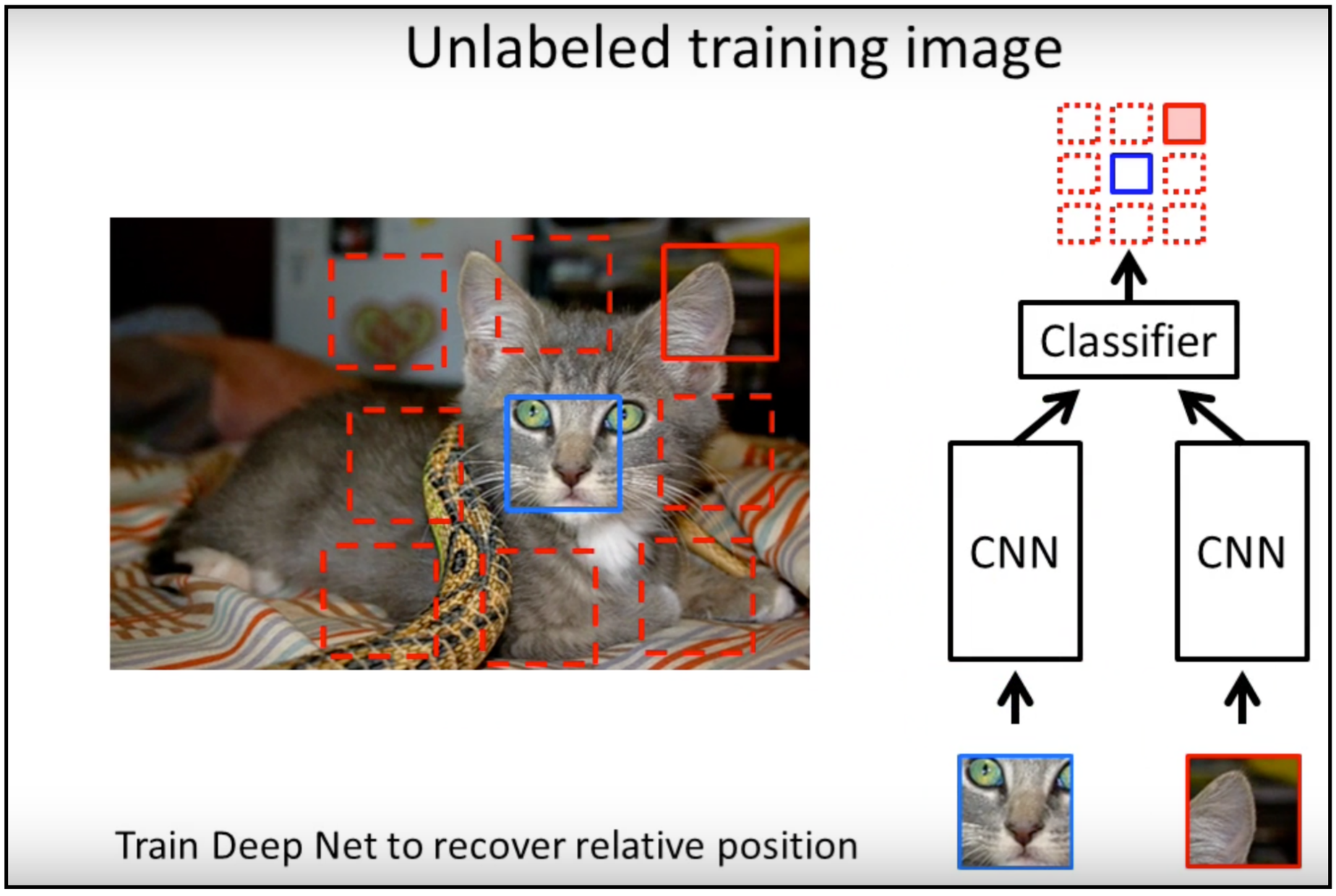
Video Prediction

- [Mathieu, Couprie, LeCun,'16]: Conditional video prediction using CNNs and an adversarial cost



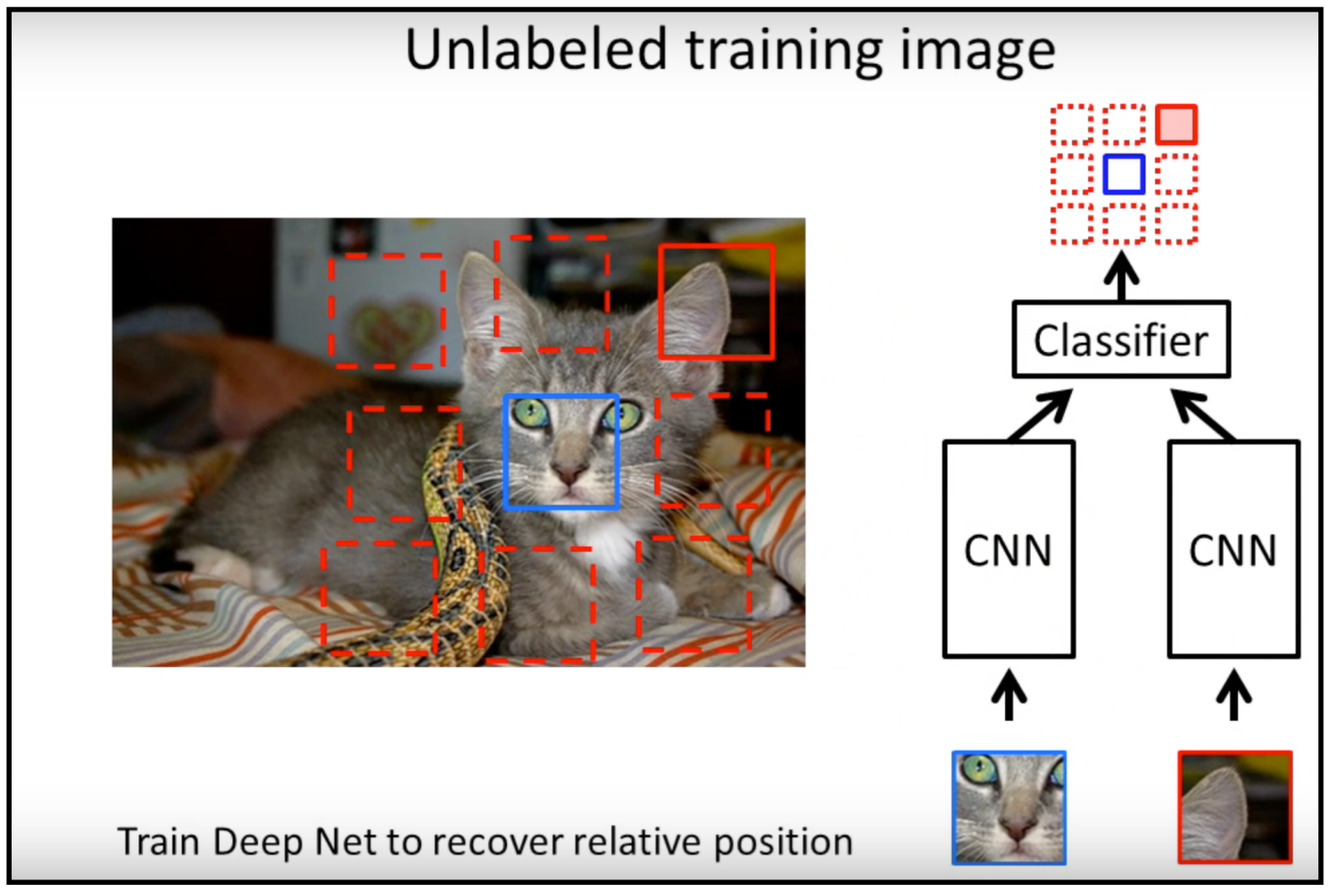
Patch Relative Configuration [Doerch et al.'15]

- Generalize the idea of positive, negative pairs to a multi-class classification problem about spatial configurations.



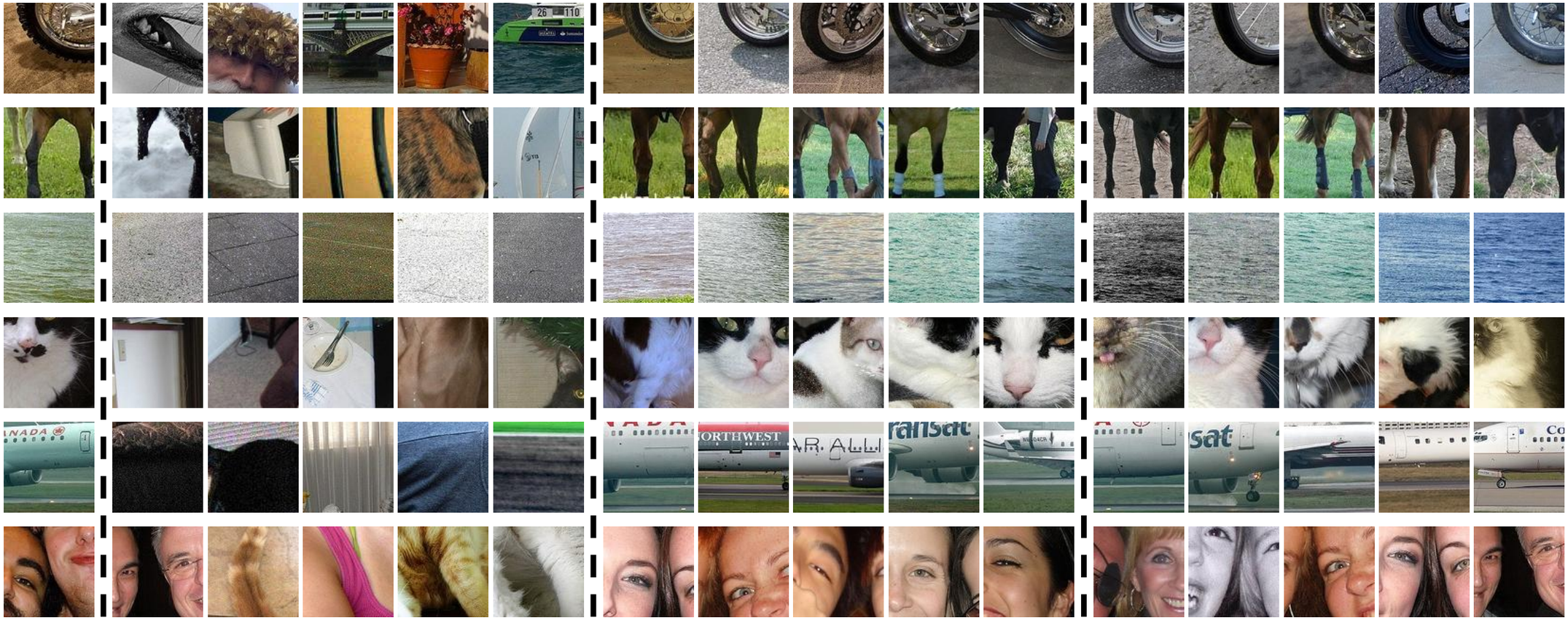
Patch Relative Configuration [Doerch et al.'15]

- Premise: A patch representation $\Phi(x)$ that does well in this task indirectly builds object priors.
- The criterion is not generative, but it retains enough information to generalize to other tasks



Patch Relative Configuration [Doerch et al.'15]

- Retrieval tasks:



- The representation captures visual similarity, leveraged in object detection, retrieval, etc.

Pixel Recurrent Networks [v.d.Oord et al'16]

- Prediction tasks of the form $\hat{x_{t+1}} = F(x_1, \ldots, x_t)$ require a loss or an associated likelihood

$$e.g.\ \|\hat{x}_{t+1} - x_{t+1}\|^2 \ \Leftrightarrow\ p(x_{t+1}|x_1, \ldots, x_t) = \mathcal{N}(F(x_1, \ldots, x_t), I)$$

- In discrete domains we simply use a multinomial loss, in continuous domains there is no principled choice.

- How about images?

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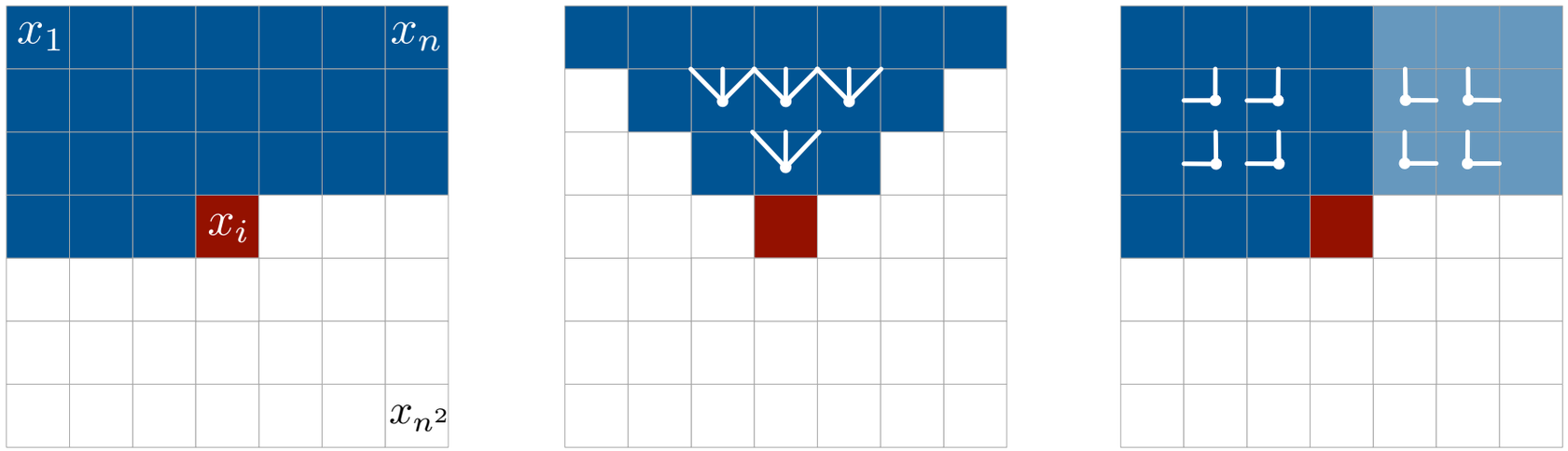
- In discrete domains we simply use a multinomial loss, in continuous domains there is no principled choice.

- How about images?
  - We can treat them as discrete two-dimensional grids $x(u) \in \{0, 255\}$
  - Model each pixel from its "past" context:

$$p(x(u)|x(v); v \in \Omega(u)) = \mathrm{softmax}\left(\Phi(x, \Omega(u))\right)$$

Pixel Recurrent Networks [v.d.Oord et al'16]

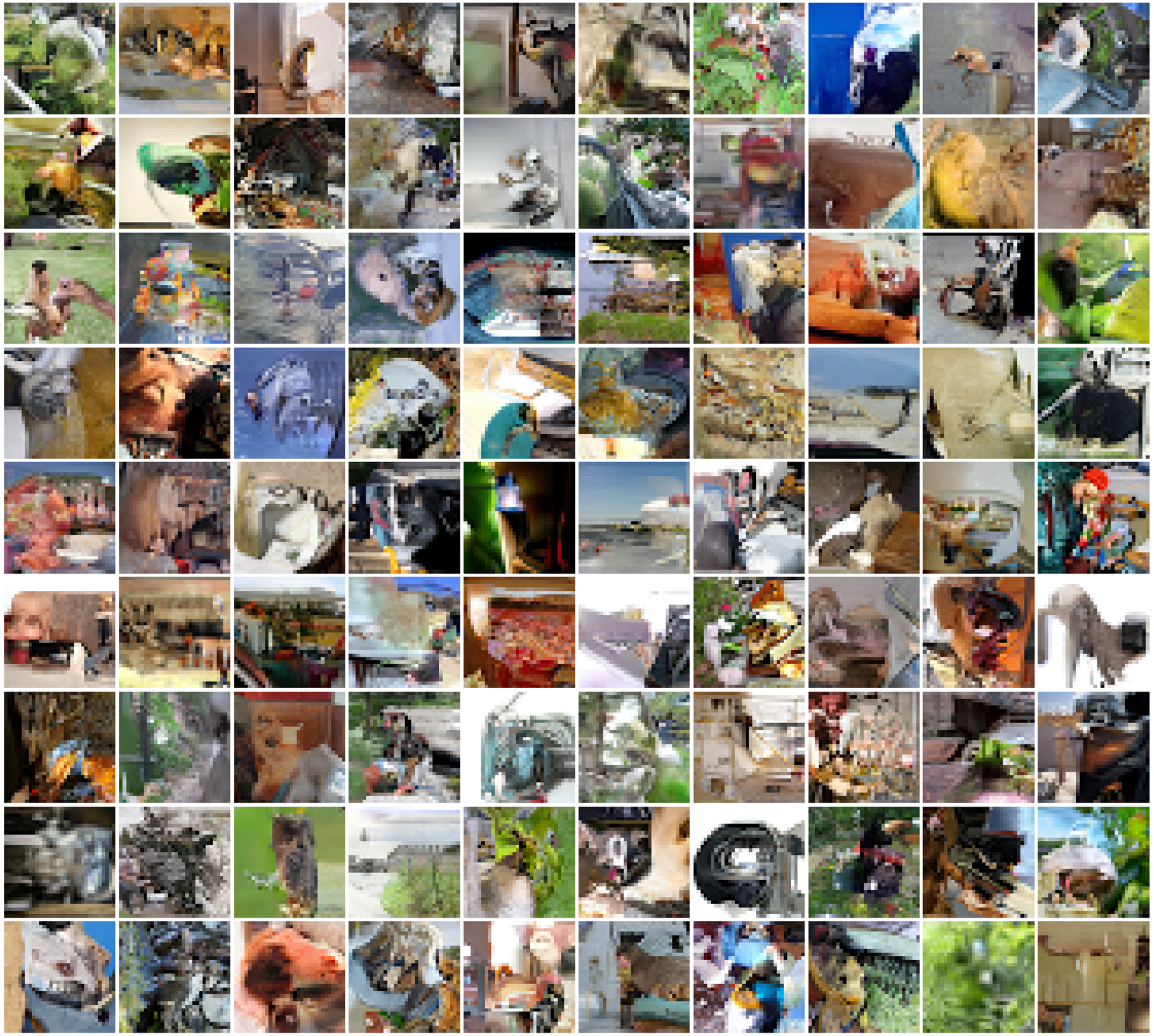
- Contexts are modeled using "diagonal BiLSTMS".



- Multi-Scale architecture conditions generations upon low-resolution samples (similarly as in LAPGANS).
- Very deep Recurrent Networks (> 10 layers).

Pixel Recurrent Networks [v.d.Oord et al'16]

- state-of-the-art image generation and modeling.



Pixel Recurrent Networks [v.d.Oord et al'16]

occluded completions original

occluded completions original

Pixel Recurrent Networks [v.d.Oord et al'16]

- MNIST and Cifar-10 log-likelihoods:

Model	NLL Test
DBM 2hl [1]:	$\approx$ 84.62
DBN 2hl [2]:	$\approx$ 84.55
NADE [3]:	88.33
EoNADE 2hl (128 orderings) [3]:	85.10
EoNADE-5 2hl (128 orderings) [4]:	84.68
DLGM [5]:	$\approx$ 86.60
DLGM 8 leapfrog steps [6]:	$\approx$ 85.51
DARN 1hl [7]:	$\approx$ 84.13
MADE 2hl (32 masks) [8]:	86.64
DRAW [9]:	$\leq$ 80.97
Diagonal BiLSTM (1 layer, $h = 32$):	**80.75**
Diagonal BiLSTM (7 layers, $h = 16$):	**79.20**

Table 4. Test set performance of different models on MNIST in *nats* (negative log-likelihood). Prior results taken from [1] (Salakhutdinov & Hinton, 2009), [2] (Murray & Salakhutdinov, 2009), [3] (Uria et al., 2014), [4] (Raiko et al., 2014), [5] (Rezende et al., 2014), [6] (Salimans et al., 2015), [7] (Gregor et al., 2014), [8] (Germain et al., 2015), [9] (Gregor et al., 2015).

Model	NLL Test (Train)
Uniform Distribution:	8.00
Multivariate Gaussian:	4.70
NICE [1]:	4.48
Deep Diffusion [2]:	4.20
Deep GMMs [3]:	4.00
RIDE [4]:	3.47
PixelCNN:	3.14 (3.08)
Row LSTM:	3.07 (3.00)
Diagonal BiLSTM:	**3.00** (2.93)

Table 5. Test set performance of different models on CIFAR-10 in *bits/dim*. For our models we give training performance in brackets. [1] (Dinh et al., 2014), [2] (Sohl-Dickstein et al., 2015), [3] (van den Oord & Schrauwen, 2014a), [4] personal communication (Theis & Bethge, 2015).

- Recently, extension to video and speech (see deepmind.com for details).

Limits of Transportation Models

- Direct learning by Optimizing the flow requires back propagation through a term of the form

$$f(\Theta) = \log \det \nabla \Phi(x_i; \Theta)$$

  - Very expensive for generic transformations Φ
  - Highly specific flows affect the flexibility of the model.

- Indirect learning by the Discriminative Adversarial Training is implicit
  - No cheap way to evaluate the density $p(x)$
  - Also, no cheap way to do inference, e.g. $p(z|x)$
- How to regularize the density estimation?

Open Challenges in Generative and Inference Tasks

- Some open directions of research:
  - Generative Models of irregular or discrete data (graphs, language)
  - Learning Markov Chain Monte-Carlo methods
  - Time-Series Models robust to noise

Generative Models for Graphs

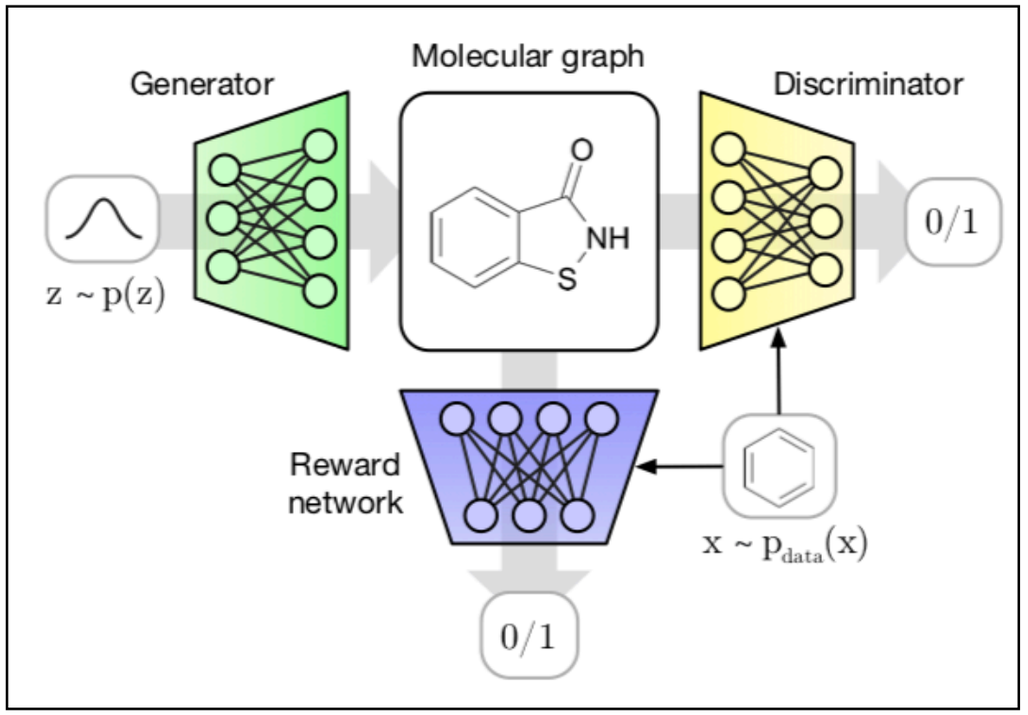
- Sequences can be generated using auto-regressive decoders, whereas images can use CNN decoders.

- How about distributions defined over general domains?
  - e.g. molecules, tweets, etc.

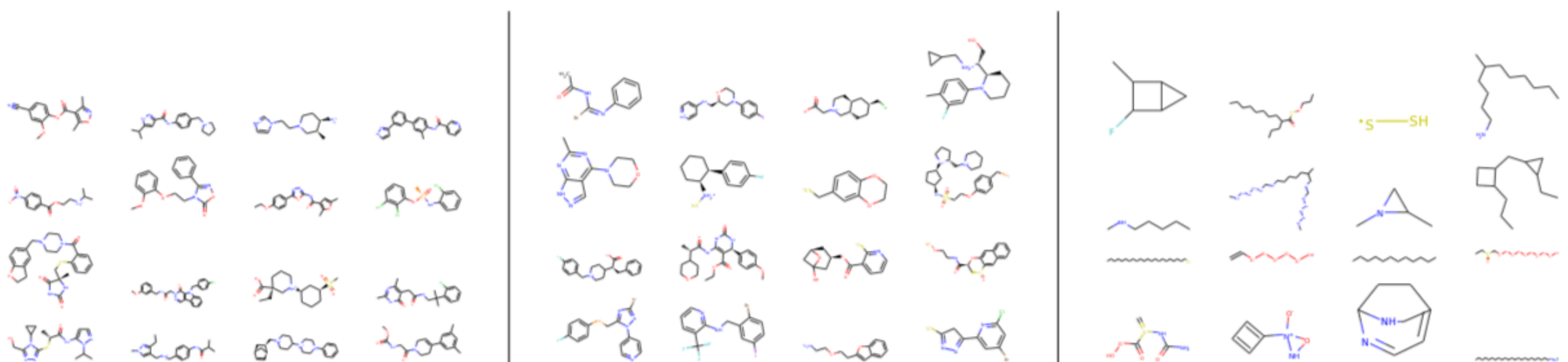
- There are several recent papers that explore the main generative paradigms over general graphs:
  - Variational Autoencoders: "Surface Nets", [Kostrikov et al.'18] "Variational Graph Autoencoders", Kipf et al. "Graphite", Grover et al.
  - Sequential Models: "GraphRNN", et.c
  - Adversarial Models: GraphGAN, MolGan.

Generative Models for Graphs

- Challenges:
  - Generation of sparse matrices in near linear time
  - generic vs specific architectures to each domain.



Learning Deep Generative Models of Graphs



Learning Markov Chain Monte-Carlo

- We saw in class that MH is a very *robust* algorithm — consistent in very general conditions, but potentially very slow in high-dimensions.

- Q: Can we leverage structural information on certain class of probability distributions to *learn* more efficient sampling schemes?

Learning Markov-Chain Monte-Carlo

- Recent papers attempting to use adversarial training to train samplers.

A-NICE-MC: Adversarial Training for MCMC

Jiaming Song
Stanford University
tsong@cs.stanford.edu

Shengjia Zhao
Stanford University
zhaosj12@cs.stanford.edu

Stefano Ermon
Stanford University
ermon@cs.stanfo

A Complete Recipe for Stochastic Gradient MCMC

Yi-An Ma, **Tianqi Chen**, and **Emily B. Fox**
University of Washington {yianma@u,tqchen@cs,ebfox@stat}.washington.edu

Metropolis-Hastings Generative Adversarial Networks

Ryan Turner Uber AI Labs
Jane Hung Uber AI Labs
Yunus Saatci Uber AI Labs
Jason Yosinski Uber AI Labs

META-LEARNING FOR STOCHASTIC GRADIENT MCMC

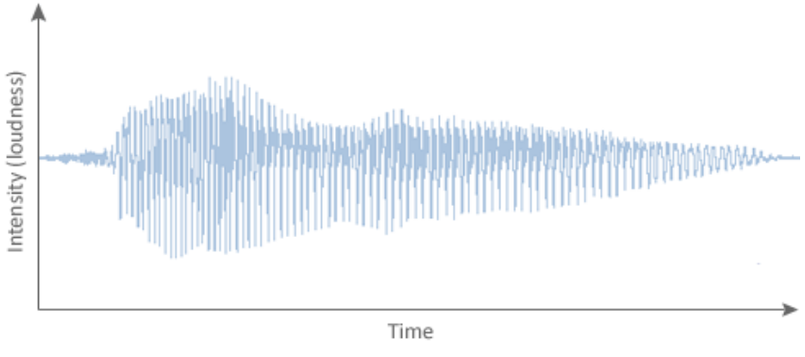
Anonymous authors
Paper under double-blind review

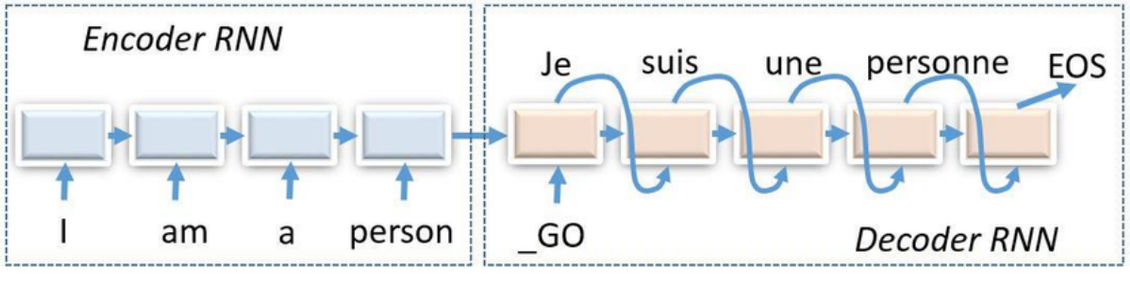
METROPOLIS-HASTINGS VIEW ON VARIATIONAL INFERENCE AND ADVERSARIAL TRAINING

Anonymous authors
Paper under double-blind review

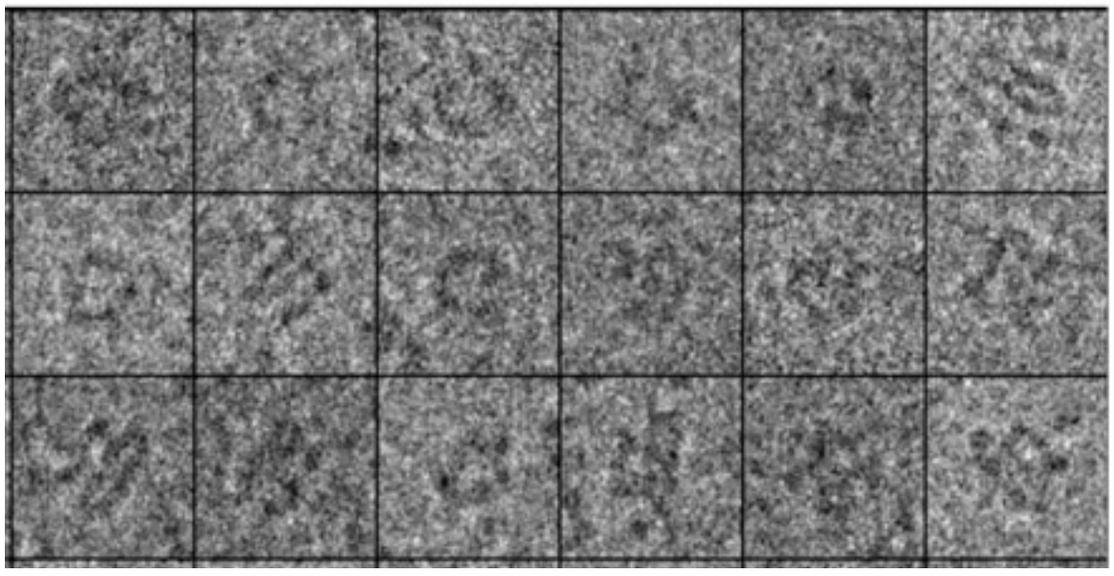
Noise in ML

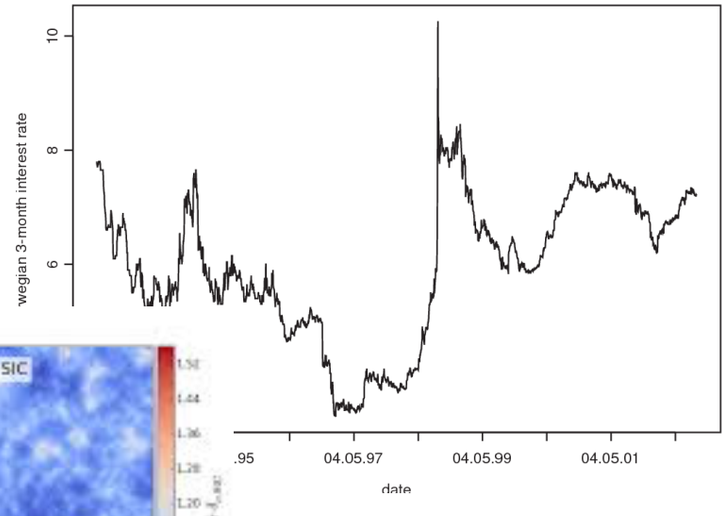
- Another major question for current research is how to deal with noise in deep, non-linear generative/predictive models.

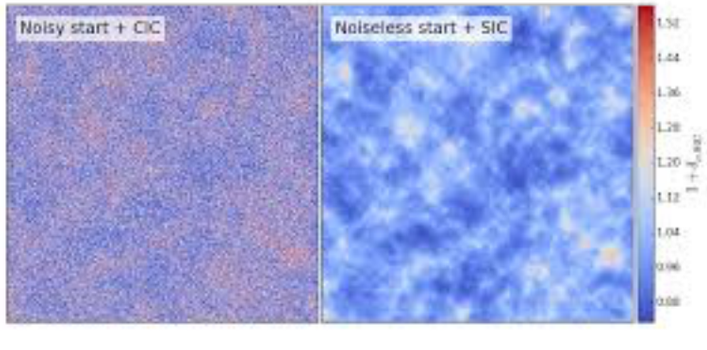




noise-free







typical real-life

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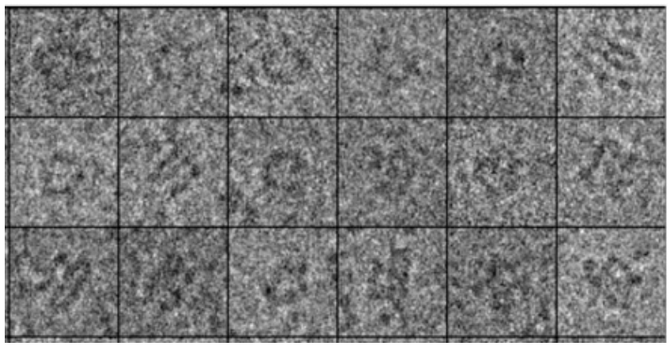

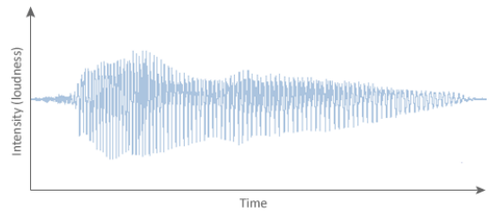

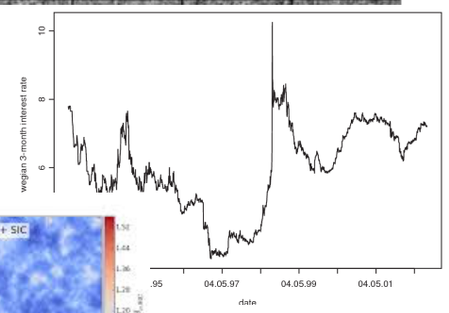

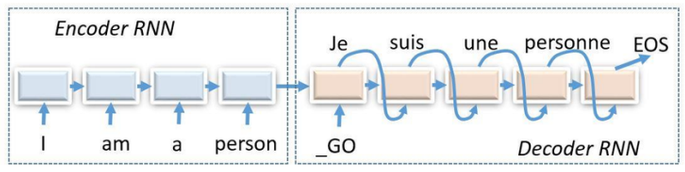

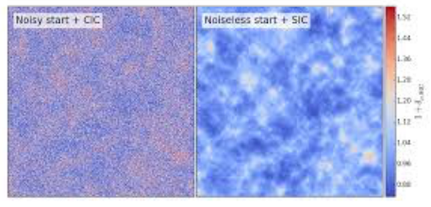

- In some regimes, one can trade-off noise with more labeled data (e.g. tags in image recognition), but this is not always scalable.
- Guarantees that deep models can find signal within noise?