Advanced topics in deep generative models

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Breaking the Surface 2019
Biograd na Moru, Croatia

Part I

Improving Variational Auto-encoders

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- **Reminder:** VAEs optimize the ELBO, with a KL divergence to bound the data log-likelihood

$$F(\mathbf{x}, \theta, \phi) = \ln p(\mathbf{x}) - D\left(q_\phi(\mathbf{z}|\mathbf{x}) || p(\mathbf{z}|\mathbf{x})\right) \tag{1}$$

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     - Hierarchical latent variables
     - Improved flexibility with flows

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- Use as likelihood estimator, **e.g**. with $k \approx 10^3$

Training procedure importance weighted autoencoders

- Gradients of importance weighted lower bound

$$\nabla F_k(\mathbf{x}) = \mathbb{E}_{\mathbf{z}_{1:k} \sim q_\phi(\mathbf{z}|\mathbf{x})} \left[\sum_{i=1}^{k} \widetilde{w}_i \nabla \big(\ln p(\mathbf{x}, \mathbf{z}_i) - \ln q_\phi(\mathbf{z}_i|\mathbf{x}) \big) \right]$$

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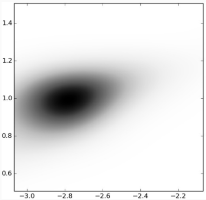
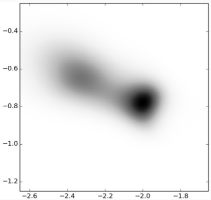
- Allows for more accurate models with complex posteriors

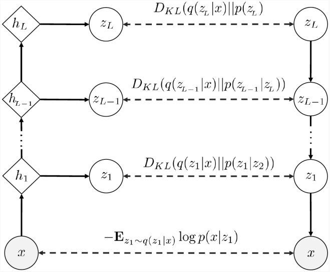




From [Burda et al., 2016]: True posterior $p(\mathbf{z}|\mathbf{x})$ VAE (left) and IW-VAE (right)

Top-down hierarchical sampling

- Multiple levels of latent variables at increasing resolutions



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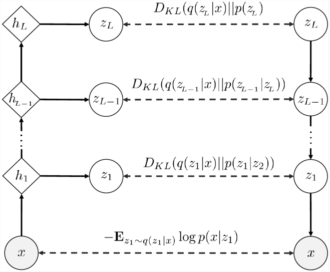

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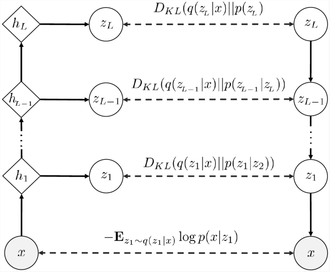

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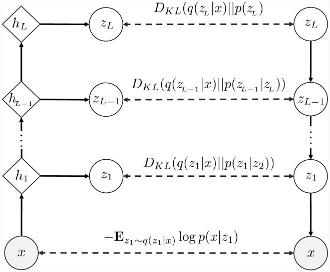

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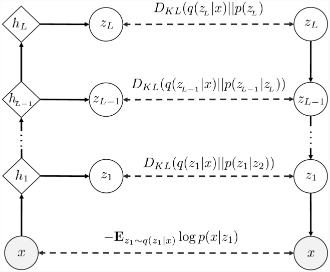
- Extended VAE log-likelihood bound



$$F = \ln p(\mathbf{x}) - D_{KL}(q(\mathbf{z}_{1:L}|\mathbf{x})||p(\mathbf{z}_{1:L}|\mathbf{x})$$
$$= \underbrace{\mathbb{E}_{q(\mathbf{z}_1|\mathbf{x})}[\ln p(\mathbf{x}|\mathbf{z}_1)]}_{\text{Reconstruction}} - \underbrace{\sum_{i=1}^{L} \mathbb{E}_{q(\mathbf{z}_{i+1})}[D_{KL}(q(\mathbf{z}_i|\mathbf{x})||p(\mathbf{z}_i|\mathbf{z}_{i+1})])}_{\text{Regularization}}$$

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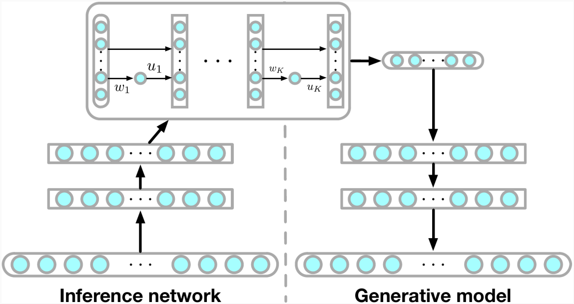

Figure from [Rezende and Mohamed, 2015]

Normalizing flows

- Let density "flow" through set of invertible transformations

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- $O(D)$ determinant, rather than $O(D^3)$, for planar and radial flows

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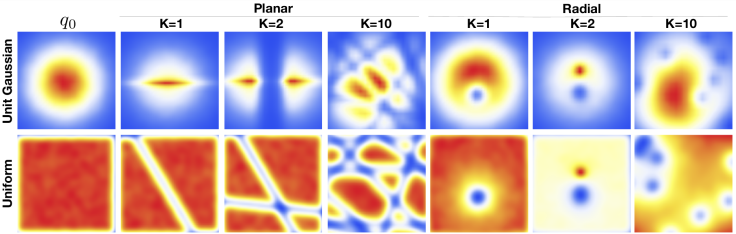
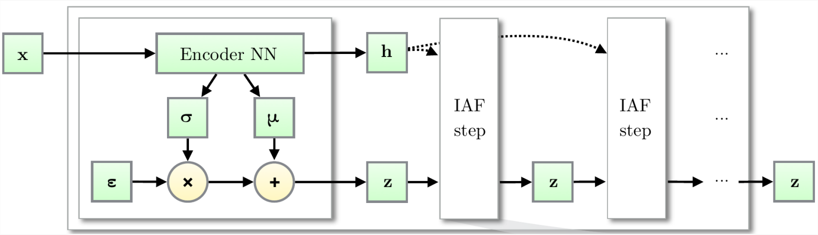


Figure from [Rezende and Mohamed, 2015]

Autoregressive flow [Kingma et al., 2016]

- Restictive flows in [Rezende and Mohamed, 2015]
  - Planar flow similar to MLP with single hidden unit
- Use autoregressive transformations in flow
  - Rich and tractable class of transformations
  - Fewer transformations needed



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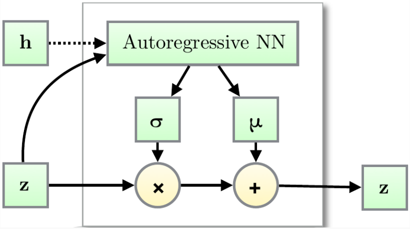

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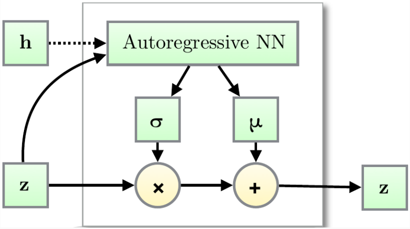

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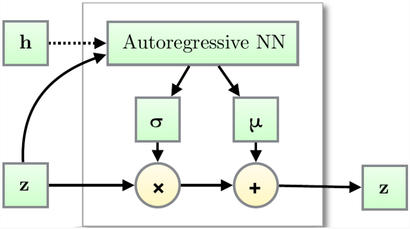
- Free to chose form of autoregressive NN dependency



Improved VAE — Recap

Ways to improve the tightness of the ELBO:

- Importance weighted autoencoder
- Hierarchical top-down sampling
- Density flow transformation

Beyond conditional independence assumption in VAE

- Standard VAE decoders assumes conditional independence

$$p(\mathbf{x}|\mathbf{z}) = \prod_{i=1}^{D} p(x_i|\mathbf{z}), \quad (3)$$

$$p(x_i|\mathbf{z}) = \mathcal{N}\left(x_i; f_\theta^\mu(\mathbf{z})_i, f_\theta^\sigma(\mathbf{z})_i\right) \quad (4)$$

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- Conditional log-likelihood is ℓ_2 reconstruction term

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- Bad metric of image similarity

Beyond conditional independence assumption in VAE

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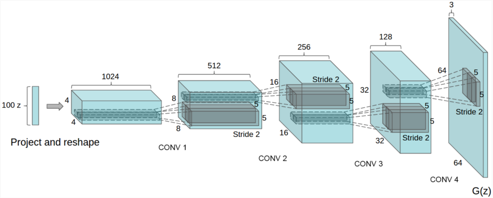

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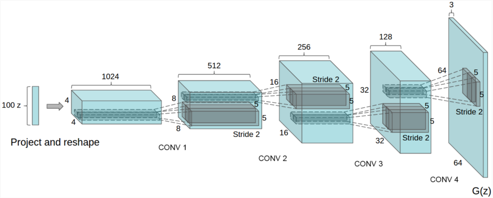
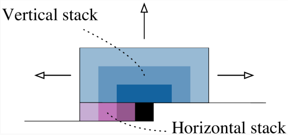
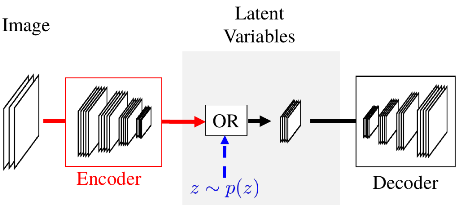


- Autoregressive PixelCNN
  - Needs many layers to induce long-range dependencies
  - Doesn't learn latent representation



Hybrid PixelVAE model [Gulrajani et al., 2017b]

- Latent var. input to deterministic upsampling decoder $f(\mathbf{z})$



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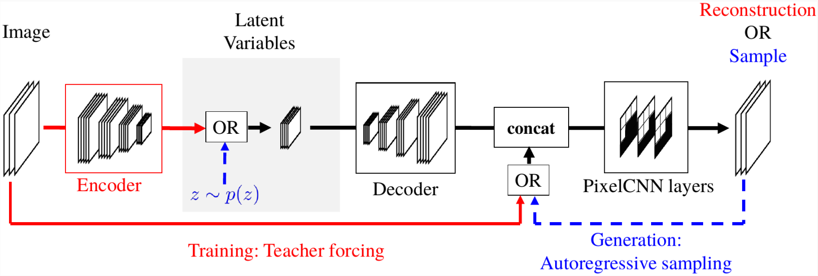

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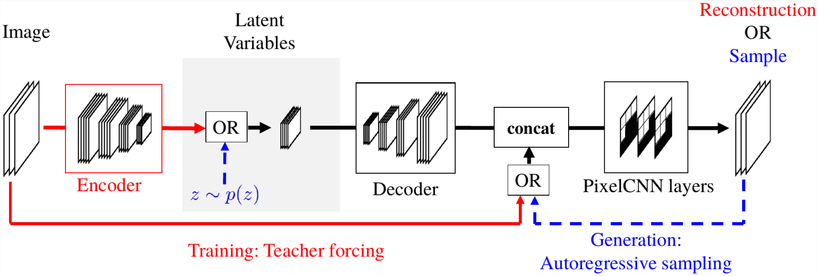
$$p(\mathbf{z}) = \mathcal{N}(\mathbf{z}; 0, I), \quad (5)$$

$$p(\mathbf{x}) = \int_{\mathbf{z}} p(\mathbf{z}) \prod_i p(x_i | \mathbf{x}_{<i}, f(\mathbf{z})) \quad (6)$$



Samples PixelVAE model LSUN dataset

- Model with three levels of stochasticity
  - Latent variables at 1×1
  - Latent variables at 8×8
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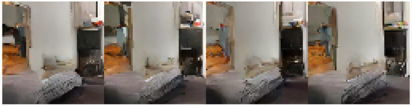

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- Hierarchical representation learning

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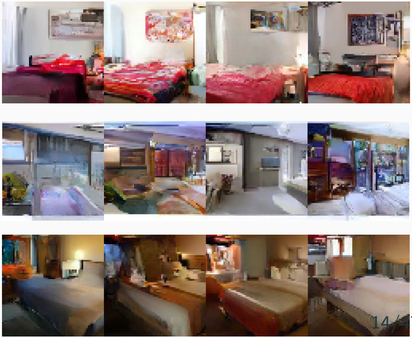
Re-sampling 8×8 + PixelCNN



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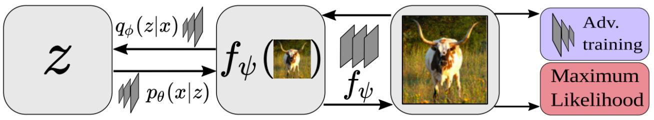

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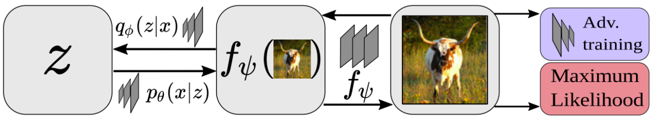

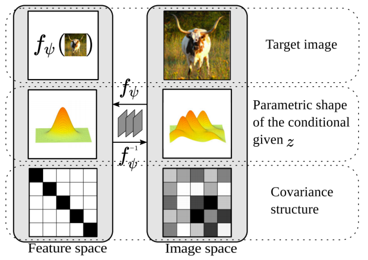

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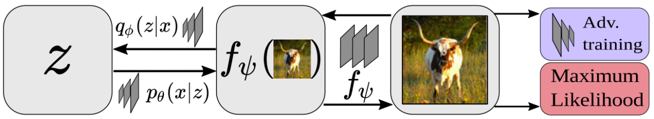

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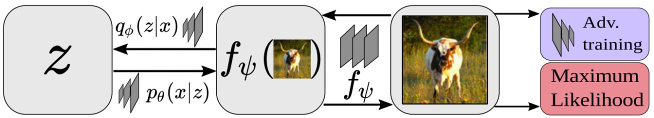

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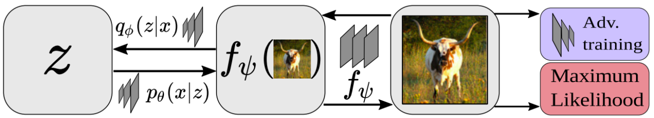

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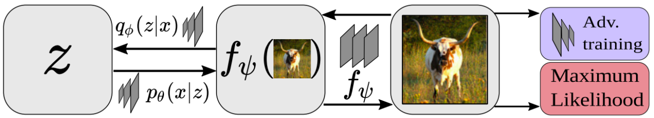
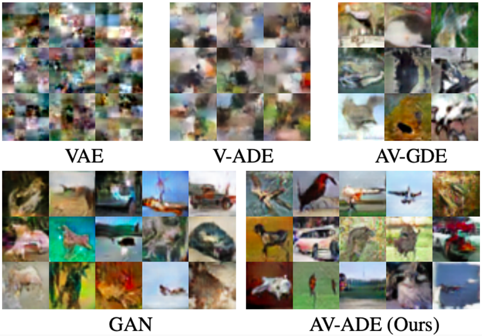
- Evidence lower-bound with change of variables

$$\ln p(\mathbf{x}) \geq \mathbb{E}_{q(\mathbf{z}|\mathbf{x})}[\ln p_{\mathbf{y}}(f(\mathbf{x})|\mathbf{z})] - D_{\mathrm{KL}}(q(\mathbf{z}|\mathbf{x})||p(\mathbf{y})) + \ln \left| \det \frac{\partial f(\mathbf{x})}{\partial \mathbf{x}} \right|$$



Hybrid VAE-Flow model - Ablation

- Adversarial training critical for good sample quality
- MLE critical for good held-out likelihoods
- Flow improves both likelihoods and sample quality



	f_ψ	Adv.	MLE	BPD ↓	IS ↑	FID ↓
GAN	×	✓	×	[7.0]	6.8	31.4
VAE	×	×	✓	4.4	2.0	171.0
V-ADE†	✓	×	✓	3.5	3.0	112.0
AV-GDE	×	✓	✓	4.4	5.1	58.6
AV-ADE†	✓	✓	✓	3.9	7.1	28.0

Table 1: Quantitative results. † : Parameter count decreased by 1.4% to compensate for f_ψ. [Square brackets] denote that the value is approximated, see Section 5.

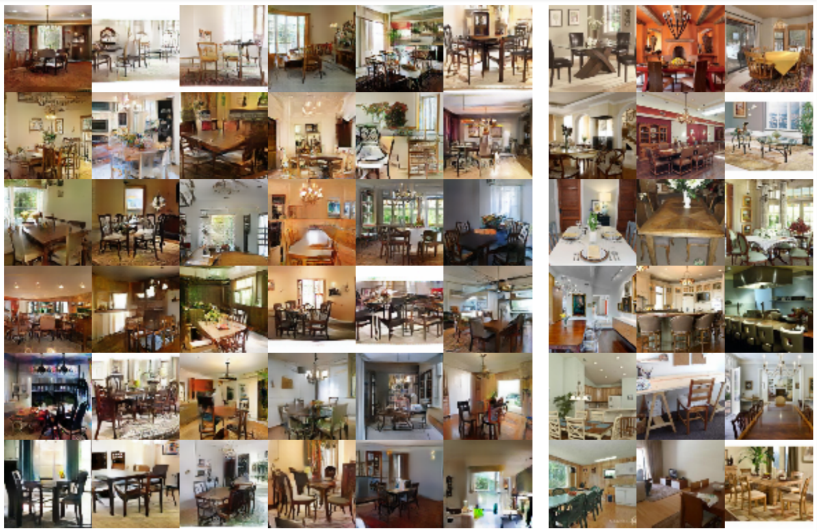
Figure 5: Samples from GAN and VAE baselines, our V-ADE, AV-GDE and AV-ADE models, all trained on CIFAR-10.

Hybrid VAE-Flow model - Comparison to Glow

- AV-ADE: better samples, worse likelihood
- Temperature annealing allows Glow to trade-off the two

LSUN 64×64: Chruches (C) and Bedrooms (B). Figure from [Lucas et al., 2019]

Hybrid VAE-Flow model - Samples and Images



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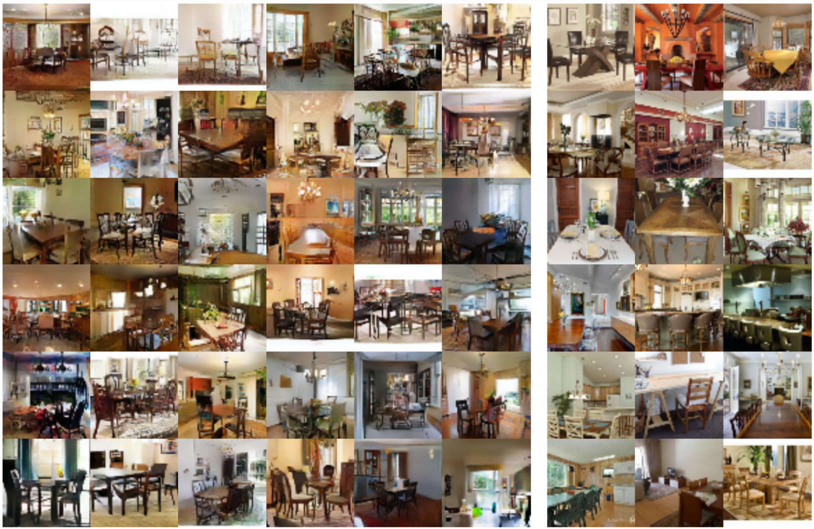

LSUN 64 × 64: Dining rooms. Samples left, training images right.
Figure from [Lucas et al., 2019]

Part II

Recent advances in flow-based generative modeling

Reduced temperature sampling [Kingma and Dhariwal, 2018]

- Sample closer to the mode of the distribution

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- Can sample from reduced Gaussian in latent space, and then project

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Increasing temperature from left to right. Figure from [Kingma and Dhariwal, 2018].

Recipes for "efficient" invertible flows

$$\mathbf{y} = f(\mathbf{x}), \qquad J_f(x) = \frac{\partial \mathbf{y}}{\partial \mathbf{x}^\top}, \tag{13}$$

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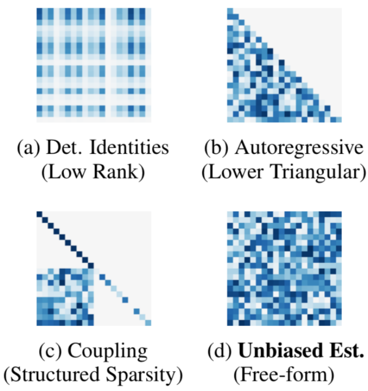

(a) Det. Identities (Low Rank)

(b) Autoregressive (Lower Triangular)

(c) Coupling (Structured Sparsity)

(d) **Unbiased Est.** (Free-form)

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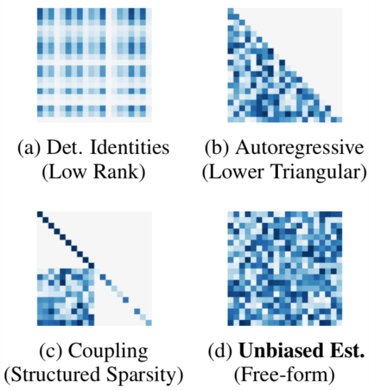

(a) Planar flow [Rezende and Mohamed, 2015]

(b) Inverse Autoregressive Flow [Kingma et al., 2016]

(c) Real-NVP [Dinh et al., 2017]

(d) **Invertible ResNet** [Behrmann et al., 2019, R.Chen et al., 2019]

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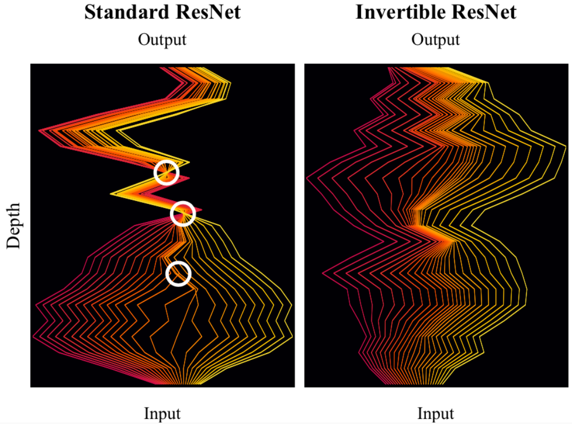

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- Possible to use ResNet for flow-based generative model

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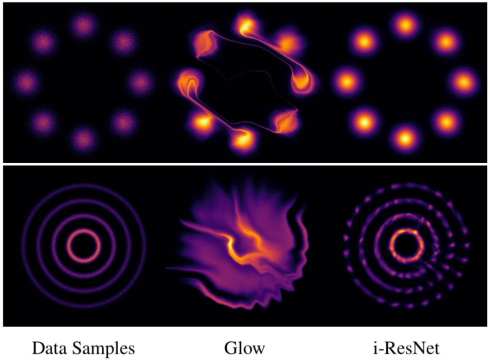

Figure from [Behrmann et al., 2019]

Invertible ResNets [Behrmann et al., 2019]

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	$\lambda = 0$	$\lambda = 1/D$		$\lambda = 1$	
Block Type	Acc↑	BPD↓	Acc↑	BPD↓	Acc↑
Coupling	89.77%	4.30	87.58%	3.54	67.62%
+ 1×1 Conv	90.82%	4.09	87.96%	3.47	67.38%
Residual	**91.78%**	**3.62**	**90.47%**	**3.39**	**70.32%**

Results on CIFAR-10 from [R.Chen et al., 2019]

Part III

Stabilizing GAN training

A discussion on the GAN training loss

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- Jensen-Shannon divergence: idealized loss approximated by the discriminator
  - Symmetric KL to mixture of p and q

$$D_{JS}(p||q) = \frac{1}{2} D_{KL}\left(p\middle|\middle|\frac{p+q}{2}\right) + \frac{1}{2} D_{KL}\left(q\middle|\middle|\frac{p+q}{2}\right) \tag{23}$$

A discussion on the GAN training loss

- Training loss for the Discriminator:

$$V(\phi, \theta) = \mathbb{E}_{x \sim p_{\text{data}}(x)}[\ln D_\phi(x)] + \mathbb{E}_{z \sim p(z)}[\ln(1 - D_\phi(f_\theta(z)))] \quad (24)$$

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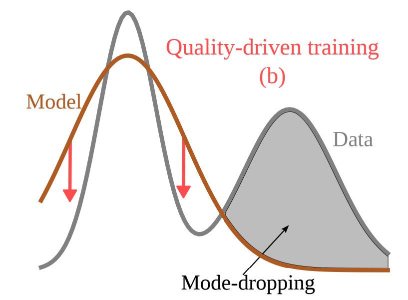

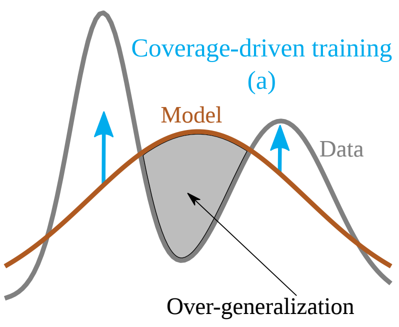

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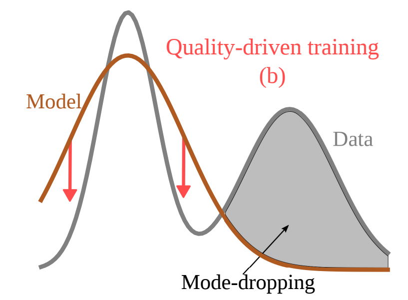

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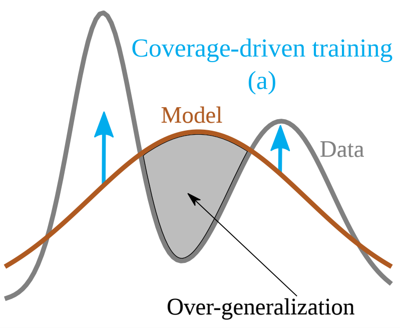

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   - Same stable points in the minimax optimization
   - Helps, but problem remains: as D_ϕ becomes strong, gradients vanish

Question:

Can we think of a better 'ideal loss'?

Wasserstein or "earth-mover" distance

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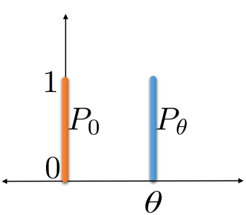
- Wasserstein distance is the cost of optimal transformation

$$D_{WS}(p||q) = \inf_{\gamma \in \Gamma(p,q)} T(\gamma) \tag{25}$$

Distributions with low dimensional support

- Simple example: support on lines in $\mathbb{R}^2$
  - p_0 uniform on $x_2 \in [0, 1]$ for $x_1 = 0$
  - p_θ uniform on $x_2 \in [0, 1]$ for $x_1 = \theta$



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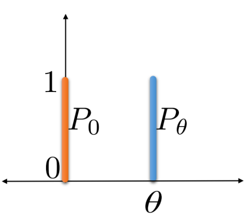

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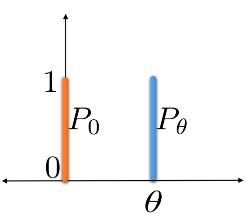

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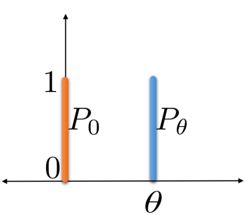

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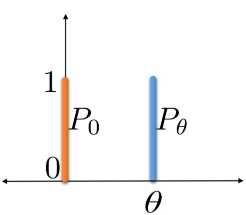

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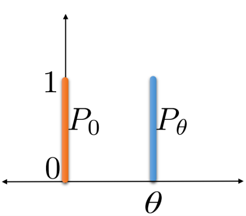

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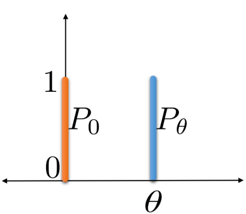

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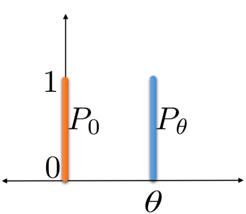

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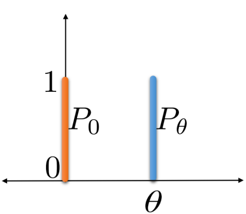

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Wasserstein GAN

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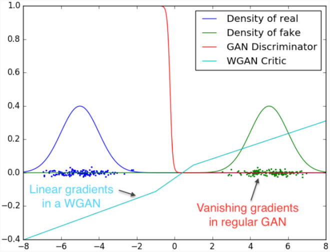

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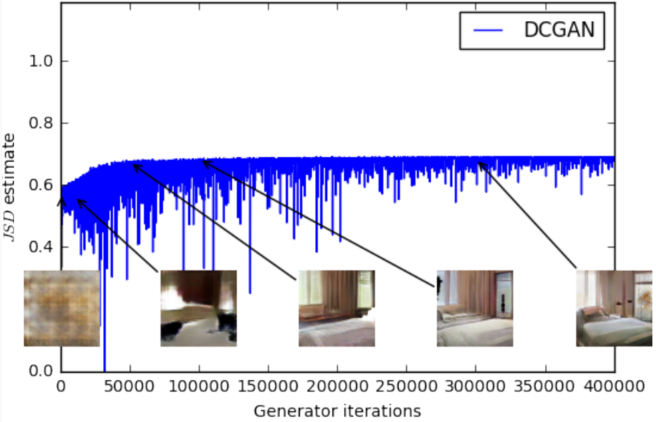

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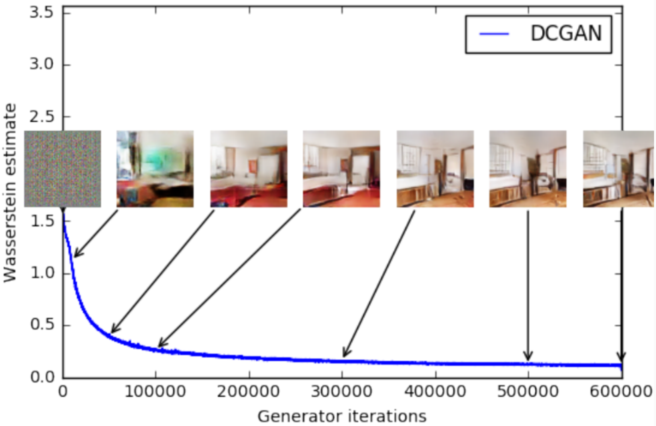

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- Removing the log avoids vanishing gradients

Lipschitz continuity as a regularizer

- **Reminder:** k-Lispschitz means $|f(x) - f(y)| \leq |x - y|$
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- Gradient penalty [Gulrajani et al., 2017a]
  - Add a penalty to the loss:

$$G_{\text{pen}} = \lambda \mathbb{E}_x[||\nabla_x D(x)||_2 - 1)^2]$$

Wrap up

- A **lot** of other losses have been develloped
- The lipschitz regularization is a widely adopted regularization
- The log is usually avoided to improve gradients when Discriminator is good.

Latent variable inference in GANs [Donahue et al., 2017]

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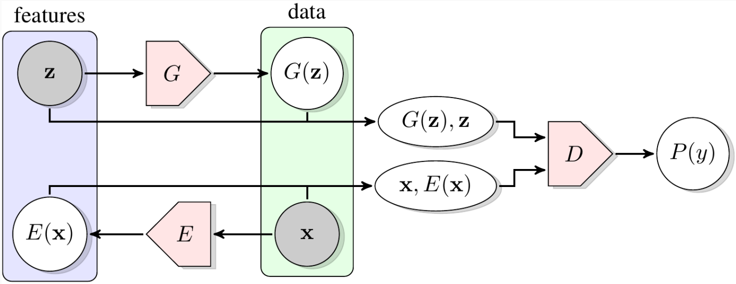
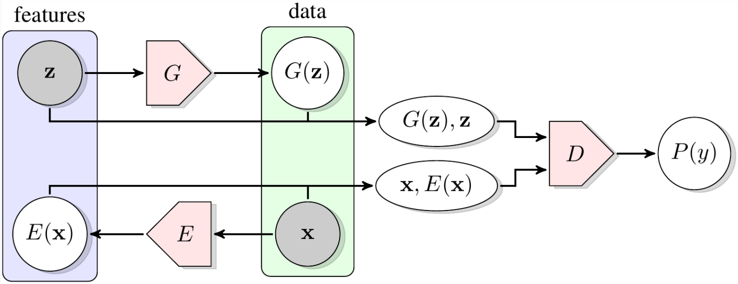


Induced joint distributions over $(\mathbf{x}, \mathbf{z})$



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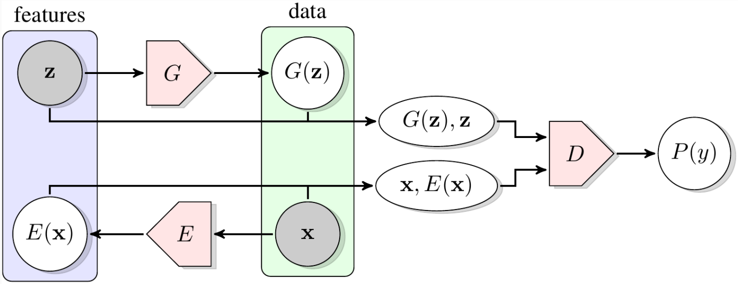

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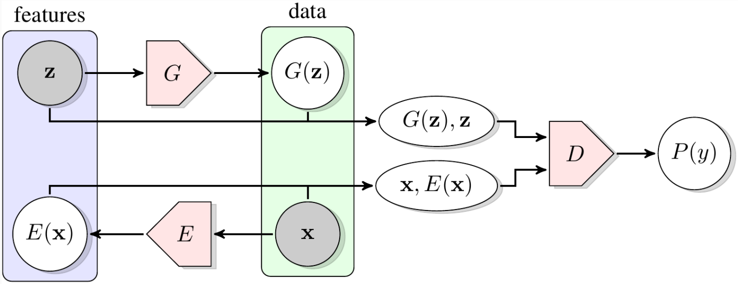

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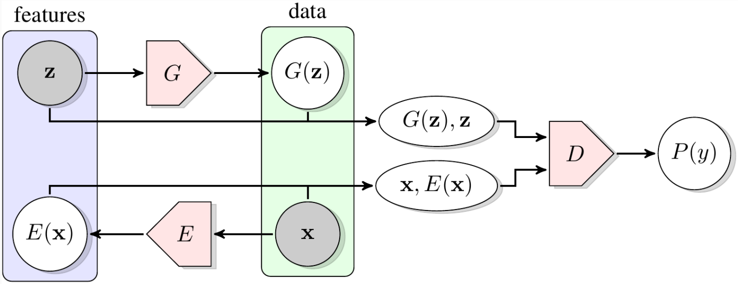

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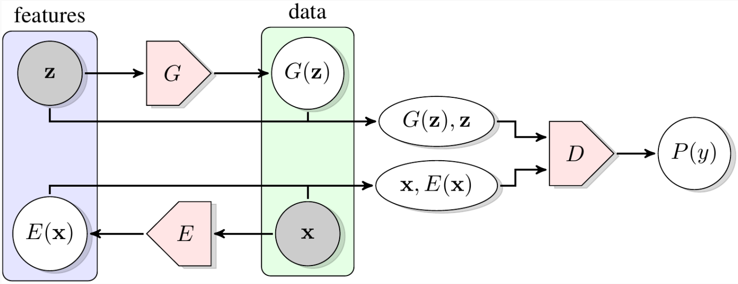
- Encoder: $p_E(\mathbf{x}, \mathbf{z}) = p_{\text{data}}(\mathbf{x})\ \delta\left(\mathbf{z} - E(\mathbf{x})\right)$
- Discriminator: pair $(\mathbf{x}, \mathbf{z})$ completed by generator or encoder?

Bidirectional GANs [Donahue et al., 2017]



$$V(D, E, G) = \mathbb{E}_{p_{\text{data}}}[\ln D(\mathbf{x}, E(\mathbf{x}))] + \mathbb{E}_{p(\mathbf{z})}[\ln(1 - D(G(\mathbf{z}), \mathbf{z}))]$$

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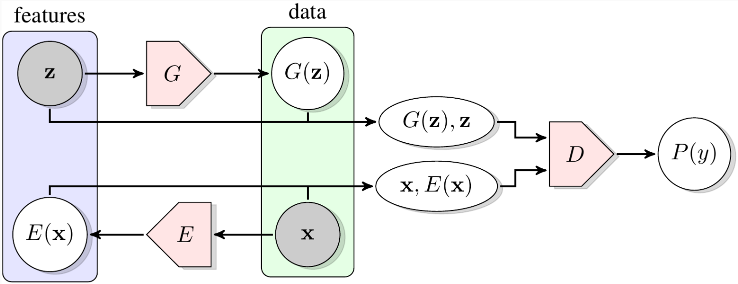

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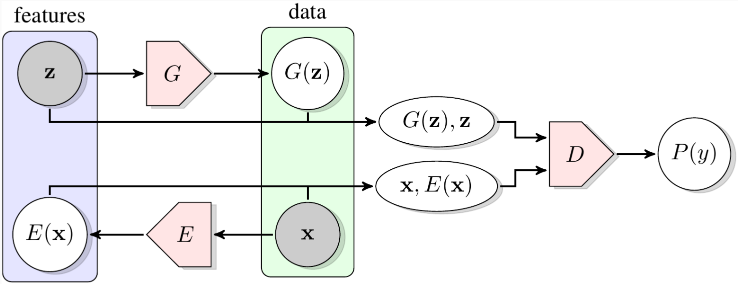

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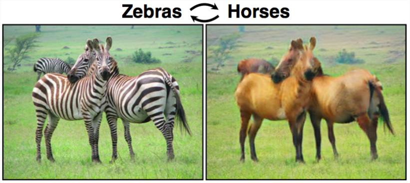
- At optimum G and E are each others inverse

Unpaired image-to-image translation [Zhu et al., 2017]



- Learn 2-way mapping between different image domains

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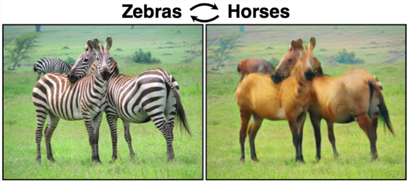

- Learn 2-way mapping between different image domains
- Without using supervised aligned training samples

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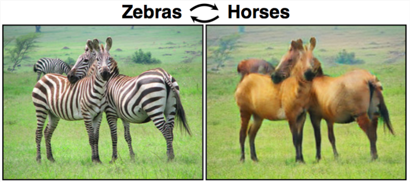

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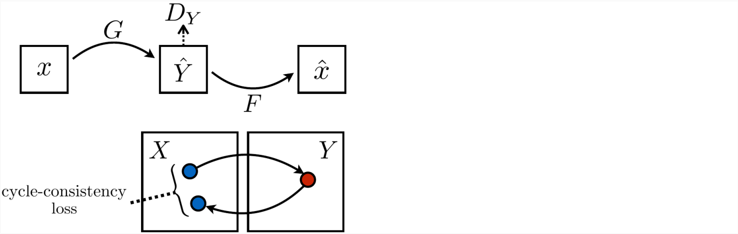

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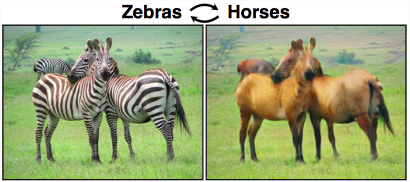

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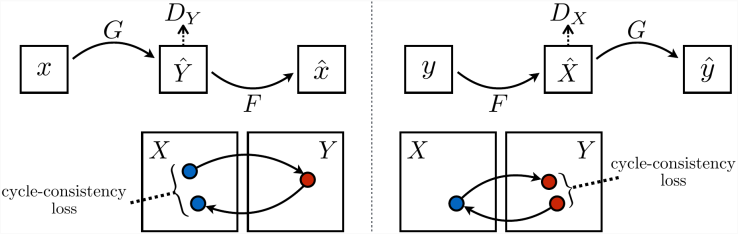
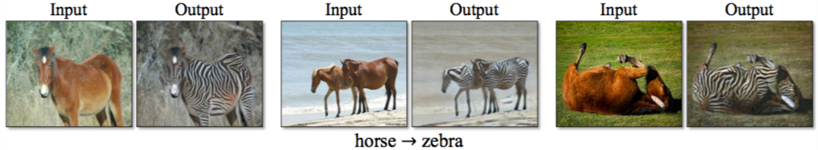
1. Discriminator ensures realistic samples in each domain
2. Cycle-consistency loss ensures alignment

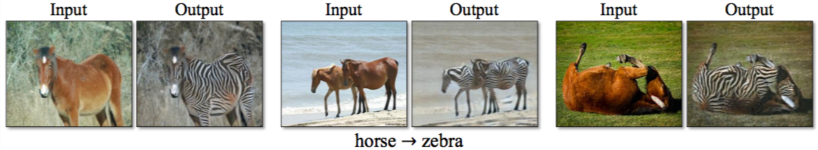


Some successful examples



Some successful examples

- Without using any supervised/aligned examples!



Some successful examples

- Without using any supervised/aligned examples!

horse → zebra

winter Yosemite → summer Yosemite

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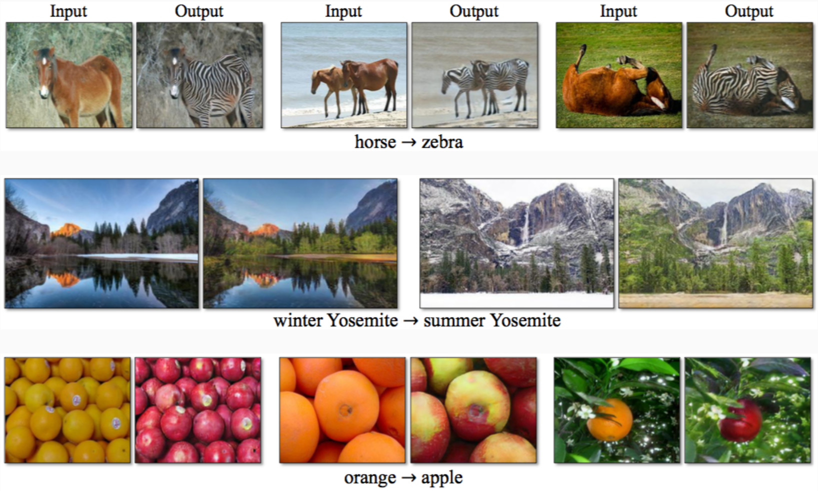

And a failure case

Wrap-up on GANs

Summary of what we discussed

- Improved losses using lipschitz constraints, inspired by earth-mover distance
- Adversarially trained inference networks.
- Style transfer

Thank you!

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