Generative models

MIPT

2023

Generative and discriminative models

Discriminative models

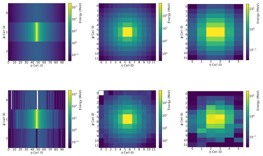
Model: $p(y|\mathbf{x})$.

Generative models

Model: $p(y, \mathbf{x})$.

Generative models:

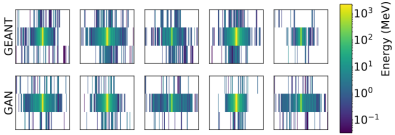
- Generate datasets (when generation is a goal)
- Synthetic dataset generation (for train or fine-tuning)
- Latent dataset properties obtaining

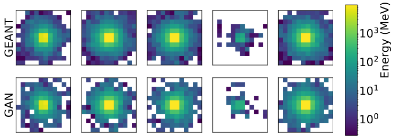


Data generation: example

Paganini et al., 2017:

- Model particle energy
- The modeling uses GAN
- Discrimination is done using GEANT software
- Result: good performance, generation is done 100-1000 times faster

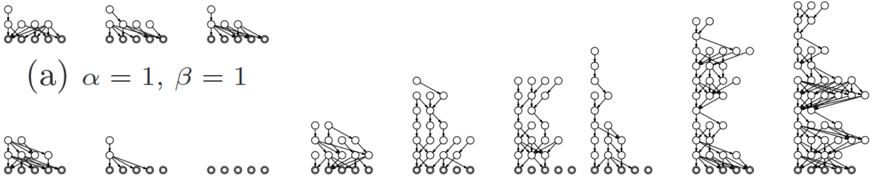




Data generation: example

Adams et al., 2010:

- The problem is to generate deep belief networks
- The model structure $\mathbf{\Gamma}$ is a sequence of adjacency matrices for each layer
- The generation is done using MCMC with Indian buffet process (α, β) as a prior
- α, β can be interpreted as a width and sparsity of the structure



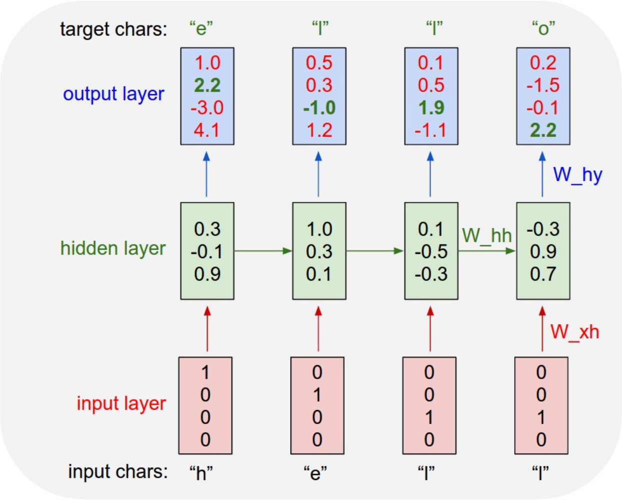
(a) $\alpha = 1, \beta = 1$ (b) $\alpha = \frac{1}{2}, \beta = 1$ (c) $\alpha = 1, \beta = 2$ (d) $\alpha = \frac{3}{2}, \beta = 1$

How to build generative models?

- **Approach 1:** assign a likelihood function (“Fully-observed likelihood”), which decomposes object likelihood into parts (“Autoregressive models”).

Example: CharRNN

Karpathy, 2015



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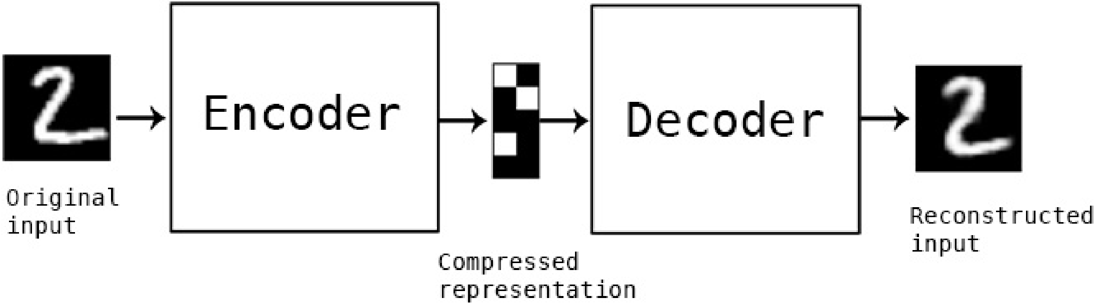
Example: autoencoder

Autoencoder is a model of dimension reduction:

$$\mathbf{H} = \boldsymbol{\sigma}(\mathbf{W}_e \mathbf{X}),$$

$$||\boldsymbol{\sigma}(\mathbf{W}_d \mathbf{H}) - \mathbf{X}||_2^2 \to \min .$$



Autoencoder: generative model?

(Alain, Bengio 2012): consider regularized autoencoder:

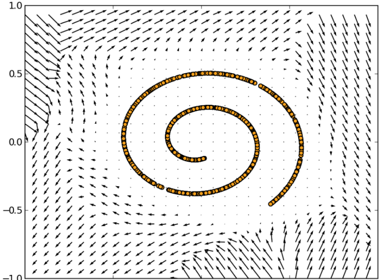
$$||\mathbf{f}(\mathbf{x}, \sigma) - \mathbf{x}||^2,$$

where σ is a noise level.

Then

$$\frac{\partial \log p(\mathbf{x})}{\partial \mathbf{x}} = \frac{||\mathbf{f}(\mathbf{x}, \sigma) - \mathbf{x}||^2}{\sigma^2} + o(1) \text{ when } \sigma \to 0.$$

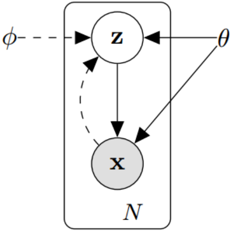
Vector field induced by reconstruction error



Variational autoencoder

Let the objects $\mathbf{X}$ be generated by latent variable $\mathbf{h} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$:

$$\mathbf{x} \sim p(\mathbf{x}|\mathbf{h}, \mathbf{w}).$$



$p(\mathbf{h}|\mathbf{x}, \mathbf{w})$ is unknown.
Maximize ELBO:

$$\log p(\mathbf{x}|\mathbf{w}) \geq \mathsf{E}_{q_\phi(\mathbf{h}|\mathbf{x})} \log p(\mathbf{x}|\mathbf{h}, \mathbf{w}) - D_{\mathrm{KL}}(q_\phi(\mathbf{h}|\mathbf{x}) || p(\mathbf{h})) \to \max.$$

Distributions $q_\phi(\mathbf{h}|\mathbf{x})$ и $p(\mathbf{x}|\mathbf{h}, \mathbf{w})$ are modeled by neural networks:

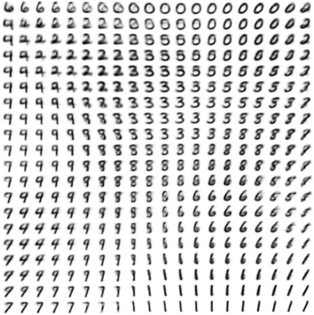
$$q_\phi(\mathbf{h}|\mathbf{x}) \sim \mathcal{N}(\boldsymbol{\mu}_\phi(\mathbf{x}), \boldsymbol{\sigma}^2_\phi(\mathbf{x})),$$

$$p(\mathbf{x}|\mathbf{h}, \mathbf{w}) \sim \mathcal{N}(\boldsymbol{\mu}_w(\mathbf{h}), \boldsymbol{\sigma}^2_w(\mathbf{h})),$$

where $\boldsymbol{\mu}$,$\boldsymbol{\sigma}$ are neural network's outputs.

Variational autoencoder: generation process

(a) Learned Frey Face manifold



(b) Learned MNIST manifold

Does good likelihood estimation leads to good sampling?
Does good sampling estimation leads to good likelihood estimation?

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- **Approach 2:** make an assumption that objects are generated by a latent variable, which is easier to analyze ("Latent variable models").
  Problems:
  - $p(\mathbf{x})$ is intractible
- Problem of both methods: high likelihhod and high sampling quality can be independent (Theis et al., 2015).
- Given a noisy mixutre:

$$p_w(x) = 0.01 p_{\text{data}}(x) + 0.99 p_{\text{noise}}(x), \log p_w(x) \geq \log p_{\text{data}}(x) - \log 100$$

- For another direction: overfitting

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- **Approach 3:** do not use likelihood and work straightforwardly with generative process (from likelihood modeling to statistical testing).

Generative-adversarial models (Goodfellow et al., 2014)

Main idea: train two models, generator G and discriminator D:

$$\min_{\mathbf{W}_G} \max_{\mathbf{w}_D} \mathrm{E}_{\mathbf{x}\in\mathfrak{D}} \log p(\mathbf{x}|\mathbf{w}_D, D) + \mathrm{E}_{\mathbf{x}\in p_G} \log(1 - p(\mathbf{x}|\mathbf{w}_D, D)).$$

The algorithm is iterative

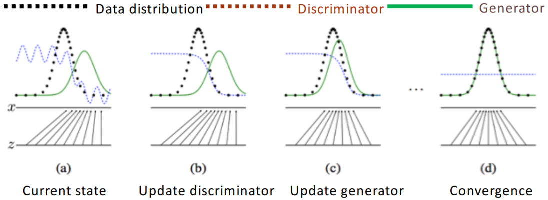
- $\mathrm{E}_{\mathbf{x}\in\mathfrak{D}} \log p(\mathbf{x}|\mathbf{w}_D, D) \to \max_{\mathbf{w}_D}$
- $\mathrm{E}_{\mathbf{x}\in p_G} \log(1 - p(\mathbf{x}|\mathbf{w}_D, D)) \to \min_{\mathbf{w}_G}$
- Alternative: $\mathrm{E}_{\mathbf{x}\in p_G} \log p(\mathbf{x}|\mathbf{w}_D, D) \to \max_{\mathbf{w}_G}$

GAN: optimality

When a discriminator is in global optimum, the generator minimizes JS:

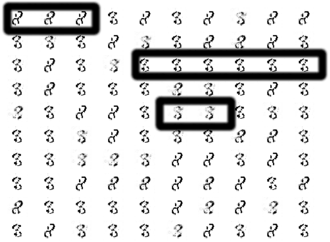
$$-\log(4) + KL\left(p(\mathbf{x}|\frac{p(\mathbf{x}) + p_G(\mathbf{x})}{2})\right) + KL\left(p_G\mathbf{x}|\frac{p(\mathbf{x}) + p_G(\mathbf{x})}{2})\right) \to \min_{\mathbf{w}_G}.$$

Consequent: the optimal generator distribution: $p_G = p(\mathbf{x})$.



Optimization details for GAN

- Generator optimization can be made in two regimes: $\mathsf{E}_{\mathbf{x} \in p_G} \log(1 - p(\mathbf{x}|\mathbf{w}_D, D)) \to \min_{\mathbf{w}_G}$ or $\mathsf{E}_{\mathbf{x} \in p_G} \log p(\mathbf{x}|\mathbf{w}_D, D) \to \max_{\mathbf{w}_G}$: the optima coincide, but for the first regime the gradient is more smooth.
- Generator can converge to a local optimum and generate only similar objects (mode collapse).



https://machinelearningmastery.com/practical-guide-to-gan-failure-modes/

Dataset shift

Dataset shift is an event when distribuition $p(\mathbf{X}, \mathbf{y})$ significantly differ for the training and test/inference phases.

- Covariate shift — difference in $p(\mathbf{X})$
- Prior probability shift — difference in $p(\mathbf{y})$
- Concept shift — difference in $p(\mathbf{y}|\mathbf{X})$

Dataset shift

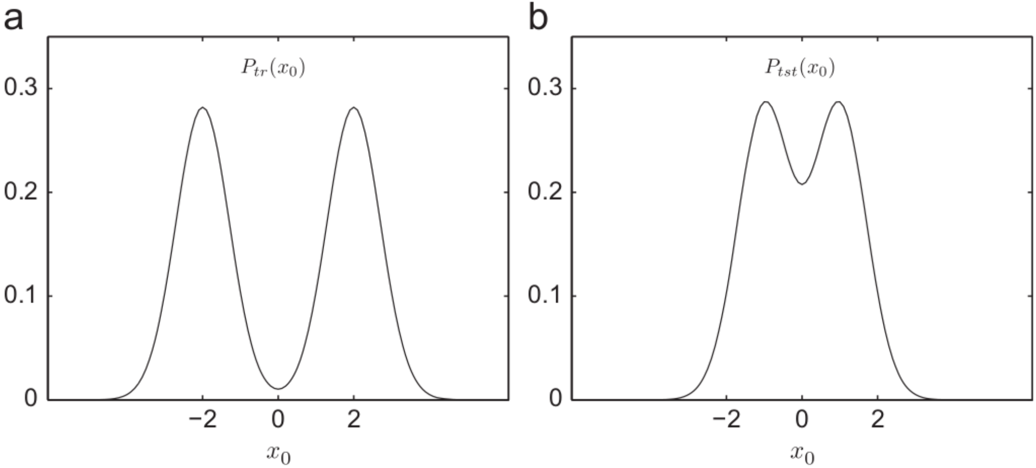
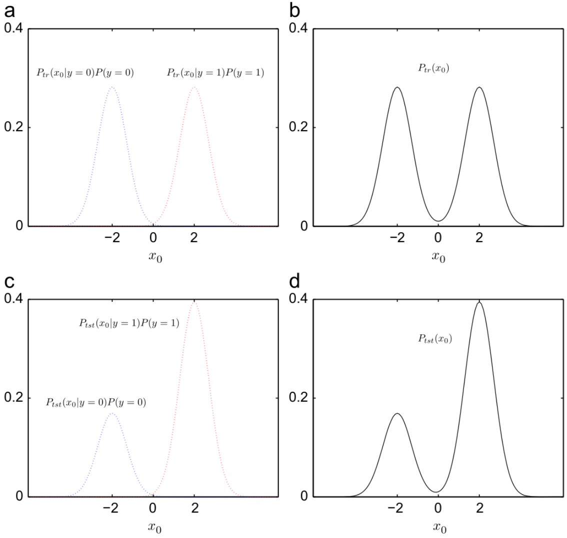


Fig. 1. Covariate shift: $P_{tst}(y|x_0) = P_{tr}(y|x_0)$ and $P_{tr}(x_0) \neq P_{tst}(x_0)$. (a) Training data and (b) test data.

Moreno-Torres et al., 2012

Dataset shift



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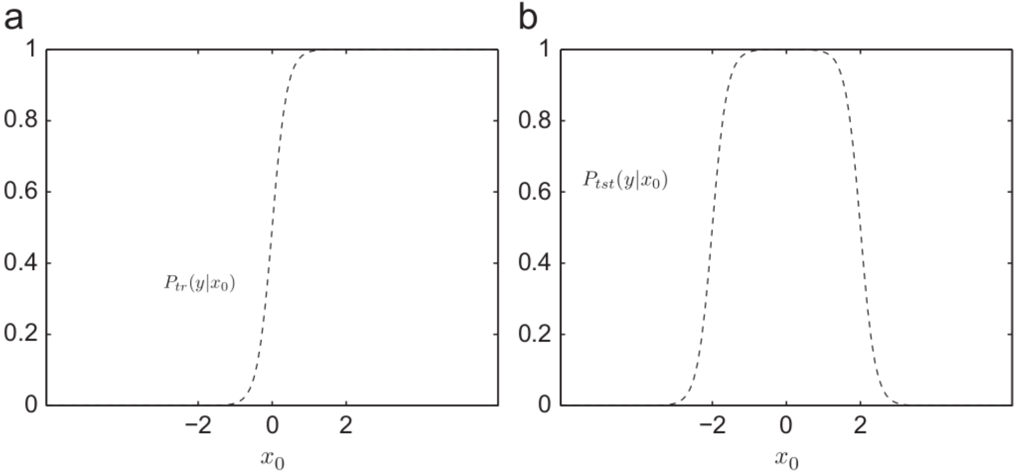

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