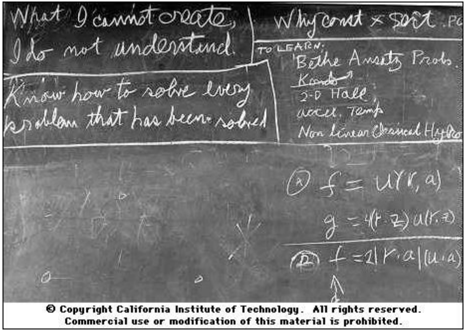
Generative vs Discriminative

MIPT

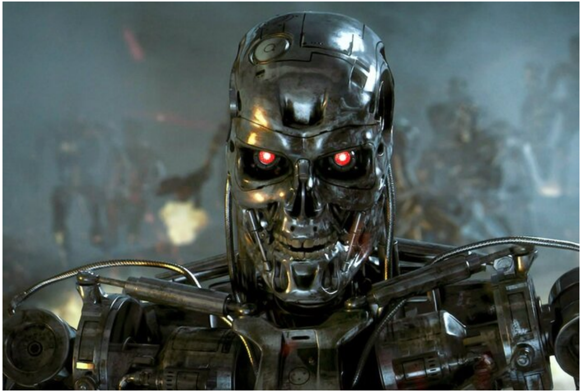
2022

Idea of generative models



Idea of discriminative models

Plato: *"A human is featherless biped"*



Sometimes it's easier to solve a target problem (i.e. classification, regression) than describe the analyzed object nature.

Generative and discriminative models

Discriminative models

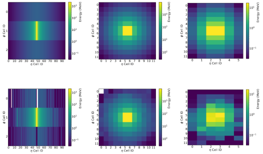
Model: $p(y|\mathrm{x})$.

Generative models

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

Why generative models:

- When dataset generation is a target problem
- Synthetic dataset generation
- Latent properties obtaining



Model selection: coherent Bayesian inference

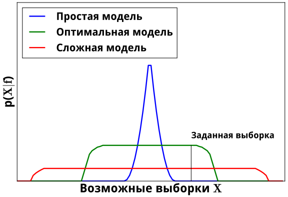
First level: find optimal parameters:

$$\mathrm{w} = \arg\max \frac{p(\mathfrak{D}|\mathrm{w})p(\mathrm{w}|\mathrm{h})}{p(\mathfrak{D}|\mathrm{h})},$$

Second level: find optimal model:

Evidence:

$$p(\mathfrak{D}|\mathrm{h}) = \int_{\mathrm{w}} p(\mathfrak{D}|\mathrm{w})p(\mathrm{w}|\mathrm{h})d\mathrm{w}.$$



What is $\mathfrak{D}$ for generative and discriminative models? Why?

Plate notation

Plate notation is an alternative visuzliation for graphical models.

Elements:

- White circles (random variables);
- Grey circels(observed variables);
- Small circles (deterministic values);
- Plates (batching).

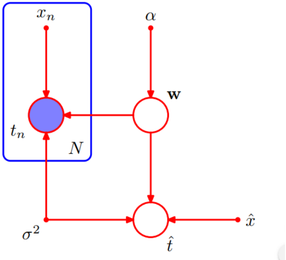
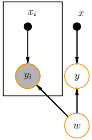


Plate notation for linear regression (Bishop)

Plate notation: discriminative and generative models

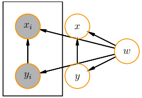
Discriminative models:

- Generate (or deterministically obtain!) x
- Generate w
- Generate $Y \sim p(y|X, w)$



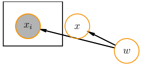
Generative model:

- Generate y
- Generate w
- Generate $x \sim p(X|y, w)$



Generative unsupervised model:

- Generate w
- Generate $x \sim p(X|w)$



Generative models and unsupervised learning

Are the generative models always unsupervised?

Generative models and unsupervised learning

Are the generative models always unsupervised?
No! Linear classification is an example

Logistic regression:

$$\mathrm{E}\left(\mathrm{y}\,|\mathrm{X}\right) \equiv g^{-1}\left(\mathrm{Xw}\right),$$

$$g^{-1}(x)\frac{e^x}{1+e^x} \in [0,1]$$

The decision function is a sigmoid.

Generative model:

$$p(y=1|x,w) = \frac{p(x|w,y=1)p(y=1)}{\sum_{k=0}^{1} p(x|w,y=k)p(y=k)},$$

$$p(x|w,y=k) \sim \mathcal{N}(w_m^k, w_s^k).$$

The decision function is a sigmoid.

Discriminative + generative

Naive approach: introduce a prior on class labels

$$p(\mathrm{x}, y|\mathrm{w}) = p(y|\mathrm{w}_y)p(x|y, \mathrm{w}_x).$$

Two optimization functions:

$$L_G = p(\mathrm{w}) \prod_{\mathrm{x},y} p(\mathrm{x}, y|\mathrm{w}),$$

$$L_D = p(\mathrm{w}) \prod_{\mathrm{x},y} p(y|\mathrm{x}, \mathrm{w}).$$

Combine them:

$$\lambda L_G + (1 - \lambda) L_D \to \max .$$

This optimization is heuristic, it does not give us ML results, nor MAP.

Discriminative + generative

(Bishop et al., 2007): introduce two probabilistic models: "discriminative" and "generative":

$$p(\mathrm{x}, y|\mathrm{w}_G, \mathrm{w}_D) = p(y|\mathrm{x}, \mathrm{w}_D)p(\mathrm{x}|\mathrm{w}_G)p(\mathrm{w}_G, \mathrm{w}_D).$$

Optimization:

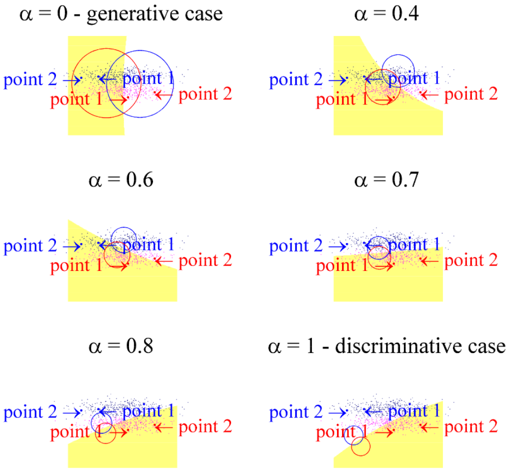
$$p(\mathrm{w}_G, \mathrm{w}_D)\prod_{\mathrm{x},y} p(y|\mathrm{x}, \mathrm{w}_D)p(\mathrm{x}|\mathrm{w}_G).$$

How to select $p(\mathrm{w}_G, \mathrm{w}_D)$?

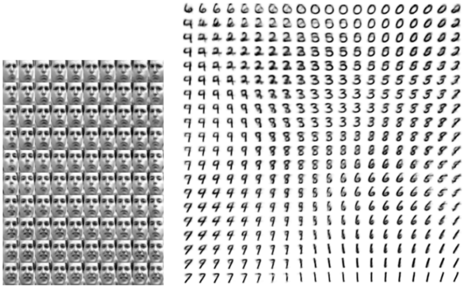
- $p(\mathrm{w}_G, \mathrm{w}_D) = p(\mathrm{w}_G)p(\mathrm{w}_D)$: obtain L_D;
- $p(\mathrm{w}_G, \mathrm{w}_D) = p(\mathrm{w}_G)\delta(\mathrm{w}_G - \mathrm{w}_D)$: obtain L_G;
- Trade-off: $p(\mathrm{w}_G, \mathrm{w}_D) \propto p(\mathrm{w}_G)p(\mathrm{w}_D)\exp(-\frac{1}{2\sigma^2}||\mathrm{w}_G - \mathrm{w}_D||^2)$.

Discriminative + generative

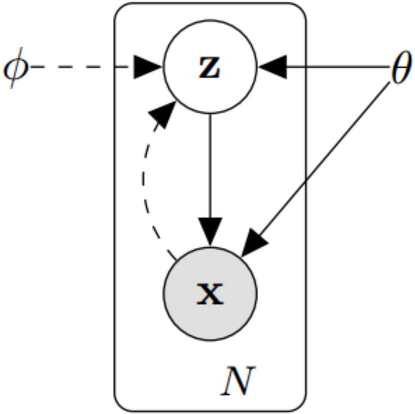
(Bishop et al., 2007): example of different combinations of these optimizations for the synthetic dataset. The dataset contains only 2 labeled objects for each class.



VAE: generation process



(a) Learned Frey Face manifold (b) Learned MNIST manifold



Semi-supervised VAE (Kingma et al., 2014)

$$\text{M1: } q_\phi(\mathbf{z}|\mathbf{x}) = \mathcal{N}(\mathbf{z}|\boldsymbol{\mu}_\phi(\mathbf{x}), \text{diag}(\boldsymbol{\sigma}^2_\phi(\mathbf{x}))), \tag{3}$$

$$\text{M2: } q_\phi(\mathbf{z}|y,\mathbf{x}) = \mathcal{N}(\mathbf{z}|\boldsymbol{\mu}_\phi(y,\mathbf{x}), \text{diag}(\boldsymbol{\sigma}^2_\phi(\mathbf{x}))); \quad q_\phi(y|\mathbf{x}) = \text{Cat}(y|\boldsymbol{\pi}_\phi(\mathbf{x})), \tag{4}$$

For this model, we have two cases to consider. In the first case, the label corresponding to a data point is observed and the variational bound is a simple extension of equation (5):

$$\log p_\theta(\mathbf{x}, y) \geq \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x},y)} \left[\log p_\theta(\mathbf{x}|y,\mathbf{z}) + \log p_\theta(y) + \log p(\mathbf{z}) - \log q_\phi(\mathbf{z}|\mathbf{x}, y)\right] = -\mathcal{L}(\mathbf{x}, y), \tag{6}$$

For the case where the label is missing, it is treated as a latent variable over which we perform posterior inference and the resulting bound for handling data points with an unobserved label y is:

$$\begin{aligned}\log p_\theta(\mathbf{x}) &\geq \mathbb{E}_{q_\phi(y,\mathbf{z}|\mathbf{x})} \left[\log p_\theta(\mathbf{x}|y,\mathbf{z}) + \log p_\theta(y) + \log p(\mathbf{z}) - \log q_\phi(y,\mathbf{z}|\mathbf{x})\right] \\ &= \sum\nolimits_y q_\phi(y|\mathbf{x})(-\mathcal{L}(\mathbf{x}, y)) + \mathcal{H}(q_\phi(y|\mathbf{x})) = -\mathcal{U}(\mathbf{x}).\end{aligned} \tag{7}$$

The bound on the marginal likelihood for the entire dataset is now:

$$\mathcal{J} = \sum\nolimits_{(\mathbf{x},y)\sim\widetilde{p}_l} \mathcal{L}(\mathbf{x}, y) + \sum\nolimits_{\mathbf{x}\sim\widetilde{p}_u} \mathcal{U}(\mathbf{x}) \tag{8}$$

Semi-supervised VAE (Kingma et al., 2014)

$$\mathcal{J}^{\alpha} = \mathcal{J} + \alpha \cdot \mathbb{E}_{\tilde{p}_l(\mathbf{x},y)}\left[-\log q_\phi(y|\mathbf{x})\right], \tag{9}$$

Algorithm 1 Learning in model M1

while generativeTraining() **do**
  $\mathcal{D} \leftarrow$ getRandomMiniBatch()
  $\mathbf{z}_i \sim q_\phi(\mathbf{z}_i|\mathbf{x}_i) \quad \forall \mathbf{x}_i \in \mathcal{D}$
  $\mathcal{J} \leftarrow \sum_n \mathcal{J}(\mathbf{x}_i)$
  $(\mathbf{g}_\theta, \mathbf{g}_\phi) \leftarrow (\frac{\partial \mathcal{J}}{\partial \theta}, \frac{\partial \mathcal{J}}{\partial \phi})$
  $(\boldsymbol{\theta}, \boldsymbol{\phi}) \leftarrow (\boldsymbol{\theta}, \boldsymbol{\phi}) + \boldsymbol{\Gamma}(\mathbf{g}_\theta, \mathbf{g}_\phi)$
end while
while discriminativeTraining() **do**
  $\mathcal{D} \leftarrow$ getLabeledRandomMiniBatch()
  $\mathbf{z}_i \sim q_\phi(\mathbf{z}_i|\mathbf{x}_i) \quad \forall \{\mathbf{x}_i, y_i\} \in \mathcal{D}$
  trainClassifier($\{\mathbf{z}_i, y_i\}$)
end while

Algorithm 2 Learning in model M2

while training() **do**
  $\mathcal{D} \leftarrow$ getRandomMiniBatch()
  $y_i \sim q_\phi(y_i|\mathbf{x}_i) \quad \forall \{\mathbf{x}_i, y_i\} \notin \mathcal{O}$
  $\mathbf{z}_i \sim q_\phi(\mathbf{z}_i|y_i, \mathbf{x}_i)$
  $\mathcal{J}^\alpha \leftarrow$ eq. (9)
  $(\mathbf{g}_\theta, \mathbf{g}_\phi) \leftarrow (\frac{\partial \mathcal{L}^\alpha}{\partial \theta}, \frac{\partial \mathcal{L}^\alpha}{\partial \phi})$
  $(\boldsymbol{\theta}, \boldsymbol{\phi}) \leftarrow (\boldsymbol{\theta}, \boldsymbol{\phi}) + \boldsymbol{\Gamma}(\mathbf{g}_\theta, \mathbf{g}_\phi)$
end while

Semi-supervised VAE (Kingma et al., 2014)

Table 1: Benchmark results of semi-supervised classification on MNIST with few labels.

N	NN	CNN	TSVM	CAE	MTC	AtlasRBF	M1+TSVM	M2	M1+M2
100	25.81	22.98	16.81	13.47	12.03	8.10 ($\pm$ 0.95)	11.82 ($\pm$ 0.25)	11.97 ($\pm$ 1.71)	**3.33** ($\pm$ 0.14)
600	11.44	7.68	6.16	6.3	5.13	–	5.72 ($\pm$ 0.049)	4.94 ($\pm$ 0.13)	**2.59** ($\pm$ 0.05)
1000	10.7	6.45	5.38	4.77	3.64	3.68 ($\pm$ 0.12)	4.24 ($\pm$ 0.07)	3.60 ($\pm$ 0.56)	**2.40** ($\pm$ 0.02)
3000	6.04	3.35	3.45	3.22	2.57	–	3.49 ($\pm$ 0.04)	3.92 ($\pm$ 0.63)	**2.18** ($\pm$ 0.04)

(a) Handwriting styles for MNIST obtained by fixing the class label and varying the 2D latent variable z

Model selection problem: recap

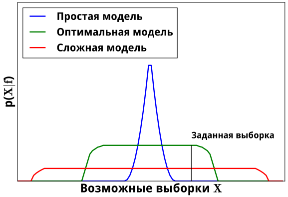
First level: find optimal parameters:

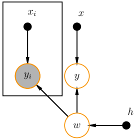
$$\mathbf{w} = \arg\max \frac{p(\mathfrak{D}|\mathbf{w})p(\mathbf{w}|\mathbf{h})}{p(\mathfrak{D}|\mathbf{h})},$$

Second level: find optimal model:

Evidence:

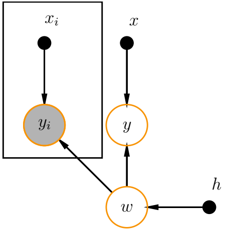
$$p(\mathfrak{D}|\mathbf{h}) = \int_{\mathbf{w}} p(\mathfrak{D}|\mathbf{w})p(\mathbf{w}|\mathbf{h})d\mathbf{w}.$$

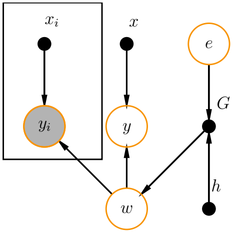




Model selection problem: recap

Can we generate target models parameters using a generative model?





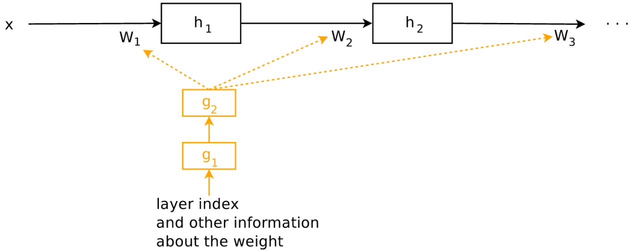
Model selection: hybrid approach

Definition

Given a set Λ.
Hypernetwork is a parametric mapping from Λ to set $\mathbb{R}^n$ of the model f parameters:

$$G : \Lambda \times \mathbb{R}^u \to \mathbb{R}^n,$$

where $\mathbb{R}^u$ is a set of hypernetwork parameters.



Ha et al., 2016

Model selection: discriminative approach

$$w_{MOE} = \langle \gamma(x), [w_1, \dots, w_n] \rangle$$

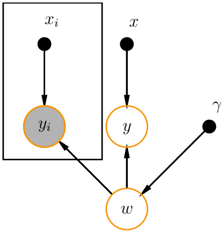


Рис. 1: Model generation scheme

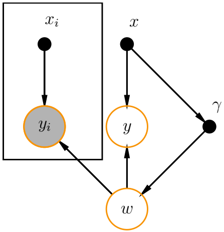


Рис. 2: MOE optimization as a discriminative model

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