Variational Autoencoders

November 13, 2020

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Overview

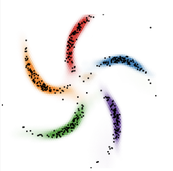
General Framework

We can compose probabilistic graphical models with neural networks to exploit their complementary strengths.

Data

GMM

GMM-SVAE



The resulting model is expressive, but also interpretable/decomposable.

Johnson, M., Duvenaud, D. K., Wiltschko, A., Adams, R. P., & Datta, S. R. (2016). Composing graphical models with neural networks for structured representations and fast inference. In Advances in neural information processing systems (pp. 2946-2954).

Parameterizing Conditional Distributions with Neural Networks

- Have neural networks output *parameters* of probability distributions, rather than predictions directly.

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- Have neural networks output *parameters* of probability distributions, rather than predictions directly.
- The cost function for optimization is now probabilistic (e.g., maximum likelihood, minimum KL-divergence) rather than minimizing a distance to the target.

Deep Latent Variable Models (DLVMs)

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How does the latent state z_i impact the data distribution for a particular sample, $x^{(i)} \sim F_{\theta_{z_i}}$?

Previously:	$\theta^{(i)} = \theta_{z_i}$	select one of K fixed parameters
Here:	$\theta^{(i)} = \texttt{NeuralNetwork}_\eta(z_i)$	flexibly create a sample-specific parameter

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   Previously: $z_i \in \{1, ..., K\}$

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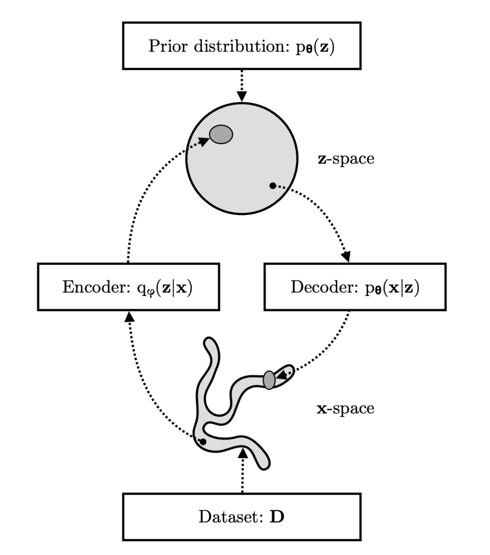
$$\begin{aligned} \text{Previously:} \quad & z_i \in \{1, ..., K\} \\ \text{Here:} \quad & z_i \in \mathbb{R}^d \end{aligned}$$

2. The parameters we need to learn, η, is still fixed in dimension.

Variational Autoencoders



Q: What does this remind you of?

Probabilistic model

Simplification

For ease of illustration, we restrict our attention to a variational autoencoder that applies i.i.d assumptions and Gaussian distributions (and therefore real-valued observations) throughout. Note that neither assumption is necessary.

Probabilistic decoder

Consider a parametric frequentist latent variable model, with

- observations $x = (x^{(i)})_{i=1}^{N}, \quad x^{(i)} \in \mathbb{R}^d$
- latent variables $z = (z^{(i)})_{i=1}^{N}, \quad z^{(i)} \in \mathbb{R}^k$
- parameter θ (fixed but to be learned)

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Since the MLP maps latent variables, z, to the parameters of a probability distribution over observed data, x, we refer to it as a **probabilistic decoder.**

Notes on notation

1. $\mathcal{N}(M, V)$ refers to the Gaussian density with mean M and covariance V.
2. $\mu_{x^{(i)}}(z^{(i)}, \theta)$ is meant to denote the mean parameter for a distribution over observed datum $x^{(i)}$; that parameter is a function of latent variable z and learnable parameter θ. Notation should be similarly interpreted throughout this section.

Probabilistic encoder

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$$q_\phi(z|x) = \prod_i q_\phi(z^{(i)}|x^{(i)})$$

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Probabilistic encoder

- We may regard the probabilistic encoder as an approximation to the posterior distribution over latent variables which results from using the probabilistic decoder as a likelihood.
- The probabilistic encoder is sometimes also referred to as a **recognition model**.

Sample Implementation

Sample Implementation

Following Appendix C.2 of the VAE paper, we provide a sample implementation for the probabilistic encoder and decoder.

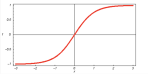
Probabilistic decoding

We may, for example, specifically assume that a latent variable $z^{(i)}$ can be probabilistically decoded into observation $x^{(i)}$ via the following process

$$h^{(i)} = \mathtt{tanh}(W_1\, z^{(i)} + b_1)$$

$$\mu_{x^{(i)}} = W_{21} h^{(i)} + b_{41}, \quad \log \sigma^2_{x^{(i)}} = W_{22} h^{(i)} + b_{22}$$

$$x|z \sim \mathcal{N}(\mu_{x^{(i)}}, \Sigma_{x^{(i)}}), \quad \text{where } \mathrm{diag}(\Sigma_{x^{(i)}}) = \sigma^2_{x^{(i)}}$$



The hyperbolic tangent (`tanh`) function

where (W_1, W_{21}, W_{22}) are the weights and (b_1, b_{21}, b_{22}) are the biases of a Multi-Layer Perceptron (MLP).

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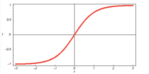

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Letting $\theta := (W_1, W_{21}, W_{22}, b_1, b_{21}, b_{22})$, we may use the trained decoder to define the likelihood, $p_\theta(x|z)$, as defined in (2.1).

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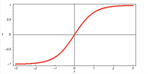

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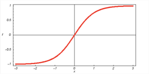

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Letting $\phi := (W_3, W_{41}, W_{42}, b_3, b_{41}, b_{42})$, we may use the trained encoder to define the approximate posterior, $q_\phi(z|x)$, as defined in (2.2).

Inference

We use variational inference to jointly optimize (θ, ϕ). For example, in our sample implementation, we have

$$\theta = (W_1, W_{21}, W_{22}, b_1, b_{21}, b_{22}) \qquad \text{generative parameters}$$

$$\phi = (W_3, W_{41}, W_{42}, b_3, b_{41}, b_{42}) \qquad \text{variational parameters}$$

In particular, we construct $\mathcal{F}(\theta, \phi; x)$, a lower-bound on the marginal likelihood, $p_\theta(x)$, via the entropy/energy decomposition which is standard in variational inference:

$$\mathcal{F}(\theta, \phi; x) = \mathbb{E}_{q_\phi(z|x)}[-\log q_\phi(z|x)) + \log p_\theta(x, z)] \tag{4.1}$$

We train the model by performing stochastic gradient descent on the variational lower bound $\mathcal{F}$. (How is this different than what we've seen?)

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During training, the objective function (4.1) is approximated by performing a Monte Carlo approximation of the expectation.

Given minibatch $x^{(i)}$, we would like to take L samples from $q_\phi(z|x^{(i)})$

$$z^{(i.l)} \sim q_\phi(z^{(i,l)}|x^{(i)})$$

and obtain the following estimator:

$$\mathcal{F}(\theta, \phi; x^{(i)}) \approx \frac{1}{L}\sum_{l=1}^{L} - \log q_\phi(z^{(i,l)}|x^{(i)}) + \log p_\theta(x^{(i)}, z^{(i,l)}) \qquad (4.2)$$

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Example	$q_\varphi(z)$	$p(\varepsilon)$	$g(\varphi, \varepsilon)$	Also...
Normal dist.	$z \sim N(\mu,\sigma)$	$\varepsilon \sim N(0,1)$	$z = \mu + \sigma * \varepsilon$	Location-scale familie: Laplace, Elliptical, Student's t, Logistic, Uniform, Triangular, ...
Exponential	$z \sim \exp(\lambda)$	$\varepsilon \sim U(0,1)$	$z = -\log(1 - \varepsilon)/\lambda$	Invertible CDF: Cauchy, Logistic, Rayleigh, Pareto,Weibull, Reciprocal, Gompertz, Gumbel and Erlan, ...
Other	$z \sim \log N(\mu,\sigma)$	$\varepsilon \sim N(0,1)$	$z = \exp(\mu + \sigma * \varepsilon)$	Gamma, Dirichlet, Beta, Chi-Squared, and F distributions

Image Credit: DP. Kingma

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Rk: In our case, the variational distribution is a multivariate normal, so $p(\epsilon)$ is simply a Gaussian with zero mean and identity covariance.

Reparametrization trick

Using the *reparameterization trick*, we construct a differentiable transformation g_ϕ of parameterless distribution $p(\epsilon)$ such that $g_\phi(\epsilon, x^{(i)})$ has the same distribution as $q_\phi(z^{(i)}|x^{(i)})$.

Using this trick, we take L samples $\{\epsilon_1, ..., \epsilon_L\}$ from $p(\epsilon)$ and obtain the estimator:

$$\mathcal{F}(\theta, \phi; x^{(i)}) \approx \frac{1}{L} \sum_{l=1}^{L} - \log q_\phi\big(g_\phi(\epsilon^{(l)}, x^{(i)})|x^{(i)}\big) + \log p_\theta\big(x^{(i)}, g_\phi(\epsilon^{(l)}, x^{(i)})\big) \tag{4.3}$$

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2. Each such sample, $z^{(i,l)}$, determines a specific form of the fitted likelihood (i.e. the decoder) by specifying its parameters,

$$p_\theta(x^{(i)} \mid z^{(i,l)}) = p_\theta\left(x^{(i)} \mid \mu_{x^{(i)}}(z^{(i,l)}) \quad , \quad \Sigma_{x^{(i)}}(z^{(i,l)})\right)$$

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3. Compute the *reconstruction probability* of the sample as the mean of these likelihoods:

$$\texttt{reconstruction probability}(x^{(i)}) := \frac{1}{L}\sum_{l=1}^{L} p_\theta\left(x^{(i)} \mid \mu_{x^{(i)}}(z^{(i,l)}), \Sigma_{x^{(i)}}(z^{(i,l)})\right)$$

An, J., & Cho, S. (2015). Variational autoencoder based anomaly detection using reconstruction probability. Special Lecture on IE, 2(1).

Evaluation

What do you think of this approach to anomaly detection?
My thoughts on VAE vs. NF for anomaly detection:

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- Thus:
  - The learned inverse is exact, rather than approximate
  - Inference is simpler – no latent variables (or variational inference) necessary!
  - Anomaly scores are exact, not approximate.
- Perhaps it's not surprising, then, that I have obtained higher quality results in practice for anomaly detection with NF's than VAE's.