Variational Autoencoders

November 13, 2020

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Overview

Deep Generative Models

- Can generate new samples (click here)
- Can interpolate across given samples
- If likelihood based, can be used to assess anomaly.

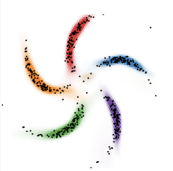
Composing PGM's with NN's

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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Previously:	$\theta^{(i)} = \theta_{z_i}$	select one of K fixed parameters
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Notes:

1. The latent variables now have continuous support (although this is an artifact of our choices for earlier examples)

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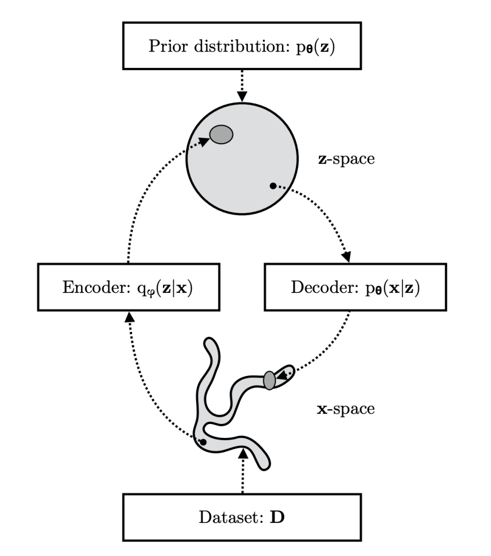
2. The parameters we need to learn, η, is fixed in dimension.

Variational Autoencoders



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 $z = (z^{(i)})_{i=1}^N, \quad z^{(i)} \in \mathbb{R}^k$
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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.

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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

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\begin{aligned}
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)}}
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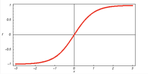

The hyperbolic tangent (`tanh`) function

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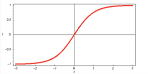

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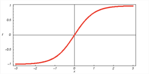

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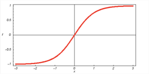

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Letting $\phi := (W_3, W_{41}, W_{42}, b_3, b_{41}, b_{42})$, we may use the trained encoder to define the approximate posterior, $q_\phi(z|x)$, as defined in (2.2).

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?

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My thoughts on VAE vs. NF for anomaly detection:

- VAE's use of latent variables, and hence the need to jointly learn the generative and variational parameters, is awkward.
- Normalizing flows learn a single invertible map (from z-space to x-space) , rather than separately learning a function and its inverse.
- 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.