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Нет возможности напрямую рассчитывать апостериорное распределение на скрытые переменные

$p(x|\theta) \to \max_\theta$ , $p(x,z|\theta)$

$$\log p(x|\theta) \geq ELBO(q,\theta) = \mathbb{E}_{q(z)} \log \frac{p(x,z|\theta)}{q(z)} \to \max_{q,\theta}$$

$$q(z) = q(z|\lambda)$$

$$ELBO(\lambda,\theta) = \mathbb{E}_{q(z|\lambda)} \log \frac{p(x,z|\theta)}{q(z)} \to \max_{\theta,\lambda}$$

$$\mathbb{E}_{p(x)} f(x) = \int f(x)p(x)\,dx \approx \frac{1}{M}\sum_{j=1}^{M} f(x_j), \quad x_j \sim p(x)$$

или оценка $f(x)$ рядом Тейлора в $\Omega(x_0)$

$$\nabla_\theta ELBO(\theta,\lambda) = \nabla_\theta \mathbb{E}_{q(z|\lambda)} \log \frac{p(x,z|\theta)}{q(z|\lambda)} =$$

$$= \mathbb{E}_{q(z|\lambda)} \nabla_\theta \mathbb{E} \log p(x,z|\theta) \approx \frac{1}{M}\sum_{j=1}^{M} \nabla_\theta \log p(x,z_j|\theta)$$

$$\nabla_\lambda ELBO(\theta,\lambda) = \nabla_\lambda \mathbb{E}_{q(z|\lambda)} \log \frac{p(x,z|\theta)}{q(z|\lambda)} \ominus$$

1) Log-derivative trick

$$\ominus \nabla_\lambda \int q(z|\lambda)(\log p(x,z|\theta) - \log q(z|\lambda))\,dz =$$

$$= \int \nabla_\lambda q(z|\lambda)(\log p(x,z|\theta) - \log q(z|\lambda))\,dz +$$

$$+ \int q(z|\lambda)(-\nabla_\lambda \log q(z|\lambda))\,dz = \left\{ \nabla_\lambda \log q(z|\lambda) = \frac{\nabla_\lambda q(z|\lambda)}{q(z|\lambda)} \right\} =$$

$$= \int q(z|\lambda)\nabla_\lambda \log q(z|\lambda)(\log p(x,z|\theta) - \log q(z|\lambda) - 1)\,dz =$$

$$= \mathbb{E}_{q(z|\lambda)}(\ldots)$$

слишком большая дисперсия оценки!

② Reparametrization Trick

$$z_0 \sim N(z_0 | 0, I), \quad z = Az_0 + b, \quad z \sim N(z | b, AA^T)$$

$$\mathbb{E} z = \mathbb{E}(Az_0 + b) = A \underbrace{\mathbb{E} z_0}_{0} + b = b$$

$$\mathbb{E}(z-b)(z-b)^T = \mathbb{E} Az_0 (Az_0)^T = A \underbrace{\mathbb{E} z_0 z_0^T}_{I} A^T = AA^T$$

$$z \sim N(z | \mu, \Sigma)$$

$$z_0 \sim N(z_0 | 0, I), \quad z = Lz_0 + \mu, \quad \Sigma = LL^T$$

$z \sim q(z|\lambda)$ репараметризуемые распределения

$\Updownarrow$

$z_0 \sim q(z_0), \quad z = f(z_0, \lambda)$

$$\nabla_\lambda ELBO(\theta, \lambda) = \nabla_\lambda \mathbb{E}_{q(z|\lambda)} \log \frac{p(x, z|\theta)}{q(z|\lambda)} =$$

$$= \nabla_\lambda \mathbb{E}_{q(z_0)} \log \frac{p(x, f(z_0, \lambda) | \theta)}{q(f(z_0, \lambda) | \lambda)} =$$

$$= \mathbb{E}_{q(z_0)} \nabla_\lambda \log \frac{p(x, f(z_0, \lambda) | \theta)}{q(f(z_0, \lambda) | \lambda)}$$

$F(x) = U[0,1]$ распр. с обр. $F^{-1}$

$\xi \sim U[0,1]$ репараметризуема

$x = F^{-1}(\xi) \quad \{F \equiv f\}$

# Relevance Vector Machine

$$\{x_i, y_i\}_{i=1}^N, \quad x_i \in \mathbb{R}^D, \quad y_i \in \{-1, +1\}$$

$$y(x) = \text{sign}(w^T x), \quad p(y_i | x_i, w) = \sigma(y_i w^T x_i)$$

$$p(w|\alpha) = N(w | 0, \text{diag}(\alpha))$$

$$p(y, w | X, \alpha) = \left[\prod_{i=1}^N p(y_i | x_i, w)\right] p(w|\alpha), \quad p(y|X, \alpha) \to \max_\alpha$$

$$\log p(y|x,\alpha) \geqslant \mathbb{E}_{q(w)} \log \frac{p(y,w|x,\alpha)}{q(w|\alpha)} =$$

$$= \left\{ q(w) = \mathcal{N}(w|\mu,\Sigma) \right\} = \sum_{i=1}^{N} \mathbb{E}_{\mathcal{N}(w|\mu,\Sigma)} \log p(y_i|x_i,w) +$$

$$+ \underbrace{\mathbb{E}_{\mathcal{N}(w|\mu,\Sigma)} \log \frac{p(w|\alpha)}{\mathcal{N}(w|\mu,\Sigma)}}_{-KL(\mathcal{N}(w|\mu,\Sigma)\,\|\,\mathcal{N}(w|0,\,diag(\alpha)))} \to \max_{\mu,\Sigma,\alpha}$$

$$\Leftrightarrow \sum_{i=1}^{N} \mathbb{E}_{\mathcal{N}(w|\mu,\Sigma)} \log \sigma(y_i w^T x_i) -$$

$$- \cancel{\tfrac{1}{2} de} - \log \det \Sigma + \frac{1}{2} \sum_i (\mu_i^2 + \Sigma_{ii}) \to \max_{\mu,\Sigma}$$

{приближение $\Sigma = diag(S)$}

$$\mathbb{E}_{\mathcal{N}(w|\mu,\Sigma)} \log \sigma(\overbrace{\underbrace{y_i w^T x_i}_{\in \mathbb{R}}}^{f(w)}) = \mathbb{E}_{\mathcal{N}(z|0,I)} \log \sigma(y_i x_i^T (Lz + \mu))$$

$\|$ {лучший способ}

$$\mathbb{E}_{\mathcal{N}(v|0,1)} \log \sigma(\underbrace{y_i}_{1} \sqrt{x_i^T \Sigma x_i}\, v + y_i \mu^T x_i)$$

$// \; w \sim \mathcal{N}(w|\mu,\Sigma) \Rightarrow u = y_i w^T x_i \sim \mathcal{N}(u | y_i \mu^T x_i,\; x_i^T \Sigma x_i)$

$\mathbb{R} \leftarrow \mathbb{R}^n$

$$\mathbb{E}u = y_i (\mathbb{E} w^T) x_i = y_i \mu^T x_i$$

$$\mathbb{E}(u - \mathbb{E}u)^2 = \mathbb{E}(y_i w^T x_i - y_i \mu^T x_i)^2 =$$

$$= \mathbb{E}(y_i (w - \mu)^T x_i)^2 =$$

$$= \mathbb{E}((w-\mu)^T x_i)^2 =$$

$$= \mathbb{E}(x_i^T (w-\mu)(w-\mu)^T x_i) =$$

$$= x_i^T [\mathbb{E}(w-\mu)(w-\mu)^T] x_i =$$

$$= x_i^T \Sigma x_i$$

**RVM + NN**

$\{x_i, y_i\}$, $y(x) = \text{sign}\, f(x,w)$ — нейросеть

$$p(y_i|x_i,w) = \sigma(y_i f(x_i,w))$$

$$p(w|\alpha) = \mathcal{N}(w|0, diag(\alpha))$$

$$p(y|x,\alpha) \to \max_{\alpha}$$

$$\mathbb{E}_{N(w|\mu, \, diag(s))} \log \sigma(y_i f(x_i, w))$$

$$x \to \boxed{\text{linear}} \to u_1 \to \boxed{g} \to a_2 \to \boxed{\text{linear}} \to u_2 \to \dots \to a_L$$

$w_1$ $w_2$

Local Reparametrization Trick LRT

$$u_{1k} = w_{1,k}^T x \quad , \quad w_{1,k} \sim N(w_{1,k} | \mu_{1,k}, diag(s_{1,k}))$$

$$u_{1,k} \sim N(u_{1,k} | \mu_{1,k}^T x, \; x^T diag(s_{1,k}) x)$$

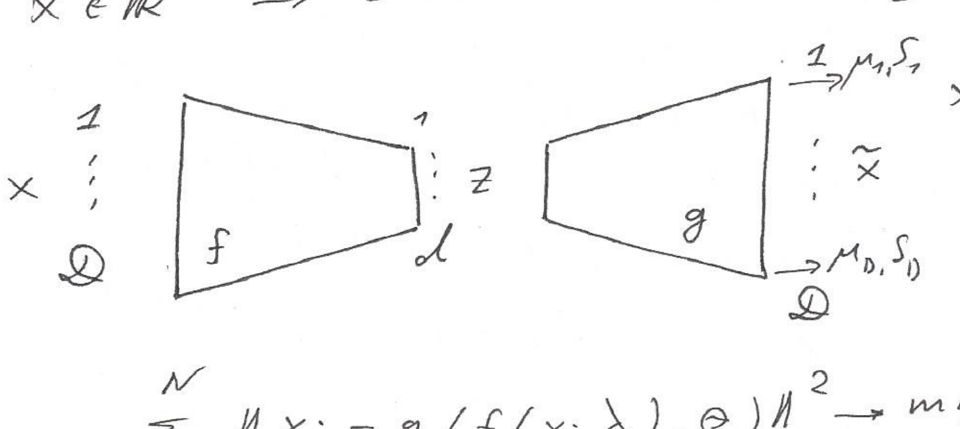
сэмплирование матрицы весов

$\Downarrow$ сэмплирование размера выхода
~~на~~ линейного слоя

разреживание весов RVM $\equiv$ вариационный дропаут

<u>Вариационный автокодировщик (VAE)</u>

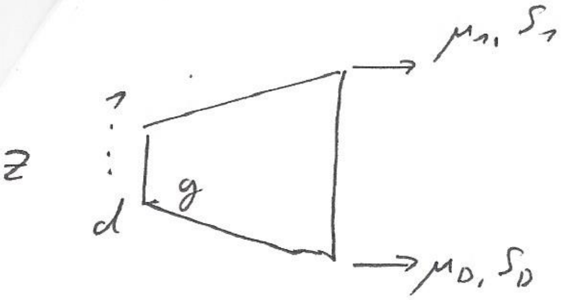
$x \in \mathbb{R}^D \to z \in \mathbb{R}^d$ $\quad z \sim N(z | 0, I)$




$x \sim N(x | \mu(z, \theta),$
$diag(s(z, \theta)))$

$$\sum_{i=1}^{N} \| x_i - g(f(x_i, \lambda), \theta) \|^2 \to \min_{\theta, \lambda}$$

вариационные нейросеть




$$p(X, Z|\Theta) = \prod_{i=1}^{D} \left[ \mathcal{N}(x_i | \mu(z_i, \Theta), \operatorname{diag}(S(z_i, \Theta))) \right] \cdot \mathcal{N}(z_i | 0, I)$$

$$\log p(X|\Theta) \geqslant \mathbb{E}_{q(Z)} \log \frac{p(X, Z|\Theta)}{q(Z)} =$$

$$= \sum_{i=1}^{N} \mathbb{E}_{q(z_i)} \log \frac{p(x_i, z_i|\Theta)}{q(z_i)} \;(=)$$

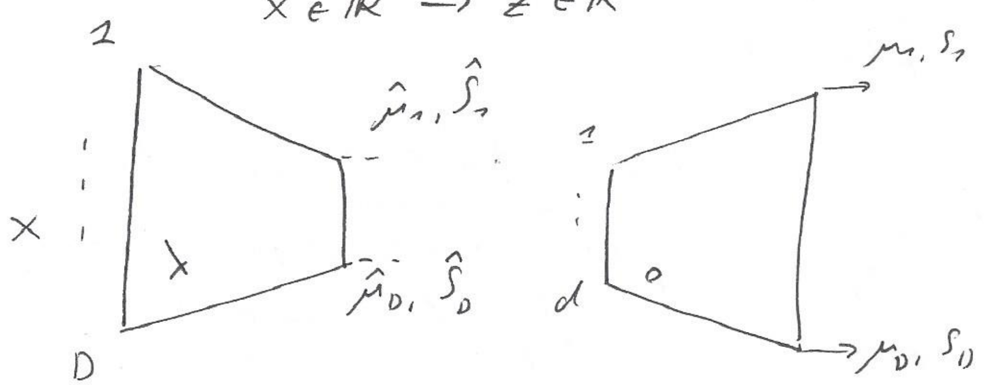
$\|$

$p(z_i|x_i, \Theta)$

в апостериорное распр. поставим сеть:

$$q(z_i|x_i, \lambda) = \mathcal{N}(z_i | \hat{\mu}(x_i, \lambda), \operatorname{diag}(\hat{S}(x_i, \lambda)))$$

$$x \in \mathbb{R}^D \to z \in \mathbb{R}^d$$




$$(=) \sum_{i=1}^{N} \mathbb{E}_{\mathcal{N}(z_i | \hat{\mu}(x_i, \lambda), \operatorname{diag}(\hat{S}(x_i, \lambda)))} \log \frac{\mathcal{N}(x_i | \mu(z_i, \Theta), \operatorname{diag}(S(x_i, \Theta)))\, \mathcal{N}(z_i | 0, I)}{q(z_i | x_i, \lambda)} \longrightarrow \max_{\Theta, \lambda}$$

$$\| -\int_a^b \ln \frac{1}{b-a} \cdot \frac{1}{b-a}\, dx = -\ln(b-a)$$

$$\| \ \mathbb{E}[(X-\hat{X})^2] \geq \frac{1}{2\pi e} e^{2h(x)}$$

$$\log p_\theta(x) = \mathbb{E}_{z\sim q_\varphi(z|x)} \log p_\theta(x) =$$

$$= \mathbb{E}_{z\sim q_\varphi(z|x)} \log \frac{p_\theta(x,z)\, q_\varphi(z|x)}{q_\varphi(z|x)\, p_\theta(z|x)} =$$

$$= \mathbb{E}_{z\sim q_\varphi(z|x)} \log \frac{p_\theta(x,z)}{q_\varphi(z|x)} + KL(q_\varphi(z|x), p_\theta(z|x)) \geq$$

$$\geq \mathbb{E}_{z\sim q_\varphi(z|x)} \log \frac{p_\theta(x|z)\, p(z)}{q_\varphi(z|x)} =$$

$$= \mathbb{E}_{z\sim \underbrace{q_\varphi(z|x)}_{\text{энкодер}}} \log \underbrace{p_\theta(x|z)}_{\text{декодер}} - \underbrace{KL(q_\varphi(z|x), p(z))}_{\text{регуляризатор}} =$$

$$= \mathcal{L}(x;\varphi,\theta) \to \max_{\varphi,\theta} \qquad \mathcal{L}_{\varphi,\theta}(x) \to \max_{\varphi,\theta}$$

$$\frac{\partial}{\partial\theta} \mathcal{L}_{\varphi,\theta}(x) = \mathbb{E}_{z\sim q_\varphi(z|x)} \frac{\partial}{\partial\theta} \log p_\theta(x,z)$$

$$\varepsilon \sim N(\varepsilon|0,I), \quad z = \mu + \sigma\varepsilon \Rightarrow N(z|\mu, \sigma^2 I)$$

$$\frac{\partial}{\partial\varphi} \mathcal{L}_{\varphi,\theta}(x) = \mathbb{E}_{\varepsilon\sim N(\varepsilon|0,I)} \frac{\partial}{\partial\varphi} \log p_\theta(x|\mu_\varphi(x) + \sigma_\varphi(x)\varepsilon) -$$

$$- \frac{\partial}{\partial\varphi} KL(q_\varphi(z|x) \| p(z))$$