



Information Theory in Deep Neural Networks

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Outline



- Preliminary of Information Theory
- Information between Data and Representation
- Information Bottleneck & Mutual Information
- Disentangled Representation via Mutual Information
- Generalization Bound from Mutual Information



Preliminary



• Uncertainty





• Shannon Entropy

$$H(X) = -\sum_{x\in\chi} p(x)logp(x)$$



• Uncertainty



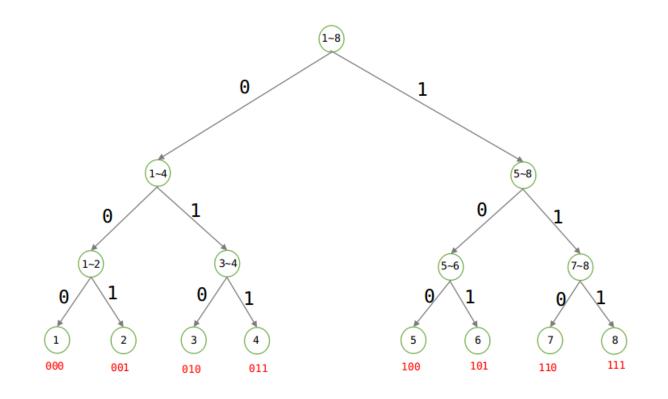
$$egin{aligned} H(X) &= -rac{1}{2} imes lograc{1}{2} - rac{1}{2} imes lograc{1}{2} = 1 \ &P\left\{Y = 1, 2, \dots, 6
ight\} = rac{1}{6} \ H(Y) = 6 imes \left(-rac{1}{6} lograc{1}{6}
ight) = log6 \ &H(X) = 1 = log2 < H(Y) = log6 \end{aligned}$$

1.2. Mean Coding Length



• Minimum MCL

$$H(x) = -\sum_{x \in X} p(x) \log p(x) = E_{x \sim P}[-\log p(X)]$$







• Coding *P* with *Q*

$$H(P,Q) = E_{x \sim P}[-\log Q(X)] = -\sum_{x \in X} \frac{p(x) \log q(x)}{1}$$

Minimize MCL

1.4. KL Divergence



• Distribution Gap

$$KL(P||Q) = \sum P(x) \log \frac{P(x)}{Q(x)} = \sum_{x \in X} p(x) \log p(x) - \sum_{x \in X} p(x) \log q(x)$$
$$= -H(P) + H(P,Q)$$
$$\uparrow$$
Data are given

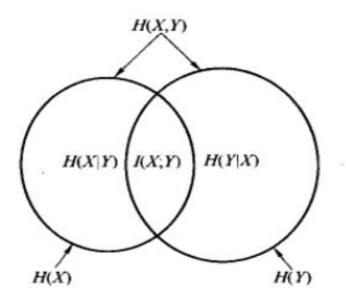




• Dependence

$$\mathrm{I}(X;Y) = \sum_{y\in\mathcal{Y}}\sum_{x\in\mathcal{X}}p(x,y)\log\left(rac{p(x,y)}{p(x)\,p(y)}
ight)$$

$$I(X;Y) = H(X) - H(X|Y).$$





Information between Data and Representation

2.1. Minimum Entropy in Data



• Information Entropy

$$\mathcal{H}_c = -\sum_{c\in\mathbb{N}^2} p_c \log p_c$$

Chinese character 9.65bit vs. English character 4.03bit

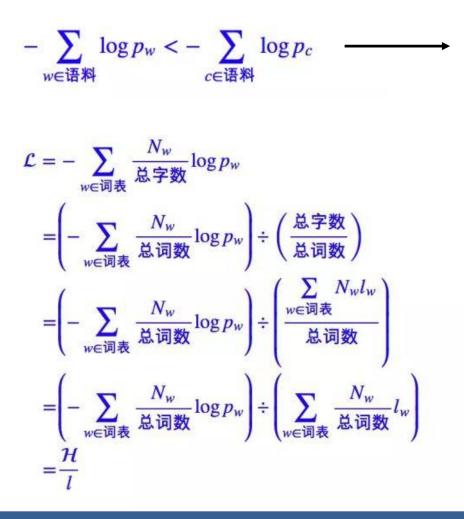
From characters to words



2.1. Minimum Entropy in Data



• Information Entropy



 $-\sum N_w \log p_w < -\sum N_c \log p_c$ we词表 c∈字表

 $-\sum_{c \in \mathbf{R}, \mathbf{k}} \frac{N_c}{\mathbf{k}^2 \mathbf{k}} \log p_c = -\sum_{c \in \mathbf{R}, \mathbf{k}} p_c \log p_c$





• Localize / Segment

$$\mathcal{H} = -\sum_{w \in ijk} p_w \log p_w, \quad l = \sum_{w \in ijk} p_w l_w$$

$$\mathcal{L} = \frac{\mathcal{H}}{l} = \frac{-\sum_{i} p_i \log p_i}{\sum_{i} p_i l_i}$$

To combine character a and b as a word

$$\begin{split} \tilde{p}_{ab} &= \frac{N_{ab}}{\tilde{N}} = \frac{p_{ab}}{1 - p_{ab}} \\ \tilde{p}_a &= \frac{\tilde{N}_a}{\tilde{N}} = \frac{p_a - p_{ab}}{1 - p_{ab}}, \ \tilde{p}_b = \frac{\tilde{N}_b}{\tilde{N}} = \frac{p_b - p_{ab}}{1 - p_{ab}} \\ \tilde{p}_i &= \frac{N_i}{\tilde{N}} = \frac{p_i}{1 - p_{ab}}, \ (i \neq a, b) \end{split}$$

2.1. Minimum Entropy in Data



• Minimize Entropy

$$\begin{split} \tilde{\mathcal{H}} &= -\frac{1}{1-p_{ab}} \left\{ p_{ab} \log\left(\frac{p_{ab}}{1-p_{ab}}\right) + \\ & \sum_{i=a,b} (p_i - p_{ab}) \log\left(\frac{p_i - p_{ab}}{1-p_{ab}}\right) + \sum_{i \neq a,b} p_i \log\left(\frac{p_i}{1-p_{ab}}\right) \right\} \\ &= \frac{1}{1-p_{ab}} (\mathcal{H} - \underline{\mathcal{F}}_{ab}) \end{split}$$

$$\mathcal{F}_{ab} = p_{ab} \log \frac{p_{ab}}{p_a p_b} - (1 - p_{ab}) \log(1 - p_{ab}) + \sum_{i=a,b} (p_i - p_{ab}) \log \left(1 - \frac{p_{ab}}{p_i}\right)$$

2.1. Minimum Entropy in Data



• Minimize Entropy

$$\begin{split} \tilde{l} &= \frac{p_{ab}}{1 - p_{ab}} (l_a + l_b) + \sum_{i=a,b} \frac{p_i - p_{ab}}{1 - p_{ab}} l_i + \sum_{i \neq a,b} \frac{p_i}{1 - p_{ab}} l_i \\ &= \frac{l}{1 - p_{ab}} \end{split}$$

After knowing the change, the change of *L*:

$$\frac{\tilde{\mathcal{H}}}{\tilde{l}} - \frac{\mathcal{H}}{l} = -\frac{\mathcal{F}_{ab}}{l}$$



• Minimize Entropy

$$\mathcal{F}_{ab} \approx F_{ab}^* = p_{ab} \left(\ln \frac{p_{ab}}{p_a p_b} - 1 \right)$$

$$\mathcal{F}_a \approx \mathcal{F}_a^* = p_a \left(\ln \frac{p_a}{\prod_{i \in a} p_i} - 1 \right)$$

$$PMI(a,b) = ln \frac{p_{ab}}{p_a p_b} > 1$$
 Segment

$$lnrac{p_{ab}}{p_ap_b} < {\sf min_pmi}$$

Split



• Library Model

 $S = \sum_{i,j} p(i) d(i)$





• What if more than one book?

$$S = \sum_{i,j} p(i)p(j|i)[d(i) + d(i,j)] = \sum_{i,j} p(i,j)[d(i) + d(i,j)]$$

• book2vec

$$S = \min_{\mathbf{v}} \sum_{i,j} p(i)p(j|i) \left[||\mathbf{v}_i|| + ||\mathbf{v}_i - \mathbf{v}_j|| \right] = \sum_{i,j} p(i,j) \left[||\mathbf{v}_i|| + ||\mathbf{v}_i - \mathbf{v}_j|| \right]$$

s.t. $\forall i, j, ||\mathbf{v}_i - \mathbf{v}_j|| \ge d_{\min}$
$$S = \sum_{i,j} p(i)p(j|i)f(\mathbf{v}_i, \mathbf{v}_j) = \sum_{i,j} p(i,j)f(\mathbf{v}_i, \mathbf{v}_j)$$



• What if more than one book?

$$S = \sum_{i,j} p(i)p(j|i)f(\mathbf{v}_i, \mathbf{v}_j) = \sum_{i,j} p(i,j)f(\mathbf{v}_i, \mathbf{v}_j)$$

• word2vec – skip gram

$$f(\mathbf{v}_i, \mathbf{v}_j) = -\log \frac{e^{-\|\mathbf{v}_i - \mathbf{v}_j\|^2}}{Z_i}, \quad Z_i = \sum_j e^{-\|\mathbf{v}_i - \mathbf{v}_j\|^2}$$

$$f(\mathbf{v}_i, \mathbf{v}_j) = -\log \frac{e^{\langle \mathbf{v}_i, \mathbf{v}_j \rangle}}{Z_i}, \quad Z_i = \sum_j e^{\langle \mathbf{v}_i, \mathbf{v}_j \rangle}$$

$$S = \sum_{i,j} p(i)p(j|i)f(\mathbf{v}_i, \mathbf{v}_j) = -\sum_{i,j} p(i)p(j|i)\log q(j|i)$$



• (t-)SNE

Let
$$P(i) = c$$

 $p(\mathbf{x}_j | \mathbf{x}_i) = \frac{e^{-\|\mathbf{x}_i - \mathbf{x}_j\|^2 / 2\sigma^2}}{\sum_{j=1}^{j \neq i} e^{-\|\mathbf{x}_i - \mathbf{x}_j\|^2 / 2\sigma^2}}$
 $S = -\sum_{i,j=1}^{i \neq j} p(\mathbf{x}_j | \mathbf{x}_i) \log q(j | i), \quad q(j | i) = \frac{e^{-\|\mathbf{v}_i - \mathbf{v}_j\|^2}}{\sum_{j=1}^{j \neq i} e^{-\|\mathbf{v}_i - \mathbf{v}_j\|^2}}$



dx

Generative model from *Z* to *X* •

$$p(X) \sim \{X_1, \dots, X_n\}$$

$$p(x) = \int p(x|z)p(z)dz, \quad p(x,z) = \underline{p(x|z)}p(z)$$

$$KL(p(x,z) ||q(x,z)) = \iint p(x,z) \ln \frac{p(x,z)}{q(x,z)}dzdx$$

$$KL(p(x,z) ||q(x,z)) = \int p(x) \left[\int p(z|x) \ln \frac{p(x,z)}{q(x,z)}dz\right]dz$$

$$= \mathbb{E}_{x \sim p(x)} \left[\int p(z|x) \ln \frac{p(z|x)p(x)}{q(x,z)}dz\right]$$



• Joint Probability Matching

$$KL(p(x,z) \| q(x,z)) = \mathbb{E}_{x \sim p(x)} \left[\int p(z|x) \ln \frac{p(z|x)p(x)}{q(x,z)} dz \right]$$
$$\ln \frac{p(z|x)p(x)}{q(x,z)} = \ln \frac{p(z|x)}{q(x,z)} + \ln p(x)$$
$$\mathbb{E}_{x \sim p(x)} \left[\int p(z|x) \ln p(x) dz \right] = \mathbb{E}_{x \sim p(x)} \left[\ln p(x) \int p(z|x) dz \right]$$
$$= \mathbb{E}_{x \sim p(x)} \left[\ln p(x) \right]$$



• Losses

$$\mathcal{L} = \mathbb{E}_{x \sim p(x)} \left[\int p(z|x) \ln \frac{p(z|x)}{q(x|z)q(z)} dz \right]$$

$$= \mathbb{E}_{x \sim p(x)} \left[-\int p(z|x) \ln q(x|z) dz + \int p(z|x) \ln \frac{p(z|x)}{q(z)} dz \right]$$

$$= \mathbb{E}_{x \sim p(x)} \left[\mathbb{E}_{z \sim p(z|x)} \left[-\ln q(x|z) \right] + \mathbb{E}_{z \sim p(z|x)} \left[\ln \frac{p(z|x)}{q(z)} \right] \right]$$

$$= \mathbb{E}_{x \sim p(x)} \left[\mathbb{E}_{z \sim p(z|x)} \left[-\ln q(x|z) \right] + KL \left(p(z|x) \| q(z) \right) \right]$$

Uniform Gaussian as a Prior
Loss for Generation





• Components

$$\mathcal{L} = \mathbb{E}_{x \sim p(x)} \begin{bmatrix} \mathbb{E}_{z \sim p(z|x)} \begin{bmatrix} -\ln q(x|z) \end{bmatrix} + KL(p(z|x) \| q(z)) \end{bmatrix}$$

Standard Gaussian
Bernoulli / Gaussian
$$\hat{p}(z|x) = q(z|x) = \frac{q(x|z)q(z)}{q(x)} = \frac{q(x|z)q(z)}{\int q(x|z)q(z)dz}$$



• P(z|x)

$$p(z|x) = \frac{1}{\prod_{k=1}^{d} \sqrt{2\pi\sigma_{(k)}^{2}(x)}} \exp\left(-\frac{1}{2} \left\|\frac{z-\mu(x)}{\sigma(x)}\right\|^{2}\right)$$

$$KL(p(z|x) \| q(z)) = \frac{1}{2} \sum_{k=1}^{d} \left(\mu_{(k)}^{2}(x) + \sigma_{(k)}^{2}(x) - \ln \sigma_{(k)}^{2}(x) - 1 \right)$$



• P(x/z) with Bernoulli distribution

$$p(\xi) = \begin{cases} \rho, \ \xi = 1; \\ 1 - \rho, \ \xi = 0 \end{cases}$$

$$q(x|z) = \prod_{k=1}^{D} \left(\rho_{(k)}(z) \right)^{x(k)} \left(1 - \rho_{(k)}(z) \right)^{1 - x(k)}$$

$$-\ln q(x|z) = \sum_{k=1}^{D} \left[-x_{(k)} \ln \rho_{(k)}(z) - (1 - x_{(k)}) \ln \left(1 - \rho_{(k)}(z) \right) \right]$$

Cross Entropy Loss



• P(x/z) with Gaussian distribution

$$q(x|z) = \frac{1}{\prod_{k=1}^{D} \sqrt{2\pi\sigma_{(k)}^{2}(z)}} \exp\left(-\frac{1}{2} \left\|\frac{x - \mu(z)}{\sigma(z)}\right\|^{2}\right)$$

$$-\ln q(x|z) = \frac{1}{2} \left\| \frac{x - \mu_k(z)}{\sigma(z)} \right\|^2 + \frac{D}{2} \ln 2\pi + \frac{1}{2} \sum_{k=1}^{D} \ln \sigma_{(k)}^2(z)$$

$$-\ln q(x|z) \sim \frac{1}{2\sigma^2} \left\| x - \mu_k(z) \right\|^2$$
MSE



Information Bottleneck & Mutual Information

3.1. Information Bottleneck



• Information Extraction

$$\max[I(Z;Y) - \beta I(X;Z)]$$



3.1. Information Bottleneck



• Loss

$$\begin{split} & \underbrace{\iint p(z|x)\tilde{p}(x)\log\frac{p(z|x)}{p(z)}dxdz}_{p(z)} \\ = & \iint p(z|x)\tilde{p}(x)\log\frac{p(z|x)}{q(z)}\frac{q(z)}{p(z)}dxdz \\ = & \iint p(z|x)\tilde{p}(x)\log\frac{p(z|x)}{q(z)} + \iint p(z|x)\tilde{p}(x)\log\frac{q(z)}{p(z)}dxdz \\ = & \iint p(z|x)\tilde{p}(x)\log\frac{p(z|x)}{q(z)} + \int p(z)\log\frac{q(z)}{p(z)}dz \\ = & \iint p(z|x)\tilde{p}(x)\log\frac{p(z|x)}{q(z)} - \int p(z)\log\frac{p(z)}{q(z)}dz \\ = & \int \tilde{p}(x)KL(p(z|x)||q(z))dx - KL(\underline{p(z)}||q(z)) \\ < & \int \tilde{p}(x)KL(p(z|x)||q(z))dx \end{aligned} > 0$$

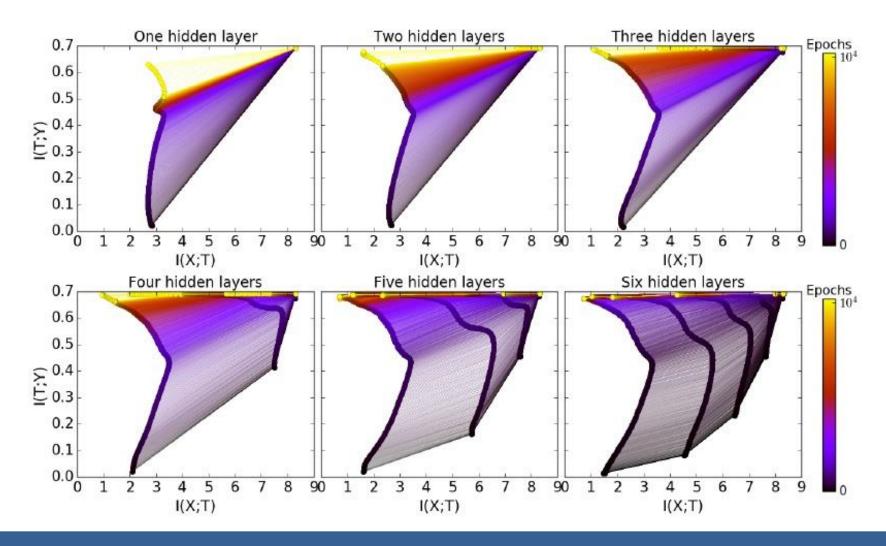
$$KLig(p(z|x) \| q(z)ig)ig]$$

Standard Gaussian

3.1. Information Bottleneck



• Two phase of learning



3.2. Deep InfoMax



• AutoEncoder – Keep key information



$$p(z|x) = \max_{p(z|x)} I(X, Z)$$



• Maximum Mutual Information

3.2. Deep InfoMax

$$I(X, Z) = \iint p(z|x)\tilde{p}(x) \log \frac{p(z|x)}{p(z)} dxdz$$

Given data distribution
$$p(z) = \int \frac{p(z|x)\tilde{p}(x)dx}{1}$$
$$p(z|x) = \max_{p(z|x)} I(X, Z)$$



• Prior Distribution

$$KL(p(z)||q(z)) = \int p(z) \log \frac{p(z)}{q(z)} dz$$

$$p(z|x) = \min_{p(z|x)} \left\{ -I(X, Z) + \lambda KL(p(z)||q(z)) \right\}$$

$$= \min_{p(z|x)} \left\{ -\iint_{p(z|x)\tilde{p}(x)} \log \frac{p(z|x)}{p(z)} \frac{dxdz}{p(z)} + \lambda \int_{p(z)} \log \frac{p(z)}{q(z)} dz \right\}$$

$$= \min_{p(z|x)} \left\{ \iint_{p(z|x)\tilde{p}(x)} \left[-(1+\lambda) \log \frac{p(z|x)}{p(z)} + \lambda \log \frac{p(z|x)}{q(z)} \right] dxdz \right\}$$

$$= \min_{p(z|x)} \left\{ -\beta \cdot I(X, Z) + \gamma \cdot \mathbb{E}_{x \sim \tilde{p}(x)} [KL(p(z|x)||q(z))] \right\}$$



• Mutual Information

$$I(X, Z) = \iint p(z|x)\tilde{p}(x)\log\frac{p(z|x)\tilde{p}(x)}{p(z)\tilde{p}(x)}dxdz$$
$$=KL(p(z|x)\tilde{p}(x)||p(z)\tilde{p}(x))$$

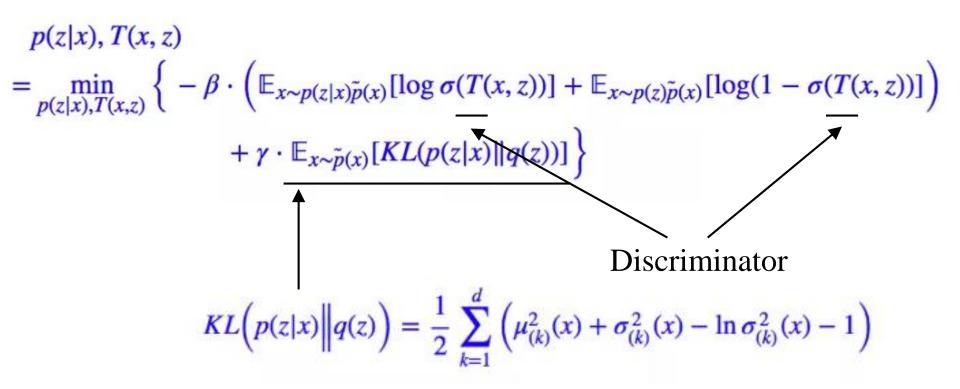
• From f-GAN

 $D_{f}(P||Q) = \max_{T} \left(\mathbb{E}_{x \sim p(x)}[T(x)] - \mathbb{E}_{x \sim q(x)}[g(T(x))] \right)$ $JS(p(z|x)\tilde{p}(x), p(z)\tilde{p}(x))$ $= \max_{T} \left(\mathbb{E}_{x \sim p(z|x)\tilde{p}(x)}[\log \sigma(T(x, z))] + \mathbb{E}_{x \sim p(z)\tilde{p}(x)}[\log(1 - \sigma(T(x, z))] \right)$



• Deep InfoMax

 $p(z|x) = \min_{p(z|x)} \left\{ -\beta \cdot JS(p(z|x)\tilde{p}(x), p(z)\tilde{p}(x)) + \gamma \cdot \mathbb{E}_{x \sim \tilde{p}(x)}[KL(p(z|x)||q(z))] \right\}$





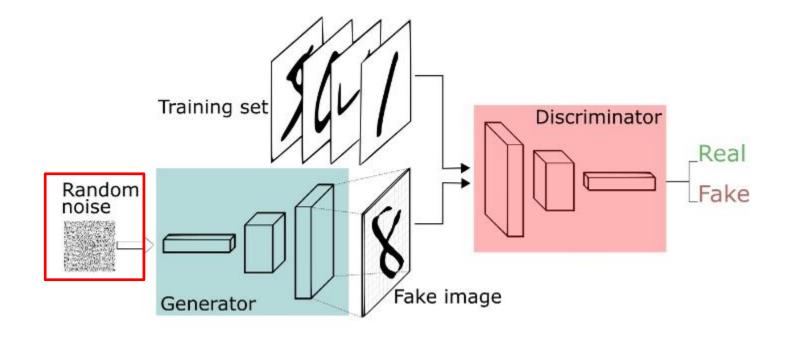
Disentangled Representation





• GAN

$$\min_{G} \max_{D} V(D,G) = E_{p(\mathbf{x})} \left[\log(D(\mathbf{x})) \right] + E_{p(\mathbf{z})} \left[\log(1 - D(G(\mathbf{z}))) \right]$$





• InfoGAN

$$\min_{G} \max_{D} V_I(D,G) = V(D,G) - \lambda I(c;G(z,c))$$

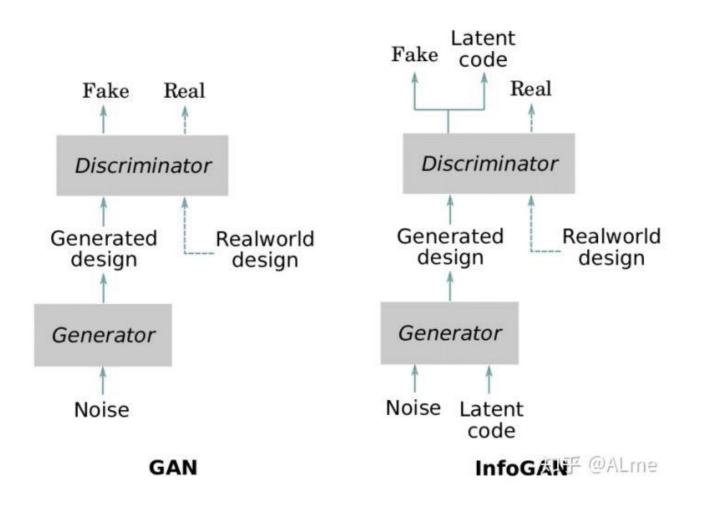
$$\begin{split} I(c;G(z,c)) &= H(c) - H(c|G(z,c)) \\ &= \mathbb{E}_{x \sim G(z,c)} [\mathbb{E}_{c' \sim P(c|x)} [\log P(c'|x)]] + H(c) \\ &= \mathbb{E}_{x \sim G(z,c)} [\underbrace{D_{\mathrm{KL}}(P(\cdot|x) \parallel Q(\cdot|x))}_{\geq 0} + \mathbb{E}_{c' \sim P(c|x)} [\log Q(c'|x)]] + H(c) \\ &\geq \mathbb{E}_{x \sim G(z,c)} [\mathbb{E}_{c' \sim P(c|x)} [\log Q(c'|x)]] + H(c) \end{split}$$

$$L_{I}(G,Q) = E_{c \sim P(c), x \sim G(z,c)} [\log Q(c|x)] + H(c)$$

Discriminator

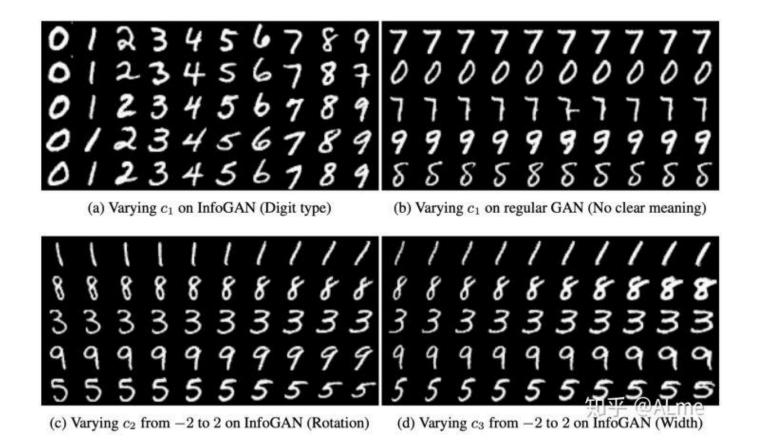


• Architecture





• Disentangled Representation





• VAE

$$\mathcal{L}(\theta,\phi;\mathbf{x},\mathbf{z}) = \mathbb{E}_{q_{\phi}(\mathbf{z}|\mathbf{x})}[\log p_{\theta}(\mathbf{x}|\mathbf{z})] - D_{KL}(q_{\phi}(\mathbf{z}|\mathbf{x}) \parallel p(\mathbf{z}))$$

• BetaVAE

 $\mathcal{L}(\theta,\phi;\mathbf{x},\mathbf{z},\beta) = \mathbb{E}_{q_{\phi}(\mathbf{z}|\mathbf{x})}[\log p_{\theta}(\mathbf{x}|\mathbf{z})] - \beta D_{KL}(q_{\phi}(\mathbf{z}|\mathbf{x}) \parallel p(\mathbf{z}))$

Standard Gaussian distribution



• Information Bottleneck

$$\max[I(Z; Y) - \beta I(X; Z)]$$
• Understanding BetaVAE
$$\mathcal{L}(\theta, \phi; \mathbf{x}, \mathbf{z}, \beta) = \mathbb{E}_{q_{\phi}(\mathbf{z}|\mathbf{x})}[\log p_{\theta}(\mathbf{x}|\mathbf{z})] - \beta D_{KL}(q_{\phi}(\mathbf{z}|\mathbf{x}) \parallel p(\mathbf{z}))$$

$$q^{(z_1|x_1)} = q^{(z_2|x_2)} q^{(z_3|x_3)}$$

4.3. Standard Gaussian Distribution



• Decomposition

$$P(x,y) = p(x)p(y)$$

• Interpolation

 $z_1+z_2\sim \mathcal{N}(\mu_1+\mu_2,\sigma_1^2+\sigma_2^2)$





Generalization Bound



Generalization Error

$$E(h; \mathcal{D}) = P_{\boldsymbol{x} \sim \mathcal{D}} (h(\boldsymbol{x}) \neq y)$$

• Empirical error

$$\widehat{E}(h; D) = \frac{1}{m} \sum_{i=1}^{m} \mathbb{I}(h(\boldsymbol{x}_i) \neq y_i)$$

• Generalization bound

 $E(h)\leqslant\epsilon_{0}$



• Probably Approximately Correct (PAC)

 $P(E(h) \leq \epsilon) \ge 1 - \delta$, $0 < \epsilon, \delta < 1$

• Sample Complexity

 $m \ge \operatorname{poly}(1/\epsilon, 1/\delta, \operatorname{size}(\boldsymbol{x}), \operatorname{size}(c))$

• Properly PAC learnable

$$\mathcal{H} = \mathcal{C}$$

• Infinity hypothesis space

$$|\mathcal{H}| = \infty$$



• If $|\mathcal{H}| \neq \infty$ and $c \in \mathcal{H}$

$$P(h(\boldsymbol{x}) = \boldsymbol{y}) = 1 - P(h(\boldsymbol{x}) \neq \boldsymbol{y})$$
$$= 1 - E(h)$$
$$< 1 - \epsilon .$$

$$P((h(\boldsymbol{x}_1) = y_1) \land \ldots \land (h(\boldsymbol{x}_m) = y_m)) = (1 - P(h(\boldsymbol{x}) \neq y))^m$$

< $(1 - \epsilon)^m$.

$$P(h \in \mathcal{H} : E(h) > \epsilon \wedge \widehat{E}(h) = 0) < |\mathcal{H}|(1-\epsilon)^m < |\mathcal{H}|e^{-m\epsilon} \leq \delta,$$

$$m \geqslant \frac{1}{\epsilon} \left(\ln |\mathcal{H}| + \ln \frac{1}{\delta} \right)$$



• If $|\mathcal{H}| \neq \infty \& c \notin \mathcal{H}$

$$P(E(h) - \min_{h' \in \mathcal{H}} E(h') \leq \epsilon) \ge 1 - \delta$$

• If $|\mathcal{H}| = \infty$

$$\operatorname{VC}(\mathcal{H}) = \max\{m: \Pi_{\mathcal{H}}(m) = 2^m\}$$

$$P\left(E(h) - \widehat{E}(h) \leqslant \sqrt{\frac{8d\ln\frac{2em}{d} + 8\ln\frac{4}{\delta}}{m}}\right) \geqslant 1 - \delta \ .$$



• Low MI => Generalization

$$|\mathbf{E}[\phi_T - \mu_T]| \le \sigma \sqrt{2I(T; \phi)},$$
$$|\mathbf{E}[\phi_T] - \mathbf{E}[\mu_T]| \le \sigma \sqrt{\frac{2I(T; \phi)}{n}}.$$
$$\mathbf{E}[L(\hat{f}) - \hat{L}(\hat{f})] \le \sqrt{\frac{I(\hat{f}(\mathbf{x}); \mathbf{Y})}{2n}}.$$

5.3. Generalization bound via CMI



- $I(T(X), X) \rightarrow \infty$, but strong generalization holds
- CMI is finite

$$CMI_D(T) = I(T(\tilde{X}_S); S|\tilde{X})$$

$$CMI_D(T) \le H(S) = \log 2^n = n$$

- Low CMI => Generalization
- CMI is bounded by VC dimension and Compression Schemes
- CMI is bounded from (ε, δ) -DP (via TV Stability)

Thank

you

