

Noise-contrastive estimation of unnormalised statistical models

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11th November 2016

Problem statement

- ▶ Task: Estimate the parameters θ of a parametric model $p(\cdot|\theta)$ of a d dimensional random vector \mathbf{x}
- ▶ Given: Data $\mathbf{X} = (\mathbf{x}_1, \dots, \mathbf{x}_n)$ (iid)
- ▶ Given: Unnormalized model $\phi(\cdot|\theta)$

$$\int_{\xi} \phi(\xi; \theta) d\xi = Z(\theta) \neq 1 \quad p(\mathbf{x}; \theta) = \frac{\phi(\mathbf{x}; \theta)}{Z(\theta)} \quad (1)$$

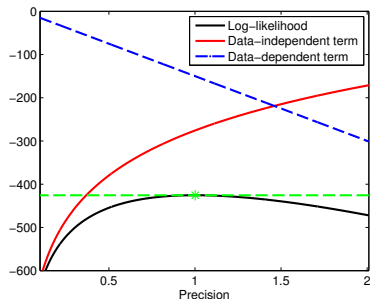
Normalizing partition function $Z(\theta)$ not known / computable.

Why does the partition function matter?

- ▶ Consider $p(x; \theta) = \frac{\phi(x; \theta)}{Z(\theta)} = \frac{\exp(-\theta \frac{x^2}{2})}{\sqrt{2\pi/\theta}}$
- ▶ Log-likelihood function for precision $\theta \geq 0$

$$\ell(\theta) = -n \log \sqrt{\frac{2\pi}{\theta}} - \theta \sum_{i=1}^n \frac{x_i^2}{2} \quad (2)$$

- ▶ Data-dependent (blue) and independent part (red) balance each other.
- ▶ If $Z(\theta)$ is intractable, $\ell(\theta)$ is intractable.



Why is the partition function hard to compute?

$$Z(\theta) = \int_{\xi} \phi(\xi; \theta) d\xi$$

- ▶ Integrals can generally not be solved in closed form.
- ▶ In low dimensions, $Z(\theta)$ can be approximated to high accuracy.
- ▶ Curse of dimensionality: Solutions feasible in low dimensions become quickly computationally prohibitive as the dimension d increases.

Why are unnormalized models important?

- ▶ Unnormalized models are widely used.
- ▶ Examples:
 - ▶ models of images (Markov random fields)
 - ▶ models of text (neural probabilistic language models)
 - ▶ models in physics (Ising model)
 - ▶ ...
- ▶ Advantage: Specifying unnormalized models is often easier than specifying normalized models.
- ▶ Disadvantage: Likelihood function is generally intractable.

Noise-contrastive estimation

- Intuition and definition

- Properties

Bregman divergence to estimate unnormalized models

- Framework

- Noise-contrastive estimation as member of the framework

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Bregman divergence to estimate unnormalized models

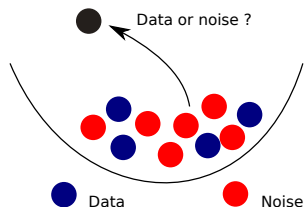
- Framework

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Intuition behind noise-contrastive estimation

- ▶ Formulate the estimation problem as a classification problem: observed data vs. auxiliary “noise” (with known properties)
- ▶ Successful classification \equiv learn the differences between the data and the noise
- ▶ differences + known noise properties \Rightarrow properties of the data

- ▶ Unsupervised learning by supervised learning
- ▶ We used (nonlinear) logistic regression for classification

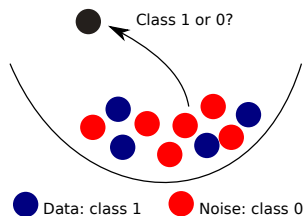


Logistic regression (1/2)

- ▶ Let $\mathbf{Y} = (\mathbf{y}_1, \dots, \mathbf{y}_m)$ be a sample from a random variable \mathbf{y} with known (auxiliary) distribution $p_{\mathbf{y}}$.
- ▶ Introduce labels and form regression function:

$$P(C = 1|\mathbf{u}; \theta) = \frac{1}{1 + G(\mathbf{u}; \theta)} \quad G(\mathbf{u}; \theta) \geq 0 \quad (3)$$

- ▶ Determine the parameters θ such that $P(C = 1|\mathbf{u}; \theta)$ is
 - ▶ large for most \mathbf{x}_i
 - ▶ small for most \mathbf{y}_i .



Logistic regression (2/2)

- ▶ Maximize (rescaled) conditional log-likelihood using the labeled data $\{(\mathbf{x}_1, 1), \dots, (\mathbf{x}_n, 1), (\mathbf{y}_1, 0), \dots, (\mathbf{y}_m, 0)\}$,

$$J_n^{\text{NCE}}(\boldsymbol{\theta}) = \frac{1}{n} \left(\sum_{i=1}^n \log P(C = 1 | \mathbf{x}_i; \boldsymbol{\theta}) + \sum_{i=1}^m \log [P(C = 0 | \mathbf{y}_i; \boldsymbol{\theta})] \right)$$

- ▶ For large sample sizes n and m , $\hat{\boldsymbol{\theta}}$ satisfying

$$G(\mathbf{u}; \hat{\boldsymbol{\theta}}) = \frac{m p_{\mathbf{y}}(\mathbf{u})}{n p_{\mathbf{x}}(\mathbf{u})} \quad (4)$$

is maximizing $J_n^{\text{NCE}}(\boldsymbol{\theta})$. **Without any normalization constraints.**

proof

Noise-contrastive estimation

(Gutmann and Hyvärinen, 2010; 2012)

- ▶ Assume unnormalized model $\phi(\cdot|\theta)$ is parametrized such that its scale can vary freely.

$$\theta \rightarrow (\theta; c) \quad \phi(\mathbf{u}; \theta) \rightarrow \exp(c)\phi(\mathbf{u}; \theta) \quad (5)$$

- ▶ Noise-contrastive estimation:
 1. Choose p_y
 2. Generate auxiliary data \mathbf{Y}
 3. Estimate θ via logistic regression with

$$G(\mathbf{u}; \theta) = \frac{m}{n} \frac{p_y(\mathbf{u})}{\phi(\mathbf{u}; \theta)}. \quad (6)$$

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- ▶ $G(\mathbf{u}; \theta) \rightarrow \frac{m}{n} \frac{p_y(\mathbf{u})}{p_x(\mathbf{u})} \Rightarrow \phi(\mathbf{u}; \theta) \rightarrow p_x(\mathbf{u})$

Example

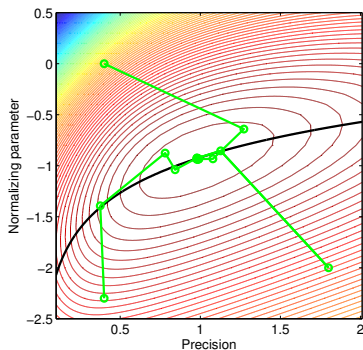
- ▶ Unnormalized Gaussian:

$$\phi(u; \boldsymbol{\theta}) = \exp(\theta_2) \exp\left(-\theta_1 \frac{u^2}{2}\right), \quad \theta_1 > 0, \theta_2 \in \mathbb{R}, \quad (7)$$

- ▶ Parameters: θ_1 (precision), $\theta_2 \equiv c$ (scaling parameter)

Contour plot of $J_n^{\text{NCE}}(\boldsymbol{\theta})$:

- ▶ Gaussian noise with $\nu = m/n = 10$
- ▶ True precision $\theta_1^* = 1$
- ▶ Black: normalized models
- ▶ Green: optimization paths



(Gutmann and Hyvärinen, 2012)

- ▶ Assume $p_x = p(\cdot|\theta^*)$
- ▶ Consistency: As n increases,

$$\hat{\theta}_n = \operatorname{argmax}_{\theta} J_n^{\text{NCE}}(\theta), \quad (8)$$

converges in probability to θ^* .

- ▶ Efficiency: As $\nu = m/n$ increases, for any valid choice of p_y , noise-contrastive estimation tends to “perform as well” as MLE (it is asymptotically Fisher efficient).

Validating the statistical properties with toy data

- ▶ Let the data follow the ICA model $\mathbf{x} = \mathbf{A}\mathbf{s}$ with 4 sources.

$$\log p(\mathbf{x}; \boldsymbol{\theta}^*) = - \sum_{i=1}^4 \sqrt{2} |\mathbf{b}_i^* \mathbf{x}| + c^* \quad (9)$$

with $c^* = \log |\det \mathbf{B}^*| - \frac{4}{2} \log 2$ and $\mathbf{B}^* = \mathbf{A}^{-1}$.

- ▶ To validate the method, estimate the unnormalized model

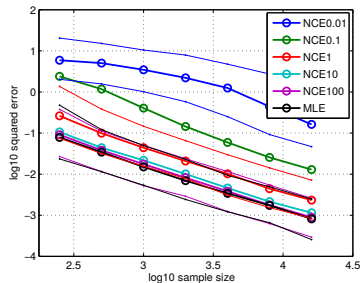
$$\log \phi(\mathbf{x}; \boldsymbol{\theta}) = - \sum_{i=1}^4 \sqrt{2} |\mathbf{b}_i \mathbf{x}| + c \quad (10)$$

with parameters $\boldsymbol{\theta} = (\mathbf{b}_1, \dots, \mathbf{b}_4, c)$.

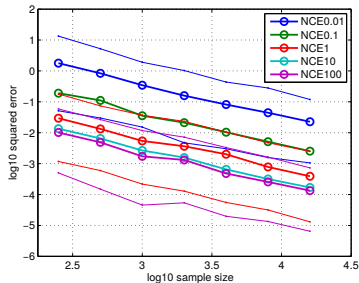
- ▶ Contrastive noise p_y : Gaussian with the same covariance as the data.

Validating the statistical properties with toy data

- ▶ Results for 500 estimation problems with random \mathbf{A} , for $\nu \in \{0.01, 0.1, 1, 10, 100\}$.
- ▶ MLE results: with properly normalized model



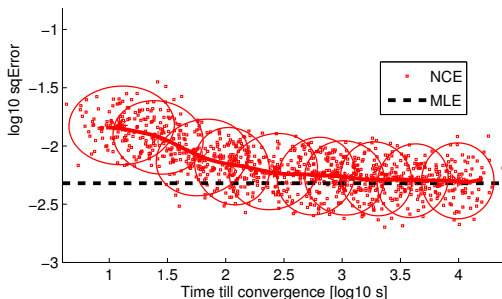
(a) Mixing matrix



(b) Normalizing constant

Computational aspects

- ▶ The estimation accuracy improves as m increases.
- ▶ Trade-off between computational and statistical performance.
- ▶ Example: ICA model as before but with 10 sources. $n = 8000$, $\nu \in \{1, 2, 5, 10, 20, 50, 100, 200, 400, 1000\}$.
Performance for 100 random estimation problems:



Computational aspects

How good is the trade-off? Compare with

1. MLE where partition function is evaluated with importance sampling. Maximization of

$$J_{\text{IS}}(\boldsymbol{\theta}) = \frac{1}{n} \sum_{i=1}^n \log \phi(\mathbf{x}_i; \boldsymbol{\theta}) - \log \left(\frac{1}{m} \sum_{i=1}^m \frac{\phi(\mathbf{y}_i; \boldsymbol{\theta})}{p_{\mathbf{y}}(\mathbf{y}_i)} \right) \quad (11)$$

2. Score matching: minimization of

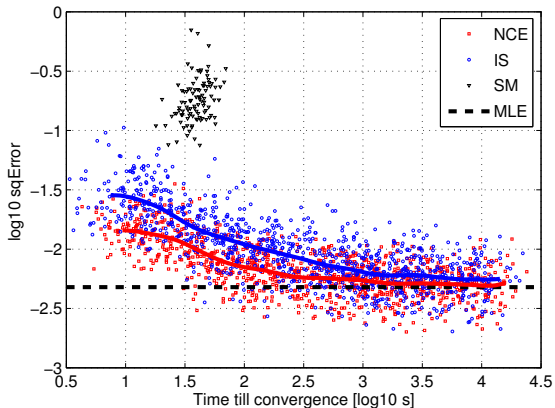
$$J_{\text{SM}}(\boldsymbol{\theta}) = \frac{1}{n} \sum_{i=1}^n \sum_{j=1}^{10} \frac{1}{2} \Psi_j^2(\mathbf{x}_i; \boldsymbol{\theta}) + \Psi_j'(\mathbf{x}_i; \boldsymbol{\theta}) \quad (12)$$

$$\text{with } \Psi_j(\mathbf{x}; \boldsymbol{\theta}) = \frac{\partial \log \phi(\mathbf{x}; \boldsymbol{\theta})}{\partial x_j} \quad (\text{here: smoothing needed!})$$

(see Gutmann and Hyvärinen, 2012, for more comparisons)

Computational aspects

- ▶ NCE is less sensitive to the mismatch of data and noise distribution than importance sampling.
- ▶ Score matching does not perform well if the data distribution is not sufficiently smooth.



Application examples

- ▶ Models of text: e.g. Mnih and Teh, 2012, *A fast and simple algorithm for training neural probabilistic language models*
- ▶ Models of images: e.g. Gutmann and Hyvärinen, 2013, *A three-layer model of natural image statistics*
- ▶ Machine translation: e.g. Zoph et al, 2016, *Simple, fast noise-contrastive estimation for large RNN vocabularies*
- ▶ Product recommendation: e.g. Tschitschek et al, 2016, *Learning probabilistic submodular diversity models via noise contrastive estimation*

Noise-contrastive estimation

- Intuition and definition

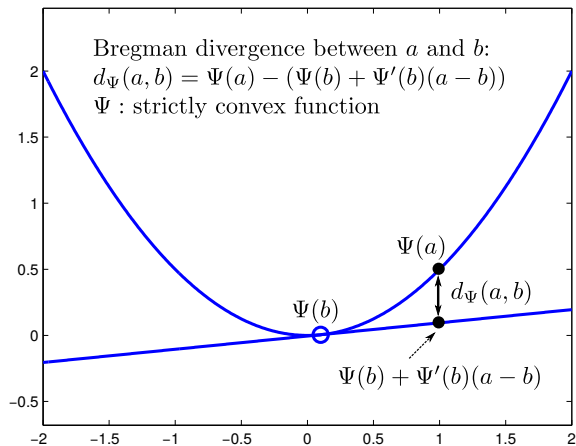
- Properties

Bregman divergence to estimate unnormalized models

- Framework

- Noise-contrastive estimation as member of the framework

Bregman divergence between two vectors a and b



$$u \log(u) - (1 + u) \log(1 + u)$$

$$-\log(u)$$

$$u \log(u)$$

$$d_{\Psi}(a, b) = 0 \Leftrightarrow a = b$$

$$d_{\Psi}(a, b) > 0 \text{ if } a \neq b$$

Bregman divergence between two functions f and g

- ▶ Compute $d_{\Psi}(f(\mathbf{u}), g(\mathbf{u}))$ for all \mathbf{u} in their domain; take weighted average

$$\tilde{d}_{\Psi}(f, g) = \int d_{\Psi}(f(\mathbf{u}), g(\mathbf{u})) d\mu(\mathbf{u}) \quad (13)$$

$$= \int \Psi(f) - [\Psi(g) + \Psi'(g)(f - g)] d\mu \quad (14)$$

- ▶ Zero iff $f = g$ (a.e.); **no normalization condition on f or g**
- ▶ Fix f , omit terms not depending on g ,

$$J(g) = \int [-\Psi(g) + \Psi'(g)g - \Psi'(g)f] d\mu \quad (15)$$

Estimation of unnormalized models

$$J(g) = \int [-\Psi(g) + \Psi'(g)g - \Psi'(g)f]d\mu$$

- ▶ Idea: Choose f , g , and μ so that we obtain a computable cost function for consistent estimation of unnormalized models.
- ▶ Choose $f = T(p_x)$ and $g = T(\phi)$ such that

$$f = g \Rightarrow p_x = \phi \tag{16}$$

Examples:

- ▶ $f = p_x, g = \phi$
 - ▶ $f = \frac{p_x}{\nu p_y}, g = \frac{\phi}{\nu p_y}$
 - ▶ ...
- ▶ Choose μ such that the integral can either be computed in closed form or approximated as sample average.

(Gutmann and Hirayama, 2011)

Estimation of unnormalized models

(Gutmann and Hirayama, 2011)

- ▶ Several estimation methods for unnormalized models are part of the framework
 - ▶ Noise-contrastive estimation
 - ▶ Poisson-transform (Barthelmé and Chopin, 2015)
 - ▶ Score matching (Hyvärinen, 2005)
 - ▶ Pseudo-likelihood (Besag, 1975)
 - ▶ ...
- ▶ Noise-contrastive estimation:

$$\Psi(u) = u \log u - (1 + u) \log(1 + u) \quad (17)$$

$$f(\mathbf{u}) = \frac{\nu p_{\mathbf{y}}(\mathbf{u})}{p_{\mathbf{x}}(\mathbf{u})} \quad d\mu(\mathbf{u}) = p_{\mathbf{x}}(\mathbf{u}) d\mathbf{u} \quad (18)$$

proof

- ▶ Point estimation for parametric models with intractable partition functions (unnormalized models)
- ▶ Noise contrastive estimation
 - ▶ Estimate the model by learning to classify between data and noise
 - ▶ Consistent estimator, has MLE as limit
 - ▶ Applicable to large-scale problems
- ▶ Bregman divergence as general framework to estimate unnormalized models.

Maximizer of the NCE objective function

Noise-contrastive estimation as member of the Bregman framework

Maximizer of the NCE objective function

Noise-contrastive estimation as member of the Bregman framework

Proof of Equation (4)

For large sample sizes n and m , $\hat{\theta}$ satisfying

$$G(\mathbf{u}; \hat{\theta}) = \frac{m p_{\mathbf{y}}(\mathbf{u})}{n p_{\mathbf{x}}(\mathbf{u})}$$

is maximizing $J_n^{\text{NCE}}(\theta)$,

$$J_n^{\text{NCE}}(\theta) = \frac{1}{n} \left(\sum_{i=1}^n \log P(C = 1 | \mathbf{x}_i; \theta) + \sum_{i=1}^m \log [P(C = 0 | \mathbf{y}_i; \theta)] \right)$$

without any normalization constraints.

Proof of Equation (4)

$$\begin{aligned} J_n^{\text{NCE}}(\boldsymbol{\theta}) &= \frac{1}{n} \left(\sum_{i=1}^n \log P(C = 1 | \mathbf{x}_i; \boldsymbol{\theta}) + \sum_{i=1}^m \log [P(C = 0 | \mathbf{y}_i; \boldsymbol{\theta})] \right) \\ &= \frac{1}{n} \sum_{t=1}^n \log P(C = 1 | \mathbf{x}_t; \boldsymbol{\theta}) + \frac{m}{n} \frac{1}{m} \sum_{t=1}^m \log [P(C = 0 | \mathbf{y}_t; \boldsymbol{\theta})] \end{aligned}$$

Fix the ratio $m/n = \nu$ and let $n \rightarrow \infty$ and $m \rightarrow \infty$. By law of large numbers, J_n^{NCE} converges to J^{NCE} ,

$$J^{\text{NCE}}(\boldsymbol{\theta}) = \mathbb{E}_{\mathbf{x}} (\log P(C = 1 | \mathbf{x}; \boldsymbol{\theta})) + \nu \mathbb{E}_{\mathbf{y}} (\log P(C = 0 | \mathbf{y}; \boldsymbol{\theta})) \quad (19)$$

With $P(C = 1 | \mathbf{x}; \boldsymbol{\theta}) = \frac{1}{1+G(\mathbf{x}; \boldsymbol{\theta})}$ and $P(C = 0 | \mathbf{y}; \boldsymbol{\theta}) = \frac{G(\mathbf{y}; \boldsymbol{\theta})}{1+G(\mathbf{y}; \boldsymbol{\theta})}$ we have

$$\begin{aligned} J^{\text{NCE}}(\boldsymbol{\theta}) &= - \mathbb{E}_{\mathbf{x}} \log(1 + G(\mathbf{x}; \boldsymbol{\theta})) + \nu \mathbb{E}_{\mathbf{y}} \log G(\mathbf{y}; \boldsymbol{\theta}) - \\ &\quad \nu \mathbb{E}_{\mathbf{y}} \log(1 + G(\mathbf{y}; \boldsymbol{\theta})) \end{aligned} \quad (20)$$

Consider the objective $J^{\text{NCE}}(\boldsymbol{\theta})$ as a function of $H = \log G$ rather than $\boldsymbol{\theta}$,

$$\begin{aligned} \mathcal{J}^{\text{NCE}}(H) &= -\mathbb{E}_{\mathbf{x}} \log(1 + \exp H(\mathbf{x})) + \nu \mathbb{E}_{\mathbf{y}} H(\mathbf{y}) - \nu \mathbb{E}_{\mathbf{y}} \log(1 + \exp H(\mathbf{y})) \\ &= -\int p_{\mathbf{x}}(\boldsymbol{\xi}) \log(1 + \exp H(\boldsymbol{\xi})) d\boldsymbol{\xi} + \nu \int p_{\mathbf{y}}(\boldsymbol{\xi}) H(\boldsymbol{\xi}) d\boldsymbol{\xi} \\ &\quad - \nu \int p_{\mathbf{y}}(\boldsymbol{\xi}) \log(1 + \exp H(\boldsymbol{\xi})) d\boldsymbol{\xi} \\ &= -\int (p_{\mathbf{x}}(\boldsymbol{\xi}) + \nu p_{\mathbf{y}}(\boldsymbol{\xi})) \log(1 + \exp H(\boldsymbol{\xi})) d\boldsymbol{\xi} + \\ &\quad \nu \int p_{\mathbf{y}}(\boldsymbol{\xi}) H(\boldsymbol{\xi}) d\boldsymbol{\xi} \end{aligned}$$

We now expand $\mathcal{J}^{\text{NCE}}(H + \epsilon q)$ around H for an arbitrary function q and a small scalar ϵ .

With

$$\begin{aligned}\log(1 + \exp [H(\xi) + \epsilon q(\xi)]) &= \log(1 + \exp H(\xi)) + \frac{\epsilon q(\xi)}{1 + \exp(-H(\xi))} \\ &+ \frac{\epsilon^2}{2} \frac{q(\xi)}{1 + \exp(-H(\xi))} \frac{q(\xi)}{1 + \exp(H(\xi))} \\ &+ O(\epsilon^3)\end{aligned}$$

we have

$$\begin{aligned}\mathcal{J}^{\text{NCE}}(H + \epsilon q) &= - \int (p_x(\xi) + \nu p_y(\xi)) \log(1 + \exp H(\xi)) d\xi \\ &- \epsilon \int \frac{p_x(\xi) + \nu p_y(\xi)}{1 + \exp(-H(\xi))} q(\xi) d\xi \\ &- \frac{\epsilon^2}{2} \int \frac{p_x(\xi) + \nu p_y(\xi)}{1 + \exp(-H(\xi))} \frac{q(\xi)^2}{1 + \exp(H(\xi))} d\xi \\ &+ \nu \int p_y(\xi) H(\xi) d\xi + \epsilon \nu \int p_y(\xi) q(\xi) d\xi + O(\epsilon^3)\end{aligned}$$

Collecting terms gives:

$$\begin{aligned} \mathcal{J}^{\text{NCE}}(H + \epsilon q) &= \mathcal{J}^{\text{NCE}}(H) + \epsilon \int \left(\nu p_y(\xi) - \frac{p_x(\xi) + \nu p_y(\xi)}{1 + \exp(-H(\xi))} \right) q(\xi) d\xi \\ &\quad - \frac{\epsilon^2}{2} \int \frac{p_x(\xi) + \nu p_y(\xi)}{1 + \exp(-H(\xi))} \frac{q(\xi)^2}{1 + \exp(H(\xi))} d\xi + O(\epsilon^3) \end{aligned}$$

The second-order term is negative for all (non-trivial) q and H .

The first-order term is zero for all q if and only if

$$\begin{aligned} \nu p_y(\xi) &= \frac{p_x(\xi) + \nu p_y(\xi)}{1 + \exp(-H^*(\xi))} \\ \nu p_y(\xi) + \nu p_y(\xi) \exp(-H^*(\xi)) &= p_x(\xi) + \nu p_y(\xi) \\ \exp(-H^*(\xi)) &= \frac{p_x(\xi)}{\nu p_y(\xi)} \end{aligned}$$

which shows that $\hat{\theta}$ such that $G(\xi; \hat{\theta}) = \exp(H^*(\xi)) = \nu \frac{p_y}{p_x}$ is maximizing $\mathcal{J}^{\text{NCE}}(\theta)$.

back

Maximizer of the NCE objective function

Noise-contrastive estimation as member of the Bregman framework

Proof

In noise-contrastive estimation, we maximize

$$J_n^{\text{NCE}}(\boldsymbol{\theta}) = \frac{1}{n} \left(\sum_{i=1}^n \log P(C = 1 | \mathbf{x}_i; \boldsymbol{\theta}) + \sum_{i=1}^m \log [P(C = 0 | \mathbf{y}_i; \boldsymbol{\theta})] \right)$$

Sample version of

$$J^{\text{NCE}}(\boldsymbol{\theta}) = \mathbb{E}_{\mathbf{x}} (\log P(C = 1 | \mathbf{x}; \boldsymbol{\theta})) + \nu \mathbb{E}_{\mathbf{y}} (\log P(C = 0 | \mathbf{y}; \boldsymbol{\theta}))$$

With

$$P(C = 1 | \mathbf{u}; \boldsymbol{\theta}) = \frac{1}{1 + G(\mathbf{u}; \boldsymbol{\theta})} \quad P(C = 0 | \mathbf{u}; \boldsymbol{\theta}) = \frac{1}{1 + 1/G(\mathbf{u}; \boldsymbol{\theta})}$$

$$J^{\text{NCE}}(\boldsymbol{\theta}) = -\mathbb{E}_{\mathbf{x}} \log(1 + G(\mathbf{x}; \boldsymbol{\theta})) - \nu \mathbb{E}_{\mathbf{y}} \log(1 + 1/G(\mathbf{y}; \boldsymbol{\theta})) \quad (21)$$

where $G(\mathbf{u}; \boldsymbol{\theta}) = \frac{\nu p_{\mathbf{y}}(\mathbf{u})}{\phi(\mathbf{u}; \boldsymbol{\theta})}$.

The general cost function in the Bregman framework is

$$J(g) = \int [-\Psi(g) + \Psi'(g)g - \Psi'(g)f] d\mu \quad (22)$$

With

$$\Psi(g) = g \log(g) - (1 + g) \log(1 + g) \quad (23)$$

$$\Psi'(g) = \log(g) - \log(1 + g) \quad (24)$$

we have

$$\begin{aligned} J(g) = \int & [-g \log(g) + (1 + g) \log(1 + g) \\ & + \log(g)g - \log(1 + g)g \\ & - \log(g)f + \log(1 + g)f] d\mu \end{aligned} \quad (25)$$

$$J(g) = \int [\log(1 + g) - \log(g)f + \log(1 + g)f] d\mu \quad (26)$$

$$= \int [\log(1 + g) + \log(1 + 1/g)f] d\mu \quad (27)$$

With

$$f(\mathbf{u}) = \frac{\nu p_y(\mathbf{u})}{p_x(\mathbf{u})} \quad g(\mathbf{u}) = G(\mathbf{u}; \boldsymbol{\theta}) \quad d\mu(\mathbf{u}) = p_x(\mathbf{u}) d\mathbf{u} \quad (28)$$

we have

$$J(G(\cdot; \boldsymbol{\theta})) = \int p_x(\mathbf{u}) \log(1 + G(\mathbf{u}; \boldsymbol{\theta})) d\mathbf{u} \\ + \nu \int p_y(\mathbf{u}) \log(1 + 1/G(\mathbf{u}; \boldsymbol{\theta})) d\mathbf{u} \quad (29)$$

$$= -J^{\text{NCE}}(\boldsymbol{\theta}) \quad (30)$$

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