## KRR - Learning the parameters of a BN

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## December 2018

We assume there is a real distribution  $P_r(\mathbf{X})$  we do not have access to. Instead we either have a collection of samples from that distribution, or we are able to sample from it. In what follows we are concerned with learning some parametric model  $P_{\theta}(\mathbf{X})$  that models as good as possible the real distribution  $P_r(\mathbf{X})$ .

We also assume the structure of a Bayesian Network that represents  $P_{\theta}(\mathbf{X})$  to be known. We are left to learn the CPDs for each variable  $X \in \mathbf{X}$ . In what follows we will use  $\mathbf{Y} \stackrel{not.}{=} Par(X)$  to denote the parents of X.

One way to ensure that we have good representations of the probabilities is learning a set of parameters  $\theta_{X|\mathbf{Y}=\mathbf{y}}$  such that  $P(X \mid \mathbf{Y} = \mathbf{y}) = \sigma\left(\theta_{X|\mathbf{Y}=\mathbf{y}}\right)$  where  $\sigma(x) = (1 + e^{-x})^{-1}$  is the *sigmoid* function. The sigmoid function is continous and differentiable in  $\mathbb{R}$  and has a nice derivative  $\sigma'(x) = \sigma(x)(1 - \sigma(x))$ .

Learning the model of a distribution. A common metric between distributions is the KL divergence. We therefore might use it to perform stochastic optimization of the parameters  $\theta$  in order to increase the cross-entropy between the two distributions.

$$\theta^* = \underset{\theta}{\operatorname{argmin}} KL\left(P_r \mid\mid P_{\theta}\right) = \underset{\theta}{\operatorname{argmin}} \mathbb{E}_{\mathbf{x} \sim P_r} \left[ \log \left( \frac{P_r\left(\mathbf{x}\right)}{P_{\theta}\left(\mathbf{x}\right)} \right) \right] = \underset{\theta}{\operatorname{argmin}} - \mathbb{E}_{\mathbf{x} \sim P_r} \left[ \log \left( P_{\theta}\left(\mathbf{x}\right) \right) \right]$$
(1)

**Stochastic Optimization.** We start with some random parameters  $\theta^{(0)}$  and for each observed sample  $\mathbf{x}^{(t)}$  we move in the direction opposed to the gradient in order to minimize our cost function.

$$KL(P_r \mid\mid P_{\theta}) \approx \sum_{\mathbf{x} \sim P_r} \log P_{\theta}(\mathbf{x}) \approx \log P_{\theta}(\mathbf{x}^{(t)})$$
 (2)

$$\theta_{X|\mathbf{Y}=\mathbf{y}}^{(t+1)} \leftarrow \theta_{X|\mathbf{Y}=\mathbf{y}}^{(t)} - \eta \cdot \nabla_{\theta_{X|\mathbf{Y}=\mathbf{y}}} \log P_{\theta} \left( \mathbf{X} = \mathbf{x}^{(t)} \right)$$
(3)

Since the joint probability  $P_{\theta}(\mathbf{X})$  is just a product of all CPDs, its logarithm becomes a sum.

$$\log P_{\theta}(\mathbf{X}) = \sum_{X \in \mathbf{X}} \log P_{\theta}(X \mid Par(X))$$
(4)

For some specific parameter  $\theta_{X|\mathbf{Y}=\mathbf{y}}$ :

$$\nabla_{\theta_{X|\mathbf{Y}=\mathbf{y}}} \log P_{\theta} \left( \mathbf{X} = \mathbf{x} \right) = \nabla_{\theta_{X|\mathbf{Y}=\mathbf{y}}} \log P_{\theta} \left( X = x \right) = \begin{cases} \frac{\sigma'(\theta_{X|\mathbf{Y}=\mathbf{y}})}{\sigma(\theta_{X|\mathbf{Y}=\mathbf{y}})} = 1 - \sigma \left( \theta_{X|\mathbf{Y}=\mathbf{y}} \right) & \text{if } x = 1 \\ = x - \sigma \left( \theta_{X|\mathbf{Y}=\mathbf{y}} \right) \\ \frac{-\sigma'(\theta_{X|\mathbf{Y}=\mathbf{y}})}{1 - \sigma(\theta_{X|\mathbf{Y}=\mathbf{y}})} = -\sigma \left( \theta_{X|\mathbf{Y}=\mathbf{y}} \right) & \text{if } x = 0 \end{cases}$$
(5)