

PREDICTIVE DISTRIBUTION ESTIMATION FOR BAYESIAN MACHINE LEARNING USING A DIRICHLET PRIOR

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Overview

- ► In Bayesian treatments of machine learning, the success or failure of the estimator/classifier hinges on how well the prior distribution selected by the designer matches the actual data-generating model
- ► Highly localized Dirichlet priors can overcome the burden of a limited training set when the prior mean is well matched to the true distribution, but will degrade the approximation if the match is poor

Objective

Make inferences about unobservable $y \in \mathcal{Y}$ given observed $x \in \mathcal{X}$ and a training set $D \in \mathcal{D} = \{\mathcal{Y} \times \mathcal{X}\}^N$

▶ Joint elements (y, x) and D_n are distributed by an *unknown* PMF θ :

$$\begin{aligned} \mathbf{P}_{\mathbf{y},\mathbf{x},\mathbf{D}\,|\boldsymbol{\theta}}(\mathbf{y},\mathbf{x},D|\boldsymbol{\theta}) &= \mathbf{P}_{\mathbf{y},\mathbf{x}\,|\boldsymbol{\theta}}(\mathbf{y},\mathbf{x}|\boldsymbol{\theta}) \prod_{n=1}^{N} \mathbf{P}_{\mathbf{D}_{n}\,|\boldsymbol{\theta}}\left(D_{n}|\boldsymbol{\theta}\right) \\ &= \boldsymbol{\theta}(\mathbf{y},\mathbf{x}) \prod_{\mathbf{y}' \in \mathcal{Y}} \prod_{\mathbf{x}' \in \mathcal{X}} \boldsymbol{\theta}(\mathbf{y}',\mathbf{x}')^{\bar{N}(\mathbf{y}',\mathbf{x}';D)} \end{aligned}$$

- ► $P_{D|\theta}$ depends on D only through the transform $\bar{N}(y,x;D) \equiv \sum_{n=1}^{N} \delta \left[(y,x), D_n \right]$
 - \Rightarrow Random process $\bar{n} \equiv \bar{N}(D) \in \bar{\bar{N}}$ is a <u>sufficient statistic</u> for θ ; decisions can depend on \bar{n} in place of D

Design a decision function $f: \overline{\mathcal{N}} \mapsto \mathcal{H}^{\mathcal{X}}$, where \mathcal{H} is the decision space.

The metric is a loss function $\mathcal{L}: \mathcal{H} \times \mathcal{Y} \mapsto \mathbb{R}_{>0}$.

Clairvoyant Risk:

$$\mathcal{R}_{\theta}(\mathit{f}) = E_{x,\bar{n}\,|\theta} \left[\left. E_{y\,|\,x,\theta} \left[\left. \mathcal{L}\left(\mathit{f}(x;\bar{n}),y\right) \right] \right] \right]$$

 \Rightarrow Optimal decisions depend on the *true predictive* distribution, $P_{y|x,\theta} = \theta(\cdot,x)/\sum_{y \in \mathcal{Y}} \theta(y,x) \equiv \tilde{\theta}(x)$

\Downarrow \Downarrow Select Prior \mathbf{p}_{θ} \Downarrow \Downarrow

Bayes Risk:

$$\mathcal{R}(f) = E_{\theta} \left[\left. \mathcal{R}_{\theta} \left(f(\mathbf{x}; \bar{\mathbf{n}}) \right) \right] = E_{\mathbf{x}, \bar{\mathbf{n}}} \left[\left. E_{\mathbf{y} \, | \, \mathbf{x}, \bar{\mathbf{n}}} \left[\, \mathcal{L} \left(f(\mathbf{x}; \bar{\mathbf{n}}), \mathbf{y} \, \right) \right] \right] \right]$$

 \Rightarrow Decisions formulated using *Bayes predictive distribution*, $P_{y|x,\bar{n}} = E_{\theta|x,\bar{n}} \left[P_{y|x,\theta} \right] = \mu_{\tilde{\theta}(x)|x,\bar{n}}$

Bayesian Prediction

Dirichlet Priors:

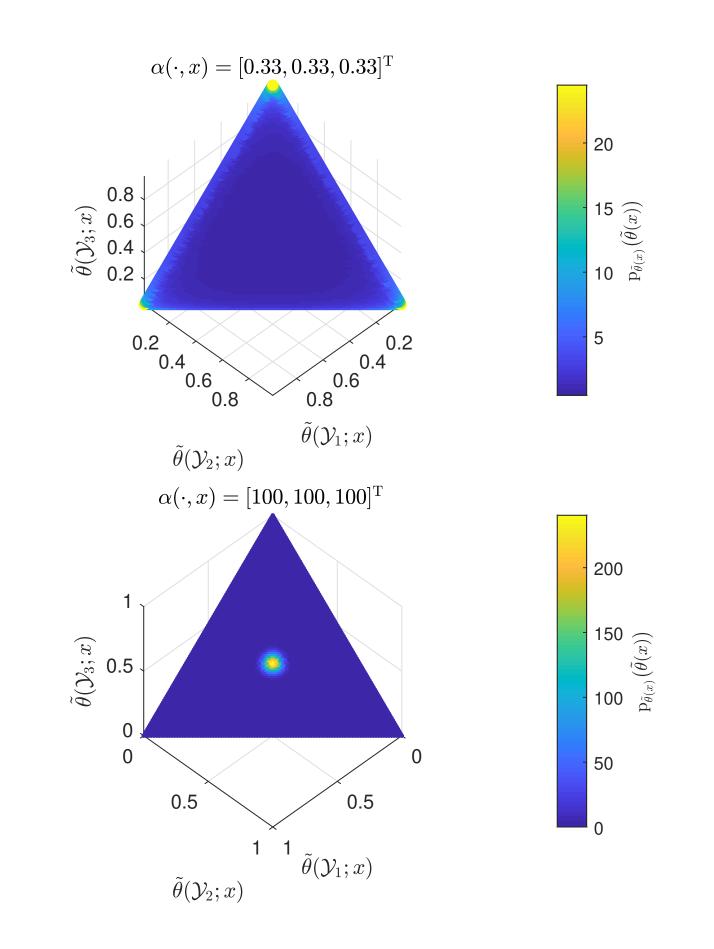
$$p_{\theta}(\theta) = \text{Dir}(\theta; \alpha)$$

$$= \beta(\alpha)^{-1} \prod_{y \in \mathcal{Y}} \prod_{x \in \mathcal{X}} \theta(y, x)^{\alpha(y, x) - 1}$$

$$\downarrow \downarrow$$

$$p_{\tilde{\theta}}(\tilde{\theta}) = \prod_{x \in \mathcal{X}} Dir(\tilde{\theta}(x); \alpha(\cdot, x))$$

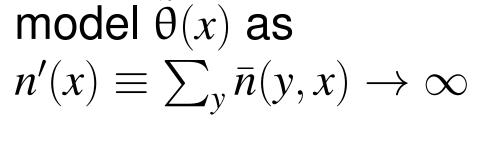
- Concentration parameters $\alpha'(x) \equiv \sum_{y \in \mathcal{Y}} \alpha(y, x)$ enable both subjective and non-informative priors
- Conjugate Prior for I.I.D. observations ⇒ Tractable Posterior

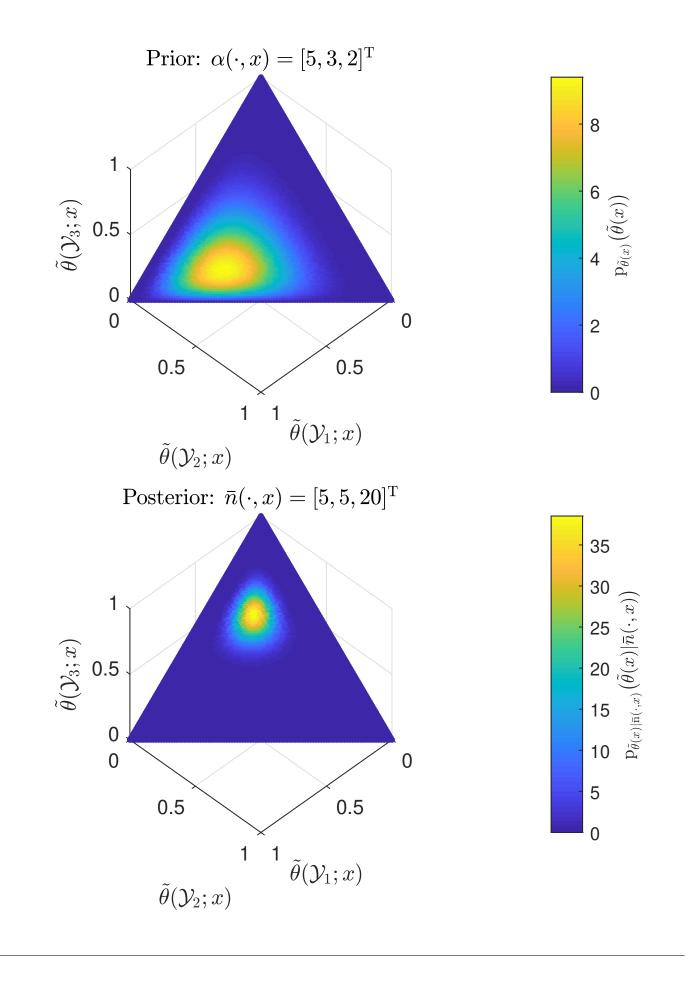


Dirichlet Posteriors:

$$\begin{aligned} & p_{\tilde{\theta}|x,\bar{n}}(\tilde{\theta}|x,\bar{n}) = p_{\tilde{\theta}|\bar{n}}(\tilde{\theta}|\bar{n}) \\ & = \prod_{x' \in \mathcal{X}} p_{\tilde{\theta}(x')|\bar{n}(\cdot,x')} \left(\tilde{\theta}(x')|\bar{n}(\cdot,x') \right)) \\ & = \prod_{x' \in \mathcal{X}} \text{Dir} \left(\tilde{\theta}(x'); \alpha(\cdot,x') + \bar{n}(\cdot,x') \right) \end{aligned}$$

Full support over distribution space ensures identification of model $\tilde{\theta}(x)$ as





Bayes Predictive Distribution:

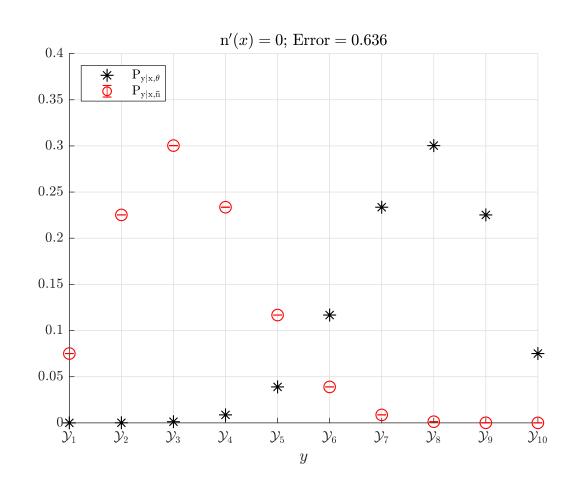
$$P_{y \mid x, \bar{n}} = \left(\frac{\alpha'(x)}{\alpha'(x) + \sum_{y} \bar{n}(y, x)}\right) \frac{\alpha(\cdot, x)}{\alpha'(x)} + \left(\frac{\sum_{y} \bar{n}(y, x)}{\alpha'(x) + \sum_{y} \bar{n}(y, x)}\right) \frac{\bar{n}(\cdot, x)}{\sum_{y} \bar{n}(y, x)}$$

- ⇒ Convex combination of data-independent PMF and conditional empirical PMF
- $\Rightarrow E_{\bar{n}\,|\,n',\theta}\,\big[\,P_{y\,|\,x,\bar{n}}\,\big] = \left(\frac{\alpha'(x)}{\alpha'(x)+n'(x)}\right)\frac{\alpha(\cdot,x)}{\alpha'(x)} + \left(\frac{n'(x)}{\alpha'(x)+n'(x)}\right)\tilde{\theta}(x)$

Density Estimation

* Density estimation accuracy assessed using the *Estimation Difference Function*:





$$Bias(x,n',\theta) = E_{\bar{n}\,|\,n',\theta}\left[\Delta(x,\bar{n},\theta)\right] = \frac{\alpha'(x)}{\alpha'(x) + n'(x)} \left(\frac{\alpha(\cdot,x)}{\alpha'(x)} - \tilde{\theta}(x)\right)$$

$$\begin{split} Cov(y,y';x,n',\theta) &= C_{\bar{n}\,|\,n',\theta} \left[\left. P_{y\,|\,x,\bar{n}}(\cdot|\,x,\bar{n}) \right](y,y') \right. \\ &= \frac{n'(x)}{\left(\alpha'(x) + n'(x)\right)^2} \left(\tilde{\theta}(y;x) \delta[y,y'] - \tilde{\theta}(y;x) \tilde{\theta}(y';x) \right) \end{split}$$

* Concentration parameter controls a Bias-Variance trade-off

Error =
$$\sqrt{\sum_{y \in \mathcal{Y}} \mathcal{E}(y, y; x, n', \theta)}$$

