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Bayesian Learning for Regression using Dirichlet Prior Distributions of Varying Localization

Paul Rademacher[1] **Miloš Doroslovački**[2]

[1] U.S. Naval Research Laboratory
Radar Division

[2] The George Washington University
Department of Electrical and Computer Engineering

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Introduction

Bayesian Learning

Bayesian approaches to statistical learning attempt to make better decisions by exploiting prior knowledge regarding the data-generating distribution:

Informative

- If the prior is localized around the true data-generating model, low-risk decisions can be made even with limited training data
- Priors that assign low weighting to the true model may not be able to realize satisfactory performance

Non-Informative

- Learners designed with minimally localized priors respond strongly to training data, avoiding the drawbacks of misinformed prior knowledge
- If the data volume is limited, high variance “overfit” solutions can occur

The Dirichlet Prior

Dirichlet prior distributions have a number of desirable properties:

- Full support over the space of data-generating distributions, guaranteeing *consistent estimation* of the true data model
- They are conjugate priors for independent, identically distributed observations[1], leading to *closed-form* posterior distributions
- Flexible parameterization enabling *both* maximally and minimally informative priors and thus a wide range of learning solutions

[1] Thomas S. Ferguson. “A Bayesian Analysis of Some Nonparametric Problems”. In: *The Annals of Statistics* (1973).

Data Model and Regression Objective

Data Representation

Observable random variable: $\mathrm{x} \in \mathcal{X} \subset \mathbb{R}$
Unobservable random variable: $\mathrm{y} \in \mathcal{Y} \subset \mathbb{R}$
Observable training data: $\mathrm{D} \in \mathcal{D} = \{\mathcal{Y} \times \mathcal{X}\}^N$

Independently, identically distributed according to an unknown probability mass function (PMF)

$$\theta \in \Theta = \left\{ \theta \in \mathbb{R}_{\geq 0}{}^{\mathcal{Y} \times \mathcal{X}} : \sum_{y \in \mathcal{Y}} \sum_{x \in \mathcal{X}} \theta(y, x) = 1 \right\} ,$$

such that $\mathrm{P}_{\mathrm{y,x}\,|\,\theta}(y, x|\theta) = \mathrm{P}_{\mathrm{D}_n\,|\,\theta}(y, x|\theta) = \theta(y, x)$.

Alternate Notation: $\theta \Leftrightarrow \left(\theta_{\mathrm{m}}, \theta_{\mathrm{c}} \right)$

- Marginal model $\theta_{\mathrm{m}} \equiv \sum_{y \in \mathcal{Y}} \theta(y, \cdot) \equiv \mathrm{P}_{\mathrm{x}\,|\,\theta_{\mathrm{m}}} \equiv \mathrm{P}_{\mathrm{x}\,|\,\theta}$
- Conditional models $\theta_{\mathrm{c}}(\mathrm{x}) \equiv \theta(\cdot, \mathrm{x}) / \theta_{\mathrm{m}}(\mathrm{x}) \equiv \mathrm{P}_{\mathrm{y}\,|\,\mathrm{x},\theta_{\mathrm{c}}} \equiv \mathrm{P}_{\mathrm{y}\,|\,\mathrm{x},\theta}$

Sufficient Statistic

Transform

Using the i.i.d. assumption,

$$\mathrm{P}_{\mathrm{D}\,|\,\theta}\left(D|\theta\right) = \left(\prod_{y\in\mathcal{Y}}\prod_{x\in\mathcal{X}}\theta(y,x)^{\Psi(y,x;D)}\right)^{N}$$

where data are represented using $\Psi : \mathcal{D} \mapsto \Psi \subset \Theta$, defined as

$$\Psi(y,x;D) = N^{-1}\sum_{n=1}^{N}\delta\big[(y,x),D_n\big] \ .$$

- Empirical distribution $\Psi(\mathrm{D})$ is a sufficient statistic[2] for the model θ
- Efficient: $|\Psi| = \binom{N+|\mathcal{Y}||\mathcal{X}|-1}{|\mathcal{Y}||\mathcal{X}|-1} \leq |\mathcal{D}|$

$\Rightarrow$ **Represent data using new random process $\psi \equiv \Psi(\mathrm{D}) \in \Psi$**

[2] Bernardo et al., *Bayesian Theory*.

Sufficient Statistic

Distribution

- Conditioned on the true model, the data statistic is an "Empirical" random process $\psi|\theta \sim \mathrm{Emp}(N, \theta)$
  - Equivalent to a normalized multinomial random process[3]
- As $N \to \infty$, the random process converges to $\psi|\theta \xrightarrow{p} \theta$
  - $\Rightarrow$ Use enables consistent estimation of model

Alternate Notation: $\psi \Leftrightarrow (\psi_\mathrm{m}, \psi_\mathrm{c})$

- Marginal $\psi_\mathrm{m} \equiv \sum_{y \in \mathcal{Y}} \psi(y, \cdot)$
- Conditional $\psi_\mathrm{c}(x) \equiv \psi(\cdot, x) / \psi_\mathrm{m}(x)$

By the aggregation property [4],

- $\psi_\mathrm{m} \,|\, \theta_\mathrm{m} \sim \mathrm{Emp}(N, \theta_\mathrm{m})$
- $\psi_\mathrm{c}(x) | \, \psi_\mathrm{m}(x), \theta_\mathrm{c}(x) \sim \mathrm{Emp}\left(N \, \psi_\mathrm{m}(x), \theta_\mathrm{c}(x)\right)$ are mutually independent

[3] Thomas P. Minka. *Bayesian inference, entropy, and the multinomial distribution*. Tech. rep. Microsoft Research, 2003.

[4] Johnson et al., *Discrete Multivariate Distributions*.

Objective

- Design a regression function $f : \Psi \mapsto \mathbb{R}^{\mathcal{X}}$ to minimize the expected squared-error with respect to θ:

$$\mathcal{R}_{\Theta}(f;\theta) = \mathrm{E}_{y,x,\psi|\theta}\left[\left(f(x;\psi) - y\right)^2\right] \equiv \underbrace{\mathrm{E}_{x\,|\,\theta_m}\left[\Sigma_{y\,|\,x,\theta_c}\right]}_{\mathcal{R}^*_{\Theta}(\theta)} + \underbrace{\mathrm{E}_{x,\psi|\theta}\left[\left(f(x;\psi) - \mu_{y\,|\,x,\theta_c}\right)^2\right]}_{\mathcal{R}_{\Theta,\mathrm{ex}}(f;\theta)}$$

- Clairvoyant[5] regressor $f_{\Theta}(x;\theta_c) = \mu_{y\,|\,x,\theta_c}$ achieves *irreducible* squared-error $\mathcal{R}^*_{\Theta}(\theta)$
- Excess squared-error can be decomposed into bias and variance terms:

$$\mathcal{R}_{\Theta,\mathrm{ex}}(f;\theta) \equiv \mathrm{E}_{x\,|\,\theta_m}\left[\left(\mathrm{E}_{\psi|\theta}\left[f(x;\psi)\right] - f_{\Theta}(x;\theta_c)\right)^2 + \mathrm{C}_{\psi|\theta}\left[f(x;\psi)\right]\right]$$

[5] Steven M. Kay. *Fundamentals of Statistical Signal Processing: Detection Theory*. Vol. 2. Prentice-Hall, 1998.

Bayesian Inference

Model unknown. Select prior p_θ and formulate Bayesian risk:

$$\mathcal{R}(f) = \mathrm{E}_\theta\left[\mathcal{R}_\Theta(f;\theta)\right] = \mathrm{E}_{\mathrm{y},\mathrm{x},\psi}\left[\left(f(\mathrm{x};\psi) - \mathrm{y}\right)^2\right]$$

$$\Downarrow \quad \Downarrow \quad \Downarrow \quad \Downarrow$$

Bayes optimal regressor:

$$f^*(\mathrm{x};\psi) = \arg\min_{y' \in \mathbb{R}} \mathrm{E}_{\mathrm{y}\,|\,\mathrm{x},\psi}\left[(y' - \mathrm{y})^2\right] = \mu_{\mathrm{y}\,|\,\mathrm{x},\psi}$$

- Observe that $\mathrm{P}_{\mathrm{y}\,|\,\mathrm{x},\psi} = \mathrm{E}_{\theta|\,\mathrm{x},\psi}\left[\mathrm{P}_{\mathrm{y}\,|\,\mathrm{x},\theta}\right] \equiv \mu_{\theta_c(\mathrm{x})|\,\mathrm{x},\psi}$

Bayesian distribution is the posterior mean[6] of the predictive model θ_c

[6] Kevin P. Murphy. *Binomial and multinomial distributions*. Tech. rep. University of British Columbia, 2006.

Distributions: Prior to Predictive

Dirichlet Prior

The probability density function of the model $\theta \in \Theta$ is Dirichlet:

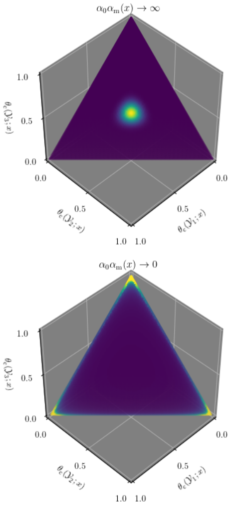
$$\mathrm{p}_\theta(\theta) = \mathrm{Dir}(\theta; \alpha_0, \alpha) \equiv \beta(\alpha_0 \alpha)^{-1} \prod_{y \in \mathcal{Y}} \prod_{x \in \mathcal{X}} \theta(y, x)^{\alpha_0 \alpha(y,x) - 1}$$

- Parameter α_0 controls localization around mean α

Alternate Notation:

- Marginal $\alpha_\mathrm{m} \equiv \sum_{y \in \mathcal{Y}} \alpha(y, \cdot)$
- Conditional $\alpha_\mathrm{c}(x) \equiv \alpha(\cdot, x) / \alpha_\mathrm{m}(x)$

∗ By the aggregation property[7], $\theta_\mathrm{m} \sim \mathrm{Dir}(\alpha_0, \alpha_\mathrm{m})$ and $\theta_\mathrm{c}(x) \sim \mathrm{Dir}\left(\alpha_0\, \alpha_\mathrm{m}(x), \alpha_\mathrm{c}(x)\right)$ are mutually independent



[7] Ferguson, "A Bayesian Analysis of Some Nonparametric Problems".

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Predictive Model Posterior

Closed-Form

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Since $\perp\!\!\!\perp_x \theta_c(x)$ and $\theta_c \perp\!\!\!\perp \theta_m$, and since the Empirical process $\theta_c(x) | \psi_m(x), \psi_c(x)$ has exponential form, Dirichlet process $\theta_c(x)$ is conjugate[8] and thus

$$\theta_c(x) | \psi_m(x), \psi_c(x) \sim \mathrm{Dir}\left(\alpha_0\, \alpha_m(x) + N\, \psi_m(x), \mu_{\theta_c(x) | \psi_m(x), \psi_c(x)}\right) ,$$

with mean functions

$$\mu_{\theta_c(x) | \psi_m(x), \psi_c(x)} = \gamma(x; \psi_m)\, \alpha_c(x) + \big(1 - \gamma(x; \psi_m)\big)\, \psi_c(x) \equiv \color{red}{\mathrm{P}_{y\,|\,x,\psi}} ,$$

where $\gamma(x; \psi_m) = \Big(1 + N\, \psi_m(x) / \big(\alpha_0\, \alpha_m(x)\big)\Big)^{-1} \in (0, 1]$.

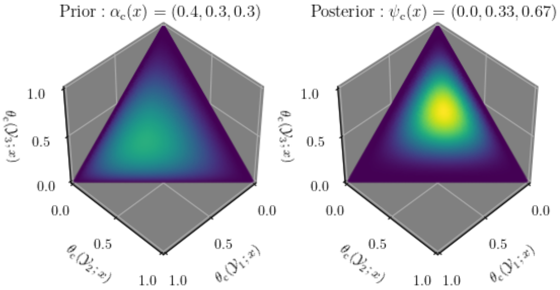
Bayesian predictions mix prior mean α_c with empirical distribution ψ_c

[8] Sergios Theodoridis. *Machine Learning: A Bayesian and Optimization Perspective*. Elsevier, 2015.

Predictive Model Posterior

Trends

- As localization α_0 increases, $\theta_c(x) \mid \psi_m(x), \psi_c(x) \xrightarrow{p} \alpha_c(x)$ and the prior is emphasized
- As training volume N increases, $\theta_c(x) \mid \psi_m(x), \psi_c(x) \xrightarrow{p} \psi_c(x)$ and data is emphasized
  - * Since $\psi_c \mid \theta_c \xrightarrow{p} \theta_c$, the true predictive model is identified



Full support prior ensures consistent estimation of model

Bayes Optimal Regressor

Regressor: $f^*(\mathrm{x};\psi) \equiv \gamma(\mathrm{x};\psi_\mathrm{m})\mu_{\mathrm{y}\,|\,\mathrm{x}} + \left(1-\gamma(\mathrm{x};\psi_\mathrm{m})\right) \sum_{y\in\mathcal{Y}} \psi_\mathrm{c}(y;\mathrm{x})\; y$

- ∗ Convexly combines first moment of $\mathrm{P}_{\mathrm{y}\,|\,\mathrm{x}} = \mu_{\theta_\mathrm{c}(\mathrm{x})} = \alpha_\mathrm{c}(\mathrm{x})$ with empirical mean
- ∗ Inherits trends from posterior distribution, allowing maximal or minimal confidence in the prior

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Excess SE: $\mathcal{R}_{\Theta,\mathrm{ex}}(f^*;\theta) \equiv \mathrm{E}_{\mathrm{x}\,|\,\theta_\mathrm{m}}\left[\lambda_{\text{Bias}}(\mathrm{x};\theta_\mathrm{m})\left(\mu_{\mathrm{y}\,|\,\mathrm{x}} - \mu_{\mathrm{y}\,|\,\mathrm{x},\theta_\mathrm{c}}\right)^2 + \lambda_{\text{Var}}(\mathrm{x};\theta_\mathrm{m})\Sigma_{\mathrm{y}\,|\,\mathrm{x},\theta_\mathrm{c}}\right]$

- ∗ $\lambda_{\text{Bias}}(x;\theta_\mathrm{m}) = \mathrm{E}_{\psi_\mathrm{m}\,|\,\theta_\mathrm{m}}\left[\gamma(x;\psi_\mathrm{m})^2\right]$ and $\lambda_{\text{Var}}(x;\theta_\mathrm{m}) = \mathrm{E}_{\psi_\mathrm{m}\,|\,\theta_\mathrm{m}}\left[\frac{\left(1-\gamma(x;\psi_\mathrm{m})\right)^2}{N\,\psi_\mathrm{m}(x)}\right]$

- Bias: proportionate to squared-difference between data-independent regressor $\mu_{\mathrm{y}\,|\,\mathrm{x}}$ and clairvoyant regressor
- Variance: proportionate to the predictive variance, adding to the irreducible risk

Trends and Results

Example

Data Model:

- $\mathcal{X} = \mathcal{Y} = \{i/127 : i = 0, \ldots, 127\}$
- $\theta_{\mathrm{m}} = |\,\mathcal{X}\,|^{-1}$
- Clairvoyant: $\mu_{\mathrm{y}\,|\,\mathrm{x},\theta_{\mathrm{c}}} = 1/\big(2 + \sin(2\pi\,\mathrm{x}\,)\big)$
- $\Sigma_{\mathrm{y}\,|\,\mathrm{x},\theta} = 0.2\,\mu_{\mathrm{y}\,|\,\mathrm{x},\theta}(1 - \mu_{\mathrm{y}\,|\,\mathrm{x},\theta})$
  $\Rightarrow\ \mathcal{R}^*_{\Theta}(\theta) \approx 0.039$

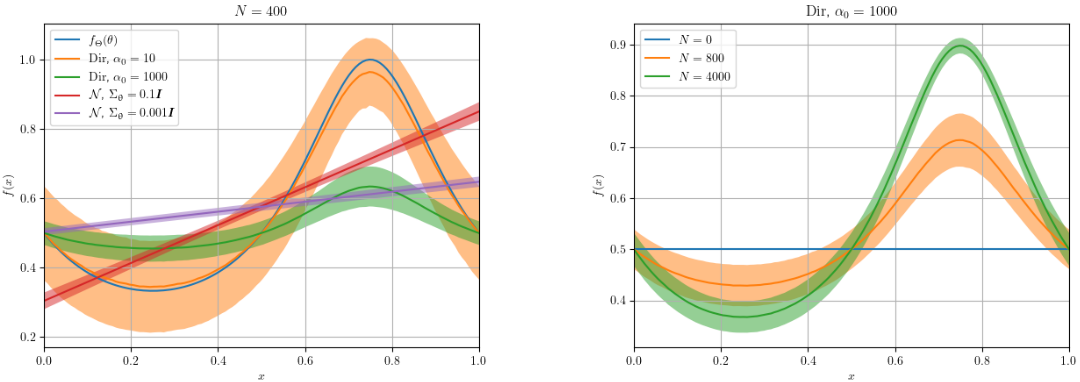
Learners:

- Dirichlet:
  - $\alpha_{\mathrm{m}} = |\,\mathcal{X}\,|^{-1}$
  - Prior $\mu_{\mathrm{y}\,|\,\mathrm{x}} = 0.5$
- Normal[9]:
  - $\mathrm{y}\,|\,\mathrm{x},\theta \sim \mathcal{N}\big([1,\mathrm{x}]\theta, 0.1\big)$
  - $\theta \sim \mathcal{N}\big([0.5, 0], \Sigma_{\theta}\big)$

- *Prior confidence* of Dirichlet and Normal learners varied using α_0 and Σ_θ
- Both learners effect the same biased untrained regressor to approximate the non-linear clairvoyant regressor

[9] Theodoridis, *Machine Learning: A Bayesian and Optimization Perspective*.

Prediction Statistics



- Lines show bias $\mathrm{E}_{\psi|\theta}\left[\mu_{\mathrm{y}\,|\,\mathrm{x},\psi}\right]$, fill regions shows variance $\mathrm{C}_{\psi|\theta}\left[\mu_{\mathrm{y}\,|\,\mathrm{x},\psi}\right]$
- Python simulation results average 50,000 learning iterations

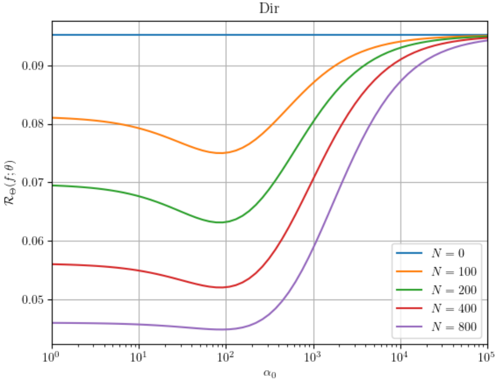
Optimal Localization

For a given conditional mean α_c, localization $\bar{\alpha}_0(x) \equiv \alpha_0\, \alpha_m(x)$ controls a Bias-Variance trade-off:

$\bar{\alpha}_0(x)$	$\lambda_{\text{Bias}}(x;\theta_m)$	$\lambda_{\text{Var}}(x;\theta_m)$
$\to \infty$	1	0
$\to 0$	$\left(1-\theta_m(x)\right)^N$	$\mathrm{E}_{\psi_m \mid \theta_m}\left[\left(N\,\psi_m(x)\right)^{-1}\right]$

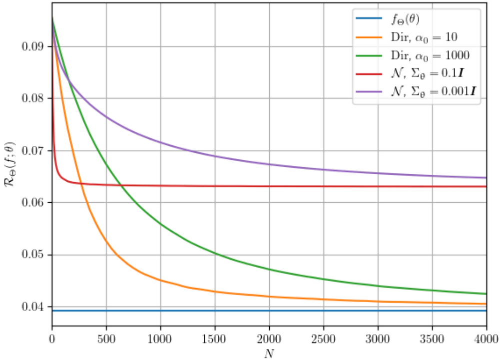
Optimal:

$$\bar{\alpha}_0(\mathrm{x}) = \frac{\Sigma_{\mathrm{y}\mid \mathrm{x},\theta_c}}{\left(\mu_{\mathrm{y}\mid \mathrm{x}} - \mu_{\mathrm{y}\mid \mathrm{x},\theta_c}\right)^2}$$



Training Volume Trends

- As $N \to \infty$, both $\lambda_{\text{Bias}}(x;\theta_{\mathrm{m}}) \to 0$ and $\lambda_{\text{Var}}(x;\theta_{\mathrm{m}}) \to 0$
  $\Rightarrow \ \mathcal{R}_{\Theta,\mathrm{ex}}(f^*;\theta) \to 0$ for any model θ
- Note that $f^*(\mathrm{x};\psi)$ converges to the clairvoyant regressor regardless of how biased the prior conditional mean α_{c} is, or how much confidence in α_{c} is indicated through the localization α_0



Conclusions

Summary

Full-support Bayesian learning with a Dirichlet prior enables:

- Asymptotically optimal performance for data-rich applications
- Maximal prior knowledge required for data-limited applications

Future Work

- Generalize these concepts for more general data models using the continuous Dirichlet process[10]
  - Practical necessity motivates the use of discretization to realize the demonstrated benefits
- Use the Dirichlet prior with different likelihood functions (e.g., mixture model) to effect limited-support priors that may be best suited for data-limited applications

[10] Samuel J. Gershman et al. “A tutorial on Bayesian nonparametric models”. In: *Journal of Mathematical Psychology* 56 (2012).