SC4/SM8 Advanced Topics in Statistical Machine Learning

Chapter 6: Bayesian Learning

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https://github.com/ywteh/advml2020

The Bayesian Learning Framework

- Bayesian learning: **treat parameter vector θ as a random variable**: process of learning is then **computation of the posterior distribution** $p(\theta|\mathcal{D})$.
- In addition to the likelihood $p(\mathcal{D}|\theta)$ need to specify a **prior distribution** $p(\theta)$.
- Posterior distribution is then given by the **Bayes Theorem**:

$$p(\theta|\mathcal{D}) = \frac{p(\mathcal{D}|\theta)p(\theta)}{p(\mathcal{D})}$$

- **Likelihood**: $p(\mathcal{D}|\theta)$
- **Prior**: $p(\theta)$
- **Posterior**: $p(\theta|\mathcal{D})$
- **Marginal likelihood**: $p(\mathcal{D}) = \int_\Theta p(\mathcal{D}|\theta)p(\theta)d\theta$

- Summarizing the posterior:
  - **Posterior mode**: $\widehat{\theta}^{\text{MAP}} = \operatorname{argmax}_{\theta\in\Theta} p(\theta|\mathcal{D})$ (maximum a posteriori).
  - **Posterior mean**: $\widehat{\theta}^{\text{mean}} = \mathbb{E}\left[\theta|\mathcal{D}\right]$.
  - **Posterior variance**: $\mathrm{Var}[\theta|\mathcal{D}]$.

Bayesian Inference on the Categorical Distribution

- Suppose we observe the with $y_i \in \{1, \ldots, K\}$, and model them as i.i.d. with pmf $\pi = (\pi_1, \ldots, \pi_K)$:

$$p(\mathcal{D}|\pi) = \prod_{i=1}^{n} \pi_{y_i} = \prod_{k=1}^{K} \pi_k^{n_k}$$

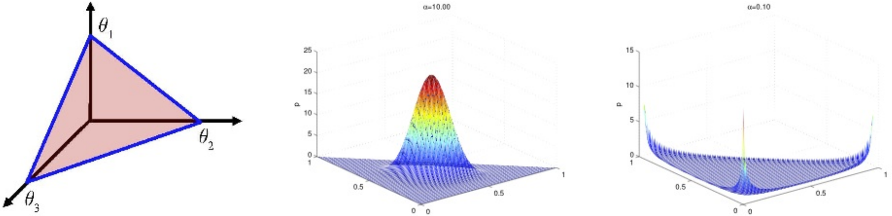
  with $n_k = \sum_{i=1}^{n} \mathbf{1}(y_i = k)$ and $\pi_k > 0$, $\sum_{k=1}^{K} \pi_k = 1$.
- The conjugate prior on π is the Dirichlet distribution $\mathrm{Dir}(\alpha_1, \ldots, \alpha_K)$ with parameters $\alpha_k > 0$, and density

$$p(\pi) = \frac{\Gamma(\sum_{k=1}^{K} \alpha_k)}{\prod_{k=1}^{K} \Gamma(\alpha_k)} \prod_{k=1}^{K} \pi_k^{\alpha_k - 1}$$

  on the probability simplex $\{\pi : \pi_k > 0, \sum_{k=1}^{K} \pi_k = 1\}$.
- The posterior is also Dirichlet $\mathrm{Dir}(\alpha_1 + n_1, \ldots, \alpha_K + n_K)$.
- Posterior mean is

$$\widehat{\pi}_k^{\text{mean}} = \frac{\alpha_k + n_k}{\sum_{j=1}^{K} \alpha_j + n_j}.$$

Dirichlet Distributions



(A) Support of the Dirichlet density for $K = 3$.
(B) Dirichlet density for $\alpha_k = 10$.
(C) Dirichlet density for $\alpha_k = 0.1$.

Naïve Bayes

- Consider the classification example with **naïve Bayes classifier**:

$$p(x_i|\phi_k) = \prod_{j=1}^{p} \phi_{kj}^{x_i^{(j)}} (1-\phi_{kj})^{1-x_i^{(j)}}.$$

- Set $n_k = \sum_{i=1}^n \mathbf{1}\{y_i = k\}$, $n_{kj} = \sum_{i=1}^n \mathbf{1}\{y_i = k, x_i^{(j)} = 1\}$. MLEs are:

$$\hat{\pi}_k = \frac{n_k}{n}, \qquad \hat{\phi}_{kj} = \frac{\sum_{i:y_i=k} x_i^{(j)}}{n_k} = \frac{n_{kj}}{n_k}.$$

- A problem: if the ℓ-th word did not appear in documents labelled as class k then $\hat{\phi}_{k\ell} = 0$ and

$$\mathbb{P}(Y = k|X = x \text{ with } \ell\text{-th entry equal to } 1) \propto \hat{\pi}_k \prod_{j=1}^{p} \left(\hat{\phi}_{kj}\right)^{x^{(j)}} \left(1-\hat{\phi}_{kj}\right)^{1-x^{(j)}} = 0$$

  i.e. we will never attribute a new document containing word ℓ to class k (regardless of other words in it).

Bayesian Inference on Naïve Bayes model

- Under the Naïve Bayes model, the joint distribution of labels $y_i \in \{1, \ldots, K\}$ and data vectors $x_i \in \{0, 1\}^p$ is

$$p(\mathcal{D}|\theta) = \prod_{i=1}^{n} p(x_i, y_i|\theta) = \prod_{i=1}^{n} \prod_{k=1}^{K} \left(\pi_k \prod_{j=1}^{p} \phi_{kj}^{x_i^{(j)}} (1 - \phi_{kj})^{1 - x_i^{(j)}} \right)^{\mathbf{1}(y_i = k)}$$
$$= \prod_{k=1}^{K} \pi_k^{n_k} \prod_{j=1}^{p} \phi_{kj}^{n_{kj}} (1 - \phi_{kj})^{n_k - n_{kj}}$$

  where $n_k = \sum_{i=1}^{n} \mathbf{1}(y_i = k)$, $n_{kj} = \sum_{i=1}^{n} \mathbf{1}(y_i = k, x_i^{(j)} = 1)$.
- For conjugate prior, we can use $\mathrm{Dir}((\alpha_k)_{k=1}^{K})$ for π, and $\mathrm{Beta}(a, b)$ for ϕ_{kj} independently.
- Because the likelihood factorises, the posterior distribution over π and (ϕ_{kj}) also factorises, and posterior for π is $\mathrm{Dir}((\alpha_k + n_k)_{k=1}^{K})$, and for ϕ_{kj} is $\mathrm{Beta}(a + n_{kj}, b + n_k - n_{kj})$.

Bayesian Inference on Naïve Bayes model

- Given $\mathcal{D} = \{(x_i, y_i)\}_{i=1}^n$, want to predict a label $\tilde{y}$ for a new document $\tilde{x}$. We can calculate

$$p(\tilde{x}, \tilde{y} = k|\mathcal{D}) = p(\tilde{y} = k|\mathcal{D})p(\tilde{x}|\tilde{y} = k, \mathcal{D})$$

with

$$p(\tilde{y} = k|\mathcal{D}) = \frac{\alpha_k + n_k}{\sum_{l=1}^K \alpha_l + n}, \quad p(\tilde{x}^{(j)} = 1|\tilde{y} = k, \mathcal{D}) = \frac{a + n_{kj}}{a + b + n_k}.$$

- Predicted class is

$$\begin{aligned} p(\tilde{y} = k|\tilde{x}, \mathcal{D}) &= \frac{p(\tilde{y} = k|\mathcal{D})p(\tilde{x}|\tilde{y} = k, \mathcal{D})}{p(\tilde{x}|\mathcal{D})} \\ &\propto \frac{\alpha_k + n_k}{\sum_{l=1}^K \alpha_l + n} \prod_{j=1}^p \left(\frac{a + n_{kj}}{a + b + n_k}\right)^{\tilde{x}^{(j)}} \left(\frac{b + n_k - n_{kj}}{a + b + n_k}\right)^{1-\tilde{x}^{(j)}} \end{aligned}$$

- Compared to ML plug-in estimator, pseudocounts help to "regularize" probabilities away from extreme values.

Bayesian Learning and Regularisation

- Consider a Bayesian approach to logistic regression: introduce a multivariate normal prior for weight vector $w \in \mathbb{R}^p$, and a uniform (improper) prior for offset $b \in \mathbb{R}$. The prior density is:

$$p(b, w) = 1 \cdot (2\pi\sigma^2)^{-\frac{p}{2}} \exp\left(-\frac{1}{2\sigma^2}\|w\|_2^2\right)$$

- The posterior is

$$p(b, w|\mathcal{D}) \propto \exp\left(-\frac{1}{2\sigma^2}\|w\|_2^2 - \sum_{i=1}^{n} \log(1 + \exp(-y_i(b + w^\top x_i)))\right)$$

- The posterior mode is equivalent to minimising the L_2-regularised empirical risk.
- Regularised empirical risk minimisation is (often) equivalent to having a prior and finding a MAP estimate of the parameters.
  - L_2 regularisation - multivariate normal prior.
  - L_1 regularisation - multivariate Laplace prior.
- From a Bayesian perspective, the MAP parameters are just one way to summarise the posterior distribution.

Bayesian Model Selection

- A model $\mathcal{M}$ with a given set of parameters $\theta_{\mathcal{M}}$ consists of both the likelihood $p(\mathcal{D}|\theta_{\mathcal{M}})$ and the prior distribution $p(\theta_{\mathcal{M}})$.
- The posterior distribution

$$p(\theta_{\mathcal{M}}|\mathcal{D},\mathcal{M}) = \frac{p(\mathcal{D}|\theta_{\mathcal{M}},\mathcal{M})p(\theta_{\mathcal{M}}|\mathcal{M})}{p(\mathcal{D}|\mathcal{M})}$$

- Marginal probability of the data under $\mathcal{M}$ (**Bayesian model evidence**):

$$p(\mathcal{D}|\mathcal{M}) = \int_{\Theta} p(\mathcal{D}|\theta_{\mathcal{M}},\mathcal{M})p(\theta_{\mathcal{M}}|\mathcal{M})d\theta$$

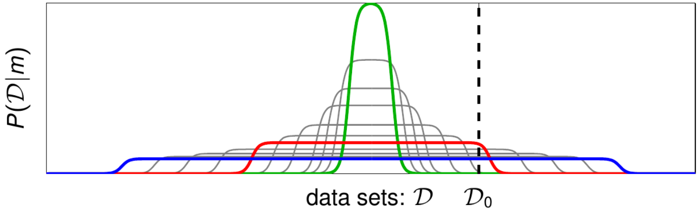
- Compare models using their **Bayes factors** $\frac{p(\mathcal{D}|\mathcal{M})}{p(\mathcal{D}|\mathcal{M}')}$

Bayesian Occam's Razor

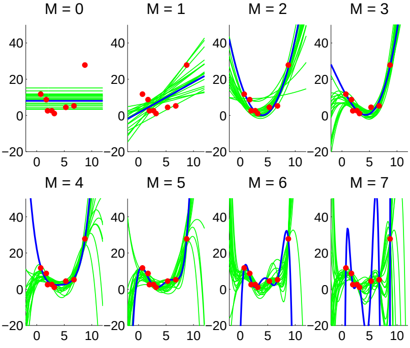
- **Occam's Razor**: of two explanations adequate to explain the same set of observations, the simpler should be preferred.

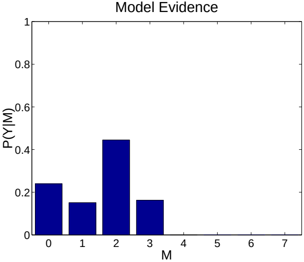
$$p(\mathcal{D}|\mathcal{M}) = \int_{\Theta} p(\mathcal{D}|\theta_{\mathcal{M}}, \mathcal{M}) p(\theta_{\mathcal{M}}|\mathcal{M}) d\theta$$

- Model evidence $p(\mathcal{D}|\mathcal{M})$ is the probability that a set of randomly selected parameter values inside the model would generate dataset $\mathcal{D}$.
- Models that are too simple are unlikely to generate the observed dataset.
- Models that are too complex can generate many possible dataset, so again, they are unlikely to generate that particular dataset at random.



Bayesian model comparison: Occam's razor at work





figures by M.Sahani

Bayesian computation

Most posteriors are intractable, and posterior approximations need to be used.

- **Laplace approximation**.
- Variational methods (**variational Bayes**, expectation propagation).
- Monte Carlo methods (MCMC and SMC).
- Approximate Bayesian Computation (ABC).

Bayesian Learning – Discussion

- Use probability distributions to reason about uncertainties of parameters (latent variables and parameters are treated in the same way).
- Model consists of the likelihood function **and** the prior distribution on parameters: allows to integrate prior beliefs and domain knowledge.
- Prior usually has hyperparameters, i.e., $p(\theta) = p(\theta|\psi)$. How to choose ψ?
  - Be Bayesian about ψ as well — choose a hyperprior $p(\psi)$ and compute $p(\psi|\mathcal{D})$: integrate the predictive posterior over hyperparameters.
  - Maximum Likelihood II — $\hat{\psi} = \mathrm{argmax}_{\psi \in \Psi}\, p(\mathcal{D}|\psi)$.

$$p(\mathcal{D}|\psi) = \int p(\mathcal{D}|\theta) p(\theta|\psi) d\theta$$

$$p(\psi|\mathcal{D}) = \frac{p(\mathcal{D}|\psi) p(\psi)}{p(\mathcal{D})}$$

Bayesian Learning – Further Reading

- Videolectures by Zoubin Ghahramani:
  Bayesian Learning
- Murphy, Chapter 5