CPSC 540: Machine Learning Empirical and Hierarchical Bayes

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Admin

- Midterm:
 - Marks posted on UBC Connect.
- Assignment 5:
 - Out soon.
 - Due April 5th.
- Remaining topics:
 - More Bayesian stats, structured prediction, variational inference, deep learning.

• For most of the course, we considered MAP estimation:

$$\begin{split} \hat{w} &= \operatorname*{argmax}_{w} p(w|X,y) \qquad \qquad \text{(train)} \\ \hat{y}^{i} &= \operatorname*{argmax}_{\hat{y}} p(\hat{y}|\hat{x}^{i},\hat{w}) \qquad \qquad \text{(test)}. \end{split}$$

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• Directly follows from rules of probability, and no separate training/testing.

Hierarchical Bayes

Beta-Bernoulli Model

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- In particular, let's assume θ comes from a beta distribution,

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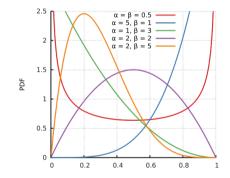
- $\bullet\,$ The parameters α and β of the prior are called hyper-parameters.
 - Similar to λ in regression, these are parameters of the prior.
- The PDF for the beta distribution has the form

$$p(\theta|\alpha,\beta) = \frac{1}{B(\alpha,\beta)} \theta^{\alpha-1} (1-\theta)^{\beta-1},$$

where the beta function is $B(\alpha,\beta) = \Gamma(\alpha)\Gamma(\beta)/\Gamma(\alpha+\beta).$

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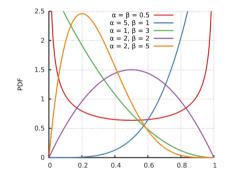
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- Uniform distribution if $\alpha = 1$ and $\beta = 1$.
- "It makes the integrals easy".

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 - Leads to Bayesian decision theory.
 - Straightforward extension: predict to minimize expected cost.

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(Bayes)
$$= \frac{\left(\theta^2(1-\theta)^1\right) \left(\frac{1}{B(\alpha,\beta)}\theta^{\alpha-1}(1-\theta)^{\beta-1}\right)}{p(HTH|\alpha, \beta)}$$
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- Understanding Bayesian inference is much easier once you can notice that:
 - The posterior is a beta distribution and the marginal likelihood integral is trivial.

• Given HTH, we've shown that posterior is

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- Probabilities sum to 1: these have same distribution and normalizing constant.
 - Posterior is a beta distribution, $p(\theta|HTH, \alpha, \beta)$ is a $\mathcal{B}(2 + \alpha, 1 + \beta)$ distribution.
 - Marginal likelihood is ratio of posterior and prior normalizing constants,

$$p(HTH|\alpha,\beta) = \frac{B(2+\alpha,1+\beta)}{B(\alpha,\beta)}.$$

Posterior Predictive

If we observe 'HHH' then our different estimates are:

• Maximum likelihood:

$$\hat{\theta} = \frac{n_H}{n} = \frac{3}{3} = 1.$$

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• Posterior predictive with Beta(1,1) prior,

$$\begin{aligned} p(H|HHH) &= \int_0^1 p(H|\theta) p(\theta|HHH) d\theta \\ &= \int_0^1 \text{Ber}(H|\theta) \text{Beta}(\theta|3+\alpha,\beta) d\theta \\ &= \int_0^1 \theta \text{Beta}(\theta|3+\alpha,\beta) d\theta = \mathbb{E}[\theta] \\ &= \frac{(3+\alpha)}{(3+\alpha)+\beta} = \frac{4}{5} = 0.8. \end{aligned}$$

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Beta Bernoulli Model Discussion

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 - $\mathcal{B}(100,1)$ prior is like seeing 100 heads and 1 tail (biased),
 - For HHH, posterior predictive is 0.990.
 - $\mathcal{B}(.01,.01)$ biases towards having unfair coin (head or tail),
 - For HHH, posterior predictive is 0.997.
 - Called "improper" prior (does not integrate to 1), but posterior can be "proper".

Baysics

Outline



2 Empirical Bayes



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- Notice that mean of posterior is the MAP estimate (not true in general).
- $\bullet\,$ Bayesian perspective gives us variability in w and optimal predictions given prior.
- But it also gives different ways to choose λ and choose basis.

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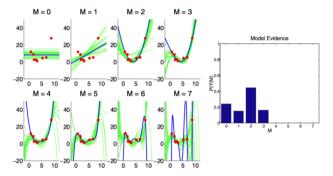
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 - Approach 2: optimize the marginal likelihood,

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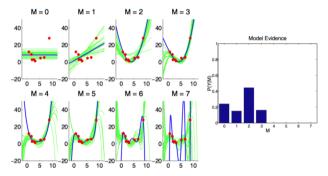
• Also called type II maximum likelihood or evidence maximization or empirical Bayes.

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http://www.cs.ubc.ca/~arnaud/stat535/slides5_revised.pdf

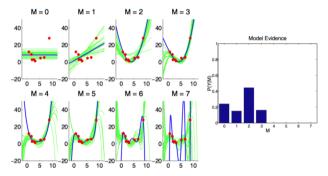
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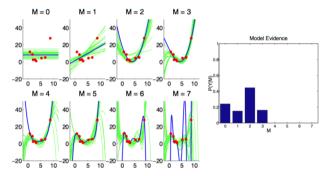
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 - Model selection criteria like BIC are approximations to marginal likelihood as $n \to \infty$.

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- We are using the data to optimize the prior.
- Even if we have a complicated model, much less likely to overfit:
 - Complicated models need to integrate over many more alternative hypotheses.

• Maximum likelihood:

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• Type II maximum likelihood:

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 - This is L2-regularization, but empirical Bayes naturally encouages sparsity.
- Non-convex and theory not well understood, but recent work shows:
 - Never performs worse than L1-regularization, and exists cases where it does better.

Bonus Slide: Overivew of Bayesian Variable Selection

- If we fix λ and use L1-regularization (Bayesian lasso), posterior is not sparse.
 - Probability that a variable is exactly 0 is zero.
 - L1-regularization only lead to sparsity because the MAP point estimate is sparse.
- Type II maximum likelihood leads to sparsity in the posterior because variance goes to zero.
- We can encourage sparsity in Bayesian models using a spike and slab prior:
 - Mixture of Dirac delta function 0 and another prior with non-zero variance.
 - Places non-zero posterior weight at exactly 0.
 - Posterior is still non-sparse, but answers the question "what is the probability that variable is non-zero"?

Hierarchical Bayes





2 Empirical Bayes



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 - Natural test, but not easy with classic methods.
 - No need for null hypothesis, p-values etc.
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 - But can only tell you which model is more likely, not whether any model is correct.

Bayesian Model Selection and Averaging

• Bayesian model selection ("type II MAP"): maximize hyper-parameter posterior,

$$\begin{split} \hat{\lambda} &= \operatorname*{argmax}_{\lambda} p(\lambda|X,y,\gamma) \\ &= \operatorname*{argmax}_{\lambda} p(y|X,\lambda) p(\lambda|\gamma), \end{split}$$

which further takes us away from overfitting (thus allowing more complex models).

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- \bullet We could do the same thing to choose order of polynomial basis, σ in RBFs, etc.
- Bayesian model averaging considers posterior over hyper-parameters,

$$\hat{y}^i = \operatorname*{argmax}_{\hat{y}} \int_{\lambda} \int_{w} p(\hat{y} | \hat{x}^i, w) p(w, \lambda | X, y, \gamma) dw.$$

• We could also maximize marginal likelihood of γ , ("type III ML"),

$$\hat{\gamma} = \operatorname*{argmax}_{\gamma} p(y|X,\gamma) = \operatorname*{argmax}_{\gamma} \int_{\lambda} \int_{w} p(y|X,w) p(w|\lambda) p(\lambda|\gamma) dw d\lambda.$$

Discussion of Hierarchical Bayes

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- Key advantage:
 - Mathematically simple to know what to do as you go up the hierarchy:
 - Same math for w , λ , γ , and so on.
- Key disadvantages:
 - It can be hard to exactly encode your prior beliefs.
 - The integrals get ugly very quickly.



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- Posterior predictive lets us directly model what we want given hyper-parameters.
- Marginal likelihood is probability seeing data given hyper-parameters.
- Empirical Bayes optimizes this to set hyper-parameters:
 - Allows tuning a large number of hyper-parameters.
 - Bayesian Occam's razor: naturally encourages sparsity and simplicity.
- Hierarchical Bayes goes even more Bayesian with prior on hyper-parameters.
 - Leads to Bayesian model selection and Bayesian model averaging.
- Next time: can we actually compute these integrals?