CPSC 540: Machine Learning

Empirical Bayes

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Motivation: Controlling Complexity

- For many of these tasks, we need very complicated models.
  - We require multiple forms of regularization to prevent overfitting.
- In 340 we saw two ways to reduce complexity of a model:
  - Model averaging (ensemble methods).
  - Regularization (linear models).
- Bayesian methods combine both of these.
  - Average over models, weighted by posterior (which includes regularizer).

Current Hot Topics in Machine Learning

Bayesian learning includes:

- Gaussian processes.
- Approximate inference.
- Bayesian nonparametrics.

Why Bayesian Learning?

- Standard L2-regularized logistic regression steup:
  - Given finite dataset containing IID samples.
    - E.g., samples (x^i, y^i) with $x^i \in \mathbb{R}^d$ and $y^i \in \{-1, 1\}$.
  - Find "best" w by minimizing NLL with a regularizer to "prevent overfitting".

$$\hat{w} \in \underset{w}{\operatorname{argmin}} - \sum_{i=1}^{n} \log p(y^i \mid x^i, w) + \frac{\lambda}{2}\|w\|^2.$$

  - Predict labels of *new* example $\tilde{x}$ using single weights $\hat{w}$,

$$\hat{y} = \operatorname{sgn}(\hat{w}^T \tilde{x}).$$

- But data was random, so weight $\hat{w}$ is a random variables.
  - This might put our trust in a $\hat{w}$ where posterior $p(\hat{w} \mid X, y)$ is tiny.

- Bayesian approach: treat w as random and predict based on rules of probability.

Problems with MAP Estimation

- Does MAP make the right decision?
  - Consider three hypothesese $\mathcal{H} = \{\text{"lands"}, \text{"crashes"}, \text{"explodes"}\}$ with posteriors:

$$p(\text{"lands"} \mid D) = 0.4, \quad p(\text{"crashes"} \mid D) = 0.3, \quad p(\text{"explodes"} \mid D) = 0.3.$$

  - The MAP estimate is "plane lands", with posterior probability 0.4.
    - But probability of dying is 0.6.
    - If we want to live, MAP estimate doesn't give us what we should do.

- Bayesian approach considers all models: says don't take plane.
- Bayesian decision theory: accounts for costs of different errors.

MAP vs. Bayes

- MAP (regularized optimization) approach maximizes over w:

$$\begin{aligned}\hat{w} &\in \operatorname*{argmax}_w p(w \mid X, y) \\ &\equiv \operatorname*{argmax}_w p(y \mid X, w)p(w) && \text{(Bayes' rule, } w \perp X) \\ \hat{y} &\in \operatorname*{argmax}_y p(y \mid \tilde{x}, \hat{w}).\end{aligned}$$

- Bayesian approach predicts by integrating over possible w:

$$\begin{aligned}p(\tilde{y} \mid \tilde{x}, X, y) &= \int_w p(\tilde{y}, w \mid \tilde{x}, X, y)dw && \text{marginalization rule} \\ &= \int_w p(\tilde{y} \mid w, \tilde{x}, X, y)p(w \mid \tilde{x}, X, y)dw && \text{product rule} \\ &= \int_w p(\tilde{y} \mid w, \tilde{x})p(w \mid X, y)dw && \tilde{y} \perp X, y \mid \tilde{x}, w\end{aligned}$$

- Considers all possible w, and weights prediction by posterior for w.

Motivation for Bayesian Learning

- Motivation for studying Bayesian learning:
  1. Optimal decisions using rules of probability (and possibly error costs).
  2. Gives estimates of variability/confidence.
     - E.g., this gene has a 70% chance of being relevant.
  3. Elegant approaches for model selection and model averaging.
     - E.g., optimize λ or optimize grouping of w elements.
  4. Easy to relax IID assumption.
     - E.g., hierarchical Bayesian models for data from different sources.
  5. Bayesian optimization: fastest rates for some non-convex problems.
  6. Allows models with unknown/infinite number of parameters.
     - E.g., number of clusters or number of states in hidden Markov model.

- Why isn't everyone using this?
  - Philosophical: Some people don't like "subjective" prior.
  - Computational: Typically leads to nasty integration problems.

Coin Flipping Example: MAP Approach

- MAP vs. Bayesian for a simple coin flipping scenario:
  1. Our likelihood is a Bernoulli,
  $$p(H \mid \theta) = \theta.$$
  2. Our prior assumes that we are in one of two scenarios:
     - The coin has a 50% chance of being fair ($\theta = 0.5$).
     - The coin has a 50% chance of being rigged ($\theta = 1$).
  3. Our data consists of three consecutive heads: 'HHH'.

- What is the probability that the next toss is a head?
  - MAP estimate is $\hat{\theta} = 1$, since $p(\theta = 1 \mid HHH) > p(\theta = 0.5 \mid HHH)$.
  - So MAP says the probability is 1.

  - But MAP overfits: we believed there was a 50% chance the coin is fair.

Coin Flipping Example: Posterior Distribution

- Bayesian method needs posterior probability over θ,

$$p(\theta = 1 \mid HHH) = \frac{p(HHH \mid \theta = 1)p(\theta = 1)}{p(HHH)} \quad \text{(Bayes rule)}$$

$$\text{(marg. rule)} = \frac{p(HHH \mid \theta = 1)p(\theta = 1)}{p(HHH \mid \theta = 0.5)p(\theta = 0.5) + p(HHH \mid \theta = 1)p(\theta = 1)}$$

$$= \frac{(1)(0.5)}{(1/8)(0.5) + (1)(0.5)} = \frac{8}{9},$$

and similarly we have $p(\theta = 0.5 \mid HHH) = \frac{1}{9}$.

- So given the data, we should believe with probability $\frac{8}{9}$ that coin is rigged.
  - There is still a $\frac{1}{9}$ probability that it is fair that MAP is ignoring.

Coin Flipping Example: Posterior Predictive

- Posterior predictive gives probability of head given data and prior,

$$
\begin{aligned}
&p(H \mid HHH) = p(H, \theta = 1 \mid HHH) + p(H, \theta = 0.5 \mid HHH) \\
&= p(H \mid \theta = 1, HHH)p(\theta = 1 \mid HHH) \\
&+ p(H \mid \theta = 0.5, HHH)p(\theta = 0.5 \mid HHH) \\
&= (1)(8/9) + (0.5)(1/9) = 0.94.
\end{aligned}
$$

- So the correct probability given our assumptions/data is 0.94, and not 1.
- Notice that there was no optimization of the parameter θ:
  - In Bayesian stats we condition on data and integrate over unknowns.
- In Bayesian stats/ML: "all parameters are nuissance parameters".

Coin Flipping Example: Discussion

Comments on coin flipping example:

- Bayesian prediction uses that HHH could come from fair coin.
- As we see more heads, posterior converges to 1.
  - MLE/MAP/Bayes usually agree as data size increases.
- If we ever see a tail, posterior of $\theta = 1$ becomes 0.

- If the prior is correct, then Bayesian estimate is optimal:
  - Bayesian decision theory gives optimal action incorporating costs.
- If the prior is incorrect, Bayesian estimate may be worse.
  - This is where people get uncomfortable about "subjective" priors.

- But MLE/MAP are also based on "subjective" assumptions.

Bayesian Model Averaging

- In 340 we saw that model averaging can improve performance.
  - E.g., random forests average over random trees that overfit.
- But should all models get equal weight?
  - What if we find a random stump that fits the data perfectly?
    - Should this get the same weight as deep random trees that likely overfit?
  - In science, research may be fraudulent or not based on evidence.
    - E.g., should we vaccines cause autism or climate change denial models?
- In these cases, naive averaging may do worse.

Bayesian Model Averaging

- Suppose we have a set of m probabilistic classifiers w_j
  - Previously our ensemble method gave all models equal weights,

$$p(\tilde{y} \mid \tilde{x}) = \frac{1}{m}p(\tilde{y} \mid \tilde{x}, w_1) + \frac{1}{m}p(\tilde{y} \mid \tilde{x}, w_2) + \cdots + \frac{1}{m}p(\tilde{y} \mid \tilde{x}, w_m).$$

- Bayesian model averaging weights by posterior,

$$p(\tilde{y} \mid \tilde{x}) = p(w_1 \mid X, y)p(\tilde{y} \mid \tilde{x}, w_1) + p(w_2 \mid X, y)(\tilde{y} \mid \hat{x}, w_2) + \cdots + p(w_m \mid X, y)p(\tilde{y} \mid \tilde{x}, w_m).$$

- So we should weight by probability that w_j is the correct model.
  - Equal weights assume all models are equally probable and fit data equally well.

Bayesian Model Averaging

- Weights are posterior, so proportional to likelihood times prior:

$$p(w_j \mid X, y) \propto \underbrace{p(y \mid X, w_j)}_{\text{likelihood}} \underbrace{p(w_j)}_{\text{prior}}.$$

- Likelihood gives more weight to models that predict y well.
- Prior should gives less weight to models that are likely to overfit.

- This is how rules of probability say we should weight models.
  - It's annoying that it requires a "prior" belief over models.
  - But as $n \to \infty$, all weight goes to "correct" model[s] w^* as long as $p(w^*) > 0$.

Bayes for Density Estimation and Generative/Discriminative

- We can use Bayesian approach to density estimation:
  - With data D and parameters θ we have:
    1. Likelihood $p(D \mid \theta)$.
    2. Prior $p(\theta)$.
    3. Posterior $p(\theta \mid D)$.

- We can use Bayesian approach to supervised learning:
  - Generative approach (naive Bayes, GDA) does density estimation of X and y:
    1. Likelihood $p(y, X \mid w)$.
    2. Prior $p(w)$.
    3. Posterior $p(w \mid X, y)$.

  - Discriminative approach (logistic regression, neural nets) just conditions on X:
    1. Likelihood $p(y \mid X, w)$.
    2. Prior $p(w)$.
    3. Posterior $p(w \mid X, y)$.

7 Ingredients of Bayesian Inference

1. Likelihood $p(y \mid X, w)$.
   - Probability of seeing data given parameters.

2. Prior $p(w \mid \lambda)$.
   - Belief that parameters are correct before we've seen data.

3. Posterior $p(w \mid X, y, \lambda)$.
   - Probability that parameters are correct after we've seen data.
   - We won't use the MAP "point estimate", we want the whole distribution.

4. Predictive $p(\tilde{y} \mid \tilde{x}, w)$.
   - Probability of test label $\tilde{y}$ given parameters w and test features $\tilde{x}$.

7 Ingredients of Bayesian Inference

4. Posterior predictive $p(\tilde{y} \mid \tilde{x}, X, y, \lambda)$.
   - Probability of new data given old, integrating over parameters.
   - This tells us which prediction is most likely given data and prior.
5. Marginal likelihood $p(y \mid X, \lambda)$ (also called "evidence").
   - Probability of seeing data given hyper-parameters.
   - We'll use this later for hypothesis testing and setting hyper-parameters.
6. Cost $C(\hat{y} \mid \tilde{y})$.
   - The penalty you pay for predicting $\hat{y}$ when it was really was $\tilde{y}$.
   - Leads to Bayesian decision theory: predict to minimize expected cost.

Review: Decision Theory

- Consider a scenario where different predictions have different costs:

Predict / True	True "spam"	True "not spam"
Predict "spam"	0	100
Predict "not spam"	10	0

- In 340 we discussed predictin $\hat{y}$ given $\hat{w}$ by minimizing expected cost:

$$\begin{aligned}\mathbb{E}[\text{Cost}(\hat{y} = \text{"spam"})] &= p(\tilde{y} = \text{"spam"} \mid \tilde{x}, \hat{w})C(\hat{y} = \text{"spam"} \mid \tilde{y} = \text{"spam"}) \\ &+ p(\tilde{y} = \text{"not spam"} \mid \tilde{x}, \hat{w})C(\hat{y} = \text{"spam"} \mid \tilde{y} = \text{"not spam"}).\end{aligned}$$

- Consider a case where $p(\tilde{y} = \text{"spam"} \mid \tilde{x}, \hat{w}) > p(\tilde{y} = \text{"not spam"} \mid \tilde{x}, \hat{w})$.
  - We might still predict "not spam" if expected cost is lower.

Bayesian Decision Theory

- Bayesian decision theory:
  - Instead of using a MAP estimate $\hat{w}$, we should use posterior predictive,

$$\mathbb{E}[\text{Cost}(\hat{y} = \text{“spam”})] = p(\tilde{y} = \text{“spam”} \mid \tilde{x}, X, y) C(\hat{y} = \text{“spam”} \mid \tilde{y} = \text{“spam”}) + p(\tilde{y} = \text{“not spam”} \mid \tilde{x}, X, y) C(\hat{y} = \text{“spam”} \mid \tilde{y} = \text{“not spam”}).$$

  - Minimizing this expected cost is the optimal action.

- Note that there is a lot going on here:
  - Expected cost depends on cost and posterior predictive.
  - Posterior predictive depends on predictive and posterior
  - Posterior depends on likelihood and prior.

Outline

Bayesian Linear Regression

- We know that L2-regularized linear regression,

$$\underset{w}{\operatorname{argmin}} \frac{1}{2\sigma^2}\|Xw - y\|^2 + \frac{\lambda}{2}\|w\|^2,$$

  corresponds to MAP estimation in the model

$$y^i \sim \mathcal{N}(w^T x^i, \sigma^2), \quad w_j \sim \mathcal{N}(0, \lambda^{-1}).$$

- By some tedious Gaussian identities, the posterior has the form

$$w \mid X, y \sim \mathcal{N}\left(\frac{1}{\sigma^2}\left(\frac{1}{\sigma^2}X^TX + \lambda I\right)^{-1} X^T y, \left(\frac{1}{\sigma^2}X^TX + \lambda I\right)^{-1}\right).$$

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

Learning the Prior from Data?

- Can we use the training data to set the hyper-parameters?
- In theory: No!
  - It would not be a "prior".
  - It's no longer the right thing to do.
- In practice: Yes!
  - Approach 1: split into training/validation set or use cross-validation as before.
  - Approach 2: optimize the marginal likelihood ("evidence"):

$$p(y \mid X, \lambda) = \int_w p(y \mid X, w) p(w \mid \lambda) dw.$$

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

Digression: Marginal Likelihood in Gaussian-Gaussian Model

- Suppose we have a Gaussian likelihood and Gaussian prior,

$$y^i \sim \mathcal{N}(w^T x^i, \sigma^2), \quad w_j \sim \mathcal{N}(0, \lambda^{-1}).$$

- The joint probability of y^i and w_j is given by

$$p(y, w \mid X, \lambda) \propto \exp\left(-\frac{1}{2\sigma^2}\|Xw - y\|^2 - \frac{\lambda}{2}\|w\|^2\right).$$

- The marginal likelihood integrates the joint over the nuisance parameter w,

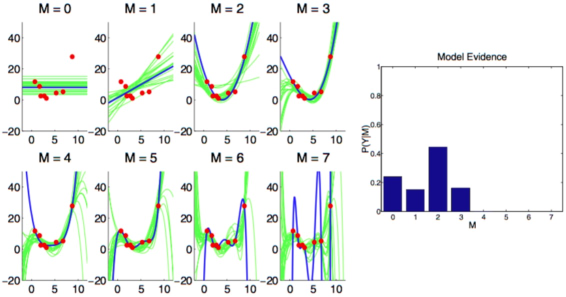
$$p(y \mid X, \lambda) = \int_w p(y, w \mid X, \lambda) dw.$$

- Solving the Gaussian integral gives a marginal likelihood of

$$p(y \mid X, \lambda) \propto |C|^{-1/2} \exp\left(-\frac{y^T C^{-1} y}{2}\right), \quad C = \sigma^2 I + \frac{1}{\lambda} X X^T.$$

Type II Maximum Likelihood for Basis Parameter

- Consider polynomial basis, and treat degree M as a hyper-parameter:



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

- Marginal likelihood (evidence) is highest for $M = 2$.
  - "Bayesian Occam's Razor": prefers simpler models that fit data well.
  - $p(y \mid X, \lambda)$ is small for $M = 7$, since 7-degree polynomials can fit many datasets.
  - It's actually non-monotonic in M: it prefers $M = 0$ and $M = 2$ over $M = 1$.
  - Model selection criteria like BIC are approximations to marginal likelihood as $n \to \infty$.

Type II Maximum Likelihood for Basis Parameter

- Why is the marginal likelihood high for degree 2 but not degree 7?
  - Marginal likelihood for degree 2:

$$p(y \mid X, \lambda) = \int_{w_0} \int_{w_1} \int_{w_2} p(y \mid X, w) p(w \mid \lambda) dw$$

  - Marginal likelihood for degree 7:

$$p(y \mid X, \lambda) = \int_{w_0} \int_{w_1} \int_{w_2} \int_{w_3} \int_{w_4} \int_{w_5} \int_{w_6} \int_{w_7} p(y \mid X, w) p(w \mid \lambda) dw.$$

  - Higher-degree integrates over high-dimensional volume:
    - A non-trivial proportion of degree 2 functions fit the data really well.
    - There are many degree 7 functions that fit the data even better, but they are a much smaller proportion of all degree 7 functions.

Bayes Factors for Bayesian Hypothesis Testing

- Suppose we want to compare hypotheses:
  - E.g., "this data is best fit with linear model" vs. a degree-2 polynomial.
- Bayes factor is ratio of marginal likelihoods,

$$\frac{p(y \mid X, \text{degree } 2)}{p(y \mid X, \text{degree } 1)}.$$

  - If very large then data is much more consistent with degree 2.
  - A common variation also puts prior on degree.
- A more direct method of hypothesis testing:
  - No need for null hypothesis, "power" of test, p-values, and so on.
  - As usual can only tell you which model is likely, not whether any are correct.

- American Statistical Assocation:
  - "Statement on Statistical Significance and P-Values".
  - http://amstat.tandfonline.com/doi/pdf/10.1080/00031305.2016.1154108
- "Hack Your Way To Scientific Glory":
  - https://fivethirtyeight.com/features/science-isnt-broken
- "Replicability crisis" in social psychology and many other fields:
  - https://en.wikipedia.org/wiki/Replication_crisis
  - http://www.nature.com/news/big-names-in-statistics-want-to-shake-up-much-maligned-p-value-1.22375
- "T-Tests Aren't Monotonic": https://www.naftaliharris.com/blog/t-test-non-monotonic
- Bayes factors don't solve problems with p-values and multiple testing.
  - But they give an alternative view, are more intuitive, and make assumptions clear.
- Some notes on various issues associated with Bayes factors:
  - http://www.aarondefazio.com/adefazio-bayesfactor-guide.pdf

Summary

- Bayesian statistics:
  - Condition on the data, integrate (rather than maximize) over posterior.
  - "All parameters are nuissance parameters".
- Marginal likelihood is probability seeing data given hyper-parameters.
- Empirical Bayes optimizes marginal likelihood to set hyper-parameters.
- Next time: putting a prior on the prior and relaxing IID