Inconsistency of Bayesian inference when the model is wrong, and how to repair it

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Outline

1. Introduction
2. Bayes when the Model is Wrong
3. Learning rates and SafeBayes
4. Discussion and Conclusion
We have one or more models:

- Each model is a set of hypotheses;
- Each hypothesis is a probability distribution
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We want to learn from the training data which of these distributions we can use to predict new data
We will consider regression models:

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\[\mathcal{M}_k = \{ p(k,\beta,\sigma^2) \mid \beta \in \mathbb{R}^{k+1}, \sigma > 0 \};\]

Hypothesis \( p(k,\beta,\sigma^2) \) expresses that

\[Y \sim \mathcal{N}\left(\beta_0 + \sum_{i=1}^{k} \beta_i g_i(X), \sigma^2\right)\]

In this presentation: \( g_i \) is a polynomial of degree \( i \)
So model \( \mathcal{M}_k \) represents all polynomials of degree up to \( k \)
Bayesian statistics

Big idea: Use probability distributions over the *models and hypotheses* to represent our uncertainty.
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- Introduce a *prior* distribution

\[ \pi(k, \beta, \sigma^2) \]
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- so that we can define the joint distribution:

\[ p_{\text{Bayes}}(Y^n, k, \beta, \sigma^2 \mid X^n) = p_{(k, \beta, \sigma^2)}(Y^n \mid X^n) \pi(k, \beta, \sigma^2) \]
Bayesian statistics: Posterior and predictive

We can use the joint distribution $p_{\text{Bayes}}$ to compute interesting things:

- The Bayesian **posterior** distribution

  $$\pi(k, \beta, \sigma^2 \mid X^n, Y^n)$$

  tells us how to update our prior beliefs after having seen the data
Bayesian statistics: Posterior and predictive

We can use the joint distribution $p_{\text{Bayes}}$ to compute interesting things:

- The Bayesian \textit{posterior} distribution

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  tells us how to update our prior beliefs after have seen the data

- The Bayesian \textit{predictive} distribution

  $$p_{\text{Bayes}}(Y_i \mid Y^{i-1}, X^i)$$

  tells what new data should look like, based on that posterior
Bayesian methods are very successful, in both theory and practice:

- Keep track of uncertainty in a very elegant way;
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Bayesian statistics: Advantages

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- Bayes avoids overfitting.
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...usually (see next section)
Experiment: Model correct

Experiment: We let Bayes choose from 51 different models (polynomials of degrees 0 up to 50); the data are actually drawn according to a distribution $P^*$ (the true distribution), which is in the simplest model:

\[
X \sim U(-1, 1);
\]
\[
Y \sim \mathcal{N}(f^*(X), 0.05)
\]

with $f^*(x) = 0$ for all $x$. 
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with $f^*(x) = 0$ for all $x$.

We use standard priors:

- More-or-less uniform on $k$;
- Gaussian with large variance on $\beta$;
- Inverse-gamma on $\sigma^2$. 
Experiment: Model correct

For these data, Bayes puts most weight on the smallest model.
For these data, Bayes puts most weight on *smallest model*
Experiment: Model correct

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New experiment:

- Same models;
- Different true distribution:
  For each data point, flip a fair coin
  - if heads, data point is drawn randomly as before;
  - if tails, data point is **exactly at (0, 0)**
Experiment: Model wrong

New experiment:

- Same models;
- Different true distribution:
  For each data point, flip a fair coin
    - if heads, data point is drawn randomly as before;
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Simplest model is still best! (in a sense we will see later)
This should just make it easier, right?
Experiment: Model wrong

- This should just make it easier, right?
- Now Bayes puts most weight on *largest models*!
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Now Bayes puts most weight on *largest models!*
Results from other experiments

We ran many more experiments, eg.

- different models;
- different priors;
- different true distributions.

The problems with Bayes occur in all of them.
We ran many more experiments, eg.
- different models;
- different priors;
- different true distributions.

The problems with Bayes occur in all of them. Problems get worse if there are more models;
- By comparison: In model-correct experiment, Bayes is hardly affected by extra models
KL divergence

If the Bayesian posterior concentrates, it is around the hypothesis \( \tilde{P} \) that is closest to \( P^* \) in terms of KL divergence among all elements in the model:

\[
D(P^* \| \tilde{P}) = \mathbb{E}_{X, Y \sim P^*} [- \log \tilde{P}(Y | X)] - C_{P^*}
\]

[Kleijn and Van der Vaart 2006]
If the Bayesian posterior concentrates, it is around the hypothesis \( \tilde{P} \) that is closest to \( P^* \) in terms of KL divergence among all elements in the model:

\[
D(P^*\|\tilde{P}) = E_{X,Y \sim P^*}[-\log \tilde{P}(Y \mid X)] - C_{P^*}
\]

[Kleijn and Van der Vaart 2006]

In our experiment, \( \tilde{P} \) is the hypothesis that
- predicts \( Y = 0 \) for all \( X \) (coincides with \( f^* \));
- sets \( \sigma^2 = 0.025 \) (\( = \) variance of \( Y \)).

This \( \tilde{P} \) also minimizes the squared risk!

Conclusion: Bayesian posterior did not concentrate!
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Introducing Generalized Bayes

Bayes:

\[ \pi(\theta \mid \text{data}) \propto p(\text{data} \mid \theta) \cdot \pi(\theta) \]

On-line prediction; PAC-Bayes; Lasso/Ridge; . . . :

\[ \pi(\theta \mid \text{data}) \propto e^{-\eta \cdot \text{loss}_\theta(\text{data})} \cdot \pi(\theta) \]

(\eta: ‘learning rate’)
Introducing Generalized Bayes

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$$\pi(\theta \mid \text{data}) \propto p(\text{data} \mid \theta) \cdot \pi(\theta)$$

$$= e^{-\text{loss}_\theta(\text{data})} \cdot \pi(\theta)$$

for $$\text{loss}_\theta(\text{data}) = -\log p(\text{data} \mid \theta)$$

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($\eta$: ‘learning rate’)

Introducing Generalized Bayes

Generalized Bayes: [Vovk 1990; Barron & Cover 1991; Walker & Hjort 2002; McAllister 2003; ...]

\[ \pi(\theta | \text{data}) \propto p(\text{data} | \theta)^{\eta} \cdot \pi(\theta) \]

\[ = e^{-\eta \cdot \text{loss}_\theta(\text{data})} \cdot \pi(\theta) \]

for \( \text{loss}_\theta(\text{data}) = - \log p(\text{data} | \theta) \)

On-line prediction; PAC-Bayes; Lasso/Ridge; ...:

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Choosing the learning rate

- $\eta = 1$: standard Bayes
- $\eta = 0$: no learning occurs (posterior remains equal to prior)
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But if $\eta$ too small, we are learning more slowly than we could
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Theoretical prescriptions for $\eta$ are often suboptimal in practice
Choosing the learning rate

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Grand aim:
Find generic method (a theory, if you will) for determining the learning rate is all such problems
Bayesian model selection

\[ p_{\text{Bayes}}(Y^n | X^n, k) \]
\[ = \int_{(\beta, \sigma^2)} p(k, \beta, \sigma^2)(Y^n | X^n) \pi(\beta, \sigma^2 | k) \, d(\beta, \sigma^2) \]

is the Bayesian marginal probability of the data given model \( \mathcal{M}_k \)

**Bayes factor model selection:** from a collection of models \( \mathcal{M}_0, \mathcal{M}_1, \ldots, c\mathcal{M}_K \), select the model \( \mathcal{M}_k \) that maximizes this quantity
Bayesian model selection as forward validation

\[- \log p_{\text{Bayes}}(Y^n | X^n, k) = \sum_{i=1}^{n} - \log p_{\text{Bayes}}(Y_i | Y^{i-1}, X^i, k)\]

Minus log likelihood = sum of logarithmic prediction errors

[Dawid 1984; Rissanen 1984]
Bayesian model selection as forward validation

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Minus log likelihood = sum of logarithmic prediction errors

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Viewed this way (‘prequential’), Bayes is similar to leave-one-out cross-validation — but goes through the data in only one direction
Can we use the same approach to learn $\eta$ instead of $k$?

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$$= \sum_{i=1}^{n} - \log E_{(k, \beta, \sigma^2) \sim \pi | Y_i^{i-1}, X_i, \eta} [p(k, \beta, \sigma^2)(Y_i)]$$
The SafeBayesian algorithm

Can we use the same approach to learn $\eta$ instead of $k$?

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$$= \sum_{i=1}^{n} - \log E_{(k,\beta,\sigma^2) \sim \pi | Y^{i-1}, X^i, \eta}[p(k,\beta,\sigma^2)(Y_i)]$$

Doesn’t work! Instead SafeBayes finds $\eta$ minimizing

$$= \sum_{i=1}^{n} E_{(k,\beta,\sigma^2) \sim \pi | Y^{i-1}, X^i, \eta} - \log[p(k,\beta,\sigma^2)(Y_i)]$$
Experiment: Wrong model (continued)
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When measured in terms of logarithmic loss 
(loss_\theta(data) = - \log p(data \mid \theta)),

- normally, Bayes learns to predict \textit{almost as well} as the best element in the model 
(slightly worse because we don’t know which element is best)
Bayes and logarithmic loss

When measured in terms of logarithmic loss
($\text{loss}_\theta(\text{data}) = -\log p(\text{data} | \theta)$),

- normally, Bayes learns to predict almost as well as the best element in the model
  (slightly worse because we don’t know which element is best)
- in our case, Bayes predicts significantly better than the best element in the model!
  (in terms of logarithmic loss; not in terms of, say, squared loss)
Bayes is ‘too good’!

Cumulative logarithmic loss of Bayesian predictive distribution, for $\eta = 1$
How is this possible?

Possible because all elements of model predict with Gaussian distributions, while Bayesian predictive can be infinite mixture of these Gaussians
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Bad and good misspecification
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Conclusion

- Standard Bayes may fail to concentrate, even on fairly innocent data
- Generalized Bayes does concentrate, *if* you know the right learning rate
- SafeBayes learns the learning rate!
Thank you!