MSML610: Advanced Machine Learning

7.5: Bayesian Model Comparison

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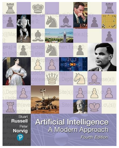
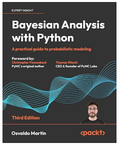
References:

- AIMA (Artificial Intelligence: a Modern Approach)
  - Chap 15: Probabilistic programming
- Martin, Bayesian Analysis with Python, 2018 (2e)




EXPERT INSIGHT
Bayesian Analysis with Python
A practical guide to probabilistic modeling
Third Edition
Osvaldo Martin
‹packt›

Models as Maps of the Real World

- Typically you need to compare models to understand which one is **"better"**
- Models are a **map, not a copy** of the real world
  - *"All models are wrong, but some are useful"* (Box, 1976)
    - "Wrong": all models are wrong since they aren't the actual territory
    - "Useful" some models describe a problem better than others
- Models have a **purpose**
  - Are approximations to understand a problem
  - A model can't reproduce all aspects equally well
  - Different models capture different data aspects

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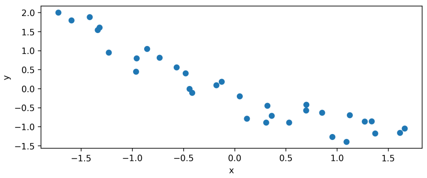
Posterior Predictive Checks

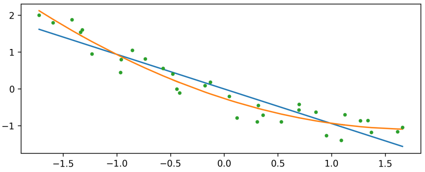
- **Goal of PPC**:
  - Evaluate model's data explanation
  - Understand model limitations
  - Improve model
- Given data from parabola + noise:
  - Fit with linear model
  - Fit with quadratic model
  - Compare predicted posterior vs observed data

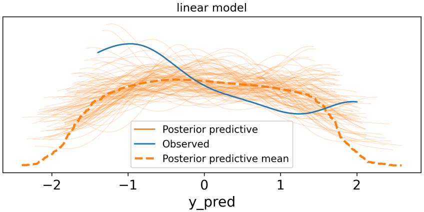


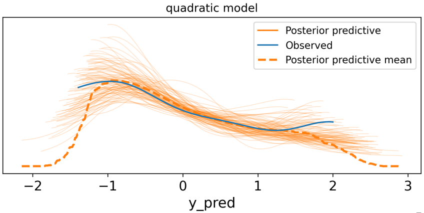
```
# Linear model.
with pm.Model() as model_l:
    # mu = alpha + beta * x
    alpha = pm.Normal('alpha', mu=0, sigma=1)
    beta = pm.Normal('beta', mu=0, sigma=10)
    mu = alpha + beta * x_c[0]
    #
    sigma = pm.HalfNormal('sigma', 5)
    #
    y_pred = pm.Normal('y_pred', mu=mu, sigma=sigma, observed=y_c)
    #
    idata_l = pm.sample(2000, idata_kwargs={"log_likelihood": True})
    idata_l.extend(pm.sample_posterior_predictive(idata_l))


# Quadratic model.
with pm.Model() as model_p:
    # mu = alpha + beta_1 * x + beta_2 * x^2
    alpha = pm.Normal('alpha', mu=0, sigma=1)
    # Beta is a 2-dim vector.
    beta = pm.Normal('beta', mu=0, sigma=10, shape=order)
    mu = alpha + pm.math.dot(beta, x_c)
    #
    sigma = pm.HalfNormal('sigma', 5)
    #
    y_pred = pm.Normal('y_pred', mu=mu, sigma=sigma, observed=y_c)
    #
    idata_q = pm.sample(2000, idata_kwargs={"log_likelihood": True})
    idata_q.extend(pm.sample_posterior_predictive(idata_q))
```

Posterior Predictive Checks

- **Compare KDE of observed and predicted data**
  - Linear model KDE doesn't match
  - Quadratic model KDE matches better
  - High uncertainty in both models, especially at tails
- Compare mean / interquartile range for data vs model
  - Plot dispersion of mean and IQR for models vs data
  - Data set provides a single point
  - Posterior provides a distribution
- Statistics "orthogonal" to model's focus are more informative, since they are less "overfit"
  - E.g., fit the mean, compare the "median"







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Bayesian P-Value for a Statistic

- A Bayesian p-value summarizes the comparison between simulated and observed data
- **Procedure**
  - Given the posterior predictive $\tilde{Y}$
  - Choose a summary statistic T (E.g., mean, median, standard deviation)
  - Compute T for:
    - The observed data T_{obs}
    - The simulated data T_{sim} from the posterior predictive
  - Compute the Bayesian p-value as the portion of simulated datasets where the test statistic is smaller than the observed data:

$$\text{Bayesian p-value} \triangleq \Pr(T_{sim} \geq T_{obs} | \tilde{Y})$$

  - If observed values agree with predicted ones, the value should be around 0.5

Bayesian P-Value for Entire Distribution

- Instead of using a summary statistic, one can compute "the probability of predicting a lower or equal value for each observed value"
- If the model is well calibrated, it captures all observations equally well, the probability should be the same for all observed values
    - The output should be a uniform distribution

Bayesian P-Value: Example

- Study the height of people in a population
- **Fit the Bayesian model**
  - Assume a normal distribution with unknown mean and variance
  - Collect observed data of heights (e.g., 100 people)
  - Specify a prior distribution for mean and variance
  - Combine observed data with prior to obtain a posterior distribution of mean and variance of population height
- **Compute Bayesian p-value**
  - From posterior distribution:
    - Generate new simulated datasets
    - For each dataset, compute mean height
  - Use test statistic T, as the difference between the mean of the replicated dataset and the observed mean
  - Compute Bayesian p-value: the proportion of replicated datasets where the test statistic is $>=$ test statistic for observed data
    - A value close to 0.5 means the observed data is covered by the model
    - A value close to 0 or 1 indicates a poor fit

Bayesian vs Frequentist P-Value

- **Frequentist p-value** is the probability of getting observed data as or more extreme, assuming the null hypothesis is true
- **Bayesian p-value** is the probability that simulated data from the model (i.e., posterior predictive check) is as or more extreme than the observed data
- P-value measures inconsistency between observed data and:
  - A null hypothesis (frequentist approach)
  - Model (Bayesian approach)
- Does p-value incorporate uncertainty?
  - (Frequentist) No, it uses single point estimates
  - (Bayesian) Yes, it incorporates uncertainty of parameter estimates

- Bayesian Model Comparison
    - ***The Balance Between Simplicity and Accuracy***
    - Measures of Predictive Accuracy
    - Bayesian Model Selection and Ensemble
    - Bayesian Hypothesis Testing
    - Regularizing Priors

Occam's Razor

- *"If you have **equivalent** explanations for the same phenomenon, you should choose the **simpler** one"*
  - Quality of explanation $\approx$ accuracy
  - Simpler $\approx$ number of model parameters
- **Complexity vs accuracy**
  - Increasing model complexity (e.g., number of model parameters) is accompanied by:
    - Increasing in-sample accuracy
    - Not necessarily out-of-sample accuracy
  - The complex model:
    - Did not "learn" from the data but just "memorize" it
    - Does a bad job generalizing to predict potentially observable data
- Ideally balance complexity and accuracy in a quantitative way

Overfitting and Underfitting

- A model is **overfit** when it has many parameters, fitting the training data well but unseen data poorly
  - Overfitting in terms of signal/noise:
    - Each dataset has “signal” and “noise”
    - We want the model to learn the signal
    - A model overfits when it learns the noise, obscuring the signal
- A model is **underfit** when it has few parameters, fitting the dataset poorly
  - An underfit model doesn’t learn the signal well
  - E.g., a constant fits a dataset, only learning the mean

Bias-Variance Trade-Off

- A model has **high bias** when:
  - It has low ability to accommodate the data
  - I.e., underfitting
  - E.g., a polynomial of degree 0
- A model has **high variance** when:
  - It has high capacity and it is sensitive to details in the data, capturing noise
  - I.e., overfitting
  - E.g., a polynomial of degree 100
- Trade-off between bias and variance
  - Goal: balance simplicity and goodness of fit
  - Aim for a model that "fits the data right," avoiding overfitting or underfitting

Accuracy Measures

- **In-sample accuracy** is measured on the data used to fit a model
- **Out-of-sample accuracy** is measured on data not used to fit a model
  - Aka "predictive accuracy"
- In-sample accuracy $>$ out-of-sample accuracy
- There is a trade-off between how much data is used for training and for evaluating true accuracy

Information Criteria: Intuition

- **Information criteria** compare models in terms of fitting the data taking into account their complexity through a penalization term
    - Out-of-sample accuracy $\approx$ in-sample accuracy $+$ a term penalizing model complexity
    - It's the VC equation

$$E_{out}[h] = E_{in}[h] + \Omega(\mathcal{H})$$

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Model Parameters for Bayesian vs Non-Bayesian Set-Up

Maximum Likelihood Estimation (MLE)

- **MLE** finds the parameter values that make the observed data most probable (given a model)
  - Denoted by $\hat{\theta}_{MLE}$
  - It's a point not a distribution
- **Procedure**:
  - Given the data $x_1, x_2, ..., x_n$
  - Assume it comes from a distribution with an unknown parameter θ
  - Pick the value of θ that makes the data most likely given a likelihood function

$$\begin{cases} L(\theta) = \log \Pr(x_1, x_2, ..., x_n|\theta) \\ \hat{\theta}_{MLE} = \text{argmax}_\theta L(\theta) \end{cases}$$

- In Bayesian terms, MLE is equivalent to the mode of θ using flat priors
  - Aka MAP (maximum a posteriori)

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Akaike Information Criterion (AIC)

- AIC is defined as

$$AIC = -2 \sum \log \Pr(y_i | \hat{\theta}_{MLE}) + 2\text{num}_{params}$$

  where:

  - $\hat{\theta}_{MLE}$ is the maximum likelihood estimation of θ
  - num_{params} is the number of parameters

- **Interpretation**:
  - The first term (log likelihood) measures how well the model fits the data
  - The second term penalizes complex models

- **Cons**:
  - Discard information about uncertainty of posterior estimation
  - MLE assumes flat priors (vs informative and weakly informative priors)
  - Number of parameters is not always a good measure of complexity
    - E.g., in hierarchical models the effective number of params is smaller

Bayesian Information Criteria

- **Bayesian Information Criteria (BIC)**
  - Like AIC, it assumes flat priors and uses MLE
  - It is not Bayesian
- **Widely Applicable Information Criteria (WAIC)**
  - Bayesian version of AIC
  - It has two terms:
    - One that measures how good the fit is
    - One that penalizes complex models
  - WAIC uses the posterior distribution to estimate both terms

Cross-Validation

- **Cross-validation** (CV)
  - **Procedure**
    - Partition data into K portions of equal size and similar statistics
    - Use $K - 1$ partitions to train the model and test on remaining partition
    - Repeat for all K folds
    - Average the results
  - **Pros**
    - Simple and effective solution to use all data to compare models
- **Leave-one-out cross-validation** (LOO-CV)
  - **Procedure**:
    - The model is fit for all data, excluding one observation
    - The model's predictive accuracy is tested on the left out observation
    - Repeat the process for all observations
    - Average the results
  - **Cons**
    - It is very computationally expensive since one needs to refit the model
- How to adapt **cross-validation to a Bayesian approach**?
  - CV and LOO require multiple model fits and fitting a Bayesian model is very expensive
  - Yes! There is a way to approximate using a single fit to the data

ELPD with LOO-CV

- 💀 Math alert
- We want to compute $ELPD_{LOO-CV}$ where:
  - "Expected Log-Pointwise predictive Density" (ELPD)
    - It should be ELPPD and not ELPD!
  - "Leave-One-Out Cross-Validation" (LOO-CV) is used to compute it
- The definition of ELPD with LOO-CV is:

$$ELPD_{LOO-CV} = \sum_{i=1}^{n} \log \int p(y_i|\theta)p(\theta|y_{-i})d\theta$$

  where:
  - Fit model using all the data without y_{-i}
  - Predict with the model the unseen y_i
  - Integrate on all the posterior values
  - Repeat for all the points
- How to compute it efficiently?
  - Use "Pareto smooth importance sampling leave-one-out cross-validation"

Pointwise Predictive Density (PPD)

- The **pointwise predictive density** for a given data point y_i is defined as the posterior predictive probability, given the rest of the data

$$PPD \triangleq \Pr(y_i|data - \{i\}) = \int p(y_i|\theta)p(\theta|y_{-i})d\theta$$

  - y_i: observed data point
  - $p(y_i|\theta)$: likelihood given model parameters θ
  - $p(\theta|y_{-i})$: posterior distribution of the model parameters given rest of data
  - Integral: averages over posterior distribution, capturing parameter uncertainty
- **Interpretation**
  - PPD measures model's predictive ability for y_i when trained on data excluding y_i
  - Similar to cross-validation, using Bayesian parameter averaging over the model parameters

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Expected Log Pointwise Predictive Density

- The ELPD is the average over unseen points of the log PPD

$$ELPD \triangleq \sum_{i=1}^{n} \log \int p(y_i|\theta_{-i})p(\theta_{-i}|y_{-i})d\theta$$

- **Interpretation**
  - It can be used to determine which model generalizes better to new data
  - ELPD measures the predictive accuracy of a Bayesian model on unseen data
  - Train on y_{-i}, i.e., all data excluding y_i
  - For each point y_i excluded from the training set, there is a new distribution of the params θ_{-i}
  - Test on y_i

PSIS-LOO-CV

- Compute the Expected Log Pointwise Predictive Density (ELPD) using Leave-One-Out Cross-Validation (LOO-CV):

$$ELPD_{LOO-CV} \triangleq \sum_i \log \int p(y_i|\theta)p(\theta|y_{-i})d\theta$$

- **Problem**: Need to train N models, one for every data point
- **Solution**:
  - Pareto-Smoothed Importance Sampling (PSIS) Leave-One-Out Cross-Validation (LOO-CV) estimates without refitting for every point
  - **Importance sampling**:
    - Use full dataset to approximate posterior distribution when one observation is left out
    - Re-weight posterior samples based on importance
  - **Pareto-smoothing**:
    - Stabilize importance weights, reducing extreme weights' impact
    - E.g., if an observation left out influences the posterior distribution
    - Provide diagnostics to assess reliability of importance weights

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- Bayesian Model Comparison
    - The Balance Between Simplicity and Accuracy
    - Measures of Predictive Accuracy
    - ***Bayesian Model Selection and Ensemble***
    - Bayesian Hypothesis Testing
    - Regularizing Priors

Bayesian Model Selection

- **Bayesian way to compare k models**
  - Calculate the evidence of each model $\Pr(Y|M_k)$, i.e., the probability of observed data Y given each model M_k
- Fitting a model and model selections are the same process in Bayesian approach
  - The VC framework considers fitting models and selecting models in the same way
  - In the frequentist approach there are different procedures
- **Model fitting**
  - Consider Bayes theorem for parameters θ and data Y, given model M_k

$$\Pr(\theta|Y, M_k) = \frac{\Pr(Y|\theta, M_k) \Pr(\theta|M_k)}{\Pr(Y|M_k)}$$

  - Find parameters θ that maximize the ratio, independently of evidence probability

$$\text{argmax}_\theta \Pr(\theta|y, M_k) = \text{argmax}_\theta \Pr(y|\theta, M_k) \Pr(\theta|M_k)$$

- **Model selection**
  - To choose the best model among $M_1, ..., M_k$, pick the one that maximizes

$$\text{argmax}_k \Pr(M_k|y) \propto \Pr(y|M_k) \Pr(M_k)$$

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Model Averaging

- What do you do when you have multiple models explaining the data?

  1. **Model selection**
     - Select one model
     - Simple solution
  2. **Report all models with their informations**
     - E.g., standard errors, posterior predictive checks
     - Express advantages and shortcomings of the models
  3. **Average all the models**
     - Build a meta-model using a weighted average of each model
     - Weight prediction by the difference between information criteria (e.g., WAIC, LOO) of the models
     - A hierarchical model is a continuous versions of multiple discrete models

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Bayes Factors

- **Bayes factors** are ratio of two marginal likelihoods of the data under competing model hypotheses M_0 and M_1

$$BF = \frac{\Pr(y|M_0)}{\Pr(y|M_1)}$$

where $BF > 1$ means model 0 explains data better than model 1

Bayes factor	Support
1-3	Anecdotal
3-10	Moderate
10-30	Strong
30-100	Very strong
>100	Extreme

- **Intuition**
  - Act as a scale weighing evidence for one theory over another

Assumption of Bayes Factors

- The assumption of Bayes factor is that the models have the same prior probability
- Otherwise we need to compute the "posterior odds" as "Bayes factors" x "prior odds"

$$\frac{\Pr(M_0|y)}{\Pr(M_1|y)} = \frac{\Pr(y|M_0)}{\Pr(y|M_1)} \frac{\Pr(M_0)}{\Pr(M_1)} = \text{Bayes factors} \times \text{prior odds}$$

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Bayes Factors: Pros and Cons

- Looking at the definition of marginal likelihood (aka evidence):

$$p(y) = \int_{\theta} p(y|\theta)p(\theta)d\theta$$

- Making the dependency of the model M_k explicit

$$p(y|M_k) = \int_{\theta_k} p(y|\theta_k, M_k)p(\theta_k, M_k)d\theta_k$$

- Pros
  - Models with more parameters have a larger prior, so the Bayes factor has a built-in Occam's Razor
- Cons
  - The marginal likelihood needs to be computed numerically over a large dimensional space
  - The marginal likelihood depends on the value of the prior
    - Changing the prior might not affect the inference of θ but have a direct effect on the marginal likelihood

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Hierarchical Models: Candies in a Jar Examples

- Each classroom has a jar filled with candies, each different but coming from the same candy shop
- Kids in each classroom need to guess the number of candies in each jar
- Individual guesses
  - Think of each jar as its own little puzzle
  - E.g., guess based on how big the jar is, how filled it is
  - Each jar has certain "parameters"
- Group learning
  - Consider what you learn from other jars since they come from the same candy shop
  - E.g., the shop prefers to use a certain type of candies, or fills the jar up to a certain level
  - The jars have certain "hyper-parameters"
- Sharing info
  - As you make more guesses, you start sharing what you have learned with your friends about each jar
  - The hierarchical model lets the info flow across models for individual jar

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Computing Bayes Factors as Hierarchical Models

- The computation of Bayes factors can be framed as a hierarchical model
    - The high-level parameter is an index assigned to each model and sampled from a categorical distribution
- We perform inference of the competing models at the same time, using a discrete variable jumping between models
    - The proportion we use to sample each model is proportional to $\Pr(M_k|y)$
- Then we compute the Bayes factors
- The models can be different in the prior, in the likelihood, or both

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Common Problems When Computing Bayes Factors

1. If one model is better than the other, then we will spend more time sampling from it
   - Cons: under-sample one of the models
2. Values of the parameters are updated, even when the parameters are not used to fit that model
   - E.g., when model 0 is chosen, the parameters in model 1 are updated, but they are only restricted by the prior
   - If the prior is too vague, the parameter values might be too far from previous accepted values and the step is rejected
   - TODO: ?

- Solutions to improve sampling
  - Force both models to be visited equally
  - Use “pseudo priors”

Using Sequential Monte Carlo to Compute Bayes Factors

- TODO

Bayes Factors and Information Criteria

-
- If we take the log of Bayes factors, we turn ratio of marginal likelihood into a difference, which is similar to comparing differences in information criteria
- We can interpret each marginal likelihood as having:
  - a fitting term (i.e., how well the model fits the data)
  - penalizing term (i.g., averaging over the prior)
    - more parameters $\rightarrow$ more diffused the prior $\rightarrow$ greater penalty
-
- TODO

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- Bayesian Model Comparison
    - The Balance Between Simplicity and Accuracy
    - Measures of Predictive Accuracy
    - Bayesian Model Selection and Ensemble
    - Bayesian Hypothesis Testing
    - ***Regularizing Priors***

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Priors and Regularization

- Using weakly/informative priors is a way of pushing a model to prevent overfitting and generalize well
- This is similar to the idea of “regularization”
- Regularization
  - Reduce information that a model can represent and reduce chances to capture noise instead of signal
  - E.g., penalize large values for the parameters in a model
  - E.g., ridge and Lasso regression applies regularization to least square method

Popular Regularization Methods in Bayesian Framework

- Ridge regression
  - Normal distribution for coefficients of linear model, pushing them toward zero
- Lasso regression
  - MAP of posterior using Laplace priors for coefficients
  - Because Laplace distribution looks like Gaussian with a sharp peak at zero, it provides “variable selection” since it induces sparsity of model