Fundamentals of Bayesian Analysis with PyMC3 and TFP

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About me



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Introduction

Statistics & Probability in ML/DL?

- Every ML model makes use of statistics.
- Libraries and frameworks tend to **mask** its details.
- Strong **prior assumptions** on data.



Do you use...? Then you assume...

Naive Bayes

Variables to be statistically independent.

Mean Squared Error

Homoscedasticity (variance remains constant and finite for assessment) .

Linear Regression

Error to be **Gaussian distributed** by default in many cases.

Pearson Correlation Coefficient

Linearity and **Homoscedasticity**.

Get to learn Statistics!

It might make the difference (or it might not)



Bayesian Analysis

Bayesian Analysis

- One approach to probabilistic modeling and inference.
- Very close to **human** (natural) decision-making.
- Allows to quantify uncertainty.
- Cares about a priori assumptions (ML tools use them a lot).
- Prior knowledge is modified by **evidence**.



Bayesian

- More intuitive, less used though.
- Parameters (Θ) are unknown.
- Evidence data (**D**) are known.
- Posterior $p(\Theta \mid \mathbf{D})$ summarizes everything about Θ . **MAP**.
- **Credible** Intervals (uncertainty relates to **Θ**).

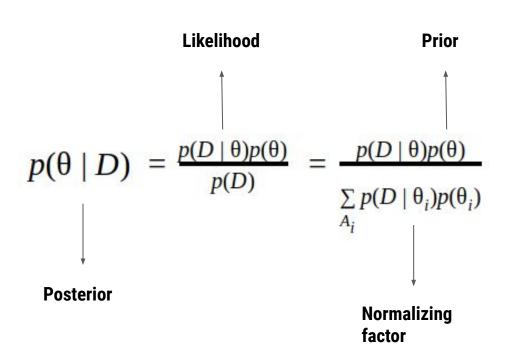
Frequentist

- Less intuitive.
- Parameters (**O**) are not RV.
- Evidence data (**D**) are unknown.
- Likelihood $p(\mathbf{D} \mid \mathbf{\Theta})$ explains the evidence. **MLE**.
- Confidence Intervals (uncertainty relates to interval itself).

Probability Rules

$$p(A \cup B) = p(A) + p(B) - p(A \cap B)$$
 Prob. of Union
$$p(A, B) = p(A \cap B) = p(A \mid B)p(B)$$
Joint prob.
$$p(A) = \sum_{b} p(A, B) = \sum_{b} p(A \mid B = b)p(B = b)$$
Marginal prob.
$$p(A \mid B) = \frac{p(A, B)}{p(B)}, \ p(B) \neq 0$$
Conditional prob.

Bayes' Theorem



Bayes' Theorem

- Bayesian → **Posterior**
- Frequentist → Likelihood (misses prior beliefs)
- Normalizing factor can be a sum
 (discrete) or an integral (continuous)
- It is difficult sometimes to calculate it analytically →Computational methods



Computational Methods

Variational Bayes Inference

- Provides exact, analytical solutions
- Locally optimal

Monte Carlo algorithms

- Draw statistically independent samples (no autocorrelation)

Markov Chain Monte Carlo algorithms

- Metropolis-Hastings \rightarrow Gibbs Sampling | Hamiltonian MC ...

Probabilistic Programming



Probabilistic Programming Tools for Python



PyMC3



TensorFlow Probability

TensorFlow Probability

- Library for probabilistic reasoning and statistical analysis in TensorFlow.
- Supports major **TF features**: *Eager* mode,
 HW acceleration, autodiff, vectorization...

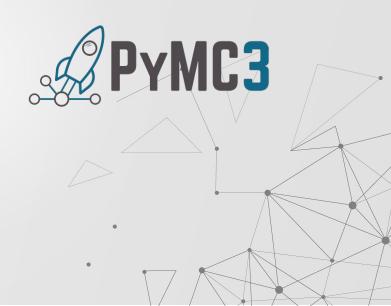
Low-level blocks: Distributions | Bijectors

High-level blocks: MCMC | Probabilistic layers | Structural time series | Edward2



PyMC3

- Library for probabilistic reasoning and statistical analysis over Theano.
- Supports **MCMC** and **Variational Bayes** inference methods.
- Easy-to-use **Python** user interface.
- Defines models as Python context managers.



Example: Bayesian Linear Regression

Conclusions

Conclusions

- **Simplicity:** PyMC3 is designed to provide a more straightforward user experience than TFP.
- Control: TFP is more open to tuning and modifications.
- **Support:** TFP has a better community support.
- **Computation:** TFP relies on top features of TF.



