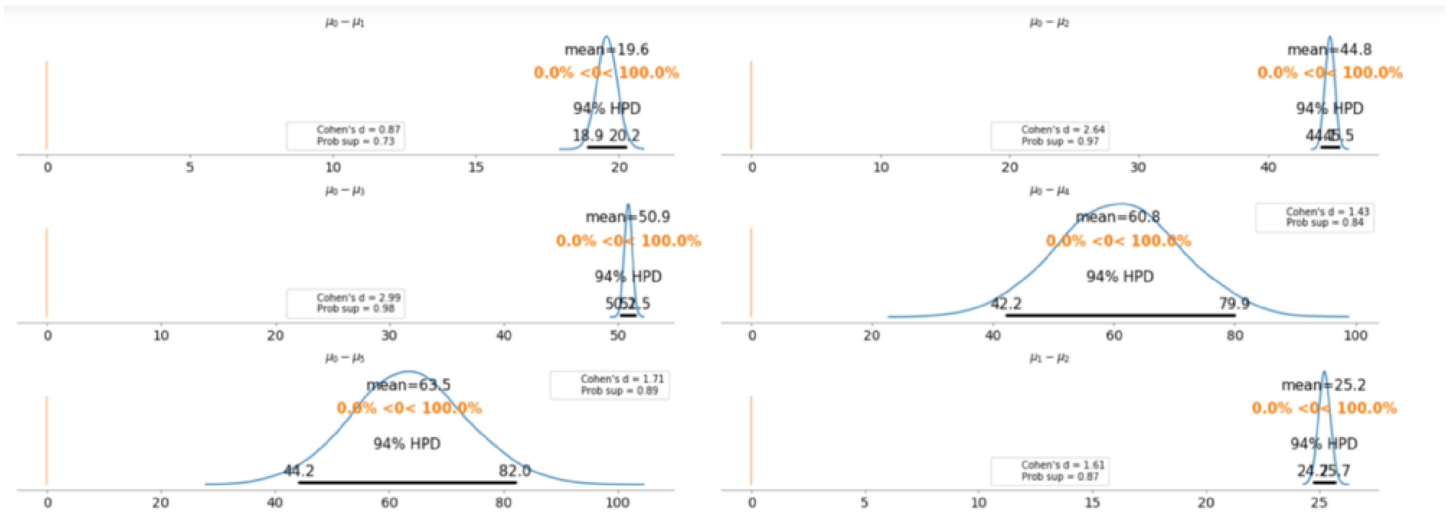


Hands On Bayesian Statistics with Python, PyMC3 & ArviZ

Gaussian Inference, Posterior Predictive Checks, Group Comparison, Hierarchical Linear Regression

Susan Li
Jul 17, 2019 · 10 min read

If you think Bayes' theorem is counter-intuitive and Bayesian statistics, which builds upon Baye's theorem, can be very hard to understand. I am with you.

There are countless reasons why we should learn Bayesian statistics, in particular, Bayesian statistics is emerging as a powerful framework to express and understand next-generation deep neural networks.

I believe that for the things we have to learn before we can do them, we learn by doing them. And nothing in life is so hard that we can't make it easier by the way we take it.

So, this is my way of making it easier: Rather than too much of theories or terminologies at the beginning, let's focus on the mechanics of Bayesian analysis, in particular, how to do Bayesian analysis and visualization with PyMC3 & ArviZ. Prior to memorizing the endless terminologies, we will code the solutions and visualize the results, and using the terminologies and theories to explain the models along the way.

PyMC3 is a Python library for probabilistic programming with a very simple and intuitive syntax. ArviZ, a Python library that works hand-in-hand with PyMC3 and can help us interpret and visualize posterior distributions.

And we will apply Bayesian methods to a practical problem, to show an end-to-end Bayesian analysis that move from framing the question to building models to eliciting prior probabilities to implementing in Python the final posterior distribution.

Before we start, let's get some basic intuitions out of the way:

Bayesian models are also known as **probabilistic models** because they are built using probabilities. And Bayesian's use probabilities as a tool to quantify uncertainty. Therefore, the answers we get are **distributions** not point estimates.

Bayesian Approach Steps

Step 1: Establish a belief about the data, including Prior and Likelihood functions.

Step 2, Use the data and probability, in accordance with our belief of the data, to update our model, check that our model agrees with the original data.

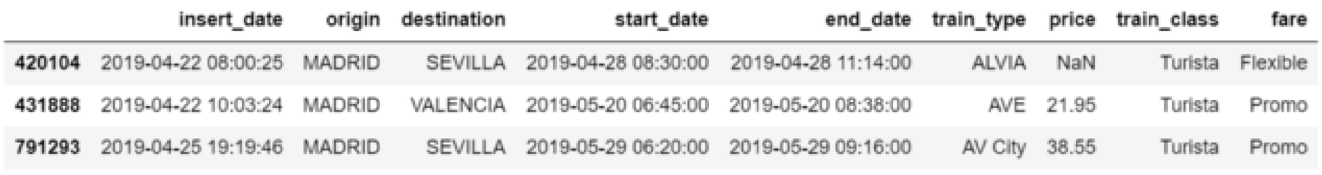
Step 3, Update our view of the data based on our model.

The Data

Since I am interested in using machine learning for price optimization, I decide to apply Bayesian methods to a Spanish High Speed Rail tickets pricing data set that can be found here. Appreciate The Gurus team for scraping the data set.

```
from scipy import stats
import arviz as az
import numpy as np
import matplotlib.pyplot as plt
import pymc3 as pm
import seaborn as sns
import pandas as pd
from theano import shared
from sklearn import preprocessing

print('Running on PyMC3 v{}'.format(pm.__version__))
```

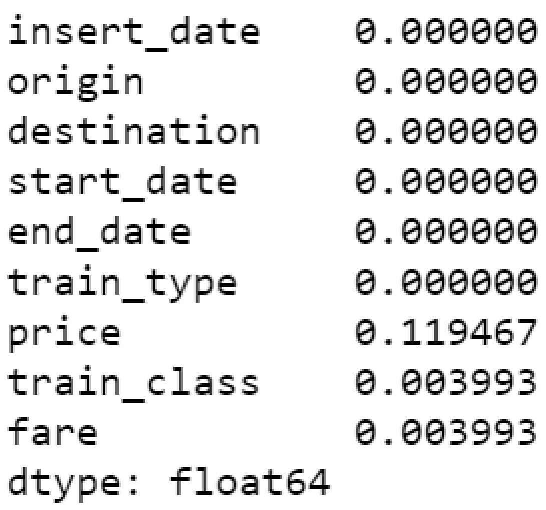
```
data = pd.read_csv('renfe.csv')
data.drop('Unnamed: 0', axis = 1, inplace=True)
data = data.sample(frac=0.01, random_state=99)
data.head(3)
```



	insert_date	origin	destination	start_date	end_date	train_type	price	train_class	fare
420104	2019-04-22 08:00:25	MADRID	SEVILLA	2019-04-28 08:30:00	2019-04-28 11:14:00	ALVIA	NaN	Turista	Flexible
431888	2019-04-22 10:03:24	MADRID	VALENCIA	2019-05-20 06:45:00	2019-05-20 08:38:00	AVE	21.95	Turista	Promo
791293	2019-04-25 19:19:46	MADRID	SEVILLA	2019-05-29 06:20:00	2019-05-29 09:16:00	AV City	38.55	Turista	Promo

Table 1

```
data.isnull().sum()/len(data)
```



```
insert_date    0.000000
origin         0.000000
destination    0.000000
start_date     0.000000
end_date       0.000000
train_type     0.000000
price          0.119467
train_class    0.003993
fare           0.003993
dtype: float64
```

Figure 1

There are 12% of values in price column are missing, I decide to fill them with the mean of the respective fare types. Also fill the other two categorical columns with the most common values.

```
data['train_class'] =
data['train_class'].fillna(data['train_class'].mode().iloc[0])
data['fare'] = data['fare'].fillna(data['fare'].mode().iloc[0])
data['price'] = data.groupby('fare').transform(lambda x:
x.fillna(x.mean()))
```

Gaussian Inferences

```
az.plot_kde(data['price'].values, rug=True)
plt.yticks([0], alpha=0);
```

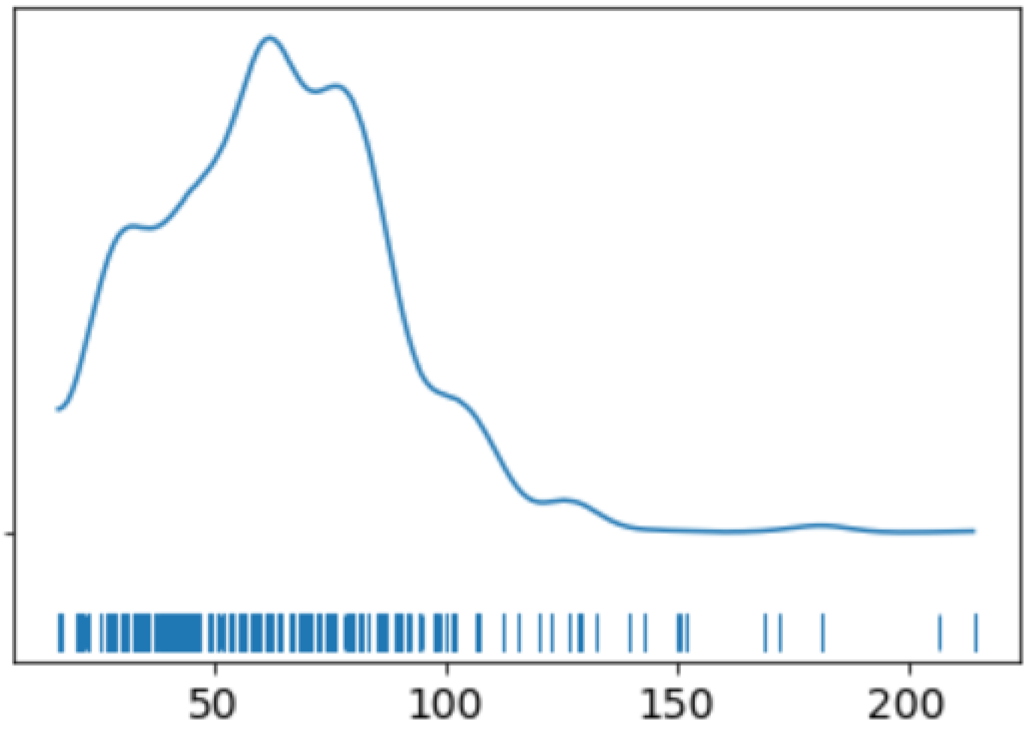


Figure 2

The KDE plot of the rail ticket price shows a Gaussian-like distribution, except for about several dozens of data points that are far away from the mean.

Let’s assume that a Gaussian distribution is a proper description of the rail ticket price. Since we do not know the mean or the standard deviation, we must set priors for both of them. Therefore, a reasonable model could be as follows.

Model

We will perform Gaussian inferences on the ticket price data. Here’s some of the modelling choices that go into this.

We would instantiate the Models in PyMC3 like this:

- Model specifications in PyMC3 are wrapped in a with-statement.

Choices of priors:

- μ, mean of a population. Normal distribution, very wide. I do not know the possible values of μ, I can set priors reflecting my ignorance. From experience I know that train ticket price can not be lower than 0 or higher than 300, so I set the boundaries of the uniform distribution to be 0 and 300. You may have different experience and set the different boundaries. That is totally fine. And if you have more reliable prior information than I do, please use it!

- σ, standard deviation of a population. Can only be positive, therefore use HalfNormal distribution. Again, very wide.

Choices for ticket price likelihood function:

- y is an observed variable representing the data that comes from a normal distribution with the parameters μ and σ.
- Draw 1000 posterior samples using NUTS sampling.

Using PyMC3, we can write the model as follows:

```python
with pm.Model() as model_g:
    μ = pm.Uniform('μ', lower=0, upper=300)
    σ = pm.HalfNormal('σ', sd=10)
    y = pm.Normal('y', mu=μ, sd=σ, observed=data['price'].values)
    trace_g = pm.sample(1000, tune=1000)
```

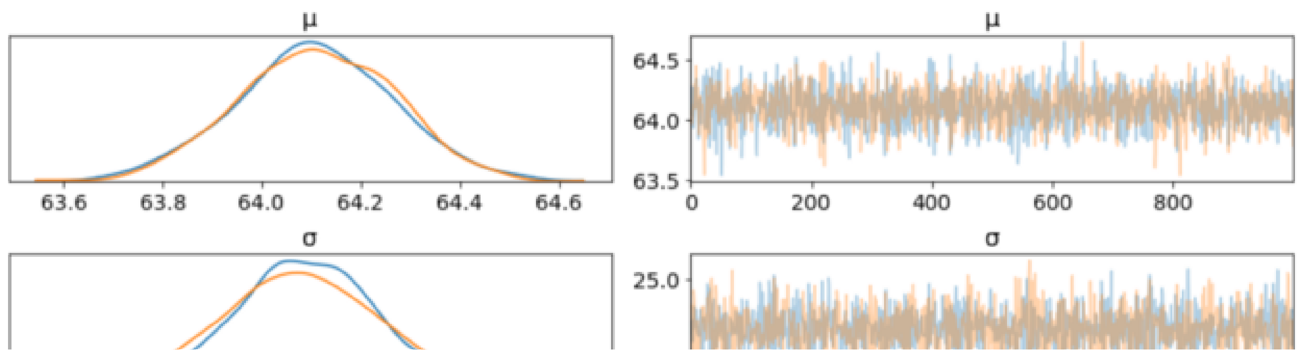
model_g.py hosted with ❤ by GitHub view raw

model_g.py

The y specifies the likelihood. This is the way in which we tell PyMC3 that we want to condition for the unknown on the knows (data).

We plot the gaussian model trace. This runs on a Theano graph under the hood.

```
az.plot_trace(trace_g);
```



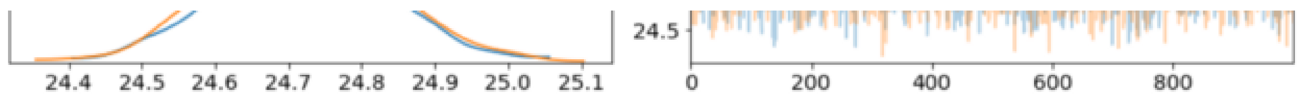


Figure 3

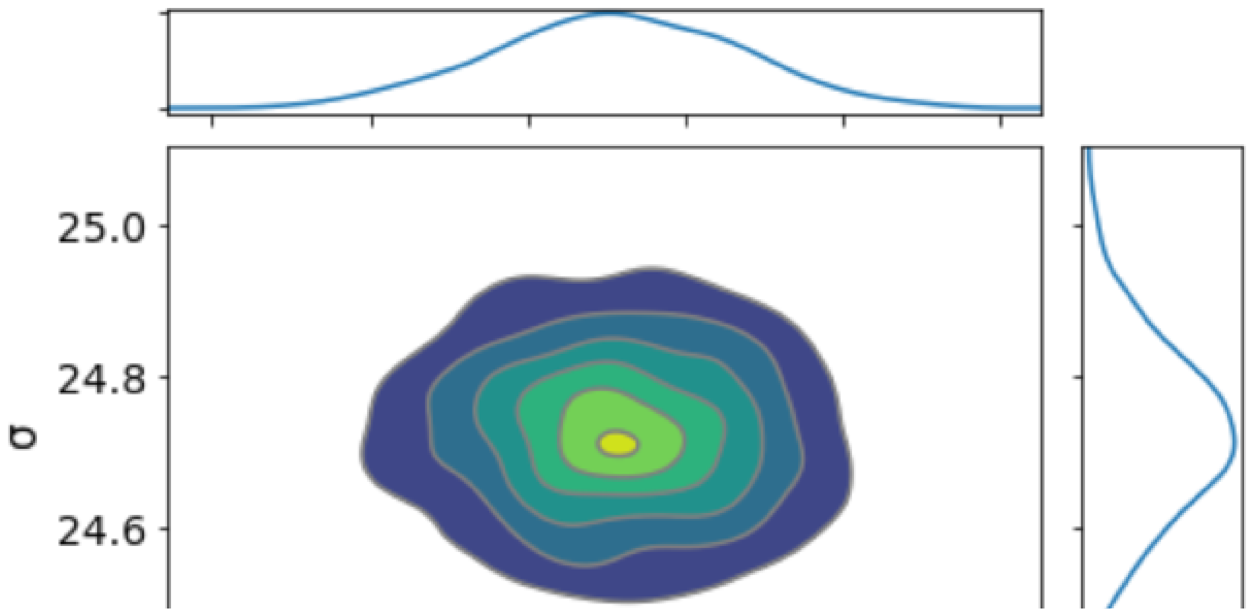
- On the left, we have a KDE plot, — for each parameter value on the x-axis we get a probability on the y-axis that tells us how likely that parameter value is.
- On the right, we get the individual sampled values at each step during the sampling. From the trace plot, we can visually get the plausible values from the posterior.
- The above plot has one row for each parameter. For this model, the posterior is bi-dimensional, and so the above figure is showing the marginal distributions of each parameter.

There are a couple of things to notice here:

- Our sampling chains for the individual parameters (left) seem well converged and stationary (there are no large drifts or other odd patterns).
- The maximum posterior estimate of each variable (the peak in the left side distributions) is very close to the true parameters.

We can plot a joint distributions of parameters.

```
az.plot_joint(trace_g, kind='kde', fill_last=False);
```



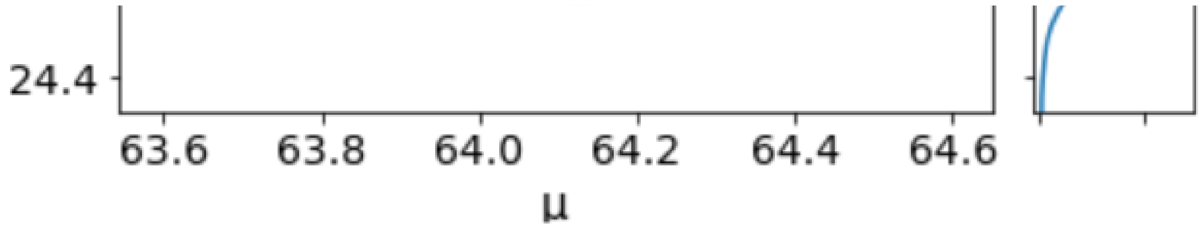
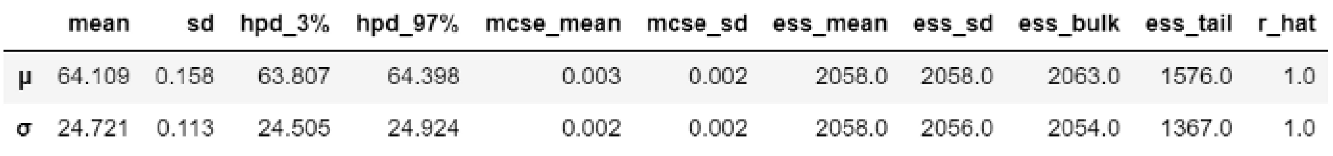


Figure 4

I don't see any correlation between these two parameters. This means we probably do not have collinearity in the model. This is good.

We can also have a detailed summary of the posterior distribution for each parameter.

```
az.summary(trace_g)
```



	mean	sd	hpd_3%	hpd_97%	mcse_mean	mcse_sd	ess_mean	ess_sd	ess_bulk	ess_tail	r_hat
μ	64.109	0.158	63.807	64.398	0.003	0.002	2058.0	2058.0	2063.0	1576.0	1.0
σ	24.721	0.113	24.505	24.924	0.002	0.002	2058.0	2056.0	2054.0	1367.0	1.0

Table 2

We can also see the above summary visually by generating a plot with the mean and Highest Posterior Density (HPD) of a distribution, and to interpret and report the results of a Bayesian inference.

```
az.plot_posterior(trace_g);
```

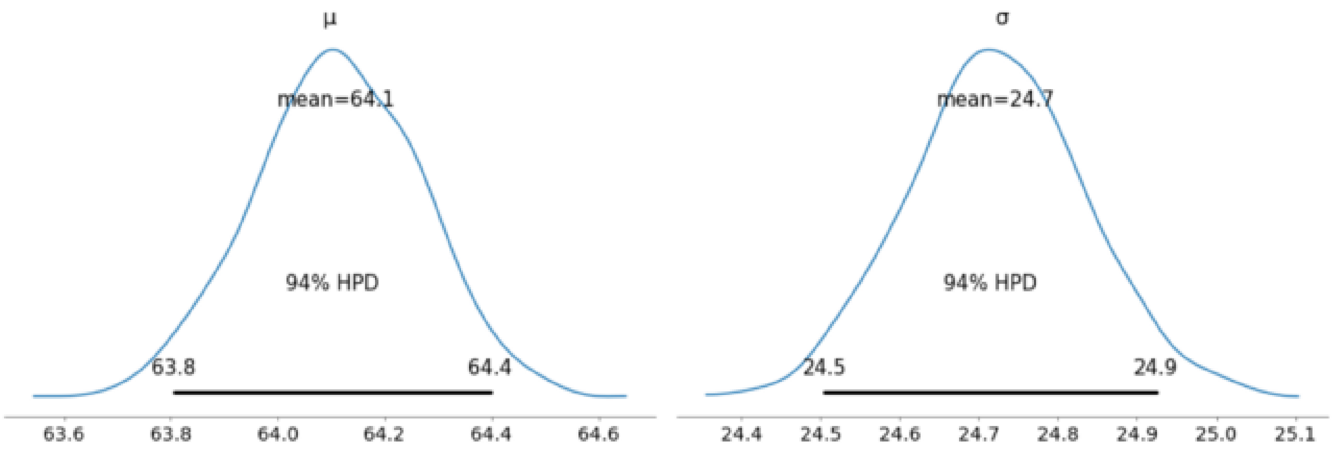


Figure 5

- Unlike Frequentist inference, in Bayesian inference, we get the entire distribution of the values.
- Every time ArviZ computes and reports a HPD, it will use, by default, a value of 94%.
- Please note that HPD intervals are not the same as confidence intervals.
- Here we can interpret as such that there is 94% probability the belief is between 63.8 euro and 64.4 euro for the mean ticket price.

We can verify the convergence of the chains formally using the Gelman Rubin test. Values close to 1.0 mean convergence.

```
pm.gelman_rubin(trace_g)
```

```
{'μ': 0.999662520982377, 'σ': 0.9996863859790907}
```

```
bfmi = pm.bfmi(trace_g)
max_gr = max(np.max(gr_stats) for gr_stats in
pm.gelman_rubin(trace_g).values())
(pm.energyplot(trace_g, legend=False, figsize=(6,
4)).set_title("BFMI = {}\nGelman-Rubin = {}".format(bfmi, max_gr)));
```

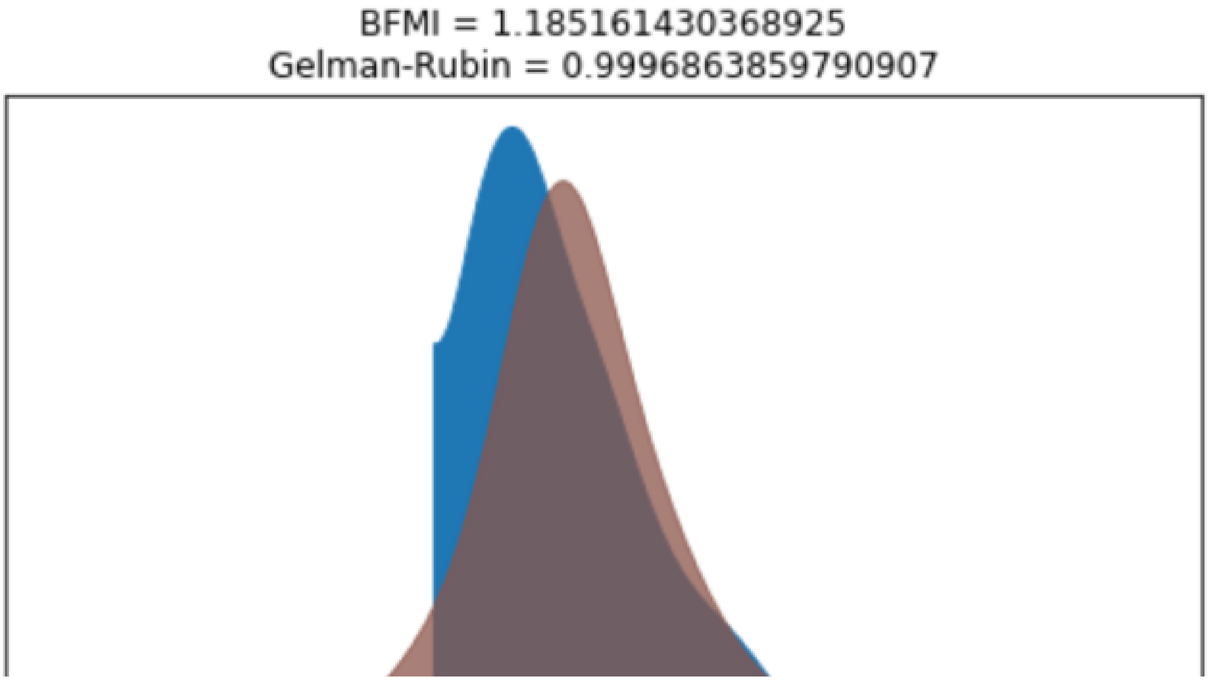


Figure 6

Our model has converged well and the Gelman-Rubin statistic looks fine.

Posterior Predictive Checks

- Posterior predictive checks (PPCs) are a great way to validate a model. The idea is to generate data from the model using parameters from draws from the posterior.
- Now that we have computed the posterior, we are going to illustrate how to use the simulation results to derive predictions.
- The following function will randomly draw 1000 samples of parameters from the trace. Then, for each sample, it will draw 25798 random numbers from a normal distribution specified by the values of μ and σ in that sample.

```
ppc = pm.sample_posterior_predictive(trace_g, samples=1000,
model=model_g)

np.asarray(ppc['y']).shape
```

```
(1000, 25798)
```

Now, ppc contains 1000 generated data sets (containing 25798 samples each), each using a different parameter setting from the posterior.

```
_, ax = plt.subplots(figsize=(10, 5))
ax.hist([y.mean() for y in ppc['y']], bins=19, alpha=0.5)
ax.axvline(data.price.mean())
ax.set(title='Posterior predictive of the mean', xlabel='mean(x)',
ylabel='Frequency');
```

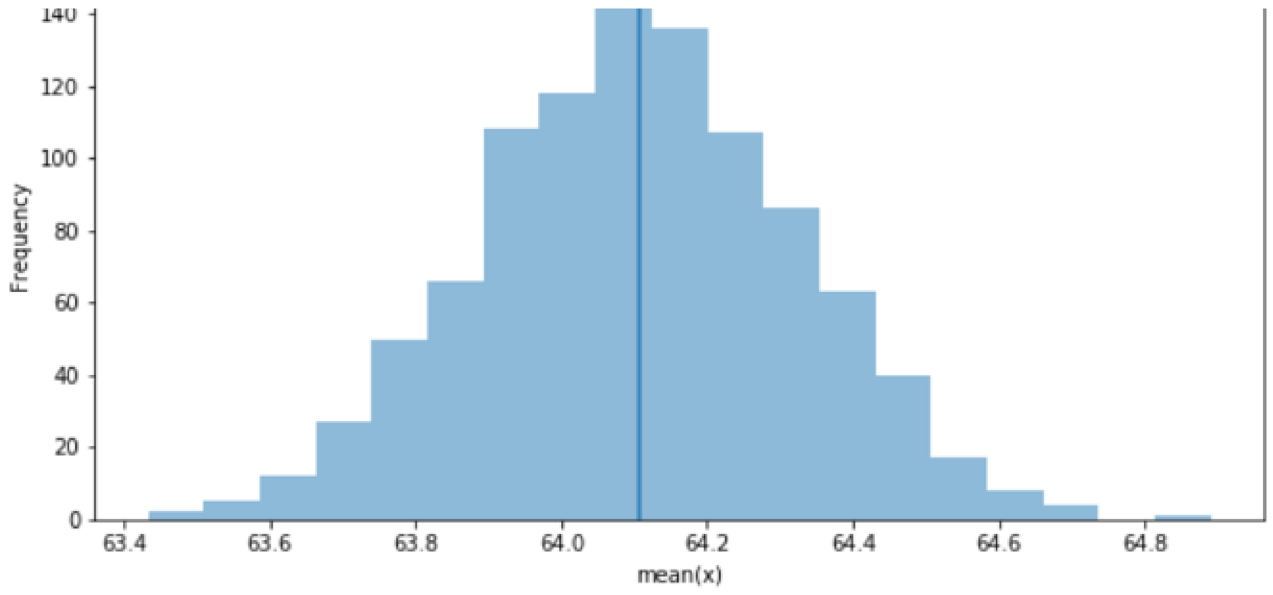


Figure 7

The inferred mean is very close to the actual rail ticket price mean.

Group Comparison

We may be interested in how price compare under different fare types. We are going to focus on estimating the effect size, that is, quantifying the difference between two fare categories. To compare fare categories, we are going to use the mean of each fare type. Because we are Bayesian, we will work to obtain a posterior distribution of the differences of means between fare categories.

We create three variables:

- The price variable, representing the ticket price.
- The idx variable, a categorical dummy variable to encode the fare categories with numbers.
- And finally the groups variable, with the number of fare categories (6)

```
price = data['price'].values
idx = pd.Categorical(data['fare'],
                     categories=['Flexible', 'Promo', 'Promo +',
'Adulto ida', 'Mesa', 'Individual-Flexible']).codes
groups = len(np.unique(idx))
```

The model for the group comparison problem is almost the same as the previous model. the only difference is that μ and σ are going to be vectors instead of scalar variables. This means that for the priors, we pass a shape argument and for the likelihood, we properly index the means and sd variables using the idx variable:

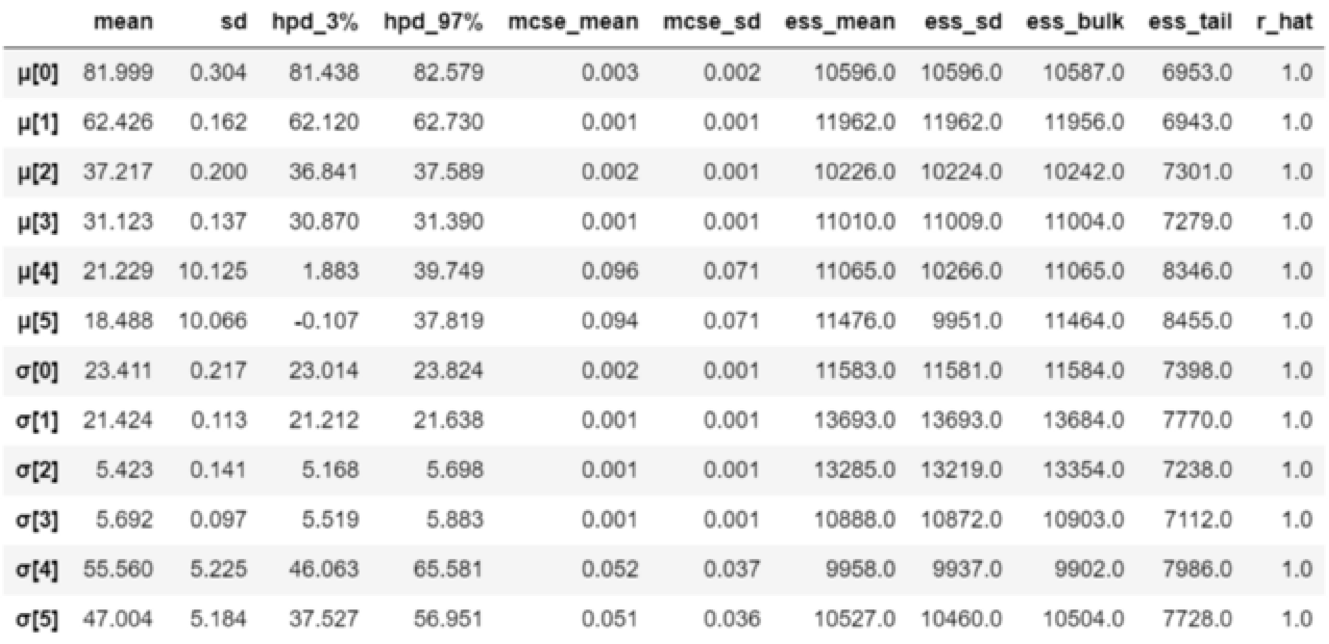
```
with pm.Model() as comparing_groups:
    μ = pm.Normal('μ', mu=0, sd=10, shape=groups)
    σ = pm.HalfNormal('σ', sd=10, shape=groups)

    y = pm.Normal('y', mu=μ[idx], sd=σ[idx], observed=price)

    trace_groups = pm.sample(5000, tune=5000)
```

comparing_groups.py hosted with ❤ by GitHub view raw

comparing_groups.py

With 6 groups (fare categories), its a little hard to plot trace plot for μ and σ for every group. So, we create a summary table:

```
flat_fares = az.from_pymc3(trace=trace_groups)
fares_gaussian = az.summary(flat_fares)
fares_gaussian
```



	mean	sd	hpd_3%	hpd_97%	mcse_mean	mcse_sd	ess_mean	ess_sd	ess_bulk	ess_tail	r_hat
μ[0]	81.999	0.304	81.438	82.579	0.003	0.002	10596.0	10596.0	10587.0	6953.0	1.0
μ[1]	62.426	0.162	62.120	62.730	0.001	0.001	11962.0	11962.0	11956.0	6943.0	1.0
μ[2]	37.217	0.200	36.841	37.589	0.002	0.001	10226.0	10224.0	10242.0	7301.0	1.0
μ[3]	31.123	0.137	30.870	31.390	0.001	0.001	11010.0	11009.0	11004.0	7279.0	1.0
μ[4]	21.229	10.125	1.883	39.749	0.096	0.071	11065.0	10266.0	11065.0	8346.0	1.0
μ[5]	18.488	10.066	-0.107	37.819	0.094	0.071	11476.0	9951.0	11464.0	8455.0	1.0
σ[0]	23.411	0.217	23.014	23.824	0.002	0.001	11583.0	11581.0	11584.0	7398.0	1.0
σ[1]	21.424	0.113	21.212	21.638	0.001	0.001	13693.0	13693.0	13684.0	7770.0	1.0
σ[2]	5.423	0.141	5.168	5.698	0.001	0.001	13285.0	13219.0	13354.0	7238.0	1.0
σ[3]	5.692	0.097	5.519	5.883	0.001	0.001	10888.0	10872.0	10903.0	7112.0	1.0
σ[4]	55.560	5.225	46.063	65.581	0.052	0.037	9958.0	9937.0	9902.0	7986.0	1.0
σ[5]	47.004	5.184	37.527	56.951	0.051	0.036	10527.0	10460.0	10504.0	7728.0	1.0

Table 3

It is obvious that there are significant differences between groups (i.e. fare categories) on the mean.

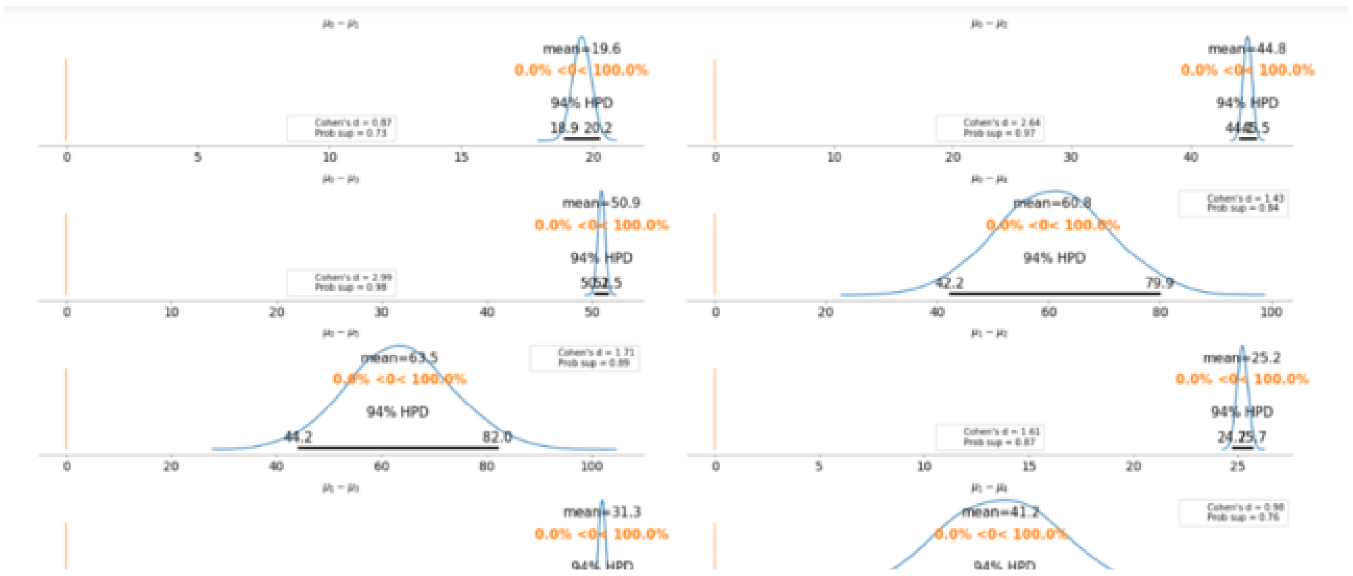
To make it clearer, we plot the difference between each fare category without repeating the comparison.

- Cohen's d is an appropriate effect size for the comparison between two means. Cohen's d introduces the variability of each group by using their standard deviations.
- probability of superiority (ps) is defined as the probability that a data point taken at random from one group has a larger value than one taken at random from another group.

```python
dist = stats.norm()

_, ax = plt.subplots(5, 2, figsize=(20, 12), constrained_layout=True)

comparisons = [(i, j) for i in range(6) for j in range(i+1, 6)]
pos = [(k, l) for k in range(5) for l in (0, 1)]

for (i, j), (k, l) in zip(comparisons, pos):
    means_diff = trace_groups['μ'][:, i] - trace_groups['μ'][:, j]
    d_cohen = (means_diff / np.sqrt((trace_groups['σ'][:, i]**2 + trace_groups['σ'][:,
    ps = dist.cdf(d_cohen/(2**0.5))
    az.plot_posterior(means_diff, ref_val=0, ax=ax[k, l])
    ax[k, l].set_title(f'$\mu_{i}-\mu_{j}$')
    ax[k, l].plot(
        0, label=f"Cohen's d = {d_cohen:.2f}\nProb sup = {ps:.2f}", alpha=0)
    ax[k, l].legend();
```

difference_plot.py hosted with ❤ by GitHub view raw

difference_plot.py



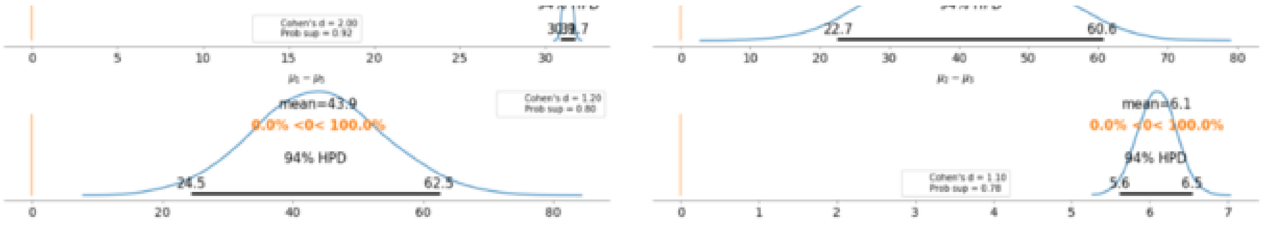


Figure 8

Basically, the above plot tells us that none of the above comparison cases where the 94% HPD includes the reference value of zero. This means for all the examples, we can rule out a difference of zero. The average differences range of 6.1 euro to 63.5 euro are large enough that it can justify for customers to purchase tickets according to different fare categories.

Bayesian Hierarchical Linear Regression

We want to build a model to estimate the rail ticket price of each train type, and, at the same time, estimate the price of all the train types. This type of model is known as a **hierarchical model** or **multilevel model.**

- Encoding the categorical variable.
- The idx variable, a categorical dummy variable to encode the train types with numbers.
- And finally the groups variable, with the number of train types (16)

```
def replace_fare(fare):

    if fare == 'Adulto ida':
        return 1
    elif fare == 'Promo +':
        return 2
    elif fare == 'Promo':
        return 3
    elif fare == 'Flexible':
        return 4
    elif fare == 'Individual-Flexible':
        return 5
    elif fare == 'Mesa':
        return 6

data['fare_encode'] = data['fare'].apply(lambda x: replace_fare(x))

label_encoder = preprocessing.LabelEncoder()
```

```
data['train_type_encode']= label_encoder.fit_transform(data['train_type'])

train_type_names = data.train_type.unique()
train_type_idx = data.train_type_encode.values

n_train_types = len(data.train_type.unique())

data[['train_type', 'price', 'fare_encode']].head()
```

encode_cat.py hosted with ❤ by GitHub view raw

encode_cat.py

	train_type	price	fare_encode
420104	ALVIA	82.077189	4
431888	AVE	21.950000	3
791293	AV City	38.550000	3
678876	LD-MD	34.350000	2
86381	AVE	45.300000	3

Table 4

The relevant part of the data we will model looks as above. And we are interested in whether different train types affect the ticket price.

Hierarchical Model

```
with pm.Model() as hierarchical_model:
    # global model parameters
    α_μ_tmp = pm.Normal('α_μ_tmp', mu=0., sd=100)
    α_σ_tmp = pm.HalfNormal('α_σ_tmp', 5.)
    β_μ = pm.Normal('β_μ', mu=0., sd=100)
    β_σ = pm.HalfNormal('β_σ', 5.)

    # train type specific model parameters
    α_tmp = pm.Normal('α_tmp', mu=α_μ_tmp, sd=α_σ_tmp, shape=n_train_types)
    # Intercept for each train type, distributed around train type mean
    β = pm.Normal('β', mu=β_μ, sd=β_σ, shape=n_train_types)
    # Model error
    eps = pm.HalfCauchy('eps', 5.)

    fare_est = α_tmp[train_type_idx] + β[train_type_idx]*data.fare_encode.values

    # Data likelihood
    fare_like = pm.Normal('fare_like', mu=fare_est, sd=eps, observed=data.price)

with hierarchical_model:
    hierarchical_trace = pm.sample(2000, tune=2000, target_accept=.9)

pm.traceplot(hierarchical_trace, var_names=['α_μ_tmp', 'β_μ', 'α_σ_tmp', 'β_σ', 'eps'])
```

hierarchical_model.py hosted with ❤ by GitHub view raw

hierarchical_model.py

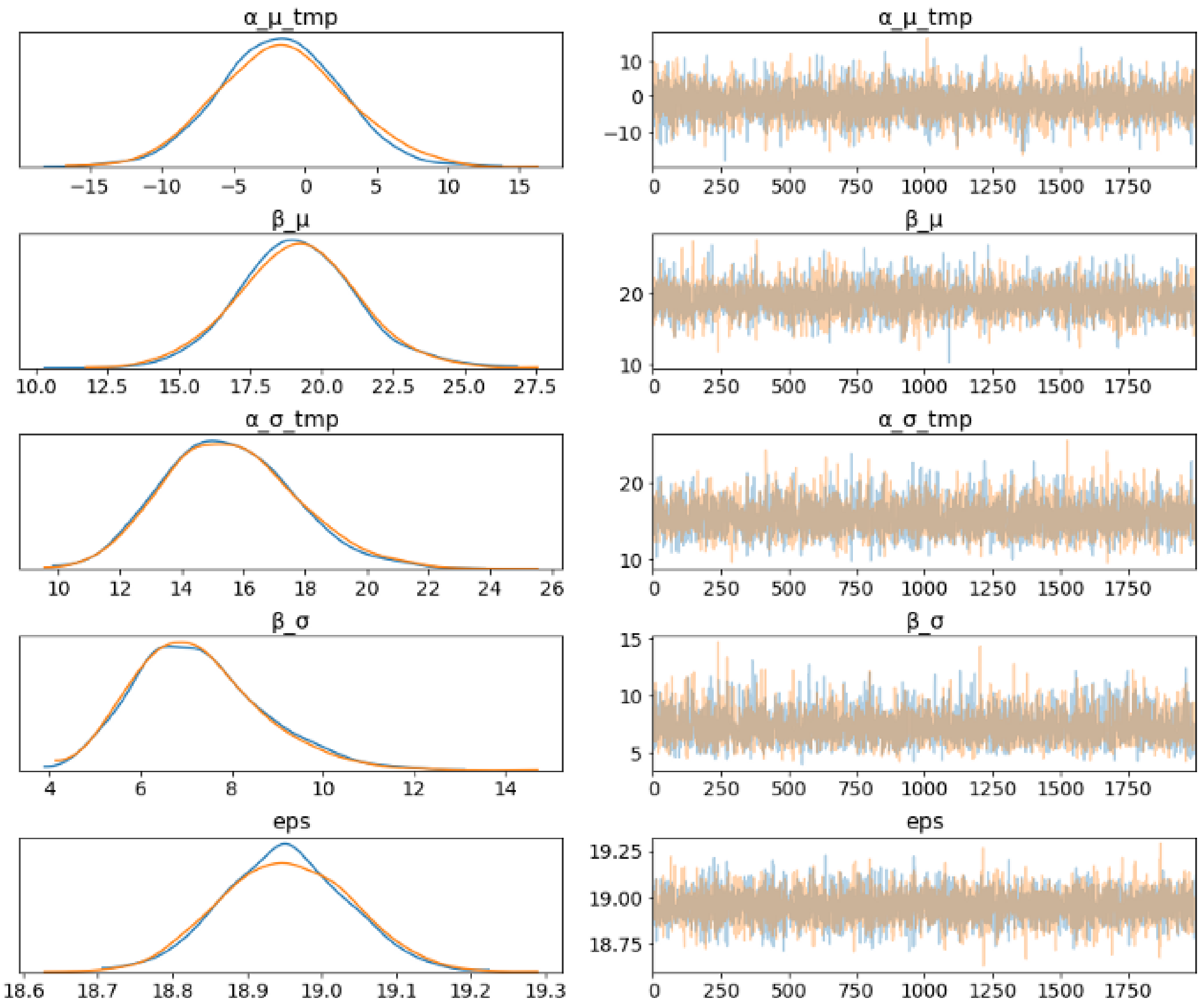


Figure 9

The marginal posteriors in the left column are highly informative, “α_μ_tmp” tells us the group mean price levels, “β_μ” tells us that purchasing fare category “Promo +” increases price significantly compare to fare type “Adulto ida”, and purchasing fare category “Promo” increases price significantly compare to fare type “Promo +”, and so on (no mass under zero).

```
pm.traceplot(hierarchical_trace, var_names=['α_tmp'], coords=
{'α_tmp_dim_0': range(5)});
```

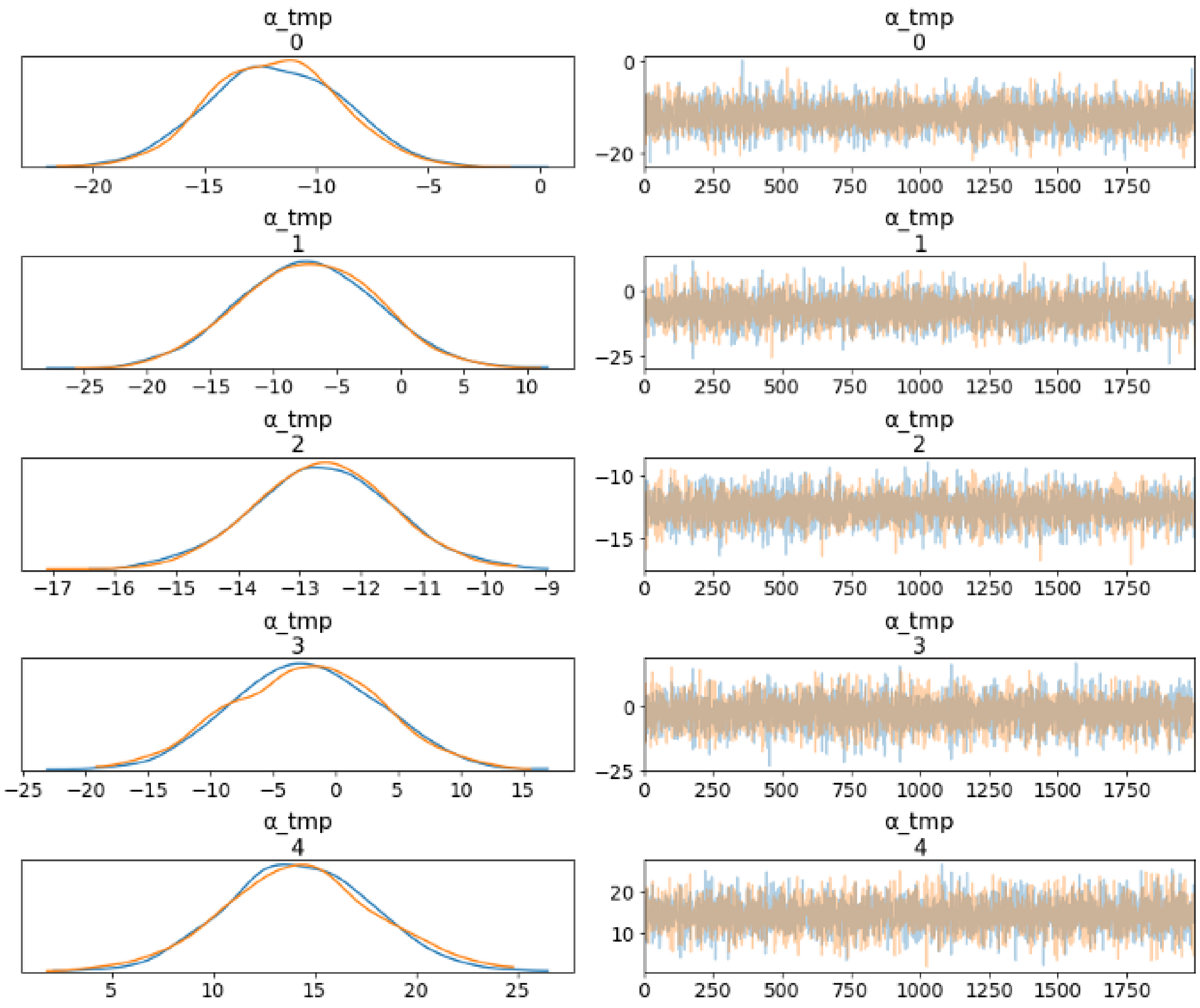


Figure 10

Among 16 train types, we may want to look at how 5 train types compare in terms of the ticket price. We can see by looking at the marginals for “α_tmp” that there is quite some difference in prices between train types; the different widths are related to how much confidence we have in each parameter estimate — the more measurements per train type, the higher our confidence will be.

Having uncertainty quantification of some of our estimates is one of the powerful things about Bayesian modelling. We’ve got a Bayesian credible interval for the price of different train types.

```
az.plot_forest(hierarchical_trace, var_names=['α_tmp', 'β'],
combined=True);
```

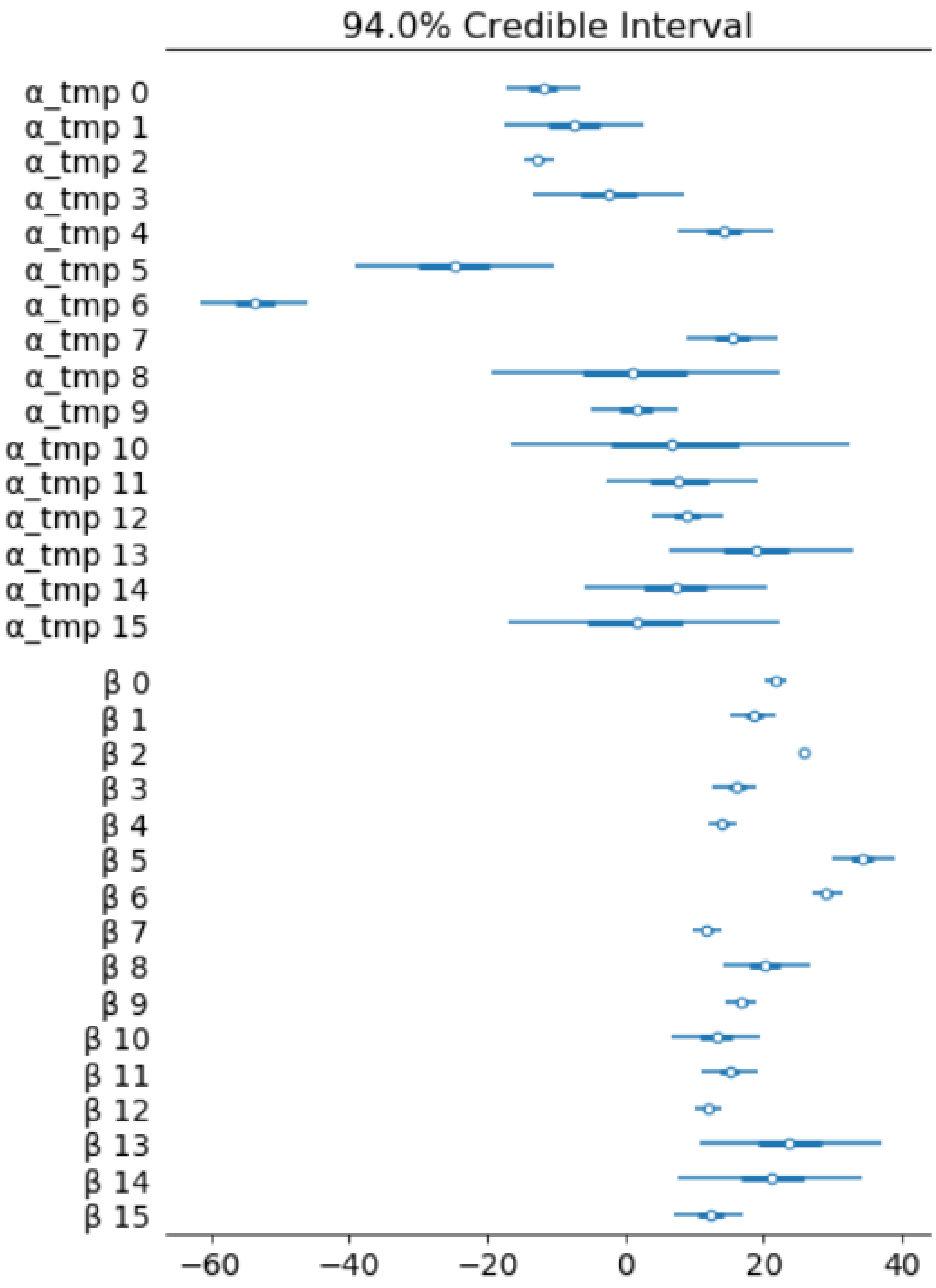


Figure 11

Lastly, we may want to compute r squared:

```
ppc = pm.sample_posterior_predictive(hierarchical_trace,
samples=2000, model=hierarchical_model)
az.r2_score(data.price.values, ppc['fare_like'])
```

```
r2        0.412089
r2_std    0.007676
dtype: float64
```

The objective of this post is to learn, practice and explain Bayesian, not to produce the best possible results from the data set. Otherwise, we would have gone with XGBoost directly.

Jupyter notebook can be found on Github, enjoy the rest of the week.

References:

GLM: Hierarchical Linear Regression - PyMC3 3.6 documentation

Gelman et al.'s (2007) radon dataset is a classic for hierarchical modeling. In this dataset the amount of the…

docs.pymc.io

A Hierarchical model for Rugby prediction - PyMC3 3.6 documentation

Edit description

docs.pymc.io

The book: Bayesian Analysis with Python

Machine Learning Data Science Bayesian Statistics Tutorial Python