# Module 10: Markov Chain Monte Carlo (MCMC) - Part 2

## **Introduction to PyMC3**

In this section we demonstrate how the Python PyMC3 library can be applied for Bayesian inference analysis and for the estimation of model parameters using the Monte Carlo Markov Chain technique.

#### References:

- <a href="https://github.com/markdregan/Bayesian-Modelling-in-Python">https://github.com/markdregan/Bayesian-Modelling-in-Python</a>)

  (https://github.com/markdregan/Bayesian-Modelling-in-Python)
- <a href="https://github.com/CamDavidsonPilon/Probabilistic-Programming-and-Bayesian-Methods-for-Hackers/">https://github.com/CamDavidsonPilon/Probabilistic-Programming-and-Bayesian-Methods-for-Hackers/</a>)
- https://docs.pymc.io (https://docs.pymc.io)

## PyMC3 installation

- via pypi: pip install pymc3
- via conda-forge: conda install -c conda-forge pymc3
- the latest (may be unstable) version can be downloaded from github.com: pip install git+https://github.com/pymc-devs/pymc3

# Bayesian method of estimating model parameters

In this example, a Bayesian approach is used to estimate model parameters. This dataset is taken from Mark Regan's chat dataset; it shows the time taken to respond to messages.

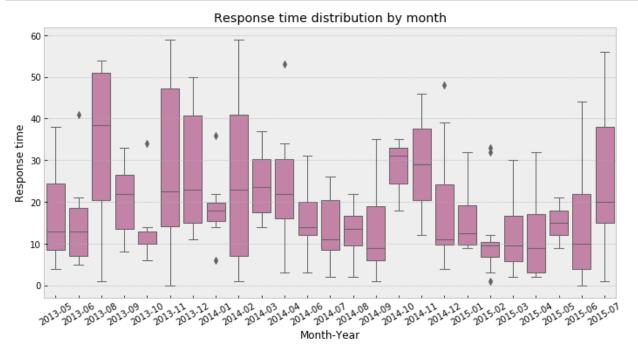
In the Bayesian approach the data is considered to be generated by a random process.

Because the response time is count data, it is natural to model it as a Poisson distribution. The goal here is to estimate the parameter of the distribution  $\lambda$  and represent the uncertainty in this parameter.

In other words we need to find the posterior distribution for the parameter  $\lambda$  using the Bayesian formula:

$$\underbrace{posterior}_{p(\lambda \mid Data)} = \underbrace{\frac{p(Data \mid \lambda) \cdot prior}{p(Data)}}_{\text{marginal likelihood}} \underbrace{\frac{prior}{p(\lambda)}}_{\text{prior}}$$

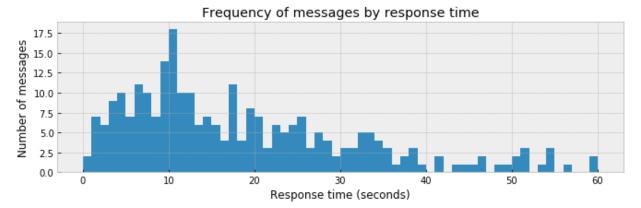
```
In [2]: # Let's plot the observed data distribution
        fig = plt.figure(figsize=(10,10))
        ax = fig.add subplot(211)
        order = np.sort(messages['year_month'].unique())
        sns.boxplot(x=messages['year month'], y=messages['time delay seconds'], ord
          = ax.set_title('Response time distribution by month')
          = ax.set xlabel('Month-Year')
          = ax.set_ylabel('Response time')
          = plt.xticks(rotation=30)
        \# ax = fig.add subplot(212)
        # plt.hist(messages['time delay seconds'].values, range=[0, 60], bins=60, h
        # = ax.set title('Response time distribution')
          = ax.set xlabel('Response time (seconds)')
        # = ax.set ylabel('Number of messages')
        plt.tight layout()
        # fig = plt.figure(figsize=(11,3))
            = plt.title('Frequency of messages by response time')
            = plt.xlabel('Response time (seconds)')
          = plt.ylabel('Number of messages')
            = plt.hist(messages['time delay seconds'].values,
                       range=[0, 60], bins=60, histtype='stepfilled')
```



```
In [3]: messages.describe()
```

#### Out[3]:

	message_length	num_participants	time_delay_seconds	time_delay_mins	day_of_week	is_we
count	266.000000	266.000000	266.000000	266.000000	266.000000	266.0
mean	31.500000	2.139098	18.041353	0.992481	2.357143	0.0
std	28.502003	0.498501	13.430821	0.086547	1.530904	0.2
min	1.000000	2.000000	0.000000	0.000000	0.000000	0.0
25%	10.000000	2.000000	8.000000	1.000000	1.000000	0.0
50%	23.000000	2.000000	14.000000	1.000000	2.000000	0.0
75%	43.750000	2.000000	25.000000	1.000000	3.000000	0.0
max	145.000000	4.000000	59.000000	1.000000	6.000000	1.(



To run this analysis, we need to choose the likelihood and the prior distribution.

- Observed data: counts of response time for each conversation;
- Likelihood: These data were generated by a random process which can be represented as a Poisson distribution;
- For the prior, the distribution of the Poisson distribution  $\lambda$  has to be chosen. From the observed data, we know that this parameter is between 0 and 60. We can start to model  $\lambda$  as a uniform distribution because we do not have an opinion as to where within this range to expect it.

To derive the posterior distribution, the MCMC sampler draws parameter  $\lambda$  values from the prior distribution and computes the likelihood that the observed data came from a distribution with these parameter values.

$$\underbrace{posterior}_{p(\lambda \mid Data)} \propto \underbrace{p(Data \mid \lambda)}_{p(\lambda)} \cdot \underbrace{prior}_{p(\lambda)}$$

As the MCMC sampler draws values from the parameter priors, it computes the likelihood of these parameters given the data - and the sampling method (for example, Metropolis) will try to guide the sampler towards parameter values of higher probability.

```
In [5]: with pm.Model() as model:
    lambda_ = pm.Uniform('lambda', lower=0, upper=60)
    likelihood = pm.Poisson('likelihood', mu=lambda_, observed=messages['ti
    start = pm.find_MAP()
    step = pm.Metropolis()
    trace = pm.sample(1000000, step, start=start, progressbar=True)
```

/anaconda3/lib/python3.7/site-packages/pymc3/tuning/starting.py:61: UserW arning: find\_MAP should not be used to initialize the NUTS sampler, simply call pymc3.sample() and it will automatically initialize NUTS in a better way.

```
warnings.warn('find_MAP should not be used to initialize the NUTS sampl
er, simply call pymc3.sample() and it will automatically initialize NUTS
in a better way.')
logp = -2,608.5, ||grad|| = 1,590.5: 100%||| 7/7 [00:00<00:00, 7
64.69it/s]
Multiprocess sampling (4 chains in 4 jobs)
Metropolis: [lambda]
Sampling 4 chains: 100%|| 402000/402000 [00:41<00:00, 9785.13dr
aws/s]
The number of effective samples is smaller than 25% for some parameters.</pre>
```

In the above code, our model is implemented with the uniform distribution for the prior distribution, and the Poisson distribution for the likelihood.

The PyMC3 method find\_MAP() was used to find the most likely value of  $\lambda$  for the starting point. This is optional, but often speeds up the computation.

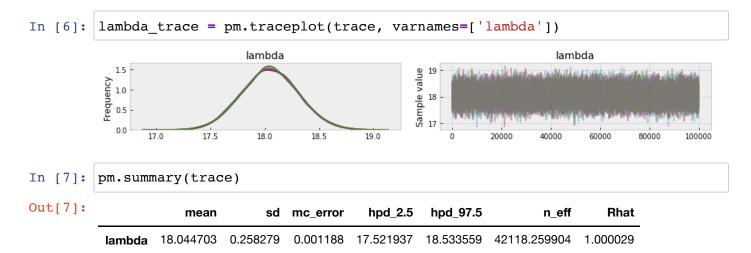
The step specifies what sampling method is used for guidance towards the most likely parameter values.

And finally, the PyMC3 function <code>sample()</code> gathers the samples (100,000 samples in this case) by traversing over the areas of the most likely parameter values. This is the main entry point to the MCMC sampling algorithms. This function takes a defined sampler passed as step, or if step is not passed will try to auto-assign the correct sampler and auto-initialize it.

The PyMC3 library has methods for graphical representation of the collected samples; below, the traceplot method is used to show the determined posterior distribution of  $\lambda$ .

The below plot (left) shows the posterior distribution of values collected for  $\lambda$ . In this case, we obtained a bell-shaped distribution for the parameter even though the prior is the uniform distribution. The mean is slightly over 18.0 sec and the obtained distribution provides a measure of uncertainty: credible values of  $\lambda$  are between 17.0 and 19.0 seconds.

This result shows the difference between the frequentist approach, where the parameter  $\lambda$  is estimated as the mean value of 'time\_delay\_seconds' and is given as a single value. In contrast, from Bayesian analysis, we get the parameter value with a measure of uncertainty. This measure of uncertainty is incredibly valuable, as we will see later. Note that the mean of posterior distribution is very close to the frequentist estimate.



## Model convergence

The *trace plots* show the history of a parameter value across iterations of the chain. It shows the value of parameters explored on each iteration step. If the model reached equilibrium there should not be any trends observed. The trace should look random around some constant value, should be jumping around and look like a "hairy caterpillar". Any trends (periodicity, upward or downward trend) indicate that the chain has not converged to stationary equilibrium state yet and the number of iteration has to be increased.

Also, it is recommended to inspect sample autocorrelation - the measure of correlation between successive samples in the chain. An autocorrelation plot should taper off to zero relatively quickly, and then oscillate around zero. If your autocorrelation plot does not taper off, the model selection (likelihood) and sampling methods should be revisited.

The effective sample size (ESS) shows the number of points that bring useful information. The effective sample size is usually given in the summary of MCMC simulation output. The ESS is related to autocorrelation. Since autocorrealtion measures the linear dependence of the current chain value on the past value (lags), it helps to estimate how much information is available. Due to autocorrelation Markov chain sampling 1000 iteration would contain less information about the distribution thag 1000 samples independently drawn from that distribution. Autocorrelation guides how iterations should be thinned out untile autocorrelation is close to 0

# **Burnin samples**

In the above code the function <code>pm.find\_MAP()</code> was used to find a good starting point for sampling. This function finds a maximum a posteriori (MAP) estimation and helps to start sampling in the area of high likelihood. But sometimes the wrong maximum can be detected, and it is recommended to discard the samples collected at the early stage (burnin samples) as they might be biased by the choice of starting point. The initial point of the chain does not affect the posterior distribution. For any starting point we expect the chain to find the bulk of posterior distribution and

get the stationary distribution. However, if chain started far from the significant regions it would take longer to find stationary distribution. From trace plot inspection, especially the initial period, it is possible to detect the time chain took to converge. The initial period is called *burn-in period* and should always be discarded form the posterior distributio. Sometimes, up to 90% of trace is discarded.

The standard practice is to simulate several chains at once. Each starting at diffeent initial value. The diagnostic method (Gelman-Rubin) was developed which calculates variability within chains, comapring that to variability between chains.

/anaconda3/lib/python3.7/site-packages/matplotlib/axes/\_base.py:3604: Mat plotlibDeprecationWarning:

The `ymin` argument was deprecated in Matplotlib 3.0 and will be removed in 3.2. Use `bottom` instead.

alternative='`bottom`', obj\_type='argument')

/anaconda3/lib/python3.7/site-packages/matplotlib/axes/\_base.py:3610: Mat plotlibDeprecationWarning:

The `ymax` argument was deprecated in Matplotlib 3.0 and will be removed in 3.2. Use `top` instead.

```
alternative='`top`', obj_type='argument')
```

/anaconda3/lib/python3.7/site-packages/matplotlib/axes/\_base.py:3604: Mat plotlibDeprecationWarning:

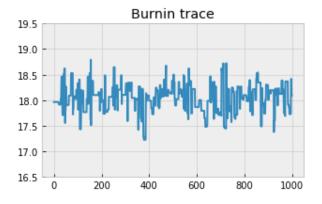
The `ymin` argument was deprecated in Matplotlib 3.0 and will be removed in 3.2. Use `bottom` instead.

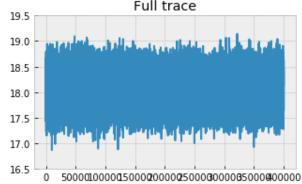
```
alternative='`bottom`', obj type='argument')
```

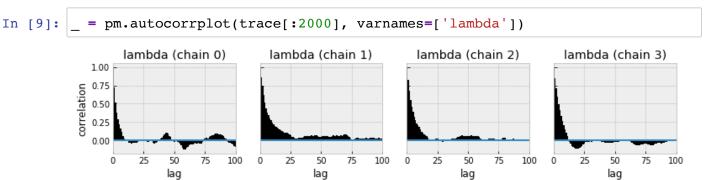
/anaconda3/lib/python3.7/site-packages/matplotlib/axes/\_base.py:3610: Mat plotlibDeprecationWarning:

The `ymax` argument was deprecated in Matplotlib 3.0 and will be removed in 3.2. Use `top` instead.

alternative='`top`', obj type='argument')





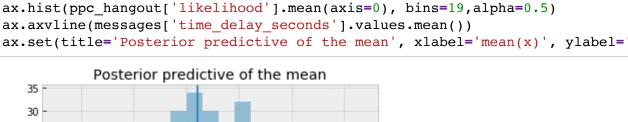


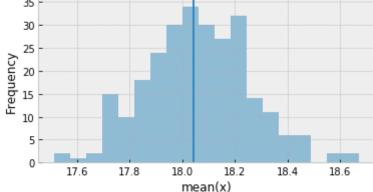
As a validation check of model performance, we shall generate the distribution of the response time.

The postrior predictive check is one of the ways to validate a model, this generate the data from the model using parameter drawn from the posterior distribution.

While plot\_posterior function plots the posterior distributions of the model parameters, the sample\_posterior\_predictive(trace, samples= N , model= ... ) will randomly draw N samples from the trace, which contains the posterior distribution. This will produce N sets of the model parameters; then for each sample of the parameters it will draw (or 'simulate') the data distribution.

This method will produce N 'simulated' datasets; these might be inspected individually or aggregate them into one distribution, for example by finding average of N distributions. Note that the function returns a dictionary {'likelihood': array of N distributions [...], [...], ... [...]}





# Logistic regression with parameters estimated from Bayesian

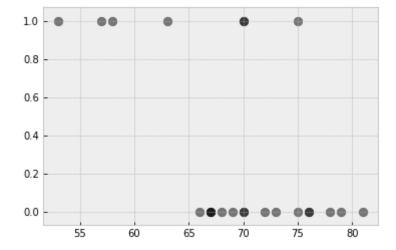
#### inference

```
In [12]:
         import theano.tensor as tt
         import numpy as np
In [13]: challenger_data = np.genfromtxt("./module10/challenger_data.csv", skip_head
In [14]:
         challenger_data = challenger_data[~np.isnan(challenger_data[:,1])]
         challenger data
Out[14]: array([[66.,
                        0.1,
                 [70.,
                        1.],
                 [69.,
                        0.],
                 [68.,
                        0.],
                 [67.,
                        0.],
                 [72.,
                        0.],
                 [73.,
                        0.],
                 [70.,
                        0.],
                 [57.,
                        1.],
                 [63.,
                        1.],
                 [70.,
                        1.],
                 [78.,
                        0.],
                 [67.,
                        0.],
                 [53.,
                        1.],
                 [67.,
                        0.],
                 [75.,
                        0.],
                 [70.,
                        0.],
                 [81.,
                        0.],
                 [76.,
                        0.],
                 [79.,
                        0.],
                 [75.,
                        1.],
                 [76.,
                        0.],
                 [58.,
                        1.]])
```

Of the previous 24 flights, data were available on failures of the O-rings on 23. Only the data corresponding to the 7 flights on which there was a damage incident were considered important, and these were thought to show no obvious trend.

```
In [15]: plt.scatter(challenger_data[:,0], challenger_data[:, 1], s=75, color="k", a
```

Out[15]: <matplotlib.collections.PathCollection at 0x1c29fb5f60>



It looks clear that the probability of damage incidents occurring increases as the outside temperature decreases. The best we can do is ask "At temperature t, what is the probability of a damage incident?".

We need a function of temperature, call it p(t), that is bounded between 0 and 1, and gradually changes as we increase temperature.

The logistic function is the most popular choice.

```
In [16]: def logistic(x, beta, alpha=0):
    return 1.0 / (1.0 + np.exp(np.dot(beta, x) + alpha))
```

```
In [17]: temperature = challenger_data[:, 0]
    D = challenger_data[:,1]

with pm.Model() as model_logit:
    beta = pm.Normal("beta", mu=0, tau=0.0001, testval = 0)
    alpha = pm.Normal("alpha", mu=0, tau=0.001, testval = 0)
    p = pm.Deterministic("p", 1.0/(1.0 + tt.exp(beta*temperature + alpha)))

observed = pm.Bernoulli("bernoulli_obs", p, observed = D)

start = pm.find_MAP()
    step = pm.Metropolis()
    trace = pm.sample(200000, start=start, step=step, progressbar=True)
    burned_trace = trace[1000000::2]
```

/anaconda3/lib/python3.7/site-packages/pymc3/tuning/starting.py:61: UserW arning: find\_MAP should not be used to initialize the NUTS sampler, simply call pymc3.sample() and it will automatically initialize NUTS in a better way.

```
warnings.warn('find_MAP should not be used to initialize the NUTS sampler, simply call pymc3.sample() and it will automatically initialize NUTS in a better way.')
logp = -20.175, ||grad|| = 9.907: 100%| 27/27 [00:00<00:00, 20 69.44it/s]
Multiprocess sampling (4 chains in 4 jobs)
CompoundStep
>Metropolis: [alpha]
>Metropolis: [beta]
Sampling 4 chains: 100%| 802000/802000 [01:40<00:00, 7968.97dr aws/s]
The number of effective samples is smaller than 10% for some parameters.
```

To connect probabilities to observed data, we use a Bernoulli random variable with parameter p. It takes value 1 with probability p, and 0 otherwise.

/anaconda3/lib/python3.7/site-packages/matplotlib/axes/\_axes.py:6521: Mat plotlibDeprecationWarning:

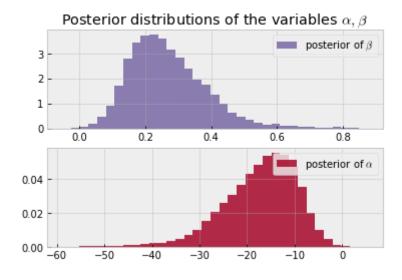
The 'normed' kwarg was deprecated in Matplotlib 2.1 and will be removed in 3.1. Use 'density' instead.

alternative="'density'", removal="3.1")

/anaconda3/lib/python3.7/site-packages/matplotlib/axes/\_axes.py:6521: Mat plotlibDeprecationWarning:

The 'normed' kwarg was deprecated in Matplotlib 2.1 and will be removed in 3.1. Use 'density' instead.

alternative="'density'", removal="3.1")

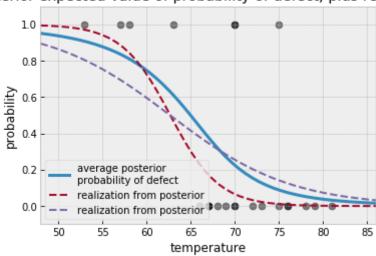


```
In [19]: t = np.linspace(temperature.min() - 5, temperature.max()+5, 50)[:, None]
    p_t = logistic(t.T, beta_samples, alpha_samples)

mean_prob_t = p_t.mean(axis=0)
```

```
In [20]: plt.plot(t, mean_prob_t, lw=3, label="average posterior \nprobability \
    of defect")
    plt.plot(t, p_t[0, :], ls="--", label="realization from posterior")
    plt.plot(t, p_t[-2, :], ls="--", label="realization from posterior")
    plt.scatter(temperature, D, color="k", s=50, alpha=0.5)
    plt.title("Posterior expected value of probability of defect; \
    plus realizations")
    plt.legend(loc="lower left")
    plt.ylim(-0.1, 1.1)
    plt.xlim(t.min(), t.max())
    plt.ylabel("probability")
    plt.xlabel("temperature");
```

#### Posterior expected value of probability of defect; plus realizations

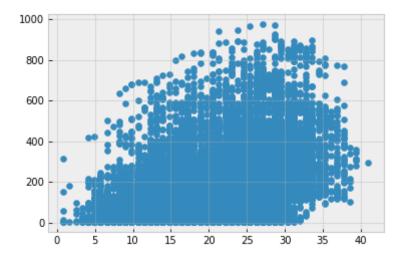


#### **Bayesian linear regression**

```
In [21]: from sklearn.linear_model import LinearRegression
In [22]: bike_sharing = pd.read_csv('./module10/bikes_sharing.csv', header=0, sep= '
In [23]: bike_sharing.isnull().values.any()
Out[23]: False
In [24]: bike_sharing.shape
Out[24]: (10886, 12)
```

```
In [25]: plt.scatter(x=bike_sharing['temp'], y=bike_sharing['count'])
```

Out[25]: <matplotlib.collections.PathCollection at 0x1c2228ef28>

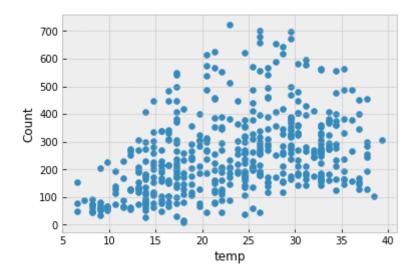


```
In [26]: bike_sharing.datetime = bike_sharing.datetime.apply(pd.to_datetime)
    bike_sharing['month'] = bike_sharing.datetime.apply(lambda x : x.month)
    bike_sharing['hour'] = bike_sharing.datetime.apply(lambda x : x.hour)
```

```
In [27]: # we want to predice bike renting at certain time (15:00 - 15:59)
bike_sharing_15 = bike_sharing.loc[bike_sharing['hour'] == 15]
```

```
In [28]: plt.scatter(x=bike_sharing_15['temp'], y=bike_sharing_15['count'])
    plt.xlabel("temp")
    plt.ylabel('Count')
```

Out[28]: Text(0, 0.5, 'Count')



Implement MCMC to find the posterior distribution of the model parameters. Rather than a single point estimate of the model weights, Bayesian linear regression will give us a posterior distribution for the model weights.

```
In [33]: with pm.Model() as linear_model:
    intercept = pm.Normal('Intercept', mu = 0, sd = 10)

    slope = pm.Normal('slope', mu = 0, sd = 10)

    sigma = pm.HalfNormal('sigma', sd = 10)

# Estimate
    mean = intercept + slope * X.loc[:, 'atemp']

Y_obs = pm.Normal('Y_obs', mu = mean, sd = sigma, observed = y.values)

#Sampler
    step = pm.NUTS()

linear_trace = pm.sample(20000, step=step, progressbar=True)
```

Multiprocess sampling (4 chains in 4 jobs)

NUTS: [sigma, slope, Intercept]

Sampling 4 chains: 100% | 82000/82000 [00:28<00:00, 2913.13draw s/s]

The acceptance probability does not match the target. It is 0.88524325428 50333, but should be close to 0.8. Try to increase the number of tuning s teps.

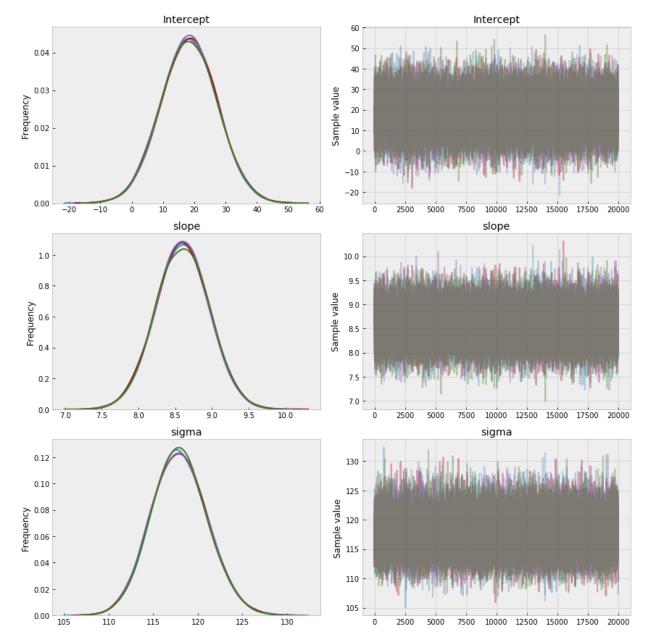
The acceptance probability does not match the target. It is 0.88544861938 28859, but should be close to 0.8. Try to increase the number of tuning s teps.

The acceptance probability does not match the target. It is 0.89454942152 51486, but should be close to 0.8. Try to increase the number of tuning s teps.

```
In [34]: linear_trace.mean_tree_accept.mean()
```

Out[34]: 0.8814988619015427

```
In [35]: pm.traceplot(linear_trace, figsize=(12,12))
```



```
In [36]: pm.plot_posterior(linear_trace, figsize=(12,10), text_size=20)
Out[36]: array([<matplotlib.axes._subplots.AxesSubplot object at 0x1c235acba8>,
                <matplotlib.axes._subplots.AxesSubplot object at 0x1c36da59b0>,
                 <matplotlib.axes._subplots.AxesSubplot object at 0x1c373c3be0>],
               dtype=object)
                        Intercept
                                                                slope
                     mean = 18.200
                                                            mean = 8.593
                                                             95% HPD
                       95% HPD
               0.715
                                   35.184
                                                      7.908
                                                                        9.309
          -20
                    Ó
                           20
                                            60
                                                 7
                                                                     9
                                    40
                                                           8
                                                                              10
                         sigma
                    mean = 117.882
                      95% HPD
            111.755
                                 123.865
```

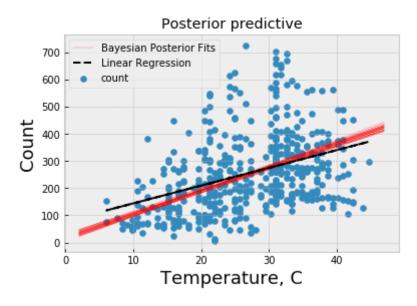
130

# **Prediction of response**

110

120

Out[37]: <matplotlib.legend.Legend at 0x1c278c4f98>



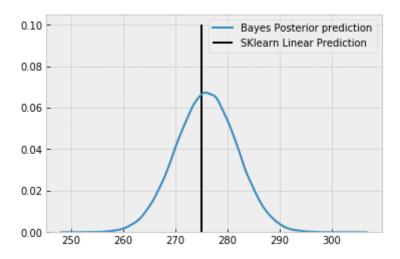
#### pm.summary(linear\_trace) In [38]: Out[38]: Rhat mean sd mc\_error hpd\_2.5 hpd\_97.5 n eff 18.199924 8.804677 0.044636 0.715397 35.184051 37300.308531 1.000008 Intercept 8.592864 0.356856 0.001777 7.908155 9.309120 37772.748131 0.999993 slope sigma 117.882196 3.092717 0.015063 111.754786 123.865028 47554.517468 1.000002

# **Prediction for single point**

/anaconda3/lib/python3.7/site-packages/scipy/stats/stats.py:1713: FutureW arning: Using a non-tuple sequence for multidimensional indexing is depre cated; use `arr[tuple(seq)]` instead of `arr[seq]`. In the future this will be interpreted as an array index, `arr[np.array(seq)]`, which will result either in an error or a different result.

return np.add.reduce(sorted[indexer] \* weights, axis=axis) / sumval

Out[39]: <matplotlib.axes. subplots.AxesSubplot at 0x1c27916518>



#### You have reached the end of this module.

If you have any questions, please reach out to your peers using the discussion boards. If you and your peers are unable to come to a suitable conclusion, do not hesitate to reach out to your instructor on the designated discussion board.

When you are comfortable with the content, and have practiced to your satisfaction, you may proceed to any related assignments, and to the next module.

```
In [ ]:
```