

Data Analytics - final project

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```
In [ ]: import cmdstanpy
import pandas as pd
import arviz as az
import numpy as np
import matplotlib.pyplot as plt
import scipy.stats as stats
```

```
In [ ]: from DA_tools.DA_tools import ribbon_plot
from DA_tools.DA_colors import *
```

Problem statement

In the project we modeled the relationship between the amount of sugar and calories in cereals.

The main point to create this model is to investigate the relationship between sugars and calories in cereals. Potential use case is for example estimate the amount of sugars knowing the number of calories.

Dataset was collected from <https://www.kaggle.com/datasets/crawford/80-cereals?select=cereal.csv>.

It contains nutrition values (like protein, fat, sugars and much more) of 77 different types of cereals.

Data preprocessing

```
In [ ]: df = pd.read_csv('cereal.csv', index_col=0)
```

```
In [ ]: df.head()
```

Out[]:

	mfr	type	calories	protein	fat	sodium	fiber	carbo	sugars	potass	vitamins	shelf
100% Bran	N	C	70	4	1	130	10.0	5.0	6	280	25	3
100% Natural Bran	Q	C	120	3	5	15	2.0	8.0	8	135	0	3
All-Bran	K	C	70	4	1	260	9.0	7.0	5	320	25	3
All-Bran with Extra Fiber	K	C	50	4	0	140	14.0	8.0	0	330	25	3
Almond Delight	R	C	110	2	2	200	1.0	14.0	8	-1	25	3

Those nutrition values are defined as per serving where serving size is given in 'weight' table in ounces. So we decided to scale it to have values for 1 ounce in every row.

```
In [ ]: df['sugars'] = df['sugars']/df['weight']
df['calories'] = df['calories']/df['weight']
```

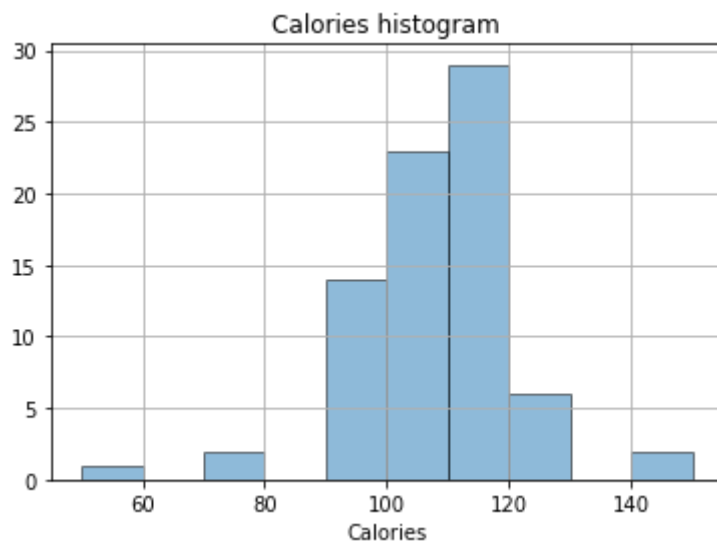
```
In [ ]: df.head()
```

Out[]:

	mfr	type	calories	protein	fat	sodium	fiber	carbo	sugars	potass	vitamins	shelf
100% Bran	N	C	70.0	4	1	130	10.0	5.0	6.0	280	25	3
100% Natural Bran	Q	C	120.0	3	5	15	2.0	8.0	8.0	135	0	3
All-Bran	K	C	70.0	4	1	260	9.0	7.0	5.0	320	25	3
All-Bran with Extra Fiber	K	C	50.0	4	0	140	14.0	8.0	0.0	330	25	3
Almond Delight	R	C	110.0	2	2	200	1.0	14.0	8.0	-1	25	3

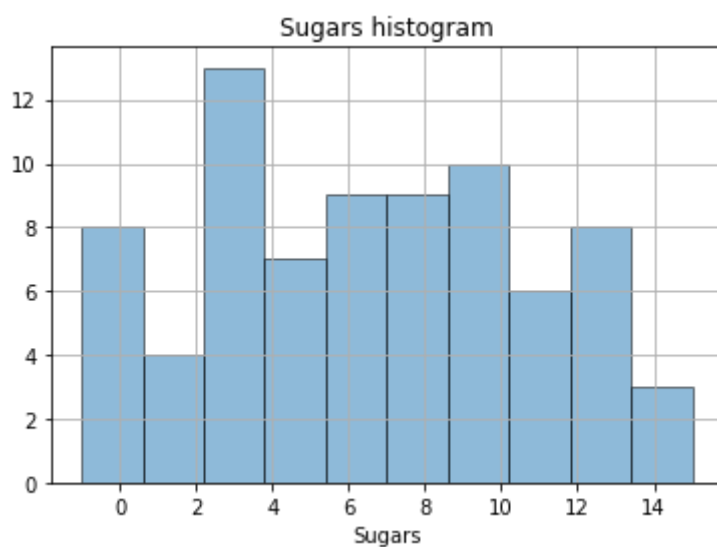
Histogram of calories

```
In [ ]: df['calories'].hist(alpha=0.5, ec='black')
plt.title('Calories histogram')
plt.xlabel('Calories')
plt.show()
```



Histogram of sugars

```
In [ ]: df['sugars'].hist(alpha=0.5, ec='black')
plt.title('Sugars histogram')
plt.xlabel('Sugars')
plt.show()
```



Creation of dataframe with values that we need (calories and sugars).

```
In [ ]: data = df[['calories' , 'sugars']]
```

```
In [ ]: data
```

Out[]:

	calories	sugars
100% Bran	70.0	6.0
100% Natural Bran	120.0	8.0
All-Bran	70.0	5.0
All-Bran with Extra Fiber	50.0	0.0
Almond Delight	110.0	8.0
...
Triples	110.0	3.0
Trix	110.0	12.0
Wheat Chex	100.0	3.0
Wheaties	100.0	3.0
Wheaties Honey Gold	110.0	8.0

77 rows × 2 columns

Next we've checked if all values are reasonable.

In []: `data['calories'].value_counts()`

Out[]:

```

110.000000    29
100.000000    19
 90.000000     7
120.000000     6
 90.225564     3
 70.000000     2
150.000000     2
 50.000000     1
 97.744361     1
 96.000000     1
107.692308     1
106.666667     1
105.263158     1
104.000000     1
 96.385542     1
 93.333333     1
Name: calories, dtype: int64

```

In []: `data['sugars'].value_counts()`

```
Out[ ]: 3.000000    13
        0.000000     7
        6.000000     7
        8.000000     6
        5.000000     5
        11.000000    5
        12.000000    5
        7.000000     3
        10.000000    3
        13.000000    3
        2.000000     3
        9.000000     3
        9.022556     2
        15.000000    2
        1.000000     1
        6.015038     1
        14.000000    1
        4.000000     1
        6.923077     1
        8.666667     1
        5.263158     1
        10.526316    1
        -1.000000     1
        9.333333     1
Name: sugars, dtype: int64
```

We've found that in sugars we have value of -1 which is an absurd. So we've decided to remove it.

```
In [ ]: data = data.drop(data[data['sugars'] == -1].index)
```

Dataframe statistics.

```
In [ ]: data.describe()
```

```
Out[ ]:
```

	calories	sugars
count	76.000000	76.000000
mean	104.049501	6.654904
std	13.936164	4.093540
min	50.000000	0.000000
25%	100.000000	3.000000
50%	107.179487	6.007519
75%	110.000000	10.000000
max	150.000000	15.000000

Models in project

1. Model using normal distribution

1.1 Model based only on calories

In our project we decided to start with simple model based only on calories.

1.2 Model with sugars as predictor

Next, we decided to add sugars as predictor. Calories will be now defined in the model as:

$$calories_i \sim Normal(\mu_i, \sigma)$$

$$\mu_i = \alpha + \beta * sugars_i$$

Where α and β have normal distribution and σ has exponential distribution.

2. Model using double exponential distribution

In the second model we decided to use double exponential distribution instead of normal distribution because as we can see on calories histogram values of calories in our dataset are stacked in the middle of the histogram and we thought that it will fit our data better than normal distribution.

$$calories_i \sim DoubleExponential(\mu_i, \sigma)$$

$$\mu_i = \alpha + \beta * sugars_i$$

Where α and β have normal distribution and σ has exponential distribution.

1. Model using normal distribution

1.1

In the first model we've considered only calories and used normal distribution.

Normal distribution

$$Normal(y|\mu, \sigma) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{1}{2}\left(\frac{y-\mu}{\sigma}\right)^2\right)$$

Prior predictive check

Prior values were chosen based on <https://kalkulatorkalorii.net/> webpage. We've checked few types of cereals that we know. Based on those values we picked values for priors, we set the value of mu to be normally distributed with mean of 105 and standard deviation of 15.

The value of sigma was set to be exponentially distributed with inverse scale beta of 0.067 (because $\frac{1}{15} \approx 0.067$).

```
In [ ]: with open('cereal_1_ppc.stan') as file:
        print(file.read())
```

```

generated quantities {
  real mu = normal_rng(105, 15);
  real sigma = exponential_rng(0.067);
  real calories = normal_rng(mu, sigma);
}

```

```
In [ ]: model_ppc=cmdstanpy.CmdStanModel(stan_file='cereal_1_ppc.stan')
```

```
INFO:cmdstanpy:found newer exe file, not recompiling
```

```
In [ ]: R = 1000
sim = model_ppc.sample(iter_sampling=R, iter_warmup=0, chains=1, fixed_param=True,
```

```
INFO:cmdstanpy:CmdStan start processing
chain 1 |          | 00:00 Status
```

```
INFO:cmdstanpy:CmdStan done processing.
```

```
In [ ]: mu_sim=sim.stan_variable('mu')
sigma_sim=sim.stan_variable('sigma')
calories_sim=sim.stan_variable('calories')
```

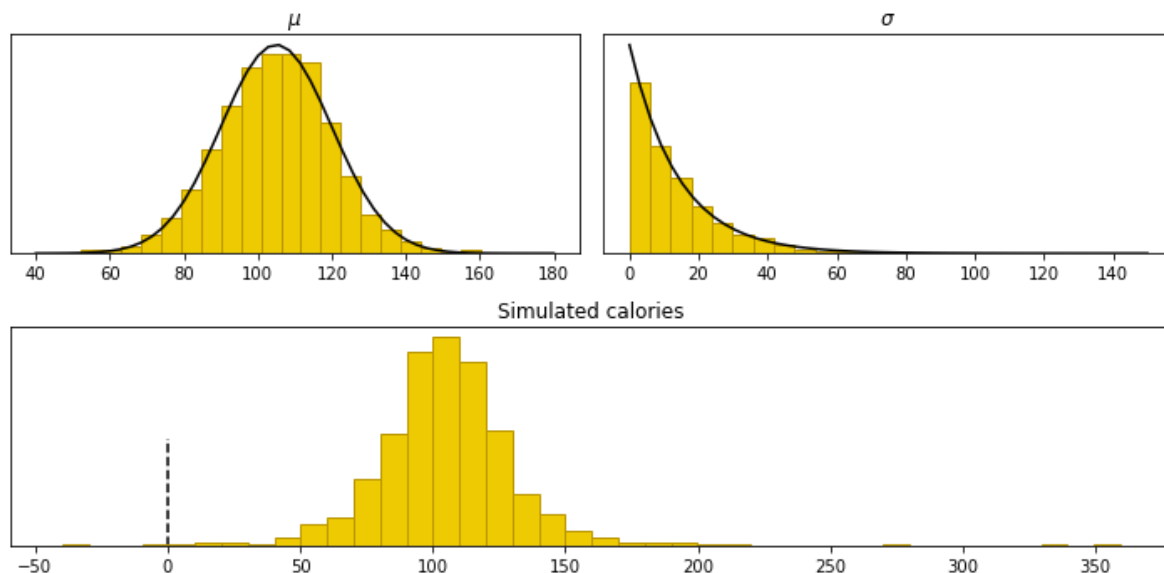
```
In [ ]: fig = plt.figure(figsize=(10,5))
gs = fig.add_gridspec(2,2)
ax1 = fig.add_subplot(gs[1,:])
ax1.vlines([0], ymin=0, ymax=1e-2, linestyle='--',color='black', zorder=1)
ax1.hist(calories_sim, bins=40, color=DARK, edgecolor=DARK_HIGHLIGHT,density=True)

ax1.set_yticks([])
ax1.set_title('Simulated calories')

ax2 = fig.add_subplot(gs[0, 0])
ax3 = fig.add_subplot(gs[0, 1])

ax2.hist(mu_sim, bins=20, color=DARK, edgecolor=DARK_HIGHLIGHT,density=True)
x=np.linspace(40,180)
y=stats.norm.pdf(x,loc=105,scale=15)
ax2.plot(x,y,'black')
ax3.set_title('$\sigma$')
ax2.set_title('$\mu$')
ax2.set_yticks([])
ax3.set_yticks([])
ax3.hist(sigma_sim, bins=20, color=DARK, edgecolor=DARK_HIGHLIGHT,density=True)
x=np.linspace(0,150)
y=stats.expon.pdf(x,scale=14)
ax3.plot(x,y,'black')

fig.tight_layout()
plt.show()
```



As we can see simulated values of parameters μ and σ were distributed well, as we expected.

Values of simulated calories are mostly distributed well (the mean is distributed where we expected) but we have some outliers which, when we add some data, will probably disappear.

Posterior analysis

```
In [ ]: with open('cereal_1_fit.stan') as file:
        print(file.read())

data {
  int N;
  real calories[N];
}

parameters {
  real mu;
  real<lower=0> sigma;
}

model {
  mu ~ normal(105, 15);
  sigma ~ exponential(0.067);
  calories ~ normal(mu, sigma);
}

generated quantities {
  real log_lik = normal_lpdf(calories | mu, sigma);
  real calorie = normal_rng(mu, sigma);
}
```

Data required for this model:

- N -> calories vector size
- calories -> calories vector

```
In [ ]: model_1_fit=cmdstanpy.CmdStanModel(stan_file='cereal_1_fit.stan')
```

INFO:cmdstanpy:found newer exe file, not recompiling


```
In [ ]: fit_1=model_1_fit.sample(data=dict(N=len(data['calories']), calories=data['calories']
```

```
INFO:cmdstanpy:CmdStan start processing
```

```
chain 1 |          | 00:00 Status
chain 2 |          | 00:00 Status
chain 3 |          | 00:00 Status
chain 4 |          | 00:00 Status
```

```
INFO:cmdstanpy:CmdStan done processing.
```

```
In [ ]: print(fit_1.diagnose())
```

```
Processing csv files: C:\GitHub\DataAnalyticsProject\Project\samples\cereal_1_fit-
20220621214924_1.csv, C:\GitHub\DataAnalyticsProject\Project\samples\cereal_1_fit-
20220621214924_2.csv, C:\GitHub\DataAnalyticsProject\Project\samples\cereal_1_fit-
20220621214924_3.csv, C:\GitHub\DataAnalyticsProject\Project\samples\cereal_1_fit-
20220621214924_4.csv
```

```
Checking sampler transitions treedepth.
Treedepth satisfactory for all transitions.
```

```
Checking sampler transitions for divergences.
No divergent transitions found.
```

```
Checking E-BFMI - sampler transitions HMC potential energy.
E-BFMI satisfactory.
```

```
Effective sample size satisfactory.
```

```
Split R-hat values satisfactory all parameters.
```

```
Processing complete, no problems detected.
```

```
No errors/issues occurred during sampling.
```

```
In [ ]: az.summary(fit_1, var_names=['mu', 'sigma'], round_to=2, kind='stats')
```

```
Out[ ]:
```

	mean	sd	hdi_3%	hdi_97%
mu	104.11	1.59	101.02	107.00
sigma	14.09	1.18	11.90	16.33

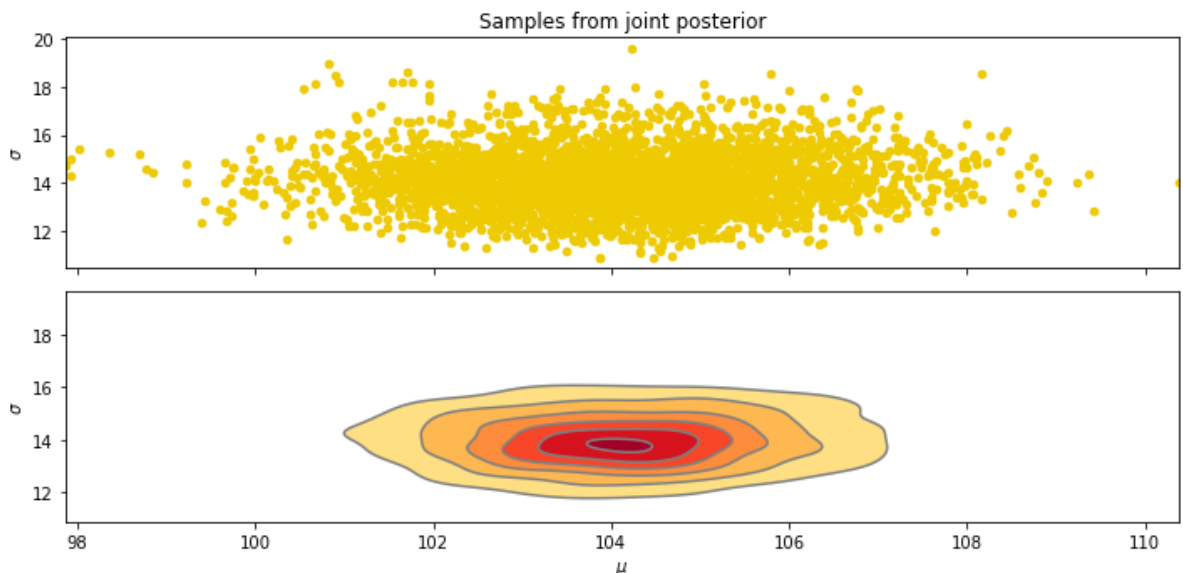
Values of mu and sigma are very close to those proposed by us in ppc.

```
In [ ]: mu_fit = fit_1.stan_variable('mu')
sigma_fit = fit_1.stan_variable('sigma')
calorie_pred = fit_1.stan_variable('calorie')
```

```
In [ ]: fig, axes = plt.subplots(2,1,figsize=(10,5), sharex=True)
ax1=axes[0]
ax1.scatter(mu_fit, sigma_fit, 20, color=DARK)
ax1.set_title("Samples from joint posterior")
ax1.set_ylabel(r'$\sigma$')
ax2=axes[1]
az.plot_kde(mu_fit, sigma_fit, ax=ax2, contourf_kwargs={'cmap':'YlOrRd'})

ax2.set_xlabel(r'$\mu$')
ax2.set_ylabel(r'$\sigma$')
```

```
fig.tight_layout()
plt.show()
```

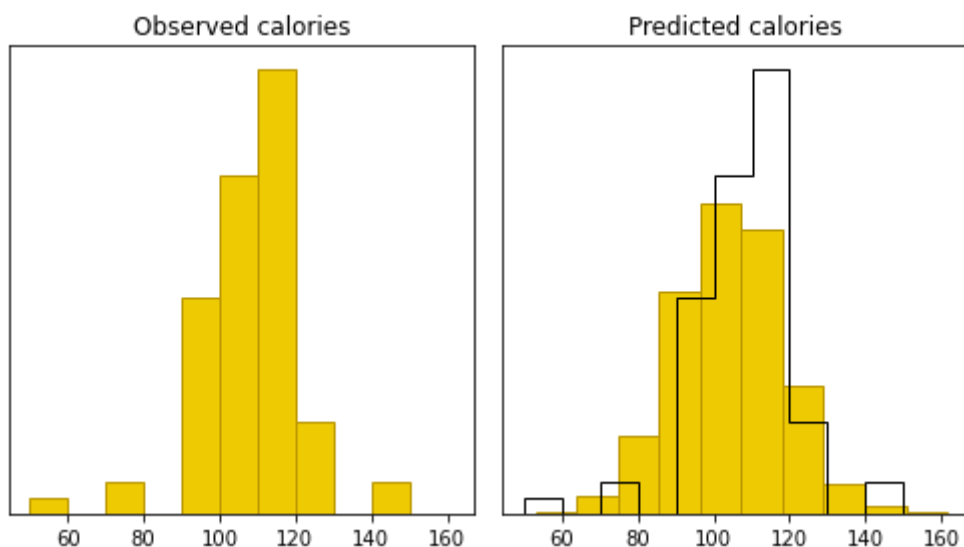


As we can see our sigma and mu samples from joint posterior are concentrated.

```
In [ ]: fig, axes = plt.subplots(1,2,figsize=(7,4),sharex=True,sharey=True)
ax=axes[0]
ax.hist(data['calories'], bins=10, color=DARK,edgecolor=DARK_HIGHLIGHT,density=True)
ax.set_title('Observed calories')
ax.set_yticks(())
ax2=axes[1]
ax2.hist(calorie_pred, bins=10, color=DARK,edgecolor=DARK_HIGHLIGHT,density=True)
ax2.hist(data['calories'], bins=10, histtype='step', color='black', density=True)

ax2.set_title('Predicted calories')
ax2.set_yticks(())
fig.tight_layout()

plt.show()
```



Outliers observed during ppc disappeared as we expected.

As we can see samples for posterior predictive did not match exactly the observed values.

Observed values are more clustered close to the mean value.

Data is not exactly similar with posterior predictive sample but it's quite close.

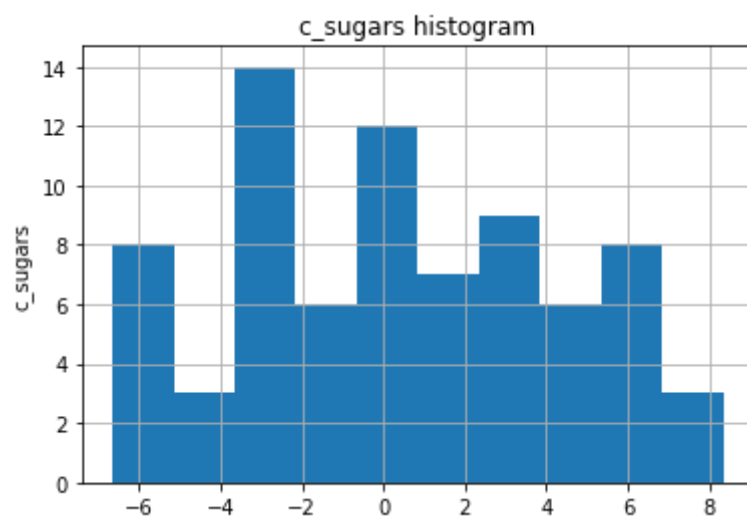
1.2

We've decided to add predictor - value of sugars.

Those values were centered to represent sugars not as grams but the difference from the mean. It was added to dataframe as 'csugars'.

$calories_i \sim \text{Normal}(\mu_i, \sigma)$
 $\mu_i = \alpha + \beta * c_sugars_i$
 α and β have normal distribution and σ has exponential distribution.

```
In [ ]: data['c_sugars'] = data['sugars'] - data['sugars'].mean()
data['c_sugars'].hist()
plt.ylabel('c_sugars')
plt.title('c_sugars histogram')
plt.show()
```



Prior predictive check

We used the same values for alpha and sigma as for mu and sigma in previous prior. The value of beta was set to be normally distributed with mean of 0 and std of 10.

```
In [ ]: with open('cereal_2a_ppc.stan') as file:
        print(file.read())

data {
  int N;
  real sugars[N];
}

generated quantities {
  real alpha = normal_rng(105, 15);
  real beta = normal_rng(0, 10);
  real sigma = exponential_rng(0.067);
  real calorie[N];
  for (i in 1:N) {
    calorie[i] = normal_rng(sugars[i]*beta+alpha, sigma);
  }
}
```

```
In [ ]: model_ppc = cmdstanpy.CmdStanModel(stan_file='cereal_2a_ppc.stan')

INFO:cmdstanpy:found newer exe file, not recompiling

In [ ]: R = 1000
data_sim = {'N': len(data), 'sugars':np.linspace(data['c_sugars'].min(),data['c_sugars'].max(),R)}
sim = model_ppc.sample(data=data_sim,iter_sampling=R, iter_warmup=0, chains=1, refresh=1000)

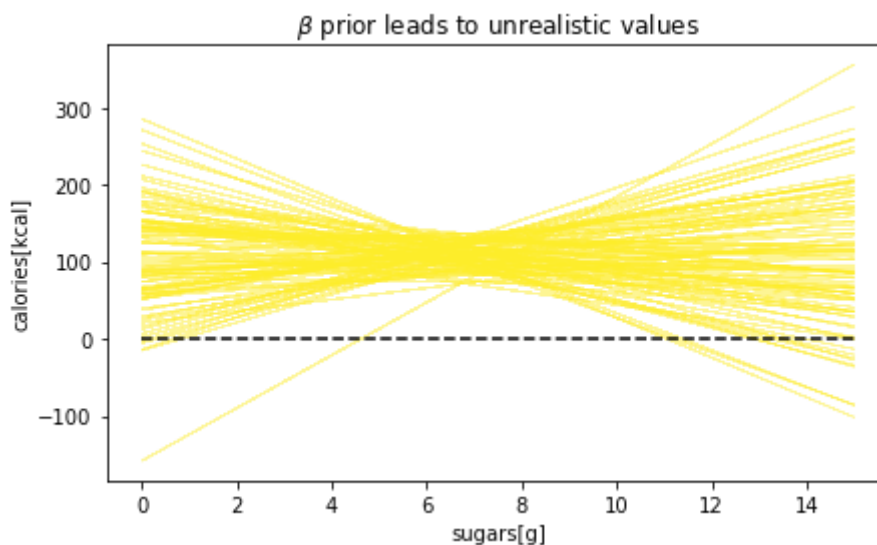
INFO:cmdstanpy:CmdStan start processing
chain 1 |          | 00:00 Status

INFO:cmdstanpy:CmdStan done processing.

In [ ]: alpha_sim = sim.stan_variable('alpha')
        beta_sim = sim.stan_variable('beta')

In [ ]: fig, axes = plt.subplots(1,1,figsize = (7,4))

        for i in range(100):
            axes.plot(data['sugars'], alpha_sim[i]+beta_sim[i]*data['c_sugars'], color=MIDNIGHTBLUE)
        axes.set_xlabel('sugars[g]')
        axes.set_ylabel('calories[kcal]')
        axes.set_title(r"$\beta$ prior leads to unrealistic values")
        axes.hlines([0],xmin=data['sugars'].min(), xmax=data['sugars'].max(), linestyle='--')
        plt.show()
```



As we can see simulated data using normal distribution for beta leads to some unrealistic values so we decided to change its distribution to lognormal with mu 0 and sigma 1. Lognormal was used because it can ensure that the values will be positive.

```
In [ ]: with open('cereal_2b_ppc.stan') as file:
        print(file.read())
```

```

data {
  int N;
  real sugars[N];
}

generated quantities {
  real alpha = normal_rng(105, 15);
  real beta = lognormal_rng(0, 1);
  real sigma = exponential_rng(0.067);
  real calorie[N];
  for (i in 1:N) {
    calorie[i] = normal_rng(sugars[i]*beta+alpha, sigma);
  }
}

```

```
In [ ]: model_ppc = cmdstanpy.CmdStanModel(stan_file='cereal_2b_ppc.stan')
```

```
INFO:cmdstanpy:found newer exe file, not recompiling
```

```
In [ ]: sim = model_ppc.sample(data=data_sim,iter_sampling=R, iter_warmup=0, chains=1, refi
```

```
INFO:cmdstanpy:CmdStan start processing
chain 1 |          | 00:00 Status
```

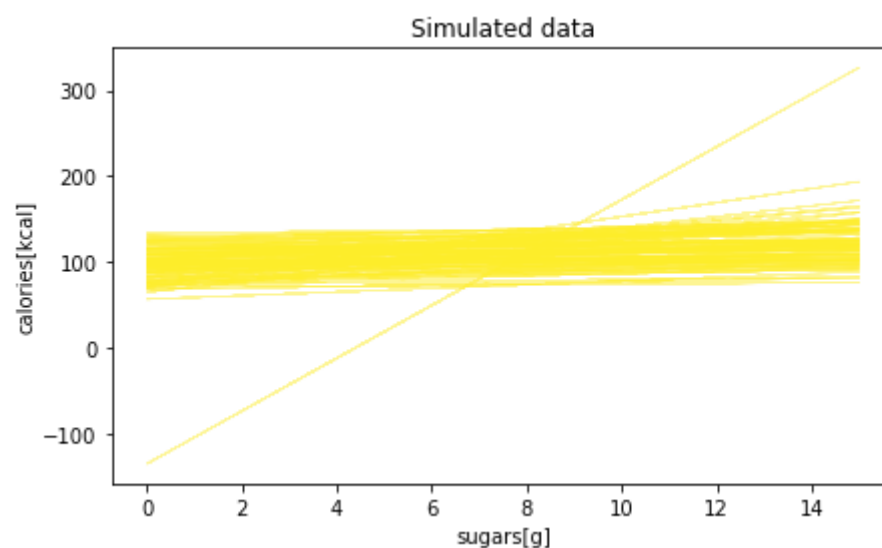
```
INFO:cmdstanpy:CmdStan done processing.
```

```
In [ ]: alpha_sim = sim.stan_variable('alpha')
        beta_sim = sim.stan_variable('beta')
```

```
In [ ]: fig, axes = plt.subplots(1,1,figsize = (7,4))

        for i in range(100):
            axes.plot(data['sugars'], alpha_sim[i]+beta_sim[i]*data['c_sugars'], color=MIDNIGHTBLUE)

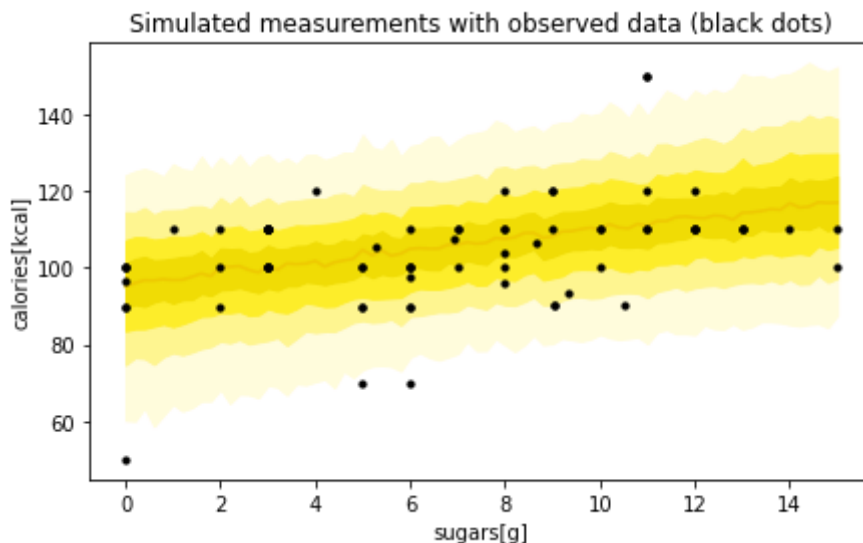
        axes.set_xlabel('sugars[g]')
        axes.set_ylabel('calories[kcal]')
        axes.set_title("Simulated data")
        plt.show()
```



Our simulated data is mostly from 60 to 140. There is one line that leads to some unrealistic values but generally it is quite well.

```
In [ ]: calorie_sim = sim.stan_variable('calorie')
```

```
In [ ]: fig, axes = plt.subplots(1,1,figsize = (7,4))
axes=ribbon_plot(data_sim['sugars']+data['sugars'].mean(),calorie_sim,axes)
axes.scatter(data['sugars'], data['calories'], color = 'black', alpha = 1, s=10)
axes.set_xlabel('sugars[g]')
axes.set_ylabel('calories[kcal]')
axes.set_title("Simulated measurements with observed data (black dots)")
plt.show()
```



As we can see observed data is well fitted inside data simulated from our model. There are 2 points that are outside of this area but they are still quite close.

```
In [ ]: fig = plt.figure(figsize=(10,5))
gs = fig.add_gridspec(2,3)
ax1 = fig.add_subplot(gs[1,:])
ax1.hist(calories_sim, bins=40, color=DARK, edgecolor=DARK_HIGHLIGHT,density=True)

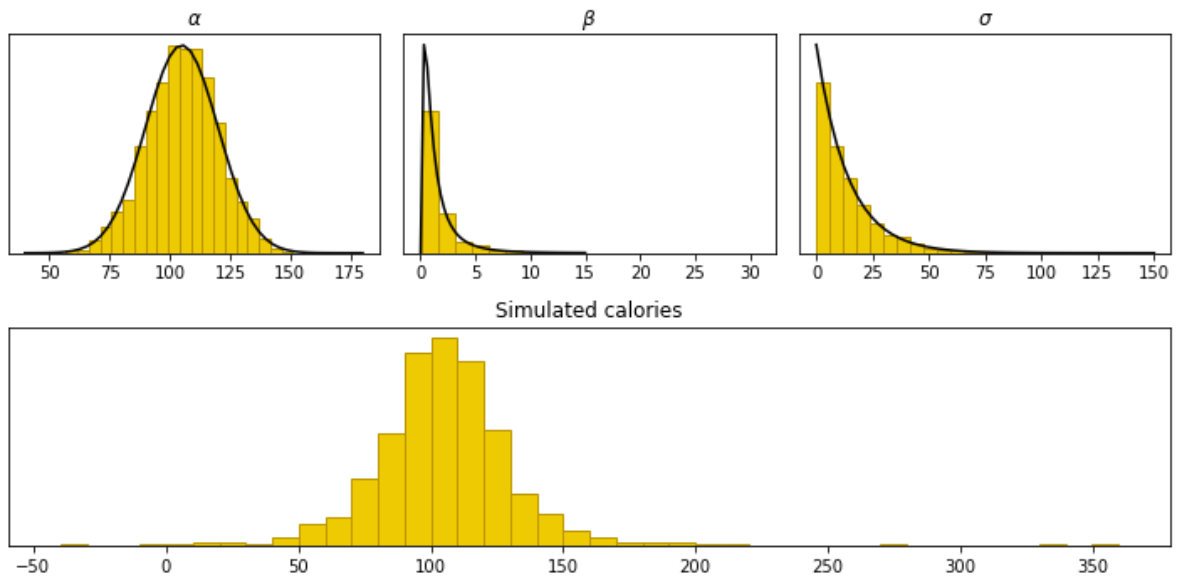
ax1.set_yticks([])
ax1.set_title('Simulated calories')

ax2 = fig.add_subplot(gs[0, 0])
ax3 = fig.add_subplot(gs[0, 1])
ax4 = fig.add_subplot(gs[0, 2])

ax2.hist(alpha_sim, bins=20, color=DARK, edgecolor=DARK_HIGHLIGHT,density=True)
x=np.linspace(40,180)
y=stats.norm.pdf(x,loc=105,scale=15)
ax2.plot(x,y,'black')
ax4.set_title('$\sigma$')
ax2.set_title(r'$\alpha$')
ax2.set_yticks([])
ax4.set_yticks([])
ax4.hist(sigma_sim, bins=20, color=DARK, edgecolor=DARK_HIGHLIGHT,density=True)
x=np.linspace(0,150)
y=stats.expon.pdf(x,scale=14)
ax4.plot(x,y,'black')

ax3.hist(beta_sim, bins=20, color=DARK, edgecolor=DARK_HIGHLIGHT,density=True)
x=np.linspace(0,15)
y=stats.lognorm.pdf(x, s=1)
ax3.plot(x,y,'black')
ax3.set_title(r'$\beta$')
ax3.set_yticks([])
```

```
fig.tight_layout()
plt.show()
```



As we can see simulated values of parameters α , β and σ were distributed well, as we expected.

Values of simulated calories are mostly distributed well (the mean is distributed where we expected) but we have some outliers which, when we add some data, will probably disappear.

Posterior

```
In [ ]: with open('cereal_2_fit.stan') as file:
        print(file.read())
```

```

data {
  int N;
  vector[N] sugars;
  real calories[N];
}

parameters {
  real alpha;
  real beta;
  real<lower=0> sigma;
}

transformed parameters {
  vector[N] mu = sugars*beta+alpha;
}

model {
  alpha ~ normal(105, 15);
  beta ~ lognormal(0, 1);
  sigma ~ exponential(0.067);
  calories ~ normal(mu, sigma);
}

generated quantities {
  vector[N] log_lik;
  real calorie[N];
  for (i in 1:N) {
    log_lik[i] = normal_lpdf(calories[i] | mu[i], sigma);
    calorie[i] = normal_rng(mu[i], sigma);
  }
}

```

Data required for this model:

- N -> calories vector size
- sugars -> sugars vector
- calories -> calories vector

```
In [ ]: model_2_fit = cmdstanpy.CmdStanModel(stan_file='cereal_2_fit.stan')
```

```
INFO:cmdstanpy:found newer exe file, not recompiling
```

```
In [ ]: data_fit = dict(N=len(data),
                        sugars=data['c_sugars'].values,
                        calories=data['calories'].values)

fit_2=model_2_fit.sample(data=data_fit, seed=12062022, output_dir='samples', adapt_
```

```
INFO:cmdstanpy:CmdStan start processing
```

```
chain 1 |           | 00:00 Status
chain 2 |           | 00:00 Status
chain 3 |           | 00:00 Status
chain 4 |           | 00:00 Status
```

```
INFO:cmdstanpy:CmdStan done processing.
```

When first running `diagnose()` we discovered the following issue.

""Checking sampler transitions for divergences. 10 of 4000 (0.25%) transitions ended with a divergence. These divergent transitions indicate that HMC is not fully able to explore the

posterior distribution. Try increasing adapt delta closer to 1. If this doesn't remove all divergences, try to reparameterize the model."""

We decide to changed "adapt_delta" parameter from 0.8 to 0.999. After this change issue was resolved.

```
In [ ]: print(fit_2.diagnose())
```

Processing csv files: C:\GitHub\DataAnalyticsProject\Project\samples\cereal_2_fit-20220621214947_1.csv, C:\GitHub\DataAnalyticsProject\Project\samples\cereal_2_fit-20220621214947_2.csv, C:\GitHub\DataAnalyticsProject\Project\samples\cereal_2_fit-20220621214947_3.csv, C:\GitHub\DataAnalyticsProject\Project\samples\cereal_2_fit-20220621214947_4.csv

Checking sampler transitions treedepth.
Treedepth satisfactory for all transitions.

Checking sampler transitions for divergences.
No divergent transitions found.

Checking E-BFMI - sampler transitions HMC potential energy.
E-BFMI satisfactory.

Effective sample size satisfactory.

Split R-hat values satisfactory all parameters.

Processing complete, no problems detected.

```
In [ ]: alpha_fit = fit_2.stan_variable('alpha')
        beta_fit = fit_2.stan_variable('beta')
        mu_fit = fit_2.stan_variable('mu')
        sigma_fit = fit_2.stan_variable('sigma')
        calorie_pred = fit_2.stan_variable('calorie')
```

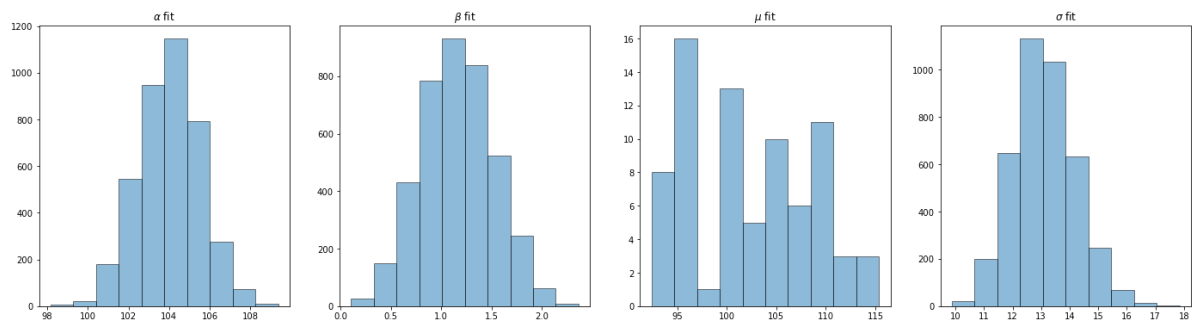
```
In [ ]: az.summary(fit_2, var_names=['alpha', 'beta', 'sigma'], round_to=2, kind='stats')
```

```
Out[ ]:
```

	mean	sd	hdi_3%	hdi_97%
alpha	104.01	1.52	101.08	106.68
beta	1.16	0.36	0.51	1.85
sigma	13.12	1.08	11.11	15.12

```
In [ ]: f, (ax1, ax2, ax3, ax4) = plt.subplots(1, 4, figsize = (24,6))

ax1.hist(alpha_fit, alpha=0.5, ec='black')
ax1.set_title(r"$\alpha$ fit")
ax2.hist(beta_fit, alpha=0.5, ec='black')
ax2.set_title(r"$\beta$ fit")
ax3.hist(mu_fit[0], alpha=0.5, ec='black')
ax3.set_title(r"$\mu$ fit")
ax4.hist(sigma_fit, alpha=0.5, ec='black')
ax4.set_title(r"$\sigma$ fit")
plt.show()
```



α values are normally distributed with values from 98 to 110 with mean somewhere around 105.

β values are normally distributed with values from 0 to 2.5 with mean somewhere around 1.

μ values are from 90 to 115.

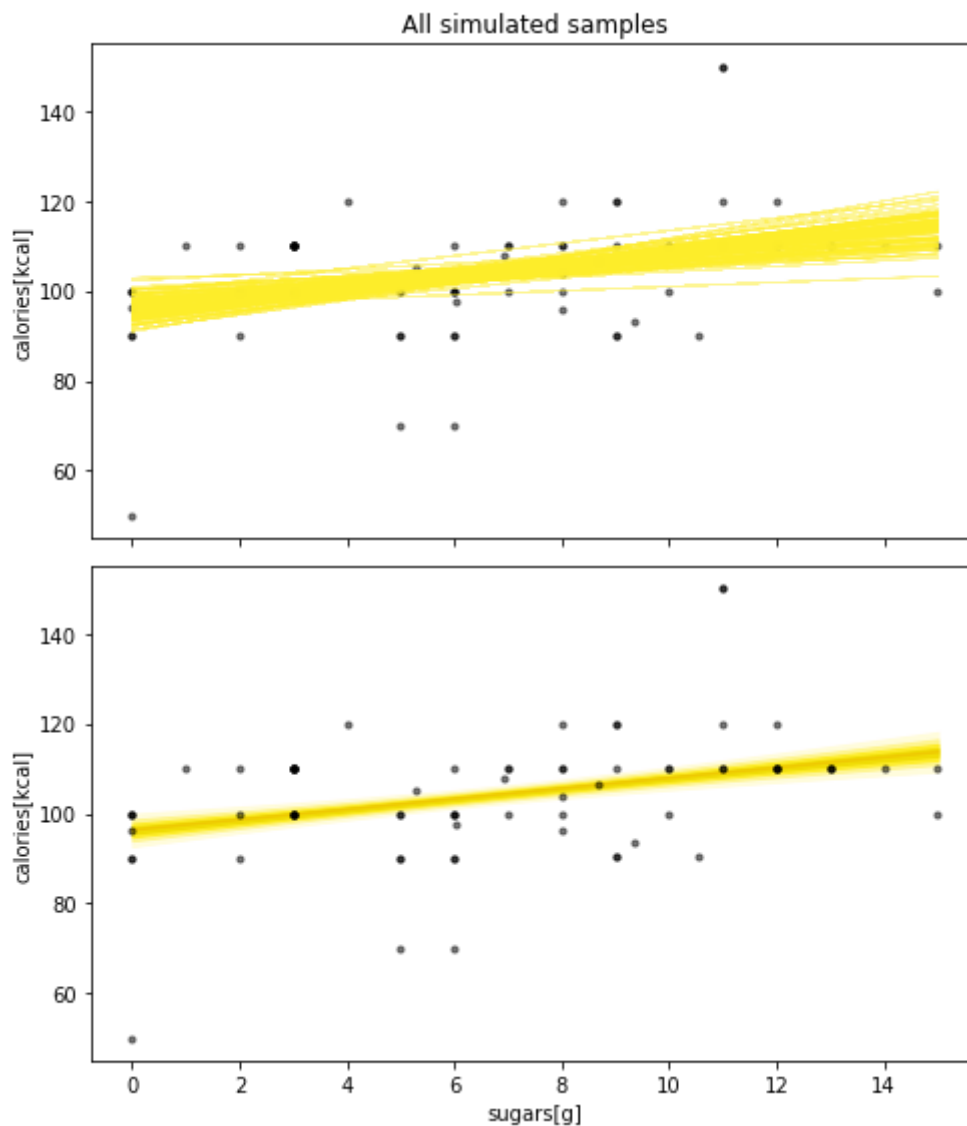
σ values are exponentially distributed with values from 10 to 18 with mean somewhere around 13.

```
In [ ]: fig, axes = plt.subplots(2,1,figsize = (7,8), sharey=True, sharex=True)
        ax0=axes[0]

        for i in range(100):
            ax0.plot(data['sugars'],
                    alpha_fit[i]+beta_fit[i]*data['c_sugars'],
                    color=MID,
                    alpha=0.5, linewidth=0.5)

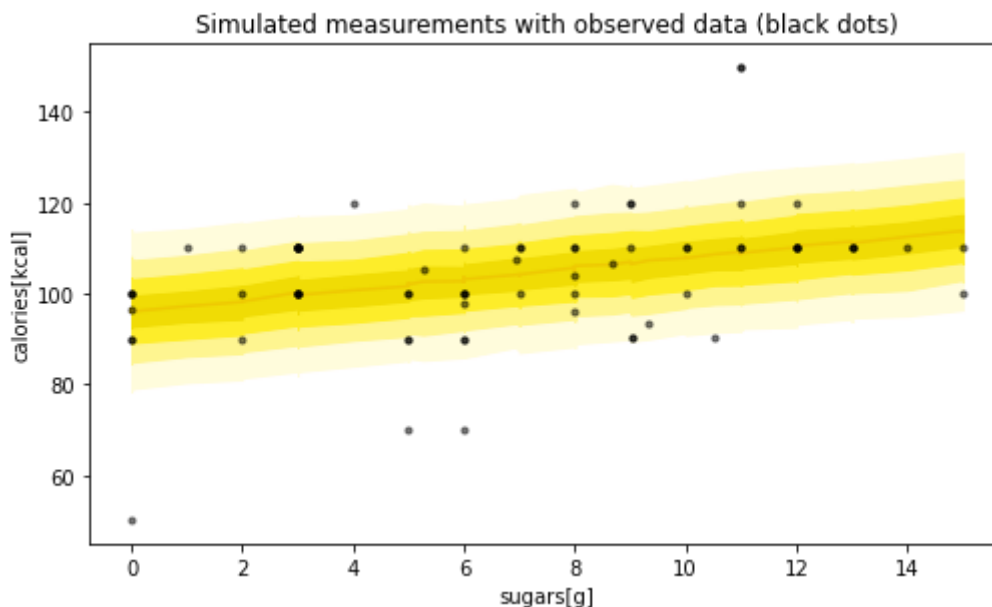
        ax0.scatter(data['sugars'], data['calories'], color='black', alpha=0.5, s=10)

        ax1=axes[1]
        ax1=ribbon_plot(data['sugars'].values, mu_fit, ax1, supress_warning=True)
        ax1.scatter(data['sugars'], data['calories'], color='black', alpha=0.5, s=10)
        ax1.set_xlabel('sugars[g]')
        ax1.set_ylabel('calories[kcal]')
        ax0.set_ylabel('calories[kcal]')
        ax0.set_title("All simulated samples")
        fig.tight_layout()
        plt.show()
```



```
In [ ]: fig, axes = plt.subplots(1,1,figsize = (7,4))

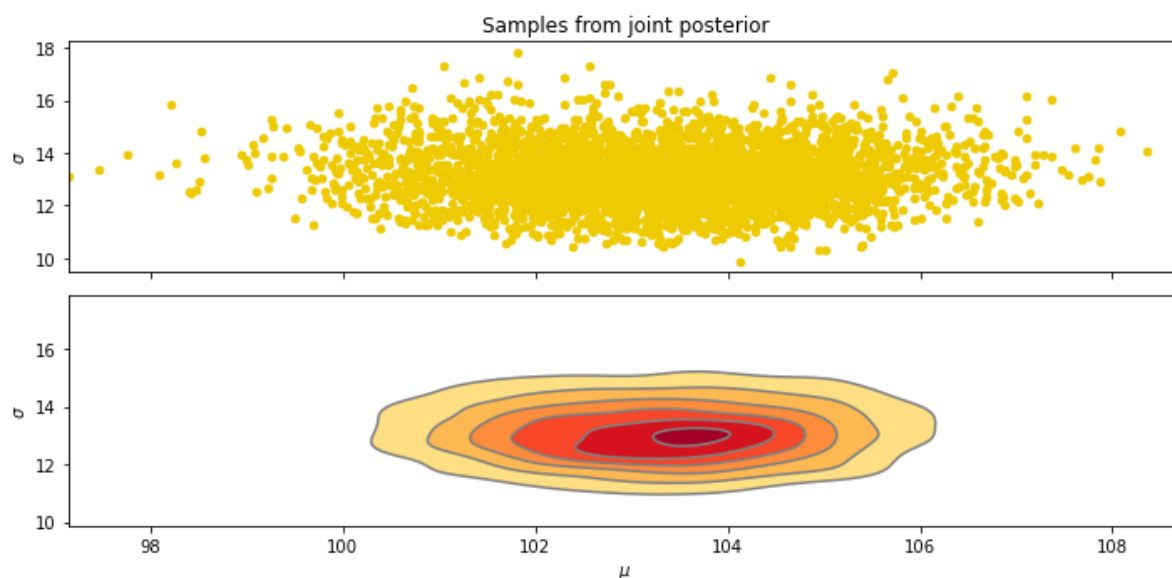
axes=ribbon_plot(data['sugars'].values, calorie_pred, axes, supress_warning=True)
axes.scatter(data['sugars'], data['calories'], color='black', alpha=0.5, s=10)
fig.tight_layout()
axes.set_xlabel('sugars[g]')
axes.set_ylabel('calories[kcal]')
axes.set_title("Simulated measurements with observed data (black dots)")
plt.show()
```



As we can see observed data is generally well fitted inside data simulated from our model. There are some points that are outside of this area.

```
In [ ]: fig, axes = plt.subplots(2,1,figsize=(10,5), sharex=True)
ax1=axes[0]
ax1.scatter(mu_fit[:,0], sigma_fit, 20, color=DARK)
ax1.set_title("Samples from joint posterior")
ax1.set_ylabel(r'$\sigma$')
ax2=axes[1]
az.plot_kde(mu_fit[:,0], sigma_fit, ax=ax2, contourf_kwargs={'cmap':'YlOrRd'})

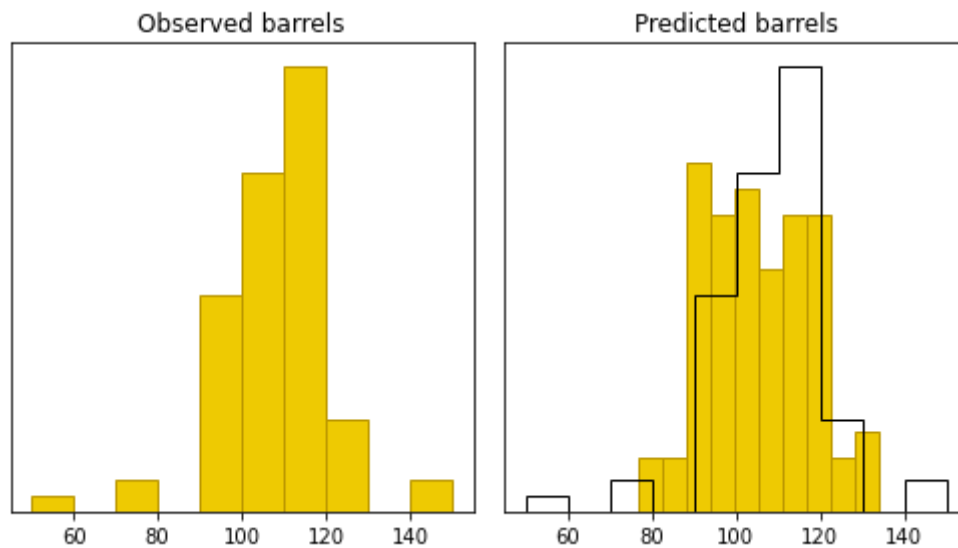
ax2.set_xlabel(r'$\mu$')
ax2.set_ylabel(r'$\sigma$')
fig.tight_layout()
plt.show()
```



```
In [ ]: fig, axes = plt.subplots(1,2,figsize=(7,4),sharex=True,sharey=True)
ax=axes[0]
ax.hist(data['calories'], bins=10, color=DARK,edgecolor=DARK_HIGHLIGHT,density=True)
ax.set_title('Observed barrels')
ax.set_yticks(())
ax2=axes[1]
ax2.hist(calorie_pred[3000], bins=10, color=DARK,edgecolor=DARK_HIGHLIGHT,density=True)
ax2.hist(data['calories'], bins=10, histtype='step', color='black', density=True)
```

```
ax2.set_title('Predicted barrels')
ax2.set_yticks(())
fig.tight_layout()

plt.show()
```



In comparison with 1.1 model values are more squeezed (previously from 60 to 160, now somewhere from 80 to 130).

As we can see our model has problem with catching values stacked in the middle so we decided to use double exponential distribution because we thought it will solve this issue.

```
In [ ]: fit_id_1 = az.from_cmdstanpy(posterior=fit_2, log_likelihood='log_lik')
```

```
In [ ]: fit_id_1
```

```
Out[ ]: arviz.InferenceData
```

- posterior
- log_likelihood
- sample_stats

Model 2

Double Exponential (Laplace) Distribution

$$DoubleExponential(y|\mu, \sigma) = \frac{1}{2\sigma} \exp\left(-\frac{|y - \mu|}{\sigma}\right)$$

Prior predictive check

We used the same values for alpha, beta and sigma as the in previous prior. We only

changed the distribution from normal distribution to double exponential distribution.

```
In [ ]: with open('cereal_3_ppc.stan') as file:
        print(file.read())
```

```
data {
  int N;
  real sugars[N];
}

generated quantities {
  real alpha = double_exponential_rng(105, 15);
  real beta = lognormal_rng(0, 1);
  real sigma = exponential_rng(0.067);
  real calorie[N];
  for (i in 1:N) {
    calorie[i] = double_exponential_rng(sugars[i]*beta+alpha, sigma);
  }
}
```

```
In [ ]: model_ppc = cmdstanpy.CmdStanModel(stan_file='cereal_3_ppc.stan')
```

```
INFO:cmdstanpy:found newer exe file, not recompiling
```

```
In [ ]: sim = model_ppc.sample(data=data_sim, iter_sampling=R, iter_warmup=0, chains=1, refi
```

```
INFO:cmdstanpy:CmdStan start processing
```

```
chain 1 |          | 00:00 Status
```

```
INFO:cmdstanpy:CmdStan done processing.
```

```
In [ ]: alpha_sim = sim.stan_variable('alpha')
        beta_sim = sim.stan_variable('beta')
        sigma_sim = sim.stan_variable('sigma')
        calories_sim=sim.stan_variable('calorie')
```

```
In [ ]: fig = plt.figure(figsize=(10,5))
        gs = fig.add_gridspec(2,3)
        ax1 = fig.add_subplot(gs[1,:])
        ax1.hist(calories_sim[579], bins=40, color=DARK, edgecolor=DARK_HIGHLIGHT,density=True)

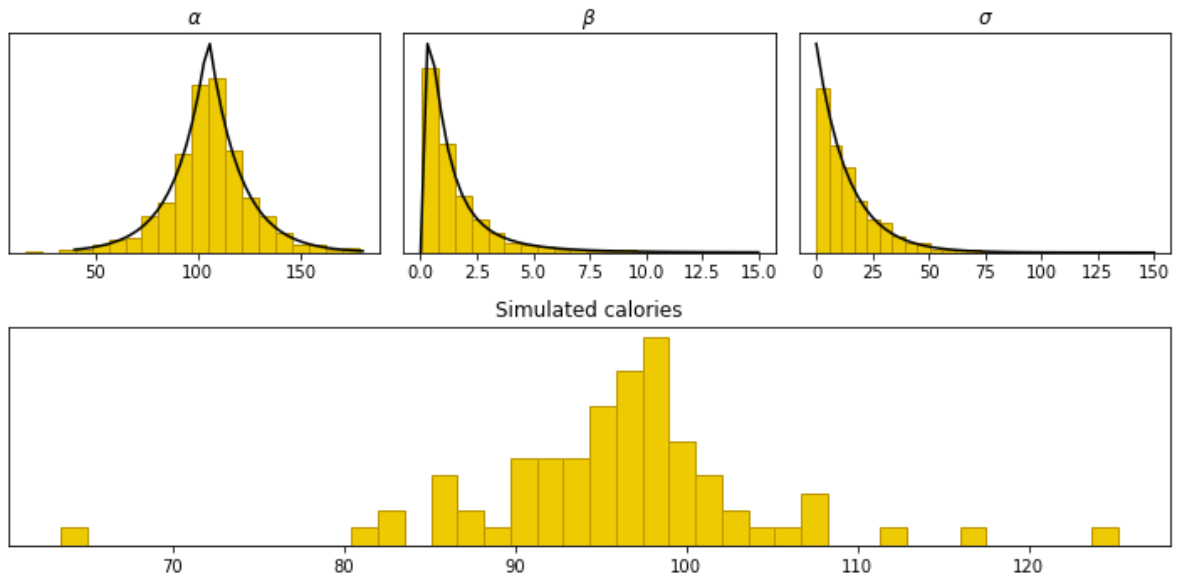
        ax1.set_yticks([])
        ax1.set_title('Simulated calories')

        ax2 = fig.add_subplot(gs[0, 0])
        ax3 = fig.add_subplot(gs[0, 1])
        ax4 = fig.add_subplot(gs[0, 2])

        ax2.hist(alpha_sim, bins=20, color=DARK, edgecolor=DARK_HIGHLIGHT,density=True)
        x=np.linspace(40,180)
        y=stats.laplace.pdf(x,loc=105,scale=15)
        ax2.plot(x,y,'black')
        ax4.set_title('$\sigma$')
        ax2.set_title(r'$\alpha$')
        ax2.set_yticks([])
        ax4.set_yticks([])
        ax4.hist(sigma_sim, bins=20, color=DARK, edgecolor=DARK_HIGHLIGHT,density=True)
        x=np.linspace(0,150)
        y=stats.expon.pdf(x,scale=14)
        ax4.plot(x,y,'black')
```

```
ax3.hist(beta_sim, bins=20, color=DARK, edgecolor=DARK_HIGHLIGHT,density=True)
x=np.linspace(0,15)
y=stats.lognorm.pdf(x, s=1)
ax3.plot(x,y, 'black')
ax3.set_title(r'$\beta$')
ax3.set_yticks([])

fig.tight_layout()
plt.show()
```



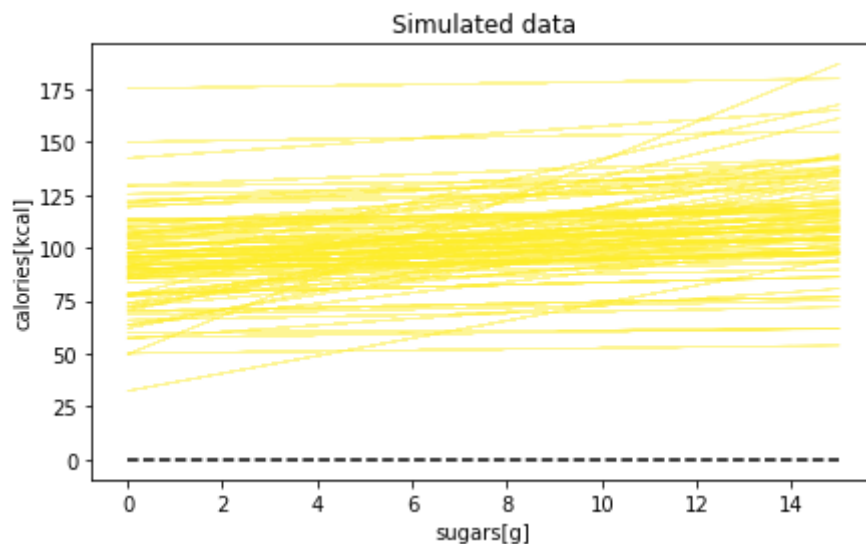
As we can see simulated values of parameters α , β and σ were distributed well, as we expected.

Values of simulated calories are mostly distributed well. In contrast to examples in 1.1 and 1.2, there are no outliers like minus values or very high values.

```
In [ ]: fig, axes = plt.subplots(1,1,figsize = (7,4))

for i in range(100):
    axes.plot(data['sugars'], alpha_sim[i]+beta_sim[i]*data['c_sugars'], color=MID)
axes.set_xlabel('sugars[g]')
axes.set_ylabel('calories[kcal]')

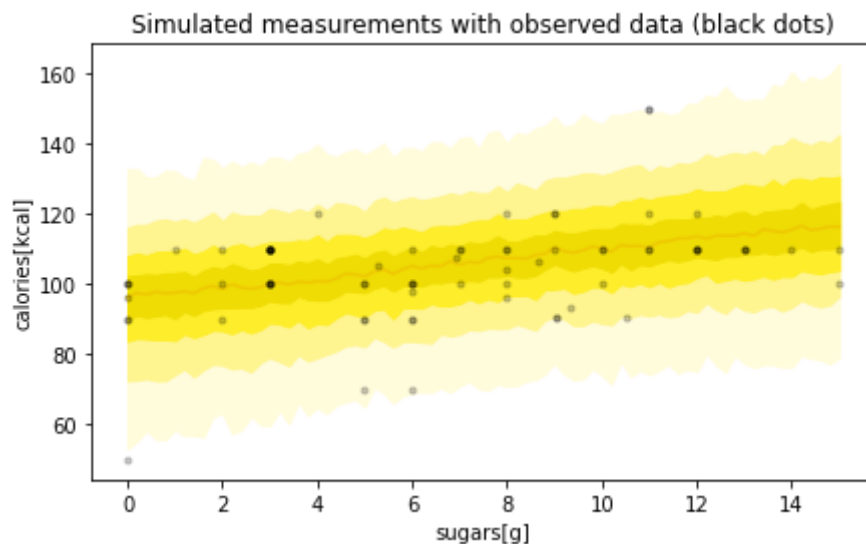
axes.hlines([0],xmin=data['sugars'].min(), xmax=data['sugars'].max(), linestyle='--')
axes.set_title("Simulated data")
plt.show()
```



Our simulated data is mostly from 50 to 150. There is no line that leads to unrealistic values like in 1.2.

```
In [ ]: calorie_sim = sim.stan_variable('calorie')
```

```
In [ ]: fig, axes = plt.subplots(1,1,figsize = (7,4))
axes=ribbon_plot(data_sim['sugars']+data['sugars'].mean(),calorie_sim,axes)
axes.scatter(data['sugars'], data['calories'], color = 'black', alpha = 0.2, s=10)
axes.set_xlabel('sugars[g]')
axes.set_ylabel('calories[kcal]')
axes.set_title("Simulated measurements with observed data (black dots)")
plt.show()
```



As we can see observed data is well fitted inside data simulated from our model.

Posterior

```
In [ ]: with open('cereal_3_fit.stan') as file:
        print(file.read())
```



```

data {
  int N;
  vector[N] sugars;
  vector[N] calories;
}

parameters {
  real alpha;
  real beta;
  real<lower=0> sigma;
}

transformed parameters {
  vector[N] mu = sugars*beta+alpha;
}

model {
  alpha ~ double_exponential(105, 15);
  beta ~ lognormal(0, 1);
  sigma ~ exponential(0.067);
  calories ~ double_exponential(mu, sigma);
}

generated quantities {
  vector[N] log_lik;
  real calorie[N];
  for (i in 1:N) {
    log_lik[i] = double_exponential_lpdf(calories[i] | mu[i], sigma);
    calorie[i] = double_exponential_rng(mu[i], sigma);
  }
}

```

Data required for this model:

- N -> size of calories vector
- sugars -> sugars vector
- calories -> calories vector

```
In [ ]: model_3_fit = cmdstanpy.CmdStanModel(stan_file='cereal_3_fit.stan')
```

```
INFO:cmdstanpy:found newer exe file, not recompiling
```

```
In [ ]: data_fit = dict(N=len(data),
                        sugars=data['c_sugars'].values,
                        calories=data['calories'].values)

fit_3=model_3_fit.sample(data=data_fit, seed=12062022, output_dir='samples')
```

```
INFO:cmdstanpy:CmdStan start processing
```

```
chain 1 |           | 00:00 Status
chain 2 |           | 00:00 Status
chain 3 |           | 00:00 Status
chain 4 |           | 00:00 Status
```

```
INFO:cmdstanpy:CmdStan done processing.
```

```
In [ ]: print(fit_3.diagnose())
```

Processing csv files: C:\GitHub\DataAnalyticsProject\Project\samples\cereal_3_fit-20220621215018_1.csv, C:\GitHub\DataAnalyticsProject\Project\samples\cereal_3_fit-20220621215018_2.csv, C:\GitHub\DataAnalyticsProject\Project\samples\cereal_3_fit-20220621215018_3.csv, C:\GitHub\DataAnalyticsProject\Project\samples\cereal_3_fit-20220621215018_4.csv

Checking sampler transitions treedepth.
Treedepth satisfactory for all transitions.

Checking sampler transitions for divergences.
No divergent transitions found.

Checking E-BFMI - sampler transitions HMC potential energy.
E-BFMI satisfactory.

Effective sample size satisfactory.

Split R-hat values satisfactory all parameters.

Processing complete, no problems detected.

No errors/issues occurred during sampling.

```
In [ ]: az.summary(fit_3, var_names=['alpha', 'beta', 'sigma'], round_to=2, kind='stats')
```

```
Out[ ]:
```

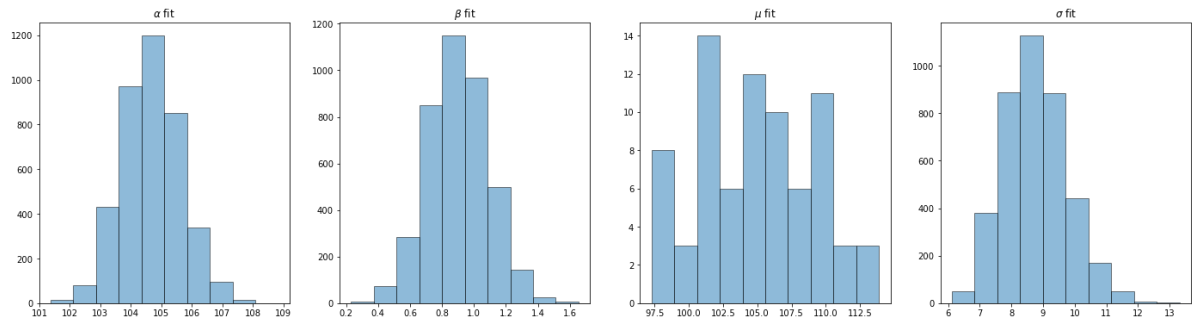
	mean	sd	hdi_3%	hdi_97%
alpha	104.68	0.97	102.93	106.54
beta	0.90	0.19	0.58	1.28
sigma	8.77	1.00	6.93	10.63

Comaring to 1.2 model mean values of beta and sigma decrease (beta from 1.16 to 0.9 and sigma from 13.12 to 8.77). Mean alpha value is similar.

```
In [ ]: alpha_fit = fit_3.stan_variable('alpha')
beta_fit = fit_3.stan_variable('beta')
mu_fit = fit_3.stan_variable('mu')
sigma_fit = fit_3.stan_variable('sigma')
calorie_pred = fit_3.stan_variable('calorie')
```

```
In [ ]: f, (ax1, ax2, ax3, ax4) = plt.subplots(1, 4, figsize = (24,6))

ax1.hist(alpha_fit, alpha=0.5, ec='black')
ax1.set_title(r"$\alpha$ fit")
ax2.hist(beta_fit, alpha=0.5, ec='black')
ax2.set_title(r"$\beta$ fit")
ax3.hist(mu_fit[0], alpha=0.5, ec='black')
ax3.set_title(r"$\mu$ fit")
ax4.hist(sigma_fit, alpha=0.5, ec='black')
ax4.set_title(r"$\sigma$ fit")
plt.show()
```



α values are normally distributed with values from 100 to 108 with mean somewhere around 105.

β values are normally distributed with values from 0 to 1.6 with mean somewhere around 0.9.

μ values are from 97.5 to 113.

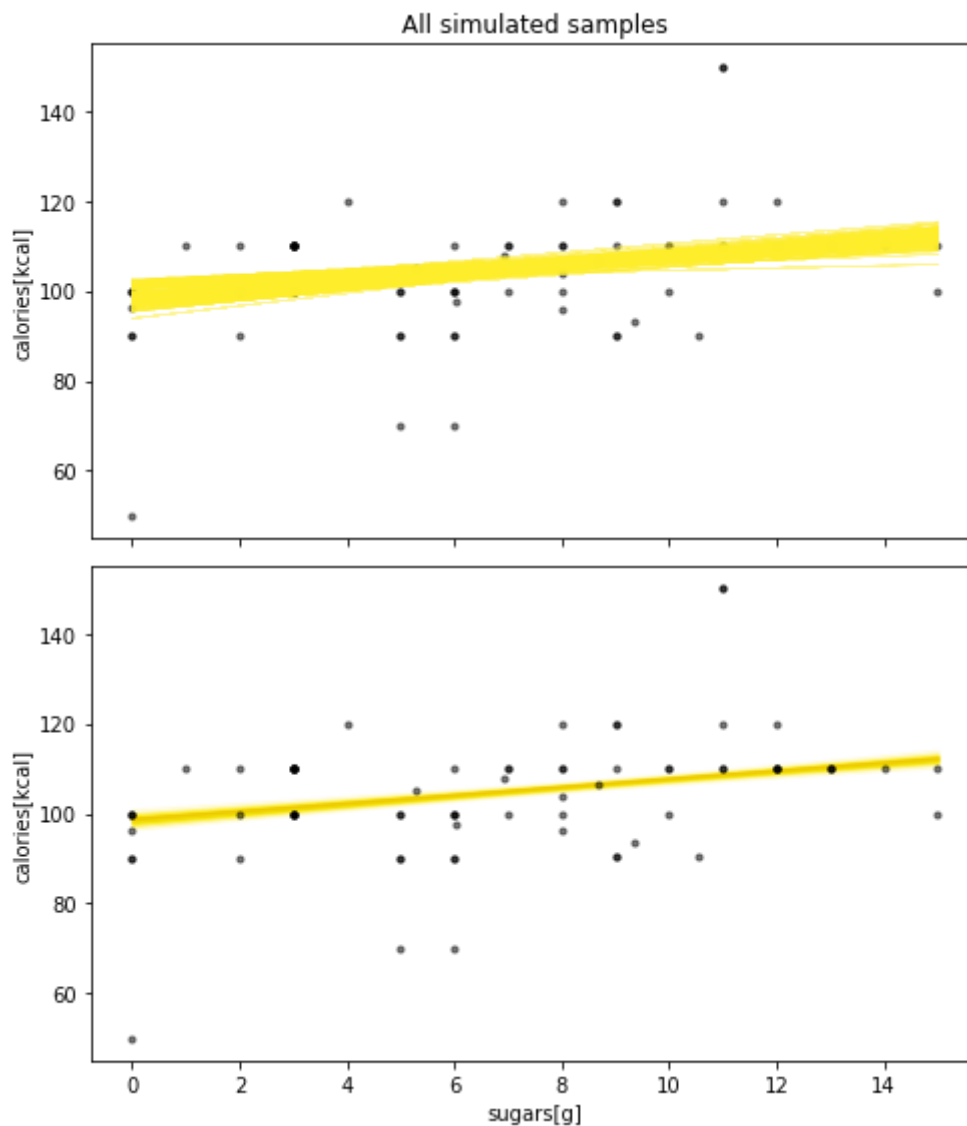
σ values are exponentially distributed with values from 6 to 13 with mean somewhere around 8.5.

```
In [ ]: fig, axes = plt.subplots(2,1,figsize = (7,8), sharey=True, sharex=True)
ax0=axes[0]

for i in range(100):
    ax0.plot(data['sugars'],
             alpha_fit[i]+beta_fit[i]*data['c_sugars'],
             color=MID,
             alpha=0.5, linewidth=0.5)

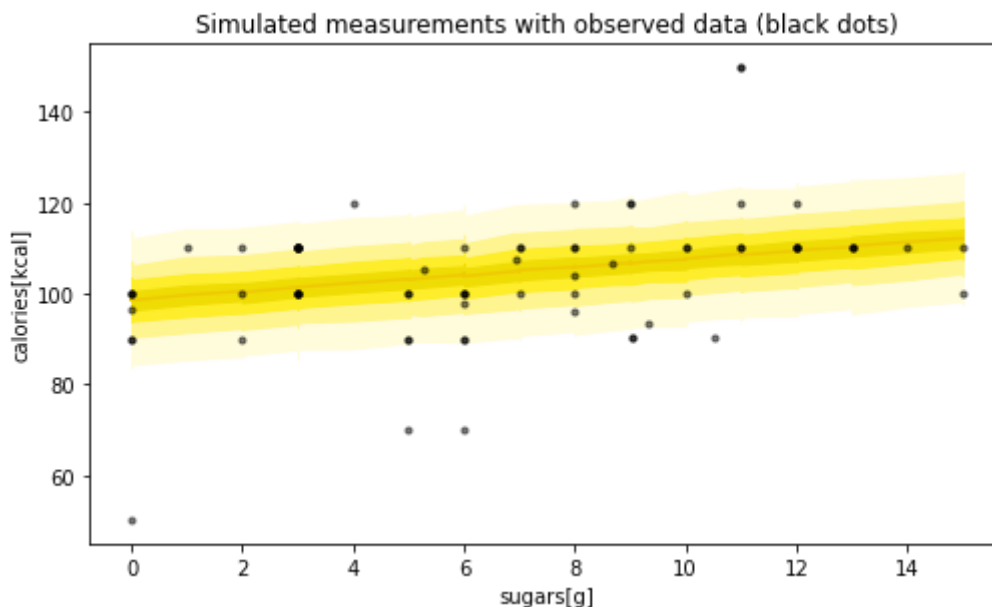
ax0.scatter(data['sugars'], data['calories'], color='black', alpha=0.5, s=10)

ax1=axes[1]
ax1=ribbon_plot(data['sugars'].values, mu_fit, ax1, suppress_warning=True)
ax1.scatter(data['sugars'], data['calories'], color='black', alpha=0.5, s=10)
ax1.set_xlabel('sugars[g]')
ax1.set_ylabel('calories[kcal]')
ax0.set_ylabel('calories[kcal]')
ax0.set_title("All simulated samples")
fig.tight_layout()
plt.show()
```



```
In [ ]: fig, axes = plt.subplots(1,1,figsize = (7,4))

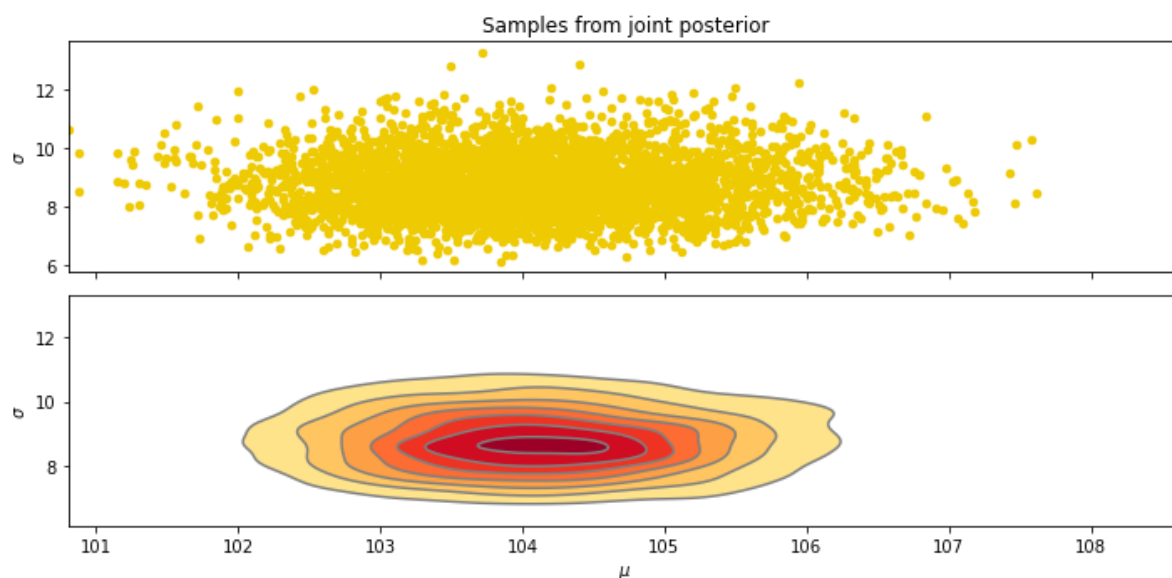
axes=ribbon_plot(data['sugars'].values, calorie_pred, axes, supress_warning=True)
axes.scatter(data['sugars'], data['calories'], color='black', alpha=0.5, s=10)
fig.tight_layout()
axes.set_xlabel('sugars[g]')
axes.set_ylabel('calories[kcal]')
axes.set_title("Simulated measurements with observed data (black dots)")
plt.show()
```



As we can see observed data is generally well fitted inside data simulated from our model. There are some points that are outside of this area.

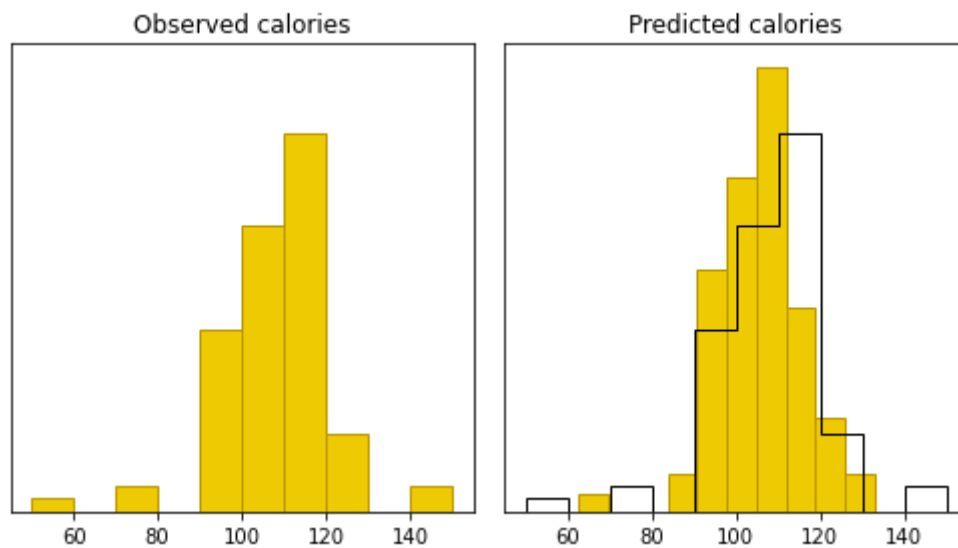
```
In [ ]: fig, axes = plt.subplots(2,1,figsize=(10,5), sharex=True)
ax1=axes[0]
ax1.scatter(mu_fit[:,0], sigma_fit, 20, color=DARK)
ax1.set_title("Samples from joint posterior")
ax1.set_ylabel(r'$\sigma$')
ax2=axes[1]
az.plot_kde(mu_fit[:,0], sigma_fit, ax=ax2, contourf_kwargs={'cmap':'YlOrRd'})

ax2.set_xlabel(r'$\mu$')
ax2.set_ylabel(r'$\sigma$')
fig.tight_layout()
plt.show()
```



```
In [ ]: fig, axes = plt.subplots(1,2,figsize=(7,4),sharex=True,sharey=True)
ax=axes[0]
ax.hist(data['calories'], bins=10, color=DARK,edgecolor=DARK_HIGHLIGHT,density=True)
ax.set_title('Observed calories')
ax.set_yticks(())
ax2=axes[1]
ax2.hist(calorie_pred[3000], bins=10, color=DARK,edgecolor=DARK_HIGHLIGHT,density=True)
ax2.hist(data['calories'], bins=10, histtype='step', color='black', density=True)
```

```
ax2.set_title('Predicted calories')
ax2.set_yticks(())
fig.tight_layout()
```



As we can see now model is able to better catch values stacked in the middle. Also values are a little bit less squeezed in compare to 1.2 model.

The one thing that can be improved are boundary values (like 60, 140).

```
In [ ]: fit_id_2 = az.from_cmdstanpy(posterior=fit_3, log_likelihood='log_lik')
```

```
In [ ]: model_compare = az.compare({'Normal distribution model': fit_id_1, 'Double exponential model': fit_id_2})
model_compare
```

```
c:\Anaconda3\envs\data_analytics\lib\site-packages\arviz\stats\stats.py:145: UserWarning: The default method used to estimate the weights for each model, has changed from BB-pseudo-BMA to stacking
  warnings.warn(
c:\Anaconda3\envs\data_analytics\lib\site-packages\arviz\stats\stats.py:212: FutureWarning: The frame.append method is deprecated and will be removed from pandas in a future version. Use pandas.concat instead.
  ics = ics.append([ic_func(dataset, pointwise=True, scale=scale)])
c:\Anaconda3\envs\data_analytics\lib\site-packages\arviz\stats\stats.py:212: FutureWarning: The frame.append method is deprecated and will be removed from pandas in a future version. Use pandas.concat instead.
  ics = ics.append([ic_func(dataset, pointwise=True, scale=scale)])
```

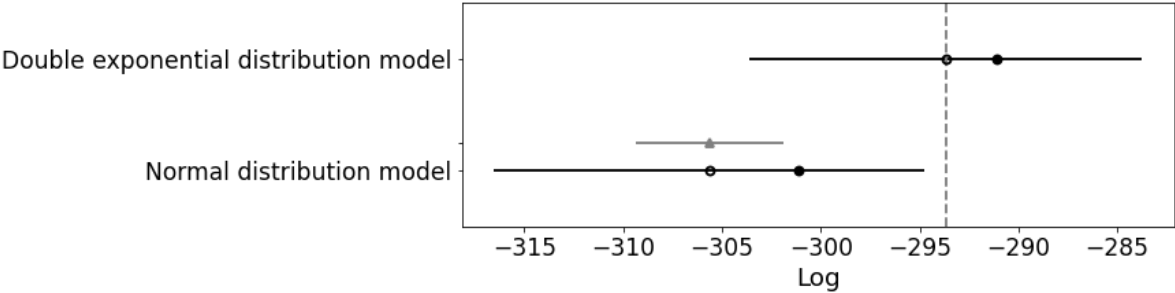
Out []:	rank	loo	p_loo	d_loo	weight	se	dse	warning	loo_score
Double exponential distribution model	0	-293.665885	2.534442	0.000000	1.0	9.929358	0.000000	False	
Normal distribution model	1	-305.648238	4.536610	11.982353	0.0	10.883787	3.732203	False	

rank -> The rank-order of the models. 0 is the best - Double exponential distribution model performs better than normal model

loo -> Higher loo indicates higher out-of-sample predictive fit ("better model") - Double exponential distribution model performs better than normal model

p_loo -> Estimated effective number of parameters
d_loo -> The difference in loo between two models
weight -> Relative weight for each model. This can be loosely interpreted as the probability of each model (among the compared model) given the data
se -> Standard error of the information criteria estimate
dse -> Standard error of the difference in information criteria between each model and the top-ranked model
warning -> A value of 1 indicates that the computation of information criteria may not be reliable. No warnings.
scale -> scale used for information criteria

```
In [ ]: az.plot_compare(model_compare, figsize = (12, 3))
plt.show()
```



When using LOO information criteria model using Laplace distribution got better result than first model. But the results were pretty close.

```
In [ ]: model_compare_2 = az.compare({'Normal distribution model':fit_id_1,'Double exponen'
model_compare_2
```

```
c:\Anaconda3\envs\data_analytics\lib\site-packages\arviz\stats\stats.py:145: UserWarning: The default method used to estimate the weights for each model, has changed from BB-pseudo-BMA to stacking
warnings.warn(
c:\Anaconda3\envs\data_analytics\lib\site-packages\arviz\stats\stats.py:1405: UserWarning: For one or more samples the posterior variance of the log predictive densities exceeds 0.4. This could be indication of WAIC starting to fail. See http://arxiv.org/abs/1507.04544 for details
warnings.warn(
c:\Anaconda3\envs\data_analytics\lib\site-packages\arviz\stats\stats.py:212: FutureWarning: The frame.append method is deprecated and will be removed from pandas in a future version. Use pandas.concat instead.
ics = ics.append([ic_func(dataset, pointwise=True, scale=scale)])
c:\Anaconda3\envs\data_analytics\lib\site-packages\arviz\stats\stats.py:212: FutureWarning: The frame.append method is deprecated and will be removed from pandas in a future version. Use pandas.concat instead.
ics = ics.append([ic_func(dataset, pointwise=True, scale=scale)])
```

Out[]:

	rank	waic	p_waic	d_waic	weight	se	dse	warning	waic_
Double exponential distribution model	0	-293.666491	2.535047	0.000000	1.0	9.929827	0.000000	False	
Normal distribution model	1	-305.663557	4.551928	11.997066	0.0	10.893591	3.739875	True	

rank -> The rank-order of the models. 0 is the best - Double exponential distribution model performs better than normal model

waic -> Higher waic indicates higher out-of-sample predictive fit ("better model") - Double exponential distribution model performs better than normal model

p_waic -> Estimated effective number of parameters

d_waic -> The difference in waic between two models

weight -> Relative weight for each model. This can be loosely interpreted as the probability of each model (among the compared model) given the data

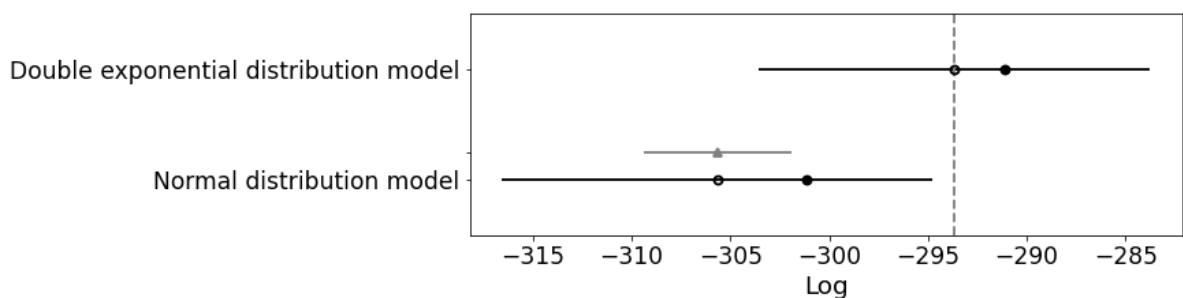
se -> Standard error of the information criteria estimate

dse -> Standard error of the difference in information criteria between each model and the top-ranked model

warning -> A value of 1 indicates that the computation of information criteria may not be reliable. Warning in "Normal distribution model" (For one or more samples the posterior variance of the log predictive densities exceeds 0.4. This could be indication of WAIC starting to fail.).

scale -> scale used for information criteria

```
In [ ]: az.plot_compare(model_compare_2, figsize = (12, 3))
plt.show()
```



When using WAIC information criteria again model using Laplace distribution got better result than first model. But the results were pretty close.

Results of comparing models using WAIC and LOO information criteria were almost the same.

In our opinion second model (using double exponential distribution) performed a little bit better than the first one because it was able to better catch values stacked close to the mean value.