Data Analytics - final project

Norbert Sak and Adam Sygut

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. Potenial 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 gien 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']
```

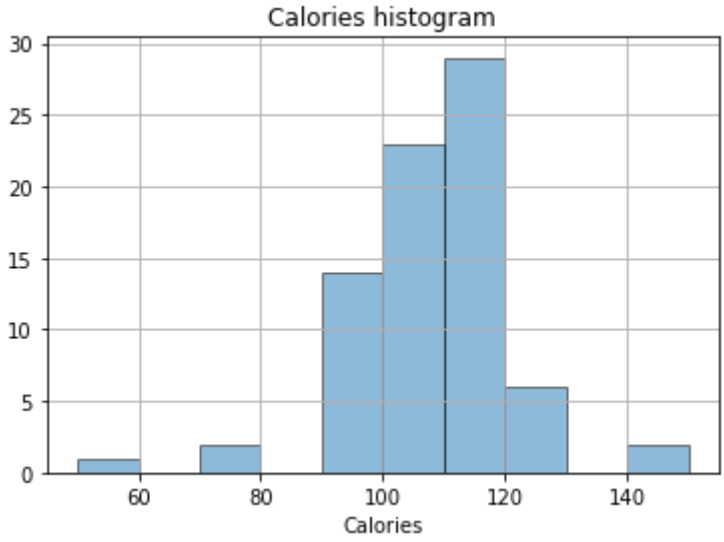
In [ ]:
```
df.head()
```

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

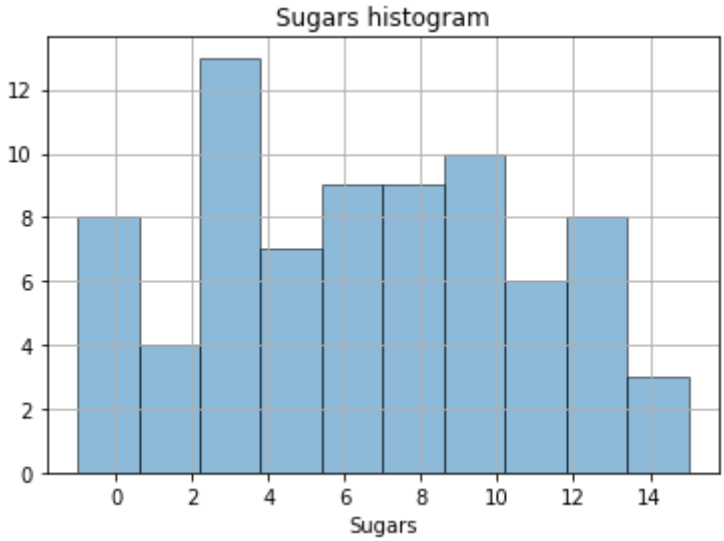
Histogram of calories

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 beacuse 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

We set the value of mu to be normally distributed with mean of 104 and standard deviation of 14 because in our dataframe mean value of calories was 104.049501 and std was 13.936164.

The value of sigma was set to be exponentially distributed with inverse scale beta of 0.071 (because $\frac{1}{14} \approx 0.071$).

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

```
generated quantities {
   real mu = normal_rng(104, 14);
   real sigma = exponential_rng(0.071);
   real calories = normal_rng(mu, sigma);
}
```

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

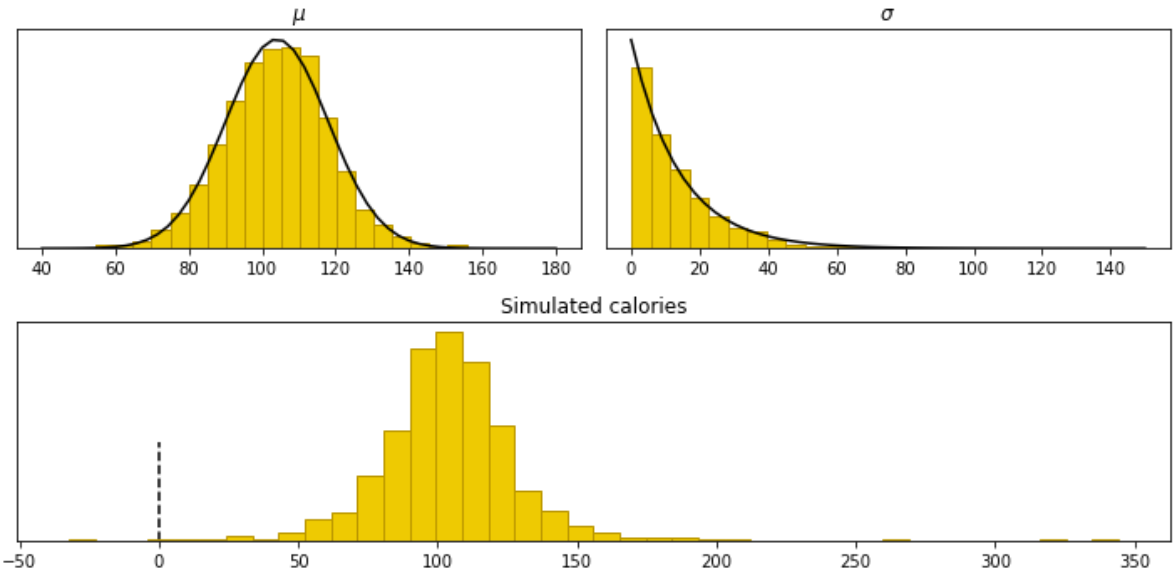
```
INFO:cmdstanpy:found newer exe file, not recompiling
```

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=104,scale=14)
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.
Values of simulated calories are mostly distributed well (the mean is distributed were we expected) but we have some outliers which, when we add some data, will probably dissapear.

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(104, 14);
   sigma ~ exponential(0.071);
   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['calorie
```

```
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-
20220619234357_1.csv, C:\GitHub\DataAnalyticsProject\Project\samples\cereal_1_fit-
20220619234357_2.csv, C:\GitHub\DataAnalyticsProject\Project\samples\cereal_1_fit-
20220619234357_3.csv, C:\GitHub\DataAnalyticsProject\Project\samples\cereal_1_fit-
20220619234357_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 occured during sampling.

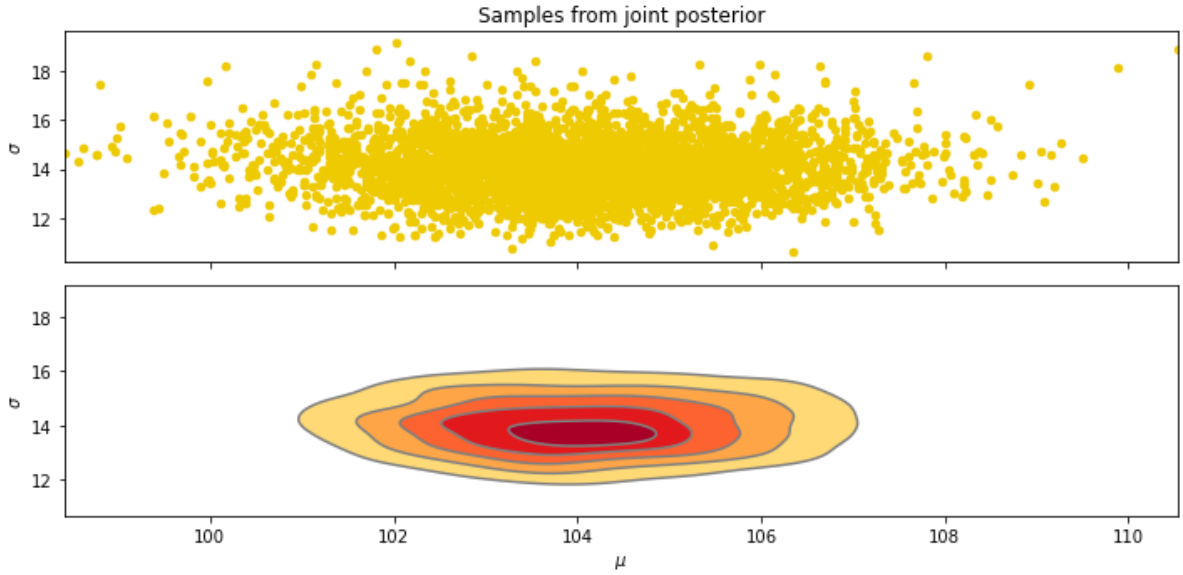
In [ ]:
```
az.summary(fit_1, var_names=['mu', 'sigma'], round_to=2, kind='stats')
```

Out[ ]:

	mean	sd	hdi_3%	hdi_97%
mu	104.00	1.63	101.01	107.05
sigma	14.07	1.15	11.94	16.20

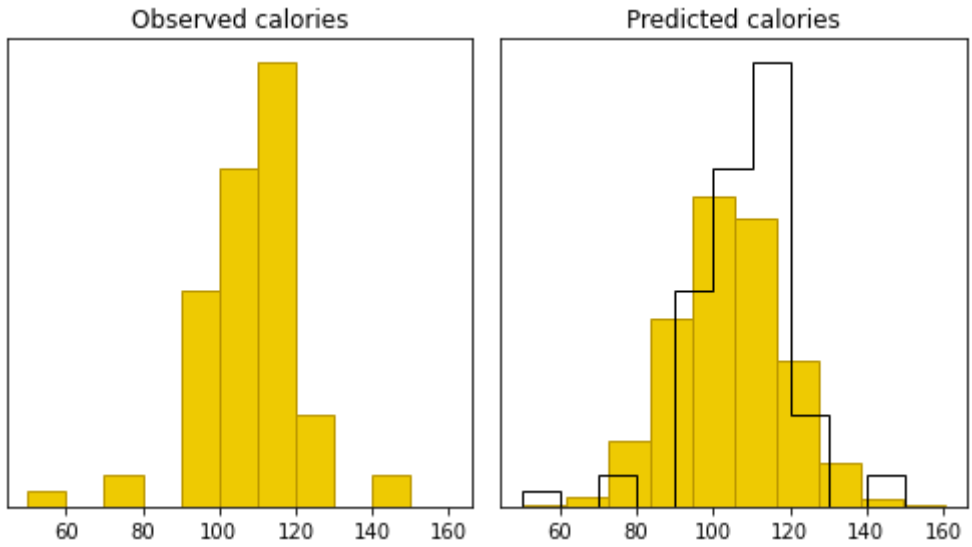
In [ ]:
```
mu_fit = fit_1.stan_variable('mu')
sigma_fit = fit_1.stan_variable('sigma')
calorie_pred = fit_1.stan_variable('calorie')
```

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 concenrated.

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=Tru
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()
```



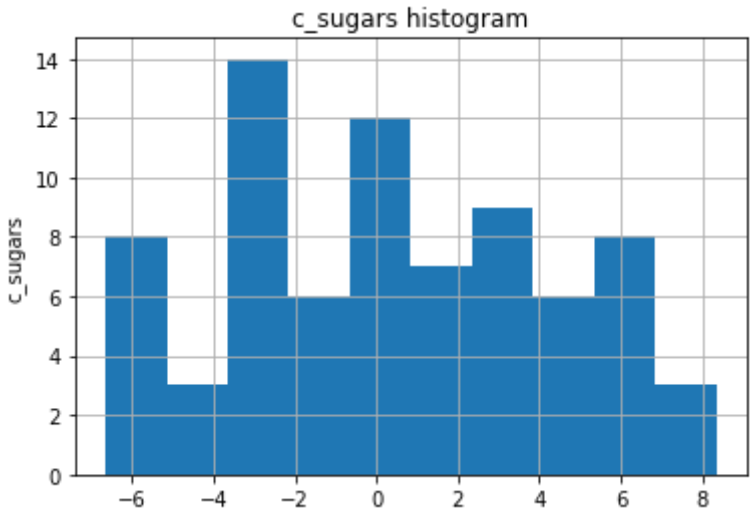
As we can see samples for posterior predictive did not match exactly the observed values.
Observed values are more clustered close to the mean value.
Data is not exactly similar with posterior predicitve sample but it's quite close.

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 'c*sugars*'.

$calories{i}\sim Normal(\mu {i}, \sigma)< br >< br >\mu {i}=\alpha + \beta *c_sugars_{i} < br >< br > Where\alphaand\betahavenormaldistributionand\sigma$ 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 distriuted 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(104, 14);
   real beta = normal_rng(0, 10);
   real sigma = exponential_rng(0.071);
   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')
```

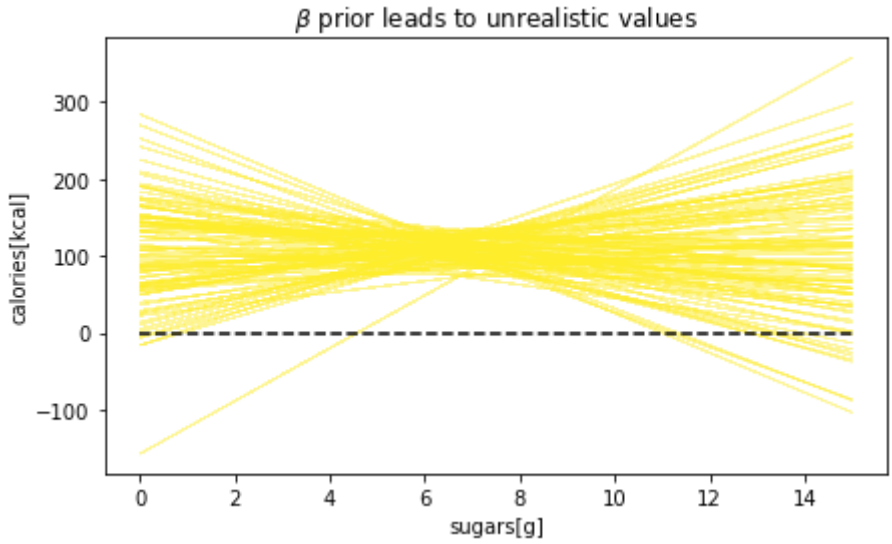
```
INFO:cmdstanpy:found newer exe file, not recompiling
```

In [ ]:
```
R = 1000
data_sim = {'N': len(data), 'sugars':np.linspace(data['c_sugars'].min(),data['c_sug

sim = model_ppc.sample(data=data_sim,iter_sampling=R, iter_warmup=0, chains=1, refr
```

```
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=MID
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()
```



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

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

generated quantities {
   real alpha = normal_rng(104, 14);
   real beta = lognormal_rng(0, 1);
   real sigma = exponential_rng(0.071);
   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')
```

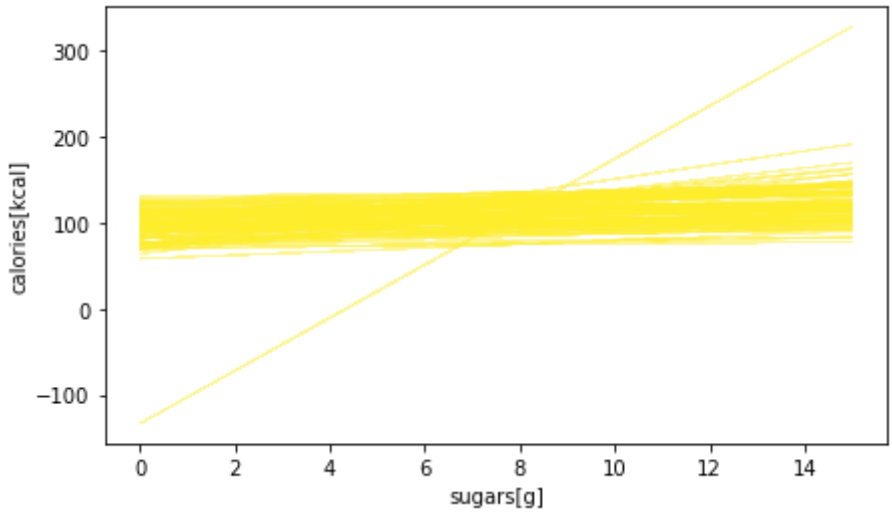
```
INFO:cmdstanpy:found newer exe file, not recompiling
```

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

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

INFO:cmdstanpy:CmdStan done processing.
```

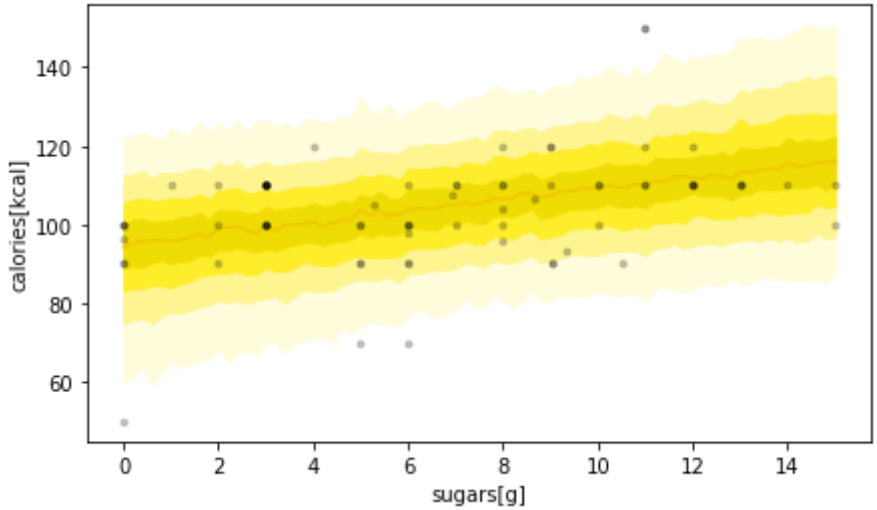
In [ ]:
```
alpha_sim = sim.stan_variable('alpha')
beta_sim = sim.stan_variable('beta')
```

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=MID_

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

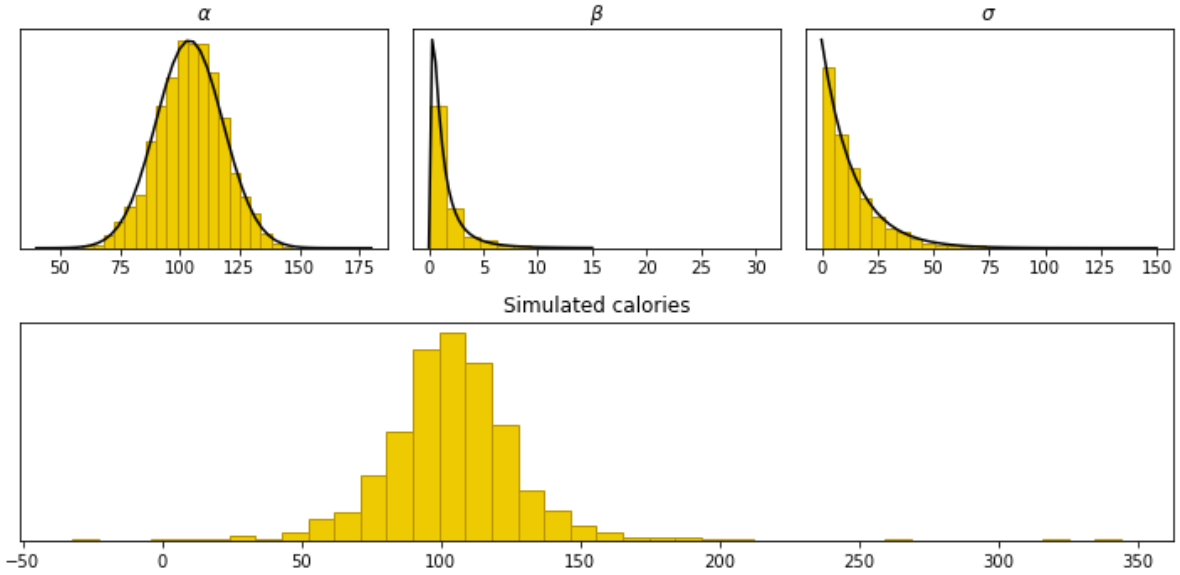


In [ ]:
```
calorie_sim = sim.stan_variable('calorie')
```

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]')
plt.show()
```



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=104,scale=14)
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()
```



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(104, 14);
   beta ~ lognormal(0, 1);
   sigma ~ exponential(0.071);
   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 0.99. After this change issue was resolved.

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

```
Processing csv files: C:\GitHub\DataAnalyticsProject\Project\samples\cereal_2_fit-
20220619234429_1.csv, C:\GitHub\DataAnalyticsProject\Project\samples\cereal_2_fit-
20220619234429_2.csv, C:\GitHub\DataAnalyticsProject\Project\samples\cereal_2_fit-
20220619234429_3.csv, C:\GitHub\DataAnalyticsProject\Project\samples\cereal_2_fit-
20220619234429_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.
```

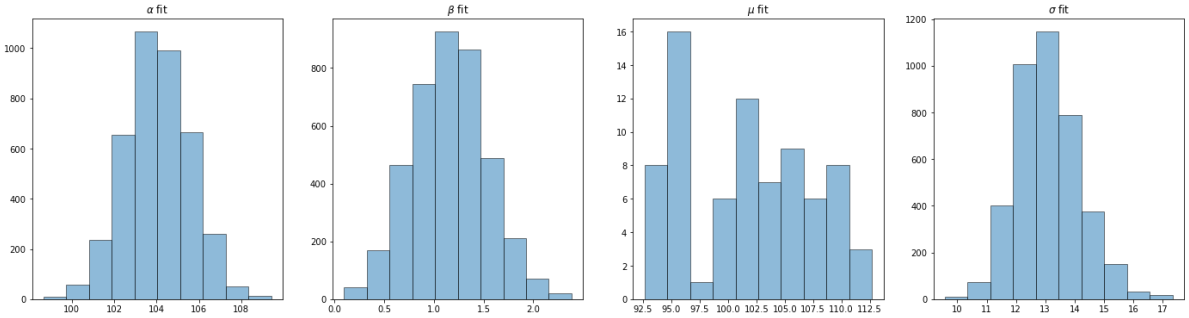
In [ ]:
```
alpha_fit = fit_2.stan_variable('alpha')
beta_fit = fit_2.stan_variable('beta')
mu_fit = fit_2.stan_variable('mu')
sigma_fit = fit_2.stan_variable('sigma')
calorie_pred = fit_2.stan_variable('calorie')
```

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

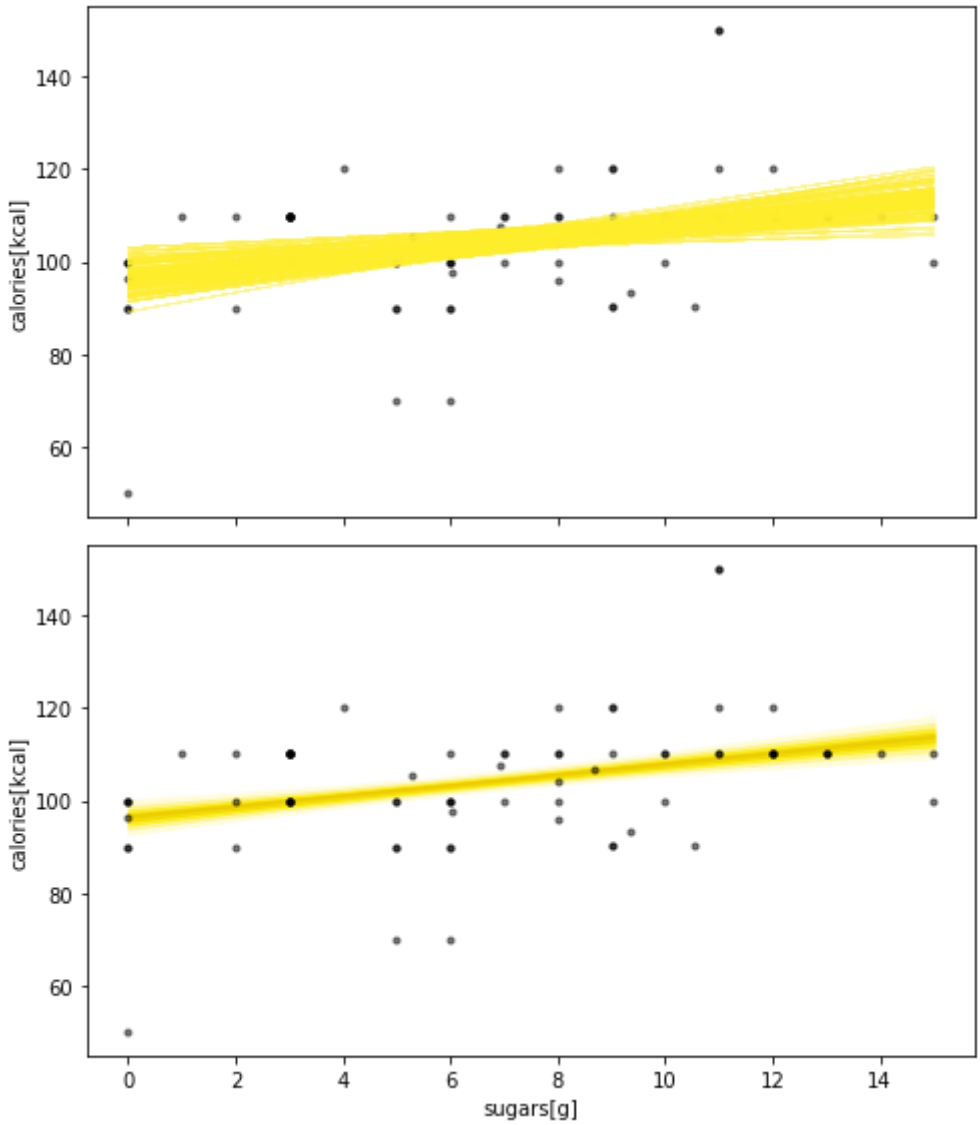
Out[ ]:

	mean	sd	hdi_3%	hdi_97%
alpha	104.05	1.53	101.33	107.04
beta	1.15	0.38	0.45	1.85
sigma	13.10	1.08	11.15	15.16

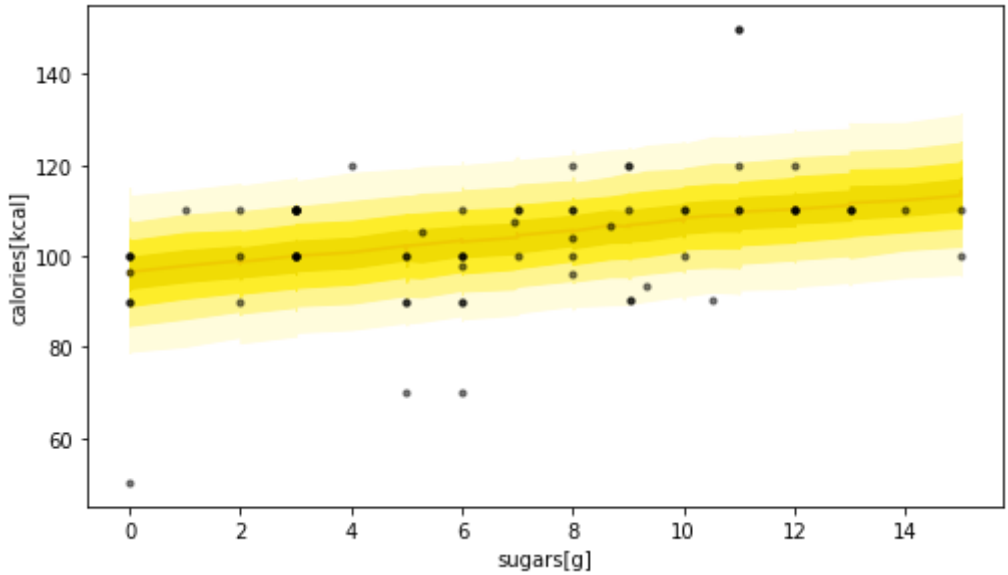
In [ ]:
```
f, (ax1, ax2, ax3, ax4) = plt.subplots(1, 4, figsize = (24,6))

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()
```



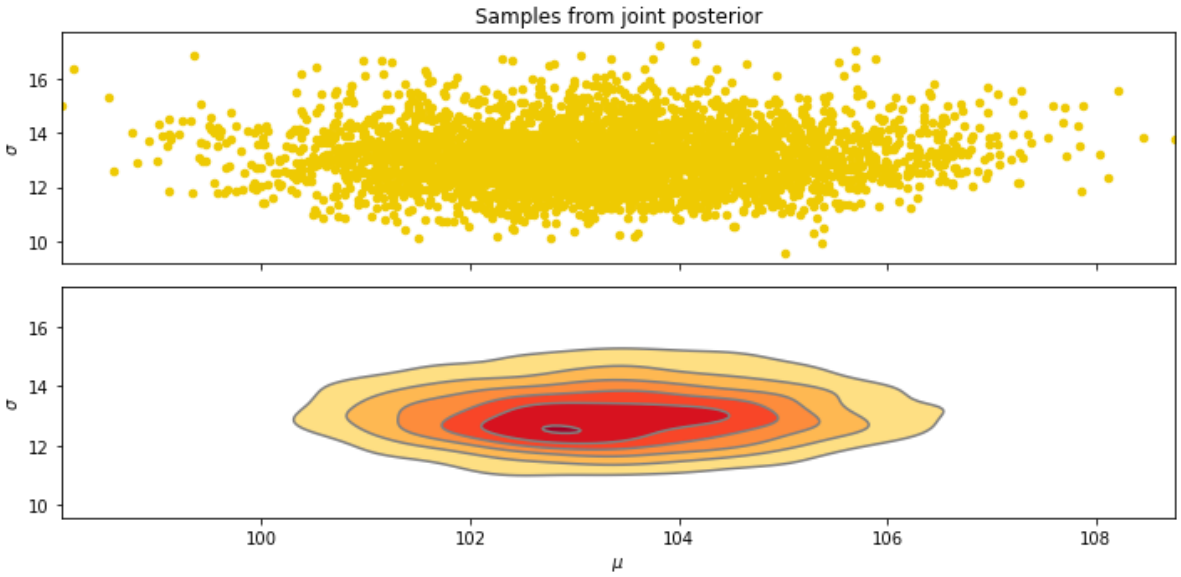
In [ ]:
```
fig, axes = plt.subplots(2,1,figsize = (7,8), sharey=True, sharex=True)
ax0=axes[0]

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



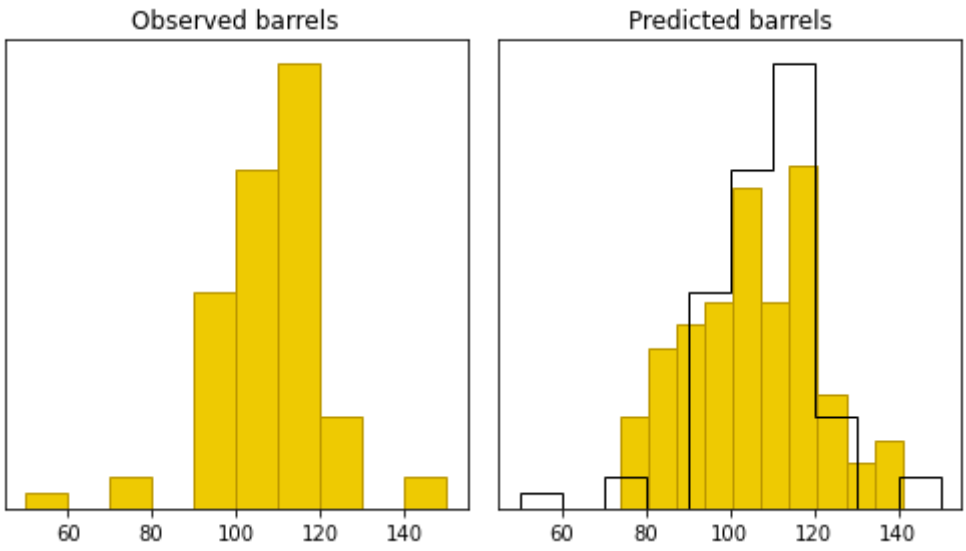
In [ ]:
```
fig, axes = plt.subplots(1,1,figsize = (7,4))

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]')
plt.show()
```



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=Tru
ax.set_title('Observed barrels')
ax.set_yticks(())
ax2=axes[1]
ax2.hist(calorie_pred[66], bins=10, color=DARK,edgecolor=DARK_HIGHLIGHT,density=Tr
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()
```



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_2 = az.from_cmdstanpy(posterior=fit_2,log_likelihood='log_lik')
```

In [ ]:
```
fit_id_2
```

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(104, 14);
   real beta = lognormal_rng(0, 1);
   real sigma = exponential_rng(0.071);
   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')
```

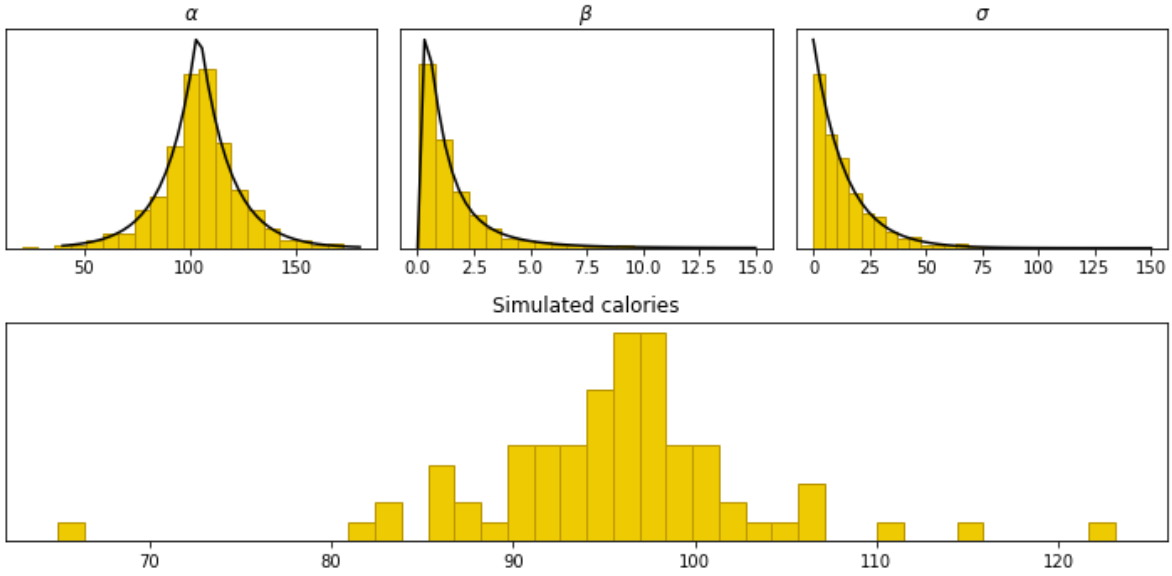
```
INFO:cmdstanpy:found newer exe file, not recompiling
```

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

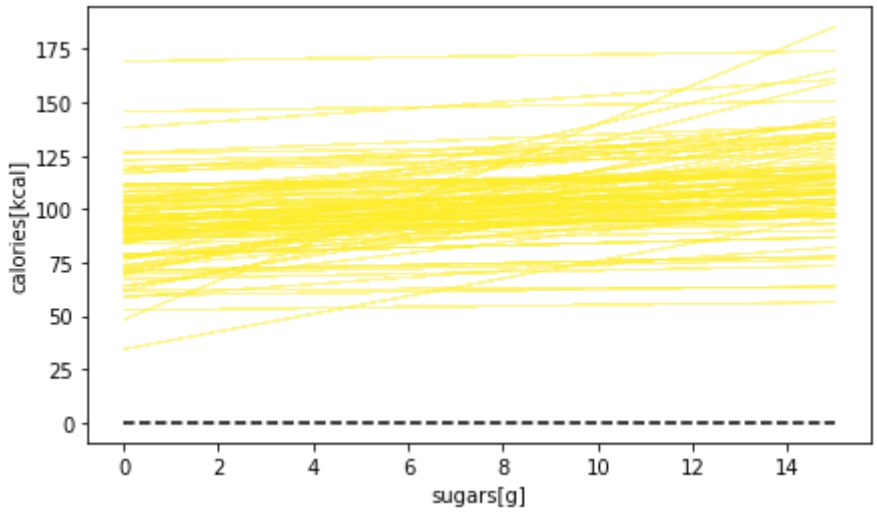
```
INFO:cmdstanpy:CmdStan start processing
chain 1 |          | 00:00 Status

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=

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=104,scale=14)
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()
```

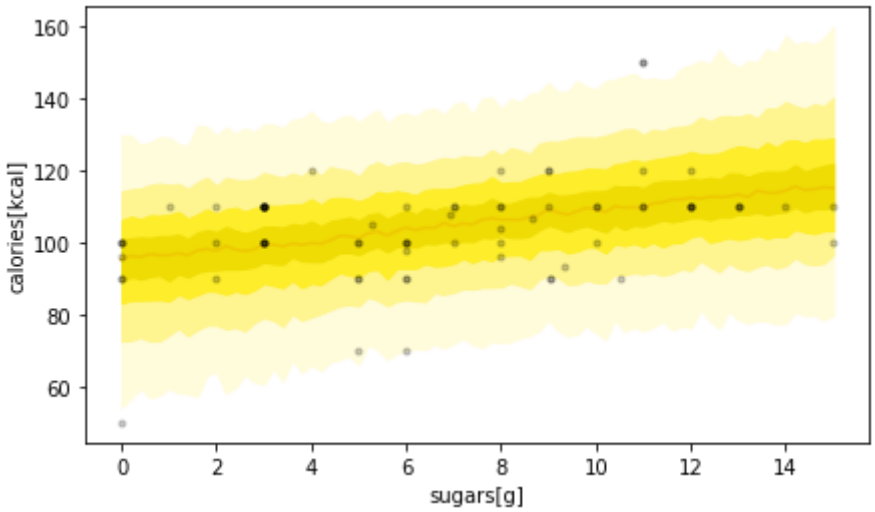


In [ ]:
```
fig, axes = plt.subplots(1,1,figsize = (7,4))

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='-
plt.show()
```



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]')
plt.show()
```



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(104, 14);
   beta ~ lognormal(0, 1);
   sigma ~ exponential(0.071);
   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 -> rozmiar wektora kalorii
- sugars -> wektor cukrów
- calories -> wektor kalorii

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-
20220619234511_1.csv, C:\GitHub\DataAnalyticsProject\Project\samples\cereal_3_fit-
20220619234511_2.csv, C:\GitHub\DataAnalyticsProject\Project\samples\cereal_3_fit-
20220619234511_3.csv, C:\GitHub\DataAnalyticsProject\Project\samples\cereal_3_fit-
20220619234511_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 occured during sampling.

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

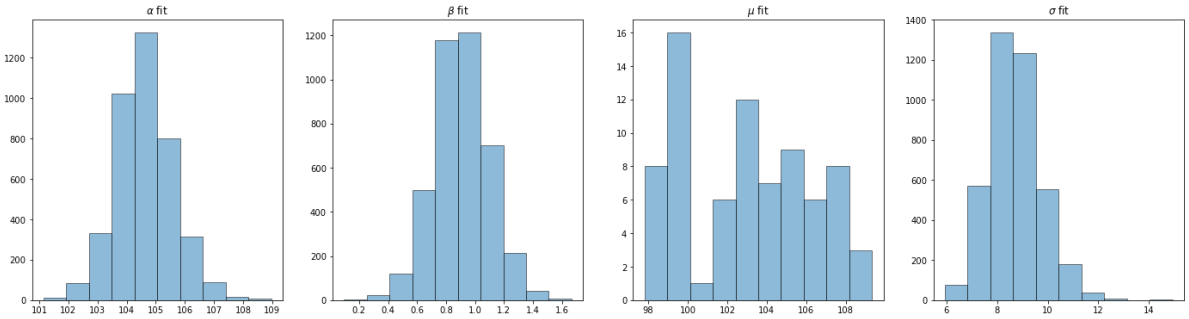
Out[ ]:

	mean	sd	hdi_3%	hdi_97%
alpha	104.63	0.98	102.90	106.63
beta	0.91	0.19	0.54	1.26
sigma	8.72	1.02	6.74	10.53

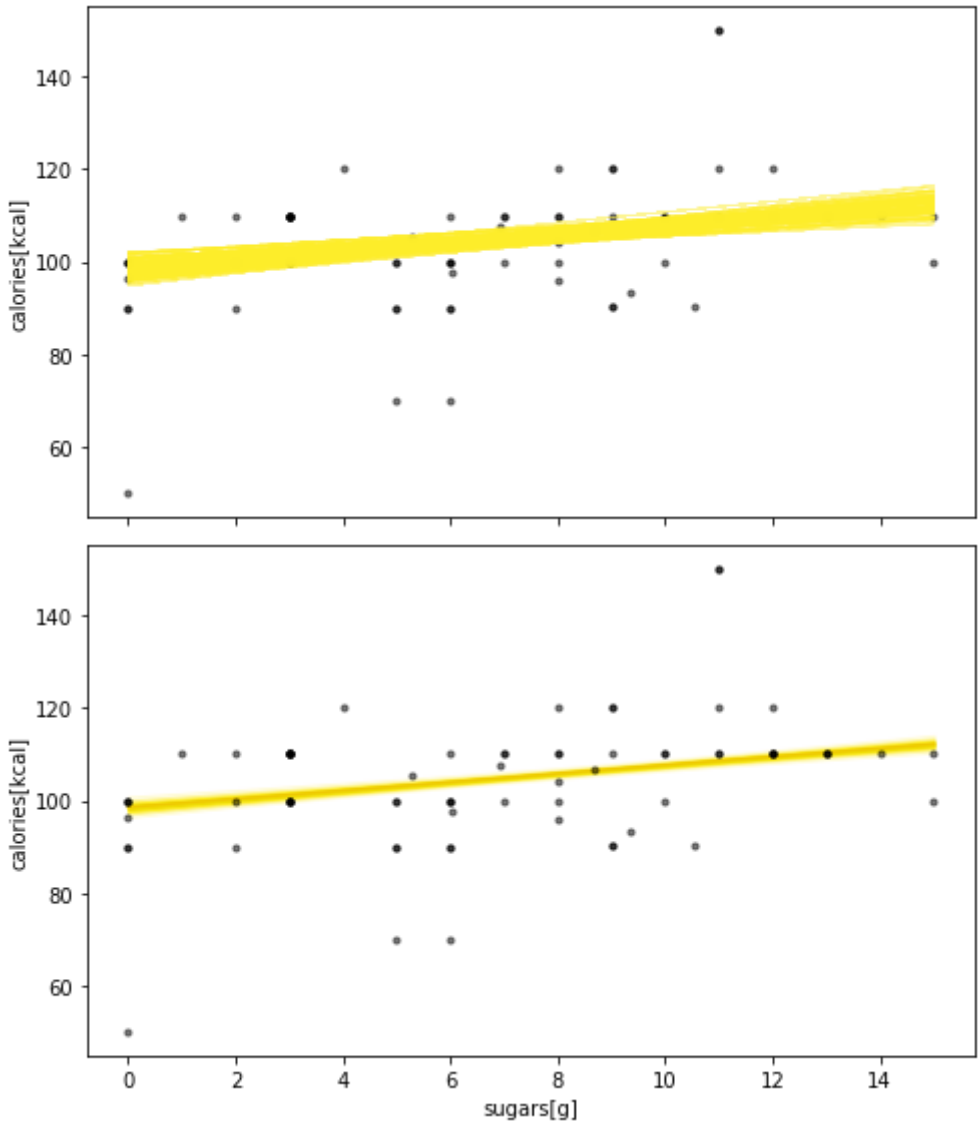
In [ ]:
```
alpha_fit = fit_3.stan_variable('alpha')
beta_fit = fit_3.stan_variable('beta')
mu_fit = fit_3.stan_variable('mu')
sigma_fit = fit_3.stan_variable('sigma')
calorie_pred = fit_3.stan_variable('calorie')
```

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

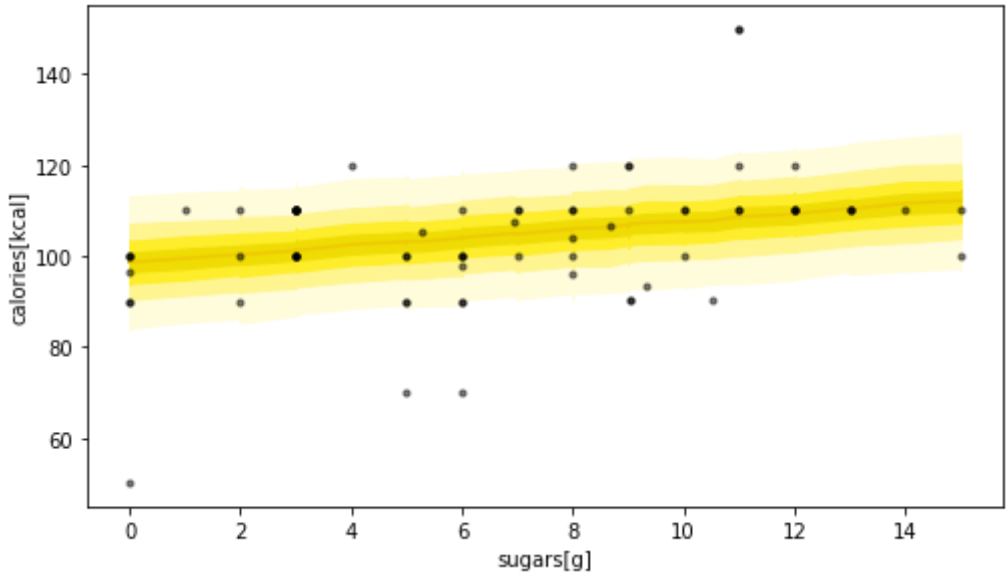
```
ax1.hist(alpha_fit, alpha=0.5, ec='black')
ax1.set_title(r"$\alpha$ fit")
ax2.hist(beta_fit, alpha=0.5, ec='black')
ax2.set_title(r"$\beta$ fit")
ax3.hist(mu_fit[0], alpha=0.5, ec='black')
ax3.set_title(r"$\mu$ fit")
ax4.hist(sigma_fit, alpha=0.5, ec='black')
ax4.set_title(r"$\sigma$ fit")
plt.show()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



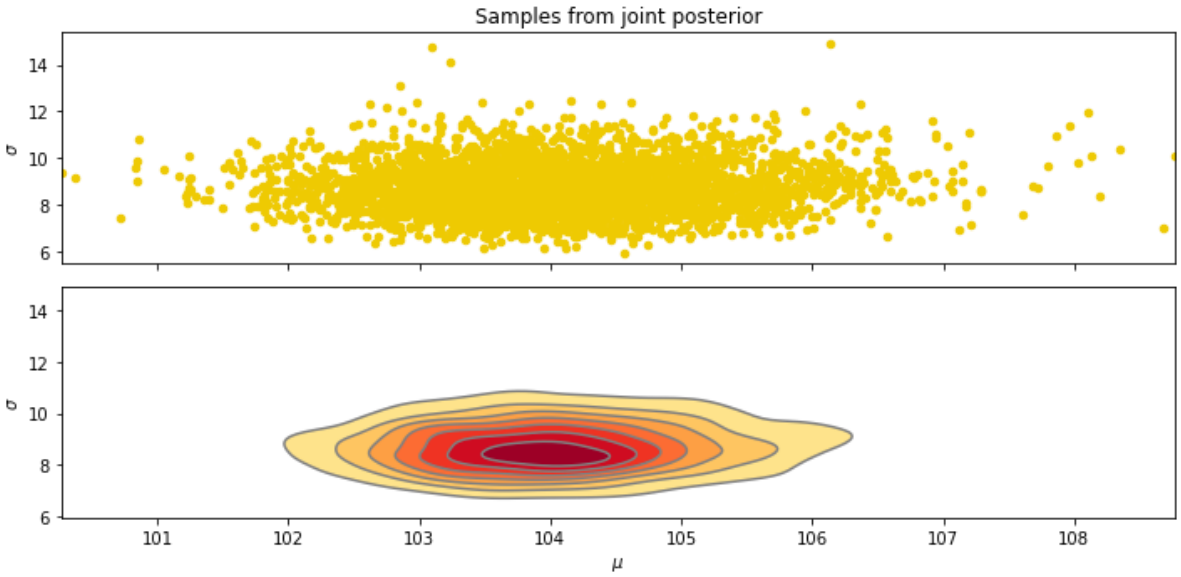
In [ ]:
```
fig, axes = plt.subplots(2,1,figsize = (7,8), sharey=True, sharex=True)
ax0=axes[0]

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



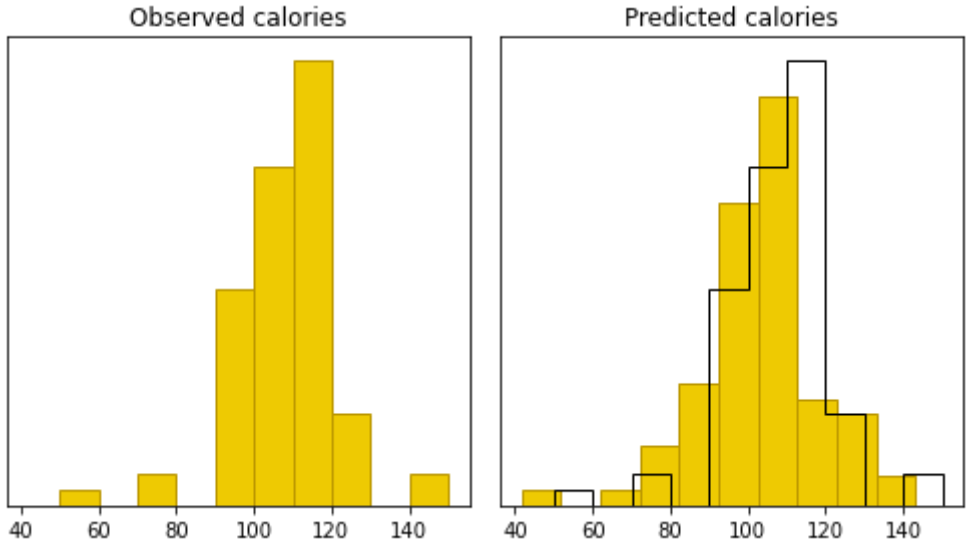
In [ ]:
```
fig, axes = plt.subplots(1,1,figsize = (7,4))

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]')
plt.show()
```



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=Tru
ax.set_title('Observed calories')
ax.set_yticks(())
ax2=axes[1]
ax2.hist(calorie_pred[99], bins=10, color=DARK,edgecolor=DARK_HIGHLIGHT,density=Tr
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.

In [ ]:
```
fit_id_3 = az.from_cmdstanpy(posterior=fit_3,log_likelihood='log_lik')
```

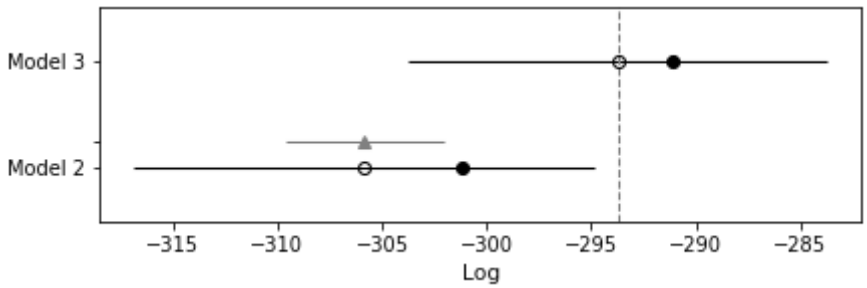
In [ ]:
```
model_compare = az.compare({'Model 2':fit_id_2,'Model 3':fit_id_3})
model_compare
```

```
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:655: UserWarning: Estimated shape parameter of Pareto distribution is greater than 0.7 for one or more samples. You should consider using a more robust model, this is because importance sampling is less likely to work well if the marginal posterior and LOO posterior are very different. This is more likely to happen with a non-robust model and highly influential observations.
  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_scale
Model 3	0	-293.733139	2.620662	0.000000	1.0	9.984329	0.000000	False	log
Model 2	1	-305.831924	4.686192	12.098785	0.0	10.998422	3.795985	True	log

In [ ]:
```
az.plot_compare(model_compare)
plt.show()
```



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

In [ ]:
```
model_compare_2 = az.compare({'Model 2':fit_id_2,'Model 3':fit_id_3}, ic='waic')
model_compare_2
```

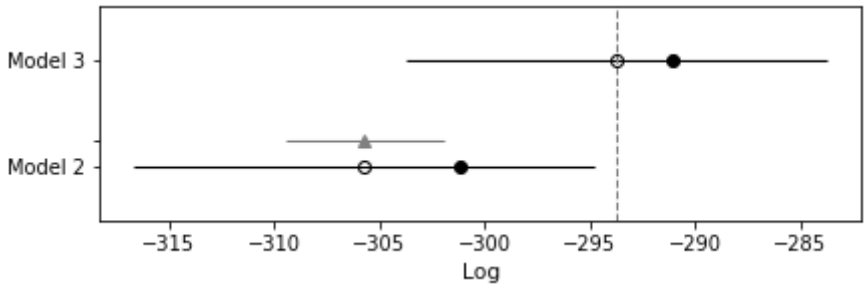
```
c:\Anaconda3\envs\data_analytics\lib\site-packages\arviz\stats\stats.py:145: UserW
arning: The default method used to estimate the weights for each model,has changed
from BB-pseudo-BMA to stacking
  warnings.warn(
c:\Anaconda3\envs\data_analytics\lib\site-packages\arviz\stats\stats.py:1405: User
Warning: For one or more samples the posterior variance of the log predictive dens
ities 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: Futur
eWarning: 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: Futur
eWarning: 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_scale
Model 3	0	-293.728342	2.615865	0.000000	1.0	9.983087	0.000000	False	log
Model 2	1	-305.720789	4.575058	11.992447	0.0	10.938185	3.751998	True	log

In [ ]:

```
az.plot_compare(model_compare_2)
plt.show()
```



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

Reults 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 fisrt one beacuse it was able to better catch values stacked close to the mean value.