report

April 17, 2023

0.1 Prerequisities

0.1.1 Install packages

We use imblearn library to solve imbalanced dataset by oversampling using SMOTE method.

This library can be installed by running the following cells.

```
Looking in indexes: https://pypi.org/simple, https://us-python.pkg.dev/colab-wheels/public/simple/
Requirement already satisfied: imblearn in /usr/local/lib/python3.9/dist-packages (0.0)
Requirement already satisfied: imbalanced-learn in /usr/local/lib/python3.9/dist-packages (from imblearn) (0.10.1)
Requirement already satisfied: scikit-learn>=1.0.2 in /usr/local/lib/python3.9/dist-packages (from imbalanced-learn->imblearn) (1.2.2)
Requirement already satisfied: scipy>=1.3.2 in /usr/local/lib/python3.9/dist-packages (from imbalanced-learn->imblearn) (1.10.1)
Requirement already satisfied: joblib>=1.1.1 in /usr/local/lib/python3.9/dist-packages (from imbalanced-learn->imblearn) (1.2.0)
Requirement already satisfied: threadpoolctl>=2.0.0 in /usr/local/lib/python3.9/dist-packages (from imbalanced-learn->imblearn) (3.1.0)
Requirement already satisfied: numpy>=1.17.3 in /usr/local/lib/python3.9/dist-packages (from imbalanced-learn->imblearn) (1.22.4)
```

We use scikeras library which contains scikit-learn wrapper for Keras models.

This library can be installed by running the following cells.

```
Looking in indexes: https://pypi.org/simple, https://us-python.pkg.dev/colab-wheels/public/simple/
Requirement already satisfied: scikeras in /usr/local/lib/python3.9/dist-packages (0.10.0)
Requirement already satisfied: packaging>=0.21 in /usr/local/lib/python3.9/dist-packages (from scikeras) (23.0)
Requirement already satisfied: scikit-learn>=1.0.0 in /usr/local/lib/python3.9/dist-packages (from scikeras) (1.2.2)
Requirement already satisfied: scipy>=1.3.2 in /usr/local/lib/python3.9/dist-packages (from scikit-learn>=1.0.0->scikeras) (1.10.1)
Requirement already satisfied: threadpoolctl>=2.0.0 in /usr/local/lib/python3.9/dist-packages (from scikit-learn>=1.0.0->scikeras)
```

```
(3.1.0)
Requirement already satisfied: numpy>=1.17.3 in /usr/local/lib/python3.9/dist-
packages (from scikit-learn>=1.0.0->scikeras) (1.22.4)
Requirement already satisfied: joblib>=1.1.1 in /usr/local/lib/python3.9/dist-
packages (from scikit-learn>=1.0.0->scikeras) (1.2.0)
```

0.1.2 Import packages

0.1.3 Fix randomness

0.1.4 Constant definitions

0.1.5 Function definitions

0.2 Problem Definition

We are performing classification of penguin species.

Our target column is named "species".

Our metrics of success is "accuracy".

0.3 Data Understanding

	species	island	bill_length_mm	bill_depth_mm	flipper_length_mm	\
0	Adelie	Torgersen	39.1	18.7	181.0	
1	Adelie	Torgersen	39.5	17.4	186.0	
2	Adelie	Torgersen	40.3	18.0	195.0	
3	Adelie	Torgersen	NaN	NaN	NaN	
4	Adelie	Torgersen	36.7	19.3	193.0	

	body_mass_g	sex	year
0	3750.0	male	2007
1	3800.0	female	2007
2	3250.0	female	2007
3	NaN	NaN	2007
4	3450.0	female	2007

Our dataset contains:

- 1 column with target variable (`species`)
- 7 columns with possible input features (`island`, `bill_length_mm`, `bill_depth_mm`, `flipper_length_mm`, `body_mass_g`, `sex`, `year`)
- 5 columns with numerical values (`bill_length_mm`, `bill_depth_mm`, `flipper_length_mm`, `body_mass_g`, `year`), out of these 4 contains floating numbers (`bill_length_mm`, `bill_depth_mm`, `flipper_length_mm`, `body_mass_g`) and 1 contain integer number (`year`)
- 3 columns with categorical values (`species`, `island`, `sex`)

```
Adelie       160
Gentoo       124
Chinstrap     79
```

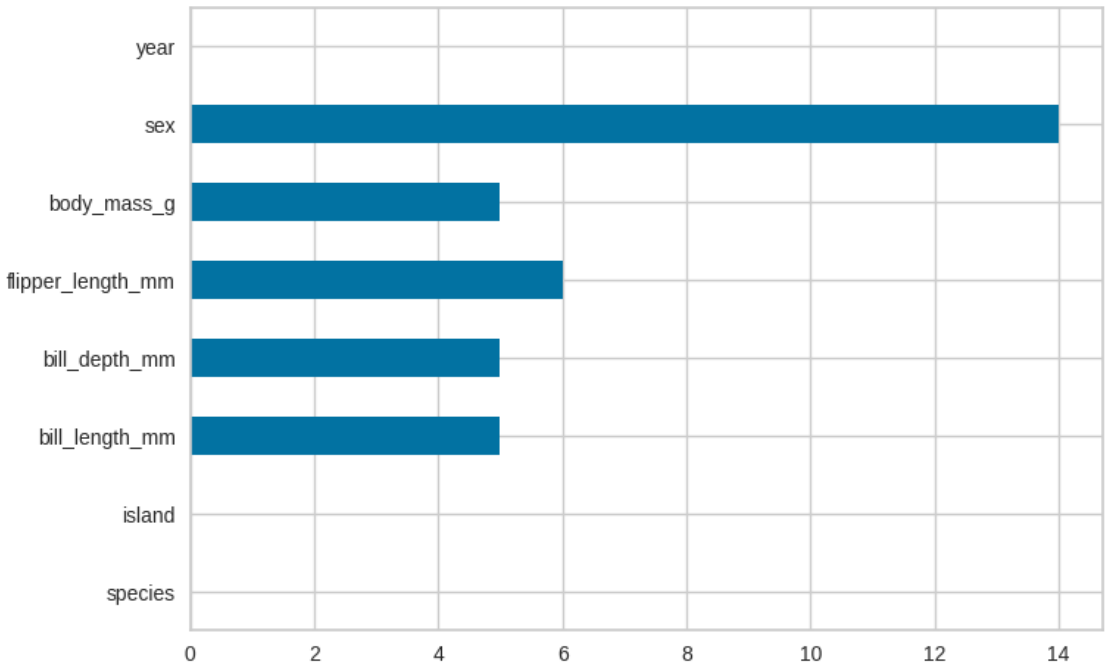
```
Name: species, dtype: int64
```

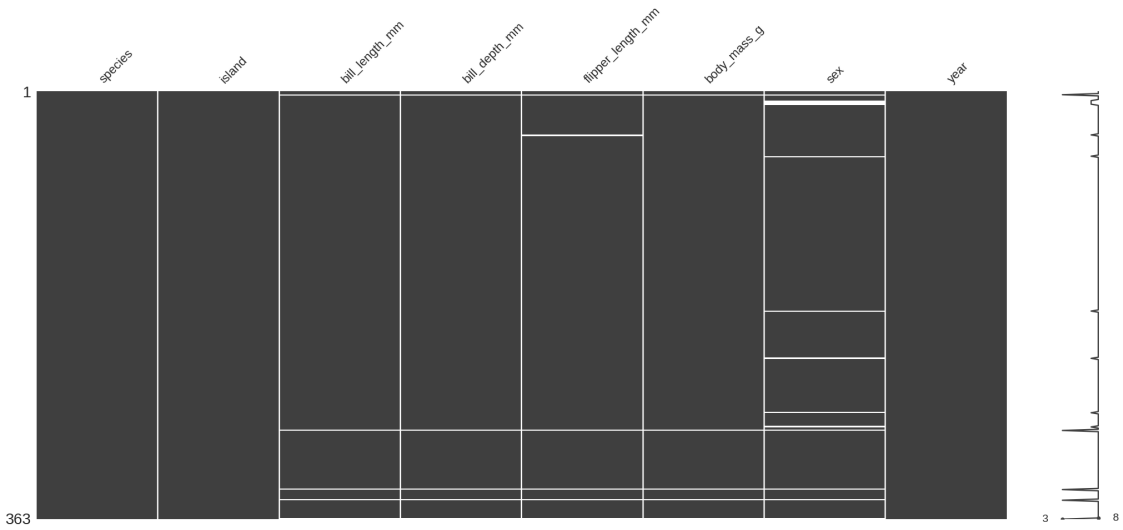
As a result of calling `value_counts()` on our target column shows:

- We are performing a multi-class classification.
- Class counts are imbalanced, therefore we need to solve class imbalance during training. We have decided to use oversampling using SMOTE method to solve class imbalance in our case.

0.3.1 Indication of missing values

	number of null values
species	0
island	0
bill_length_mm	5
bill_depth_mm	5
flipper_length_mm	6
body_mass_g	5
sex	14
year	0





Our dataset contains a small amount of missing values in columns `bill_length_mm`, `bill_depth_mm`, `flipper_length_mm`, `body_mass_g`, `sex`.

0.3.2 Descriptive statistics

`Dataset contains 363 rows and 8 columns.`

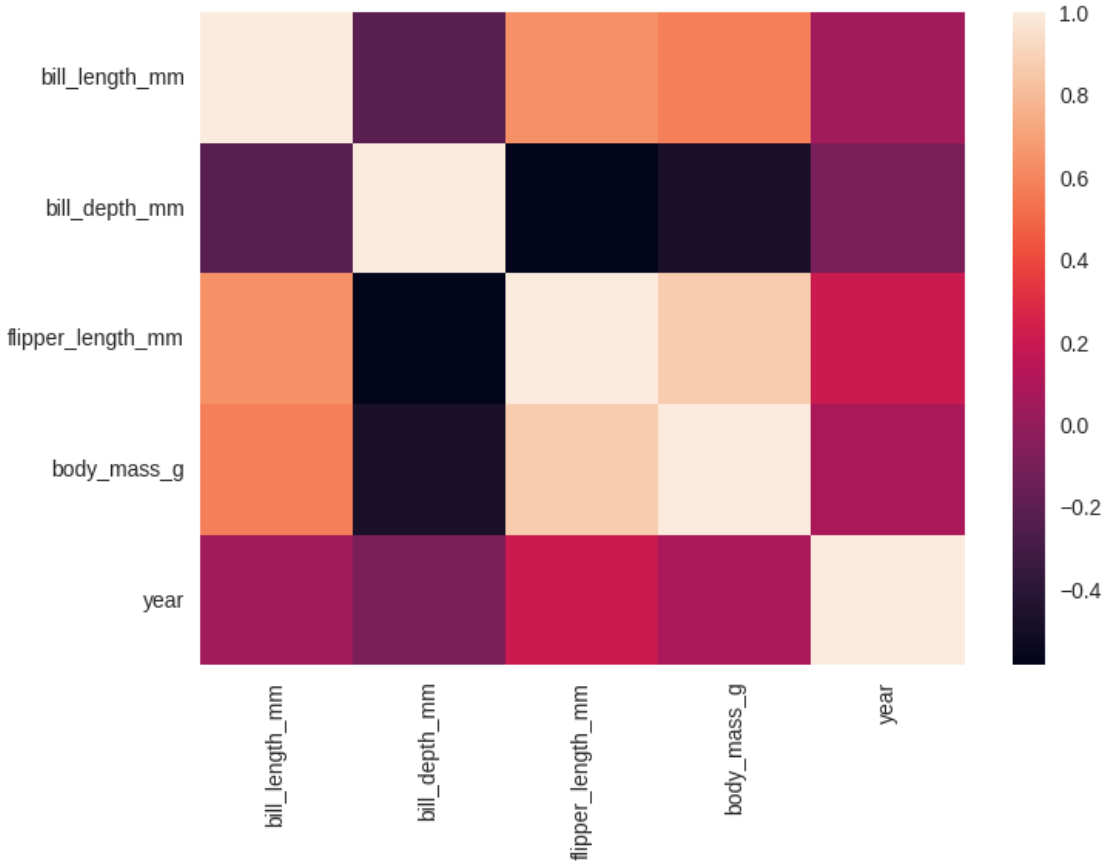
	species	island	bill_length_mm	bill_depth_mm	flipper_length_mm	\
count	363	363	358.000000	358.000000	357.000000	
unique	3	3	NaN	NaN	NaN	
top	Adelie	Biscoe	NaN	NaN	NaN	
freq	160	170	NaN	NaN	NaN	
mean	NaN	NaN	43.926257	17.205587	200.451261	
std	NaN	NaN	5.441240	1.951749	14.000754	
min	NaN	NaN	32.100000	13.100000	172.000000	
25%	NaN	NaN	39.350000	15.700000	190.000000	
50%	NaN	NaN	44.450000	17.500000	197.000000	
75%	NaN	NaN	48.500000	18.700000	213.000000	
max	NaN	NaN	59.600000	21.500000	231.000000	

	body_mass_g	sex	year
count	358.000000	349	363.000000
unique	NaN	2	NaN
top	NaN	female	NaN
freq	NaN	175	NaN
mean	4173.743017	NaN	2007.991736
std	796.395388	NaN	0.829323
min	2700.000000	NaN	2007.000000
25%	3550.000000	NaN	2007.000000
50%	3950.000000	NaN	2008.000000

```
75%      4743.750000      NaN  2009.000000
max      6300.000000      NaN  2009.000000
```

0.3.3 Correlation analysis

```
<ipython-input-15-2f9a9ba54672>:1: FutureWarning: The default value of
numeric_only in DataFrame.corr is deprecated. In a future version, it will
default to False. Select only valid columns or specify the value of numeric_only
to silence this warning.
  sns.heatmap(data_raw.corr())
```



0.3.4 Duplicates

```
Number of duplicate rows to delete: 13
```

0.4 Data Preparation

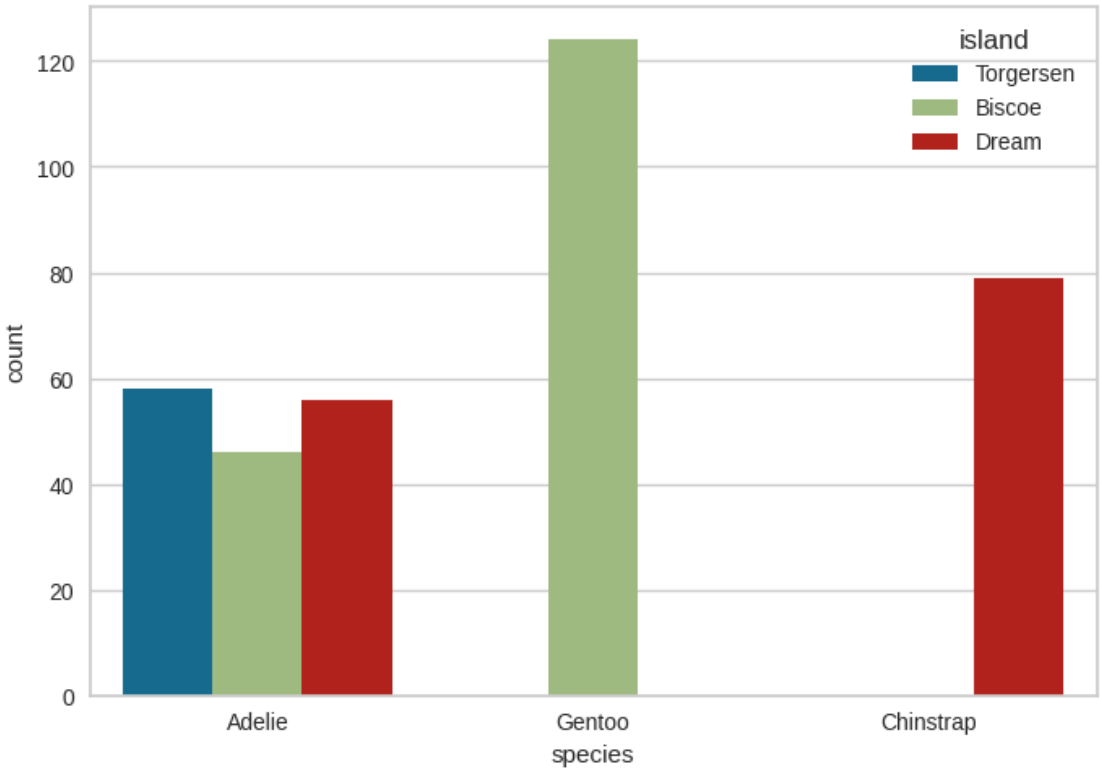
We would like to make a decision about penguin species based on physical characteristics of the penguin and on which island he has been found. That should both be available at the time of prediction.

We would not like to make a prediction of penguin species based on year as years change and we might want to make a prediction of penguin species in future, where year can be some value not found in training data. That would degrade the quality of predictions. Therefore we remove year column.

```
Best params: {'clf__criterion': 'gini', 'clf__max_depth': None,
'clf__min_samples_leaf': 2, 'clf__min_samples_split': 2, 'clf__n_estimators':
50}
Best accuracy: 0.8923130677847659
Best params: {'clf__criterion': 'gini', 'clf__max_depth': None,
'clf__min_samples_leaf': 2, 'clf__min_samples_split': 5, 'clf__n_estimators':
50}
Best accuracy: 0.9120879120879121
```

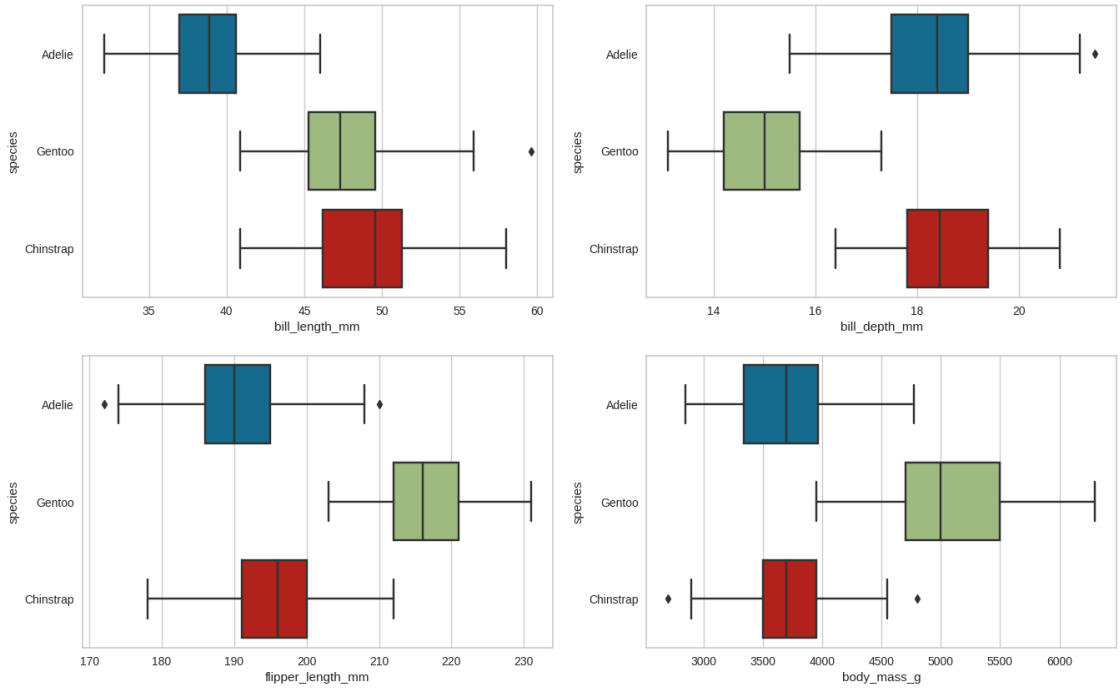
0.5 Data Visualization

0.5.1 Island habitability

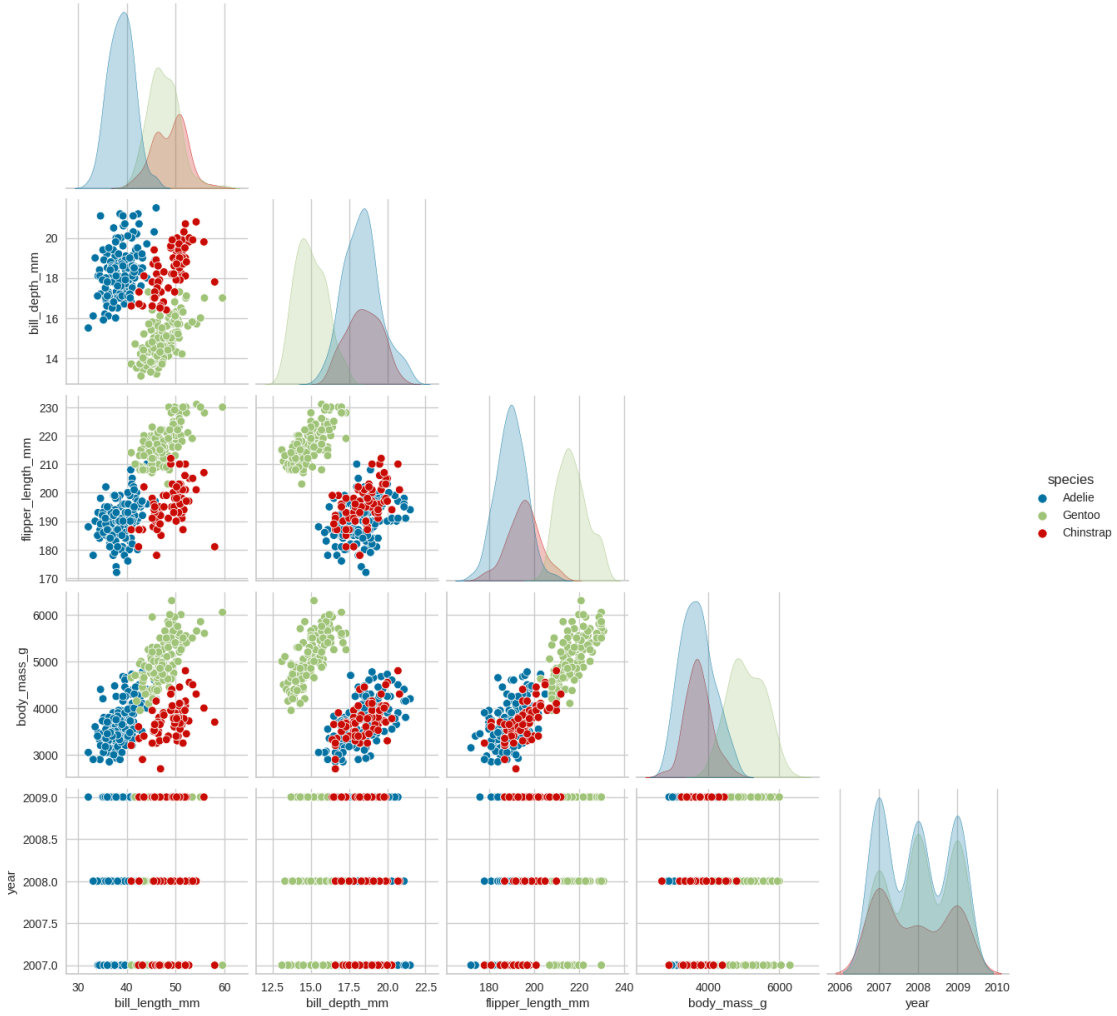


- Adelie species are found on all three islands, but Gentoo and Chinstrap are separated.
- Gentoo lives on Biscoe Island
- Chinstrap lives on Dream Island

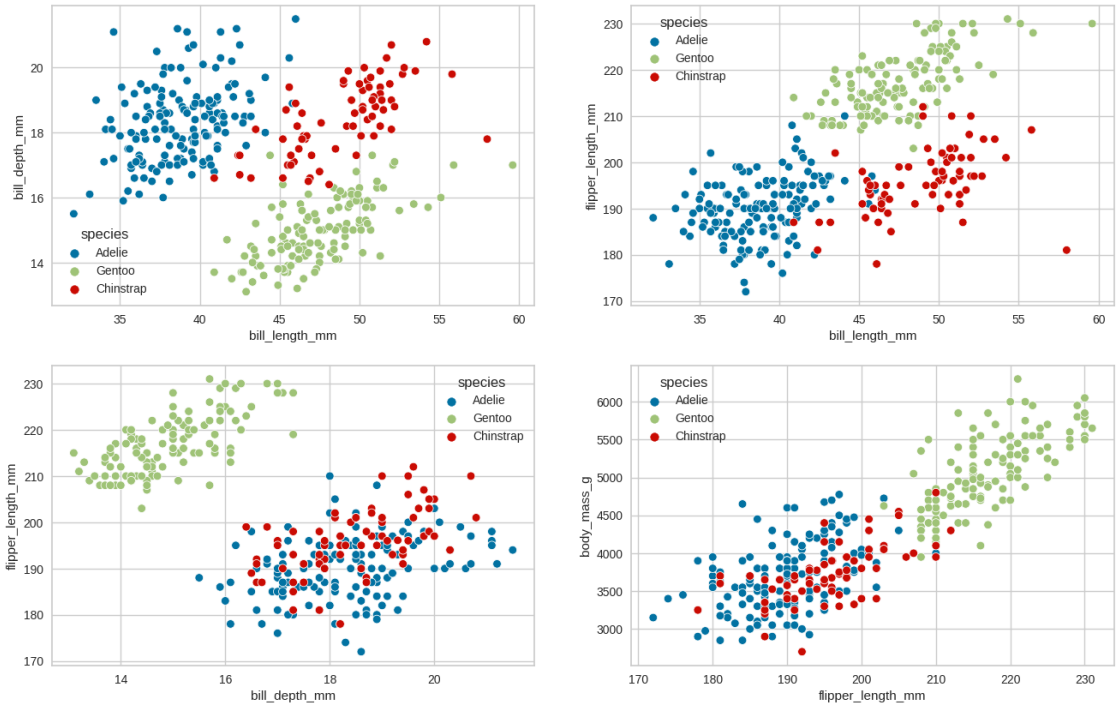
0.5.2 Boxplots



0.5.3 Pairplot

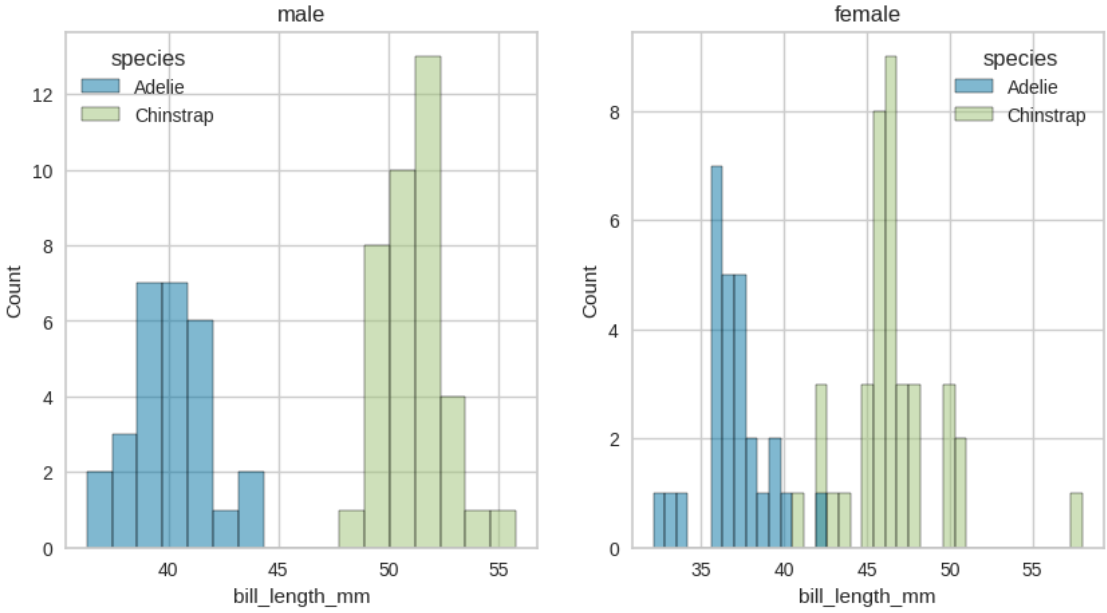


0.5.4 Scatterplots



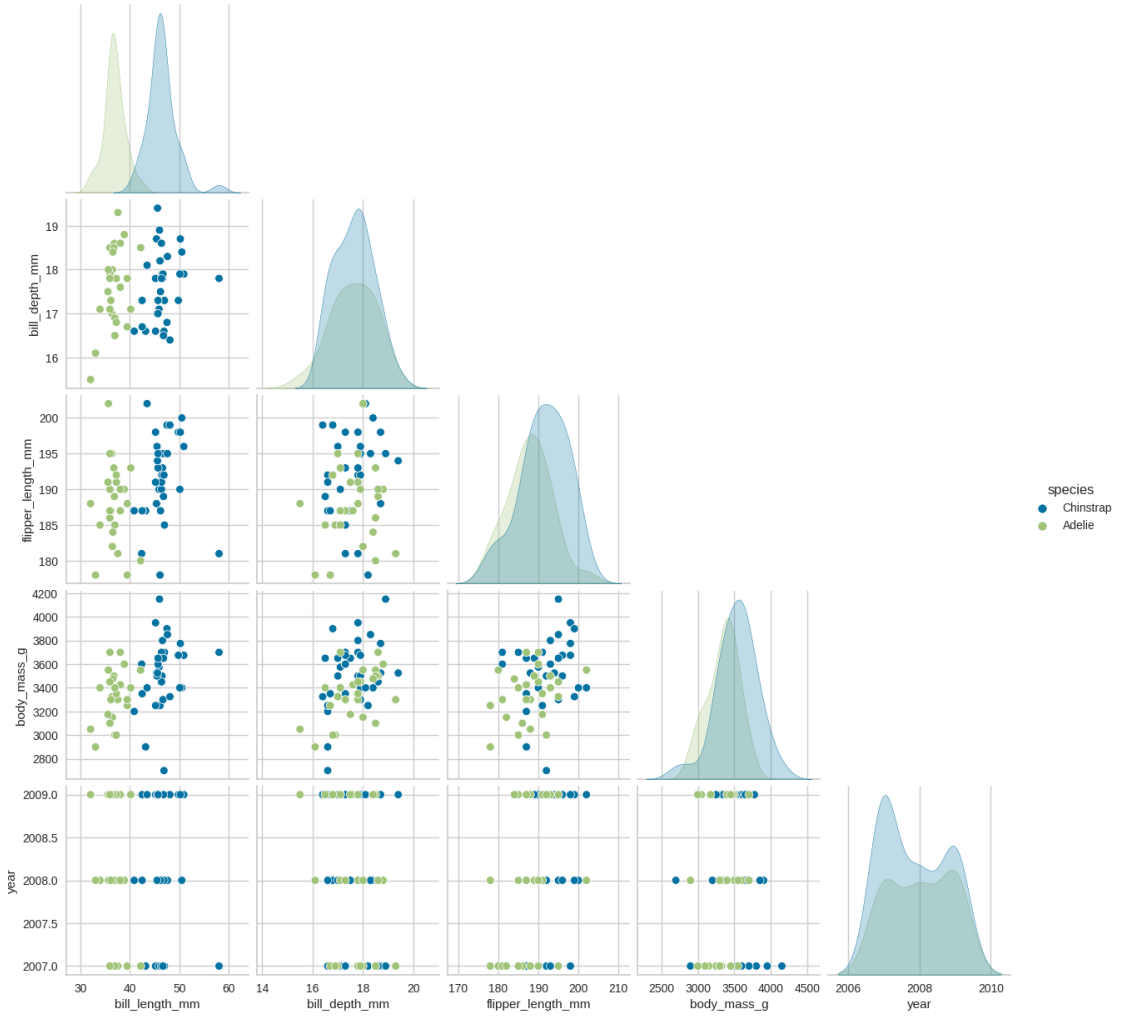
0.5.5 Adelie vs Chinstrap

Let's try to find the differences between Adelie and Chinstrap We will use the bill_lenth_mm attribute for this, since it is the only attribute that shows significant differences based on the graph of pairwise dependencies.



We can see that Adelie and Chinstrap can be easily separeted if sex = male, but not so easily if value of sex = female.

Let's look at the female gender in more detail and use a graph of pairwise dependencies.



The best linear separation on the surface we can observe with the attributes x = bill_length_mm y = flipper_length_mm

0.6 Modeling

We decided to try few different models, mainly the ones mentioned in class. Therefore we have tried:

- Support vector classifier
- Tree model

- Random Forest model
- Neural Network model (in Keras using Scikit-learn compatible wrapper)
- Bagging classifier

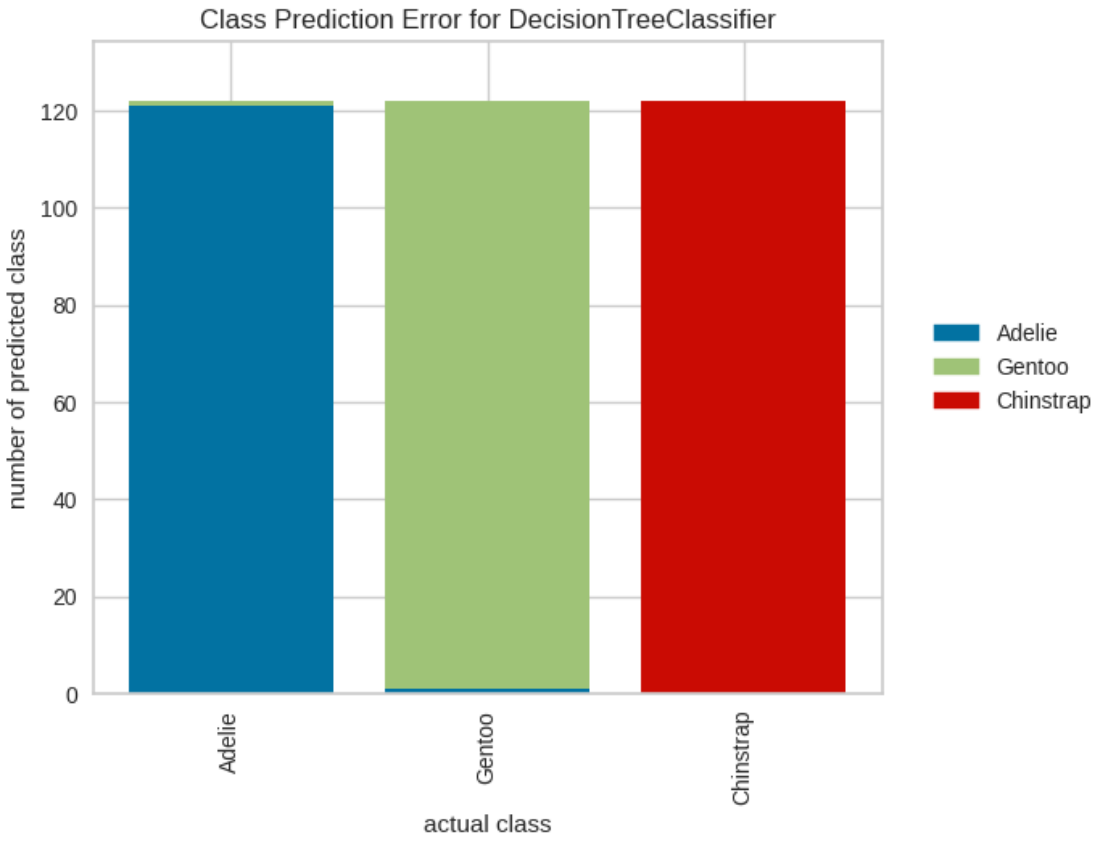
0.6.1 Model support vector classifier

```
Best params: {'clf__C': 0.5}
Best accuracy: 0.9972602739726029
```

0.6.2 Model tree

```
Best params: {'clf__criterion': 'gini', 'clf__max_depth': 4}
Best accuracy: 0.9781562384302112
```

```
/usr/local/lib/python3.9/dist-packages/yellowbrick/classifier/base.py:232:
YellowbrickWarning: could not determine class_counts_ from previously fitted
classifier
  warnings.warn(
```




```
<Axes: title={'center': 'Class Prediction Error for DecisionTreeClassifier'},
xlabel='actual class', ylabel='number of predicted class'>
```

0.6.3 Model random forest

```
Best params: {'clf__criterion': 'gini', 'clf__max_depth': None,
'clf__min_samples_leaf': 1, 'clf__min_samples_split': 5, 'clf__n_estimators':
50}
Best accuracy: 0.9890781192151055
```

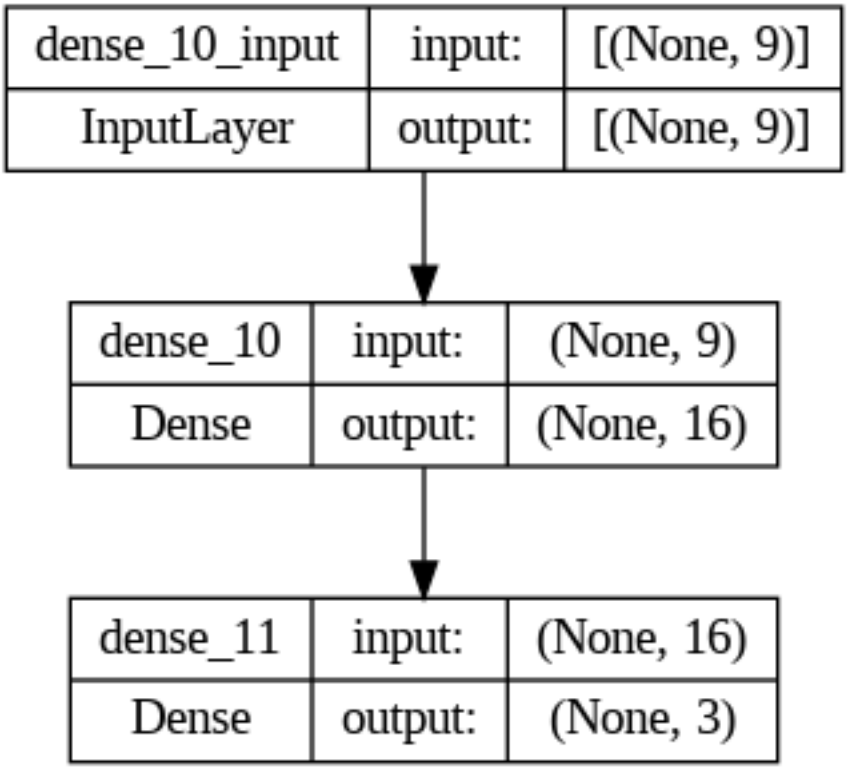
0.6.4 Model bagging classifier

```
Best params: {'clf__max_features': 0.6, 'clf__max_samples': 0.6}
Best accuracy: 0.9890781192151055
```

0.6.5 Model neural network

```
WARNING:tensorflow:5 out of the last 13 calls to <function
Model.make_predict_function.<locals>.predict_function at 0x7f04c17549d0>
triggered tf.function retracing. Tracing is expensive and the excessive number
of tracings could be due to (1) creating @tf.function repeatedly in a loop, (2)
passing tensors with different shapes, (3) passing Python objects instead of
tensors. For (1), please define your @tf.function outside of the loop. For (2),
@tf.function has reduce_retracing=True option that can avoid unnecessary
retracing. For (3), please refer to
https://www.tensorflow.org/guide/function#controlling_retracing and
https://www.tensorflow.org/api_docs/python/tf/function for  more details.
```

```
Best params: {}
Best accuracy: 1.0
```



0.6.6 Model accuracies

	model	accuracy
4	neural_network	1.000000
0	linearsvc	0.997260
2	random forest	0.989078
3	bagging	0.989078
1	tree	0.978156

0.6.7 Conclusion on selecting the best model

As we can see, the best accuracy has neural network. That is great also because the assignment explicitly mentions we must save model in `h5` format, and we know an easy way how to do it in Keras (which we use in our neural network model) described here for Keras and here in Chapter 4.2 for scikeras, so we have decided to select neural network as the best model.

Our model is limited by following factors:

- The architecture is limited by number of input features, which places a restriction on the number of neurons in input layer, which must be same as number of input features. We do this by setting `input_dim` parameter of first `Dense` layer, however we probably could achieve the same result by using separate `Input` layer with required number of neurons.
- The architecture is limited by performed task, which is a multi class classification, which places the following restrictions on the network: a) the number of neurons in output layer must be the same as number of predicted classes b) we must use softmax activation function on the last layer, which returns a sequence of predicted class probability scores between `0` and `1` which summs up to `1`, where the class with maximum probability score is the class which should be predicted.

Model could be improved by following ways:

- Using `Dropout` layer would prevent overfitting.

Values of hyperparameters (such as number of layers or number of neurons in layer) are hardcoded in our `make_model()` function and were chosen in such a way that we wanted to start with some small number of layers and neurons and if it would not work well, increase the number of layers or neurons. However, because chosen values worked well, we have not needed to use more complicated networks.

0.6.8 Save and load trained model

0.7 Evaluation

0.7.1 Make predictions on test set using best model

```
WARNING:tensorflow:5 out of the last 13 calls to <function
Model.make_predict_function.<locals>.predict_function at 0x7f04b84a89d0>
triggered tf.function retracing. Tracing is expensive and the excessive number
of tracings could be due to (1) creating @tf.function repeatedly in a loop, (2)
```

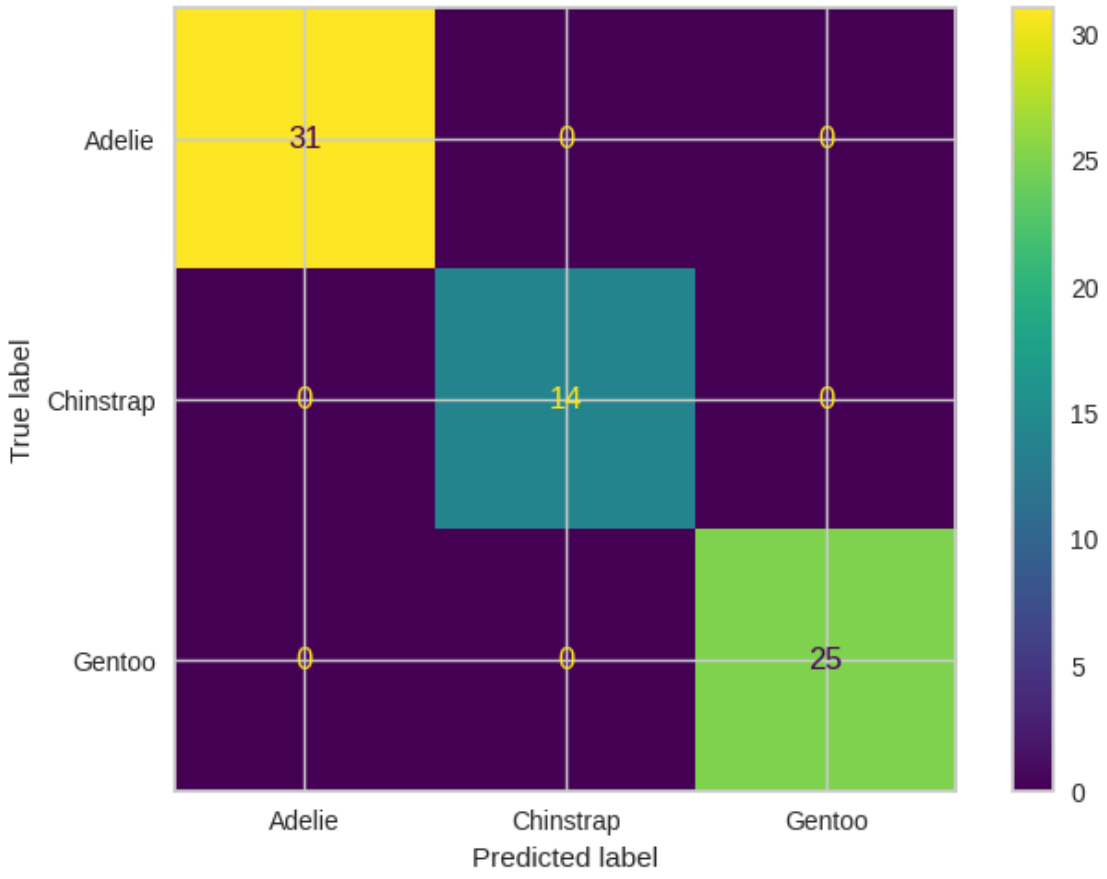
```
passing tensors with different shapes, (3) passing Python objects instead of
tensors. For (1), please define your @tf.function outside of the loop. For (2),
@tf.function has reduce_retracing=True option that can avoid unnecessary
retracing. For (3), please refer to
https://www.tensorflow.org/guide/function#controlling_retracing and
https://www.tensorflow.org/api_docs/python/tf/function for  more details.

3/3 [==============================] - 0s 4ms/step
```

0.7.2 Show classification report

	precision	recall	f1-score	support
Adelie	1.00	1.00	1.00	31
Chinstrap	1.00	1.00	1.00	14
Gentoo	1.00	1.00	1.00	25
accuracy			1.00	70
macro avg	1.00	1.00	1.00	70
weighted avg	1.00	1.00	1.00	70

0.7.3 Show confusion matrix



As we can see from classification report and confusion matrix, our model achieves 100% accuracy.

0.8 Development Environment Characteristics

0.8.1 Python version

We use the following Python version:

```
3.9.16 (main, Dec  7 2022, 01:11:51)
[GCC 9.4.0]
```

0.8.2 Packages utilized and their versions

We directly use the following packages:

- `imblearn` - for oversampling using SMOTE method
- `numpy` - for seeding random number for Keras
- `matplotlib` - for visualization
- `pandas` - for working with data in table form
- `scikeras` - contains scikit-learn compatible wrapper which we use
- `seaborn` - for visualization
- `scikit-learn` - for non-neural network models
- `tensorflow` - for neural network models using Keras API
- `yellowbrick` - for visualization of class prediction error

The full list of packages installed in our Google Collab environment and their versions can be found in the following commands output:

```
absl-py==1.4.0
alabaster==0.7.13
albumentations==1.2.1
altair==4.2.2
anyio==3.6.2
appdirs==1.4.4
argon2-cffi==21.3.0
argon2-cffi-bindings==21.2.0
arviz==0.15.1
astropy==5.2.2
astunparse==1.6.3
attrs==22.2.0
audioread==3.0.0
autograd==1.5
Babel==2.12.1
backcall==0.2.0
beautifulsoup4==4.11.2
bleach==6.0.0
blis==0.7.9
blosc2==2.0.0
```

```
bokeh==2.4.3
branca==0.6.0
CacheControl==0.12.11
cached-property==1.5.2
cachetools==5.3.0
catalogue==2.0.8
certifi==2022.12.7
cffi==1.15.1
chardet==4.0.0
charset-normalizer==2.0.12
chex==0.1.7
click==8.1.3
cloudpickle==2.2.1
cmake==3.25.2
cmdstanpy==1.1.0
colorcet==3.0.1
colorlover==0.3.0
community==1.0.0b1
confection==0.0.4
cons==0.4.5
contextlib2==0.6.0.post1
contourpy==1.0.7
convertdate==2.4.0
cryptography==40.0.1
cufflinks==0.17.3
cvxopt==1.3.0
cvxpy==1.3.1
cycler==0.11.0
cymem==2.0.7
Cython==0.29.34
dask==2022.12.1
datascience==0.17.6
db-dtypes==1.1.1
dbus-python==1.2.16
debugpy==1.6.6
decorator==4.4.2
defusedxml==0.7.1
distributed==2022.12.1
dlib==19.24.1
dm-tree==0.1.8
docutils==0.16
dopamine-rl==4.0.6
earthengine-api==0.1.348
easydict==1.10
ecos==2.0.12
editdistance==0.6.2
en-core-web-sm @ https://github.com/explosion/spacy-
models/releases/download/en_core_web_sm-3.5.0/en_core_web_sm-3.5.0-py3-none-
```

```
any.whl
entrypoints==0.4
ephem==4.1.4
et-xmlfile==1.1.0
etils==1.2.0
etuples==0.3.8
exceptiongroup==1.1.1
fastai==2.7.12
fastcore==1.5.29
fastdownload==0.0.7
fastjsonschema==2.16.3
fastprogress==1.0.3
fastrlock==0.8.1
filelock==3.11.0
firebase-admin==5.3.0
Flask==2.2.3
flatbuffers==23.3.3
flax==0.6.8
folium==0.14.0
fonttools==4.39.3
frozendict==2.3.7
fsspec==2023.4.0
future==0.18.3
gast==0.4.0
GDAL==3.3.2
gdown==4.6.6
gensim==4.3.1
geographiclib==2.0
geopy==2.3.0
gin-config==0.5.0
glob2==0.7
google==2.0.3
google-api-core==2.11.0
google-api-python-client==2.84.0
google-auth==2.17.2
google-auth-httplib2==0.1.0
google-auth-oauthlib==1.0.0
google-cloud-bigquery==3.9.0
google-cloud-bigquery-storage==2.19.1
google-cloud-core==2.3.2
google-cloud-datastore==2.15.1
google-cloud-firestore==2.11.0
google-cloud-language==2.9.1
google-cloud-storage==2.8.0
google-cloud-translate==3.11.1
google-colab @ file:///colabtools/dist/google-colab-1.0.0.tar.gz
google-crc32c==1.5.0
google-pasta==0.2.0
```

```
google-resumable-media==2.4.1
googleapis-common-protos==1.59.0
googledrivedownloader==0.4
graphviz==0.20.1
greenlet==2.0.2
grpcio==1.53.0
grpcio-status==1.48.2
gspread==3.4.2
gspread-dataframe==3.0.8
gym==0.25.2
gym-notices==0.0.8
h5netcdf==1.1.0
h5py==3.8.0
HeapDict==1.0.1
hijri-converter==2.2.4
holidays==0.22
holoviews==1.15.4
html5lib==1.1
httpimport==1.3.0
httplib2==0.21.0
humanize==4.6.0
hyperopt==0.2.7
idna==3.4
imageio==2.25.1
imageio-ffmpeg==0.4.8
imagesize==1.4.1
imbalanced-learn==0.10.1
imblearn==0.0
imgaug==0.4.0
importlib-metadata==6.3.0
importlib-resources==5.12.0
imutils==0.5.4
inflect==6.0.4
iniconfig==2.0.0
intel-openmp==2023.1.0
ipykernel==5.5.6
ipython==7.34.0
ipython-genutils==0.2.0
ipython-sql==0.4.1
ipywidgets==7.7.1
itsdangerous==2.1.2
jax==0.4.8
jaxlib @ https://storage.googleapis.com/jax-
releases/cuda11/jaxlib-0.4.7+cuda11.cudnn86-cp39-cp39-manylinux2014_x86_64.whl
jieba==0.42.1
Jinja2==3.1.2
joblib==1.2.0
jsonpickle==3.0.1
```

```
jsonschema==4.3.3
jupyter-client==6.1.12
jupyter-console==6.1.0
jupyter-server==1.23.6
jupyter_core==5.3.0
jupyterlab-pygments==0.2.2
jupyterlab-widgets==3.0.7
kaggle==1.5.13
keras==2.12.0
keras-vis==0.4.1
kiwisolver==1.4.4
korean-lunar-calendar==0.3.1
langcodes==3.3.0
lazy_loader==0.2
libclang==16.0.0
librosa==0.10.0.post2
lightgbm==3.3.5
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