pyGAM : Getting Started with Generalized Additive Models in Python

Pablo Oberhauser · Follow

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I came across pyGAM a couple months ago, but found few examples online. Below is a more practical extension to the documentation found in the pyGAM homepage.

dswah/pyGAM

pyGAM - [SEEKING FEEDBACK] Generalized Additive Models in Python

github.com

Generalized additive models are an extension of generalized linear models. They provide a modeling approach that combines powerful statistical learning with interpretability, smooth functions, and flexibility. As such, they are a solid addition to the data scientist's toolbox.

FYI: This tutorial will not focus on the theory behind GAMs. For more information on that there is an amazing blog post by Kim Larsen here:

GAM: The Predictive Modeling Silver Bullet | Stitch Fix Technology - Multithreaded

Imagine that you step into a room of data scientists; the dress code is casual and the scent of strong coffee is...

multithreaded.stitchfix.com

Or for a much more in depth read check out Simon. N. Wood's great book, "Generalized Additive Models: an Introduction in R"

Some of the major development in GAMs has happened in the R front lately with the `mgcv` package by Simon N. Wood. At our company, we had been using GAMs with modeling success, but needed a way to integrate it into our python-based "machine learning for production" framework.

Enter pyGAM

Installation

Installation is simple

```
pip install pygam
```

pyGAM also makes use of scikit-sparse which you can install via conda. Not doing so will result in a warning and potential problems with the slowing down of optimization for models with monotonicity/convexity penalties.

Classification Example

Let's walk through a classification example...

We import `LogisticGAM` to begin the classification training process, and `load_breast_cancer` for the data. This data contains 569 observations and 30 features. The target variable in this case is whether the tumor of malignant or benign, and the features are several measurements of the tumor. For showcasing purposes, we keep the first 6 features only.

```
import pandas as pd
from pygam import LogisticGAM
```

```
from sklearn.datasets import load_breast_cancer
#load the breast cancer data set

data = load_breast_cancer()
#keep first 6 features only

df = pd.DataFrame(data.data, columns=data.feature_names)[['mean
radius', 'mean texture', 'mean perimeter', 'mean area','mean
smoothness', 'mean compactness']]
target_df = pd.Series(data.target)
df.describe()
```

	mean radius	mean texture	mean perimeter	mean area	mean smoothness	mean compactness
count	569.000000	569.000000	569.000000	569.000000	569.000000	569.000000
mean	14.127292	19.289649	91.969033	654.889104	0.096360	0.104341
std	3.524049	4.301036	24.298981	351.914129	0.014064	0.052813
min	6.981000	9.710000	43.790000	143.500000	0.052630	0.019380
25%	11.700000	16.170000	75.170000	420.300000	0.086370	0.064920
50%	13.370000	18.840000	86.240000	551.100000	0.095870	0.092630
75%	15.780000	21.800000	104.100000	782.700000	0.105300	0.130400
max	28.110000	39.280000	188.500000	2501.000000	0.163400	0.345400

Description of sample classification data

Building the model

Since this is a classification problem, we want to make sure we use pyGam's `LogisticGAM()` function.

```
X = df[['mean radius', 'mean texture', 'mean perimeter', 'mean
area','mean smoothness', 'mean compactness']]
y = target_df

#Fit a model with the default parameters

gam = LogisticGAM().fit(X, y)
```

The `summary()` function provides a statistical summary of the model. In the diagnostics below, we can see statistical metrics such as AIC, UBRE, log likelihood, and pseudo-R^2 measures.

```
Model Statistics
------------------------
edof                22.822
AIC                145.995
AICc               148.168
UBRE                 2.289
loglikelihood      -50.175
deviance            100.35
scale                  1.0

Pseudo-R^2
----------------------------
explained_deviance     0.866
McFadden               0.866
McFadden_adj           0.806
```

Model summary

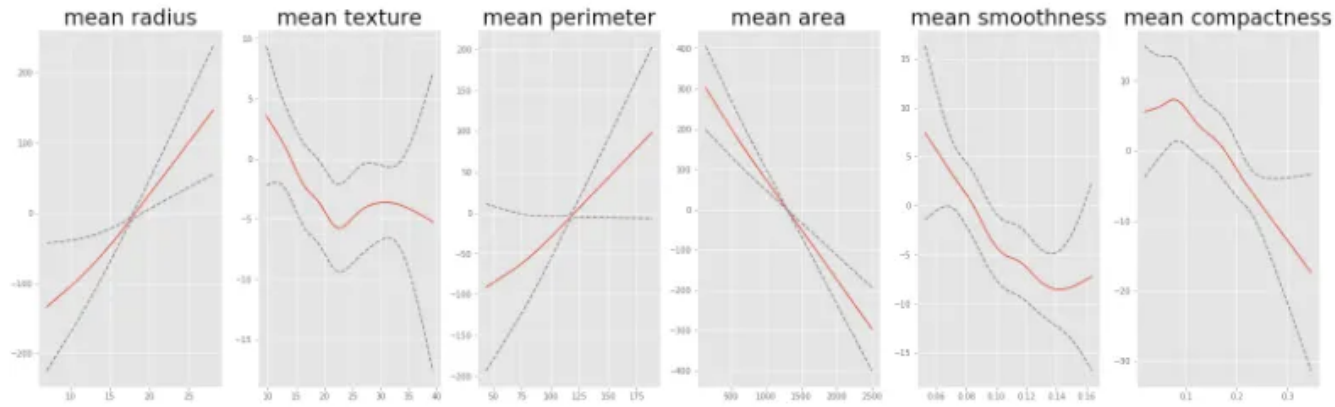
To get the training accuracy we simply run

```
gam.accuracy(X, y)
```

And we get a **.961335676625659 accuracy** right off the bat.

One of the nice things about GAMs is that their additive nature allows us to **explore and interpret individual features** by holding others at their mean. The snippet of code below shows these plots for the features included in the trained model. `generate_X_grid` helps us build a grid for nice plotting.

```
XX = generate_X_grid(gam)
plt.rcParams['figure.figsize'] = (28, 8)
fig, axs = plt.subplots(1, len(data.feature_names[0:6]))
titles = data.feature_names
for i, ax in enumerate(axs):
    pdep, confi = gam.partial_dependence(XX, feature=i+1, width=.95)
    ax.plot(XX[:, i], pdep)
    ax.plot(XX[:, i], confi[0][:, 0], c='grey', ls='--')
    ax.plot(XX[:, i], confi[0][:, 1], c='grey', ls='--')
    ax.set_title(titles[i])

plt.show()
```



Partial dependency plots with confidence intervals

We can already see some very interesting results. It is clear that some features have a fairly simple linear relationship with the target variable. There are about three features that seem to have strong non-linear relationships though. We will want to combine the interpretability of these plots, and the power to prevent over fitting in GAMs to come up with a model that generalizes well to a holdout set of data.

Partial dependency plots are extremely useful because they are highly interpretable and easy to understand. For example at first examination we can tell that there is a very strong relationship between the mean radius of the tumor and the response variable. The bigger the radius of the tumor, the more likely it is to be malignant. Other features like the mean texture are harder to decipher, and we can already infer that we might want to make that a smoother line (we walk through smoothing parameters in the next section).

Tuning Smoothness and Penalties

This is where the functionality of pyGAM begins to really shine through. We can choose to build a grid for parameter tuning or we can use intuition and domain expertise to find optimal smoothing penalties for the model.

Main parameters to keep in mind are:

`n_splines` , `lam` , and `constraints`

`n_splines` refers to the number of splines to use in each of the smooth function that is going to be fitted.

`lam` is the penalization term that is multiplied to the second derivative in the overall objective function.

`constraints` is a list of constraints that allows the user to specify whether a function should have a monotonically constraint. This needs to be a string in [‘convex’, ‘concave’, ‘monotonic_inc’, ‘monotonic_dec’,’circular’, ‘none’]

The default parameters that are being used in the model presented above are the following….

`n_splines` = 25

`lam` = 0.6

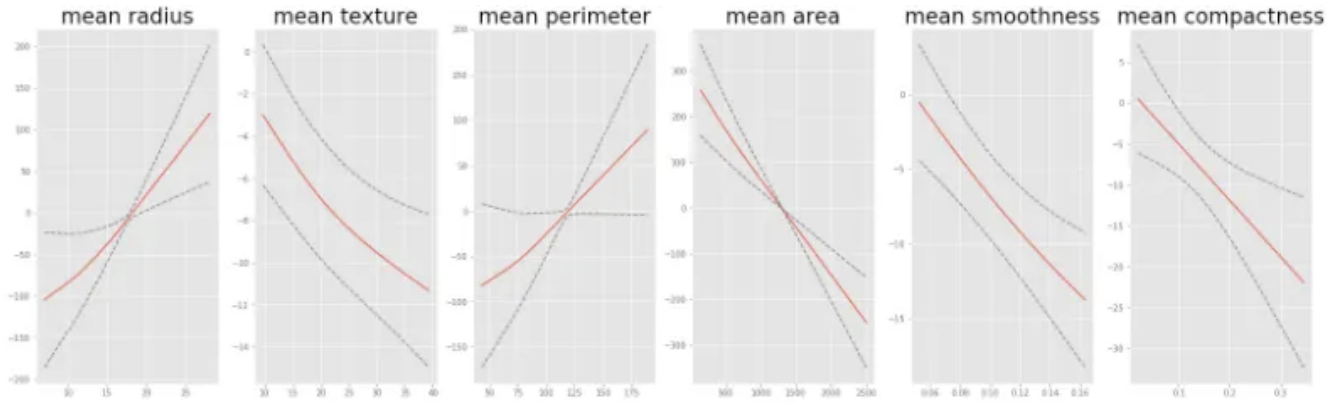
`constraints` = None

So let’s play around with `n_splines` . Let’s say for example we think mean texture is too “un-smooth” at the moment. We change parameter list to the following: (Note that another cool thing about pyGAM is that we can specify one single value of lambda and it will be copied to all of the functions. Otherwise, we can specify each one in a list…)

```
lambda_ = 0.6
n_splines = [25, 6, 25, 25, 6, 4]
constraints = None
gam = LogisticGAM(constraints=constraints,
          lam=lambda_,
         n_splines=n_splines).fit(X, y)
```

Which changes our training accuracy to **0.9507**

And now the partial dependency plots look like so:



Mean texture, mean smoothness, and mean compactness changed

The drop in accuracy tells us that there is some information we are not capturing by smoothing the mean texture estimator that much, but it highlights how the analyst can encode intuition into the modeling process.

Keep in mind that `n_splines` is only one parameter to change. Lambda controls how much we penalize 'wiggliness', so even if we keep a large value for `n_splines` we could get a straight line if lambda is large enough. Tuning these can be labor intensive, but there is an automated way to do this in pyGAM.

Grid search with pyGAM

The `gridsearch()` function creates a grid to search over smoothing parameters. This is one of the coolest functionalities in pyGAM because it is very easy to create a custom grid search. One can easily add parameters and ranges. For example, the default arguments are a dictionary of possible lambdas to create a grid search `{'lam':np.logspace(-3,3,11)}`

And just like the default argument is shows, we can add more and more arguments to the function and thus create a custom grid search.

```
gam = LogisticGAM().gridsearch(X, y)
```

Generalizing a GAM

Using a holdout set is the best way to balance bias-variance trade off in models. GAMs do a very good job at allowing the analyst to directly control over fitting in a statistical learning model.

pyGAM really plays nice with the sklearn workflow, so once it is installed it's basically like fitting a sklearn model.

We can split the data just like we usually would:

```
import numpy as np
from sklearn.model_selection import train_test_split
X_train, X_test, y_train, y_test = train_test_split(X, y,
test_size=0.33, random_state=42)
gam = LogisticGAM().gridsearch(X_train, y_train)
```

Predict classes or probabilities and use sklearn metrics for accuracy;

```
from sklearn.metrics import accuracy_score
from sklearn.metrics import log_loss
predictions = gam.predict(X_test)
print("Accuracy: {} ".format(accuracy_score(y_test, predictions)))
probas = gam.predict_proba(X_test)
print("Log Loss: {} ".format(log_loss(y_test, probas)))
```

Accuracy: 0.957446808511

Log Loss: 0.126179009744

Let's try a model that better generalizes. To do so, we can reduce the number of splines and see how the holdout set errors turn out.

```
lambda_ = [0.6, 0.6, 0.6, 0.6, 0.6, 0.6]
n_splines = [4, 14, 4, 6, 12, 12]
constraints = [None, None, None, None, None, None]
X_train, X_test, y_train, y_test = train_test_split(X, y,
test_size=0.33, random_state=42)
gam = LogisticGAM(constraints=constraints,
                  lam=lambda_,
                 n_splines=n_splines).train(X_train, y_train)
predictions = gam.predict(X_test)
print("Accuracy: {} ".format(accuracy_score(y_test, predictions)))
```

```
probas = gam.predict_proba(X_test)
print("Log Loss: {} ".format(log_loss(y_test, probas)))
```

Accuracy: 0.968085106383

Log Loss: 0.0924671883985

Regression

Switching to a regression context is simple:

```
from sklearn.datasets import load_boston
boston = load_boston()
df = pd.DataFrame(boston.data, columns=boston.feature_names)
target_df = pd.Series(boston.target)
df.head()
```

	CRIM	ZN	INDUS	CHAS	NOX	RM	AGE	DIS	RAD	TAX	PTRATIO	B	LSTAT
0	0.00632	18.0	2.31	0.0	0.538	6.575	65.2	4.0900	1.0	296.0	15.3	396.90	4.98
1	0.02731	0.0	7.07	0.0	0.469	6.421	78.9	4.9671	2.0	242.0	17.8	396.90	9.14
2	0.02729	0.0	7.07	0.0	0.469	7.185	61.1	4.9671	2.0	242.0	17.8	392.83	4.03
3	0.03237	0.0	2.18	0.0	0.458	6.998	45.8	6.0622	3.0	222.0	18.7	394.63	2.94
4	0.06905	0.0	2.18	0.0	0.458	7.147	54.2	6.0622	3.0	222.0	18.7	396.90	5.33

Data for regression problem

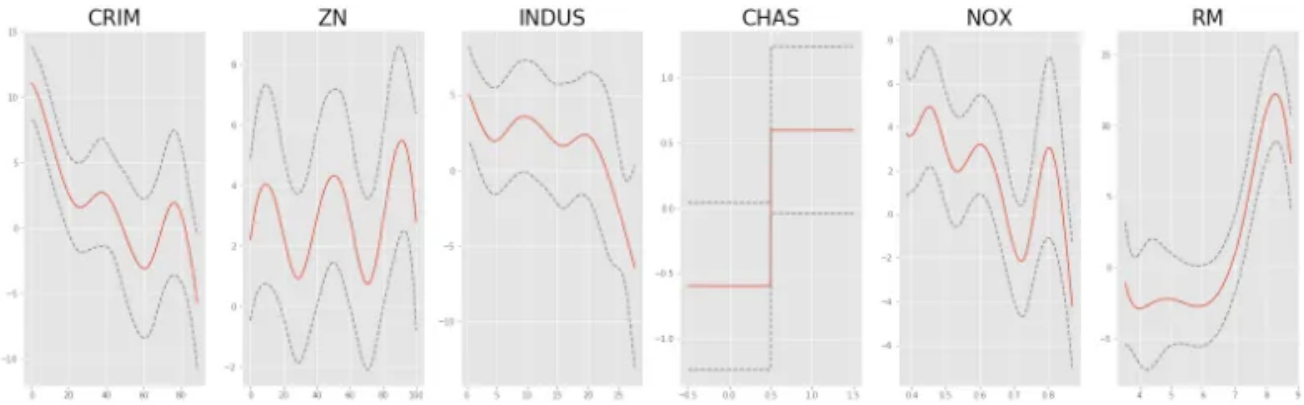
```
X = df
y = target_df

gam = LinearGAM(n_splines=10).gridsearch(X, y)
gam.summary()
```

```
Model Statistics
--------------------------
edof                 83.363
AIC                2687.268
AICc               2721.509
GCV                  14.135
loglikelihood     -1259.271
deviance            422.637
scale                10.016

Pseudo-R^2
---------------------------
explained_deviance     0.901
McFadden               0.604
McFadden_adj           0.578
```

Regression GAM summary

And we can similarly plot the feature dependencies:

```
XX = generate_X_grid(gam)
plt.rcParams['figure.figsize'] = (28, 8)
fig, axs = plt.subplots(1, len(boston.feature_names[0:6]))
titles = boston.feature_names
for i, ax in enumerate(axs):
    pdep, confi = gam.partial_dependence(XX, feature=i+1, width=.95)
    ax.plot(XX[:, i], pdep)
    ax.plot(XX[:, i], confi[0][:, 0], c='grey', ls='--')
    ax.plot(XX[:, i], confi[0][:, 1], c='grey', ls='--')
    ax.set_title(titles[i],fontsize=26)

plt.show()
```



Regression partial dependency plots

There are many more features and knobs to turn when building a GAM. Stay tuned for the advanced tutorial on further generalizing a GAM, CV for feature and smoothness selection, residual diagnostics, and more.

Machine Learning Statistics Python

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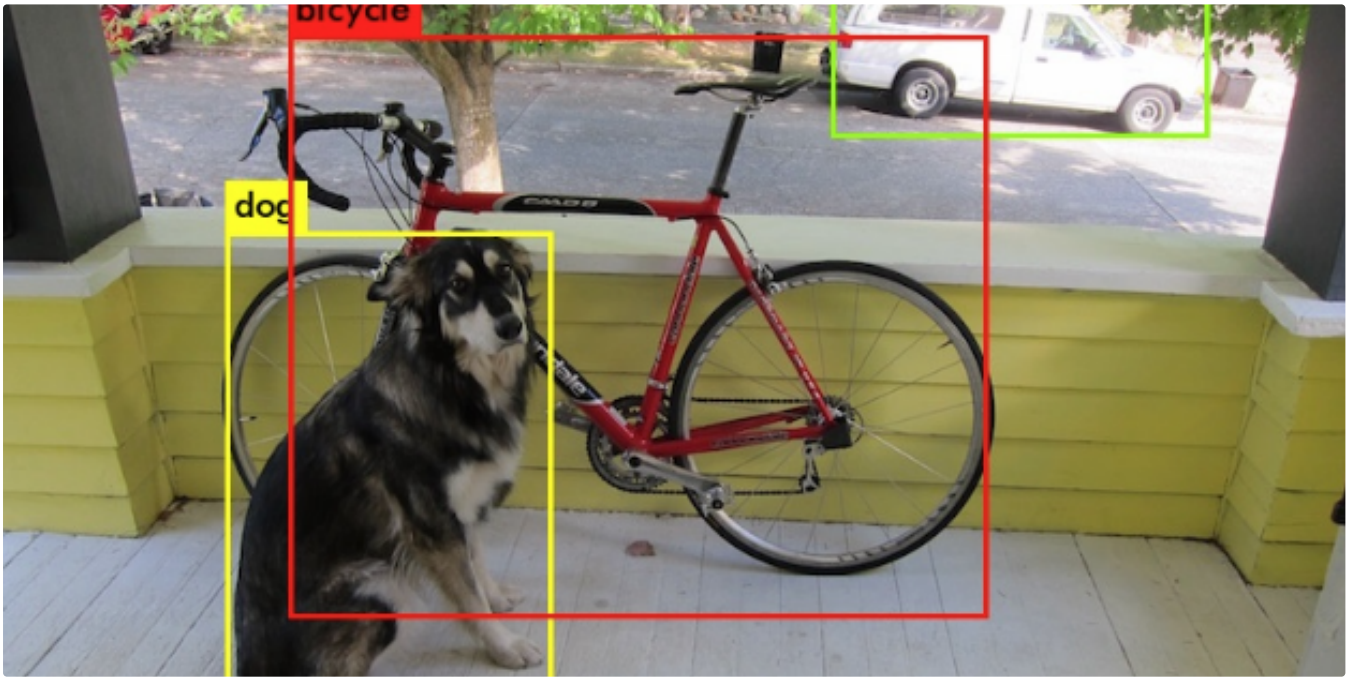

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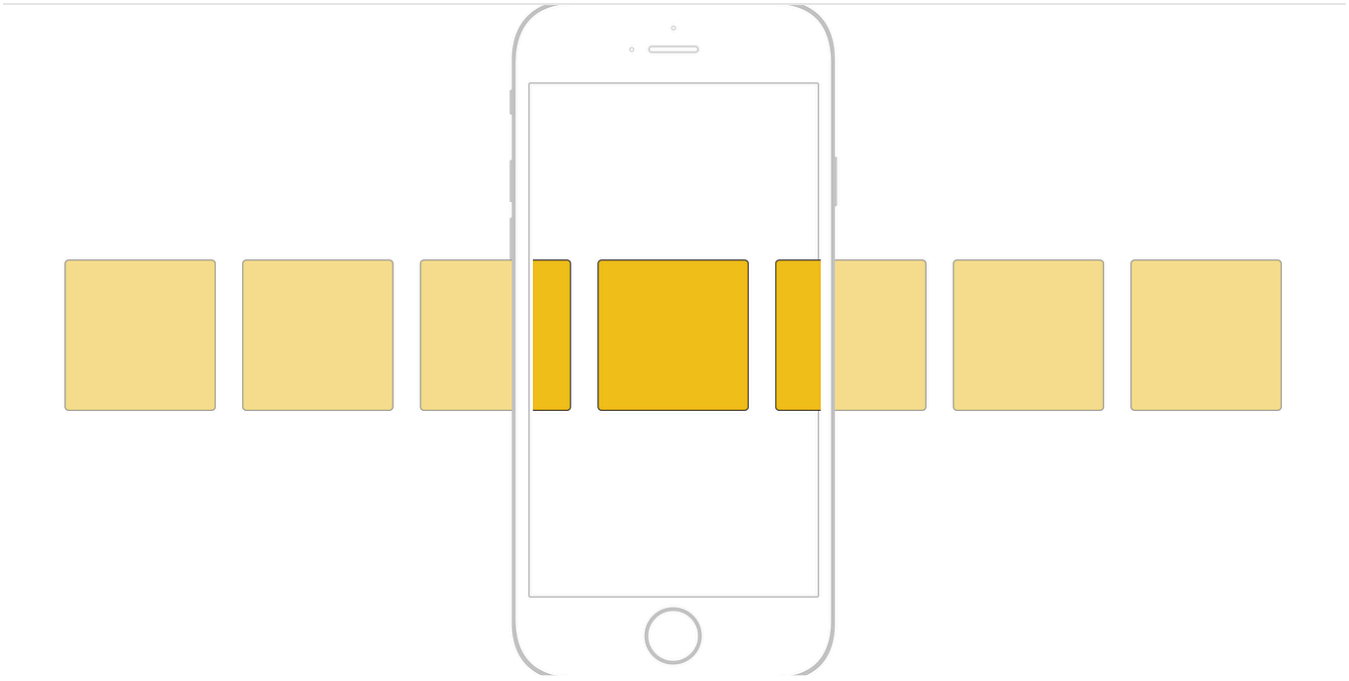

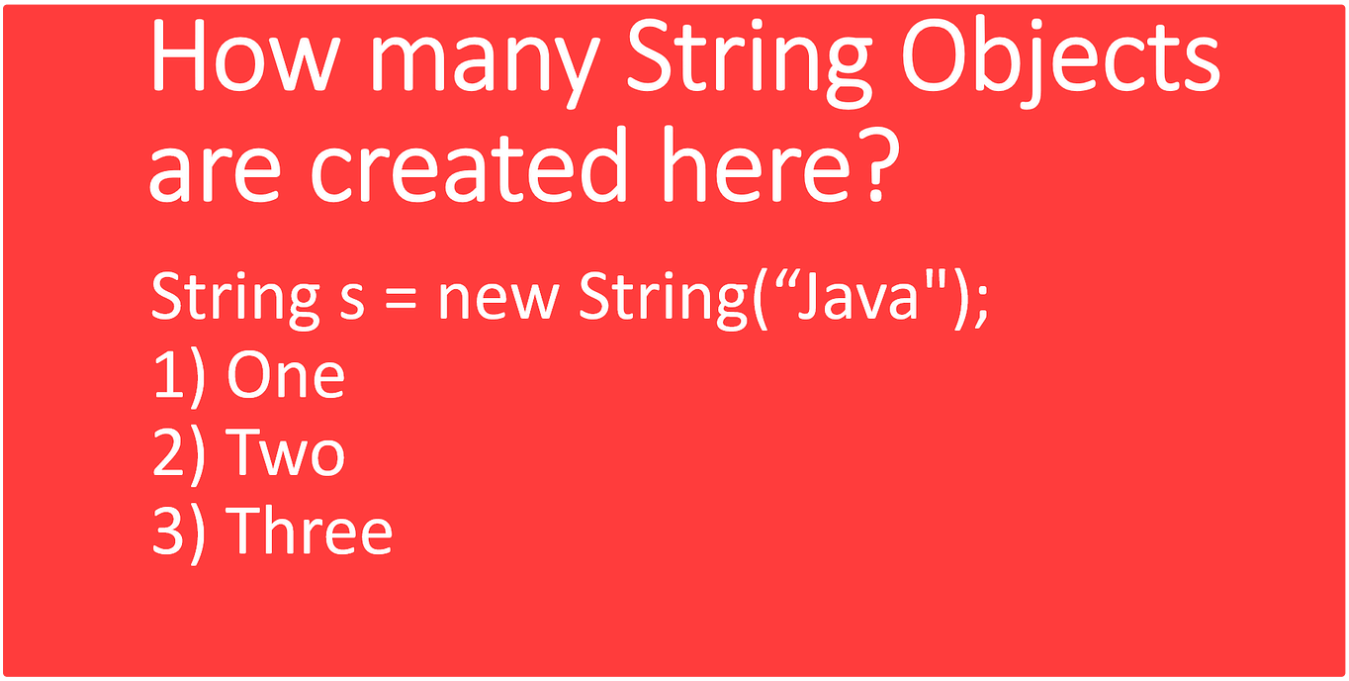

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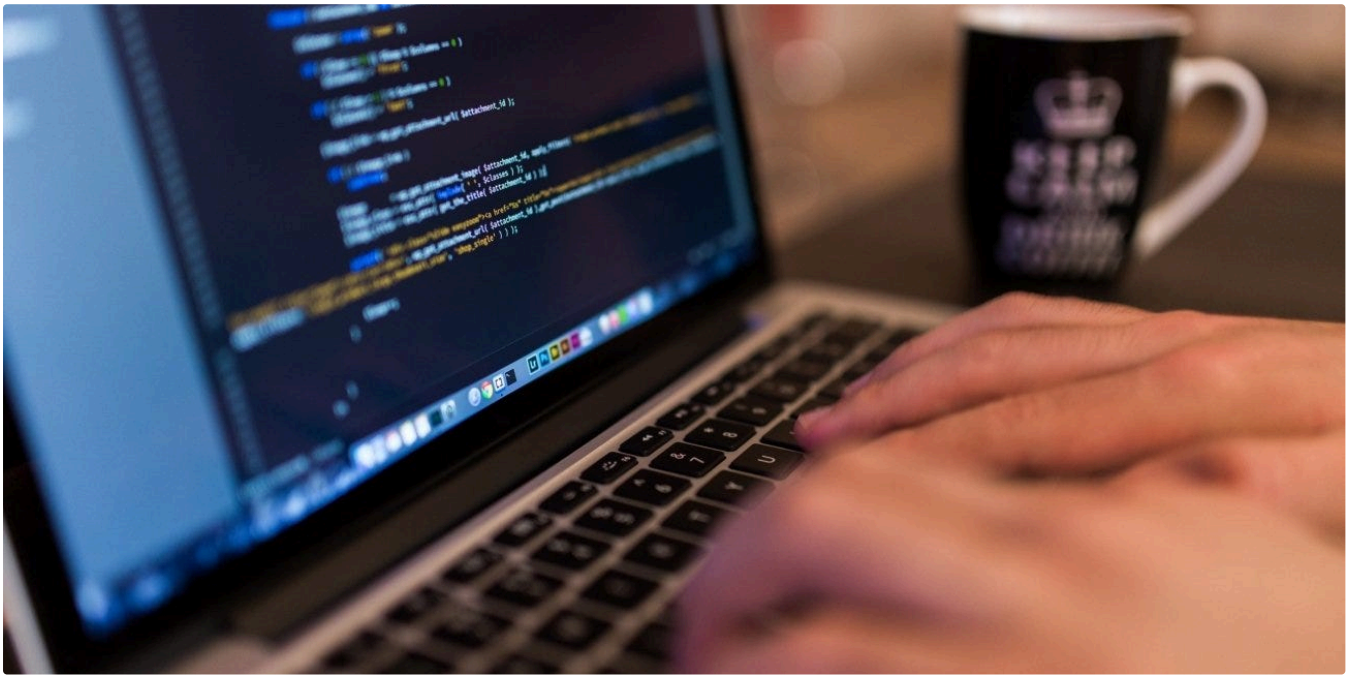

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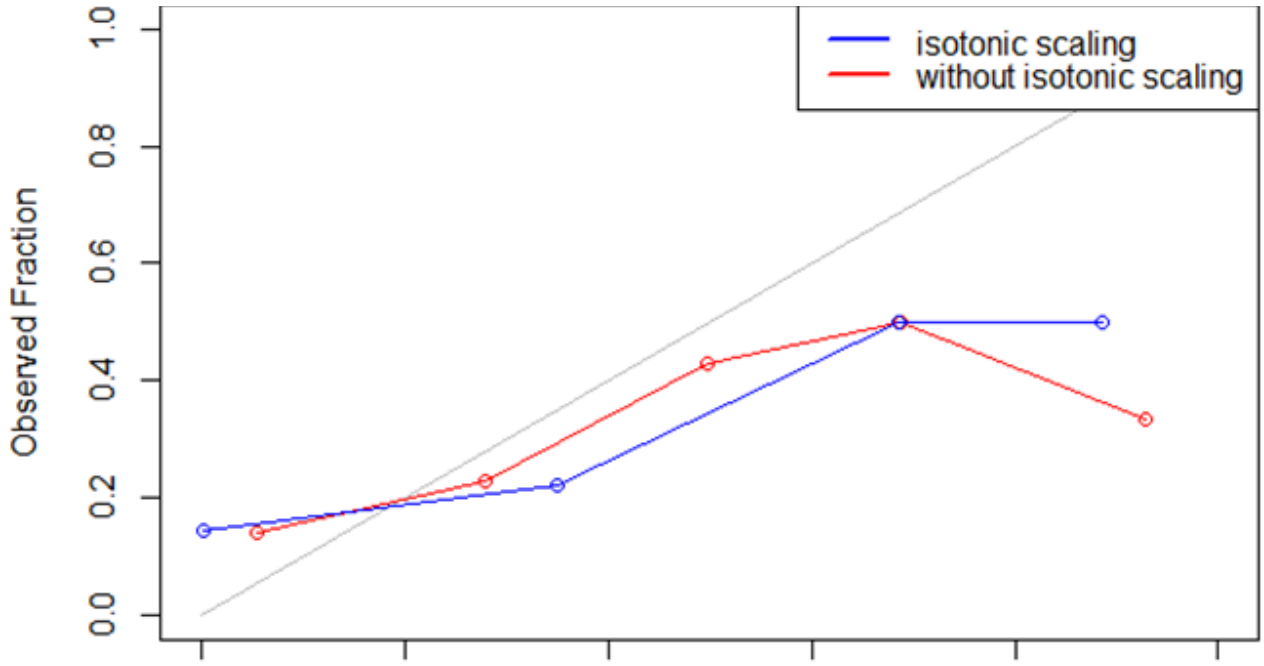

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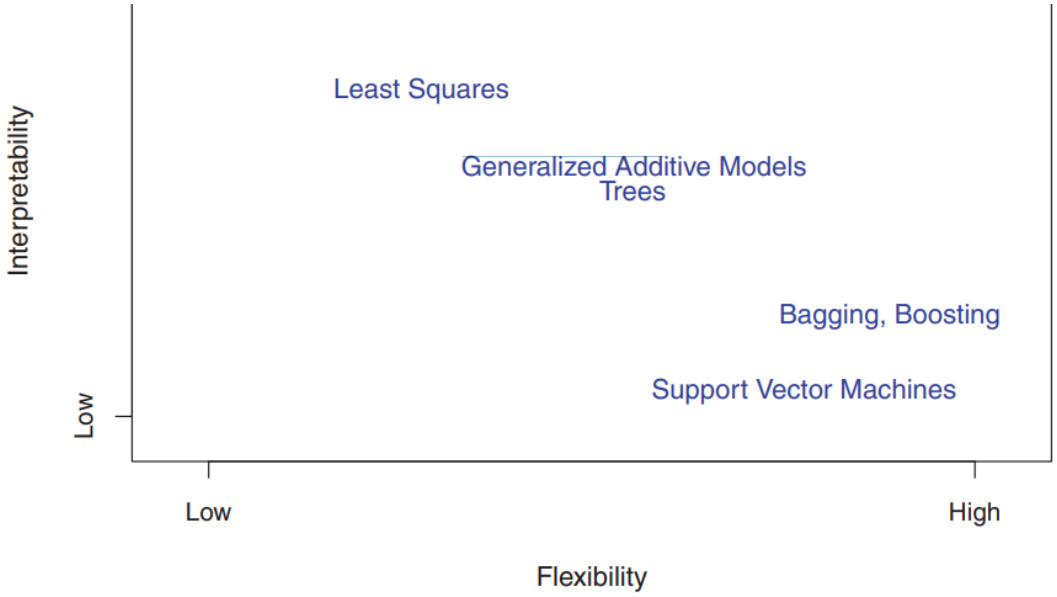

FIGURE 2.7. *A representation of the tradeoff between flexibility and inter-*

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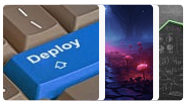

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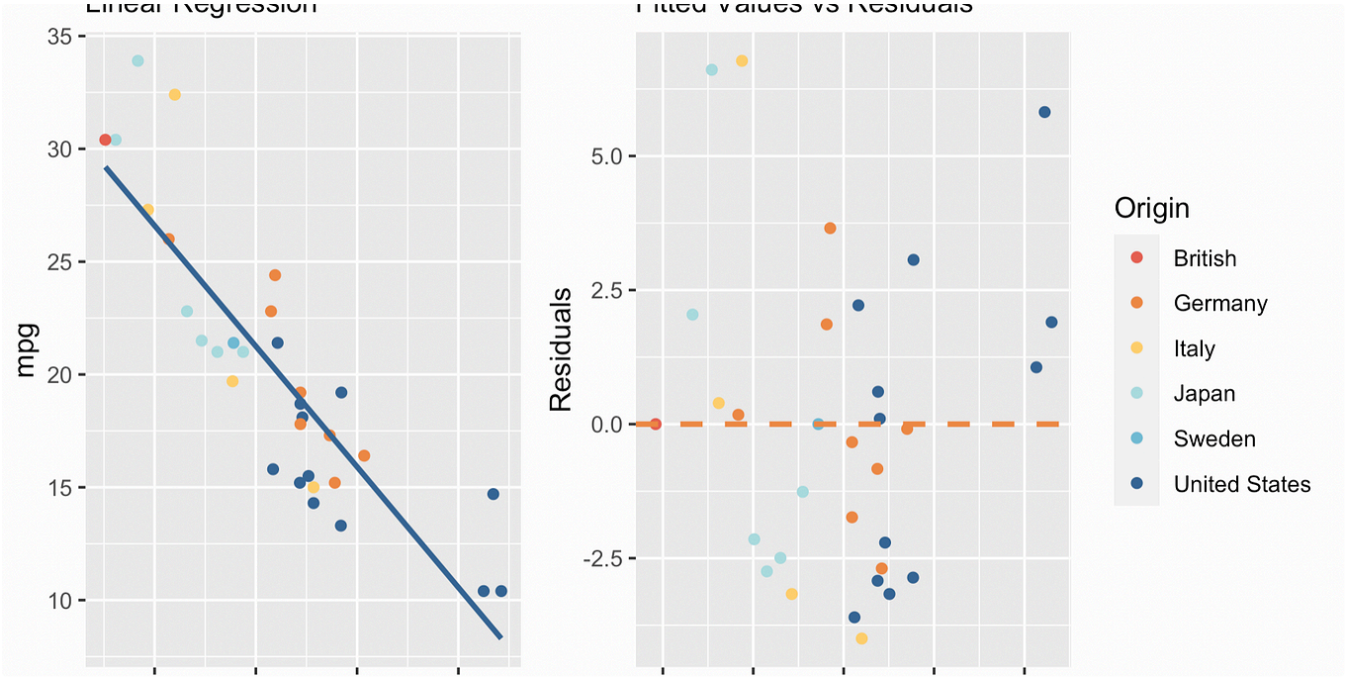

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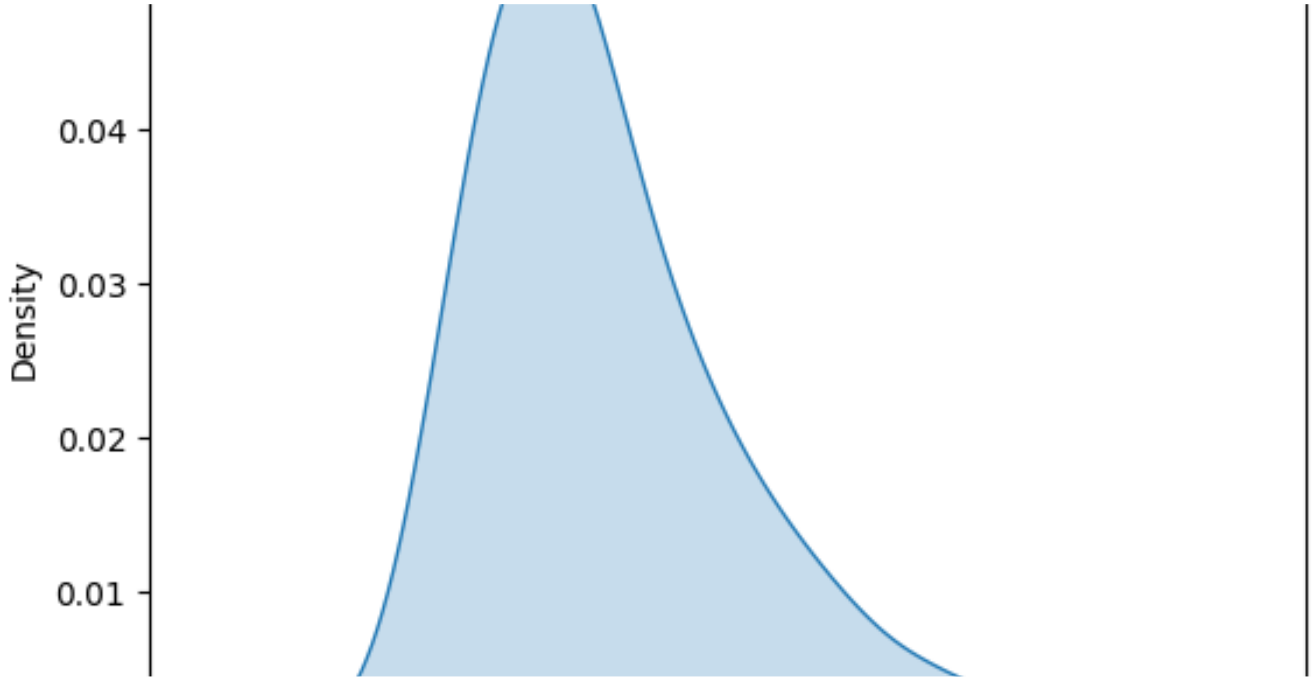

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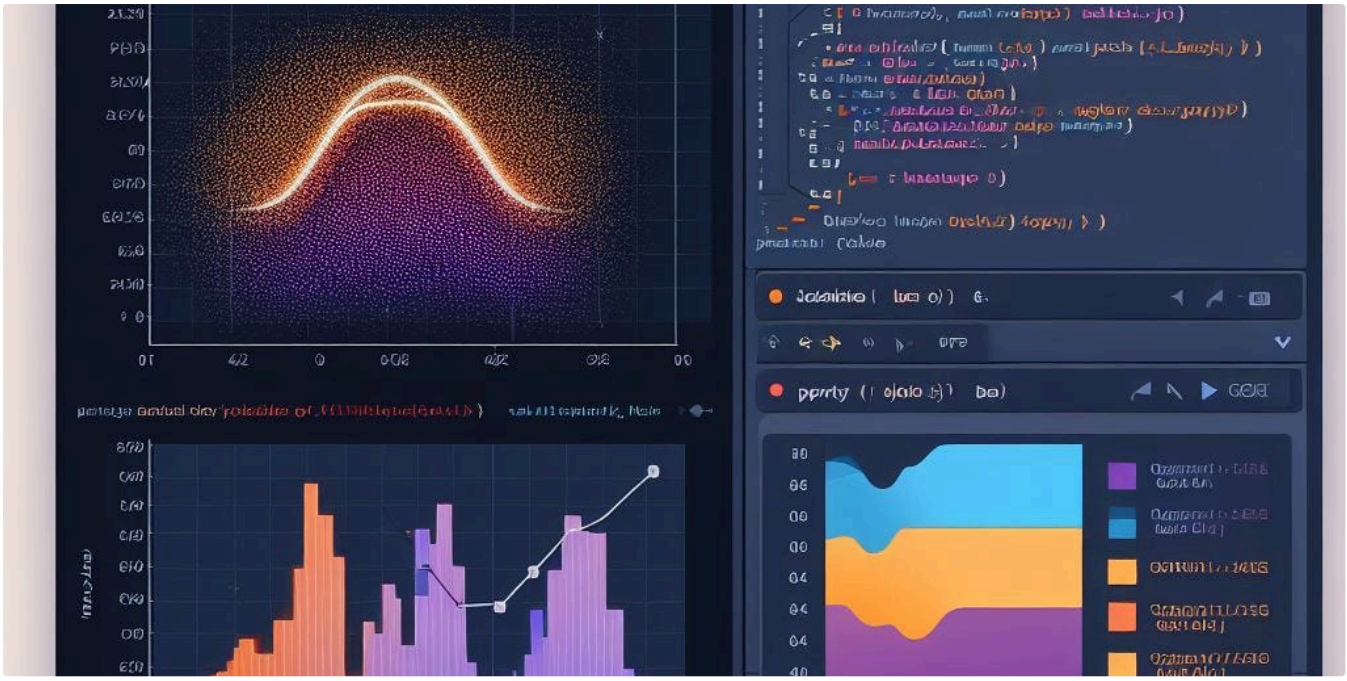

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