

PSY9511: Seminar 4

Model selection, validation and testing

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Strategies for model evaluation



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Statistical inference:

Goal: In-sample quantification

Predictive modelling:

Goal: Out-of-sample generalization

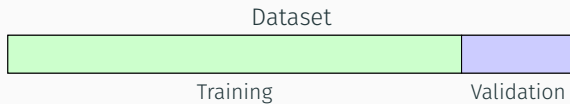
- How can we test how good our model is on **unseen data** and **be certain that performance holds if we present even more new data**

Model evaluation: Validation set

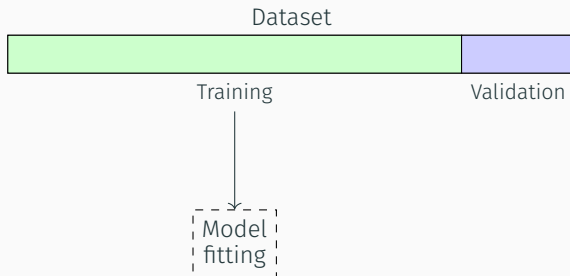
Dataset



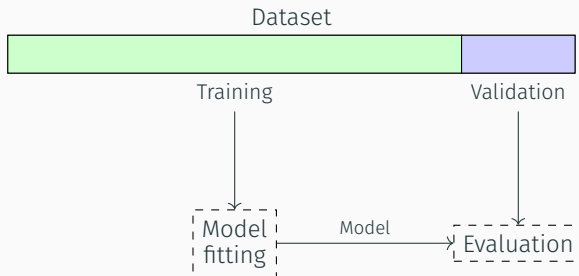
Model evaluation: Validation set



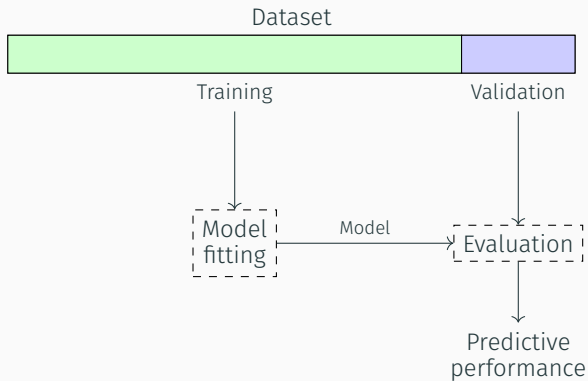
Model evaluation: Validation set



Model evaluation: Validation set



Model evaluation: Validation set



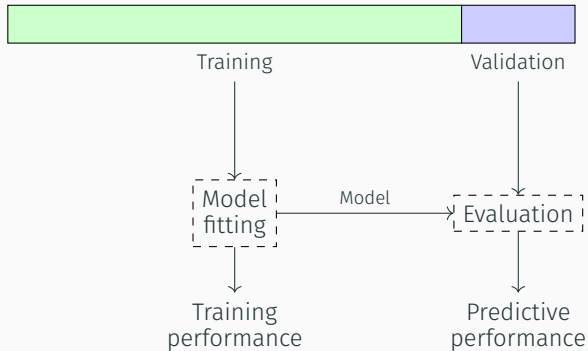
Model evaluation: Validation set

In the validation set approach we split the dataset into two subsets (commonly $\sim 80\%/20\%$), use the first for training the model and the second to test its performance.

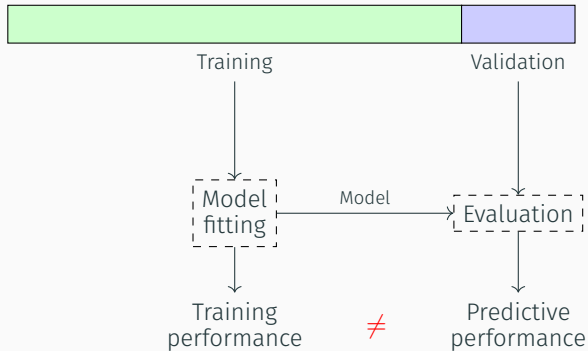
- + Accurate estimate of out-of-sample error
- + Simple
- Variable results depending on the exact split
- Only uses a subset of data for training models
- Gives a point estimate of the error, without confidence intervals



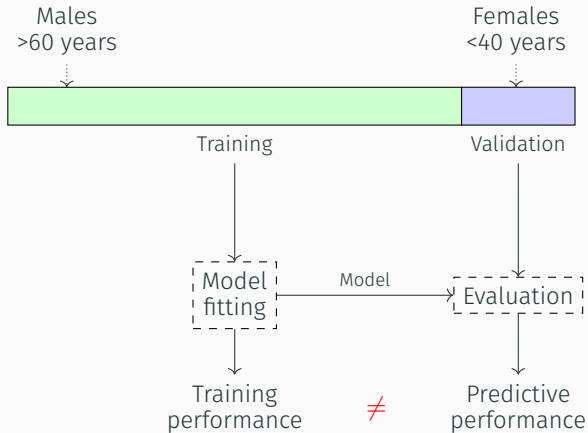
Model evaluation: Validation set



Model evaluation: Validation set



Model evaluation: Validation set



Stratification:

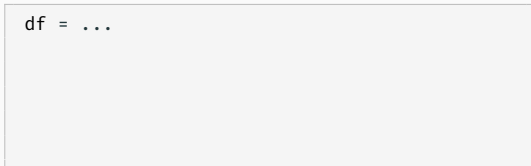
Ensuring all folds of the dataset are similar with respect to some given characteristics.

Model evaluation: Stratification

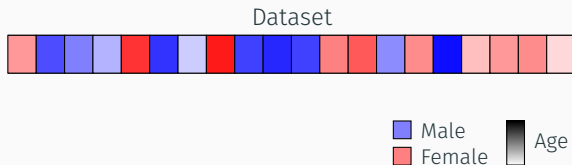
Dataset



```
In[1]: df = ...
```

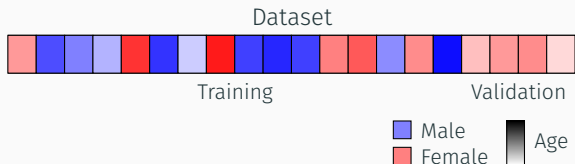


Model evaluation: Stratification



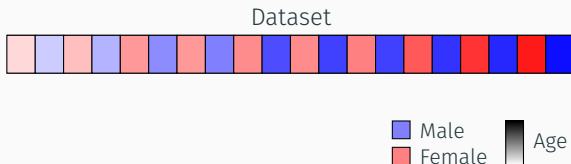
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Model evaluation: Stratification



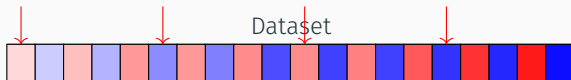
```
In[1]: df = ...  
  
train = df.iloc[:int(len(df) * 0.8)]  
validation = df.iloc[int(len(df) * 0.8):]
```


Model evaluation: Stratification



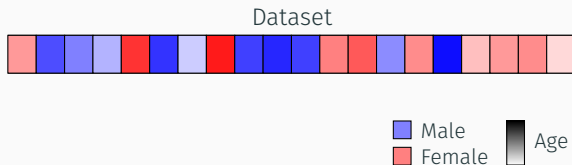
```
In[1]: df = ...  
df = df.sort_values(['sex', 'age'])
```

Model evaluation: Stratification



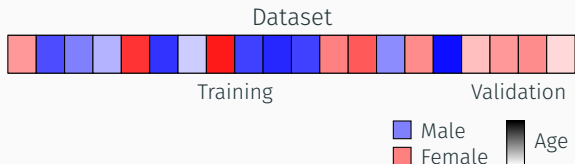
```
In[1]: df = ...  
df = df.sort_values(['sex', 'age'])  
  
df['fold'] = np.arange(len(df)) % (1 / 0.2)  
train = df[df['fold'] != 0]  
val = df[df['fold'] == 0]
```

Model evaluation: Stratification



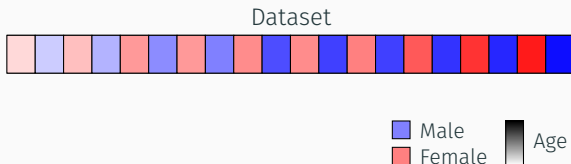
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Model evaluation: Stratification



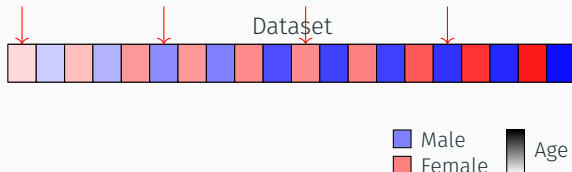
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Model evaluation: Stratification

Stratification:

Ensuring all folds of the dataset are similar with respect to some given characteristics.

- Helps alleviate the risk of training performance \gg validation performance
- **Always** stratify on target variable first
- Also good idea to stratify on other core characteristics, e.g. sex and age

```
In[1]: from sklearn.model_selection import train_test_split
```

```
library(splitstackshape)  
stratified(data, columns, split)
```

