AARHUS UNIVERSITY

LESSON 4: Data analyse

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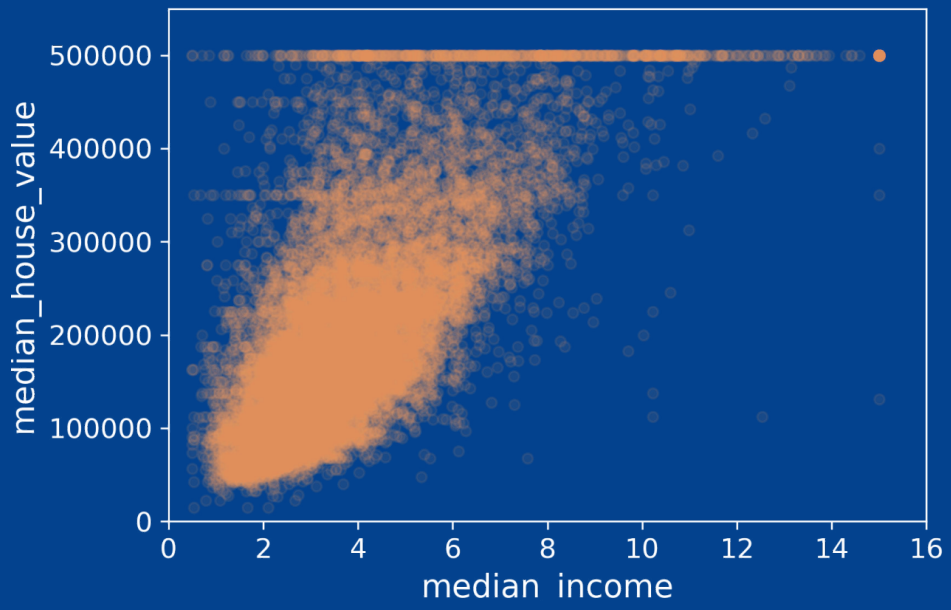
AUTUMN 2024



Agenda

Data analyse

1. Admin
   - ~~VSCode update i fremtidige `.ipynb` filer~~ (E23),
   - feedback på O1
     (een aflv. fil + `nbmerge`, ingen tekst fra opg.).
2. Datasæt og Jeres O4 projekt.
   - Opgave: `L04/dataanalyse.ipynb`
3. Statestik og visualisering.
4. Pipelines
   - Opgave: `L04/pipelines.ipynb`

'Demo' datasæt

MNIST, Iris og Moon

Iris:

Sepal/petal længde/bredde,
Mr. Fisher, 1936,
"Anderson's Iris data set"
`sklearn.datasets.load_iris(..)`

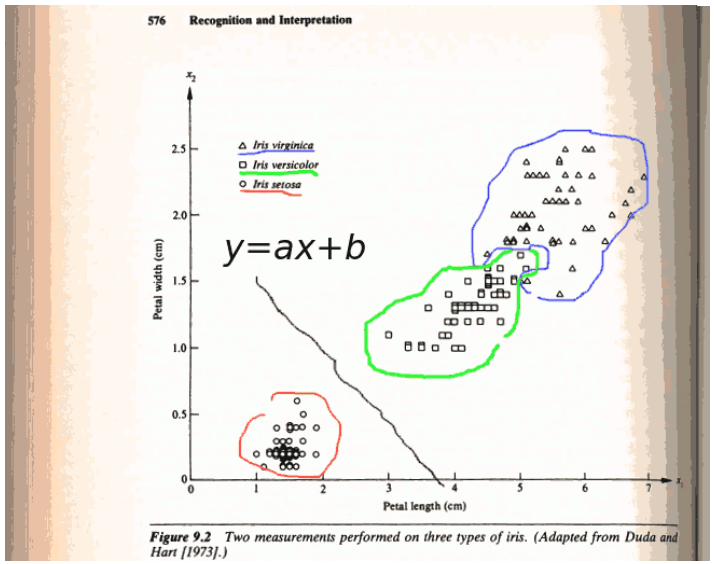
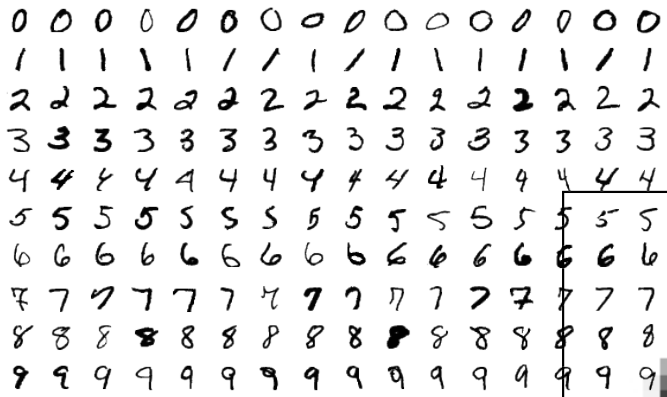
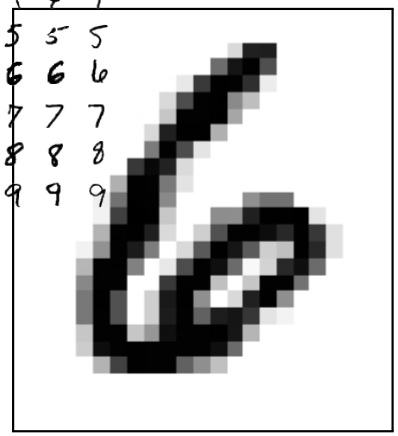


Figure 9.2 Two measurements performed on three types of iris. (Adapted from Duda and Hart [1973].)

MNIST:

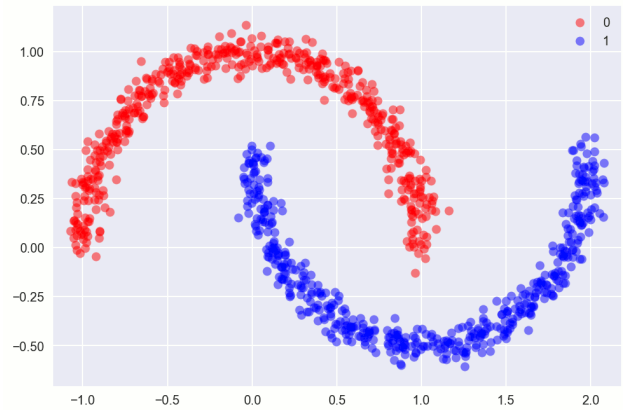
Håndskrevne tal,
preprocesseret, centrerede,
`sklearn.datasets.fetch_openml('mnist_784'..`





Moon:

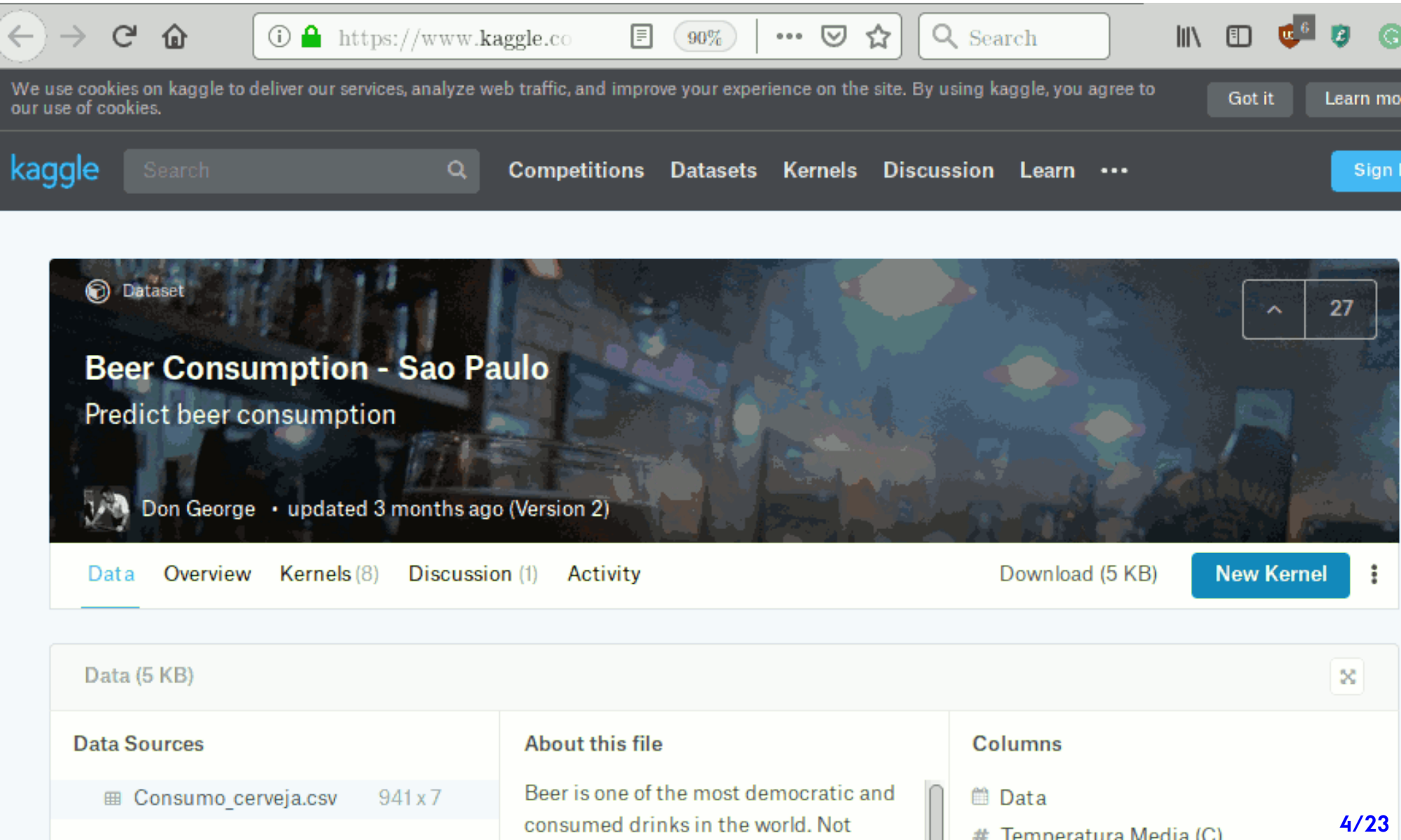
'XOR' lign.,
non-linear decision boundary,
`sklearn.datasets.make_moons(..)`



Opg. L04 Beskrivelse af eget projekt (O4)

Dit datasæt fra f.eks. `https://www.kaggle.com`...

(brug min login: user=cef@ase.au.dk, password=test123)



Opg. L04 Beskrivelse af eget projekt (O4)

..eller UCI `https://archive.ics.uci.edu/ml/index.php`..

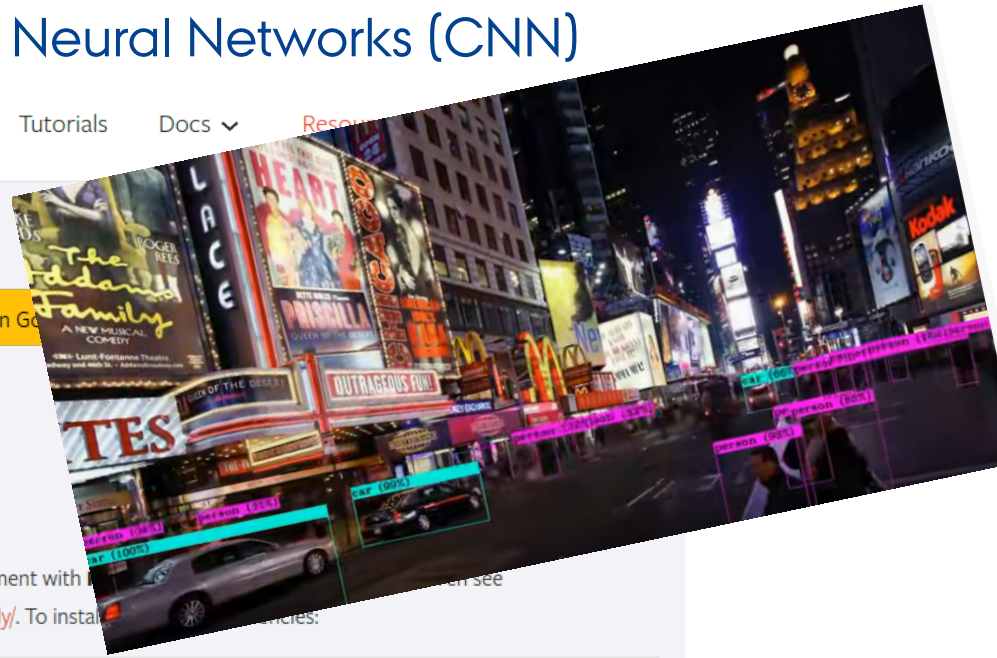
Intro til YOLOV5..

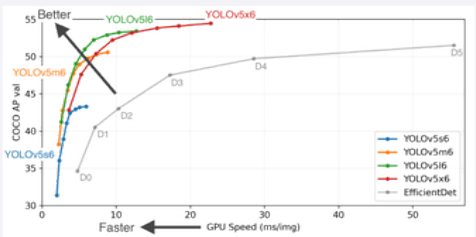
YOLOV3/4/5 Family and Convolutional Neural Networks (CNN)

PyTorch Get Started Ecosystem Mobile Blog Tutorials Docs

YOLOV5

View on Github Open on G





BEFORE YOU START

Start from a **Python>=3.8** environment with

https://pytorch.org/get-started/locally/. To instal

```
pip install -qr https://raw.githubusercontent.com/ultralytics/yolov5/master/req
```

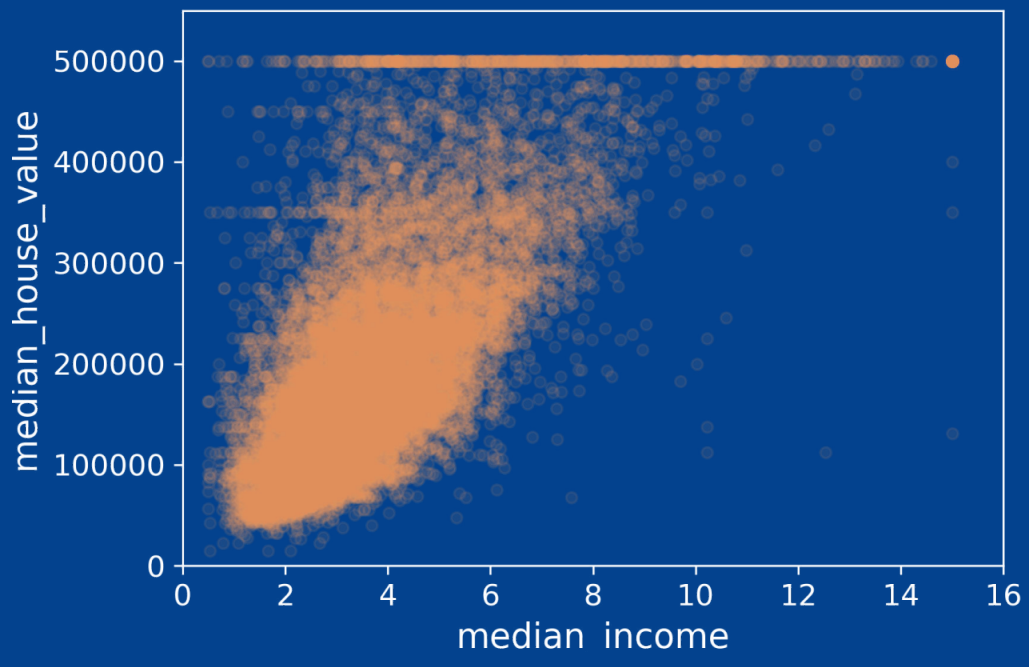
MODEL DESCRIPTION

Nano	Small	Medium	Large	XLarge
YOLOv5n	YOLOv5s	YOLOv5m	YOLOv5l	YOLOv5x
4 MB$_{FP16}$	14 MB$_{FP16}$	41 MB$_{FP16}$	89 MB$_{FP16}$	166 MB$_{FP16}$
6.3 ms$_{V100}$	6.4 ms$_{V100}$	8.2 ms$_{V100}$	10.1 ms$_{V100}$	12.1 ms$_{V100}$
28.4 mAP$_{COCO}$	37.2 mAP$_{COCO}$	45.2 mAP$_{COCO}$	48.8 mAP$_{COCO}$	50.7 mAP$_{COCO}$

YOLOV5: [https://pytorch.org/hub/ultralytics_yolov5/]
Demo video: [https://www.youtube.com/watch?v=1_SiU0YUoOI]

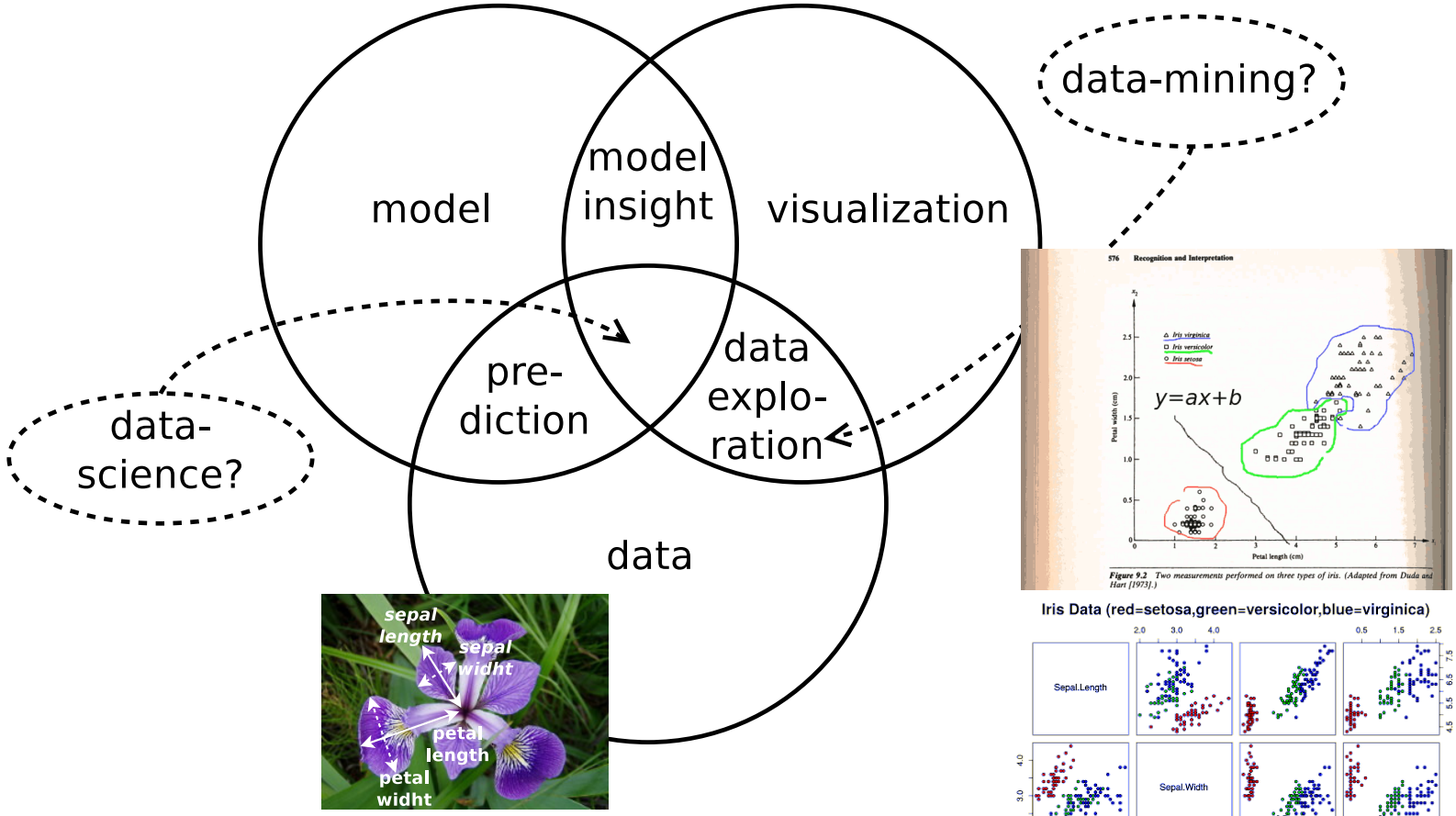
STATISTICS AND VISUALIZATION

μ, σ and being a Data Science Expert..



Machine learning baggrund

Machine learning: data science ekspert (fra L01)



Mean and Variance

The mean and variance (and hence the standard deviation) for a random variable X can for a population of N samples be estimated as

$$
\begin{aligned}
E[X] &= \frac{1}{N}\sum_{i=1}^{N} X_i &&= \mu_X \\
V[X] &= E[(X_i - E[X])(X_i - E[X])] \\
&= E[X_i X_i] - E[X]^2 \\
&= \left(\frac{1}{N}\sum_{i=1}^{N} X_i X_i\right) - \mu_X^2 &&= \sigma_X^2 \\
\sigma &= \sqrt{V}
\end{aligned}
$$

Notice that the $1/N$ factor most often appears as $1/(N-1)$ for the variance estimation.

When using the factor $1/(N-1)$, $\hat{V}$ is said to be the best unbiased estimator, when it is $1/N$ it will be biased, both assuming an underlying normal distribution.

Auto- and Cross-covariance

Now let's goto full matrix notation for the covariance. For a data matrix $\mathbf{X}$

$$\mathbf{X} = \begin{bmatrix} x_1^{(1)} & x_2^{(1)} & \cdots & x_d^{(1)} \\ x_1^{(2)} & x_2^{(2)} & \cdots & x_d^{(2)} \\ \vdots & & & \\ x_1^{(n)} & x_2^{(n)} & \cdots & x_d^{(n)} \end{bmatrix}$$

the previous one-dimensional random variable X can now be seen as a d-dimensional vector $\mathbf{x}^{(i)}$, that is one of the data rows in the full data matrix

$$X_i \rightarrow \mathbf{x}^{(i)} = \begin{bmatrix} x_1^{(i)} & x_2^{(i)} & \cdots & x_d^{(i)} \end{bmatrix}^\top$$

Auto- and Cross-covariance

The (biased) auto–covariance matrix can be estimated as

$$\begin{aligned} E[\mathbf{X}] &= \mu_{\mathbf{X}} \\ &= \frac{1}{N}\sum_{i=1}^{N} \mathbf{x}^{(i)} \end{aligned}$$

$$\begin{aligned} \mathbf{\Sigma}(\mathbf{X}) &= \mathrm{cov}(\mathbf{X}, \mathbf{X}) \\ &= \frac{1}{N}\sum_{i=1}^{N} \mathbf{x}^{(i)}\mathbf{x}^{(i)T} - \mu_{\mathbf{x}^{(i)}}\mu_{\mathbf{x}^{(i)}}^{\top} \end{aligned}$$

with implicit $1/N$ factor here (inside the first $E[\cdot]$), so the definition is a biased covariance. You may opt to use the factor $1/(N-1)$ instead.

For yet another data matrix $\mathbf{Z}$ the (biased) cross-covariance matrix is given by

$$\begin{aligned} \mathbf{\Sigma}(\mathbf{X}, \mathbf{Z}) &= \mathrm{cov}(\mathbf{X}, \mathbf{Z}) \\ &= \frac{1}{N}\sum_{i=1}^{N} \mathbf{x}^{(i)}\mathbf{z}^{(i)T} - \mu_{\mathbf{x}^{(i)}}\mu_{\mathbf{z}^{(i)}}^{\top} \end{aligned}$$

Auto-Covariance Matrix, Binary Classifier

For a dataset, $\mathbf{X}$; features λ_{cat} and λ_{dog}; classifying cat/non-cat

Auto-covariance matrix (dim = features x features)

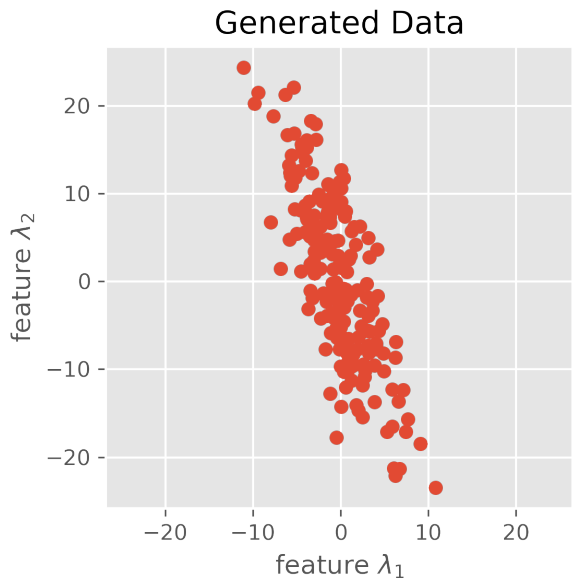
$$\mathbf{\Sigma}(\mathbf{X}) = \begin{bmatrix} \sigma_{\text{cat,cat}} & \sigma_{\text{cat,dog}} \\ \sigma_{\text{dog,cat}} & \sigma_{\text{dog,dog}} \end{bmatrix} =$$

	cat	dog
cat	σ^2_{cat}	$\sigma_{\text{cat,dog}}$
dog	$\sigma_{\text{dog,cat}}$	σ^2_{dog}

co-variance

$$\sigma_{\text{cat,dog}} = \frac{1}{N}\sum_{i=1}^{N}(x^{(i)}_{\text{cat}} - \mu_{\text{cat}})(x^{(i)}_{\text{dog}} - \mu_{\text{dog}})$$

Example $\mathbf{\Sigma}(\mathbf{X}) = \begin{bmatrix} 13.2 & -28.8 \\ -28.8 & 93.3 \end{bmatrix}$



Confusion matrix, cats only, cat/non-cat (dim = classes x classes)

$$\mathbf{M} = \begin{bmatrix} \text{TP} & \text{FP} \\ \text{FN} & \text{TN} \end{bmatrix} =$$

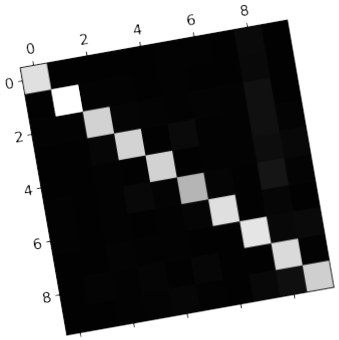
	actual cat	*actual* non-cat
cat	T, cat	F, cat
dog	F, dog	T, non-cat

Looking for Correlations

..using the auto-covariance matrix,

..for regression: the standard correlation coefficient, Pearson's r,

..or for classification: the confusion matrix



	Grade 3	Grade 4	Grade 5	Grade 6	Grade 7	Grade 8
Grade 3	1.0000	0.7598	0.7199	0.6940	0.6869	0.6432
Grade 4	0.7598	1.004	0.7975	0.7675	0.7574	0.7189
Grade 5	0.7198	0.7975	0.9933	0.7813	0.7639	0.7218
Grade 6	0.6940	0.7675	0.7813	0.9899	0.7958	0.7579
Grade 7	0.6869	0.7574	0.7639	0.7958	0.9820	0.7884
Grade 8	0.6432	0.7189	0.7218	0.7579	0.7884	0.9826

Looking for Correlations

Since the dataset is not too large, you can easily compute the *standard correlation coefficient* (also called *Pearson's r*) between every pair of attributes using the `corr()` method:

```
corr_matrix = housing.corr()
```

Now let's look at how much each attribute

```
>>> corr_matrix["median_house_value"]
median_house_value    1.000000
median_income         0.687170
total_rooms           0.135231
housing_median_age    0.114220
households            0.064702
total_bedrooms        0.047865
population           -0.026699
longitude            -0.047279
latitude             -0.142826
Name: median_house_value, dtype: float64
```

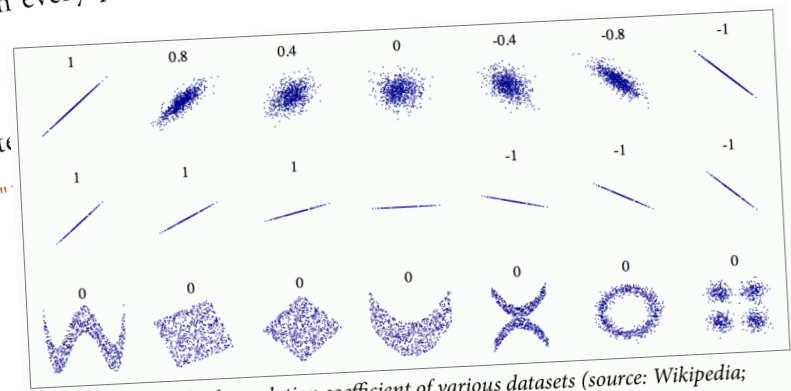


Figure 2-14. Standard correlation coefficient of various datasets (source: Wikipedia; public domain image)

The correlation coefficient ranges from –1 to 1. When it is close to 1, it means that there is a strong positive correlation; for example, the median house value tends to go up when the median income goes up. When the coefficient is close to –1, it means that there is a strong negative correlation; you can see a small negative correlation

Data Science: Visualization

Take a Quick Look at the Data Structure

Let's take a look at the top five rows using the DataFrame's `head()` method (see Figure 2-5).

```
In [5]: housing = load_housing_data()
        housing.head()
```

Out[5]:

	longitude	lati
0	-122.23	37.
1	-122.22	37.
2	-122.24	37.
3	-122.25	37.
4	-122.25	37.

Figure 2-5. Top five rows in t

Figure 2-8. A histogram fo

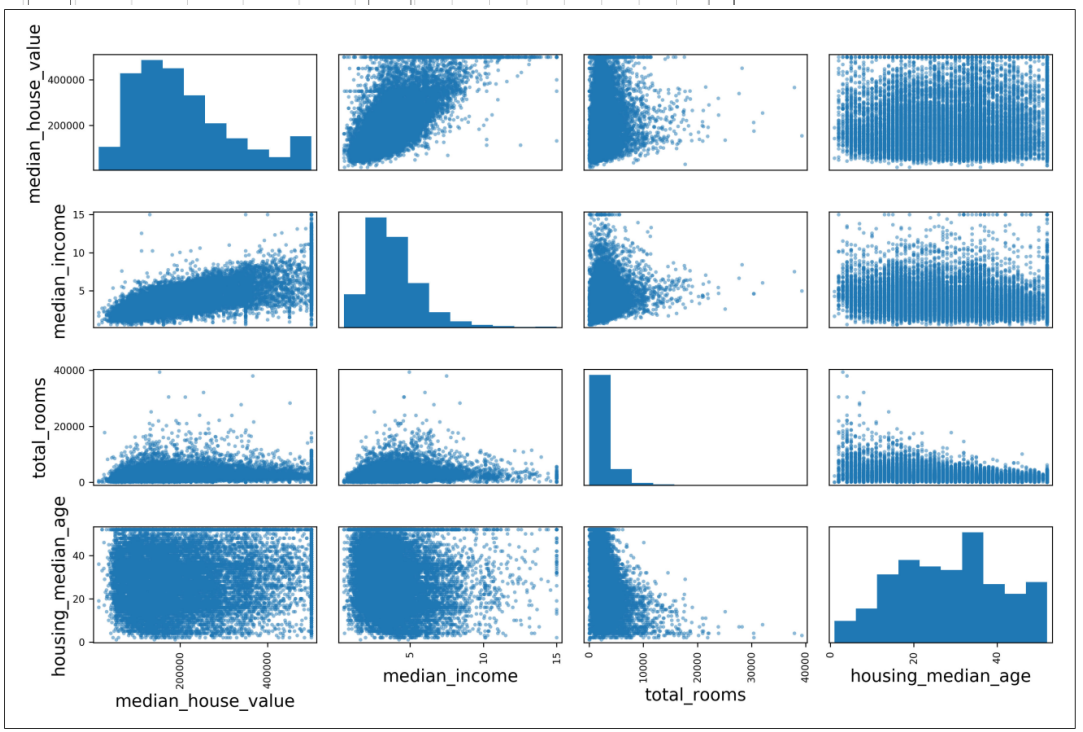


Figure 2-15. Scatter matrix

Data Science: Visualization

..why so many sales at `median_house_value` = 350 K$ and 500 *K*$??

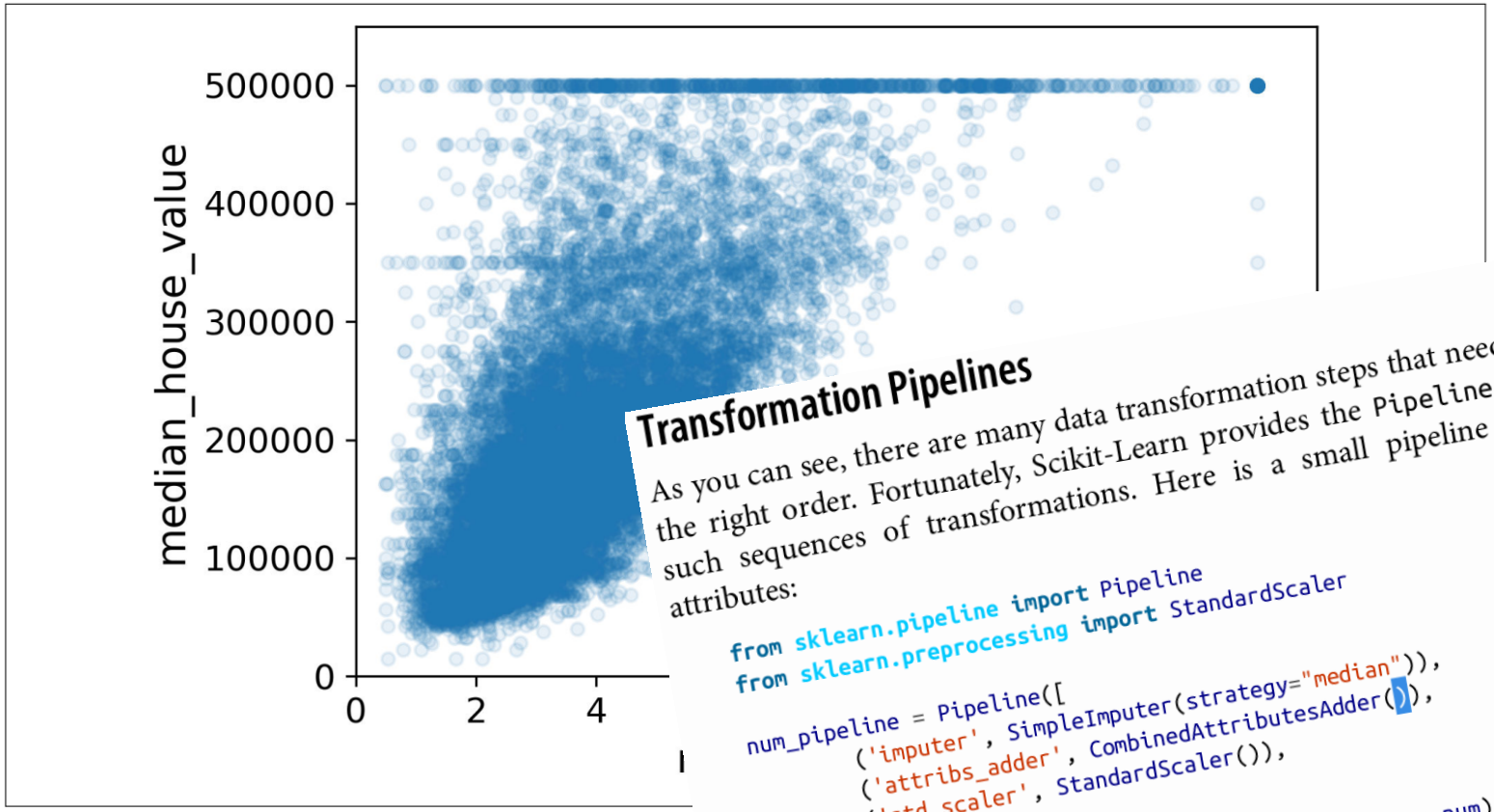


Figure 2-16. Median income versus media

Transformation Pipelines

As you can see, there are many data transformation steps that need to be executed in the right order. Fortunately, Scikit-Learn provides the `Pipeline` class to help with such sequences of transformations. Here is a small pipeline for the numerical attributes:

```
from sklearn.pipeline import Pipeline
from sklearn.preprocessing import StandardScaler

num_pipeline = Pipeline([
        ('imputer', SimpleImputer(strategy="median")),
        ('attribs_adder', CombinedAttributesAdder()),
        ('std_scaler', StandardScaler()),
    ])

housing_num_tr = num_pipeline.fit_transform(housing_num)
```

The `Pipeline` constructor takes a list of name/estimator pairs defining a sequenc steps. All but the last estimator must be transformers (i.e., they must ha `fit_transform()` method). The names can be anything you like (as long as the don't contain double underscores "__"): they will come in handy lat

..fixing data via pipelines..

PIPELINES

Putting it all together in Python code...

Pipelines and Preprocessing of Data

Normalization via Scaling or Standardization

Why the need for preprocessing?

> *Standardization of datasets is a* **common requirement for many machine learning estimators** *[..]; they might* **behave badly** *if the individual features do not more or less look like standard normally distributed data. [..]*
>
> *[*`https://scikit-learn.org/stable/modules/preprocessing.html`*]*

Standardization of a feature vector $\mathbf{x}$, giving $\mathbf{x}'$ mean zero, and standard deviation one

$$\mathbf{x}' = \frac{\mathbf{x} - \mu_{\mathbf{x}}}{\sigma_{\mathbf{x}}}$$

What kind of estimators needs preprocessing?

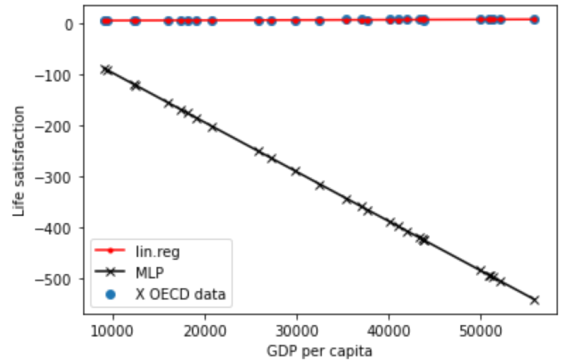
$\rightarrow$ **Neural networks (NNs=MLPs) in particular!**

What is the difference between Standardization and Scaling?

Pipelinesand Polynomial Regression

Exercise: `pipelines.ipynb`: Revisit the OECD data in O1s for MLPs

Feature: GDP per capita feature in range $10K to $50K.
But MLP expects input in the range [0;1] or perhaps [-1;1].




```
1   # Manual scaling..
2   X_min = np.min(X)
3   X_max = np.max(X)
4   s = X_max – X_min
5
6   print(f"X_min={X_min:.0f},  X_max={X_max:.0f},  s={s:.0f}")
7
8   X_scaled = (X–X_min)/s
9   print(f"X_scaled.shape={X_scaled.shape}")
10  print(f"np.min(X_scaled)={np.min(X_scaled)}")
11  print(f"np.max(X_scaled)={np.max(X_scaled)}")
12
13  mlp.fit(X_scaled ,y.ravel())
14  y_pred_mlp = mlp.predict((M–X_min)/s)
15
16  plt.plot(m, y_pred_lin, "r")
17  plt.plot(m, y_pred_mlp, "k")
18
19  print(f"mpl.score={mlp.score(X_scaled, y.ravel()):0.2f}")
```

```
Prints:
X_min=9055,
X_max=55805, s=46750
X_scaled.shape=(29, 1)
np.min(X_scaled)=0.0
np.max(X_scaled)=1.0
mpl.score=0.70
```

Pipelines

OECD Data and MLPs: introducing a `MinMaxScaler`

```
# Now, do the same but via a pipeline..
from sklearn.preprocessing import MinMaxScaler

scaler = MinMaxScaler()
scaler.fit(X)
X_scaled = scaler.transform(X)
M_scaled = scaler.transform(M)

mlp.fit(X_scaled, y)
y_pred_mlp = mlp.predict(M_scaled)

print(f"mpl.score={mlp.score(X_scaled, y):0.2f}")

# PRINTS: mpl.score=0.71
```

Pipelines

OECD Data and MLPs: putting everything in a Full Pipeline

```
# Or even better, in a full pipeline..
from sklearn.pipeline import Pipeline

pipe = Pipeline( # indent pipeline as VHDL port mappings!
  [
    ('scaler', MinMaxScaler()),
    ('mlp', mlp)
  ]
)

pipe.fit(X, y)

print(f"pipe.score(..)={pipe.score(X, y):0.2f}"

# PRINTS: pipe.score(..)=0.68
```

Pipelines and Polynomial Regression

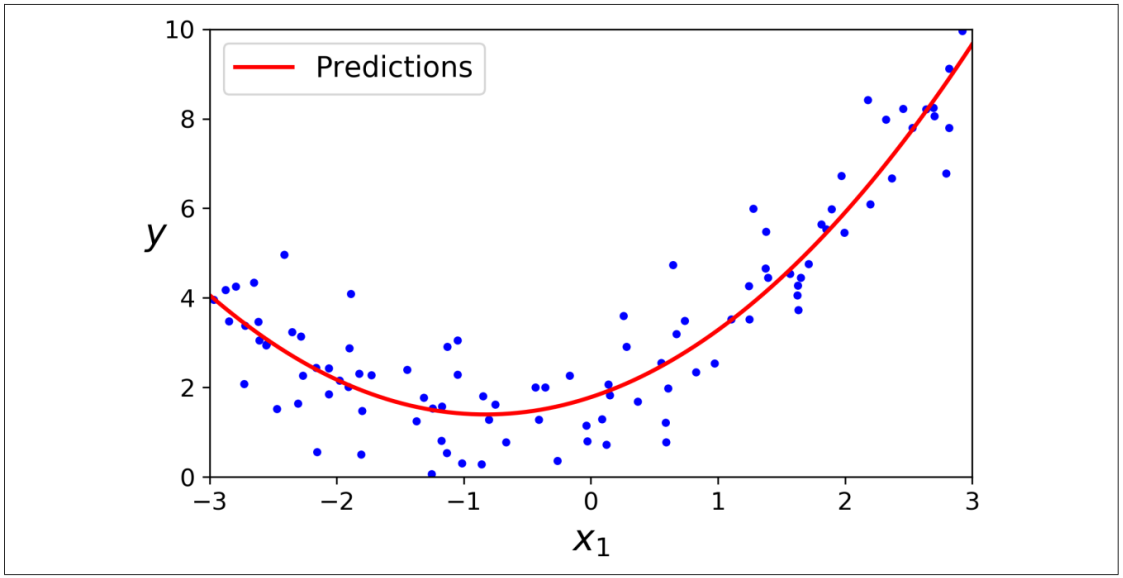


Figure 4-13. Polynomial Regression model predictions

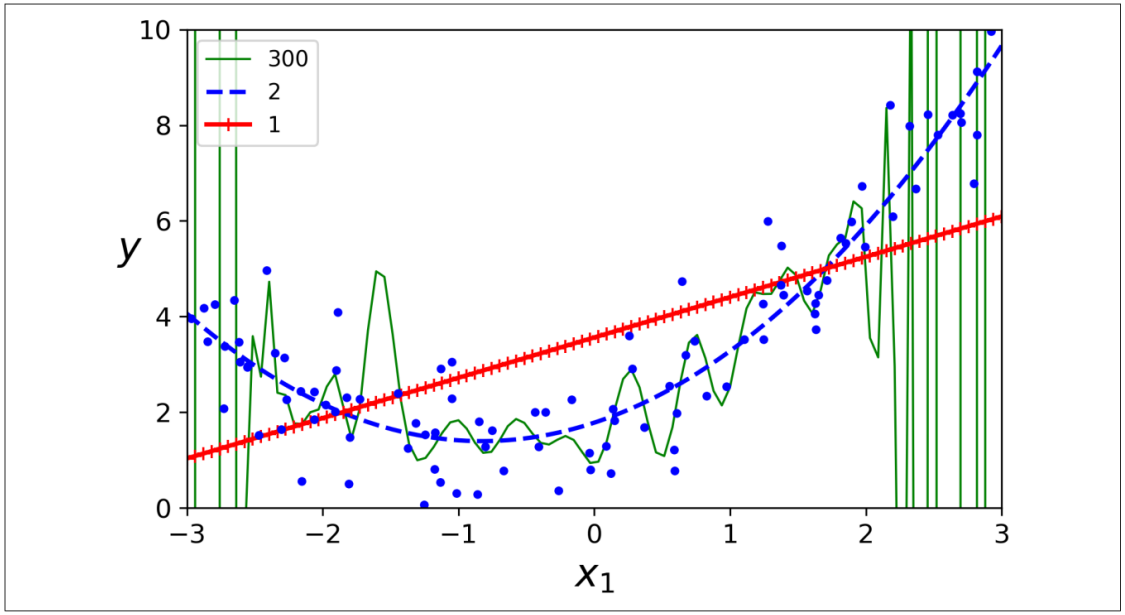


Figure 4-14. High-degree Polynomial Regression

Pipelines and Polynomial Regression

Python code from Opgave: L07/capacity_under_overfitting.ipynb

```
from sklearn.pipeline import Pipeline
from sklearn.preprocessing import PolynomialFeatures
from sklearn.linear_model import LinearRegression
from sklearn.model_selection import cross_val_score
..
polynomial_features = PolynomialFeatures(degree=degrees[i], ..
linear_regression = LinearRegression()

pipeline = Pipeline(
  [
    ("polynomial_features", polynomial_features),
    ("linear_regression", linear_regression)
  ]
)

pipeline.fit(X[:, np.newaxis], y) # done in cross_val_score()?

scores = cross_val_score(
    pipeline, X[:, np.newaxis], y,
    scoring="neg_mean_squared_error", cv=10
  )
score_mean = -scores.mean()
```

Pipelines and K-fold CV

Evaluate a score by cross-validation: `cross_val_score(..)`

sklearn.model_selection.cross_val_score

sklearn.model_selection.**cross_val_score**(*estimator*, *X*, *y=None*, ***, *groups=None*, *scoring=None*, *cv=None*, *n_jobs=None*, *verbose=0*, *fit_params=None*, *pre_dispatch='2*n_jobs'*, *error_score=nan*) [source]

Evaluate a score by cross-validation

Read more in the User Guide.

Parameters:

estimator : *estimator object implementing 'fit'*
The object to use to fit the data.

X : *array-like of shape (n_samples, n_features)*
The data to fit. Can be for example a list, or an array.

y : *array-like of shape (n_samples,) or (n_samples, n_outputs), default=None*
The target variable to try to predict in the case of supervised learning.

groups : *array-like of shape (n_samples,), default=None*
Group labels for the samples used while splitting the dataset into train/test set. Only used in conjunction with a "Group" cv instance (e.g., `GroupKFold`).

scoring : *str or callable, default=None*
A str (see model evaluation documentation) or a scorer callable object / function with signature `scorer(estimator, X, y)` which should return only a single value.

Similar to `cross_validate` but only a single metric is permitted.

If None, the estimator's default scorer (if available) is used.

cv : *int, cross-validation generator or an iterable, default=None*