Linear and Logistic Regression

Simple, yet powerful predictors

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#MachineLearning

Table of Contents

- Machine learning basics
  - Objective function, cost function, optimization
- Linear regression
  - Problem description, motivation
  - Algorithm
  - Usage
- RANSAC
- Extensions: polynomial regression
- Logistic regression
  - Problem description
  - Algorithm
  - Usage

Linear Regression

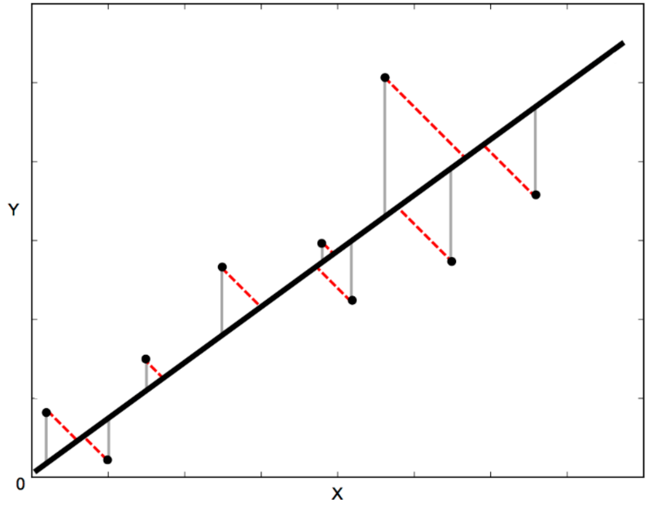
Predict continuous values…
and torture first-semester students

Linear Regression Intuition

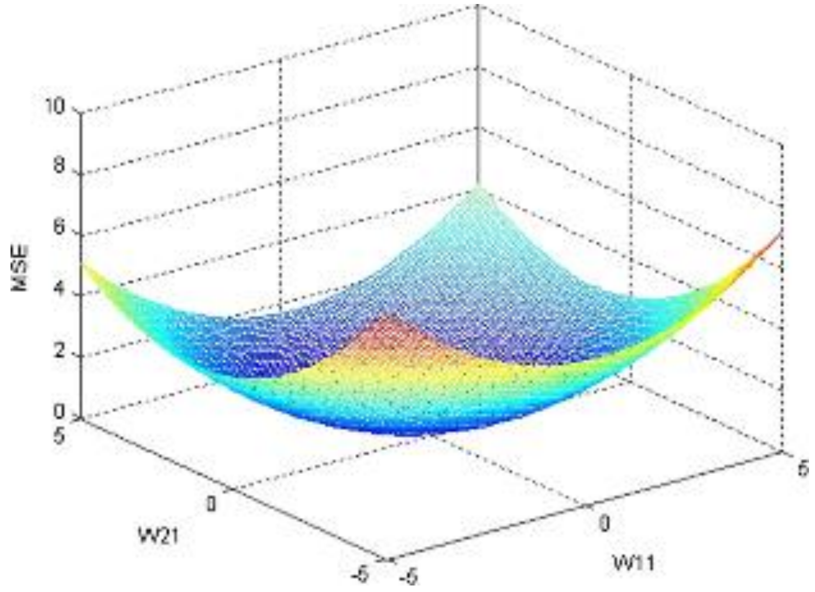
- Regression – predicting a continuous variable
- Problem statement
  - Given pairs of $(x; y)$ points, create a model
    - Input x, output y; goal: predict y given x
      - Under the assumption that y depends linearly on x (and nothing else)
- Modelling function
  - $\tilde{y} = ax + b$
  - Many samples: for each sample $(x_1, y_1), \dots, (x_n, y_n)$:
    - $\tilde{y}_i = ax_i + b,\ i \in [1; n]$
  - Many variables: $\tilde{y} = a_1 x_1 + a_2 x_2 + \cdots + a_n x_n + b \equiv a^T X + b$
    - Trick: $a_0 \equiv b; x_0 \equiv 1 \Rightarrow \tilde{y} = a_0 . 1 + a_1 x_1 + \cdots + a_n x_n = a^T x$

Training

- Loss function
  - For each sample i, $i \in [1, m]$
  - $d_i = (\tilde{y}_i - y_i)^2$
- Total cost function
  - Also called simply "cost function"
  - $J = \frac{1}{n}\sum_{i=1}^{n}(\tilde{y}_i - y_i)^2$
  - J depends on a, b, x, y
- Training process
  - Minimize the cost function
    - We're looking for parameters a, b that lead to $\min J$
    - Written as $\underset{a,b}{\arg\min}\, J$



Gradient Descent



- Input: a, b; output J
- Paraboloid (3D parabola)
  - It has exactly one min value
    - And we can see it
- Intuition
  - If the plot was a real object (say, a sheet of some sort), we could slide a ball bearing on it
  - After a while, the ball bearing will settle at the “bottom” due to gravity
  - We can "simulate" this: **gradient descent**
- Reminder: gradient
  - "Multi-dimensional derivative"

$$\nabla J = \begin{pmatrix} \frac{\partial J}{\partial a} \\ \\ \frac{\partial J}{\partial b} \end{pmatrix}$$

Gradient Descent (2)

- Iterative algorithm – perform as long as needed
  - Start from some point in the $(a; b)$ space: $(a_0; b_0)$
  - Decide how big steps to take: number α
    - Called learning rate in ML terminology
  - Use the current a, b and x, y to compute ∇J
    - $-\nabla J_a$ tells us how much to move in the a direction in order to get to the minimum
    - Similar for $-\nabla J_b$
  - Take a step with size α in each direction
    - $a_1 = a_0 - \alpha \nabla J_a; b_1 = b_0 - \alpha \nabla J_b$
    - $(a_1; b_1)$ are the new coordinates
  - Repeat the two preceding steps as needed
    - Usually, we do this for a fixed number of iterations

Example: Housing Prices

- Multiple linear regression
  - Many predictor variables
- Let's use this model to try and predict housing prices (a classical dataset located here)

```
housing.columns = ["crime_rate", "zoned_land", "industry", "bounds_river",
"nox_conc", "rooms", "age", "distance",  "highways", "tax", "pt_ratio",
"b_estimator", "pop_status", "price"]
```

- First, we want to explore the datasets
  - A more thorough exploration is "left as an exercise to the reader"
  - But we want to see what model would be appropriate
    - In addition to usual data analysis techniques, let's plot all correlations between any pair of features

Creating a Model

- Modelling is very simple
  - Like in the 2D example

```
housing_model = LinearRegression()
predictor_attributes = housing.drop("price", axis = 1)
housing_model.fit(predictor_attributes, housing.price)
print(housing_model.coef_)
print(housing_model.intercept_)
```

- So what?
  - We might want to predict some prices
  - Let's just pass some random rows and see the result
  - **Note: Never test on the training dataset!**

```
test_houses = housing.sample(10)
predicted = housing_model.predict(
  test_houses.drop("price", axis = 1))
print(predicted)
print(test_houses.price)
```

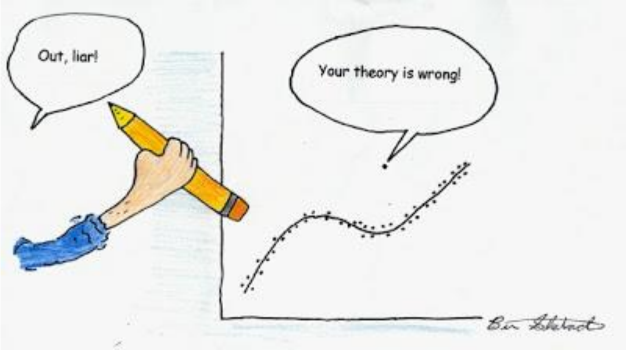
Delving Deeper into Matrices

- Dataset: $y = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \\ \vdots \\ y_n \end{bmatrix}; X = \begin{array}{cl} \begin{bmatrix} 1 & x_{11} & x_{12} & \cdots & x_{1m} \\ 1 & x_{21} & x_{22} & \cdots & x_{2m} \\ 1 & x_{31} & x_{32} & \cdots & x_{3m} \\ 1 & x_{41} & x_{42} & \cdots & x_{4m} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_{n1} & x_{n2} & \cdots & x_{nm} \end{bmatrix} & \text{third observation} \\ \text{second variable} & \end{array}$

- Parameters: $a = \begin{bmatrix} a_0 \\ a_1 \\ \vdots \\ a_m \end{bmatrix}$

- Modelling function: $\tilde{y} = Xa$

Regression with Outliers



- As we saw, the data has outliers
  - A few points which are far from the others
- Our goal is to exclude outliers
  - There are several methods
  - One very common – RANSAC (**RAN**dom **SA**mple **C**onsensus)
- Algorithm
  1. Fit a model to a random subsample ("inliers")
  2. Test all data points and include those which are "near" the model
     - Small enough error, tolerance provided by developer
  3. Fit the model again
  4. Estimate the error of the model (difference between first and second)
  5. Iterate steps 1-4 until performance reaches a threshold or number of iterations

Lab: RANSAC on the Housing Dataset

- Usage: similar to the linear regression model

```
from sklearn.linear_model import RANSACRegressor
ransac = RANSACRegressor()
ransac.fit(housing.drop("price", axis = 1), housing.price)
print(ransac.estimator_.coef_, ransac.estimator_.intercept_)
```

- We can also provide parameters, e.g. min number of random samples, max iterations, threshold (to include data points)
  - We can also provide the type of model we want to perform RANSAC on
    - Linear regression by default but we may use other regression models

```
ransac = RANSACRegressor(LinearRegression(), min_samples = 50,
 max_trials = 100, residual_threshold = 5.0)
```

- View inliers and outliers

```
inliers = housing[ransac.inlier_mask_]
outliers = housing[~ranplt.scatter(inliers.rooms, inliers.price)
plt.scatter(outliers.rooms, outliers.price)
sac.inlier_mask_]
```

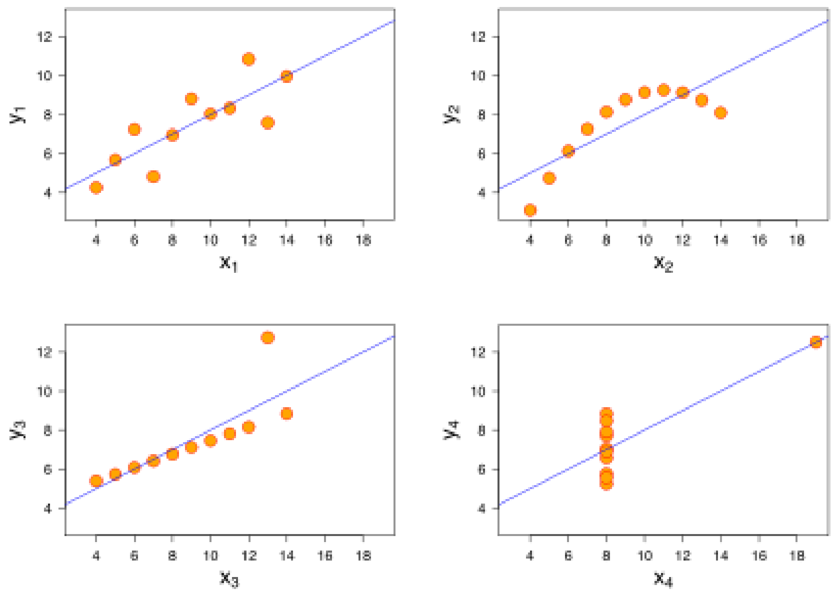
Polynomial Regression

- Extension of the linear regression algorithm
  - We can use the linear regression algorithm to perform polynomial regression (e.g. fitting a quadratic curve)
    - Just precompute the columns
    - Example: if we have columns x, y and z, compute `x * z, y * z, x * z` and perform linear regression on these 6 features
    - Example 2: polynomial terms: multiply x by itself: `x * x`, `x * x * x`, etc.
- This can be achieved easily with `scikit-learn`

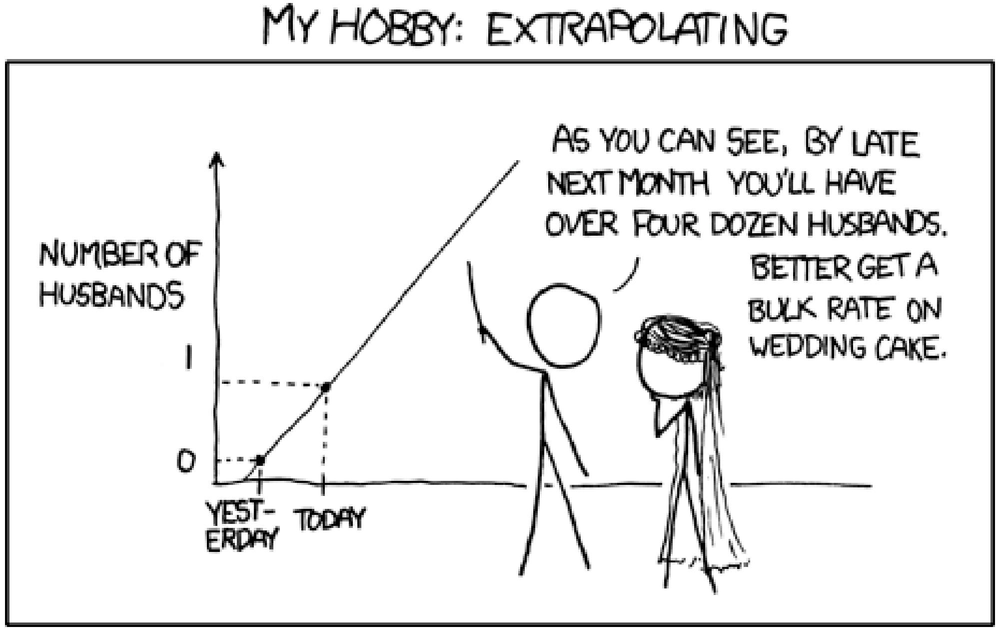
```
from sklearn.preprocessing import PolynomialFeatures

x = np.arange(6).reshape(3, 2)
poly = PolynomialFeatures(2)
x_transformed = poly.fit_transform(x)
print(poly.get_feature_names())
print(poly.n_input_features_)
print(poly.n_output_features_)
# Now we can perform linear regression with x_transformed as the input
```

Common Mistakes

- There are two main types of errors we can make while trying regression models
  - Use a **wrong model**
    - Anscombe's quartet



  - **Extrapolate** without knowing (especially if we have interacting features)



Logistic Regression

Use a regression model to classify

Classification

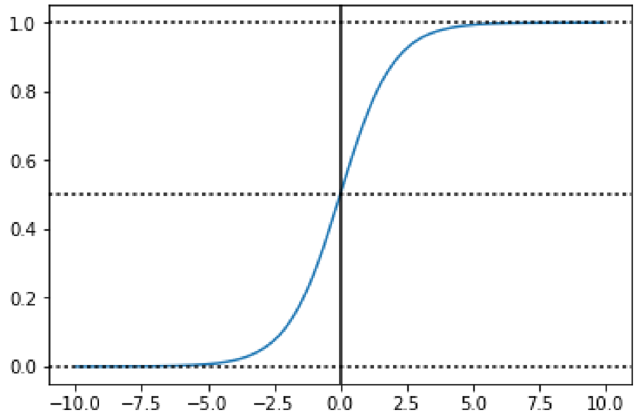
- Predict **one of several known classes**
  - Based on the input parameters
  - Example: classify whether a picture is of a cat or a dog
- Regression and classification make up most of the machine learning problems
- Choosing an algorithm
  - "No free lunch": **no single algorithm** works best
  - It's best to compare some algorithms to select the best for a particular model
    - Also, we might want to tune them first
- Reminder: ML process
  - Select features, choose a performance metric (cost function), choose a classifier, evaluate and fine-tune the performance

Logistic Regression

- Classification algorithm (despite its name)
- Two classes: negative (0) and positive (1)
  - Can be extended to more classes
- How does it work?
  - Linear regression can give us all kinds of values
  - We want to constrain them between 0 and 1
  - Approach
    - Perform linear regression: $\tilde{y} = \vec{a}x$
    - Use the sigmoid function to constrain the output:

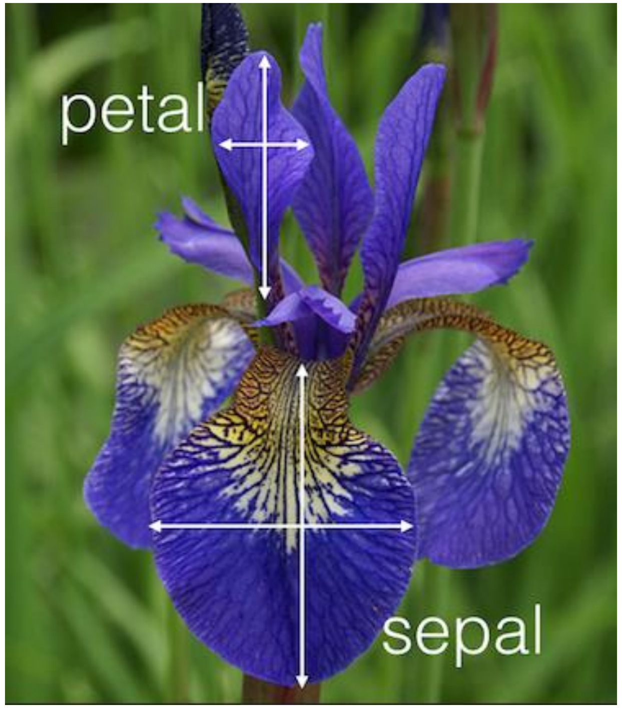
$$\sigma(\tilde{y}) = \frac{1}{1 + e^{-\tilde{y}}} = \frac{1}{1 + e^{-\vec{a}x}}$$

    - Quantization: if $\sigma > 0.5$ return 1, and 0 otherwise
      - Remember that we only need to return 0 or 1
      - We can also use the raw values as probability measures



Example: Classifying Iris Flowers

- A classic dataset for classification is the Iris dataset
  - Located here
  - **3 classes** (setosa, virginica, versicolor)
  - **4 attributes**: petal width / height; sepal width / height (all in cm)
    - Some features are highly correlated to the class
  - Explore and inspect the data before modelling



Example: Classifying Iris Flowers (2)

- Perform logistic regression

```
from sklearn.linear_model import LogisticRegression
model = LogisticRegression(C = 1e6)
model.fit(iris_train_data, iris_train_labels)
```

- Test (output classes or probabilities)

```
print(model.predict(iris_test))
print(model.predict_proba(iris_test))
```

- In the model, there's a "mysterious" parameter `C`
  - Regularization: how powerful the data is (more – next time)
  - A large number means no regularization
    - We just take the data "as-is", with no other constraints

Many Classes

- Two main approaches
  - One-vs-all: several predictors
    - One predictor for each class vs. the others
  - Overall: calculate probabilities of each class
- `scikit-learn` takes care of multiple classes (multinomial logistic regression) by default
  - We don't even need to transform the labels
  - This applies to all algorithms in the library

Summary

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Questions?