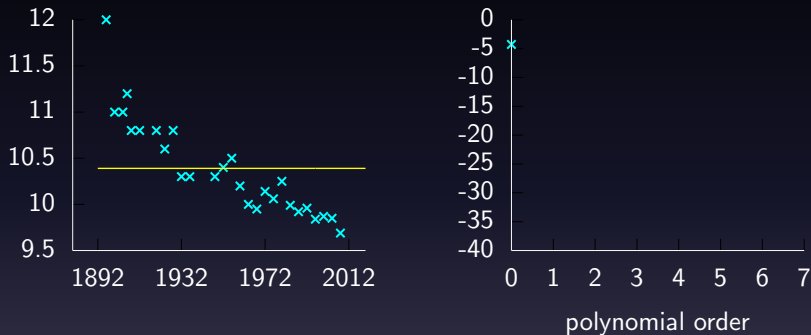# Generalization

MLAI Lecture 7

Neil D. Lawrence

Department of Computer Science
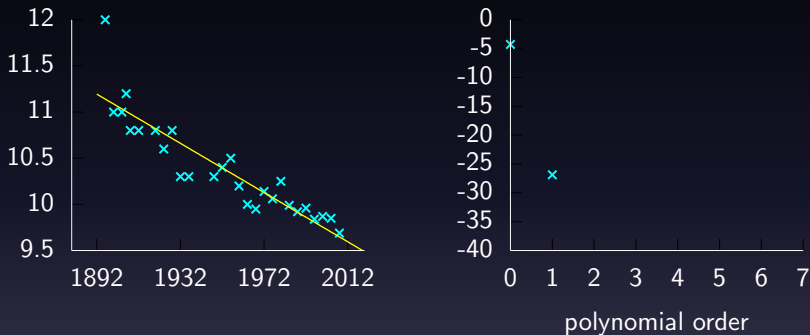Sheffield University

9th October 2012

Generalization

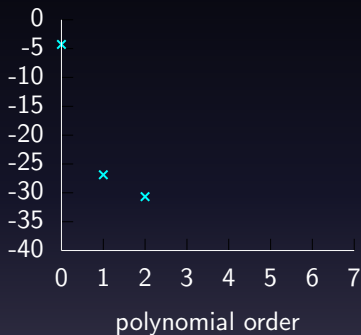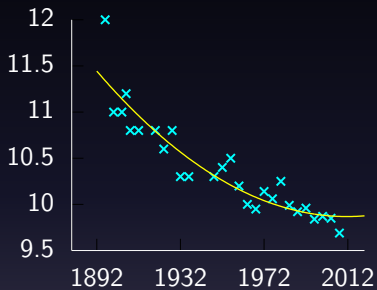# Polynomial Fits to Olympics Data

Left: fit to data, *Right*: model error. Polynomial order 0, model error -4.2717, $\sigma^2 = 0.268$, $\sigma = 0.518$.
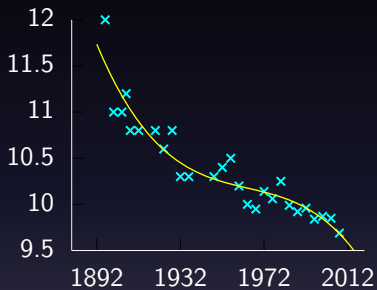
Polynomial Fits to Olympics Data

Left: fit to data, *Right*: model error. Polynomial order 1, model error -26.86, $\sigma^2 = 0.0503$, $\sigma = 0.224$.
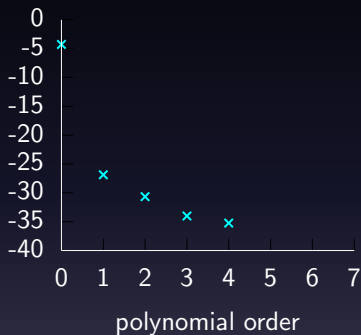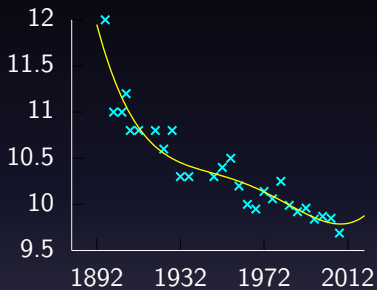
Polynomial Fits to Olympics Data

Left: fit to data, *Right*: model error. Polynomial order 2, model error -30.662, $\sigma^2 = 0.0380$, $\sigma = 0.195$.

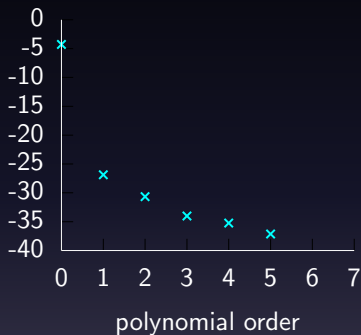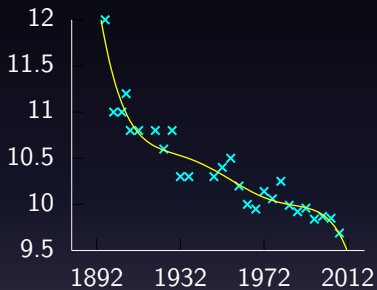# Polynomial Fits to Olympics Data

Left: fit to data, *Right*: model error. Polynomial order 3, model error -34.015, $\sigma^2 = 0.0296$, $\sigma = 0.172$.

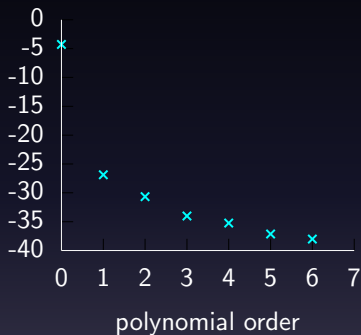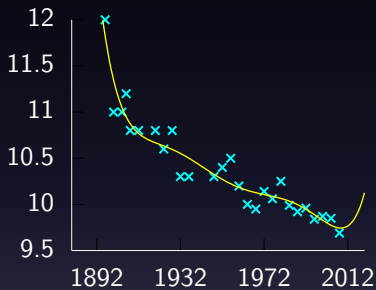# Polynomial Fits to Olympics Data

Left: fit to data, *Right*: model error. Polynomial order 4, model error -35.231, $\sigma^2 = 0.0271$, $\sigma = 0.165$.

Polynomial Fits to Olympics Data

Left: fit to data, *Right*: model error. Polynomial order 5, model error -37.138, $\sigma^2 = 0.0235$, $\sigma = 0.153$.

Polynomial Fits to Olympics Data

Left: fit to data, *Right*: model error. Polynomial order 6, model error -38.016, $\sigma^2 = 0.0220$, $\sigma = 0.148$.

- Increase number of basis functions, we obtain a better 'fit' to the data.
- How will the model perform on previously unseen data?

Training and Test Sets

- We call the data used for fitting the model the 'training set'.
- Data not used for training, but when the model is applied 'in the field' is called the 'test data'.
- Challenge for generalization is to ensure a good performance on test data given only training data.
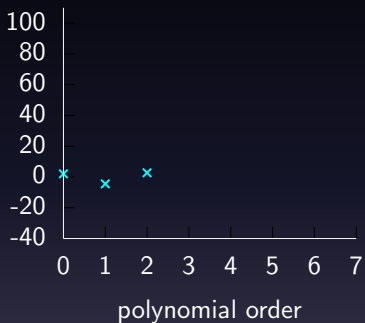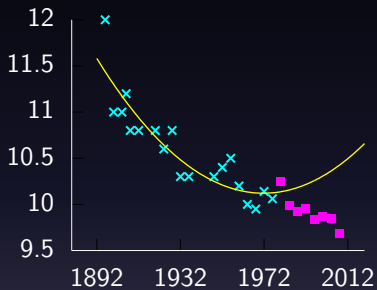
Validation Set
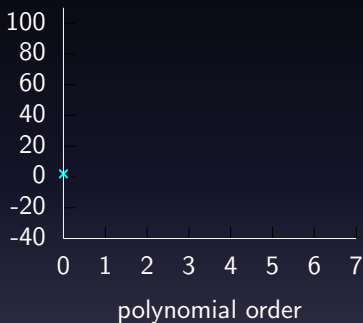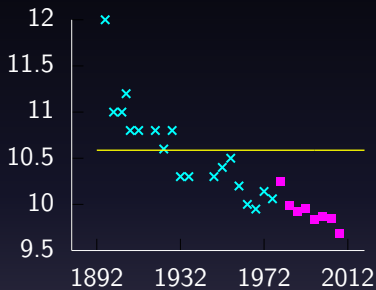
Left: fit to data, *Right*: model error. Polynomial order 0, training error 2.0524, validation error 2.0524, $\sigma^2 = 0.240$, $\sigma = 0.490$.
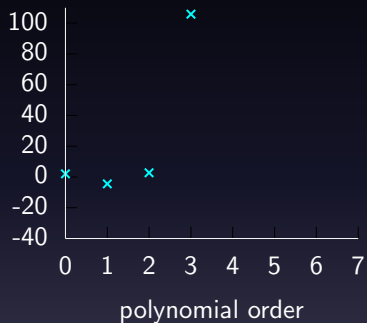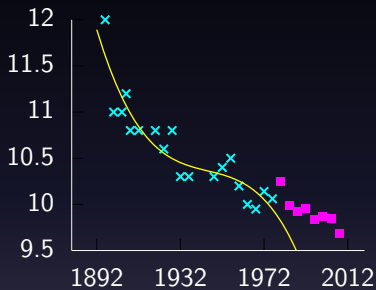
Validation Set
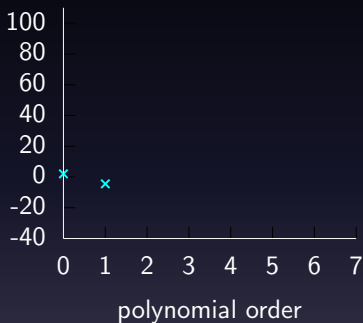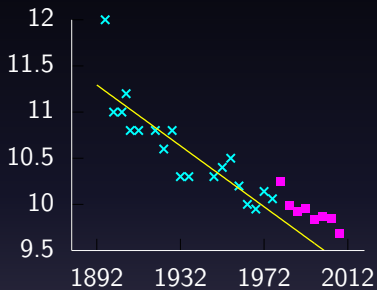
Left: fit to data, *Right*: model error. Polynomial order 1, training error -4.4127, validation error -4.4127, $\sigma^2 = 0.0582$, $\sigma = 0.241$.
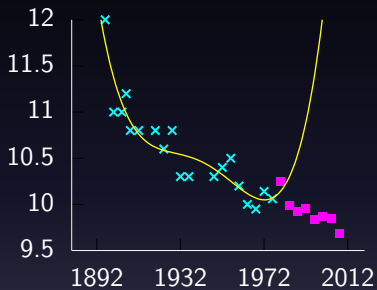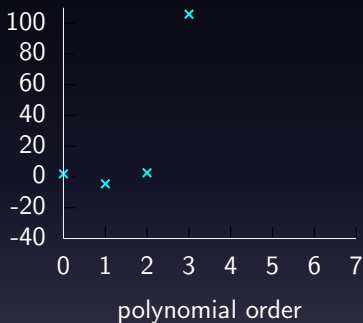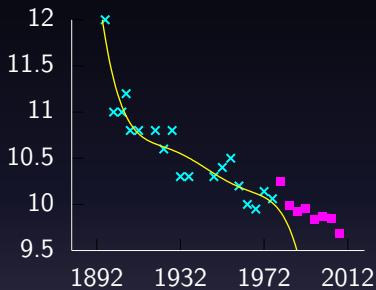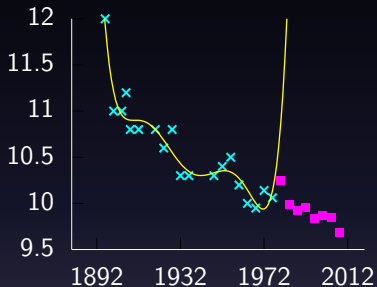
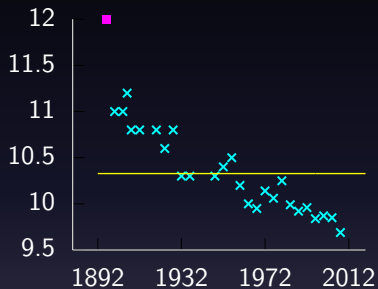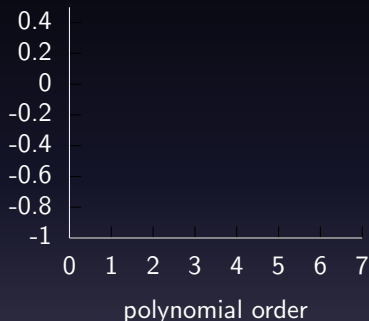# Validation Set

Left: fit to data, *Right*: model error. Polynomial order 2, training error 2.7275, validation error 2.7275, $\sigma^2 = 0.0441$, $\sigma = 0.210$.

Validation Set

Left: fit to data, *Right*: model error. Polynomial order 3, training error 105.8, validation error 105.8, $\sigma^2 = 0.0357$, $\sigma = 0.189$.

Validation Set

Left: fit to data, *Right*: model error. Polynomial order 4, training error 578.29, validation error 578.29, $\sigma^2 = 0.0301$, $\sigma = 0.173$.

Validation Set

Left: fit to data, *Right*: model error. Polynomial order 5, training error 746.57, validation error 746.57, $\sigma^2 = 0.0290$, $\sigma = 0.170$.

Left: fit to data, *Right*: model error. Polynomial order 6, training error 3.3585e+05, validation error 3.3585e+05, $\sigma^2 = 0.0183$, $\sigma = 0.135$.

Leave One Out Error

- Take training set and remove one point.
- Train on the remaining data.
- Compute the error on the point you removed (which wasn't in the training data).
- Do this for each point in the training set in turn.
- Average the resulting error. This is the leave one out error.

Leave One Out Error

Polynomial order 0, training error -4.1755, leave one out error -0.014727.
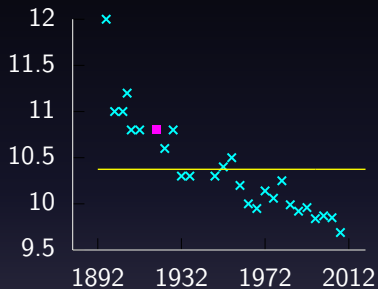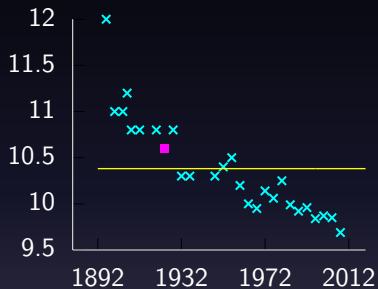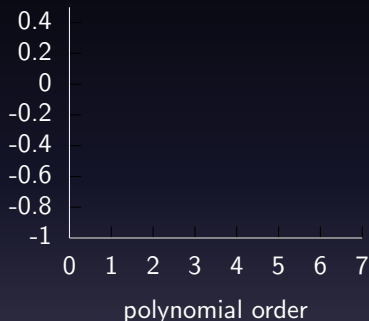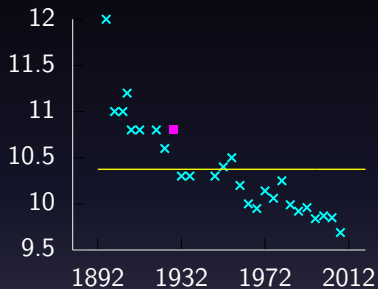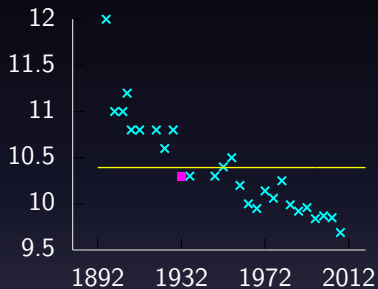
Leave One Out Error

Polynomial order 0, training error -4.1755, leave one out error -0.014727.
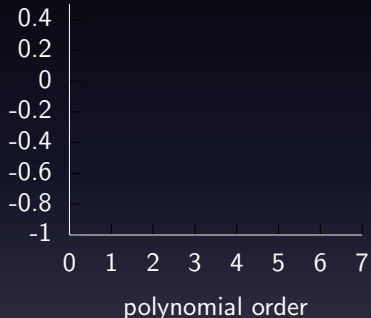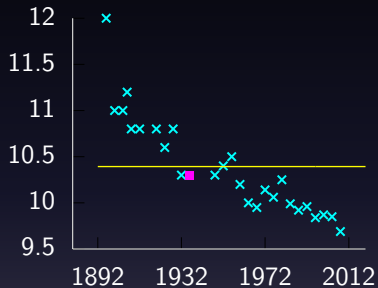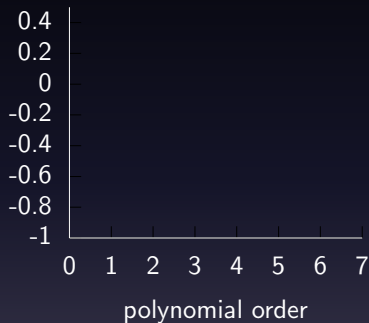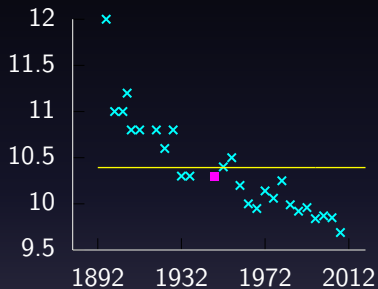
Leave One Out Error

Polynomial order 0, training error -4.1755, leave one out error -0.014727.

Leave One Out Error

Polynomial order 0, training error -4.1755, leave one out error -0.014727.
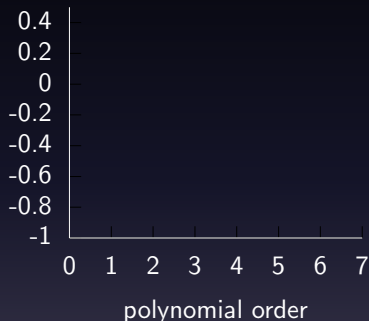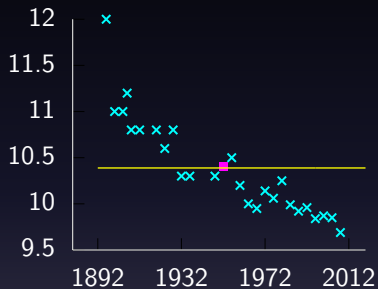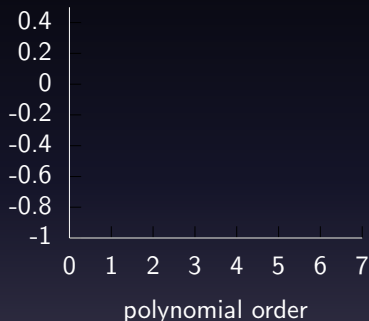
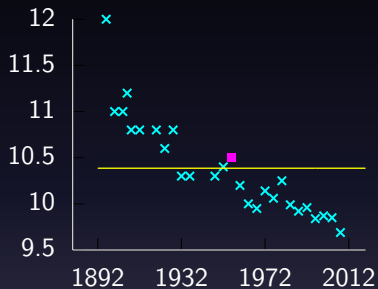# Leave One Out Error
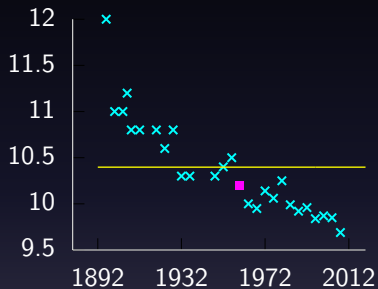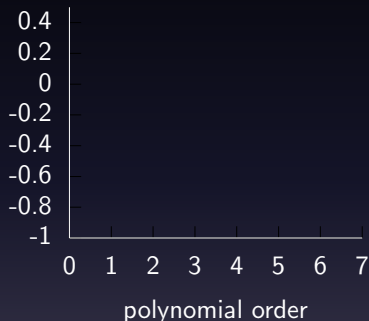

Polynomial order 0, training error -4.1755, leave one out error -0.014727.

Leave One Out Error
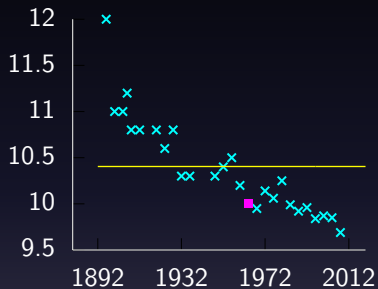

Polynomial order 0, training error -4.1755, leave one out error -0.014727.

Leave One Out Error
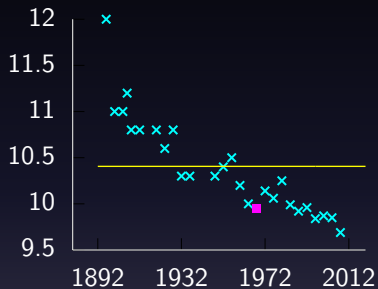

Polynomial order 0, training error -4.1755, leave one out error -0.014727.
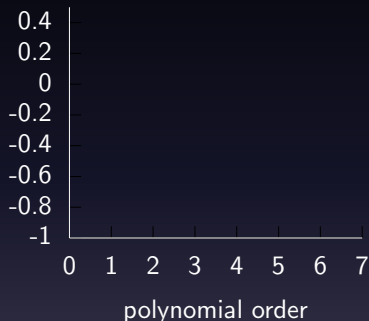
Leave One Out Error
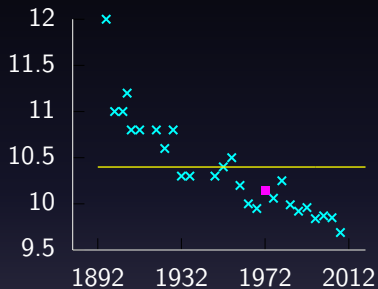

Polynomial order 0, training error -4.1755, leave one out error -0.014727.

Leave One Out Error

Polynomial order 0, training error -4.1755, leave one out error -0.014727.

Polynomial order 0, training error -4.1755, leave one out error -0.014727.

Leave One Out Error

Polynomial order 0, training error -4.1755, leave one out error -0.014727.
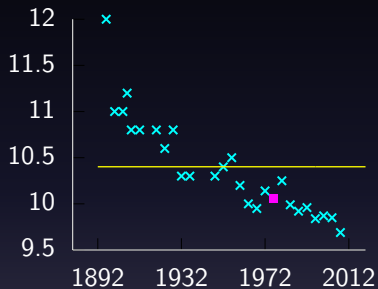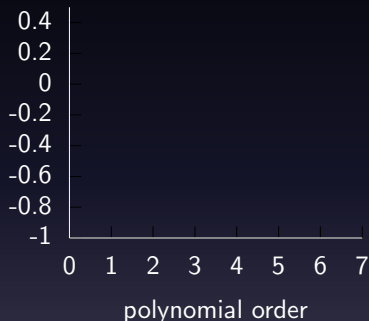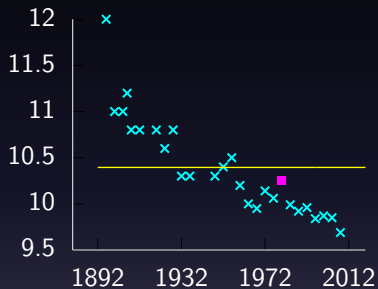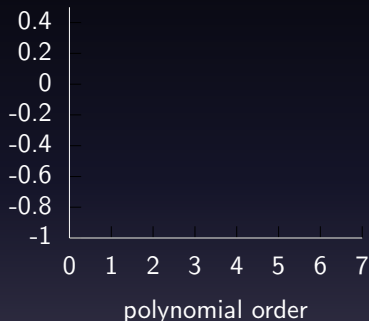
Leave One Out Error
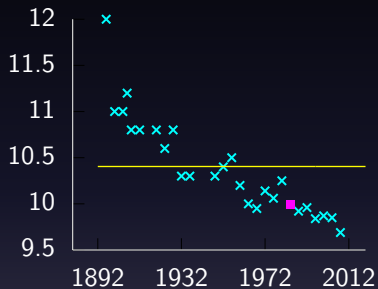

Polynomial order 0, training error -4.1755, leave one out error -0.014727.

Leave One Out Error

Polynomial order 0, training error -4.1755, leave one out error -0.014727.
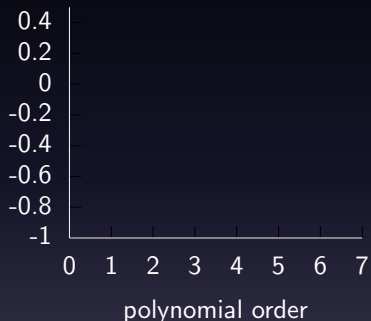
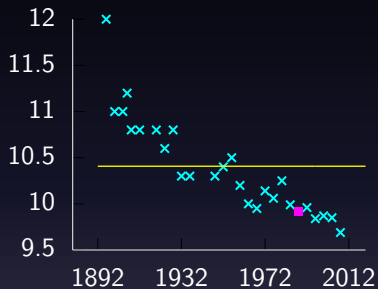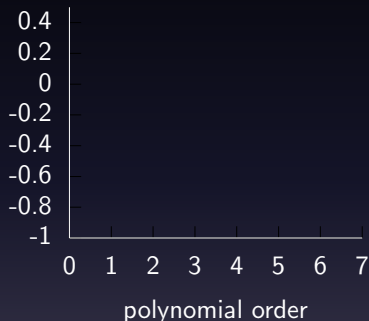# Leave One Out Error
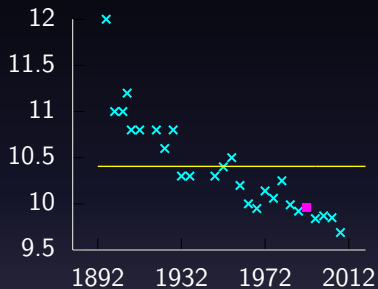

Polynomial order 0, training error -4.1755, leave one out error -0.014727.

Leave One Out Error

Polynomial order 0, training error -4.1755, leave one out error -0.014727.

Polynomial order 0, training error -4.1755, leave one out error -0.014727.
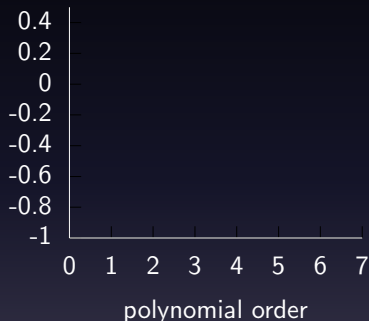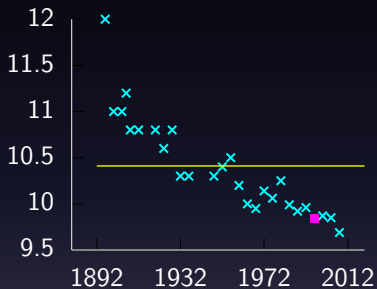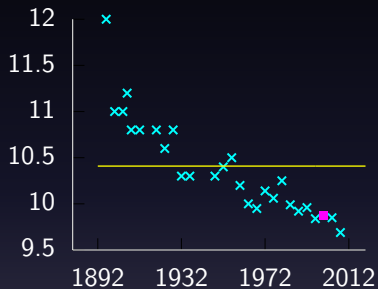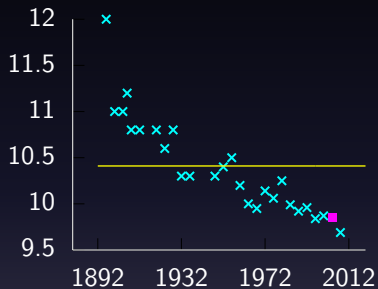
Polynomial order 0, training error -4.1755, leave one out error -0.014727.

Leave One Out Error

Polynomial order 0, training error -4.1755, leave one out error -0.014727.

Leave One Out Error

Polynomial order 0, training error -4.1755, leave one out error -0.014727.
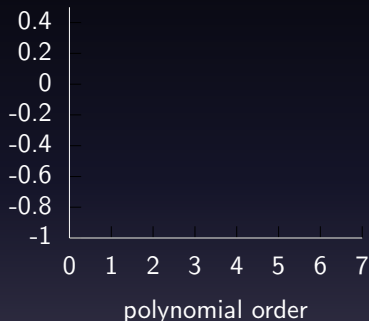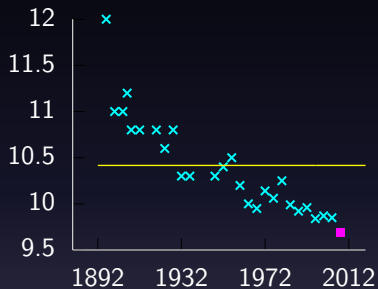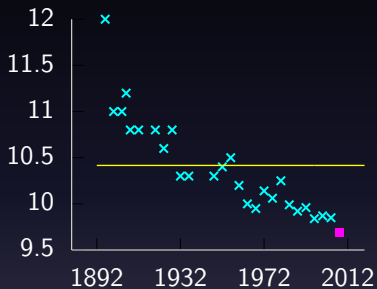
Polynomial order 0, training error -4.1755, leave one out error -0.014727.

Leave One Out Error

Polynomial order 0, training error -4.1755, leave one out error -0.014727.
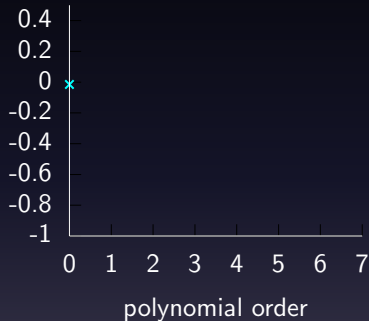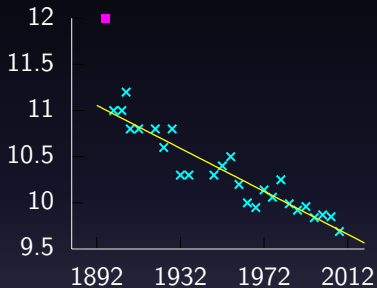
Leave One Out Error

Polynomial order 0, training error -4.1755, leave one out error -0.014727.

Leave One Out Error

Polynomial order 0, training error -4.1755, leave one out error -0.014727.
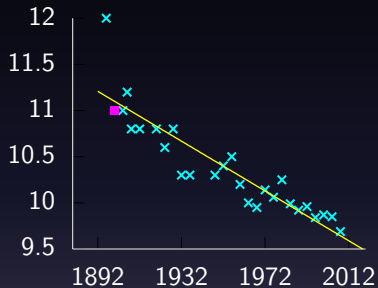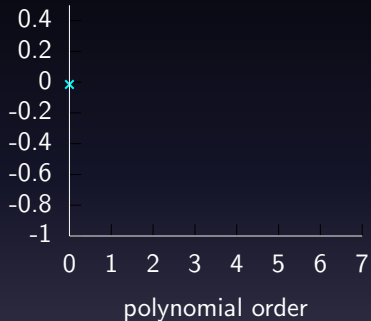
Leave One Out Error

Polynomial order 0, training error -4.1755, leave one out error -0.014727.

Leave One Out Error

Polynomial order 0, training error -4.1755, leave one out error -0.014727.
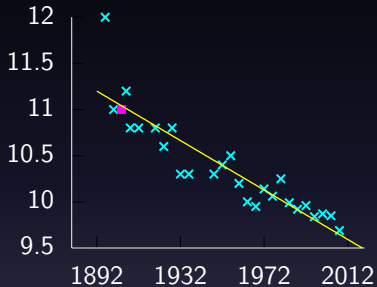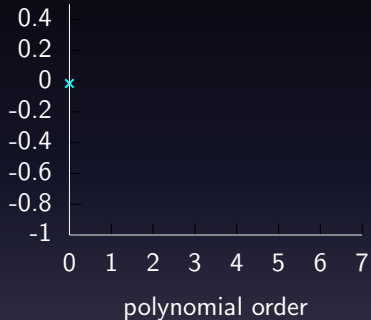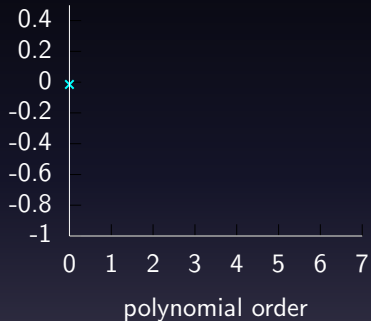
Leave One Out Error

Polynomial order 0, training error -4.1755, leave one out error -0.014727.

Leave One Out Error

Polynomial order 0, training error -4.1755, leave one out error -0.014727.

Polynomial order 0, training error -4.1755, leave one out error
-0.014727.

Polynomial order 1, training error -26.089, leave one out error -0.30898.

Polynomial order 1, training error -26.089, leave one out error -0.30898.
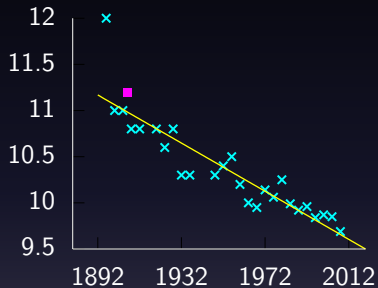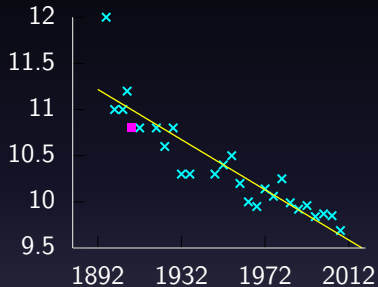
Leave One Out Error

Polynomial order 1, training error -26.089, leave one out error -0.30898.
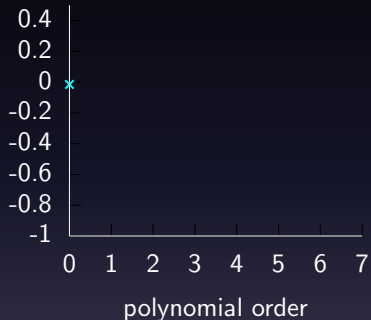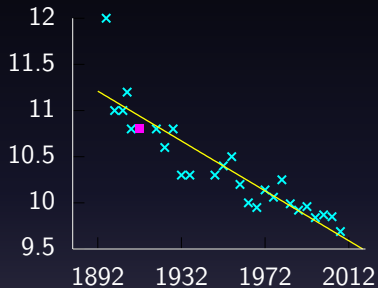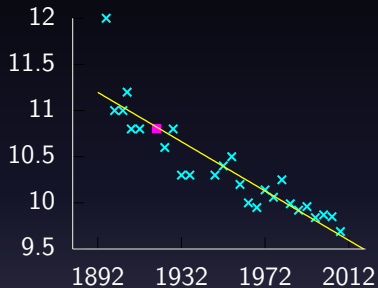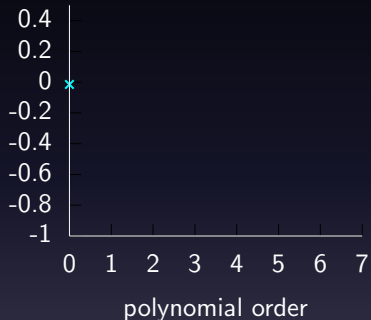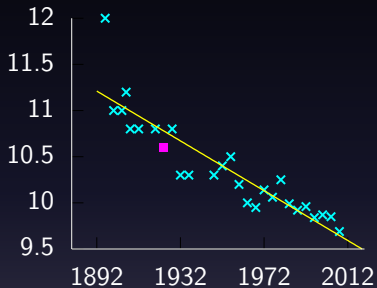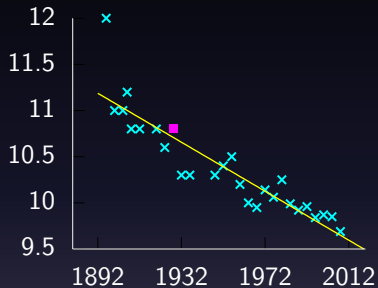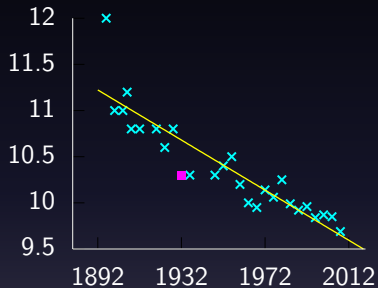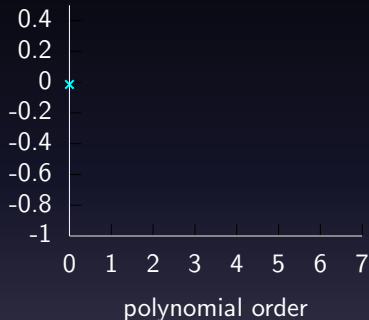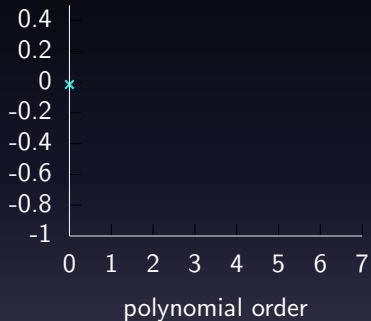
Leave One Out Error

Polynomial order 1, training error -26.089, leave one out error -0.30898.

Leave One Out Error

Polynomial order 1, training error -26.089, leave one out error -0.30898.
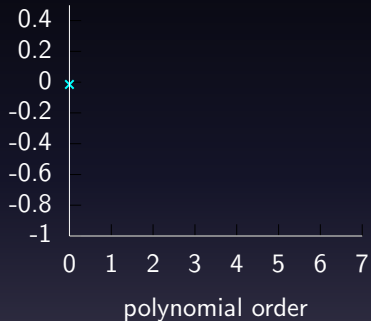
Leave One Out Error
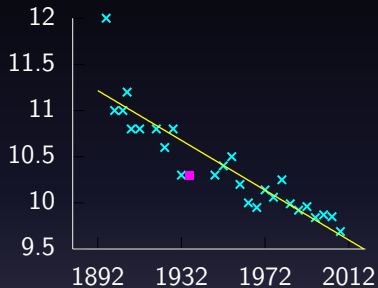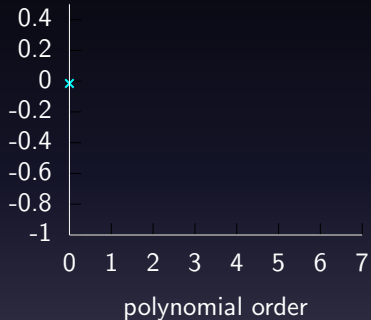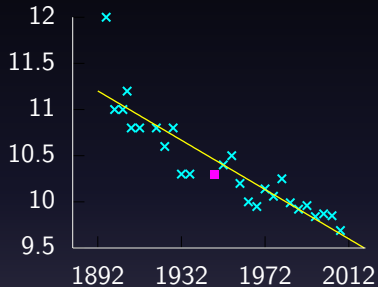

Polynomial order 1, training error -26.089, leave one out error -0.30898.

Leave One Out Error
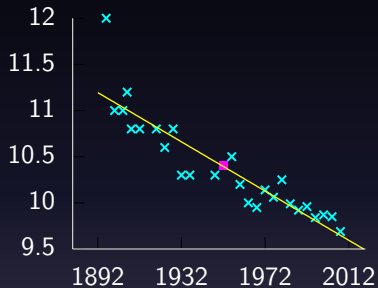

Polynomial order 1, training error -26.089, leave one out error -0.30898.

Leave One Out Error
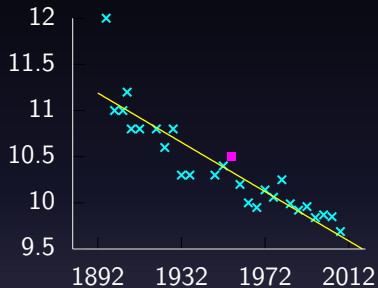

Polynomial order 1, training error -26.089, leave one out error -0.30898.

Leave One Out Error

Polynomial order 1, training error -26.089, leave one out error -0.30898.

Leave One Out Error

Polynomial order 1, training error -26.089, leave one out error -0.30898.

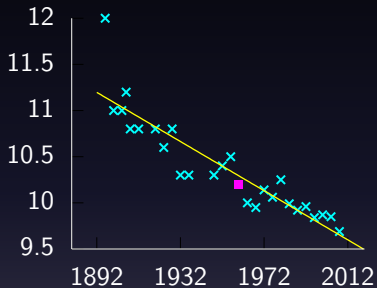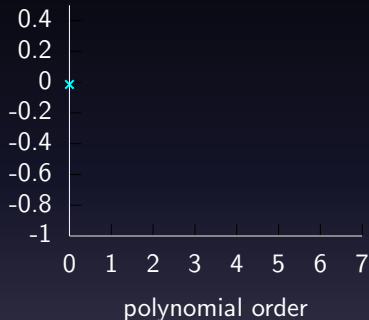# Leave One Out Error

Polynomial order 1, training error -26.089, leave one out error -0.30898.

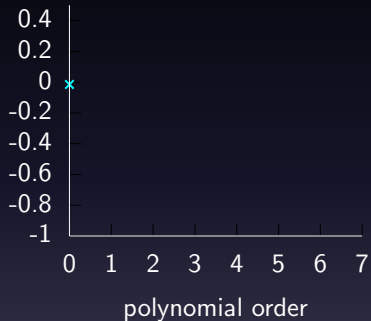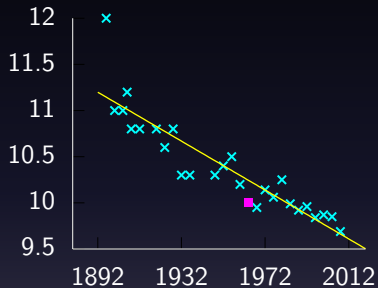# Leave One Out Error

Polynomial order 1, training error -26.089, leave one out error -0.30898.

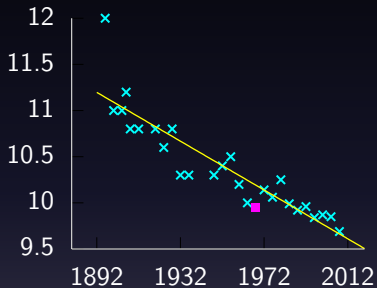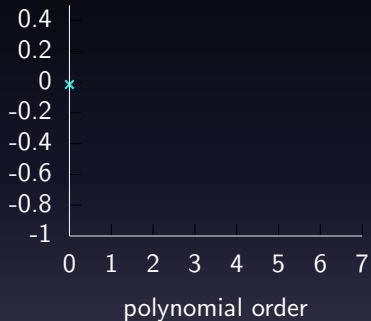# Leave One Out Error

Polynomial order 1, training error -26.089, leave one out error -0.30898.

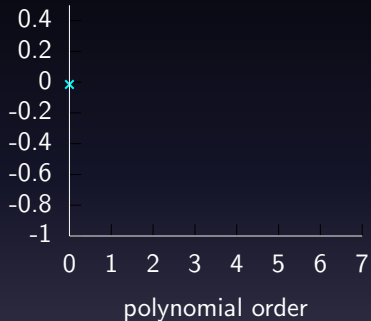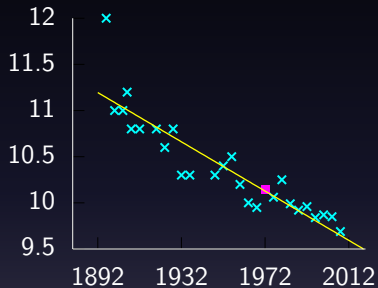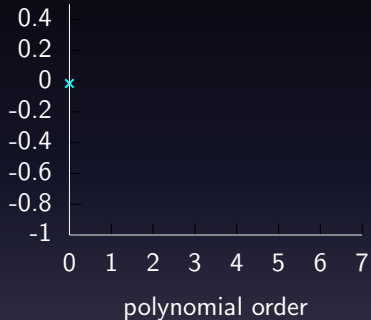# Leave One Out Error
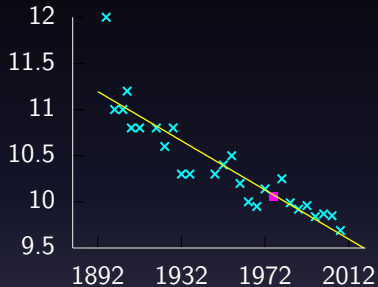

Polynomial order 1, training error -26.089, leave one out error -0.30898.

Leave One Out Error

Polynomial order 1, training error -26.089, leave one out error -0.30898.

Leave One Out Error

Polynomial order 1, training error -26.089, leave one out error -0.30898.
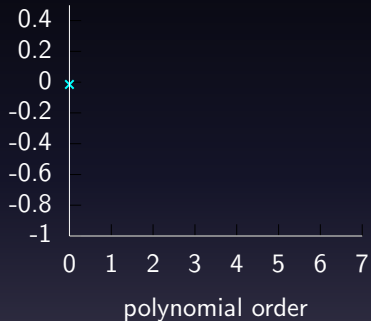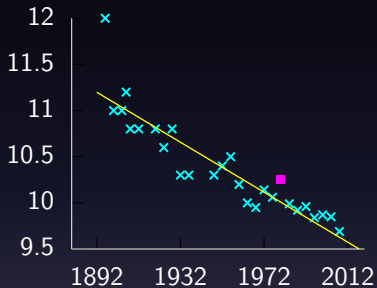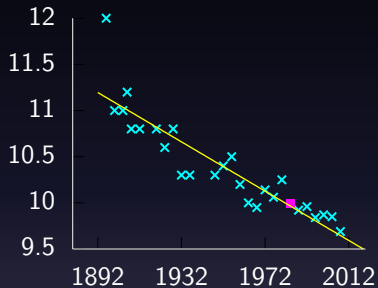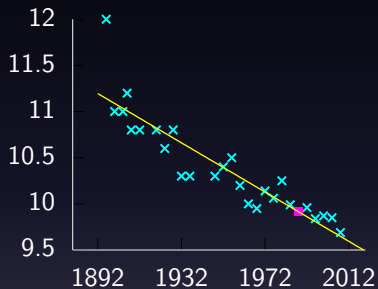
Leave One Out Error

Polynomial order 1, training error -26.089, leave one out error -0.30898.

Leave One Out Error

Polynomial order 1, training error -26.089, leave one out error -0.30898.
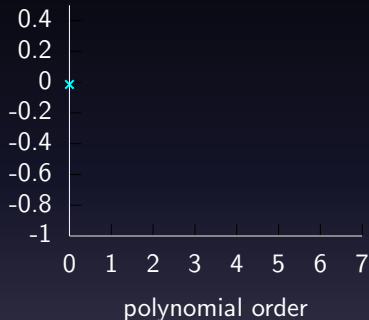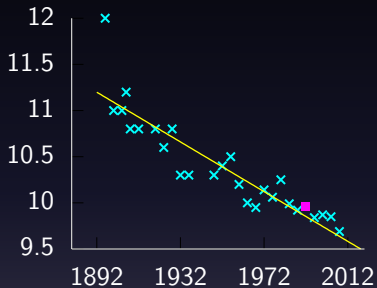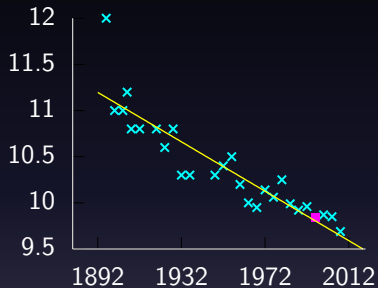
Leave One Out Error

Polynomial order 1, training error -26.089, leave one out error -0.30898.

Leave One Out Error

Polynomial order 1, training error -26.089, leave one out error -0.30898.

Leave One Out Error

Polynomial order 1, training error -26.089, leave one out error -0.30898.

Leave One Out Error

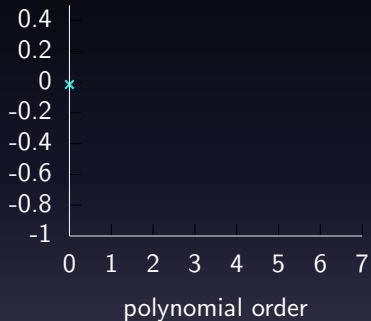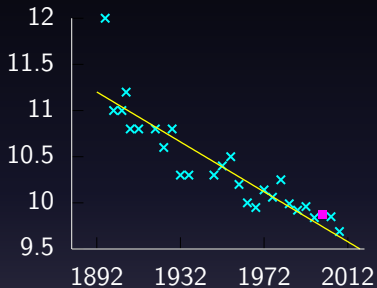Polynomial order 1, training error -26.089, leave one out error -0.30898.
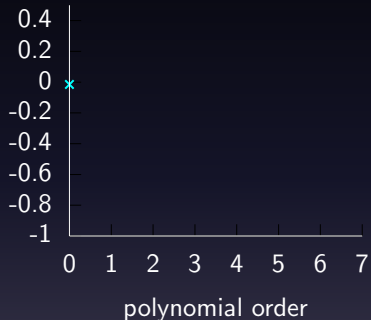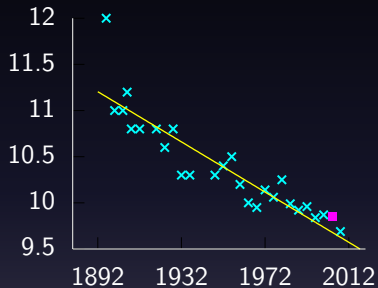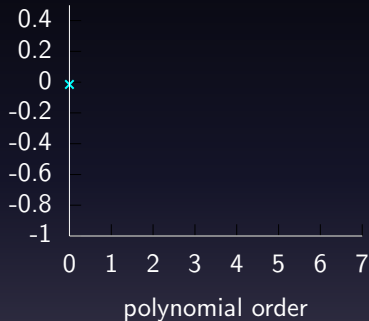
Leave One Out Error

Polynomial order 1, training error -26.089, leave one out error -0.30898.
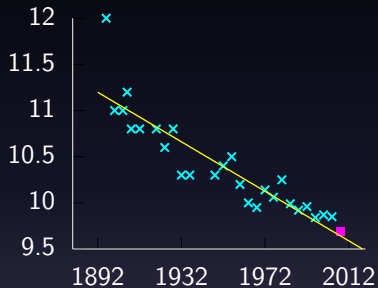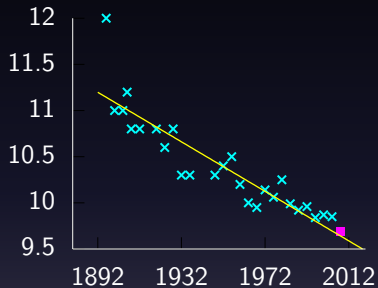
Leave One Out Error

Polynomial order 1, training error -26.089, leave one out error -0.30898.

Leave One Out Error

Polynomial order 1, training error -26.089, leave one out error -0.30898.

Leave One Out Error

Polynomial order 1, training error -26.089, leave one out error -0.30898.
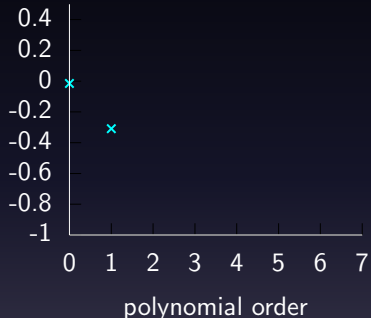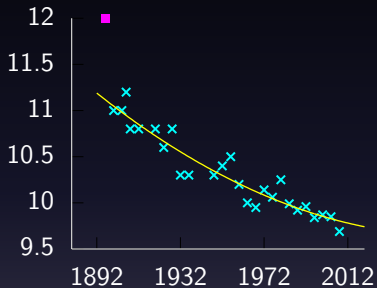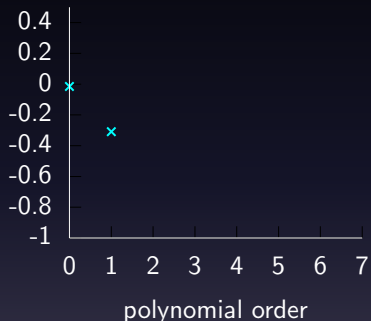
Leave One Out Error

Polynomial order 1, training error -26.089, leave one out error -0.30898.
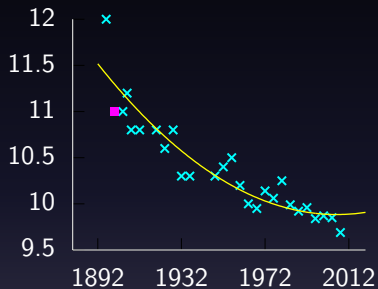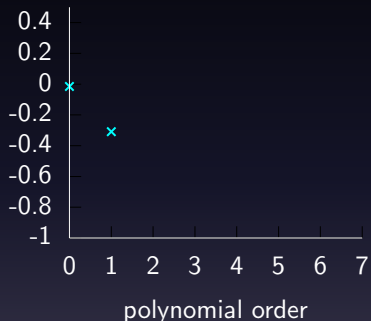
Polynomial order 1, training error -26.089, leave one out error -0.30898.

Leave One Out Error

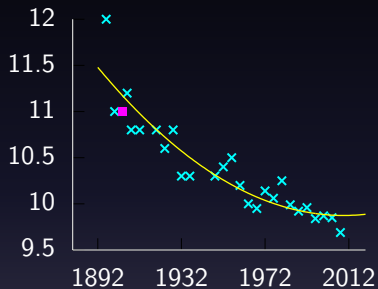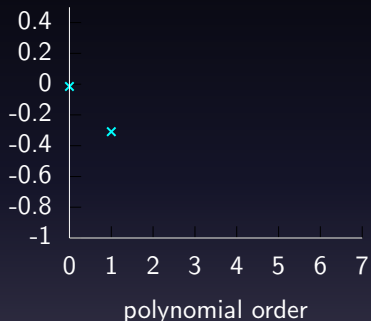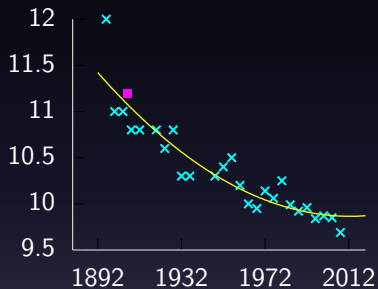Polynomial order 2, training error -29.761, leave one out error -0.4251.

Polynomial order 2, training error -29.761, leave one out error -0.4251.

Leave One Out Error

Polynomial order 2, training error -29.761, leave one out error -0.4251.
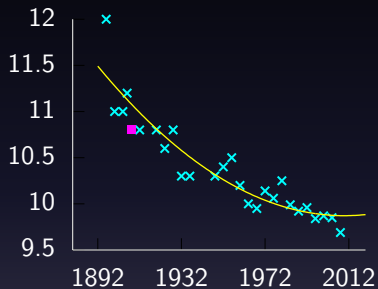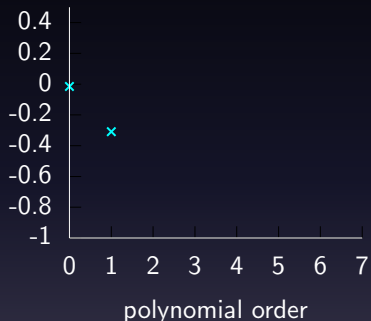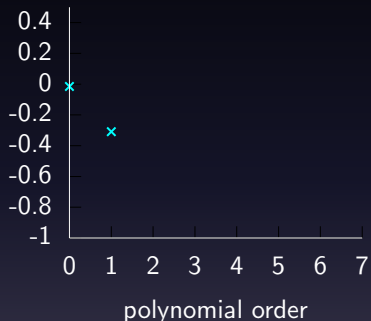
Leave One Out Error

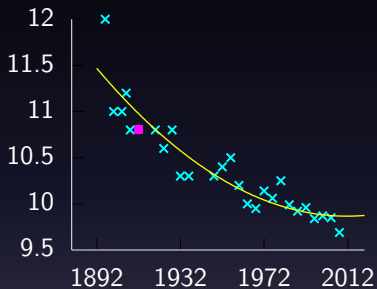Polynomial order 2, training error -29.761, leave one out error -0.4251.

Polynomial order 2, training error -29.761, leave one out error -0.4251.

Leave One Out Error

Polynomial order 2, training error -29.761, leave one out error -0.4251.

Polynomial order 2, training error -29.761, leave one out error -0.4251.

Leave One Out Error

Polynomial order 2, training error -29.761, leave one out error -0.4251.
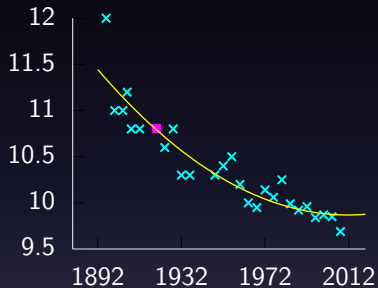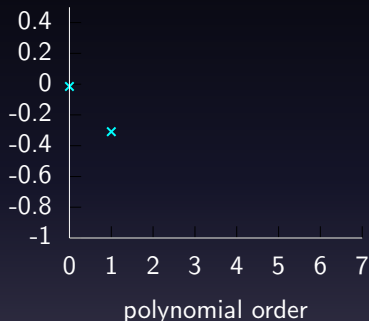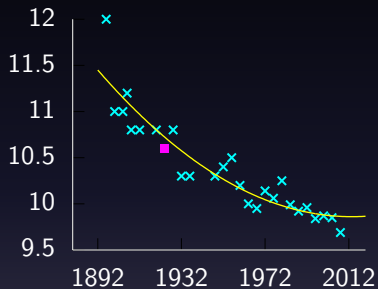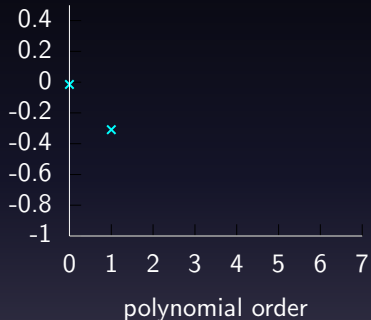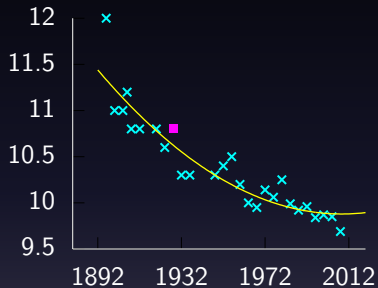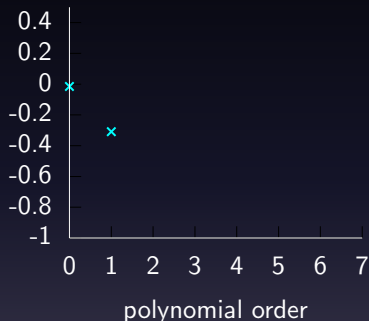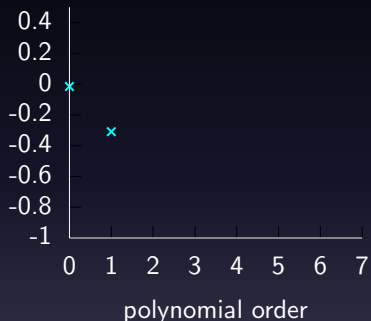
Leave One Out Error

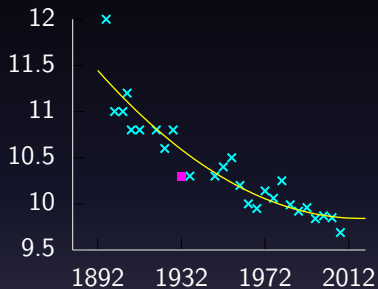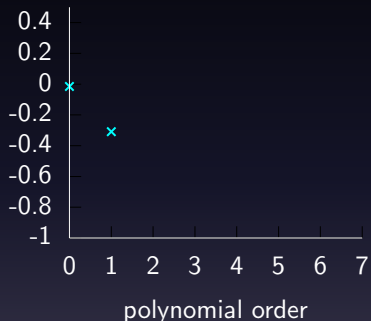Polynomial order 2, training error -29.761, leave one out error -0.4251.

Polynomial order 2, training error -29.761, leave one out error -0.4251.

Leave One Out Error

Polynomial order 2, training error -29.761, leave one out error -0.4251.

Polynomial order 2, training error -29.761, leave one out error -0.4251.
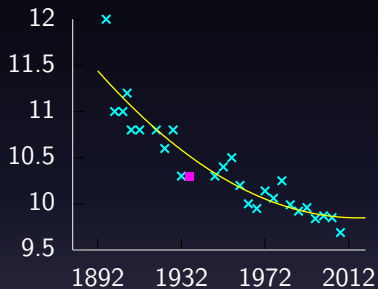
Polynomial order 2, training error -29.761, leave one out error -0.4251.

Leave One Out Error

Polynomial order 2, training error -29.761, leave one out error -0.4251.

Polynomial order 2, training error -29.761, leave one out error -0.4251.

Leave One Out Error

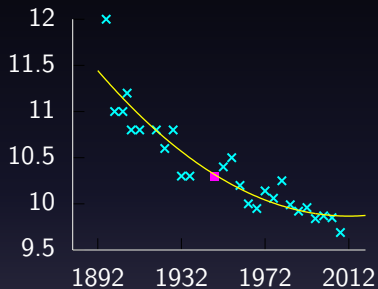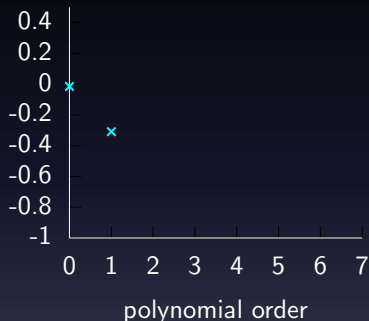Polynomial order 2, training error -29.761, leave one out error -0.4251.
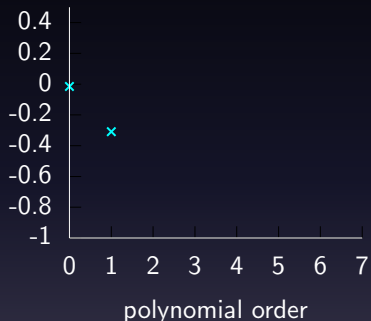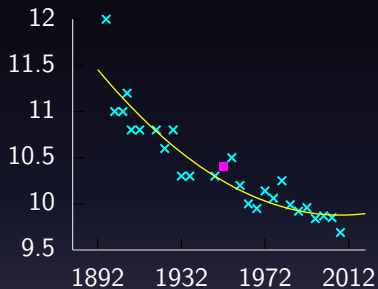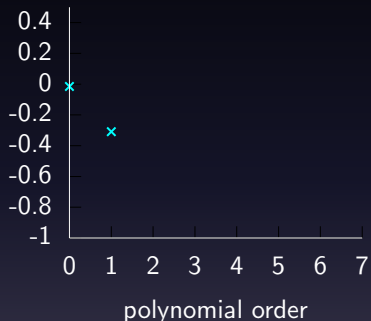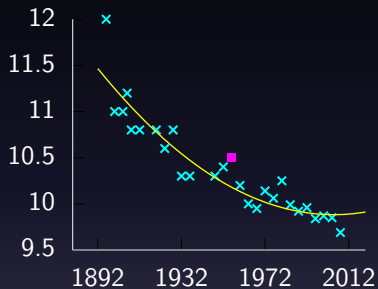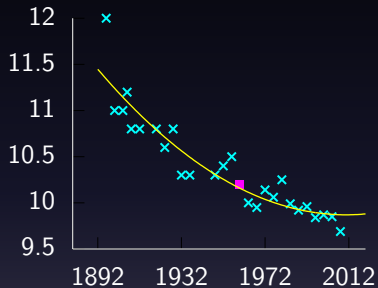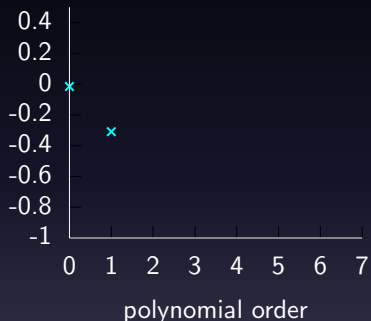
Leave One Out Error

Polynomial order 2, training error -29.761, leave one out error -0.4251.

Leave One Out Error

Polynomial order 2, training error -29.761, leave one out error -0.4251.

Leave One Out Error

Polynomial order 2, training error -29.761, leave one out error -0.4251.
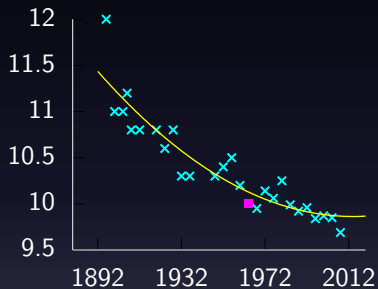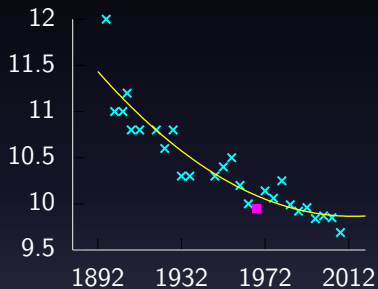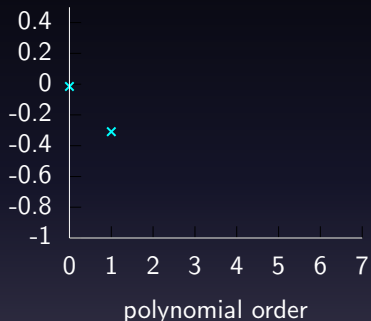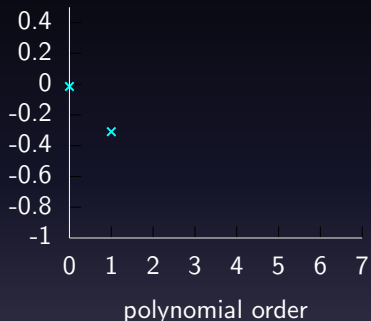
Leave One Out Error

Polynomial order 2, training error -29.761, leave one out error -0.4251.

Leave One Out Error

Polynomial order 2, training error -29.761, leave one out error -0.4251.
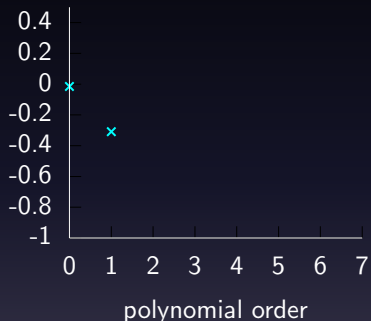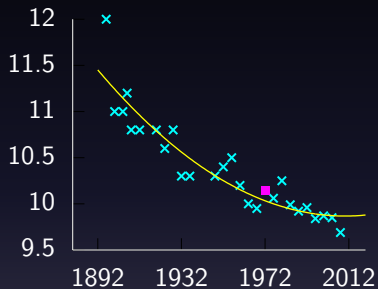
Leave One Out Error

Polynomial order 2, training error -29.761, leave one out error -0.4251.

Leave One Out Error

Polynomial order 2, training error -29.761, leave one out error -0.4251.
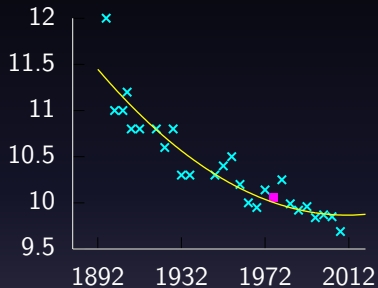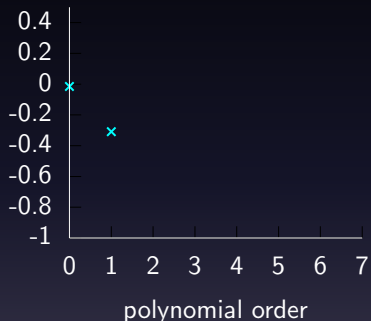
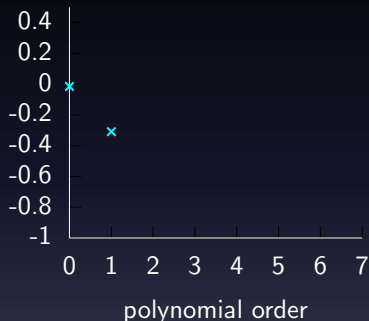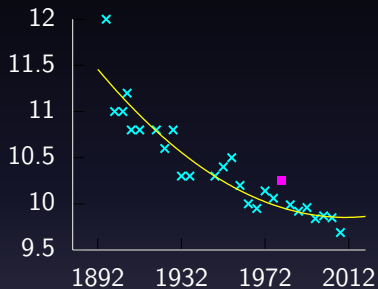# Leave One Out Error
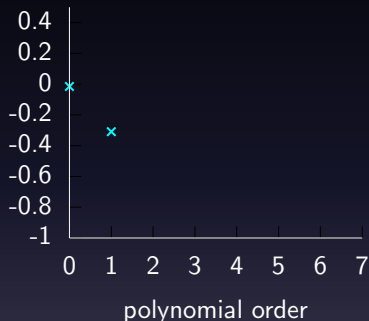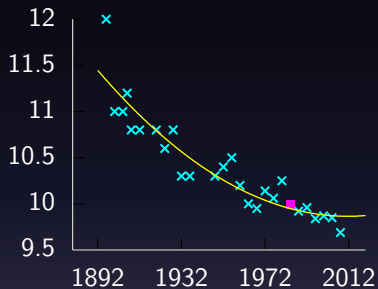

Polynomial order 2, training error -29.761, leave one out error -0.4251.

Leave One Out Error
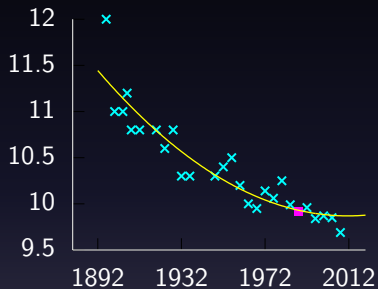

Polynomial order 2, training error -29.761, leave one out error -0.4251.

Leave One Out Error

Polynomial order 2, training error -29.761, leave one out error -0.4251.

Leave One Out Error

Polynomial order 2, training error -29.761, leave one out error -0.4251.

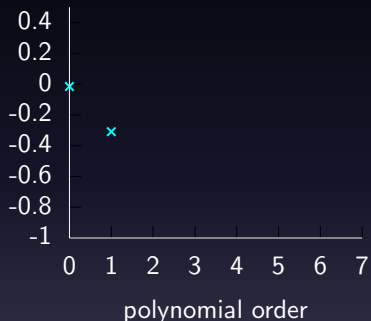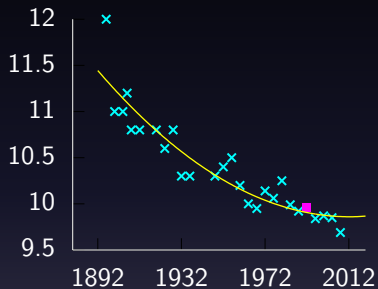# Leave One Out Error

Polynomial order 2, training error -29.761, leave one out error -0.4251.

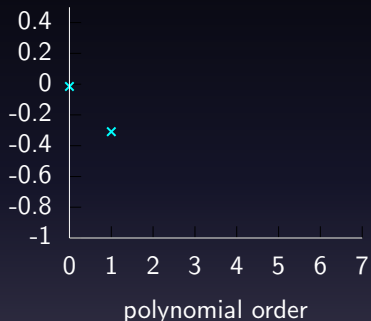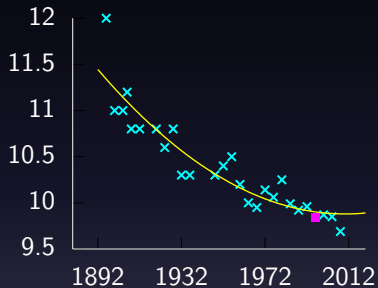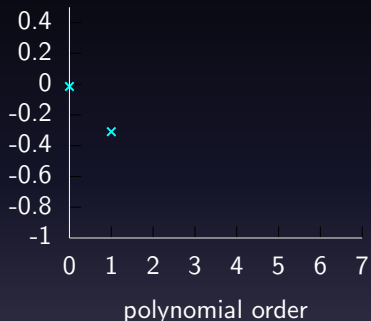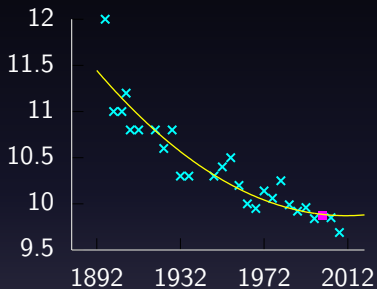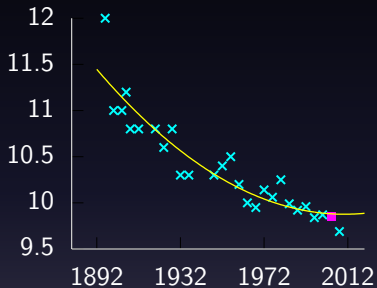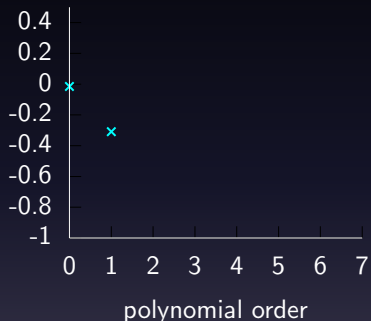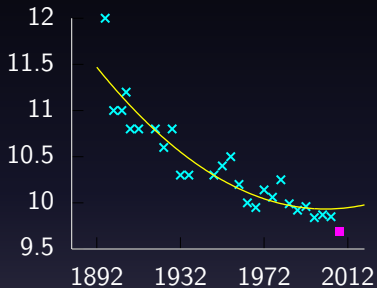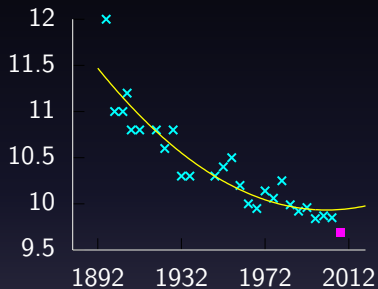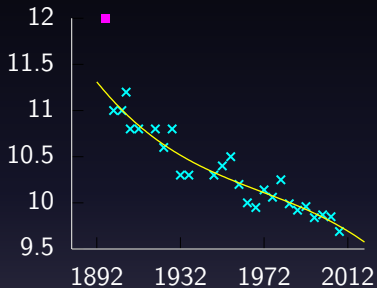# Leave One Out Error

Polynomial order 3, training error -32.998, leave one out error -0.51204.

Leave One Out Error

Polynomial order 3, training error -32.998, leave one out error -0.51204.

Leave One Out Error

Polynomial order 3, training error -32.998, leave one out error -0.51204.

Leave One Out Error

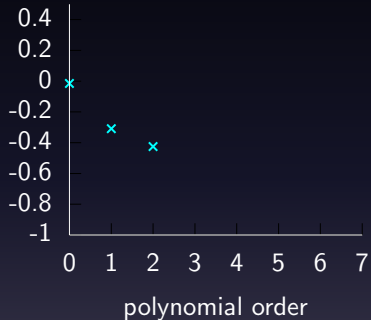Polynomial order 3, training error -32.998, leave one out error -0.51204.

Polynomial order 3, training error -32.998, leave one out error -0.51204.

Leave One Out Error

Polynomial order 3, training error -32.998, leave one out error -0.51204.
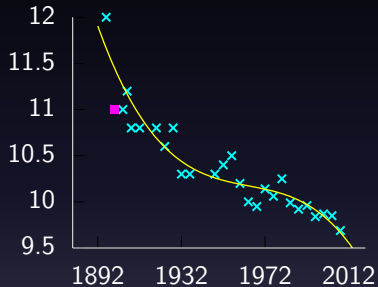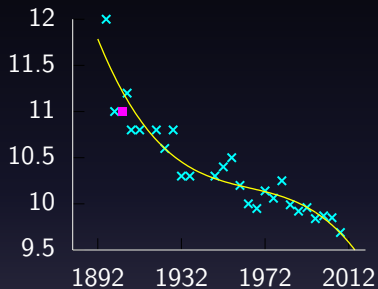
Polynomial order 3, training error -32.998, leave one out error -0.51204.
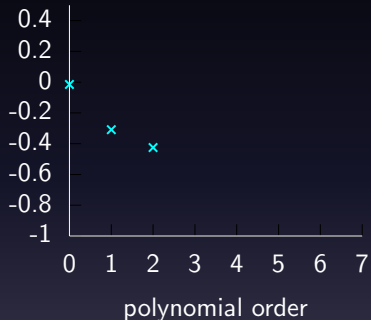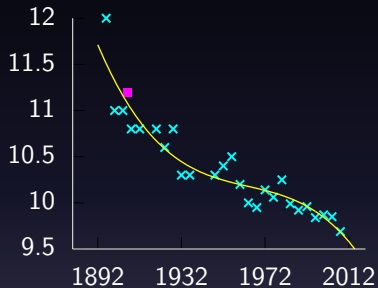
Leave One Out Error

Polynomial order 3, training error -32.998, leave one out error -0.51204.

Leave One Out Error
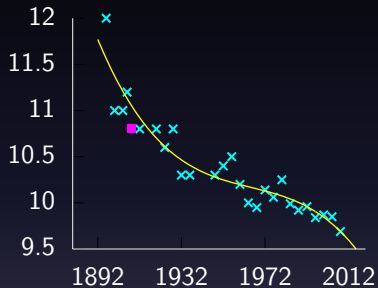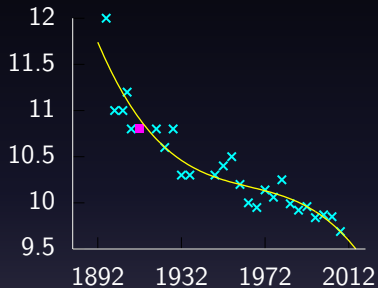

Polynomial order 3, training error -32.998, leave one out error -0.51204.

Leave One Out Error

Polynomial order 3, training error -32.998, leave one out error -0.51204.

Leave One Out Error

Polynomial order 3, training error -32.998, leave one out error -0.51204.
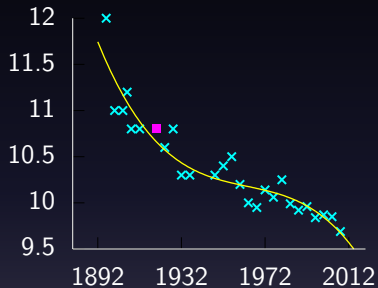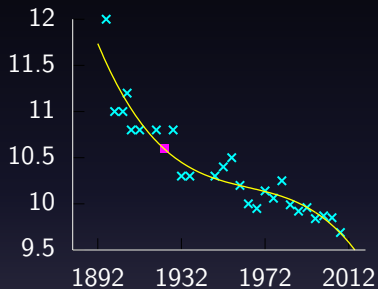
Polynomial order 3, training error -32.998, leave one out error -0.51204.
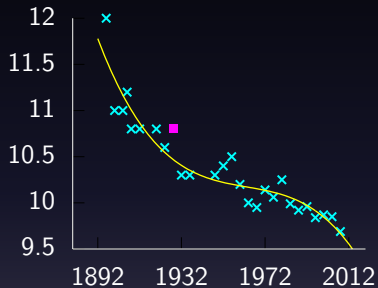
Leave One Out Error

Polynomial order 3, training error -32.998, leave one out error -0.51204.
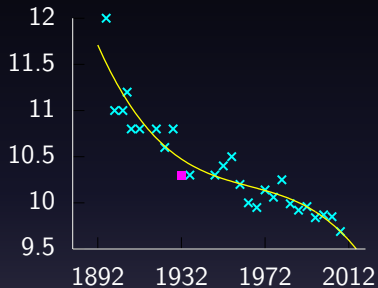
Leave One Out Error
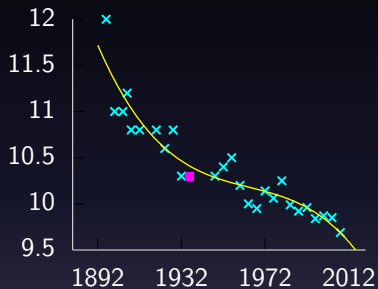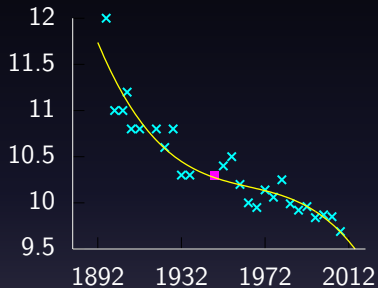

Polynomial order 3, training error -32.998, leave one out error -0.51204.

Leave One Out Error

Polynomial order 3, training error -32.998, leave one out error -0.51204.

Leave One Out Error
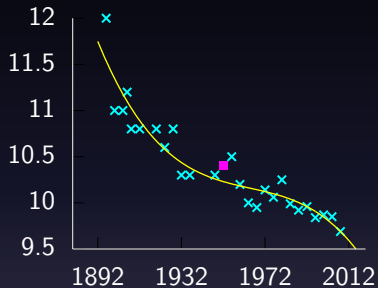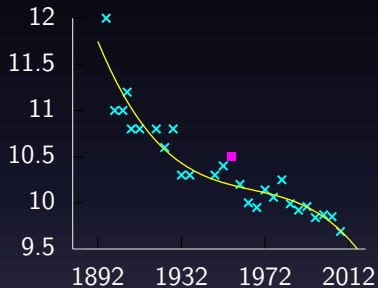

Polynomial order 3, training error -32.998, leave one out error -0.51204.

Leave One Out Error
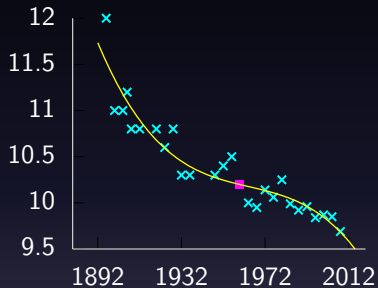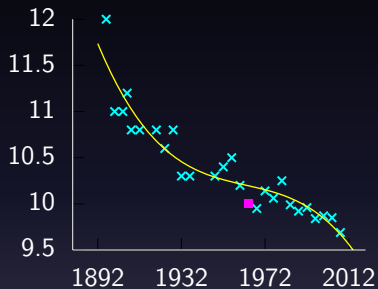

Polynomial order 3, training error -32.998, leave one out error -0.51204.

Leave One Out Error
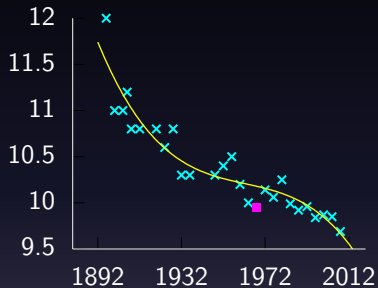

Polynomial order 3, training error -32.998, leave one out error -0.51204.

Leave One Out Error
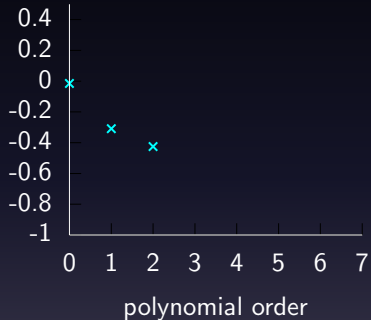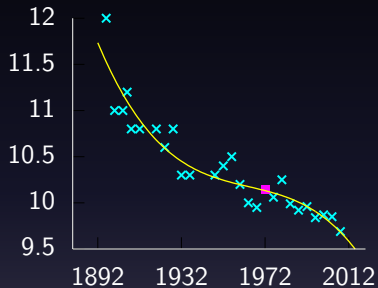

Polynomial order 3, training error -32.998, leave one out error -0.51204.

Leave One Out Error
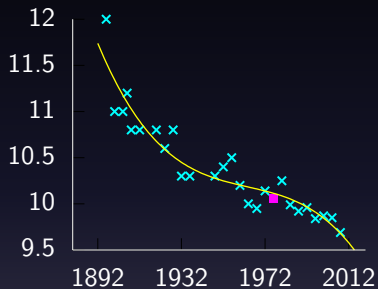

Polynomial order 3, training error -32.998, leave one out error -0.51204.

Leave One Out Error
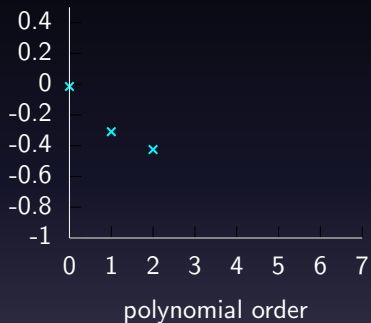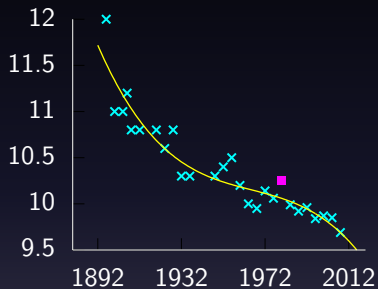

Polynomial order 3, training error -32.998, leave one out error -0.51204.

Leave One Out Error

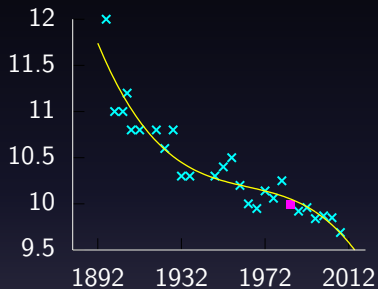Polynomial order 3, training error -32.998, leave one out error -0.51204.

Polynomial order 3, training error -32.998, leave one out error -0.51204.
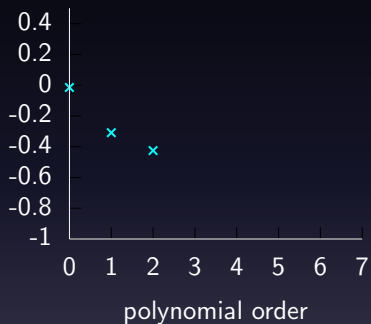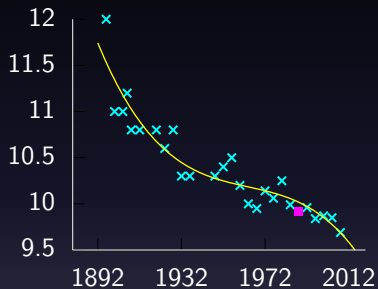
Leave One Out Error

Polynomial order 3, training error -32.998, leave one out error -0.51204.

Leave One Out Error

Polynomial order 3, training error -32.998, leave one out error -0.51204.

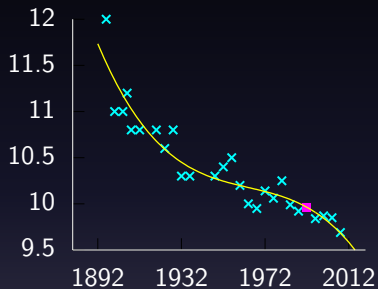Polynomial order 3, training error -32.998, leave one out error -0.51204.
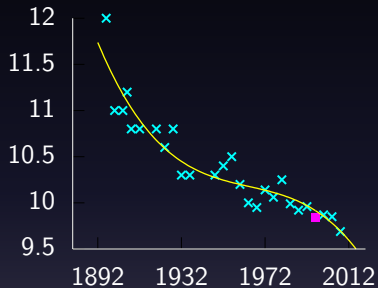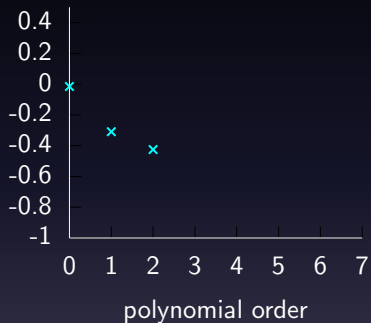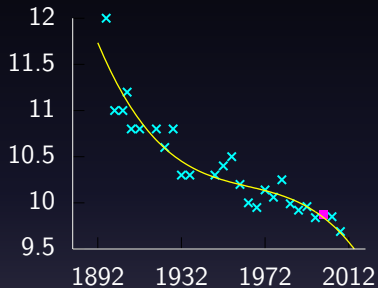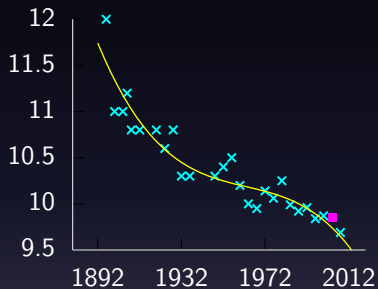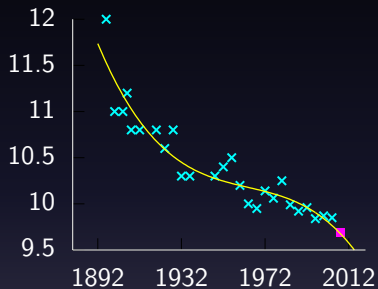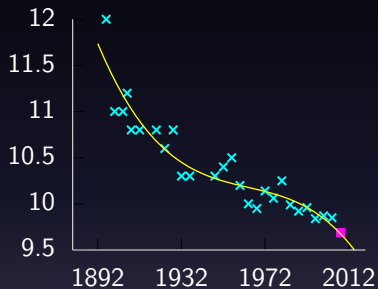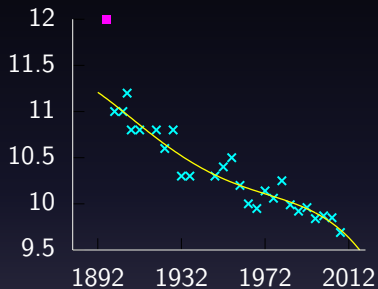
Polynomial order 3, training error -32.998, leave one out error -0.51204.
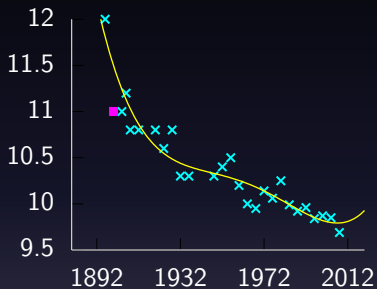
Leave One Out Error

Polynomial order 3, training error -32.998, leave one out error -0.51204.

Leave One Out Error

Polynomial order 4, training error -34.219, leave one out error -0.27864.

Leave One Out Error

Polynomial order 4, training error -34.219, leave one out error -0.27864.

Leave One Out Error

Polynomial order 4, training error -34.219, leave one out error -0.27864.

Leave One Out Error

Polynomial order 4, training error -34.219, leave one out error -0.27864.

Leave One Out Error
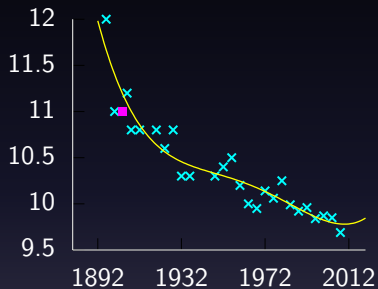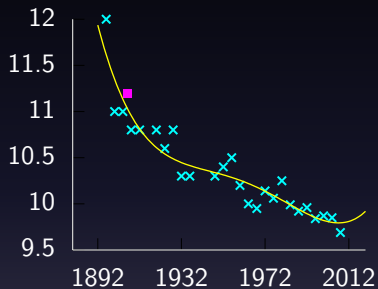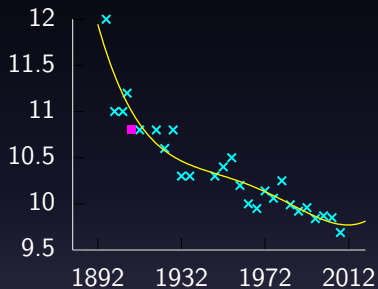

Polynomial order 4, training error -34.219, leave one out error -0.27864.

Leave One Out Error
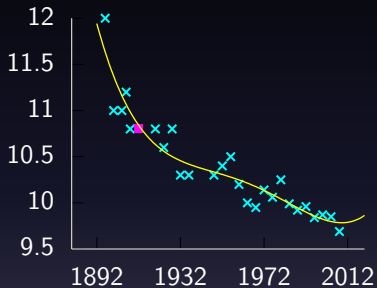

Polynomial order 4, training error -34.219, leave one out error -0.27864.

Leave One Out Error

Polynomial order 4, training error -34.219, leave one out error -0.27864.

Polynomial order 4, training error -34.219, leave one out error -0.27864.

Leave One Out Error

Polynomial order 4, training error -34.219, leave one out error -0.27864.
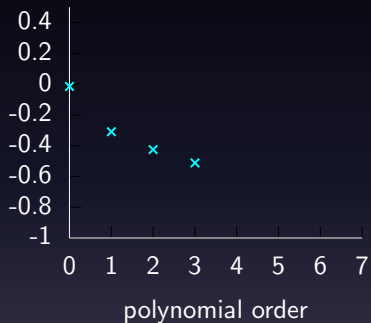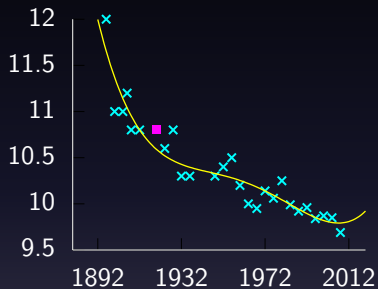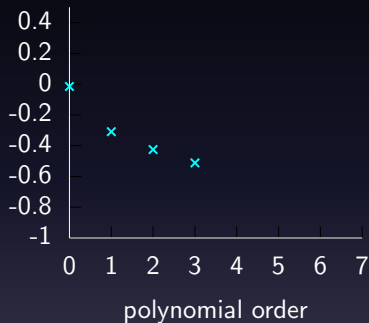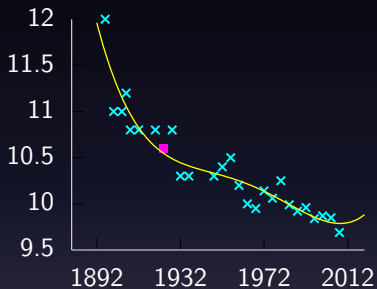
Leave One Out Error

Polynomial order 4, training error -34.219, leave one out error -0.27864.
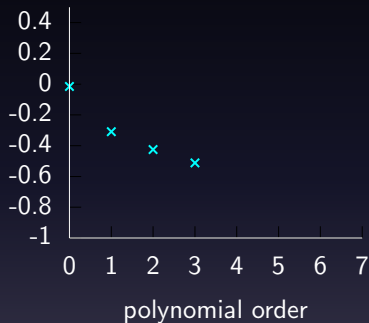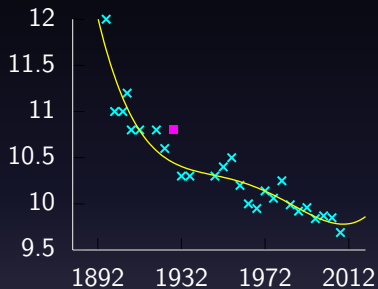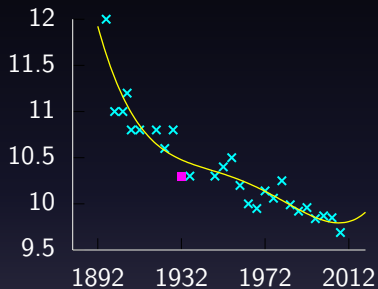
Polynomial order 4, training error -34.219, leave one out error -0.27864.

Leave One Out Error

Polynomial order 4, training error -34.219, leave one out error -0.27864.
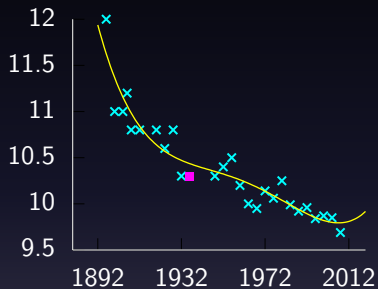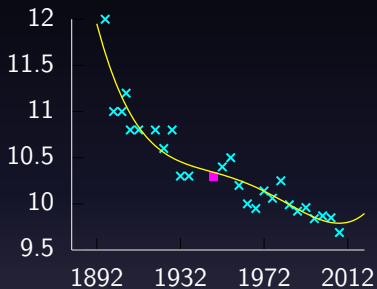
Polynomial order 4, training error -34.219, leave one out error -0.27864.
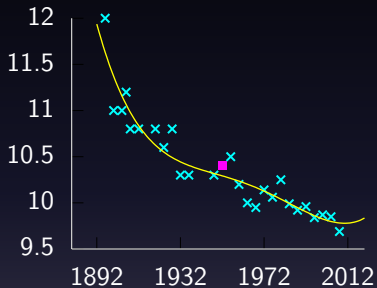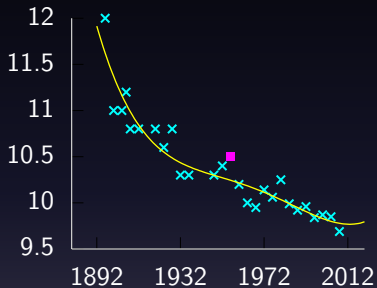
Leave One Out Error

Polynomial order 4, training error -34.219, leave one out error -0.27864.

Leave One Out Error

Polynomial order 4, training error -34.219, leave one out error -0.27864.

Polynomial order 4, training error -34.219, leave one out error -0.27864.
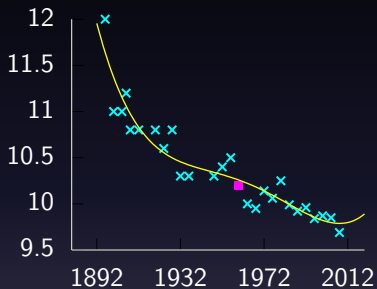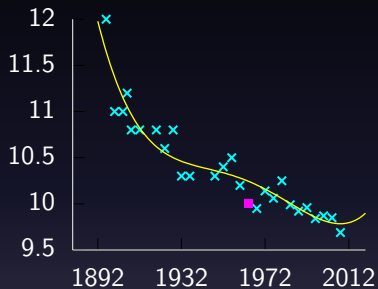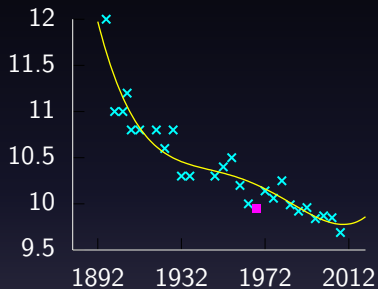
Polynomial order 4, training error -34.219, leave one out error -0.27864.

Leave One Out Error

Polynomial order 4, training error -34.219, leave one out error -0.27864.
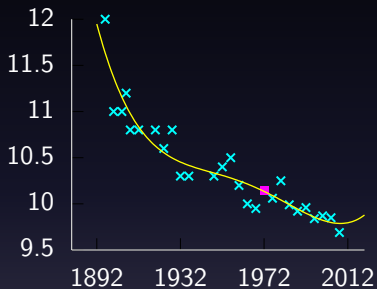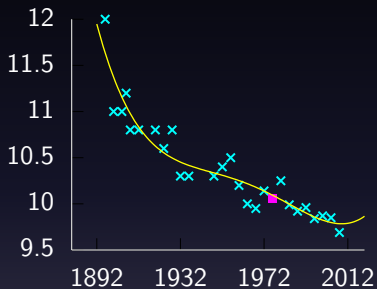
Leave One Out Error

Polynomial order 4, training error -34.219, leave one out error -0.27864.

Leave One Out Error

Polynomial order 4, training error -34.219, leave one out error -0.27864.
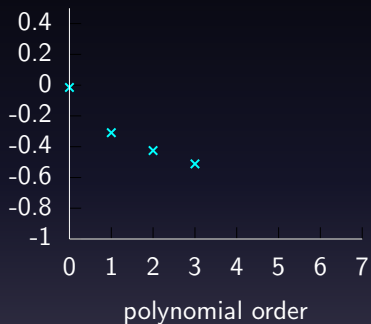
Leave One Out Error
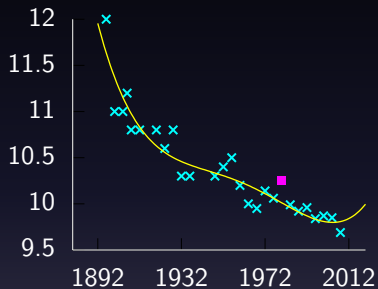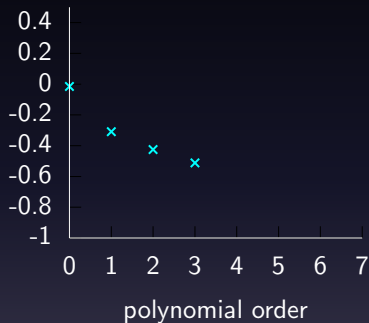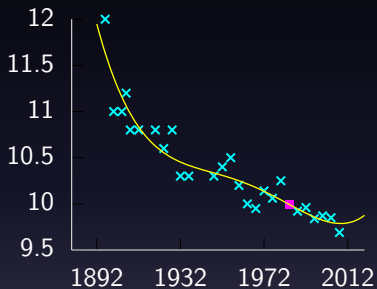

Polynomial order 4, training error -34.219, leave one out error -0.27864.

Leave One Out Error

Polynomial order 4, training error -34.219, leave one out error -0.27864.

Polynomial order 4, training error -34.219, leave one out error -0.27864.
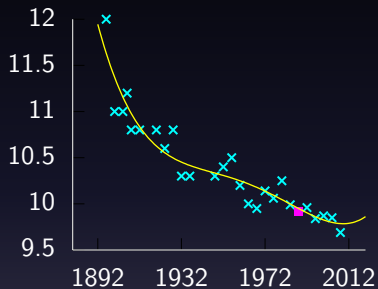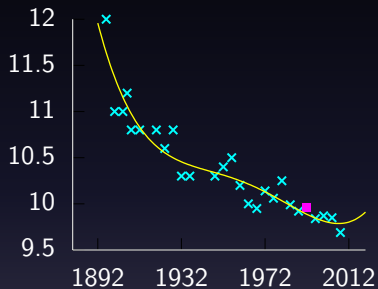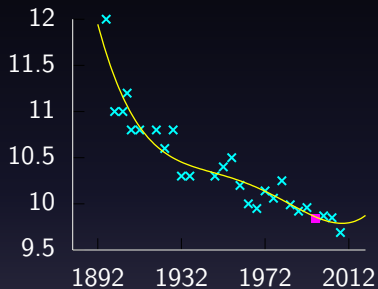
Polynomial order 4, training error -34.219, leave one out error -0.27864.

Leave One Out Error

Polynomial order 4, training error -34.219, leave one out error
-0.27864.

Leave One Out Error

Polynomial order 4, training error -34.219, leave one out error -0.27864.
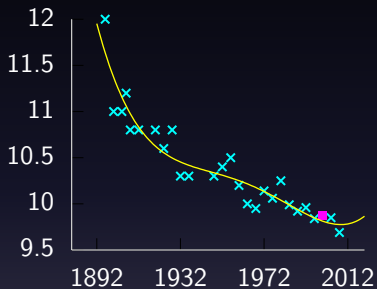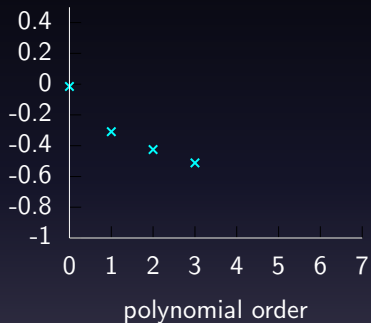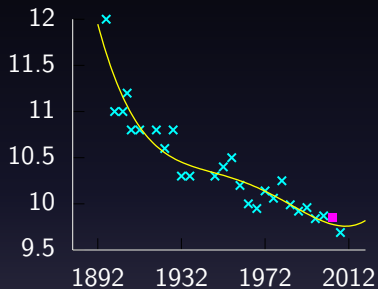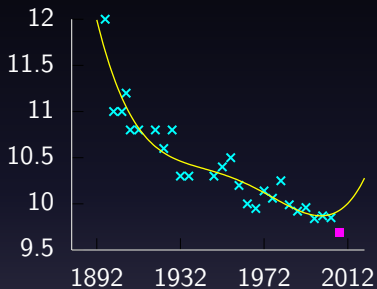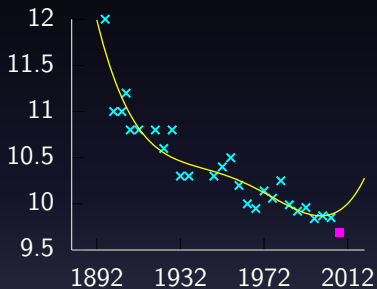
Polynomial order 4, training error -34.219, leave one out error -0.27864.

Leave One Out Error

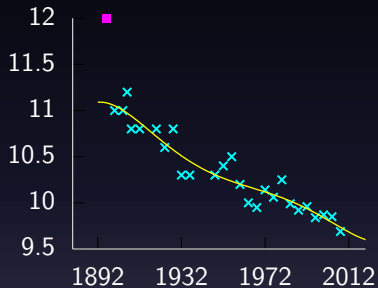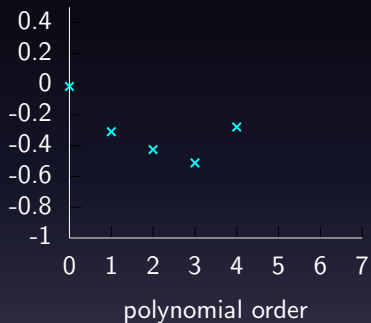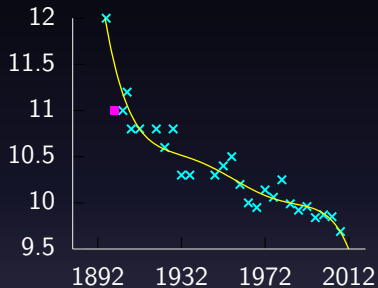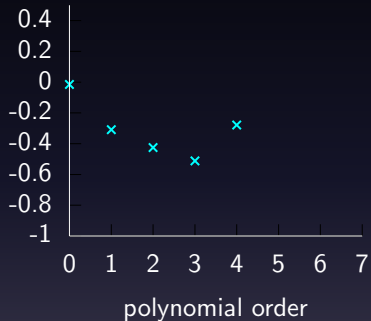Polynomial order 4, training error -34.219, leave one out error -0.27864.

Leave One Out Error

Polynomial order 5, training error -36.062, leave one out error -0.11715.

Leave One Out Error

Polynomial order 5, training error -36.062, leave one out error -0.11715.
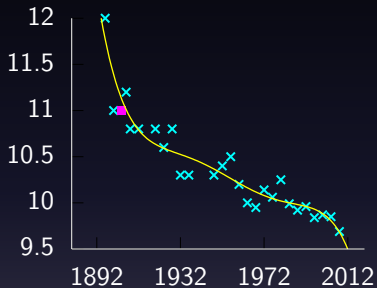
Leave One Out Error

Polynomial order 5, training error -36.062, leave one out error -0.11715.

Leave One Out Error

Polynomial order 5, training error -36.062, leave one out error -0.11715.

Leave One Out Error

Polynomial order 5, training error -36.062, leave one out error -0.11715.

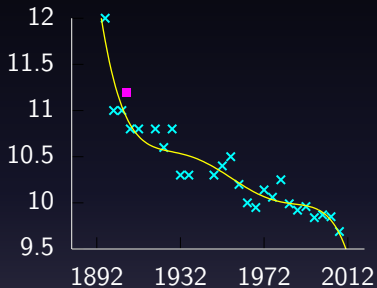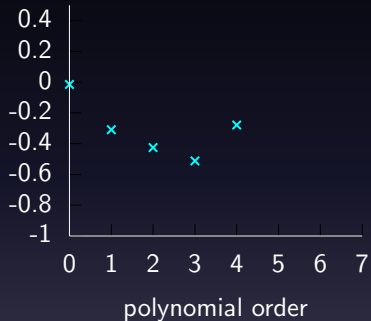# Leave One Out Error

Polynomial order 5, training error -36.062, leave one out error -0.11715.

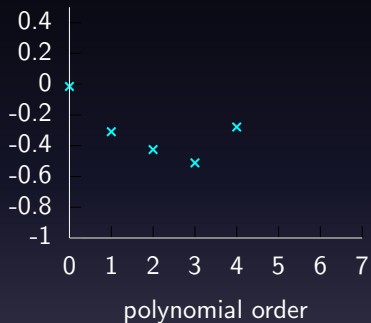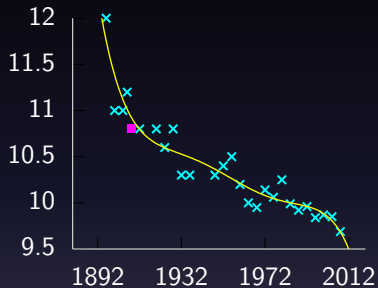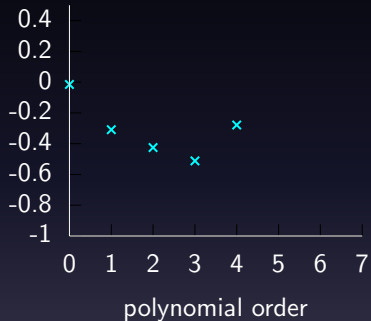# Leave One Out Error

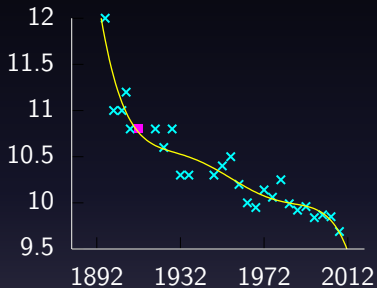Polynomial order 5, training error -36.062, leave one out error -0.11715.

Polynomial order 5, training error -36.062, leave one out error
-0.11715.

Leave One Out Error

Polynomial order 5, training error -36.062, leave one out error -0.11715.
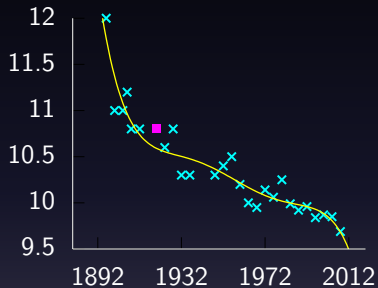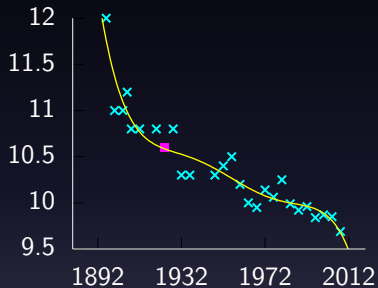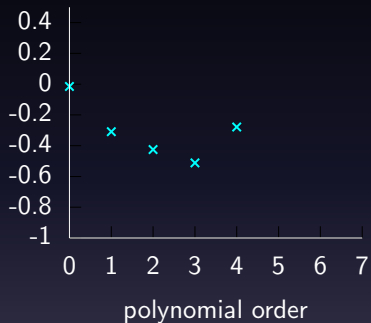
Polynomial order 5, training error -36.062, leave one out error -0.11715.
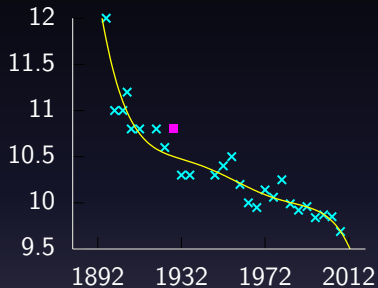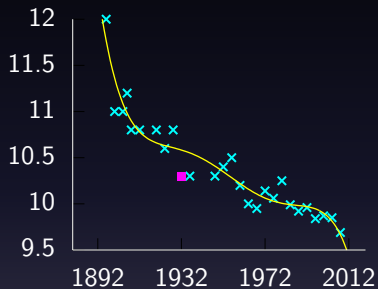
Leave One Out Error

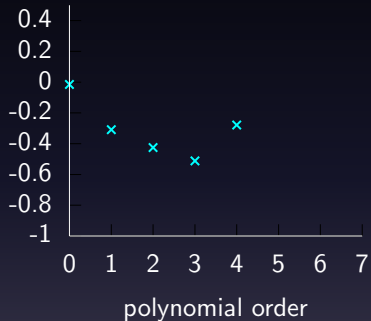Polynomial order 5, training error -36.062, leave one out error -0.11715.

Leave One Out Error

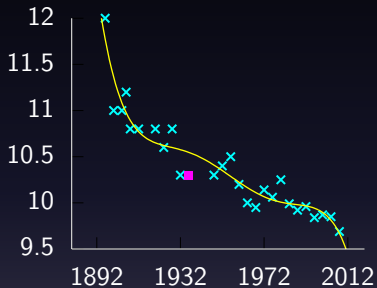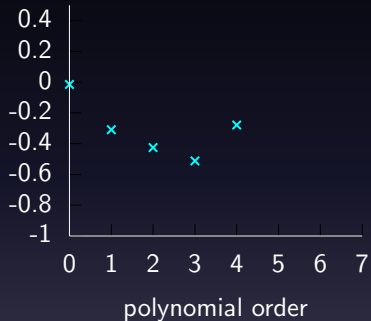Polynomial order 5, training error -36.062, leave one out error -0.11715.

Polynomial order 5, training error -36.062, leave one out error -0.11715.

Leave One Out Error

Polynomial order 5, training error -36.062, leave one out error -0.11715.
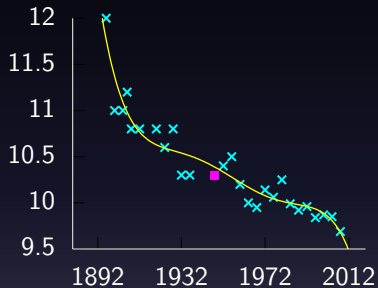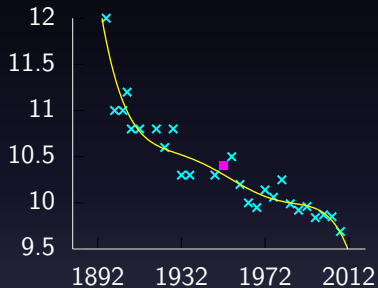
Polynomial order 5, training error -36.062, leave one out error -0.11715.
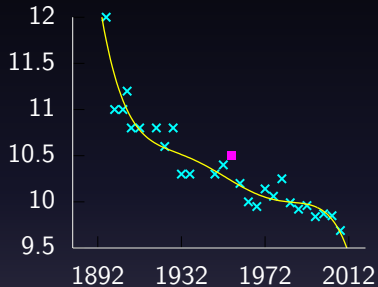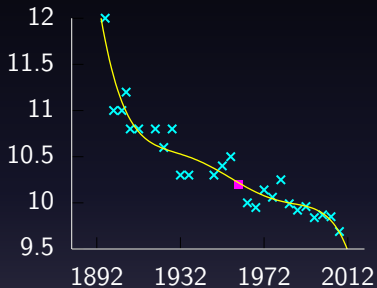
Leave One Out Error

Polynomial order 5, training error -36.062, leave one out error -0.11715.

Leave One Out Error
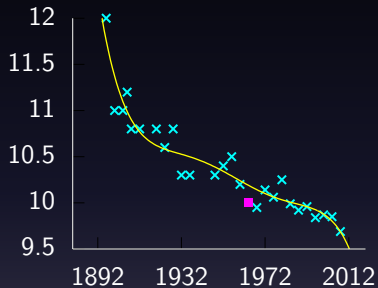

Polynomial order 5, training error -36.062, leave one out error -0.11715.

Leave One Out Error

Polynomial order 5, training error -36.062, leave one out error -0.11715.
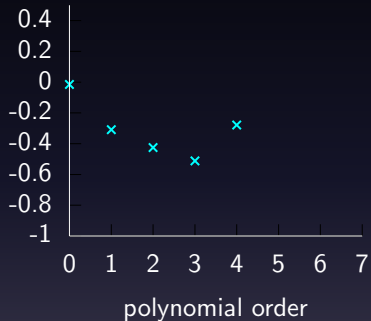
Leave One Out Error
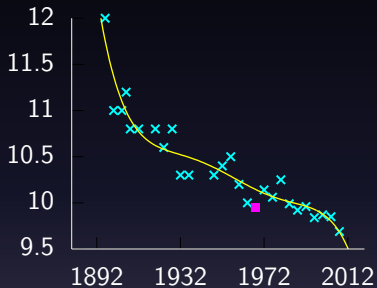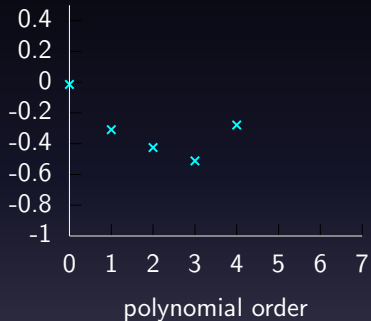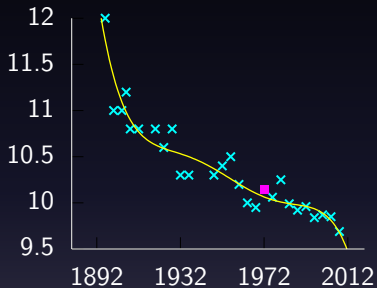

Polynomial order 5, training error -36.062, leave one out error -0.11715.

Leave One Out Error
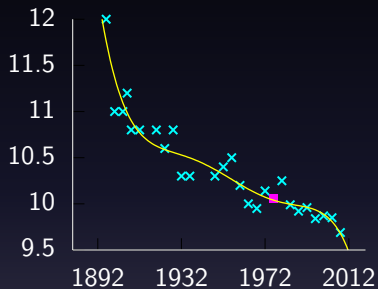

Polynomial order 5, training error -36.062, leave one out error -0.11715.

Leave One Out Error
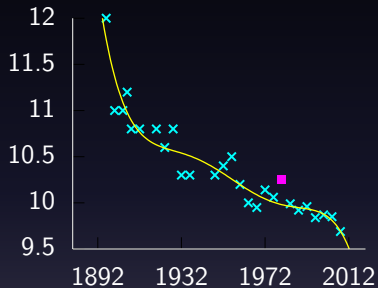

Polynomial order 5, training error -36.062, leave one out error -0.11715.

Leave One Out Error
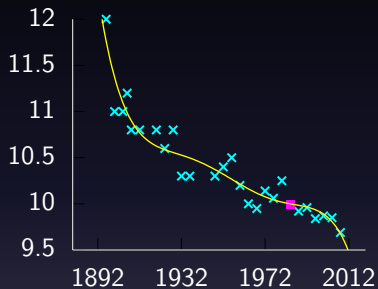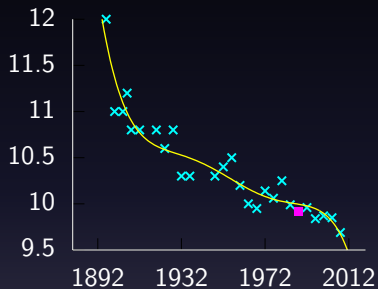

Polynomial order 5, training error -36.062, leave one out error -0.11715.

Leave One Out Error
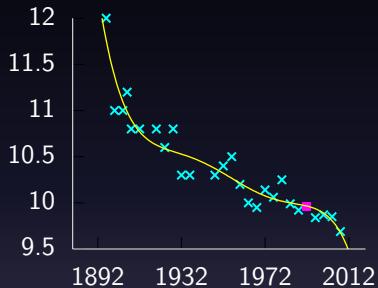

Polynomial order 5, training error -36.062, leave one out error -0.11715.

Leave One Out Error
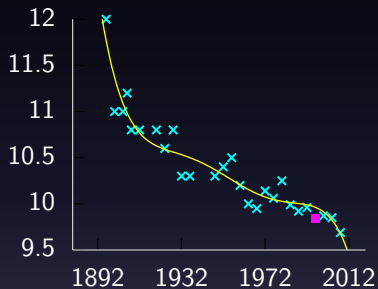

Polynomial order 5, training error -36.062, leave one out error -0.11715.

Leave One Out Error
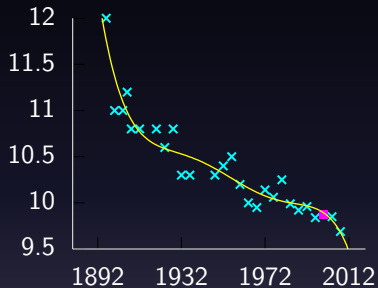

Polynomial order 5, training error -36.062, leave one out error -0.11715.

Leave One Out Error

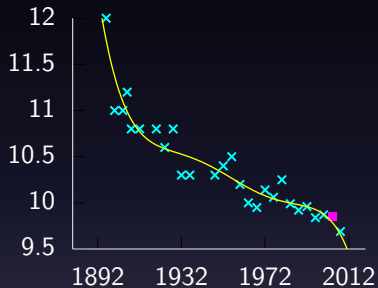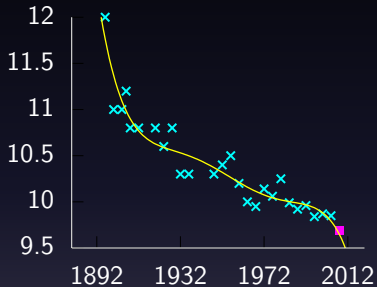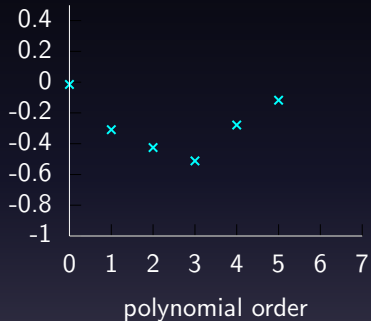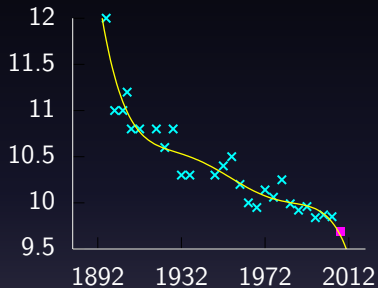Polynomial order 5, training error -36.062, leave one out error -0.11715.
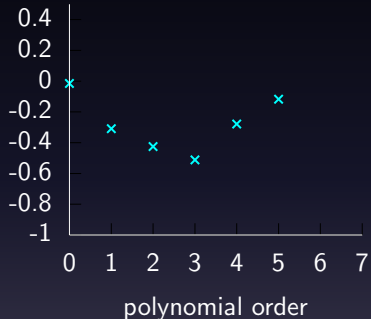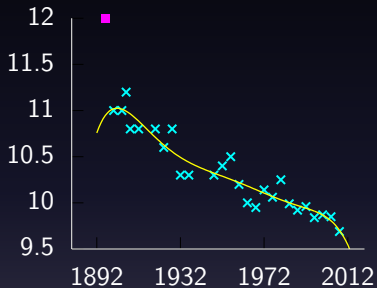
Polynomial order 5, training error -36.062, leave one out error -0.11715.

Leave One Out Error

Polynomial order 5, training error -36.062, leave one out error -0.11715.

Polynomial order 6, training error -36.942, leave one out error 0.35878.
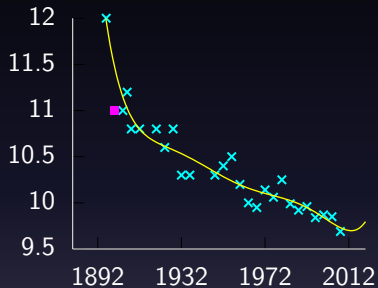
Leave One Out Error

Polynomial order 6, training error -36.942, leave one out error 0.35878.
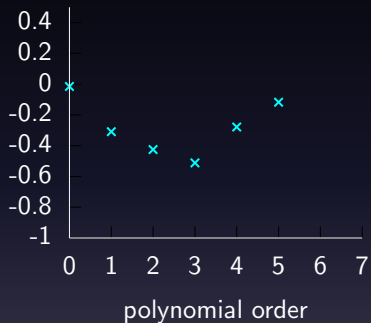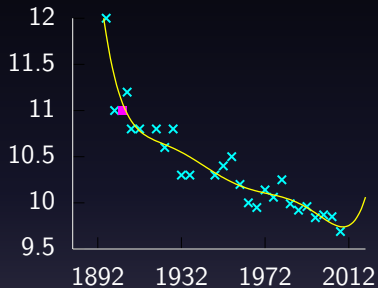
Leave One Out Error

Polynomial order 6, training error -36.942, leave one out error 0.35878.

Leave One Out Error

Polynomial order 6, training error -36.942, leave one out error 0.35878.

Leave One Out Error
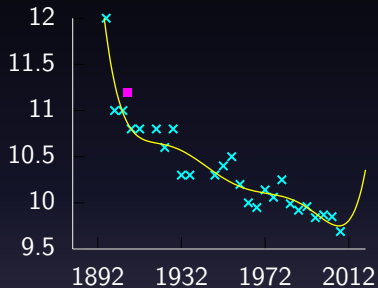

Polynomial order 6, training error -36.942, leave one out error 0.35878.

Leave One Out Error

Polynomial order 6, training error -36.942, leave one out error 0.35878.

Polynomial order 6, training error -36.942, leave one out error 0.35878.

Leave One Out Error

Polynomial order 6, training error -36.942, leave one out error 0.35878.
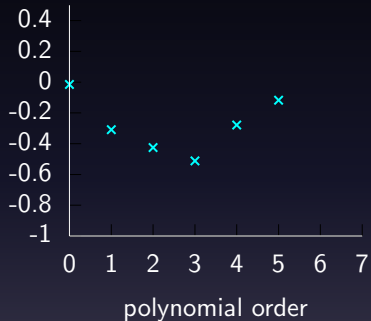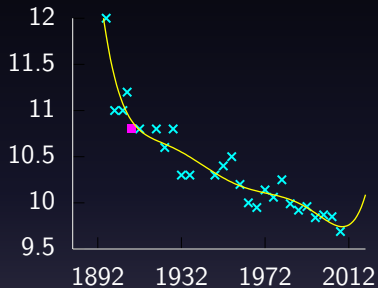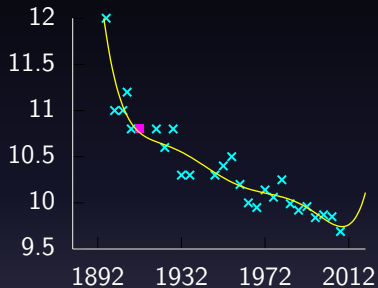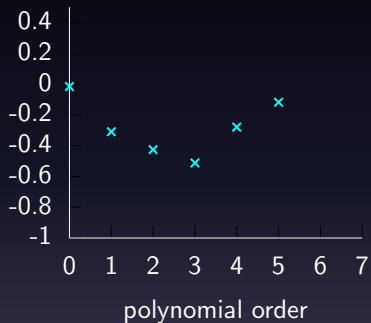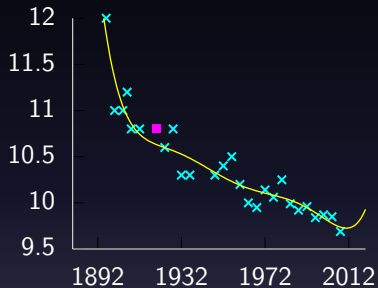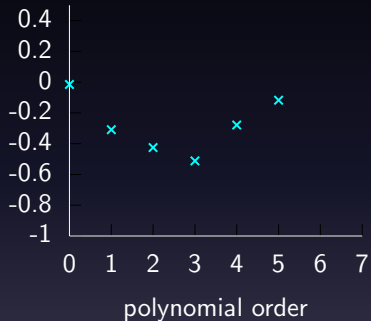
Leave One Out Error
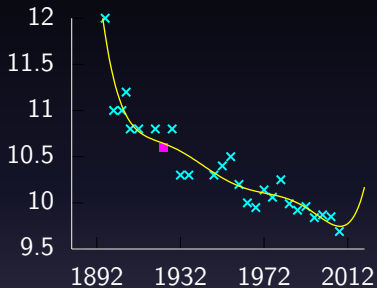

Polynomial order 6, training error -36.942, leave one out error 0.35878.

Leave One Out Error

Polynomial order 6, training error -36.942, leave one out error 0.35878.
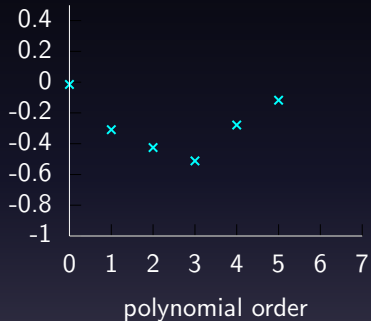
Leave One Out Error
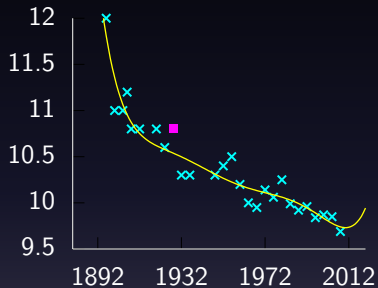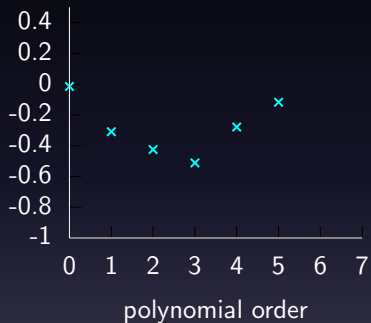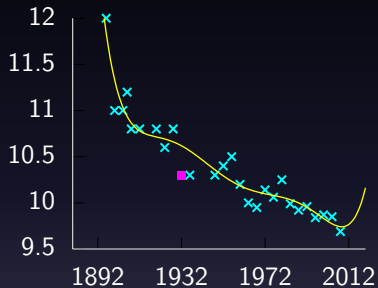

Polynomial order 6, training error -36.942, leave one out error
0.35878.

Leave One Out Error
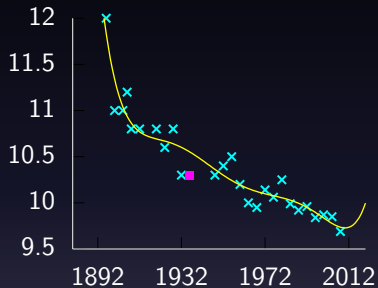

Polynomial order 6, training error -36.942, leave one out error 0.35878.

Leave One Out Error

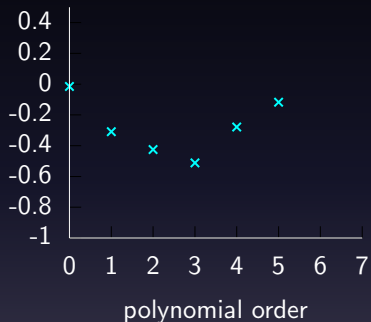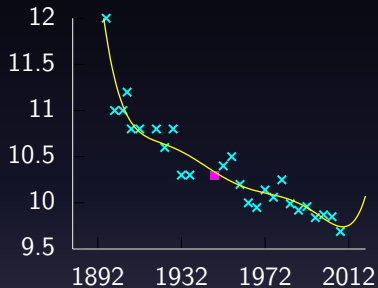Polynomial order 6, training error -36.942, leave one out error 0.35878.

Polynomial order 6, training error -36.942, leave one out error 0.35878.

Leave One Out Error

Polynomial order 6, training error -36.942, leave one out error 0.35878.
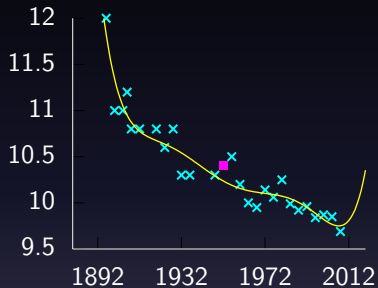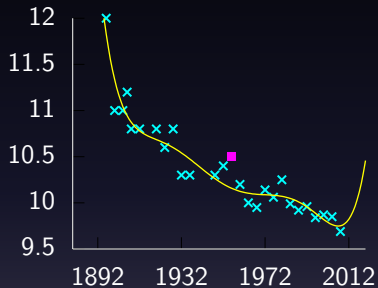
Leave One Out Error
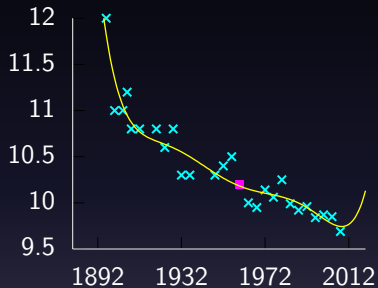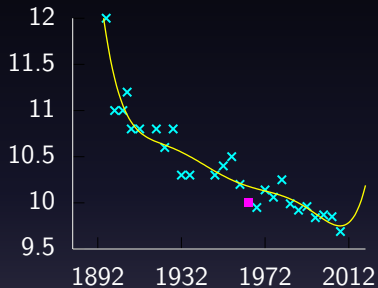

Polynomial order 6, training error -36.942, leave one out error 0.35878.

Leave One Out Error

Polynomial order 6, training error -36.942, leave one out error 0.35878.

Polynomial order 6, training error -36.942, leave one out error 0.35878.

Leave One Out Error

Polynomial order 6, training error -36.942, leave one out error 0.35878.
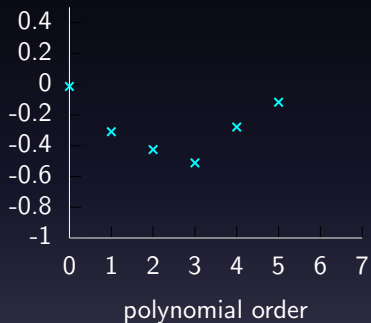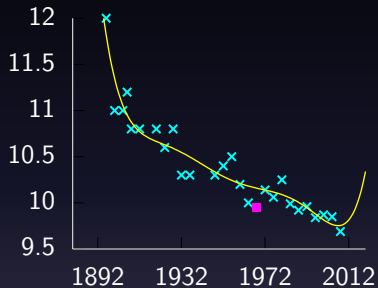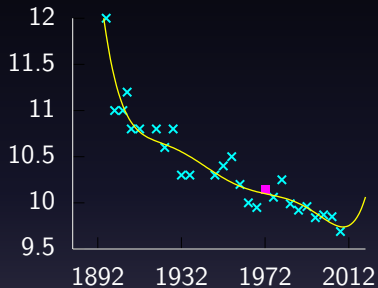
Polynomial order 6, training error -36.942, leave one out error 0.35878.

Leave One Out Error

Polynomial order 6, training error -36.942, leave one out error 0.35878.

Polynomial order 6, training error -36.942, leave one out error 0.35878.

Leave One Out Error

Polynomial order 6, training error -36.942, leave one out error
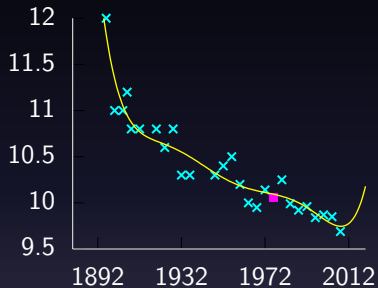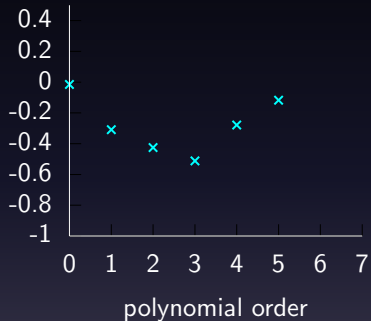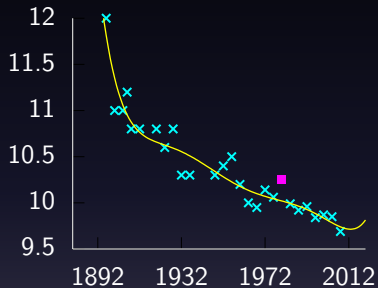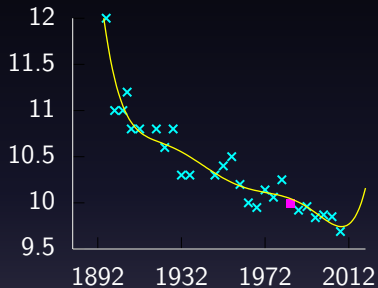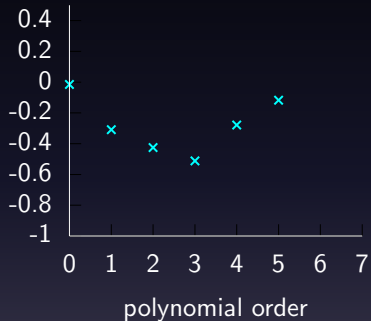0.35878.

Leave One Out Error

Polynomial order 6, training error -36.942, leave one out error 0.35878.

Leave One Out Error

Polynomial order 6, training error -36.942, leave one out error 0.35878.
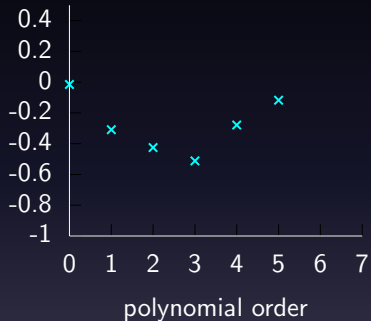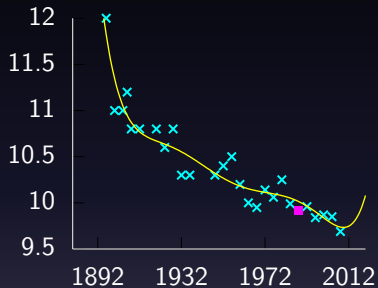
Leave One Out Error
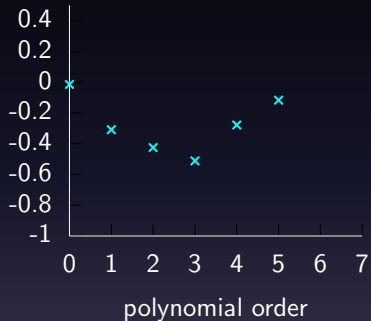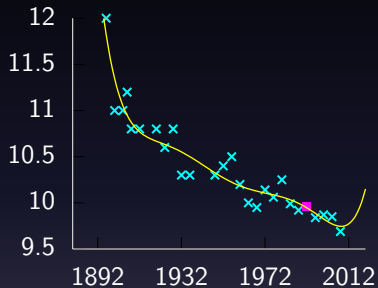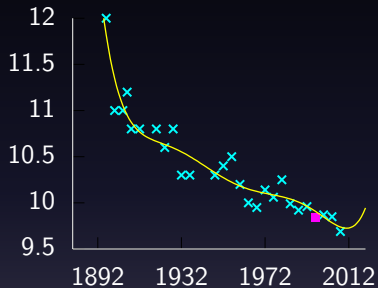

Polynomial order 6, training error -36.942, leave one out error 0.35878.

Leave One Out Error
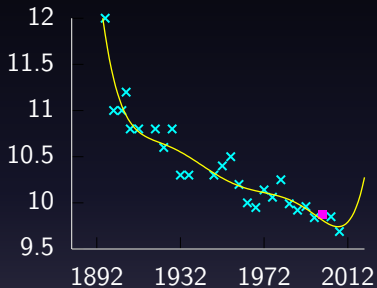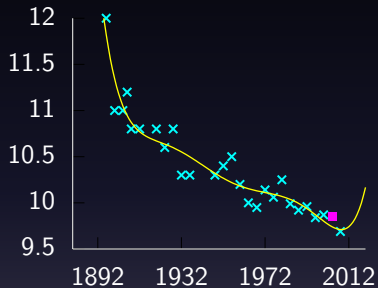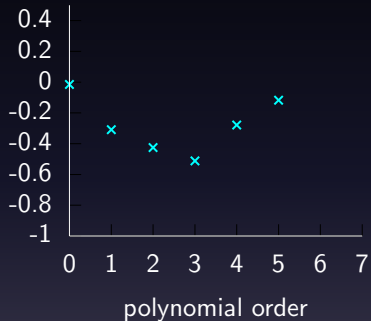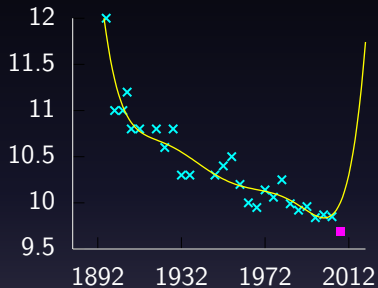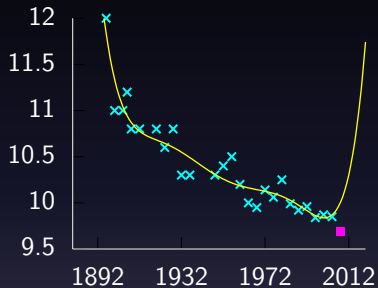

Polynomial order 6, training error -36.942, leave one out error 0.35878.
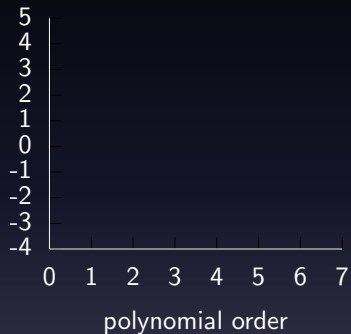
Leave One Out Error

Polynomial order 6, training error -36.942, leave one out error 0.35878.

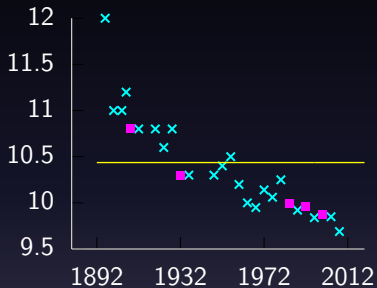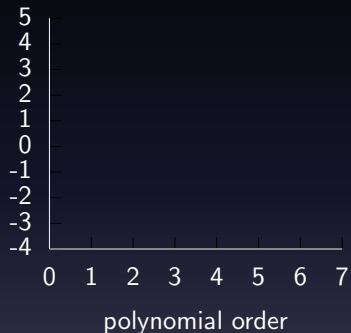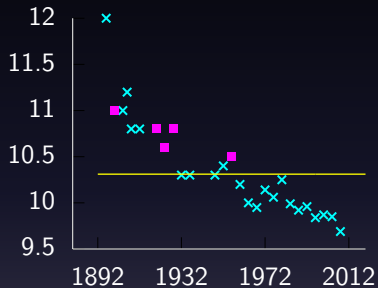- Leave one out cross validation can be very time consuming!
- Need to train your algorithm N times.
- An alternative: k fold cross validation.

Cross Validation Error

Polynomial order 0, training error -3.8547, leave one out error -0.014727.

Cross Validation Error

Polynomial order 0, training error -3.8547, leave one out error -0.014727.

Cross Validation Error

Polynomial order 0, training error -3.8547, leave one out error -0.014727.

Cross Validation Error

Polynomial order 0, training error -3.8547, leave one out error -0.014727.

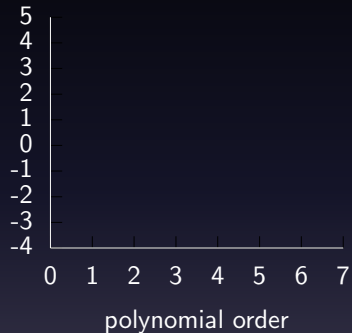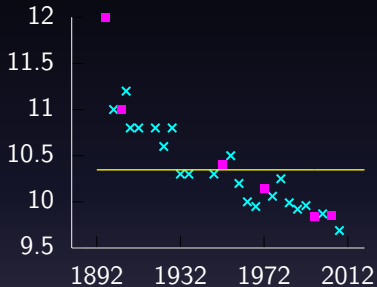# Cross Validation Error
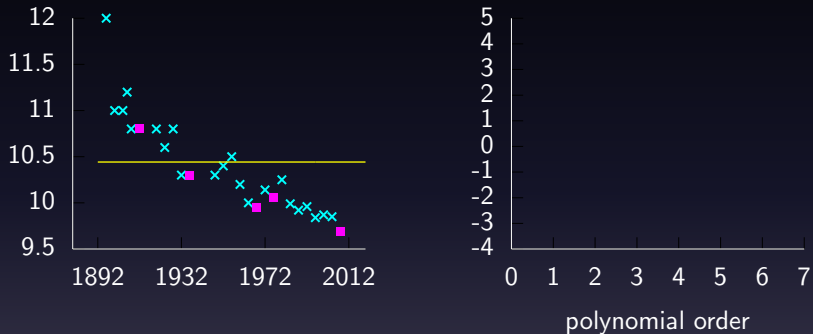

Polynomial order 0, training error -3.8547, leave one out error -0.014727.
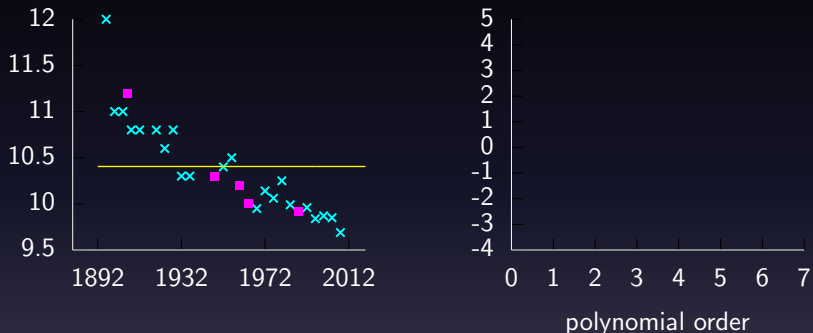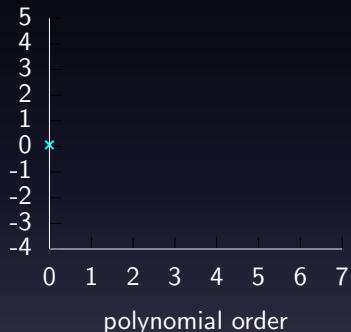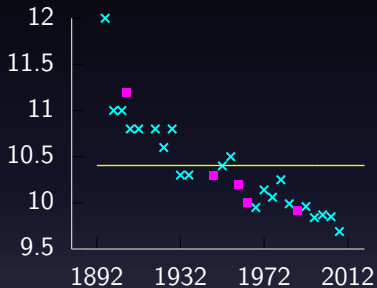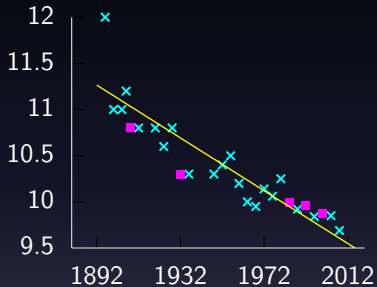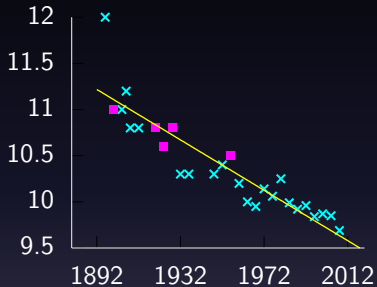
Cross Validation Error

Polynomial order 0, training error -3.8547, leave one out error -0.014727.

Cross Validation Error

Polynomial order 1, training error -22.56, leave one out error -0.30898.

Cross Validation Error

Polynomial order 1, training error -22.56, leave one out error -0.30898.
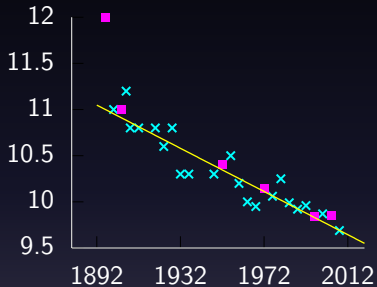
Cross Validation Error

Polynomial order 1, training error -22.56, leave one out error -0.30898.

Cross Validation Error

Polynomial order 1, training error -22.56, leave one out error -0.30898.

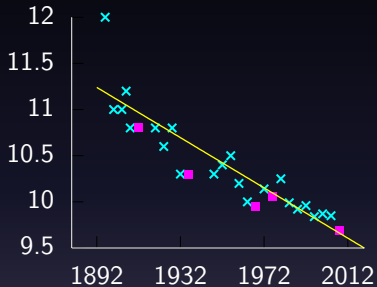# Cross Validation Error
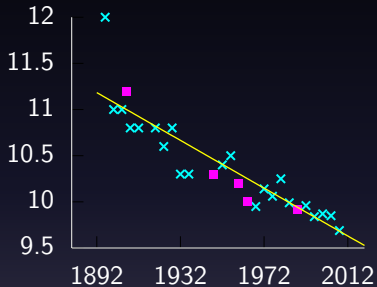

Polynomial order 1, training error -22.56, leave one out error -0.30898.
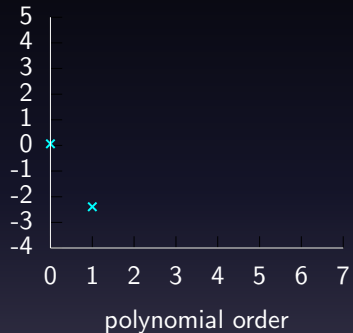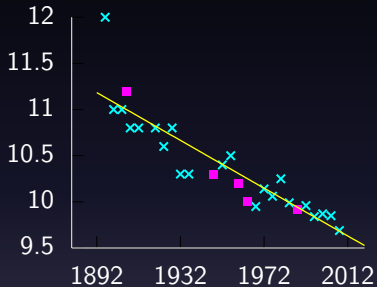
Cross Validation Error

Polynomial order 1, training error -22.56, leave one out error -0.30898.
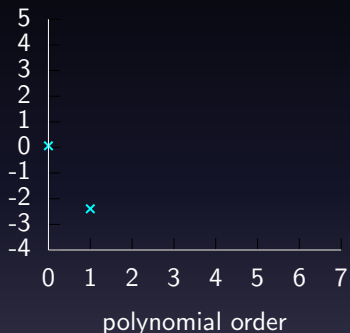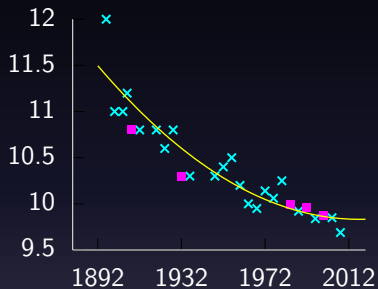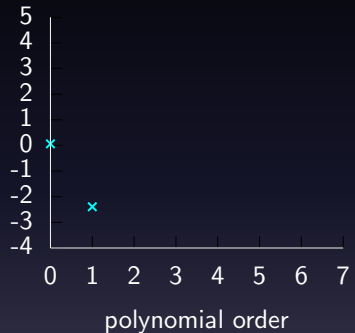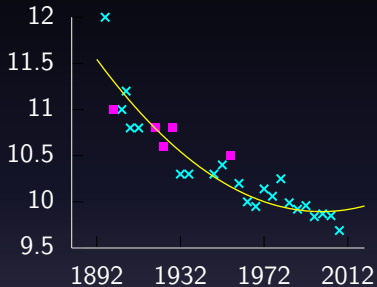
Cross Validation Error

Polynomial order 2, training error -25.533, leave one out error -0.4251.

Cross Validation Error

Polynomial order 2, training error -25.533, leave one out error -0.4251.
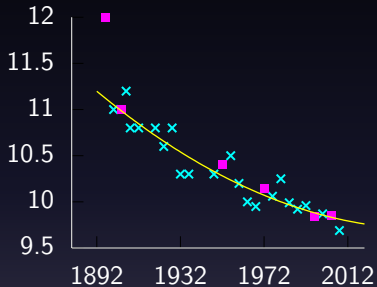
Cross Validation Error

Polynomial order 2, training error -25.533, leave one out error -0.4251.

Cross Validation Error

Polynomial order 2, training error -25.533, leave one out error -0.4251.

Cross Validation Error

Polynomial order 2, training error -25.533, leave one out error -0.4251.

Cross Validation Error

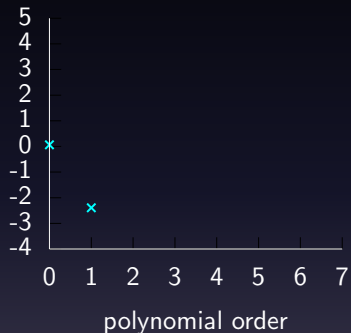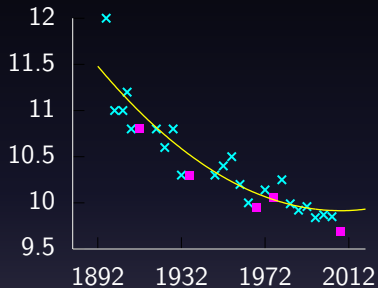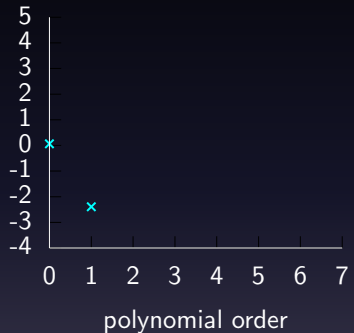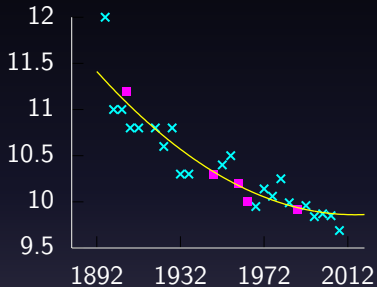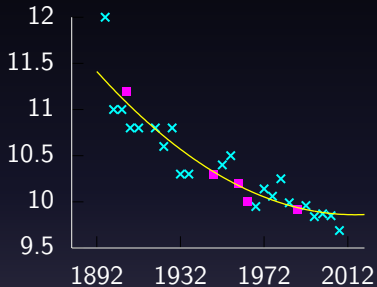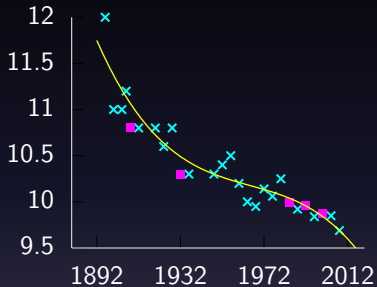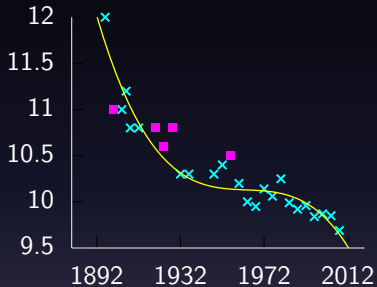
Polynomial order 2, training error -25.533, leave one out error -0.4251.

Cross Validation Error

Polynomial order 3, training error -28.792, leave one out error -0.51204.

Cross Validation Error

Polynomial order 3, training error -28.792, leave one out error -0.51204.
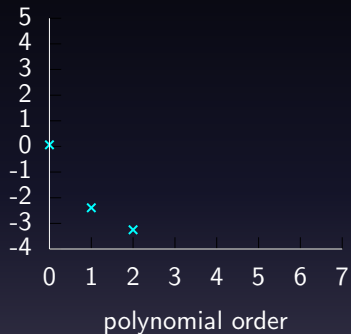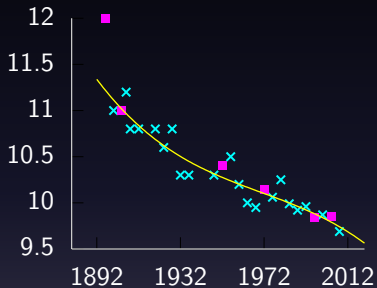
Cross Validation Error

Polynomial order 3, training error -28.792, leave one out error -0.51204.

Cross Validation Error

Polynomial order 3, training error -28.792, leave one out error -0.51204.

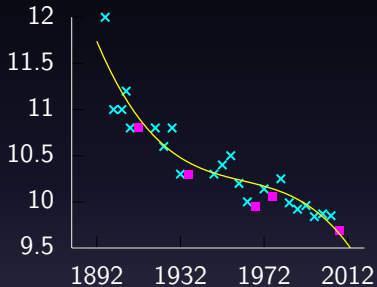# Cross Validation Error
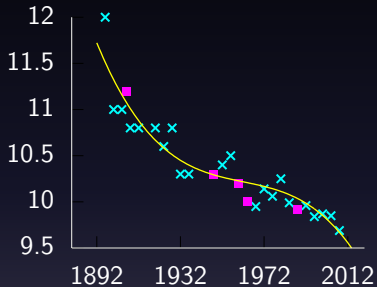

Polynomial order 3, training error -28.792, leave one out error -0.51204.
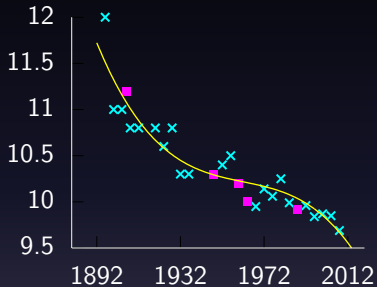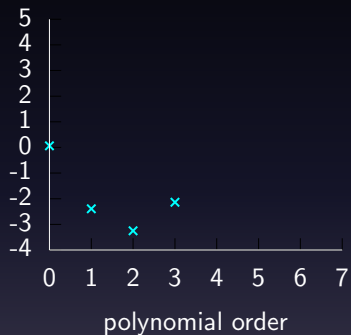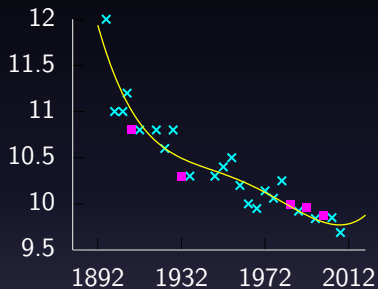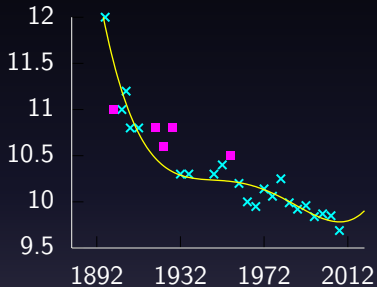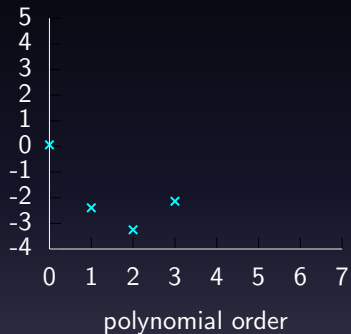
Cross Validation Error

Polynomial order 3, training error -28.792, leave one out error -0.51204.

Cross Validation Error

Polynomial order 4, training error -30.532, leave one out error -0.27864.

Cross Validation Error

Polynomial order 4, training error -30.532, leave one out error -0.27864.
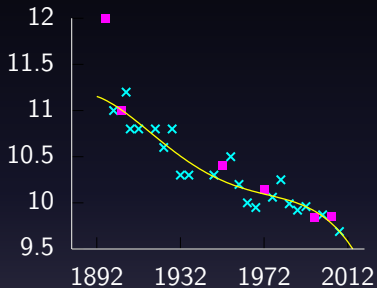
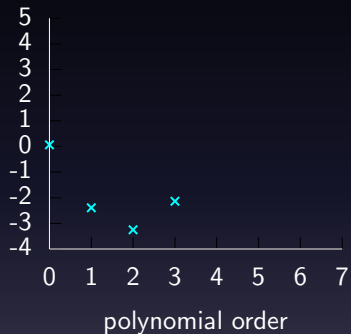# Cross Validation Error

Polynomial order 4, training error -30.532, leave one out error -0.27864.

Cross Validation Error

Polynomial order 4, training error -30.532, leave one out error -0.27864.
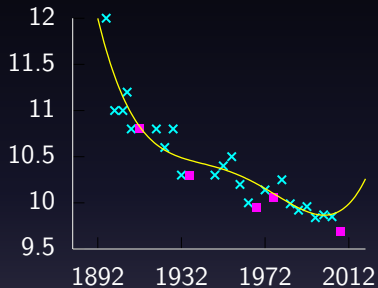
Polynomial order 4, training error -30.532, leave one out error -0.27864.

Cross Validation Error

Polynomial order 4, training error -30.532, leave one out error -0.27864.
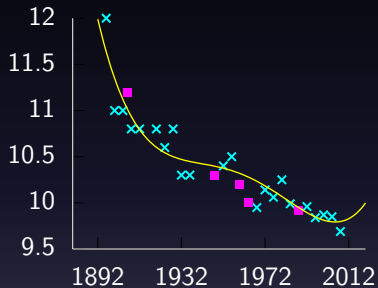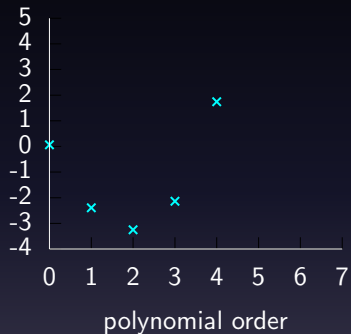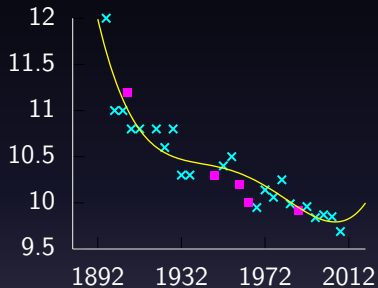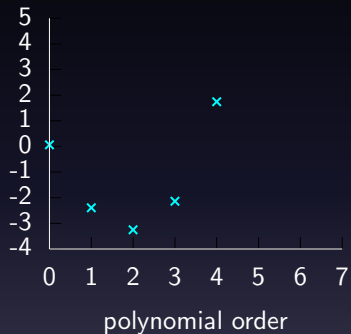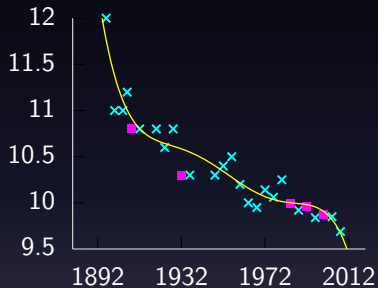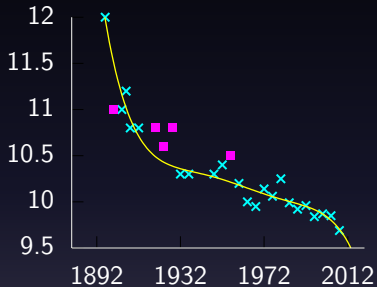
Cross Validation Error

Polynomial order 5, training error -32.022, leave one out error -0.11715.

Cross Validation Error

Polynomial order 5, training error -32.022, leave one out error -0.11715.
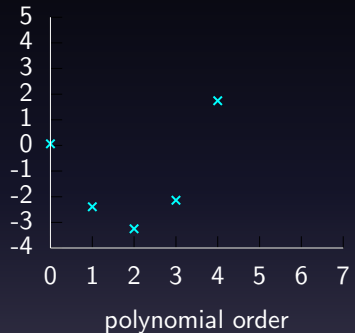
Cross Validation Error

Polynomial order 5, training error -32.022, leave one out error -0.11715.

Cross Validation Error

Polynomial order 5, training error -32.022, leave one out error -0.11715.
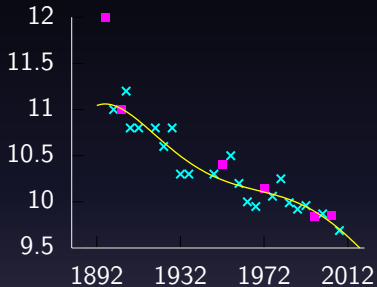
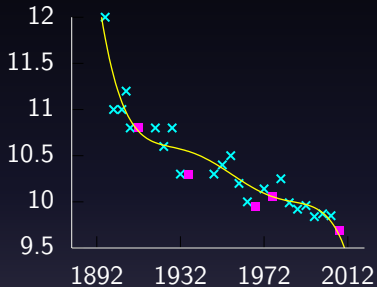# Cross Validation Error

Polynomial order 5, training error -32.022, leave one out error -0.11715.

Cross Validation Error

Polynomial order 5, training error -32.022, leave one out error -0.11715.
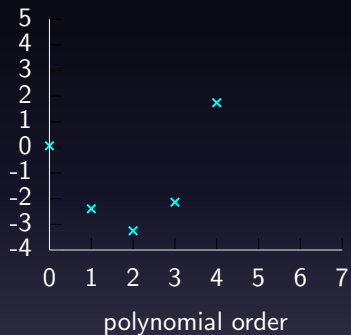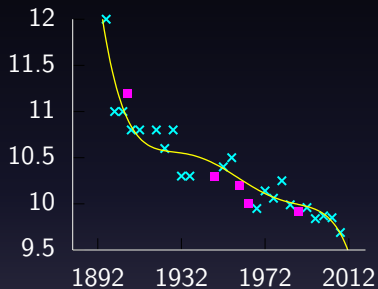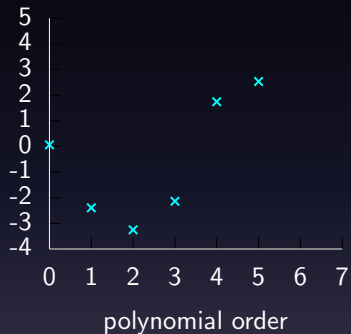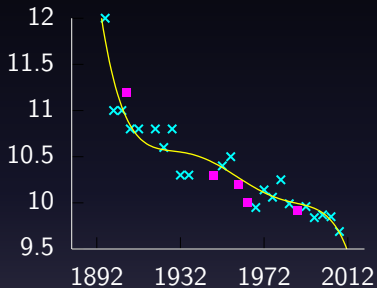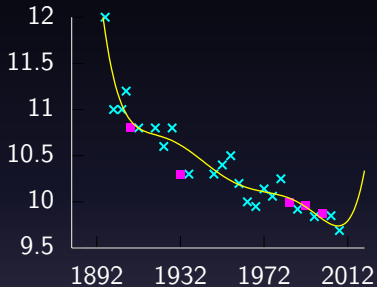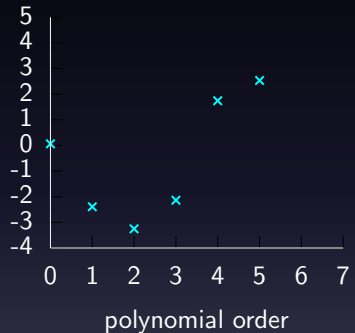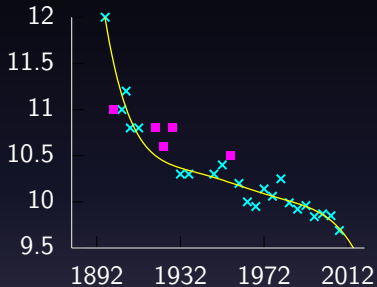
Cross Validation Error

Polynomial order 6, training error -32.792, leave one out error 0.35878.

Cross Validation Error

Polynomial order 6, training error -32.792, leave one out error 0.35878.
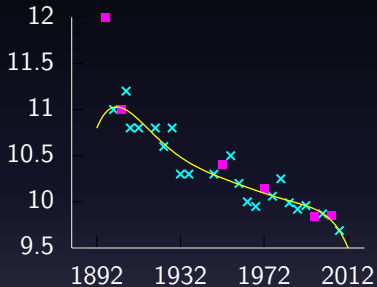
Cross Validation Error

Polynomial order 6, training error -32.792, leave one out error 0.35878.

Cross Validation Error

Polynomial order 6, training error -32.792, leave one out error 0.35878.

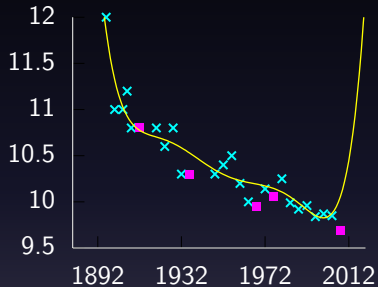# Cross Validation Error
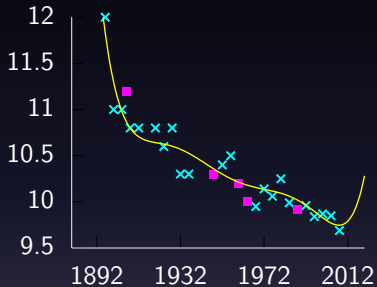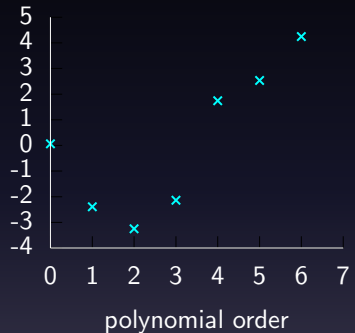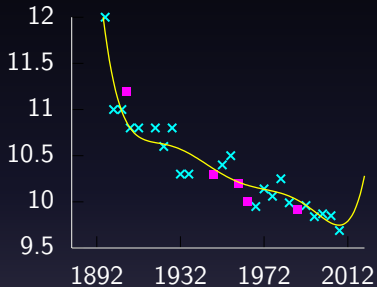

Polynomial order 6, training error -32.792, leave one out error 0.35878.

Cross Validation Error

Polynomial order 6, training error -32.792, leave one out error 0.35878.

Reading

- Section 1.5 of **?**.

S. Rogers and M. Girolami. *A First Course in Machine Learning*. CRC Press, 2011. [Google Books] .