Generalization

Neil D. Lawrence

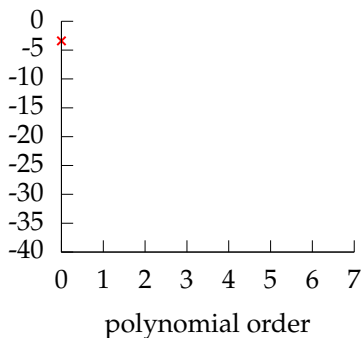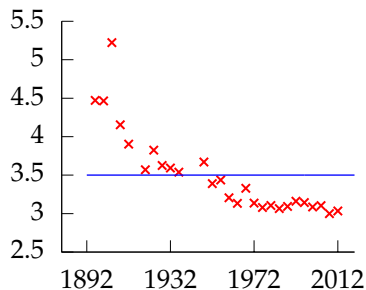Department of Computer Science
Sheffield University

4th November 2014

Review

- Last time: Looked at univariate and multivariate linear regression.
- Showed how to maximize the likelihood of a multivariate model.
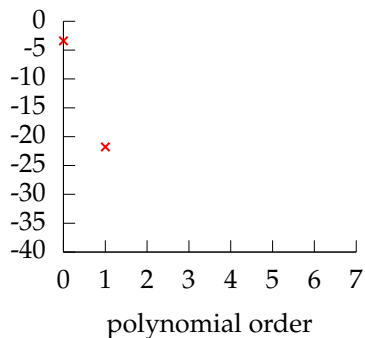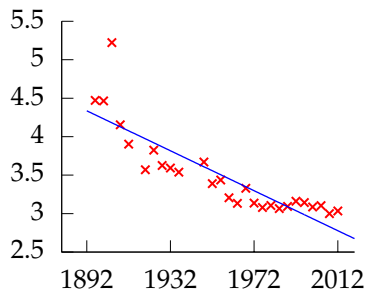- Introduced basis functions to make the model non-linear.

Generalization

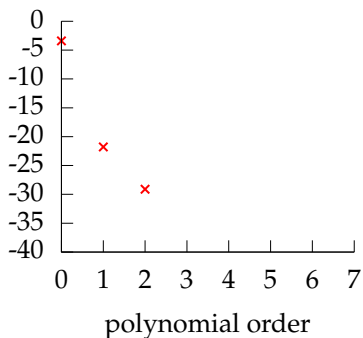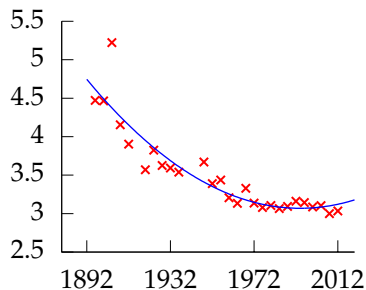# Polynomial Fits to Olympics Data

Left: fit to data, *Right*: model error. Polynomial order 0, model error -3.3989, $\sigma^2 = 0.286$, $\sigma = 0.535$.
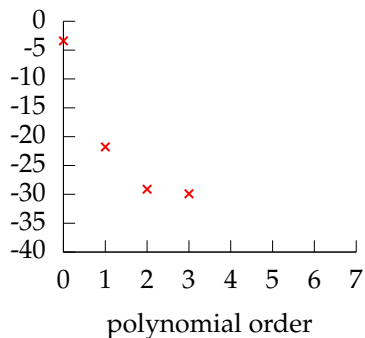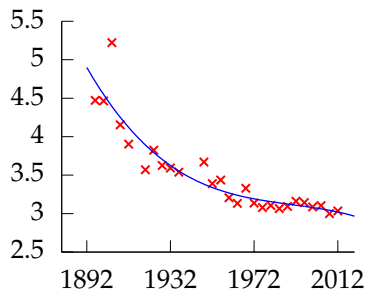
Polynomial Fits to Olympics Data

Left: fit to data, *Right*: model error. Polynomial order 1, model error -21.772, $\sigma^2 = 0.0733$, $\sigma = 0.271$.

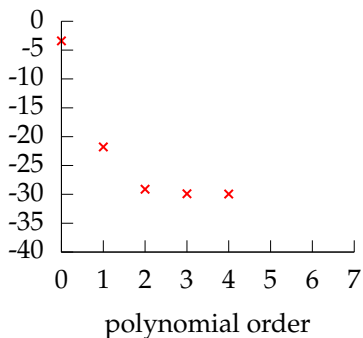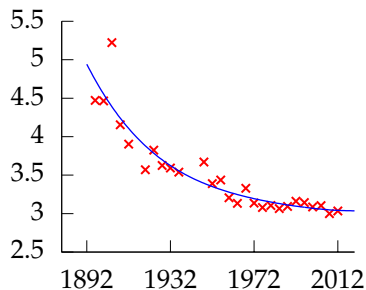# Polynomial Fits to Olympics Data

Left: fit to data, *Right*: model error. Polynomial order 2, model error -29.101, $\sigma^2 = 0.0426$, $\sigma = 0.206$.

Polynomial Fits to Olympics Data

Left: fit to data, *Right*: model error. Polynomial order 3, model error -29.907, $\sigma^2 = 0.0401$, $\sigma = 0.200$.
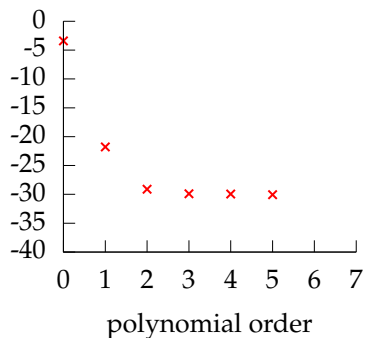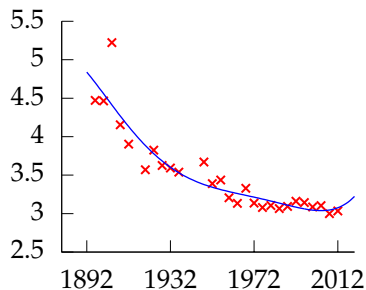
Polynomial Fits to Olympics Data

Left: fit to data, *Right*: model error. Polynomial order 4, model error -29.943, $\sigma^2 = 0.0400$, $\sigma = 0.200$.
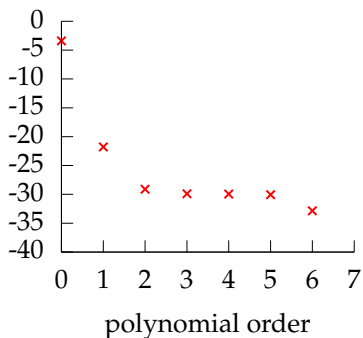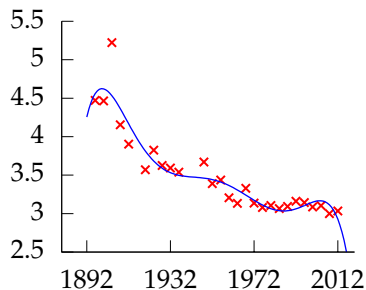
Polynomial Fits to Olympics Data

Left: fit to data, *Right*: model error. Polynomial order 5, model error -30.056, $\sigma^2 = 0.0397$, $\sigma = 0.199$.

Polynomial Fits to Olympics Data

Left: fit to data, *Right*: model error. Polynomial order 6, model error -32.866, $\sigma^2 = 0.0322$, $\sigma = 0.180$.

Overfitting

- 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
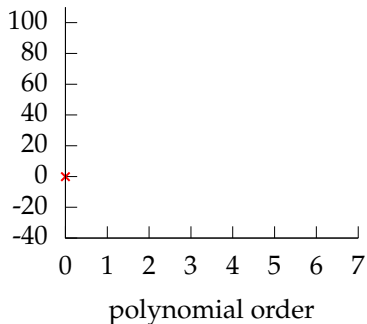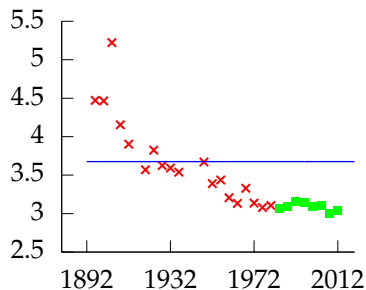
Left: fit to data, *Right*: model error. Polynomial order 0, training error -1.8774, validation error -0.13132, $\sigma^2 = 0.302$, $\sigma = 0.549$.
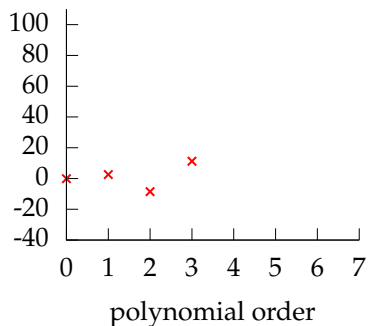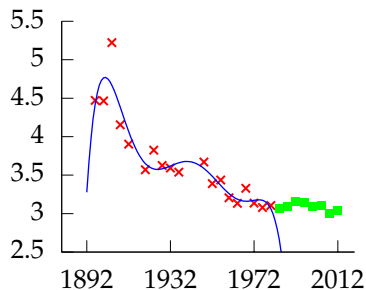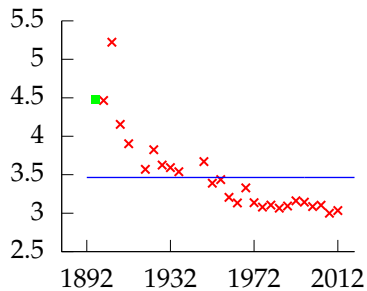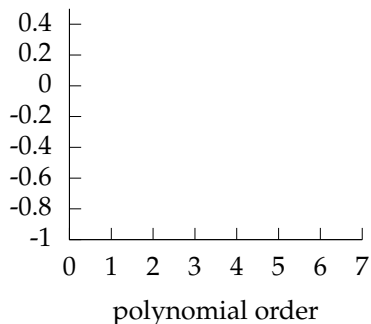
Validation Set
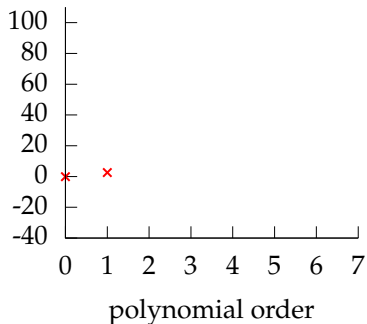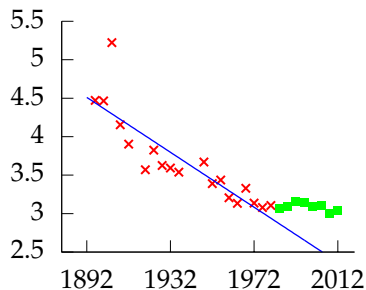
Left: fit to data, *Right*: model error. Polynomial order 1, training error -15.325, validation error 2.5863, $\sigma^2 = 0.0733$, $\sigma = 0.271$.

Validation Set
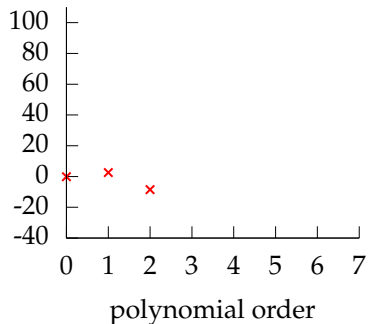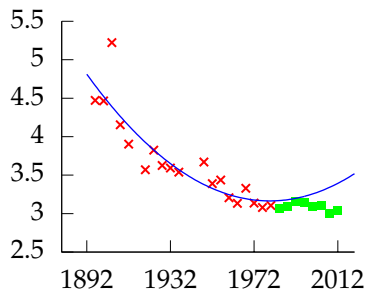
Left: fit to data, *Right*: model error. Polynomial order 2, training error -17.579, validation error -8.4831, $\sigma^2 = 0.0578$, $\sigma = 0.240$.

Validation Set
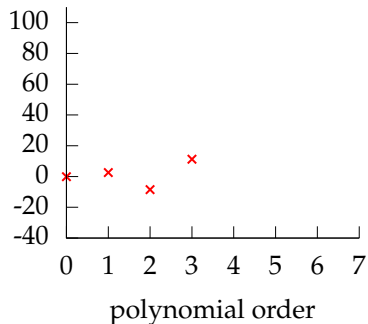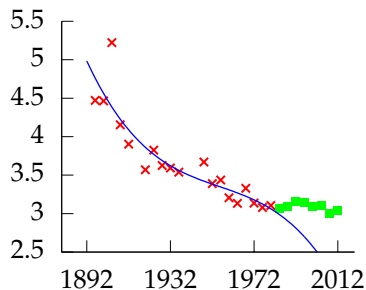
Left: fit to data, *Right*: model error. Polynomial order 3, training error -18.064, validation error 11.27, $\sigma^2 = 0.0549$, $\sigma = 0.234$.

Validation Set
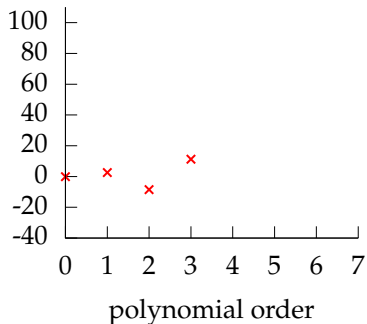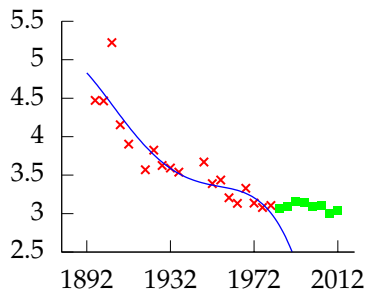
Left: fit to data, *Right*: model error. Polynomial order 4, training error -18.245, validation error 232.92, $\sigma^2 = 0.0539$, $\sigma = 0.232$.

Validation Set
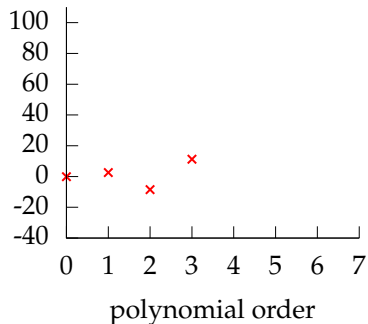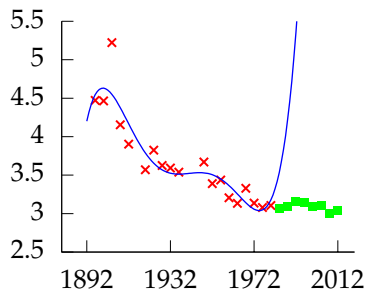
Left: fit to data, *Right*: model error. Polynomial order 5, training error -20.471, validation error 9898.1, $\sigma^2 = 0.0426$, $\sigma = 0.207$.

Validation Set

Left: fit to data, *Right*: model error. Polynomial order 6, training error -22.881, validation error 67775, $\sigma^2 = 0.0331$, $\sigma = 0.182$.

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.
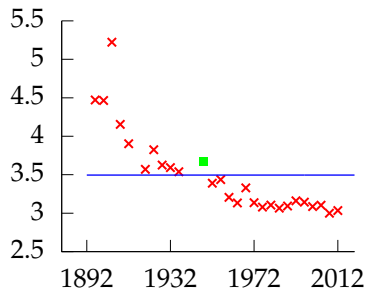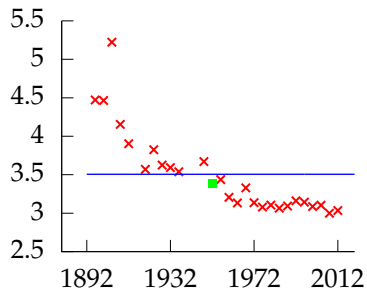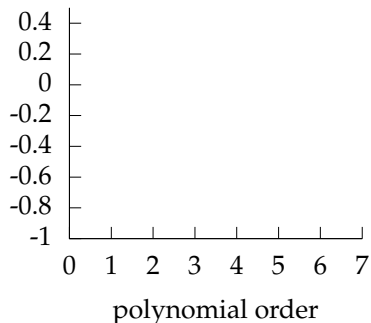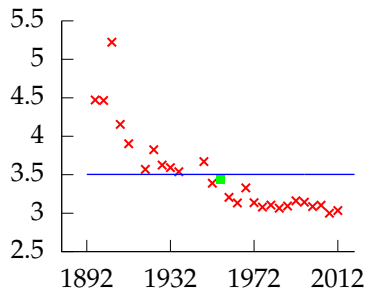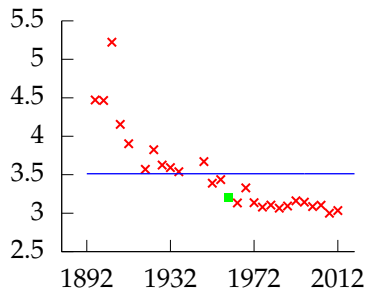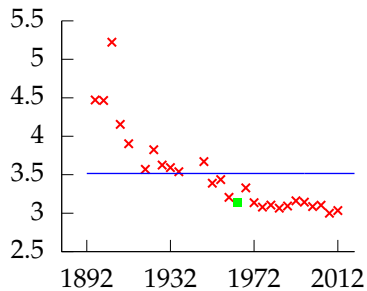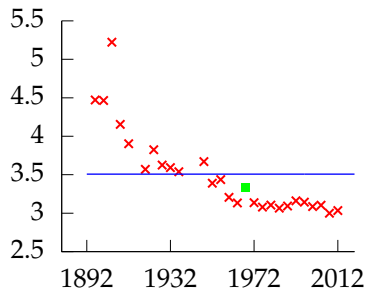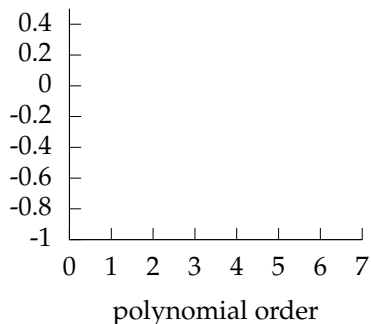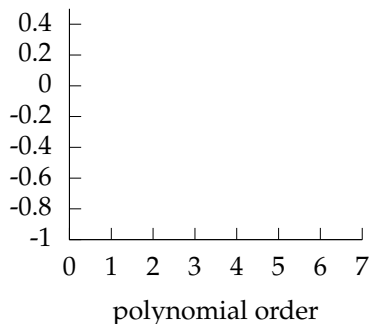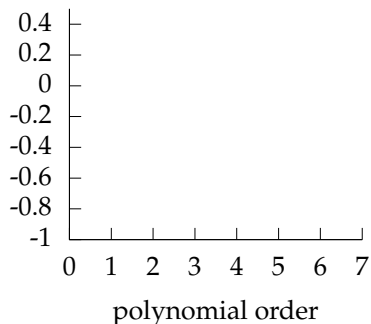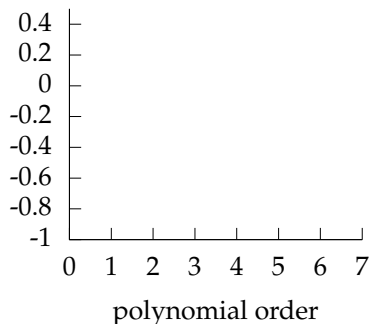
Leave One Out Error

Polynomial order 0, training error -3.346, leave one out error 0.045811.

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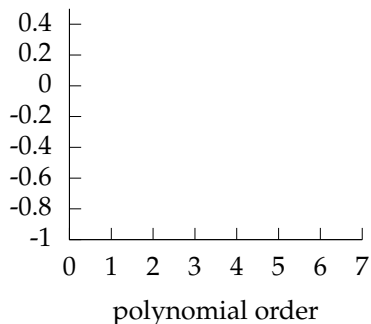Polynomial order 0, training error -3.346, leave one out error 0.045811.
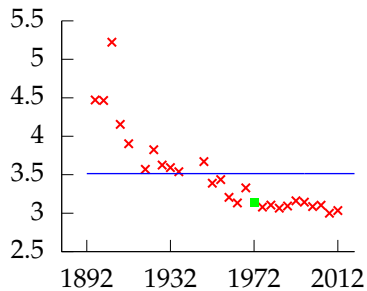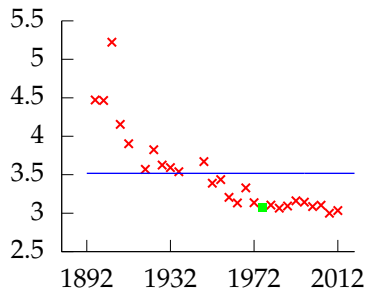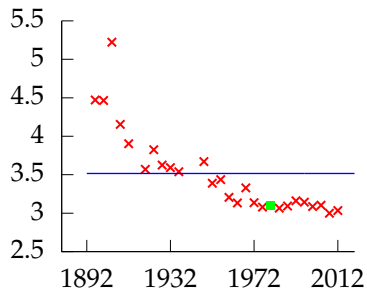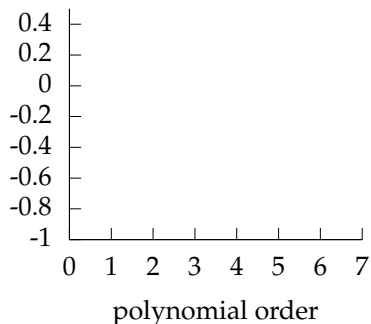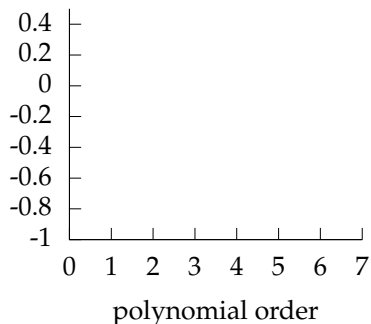
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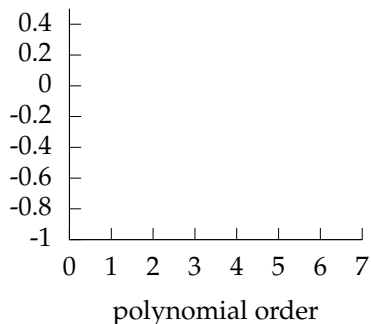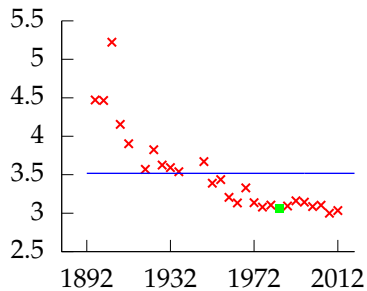
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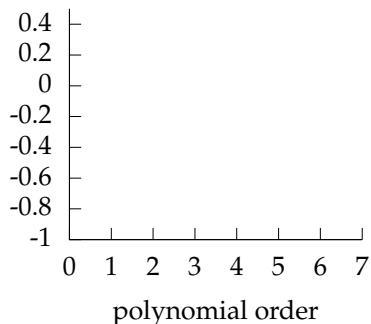
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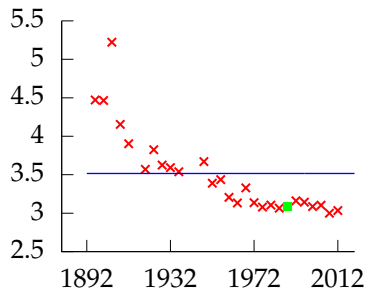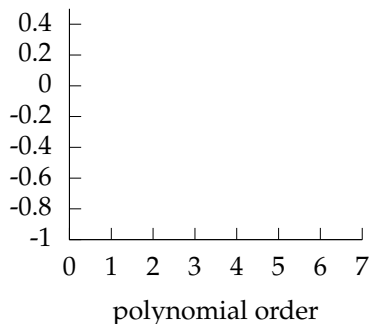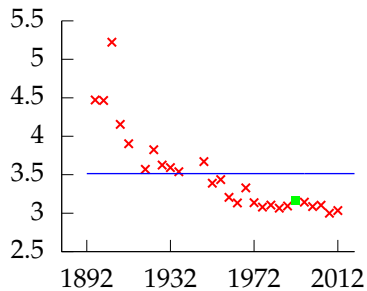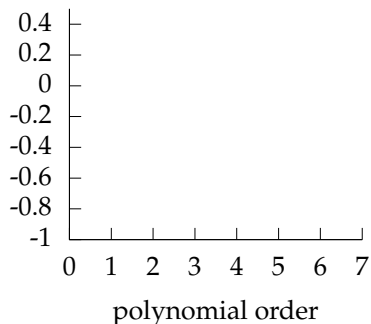
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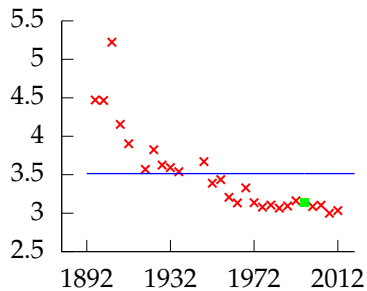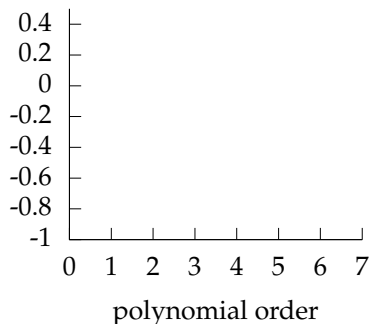
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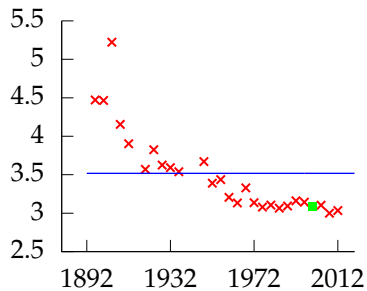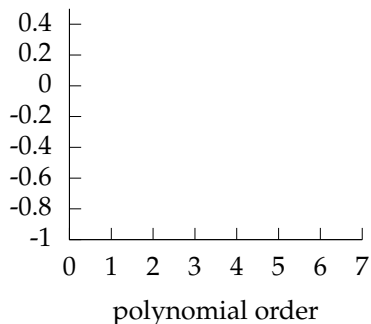

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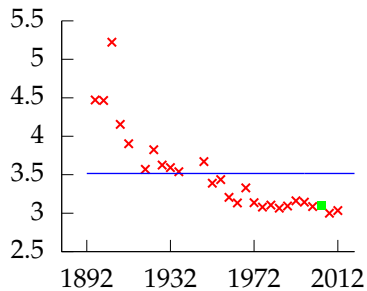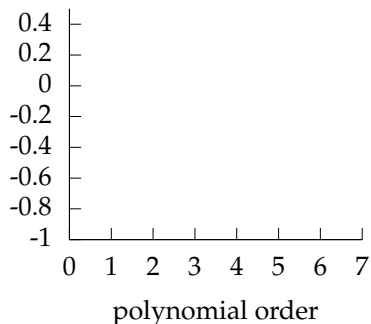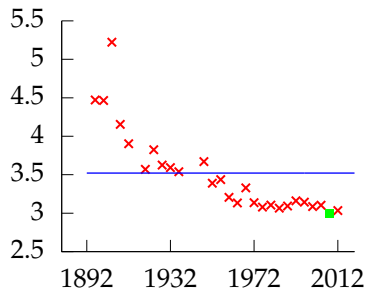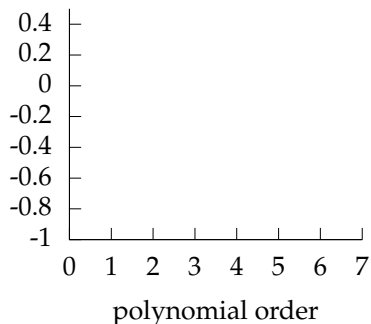

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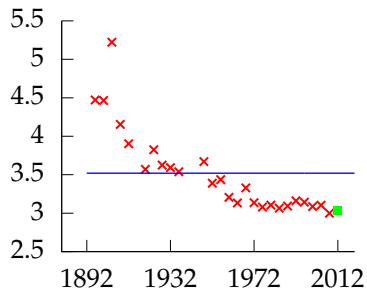

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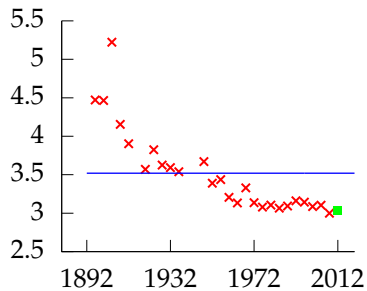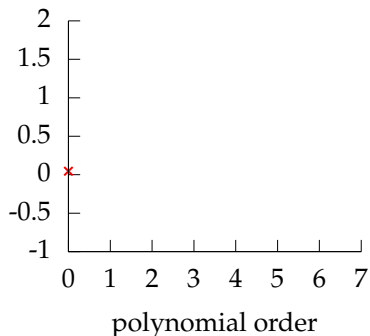

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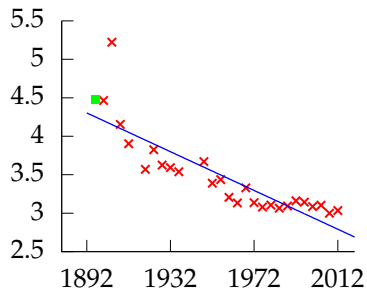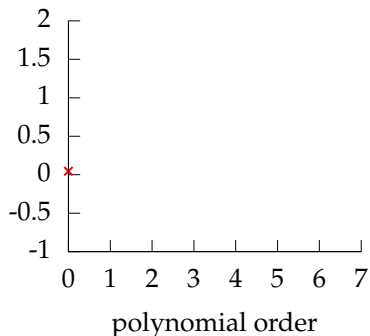
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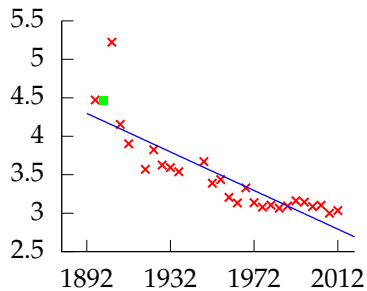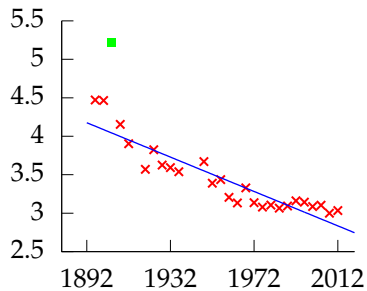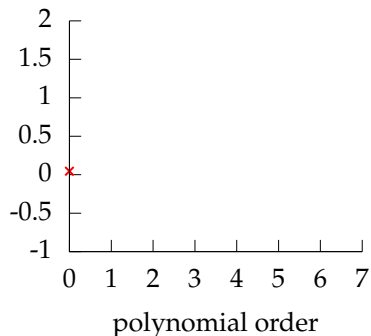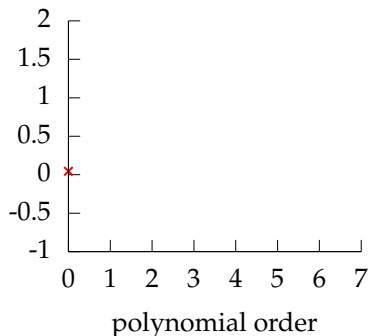
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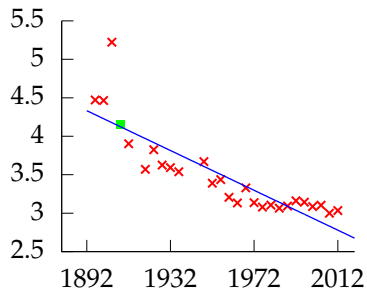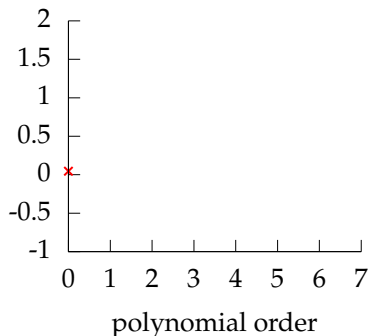
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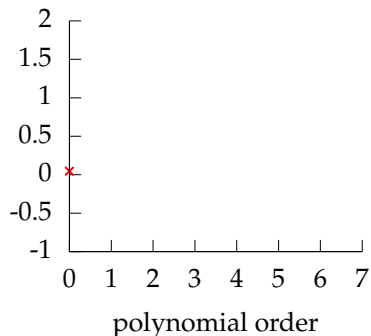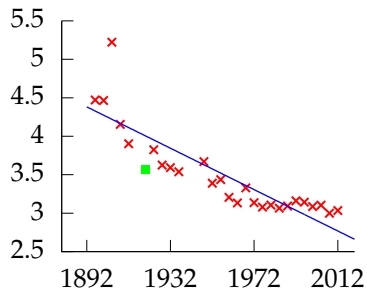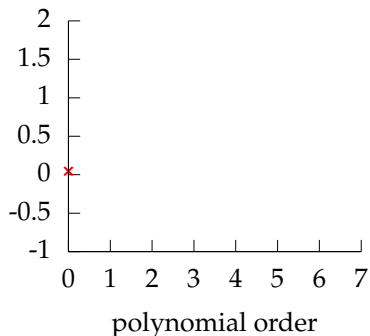Polynomial order 0, training error -3.346, leave one out error 0.045811.

Leave One Out Error

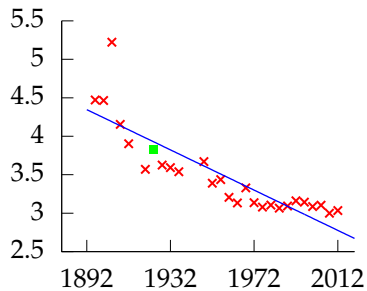Polynomial order 0, training error -3.346, leave one out error 0.045811.
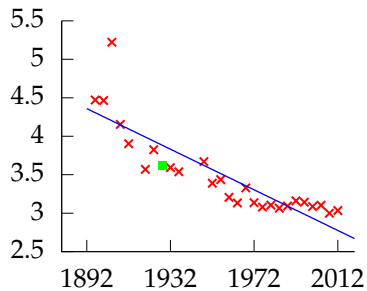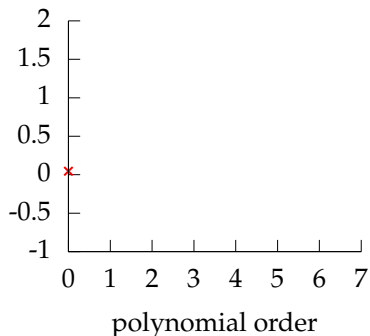
Leave One Out Error

Polynomial order 0, training error -3.346, leave one out error 0.045811.

Leave One Out Error

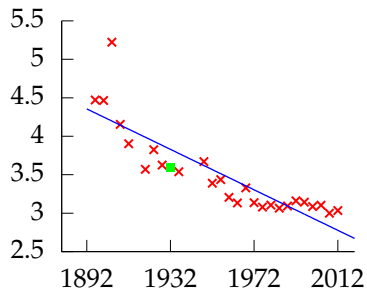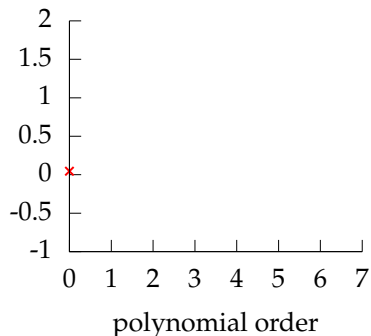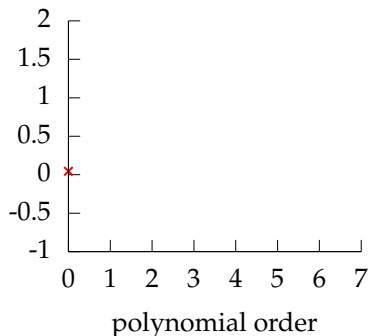Polynomial order 0, training error -3.346, leave one out error 0.045811.

Leave One Out Error

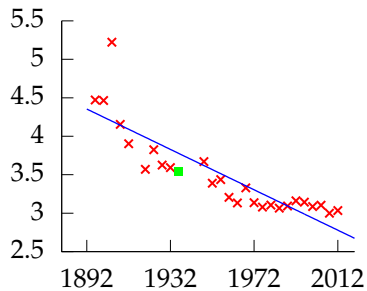Polynomial order 0, training error -3.346, leave one out error 0.045811.
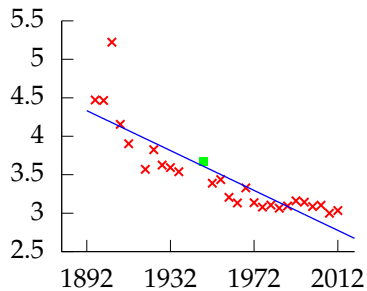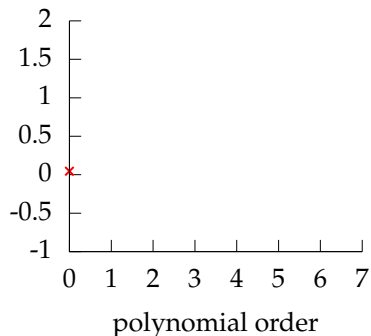
Leave One Out Error

Polynomial order 0, training error -3.346, leave one out error
0.045811.

Leave One Out Error

Polynomial order 0, training error -3.346, leave one out error 0.045811.

Leave One Out Error

Polynomial order 0, training error -3.346, leave one out error 0.045811.

Leave One Out Error

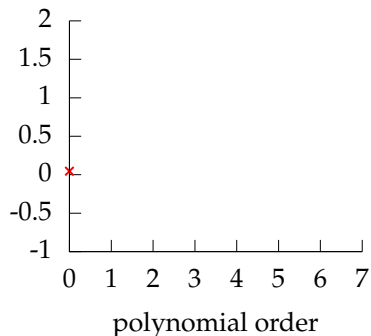Polynomial order 0, training error -3.346, leave one out error 0.045811.

Leave One Out Error

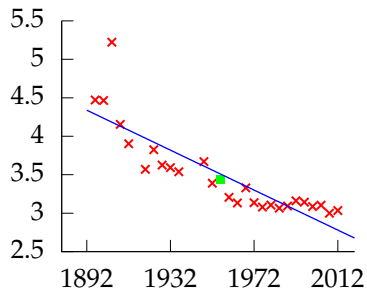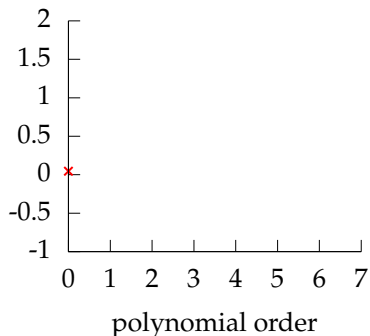Polynomial order 1, training error -21.183, leave one out error -0.15413.

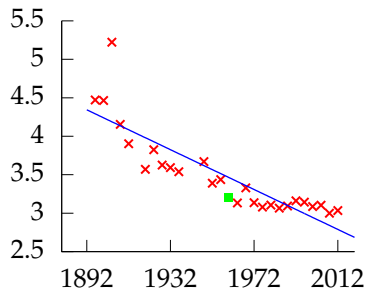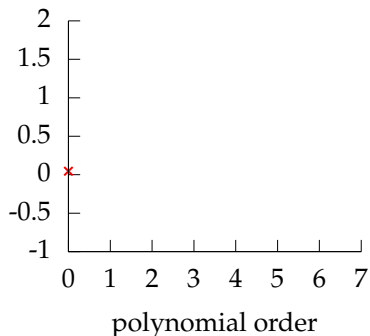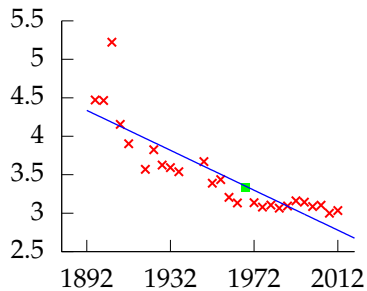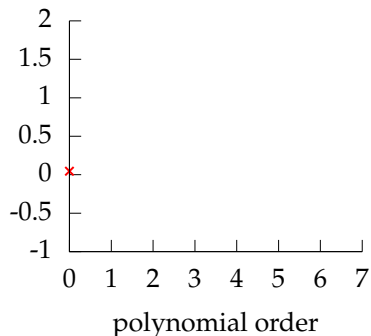Polynomial order 1, training error -21.183, leave one out error -0.15413.
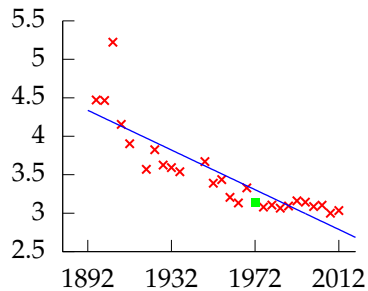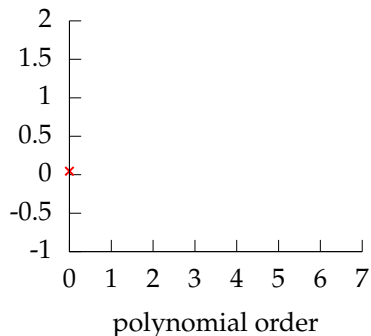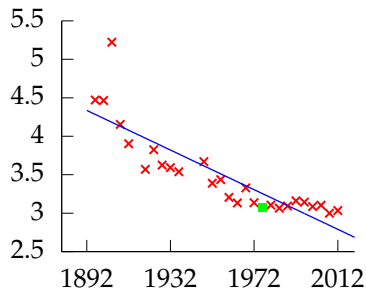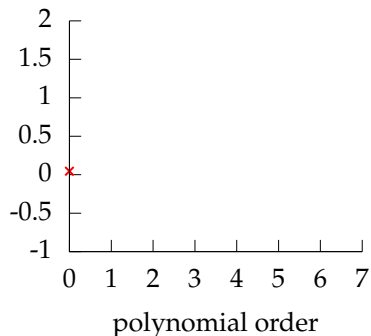
Leave One Out Error

Polynomial order 1, training error -21.183, leave one out error -0.15413.
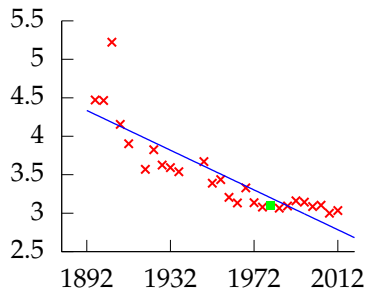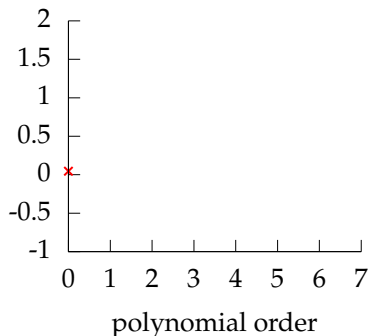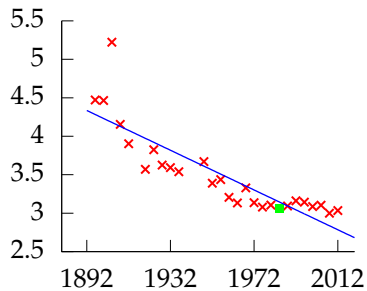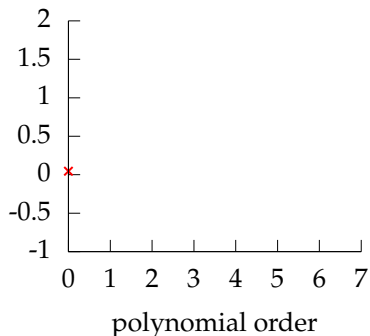
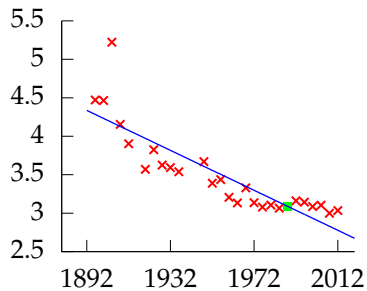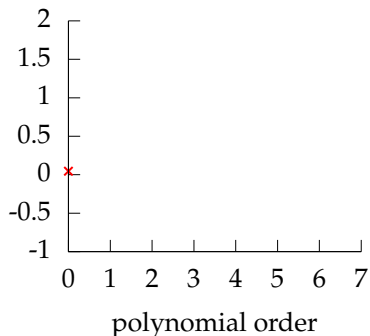# Leave One Out Error

Polynomial order 1, training error -21.183, leave one out error -0.15413.

Leave One Out Error

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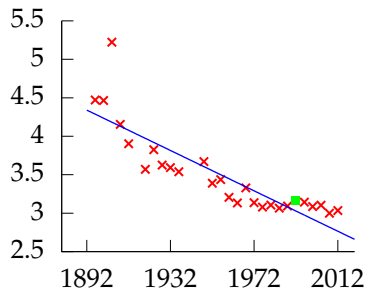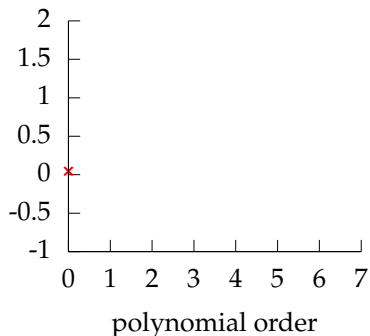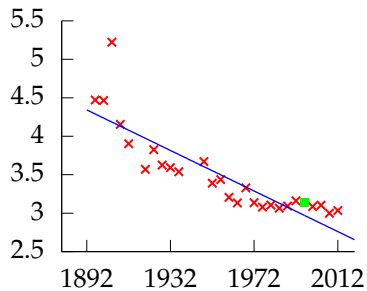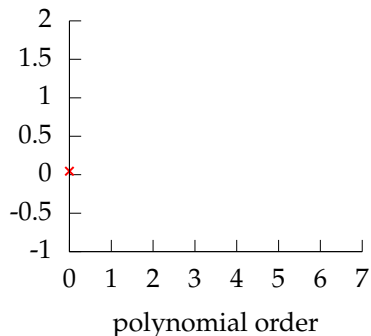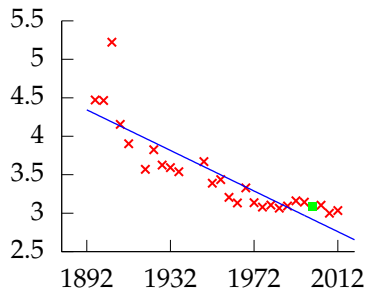Polynomial order 1, training error -21.183, leave one out error -0.15413.

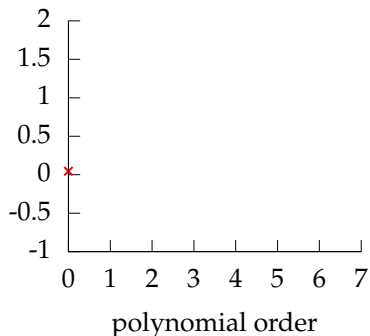Polynomial order 1, training error -21.183, leave one out error -0.15413.

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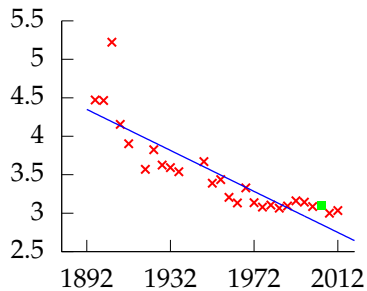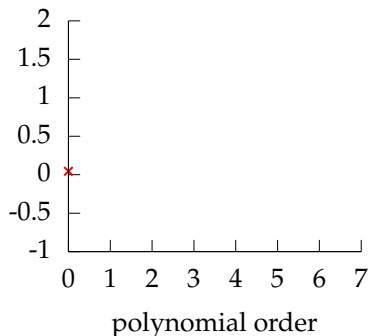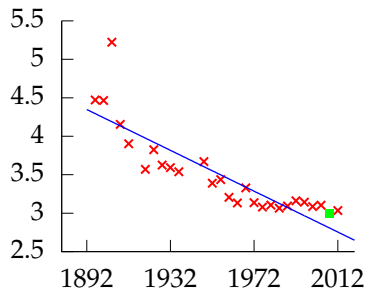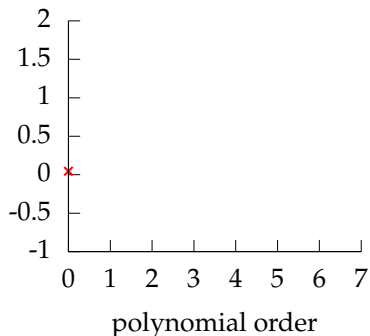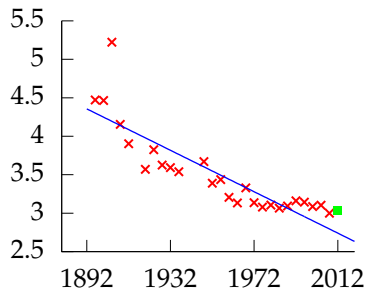
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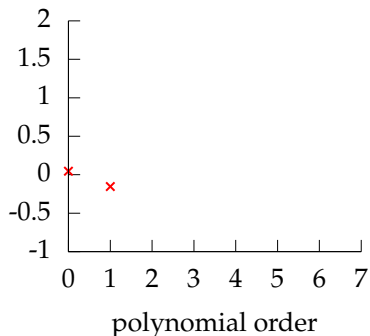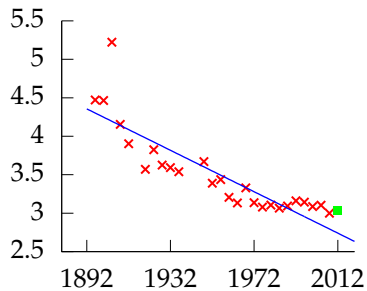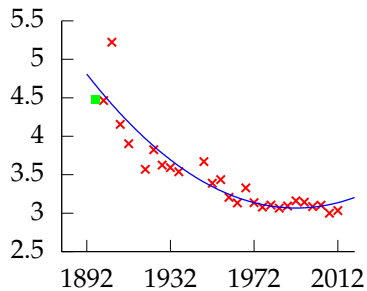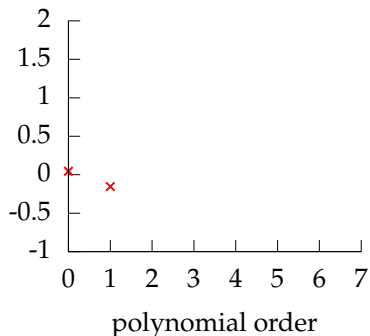

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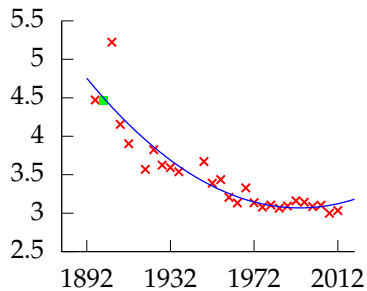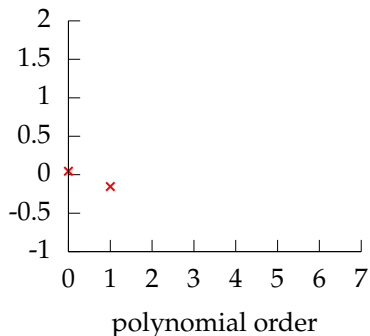Polynomial order 1, training error -21.183, leave one out error -0.15413.

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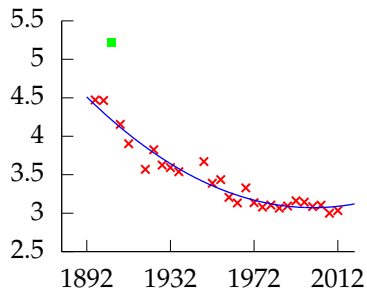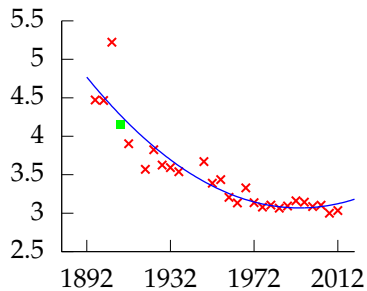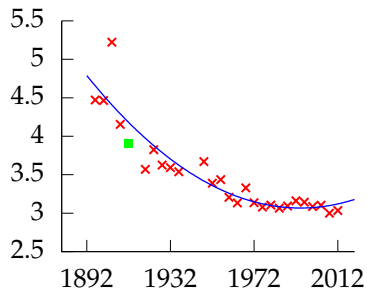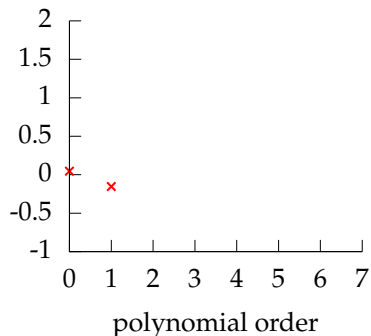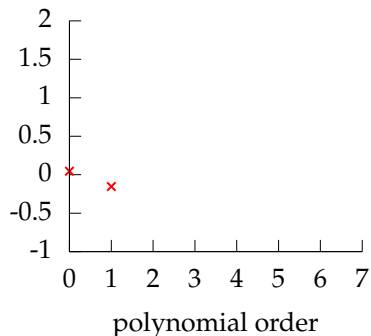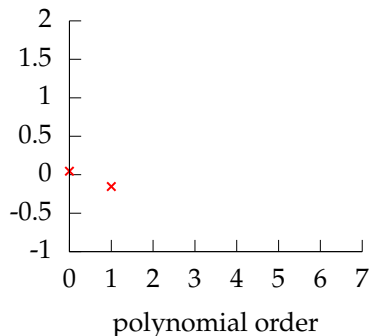
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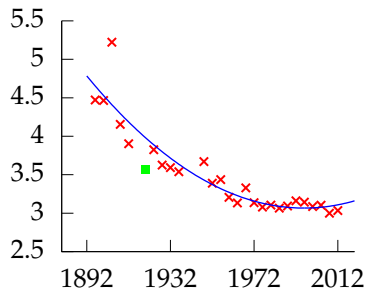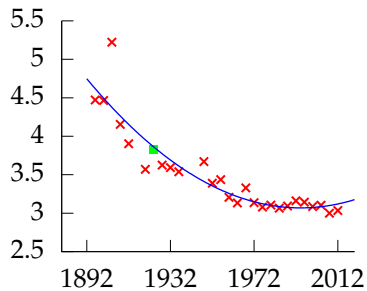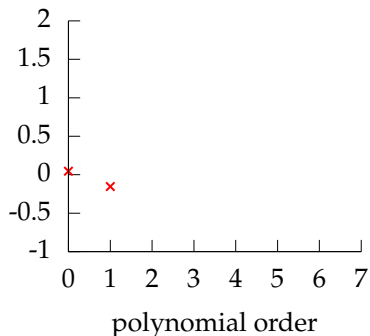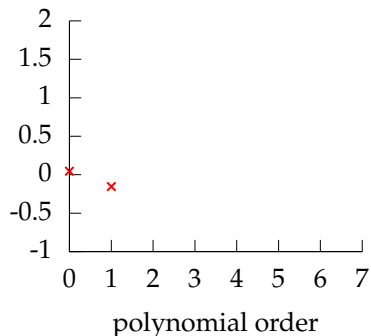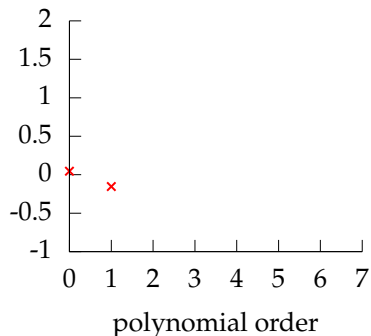Polynomial order 1, training error -21.183, leave one out error -0.15413.

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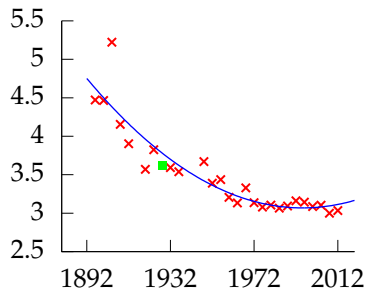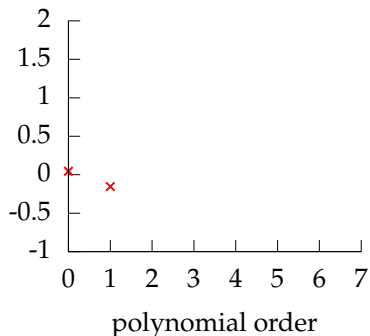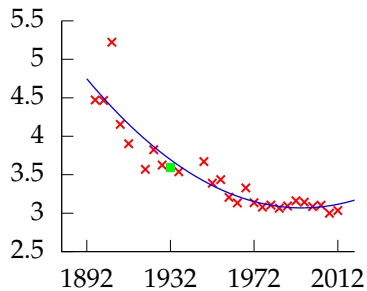
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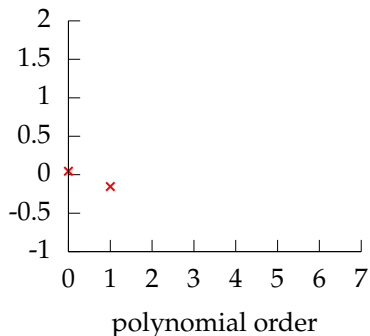
Leave One Out Error

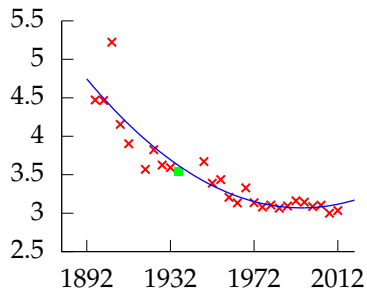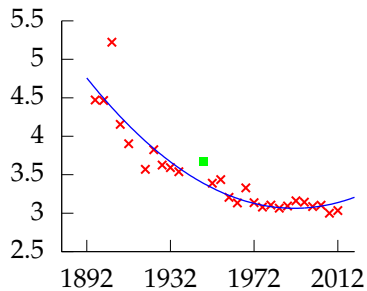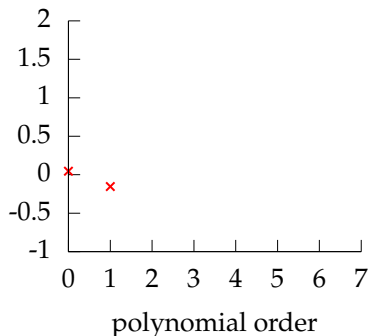Polynomial order 1, training error -21.183, leave one out error -0.15413.
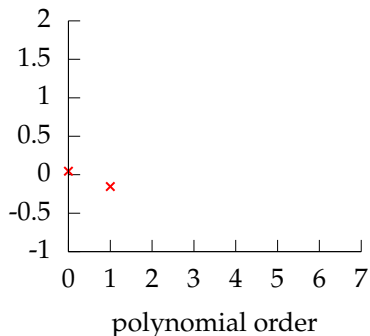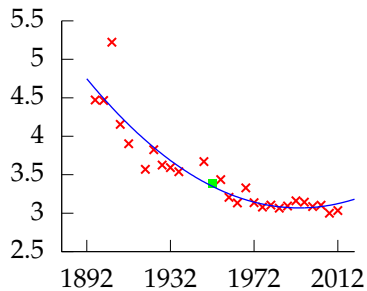
Polynomial order 2, training error -28.403, leave one out error 0.34669.
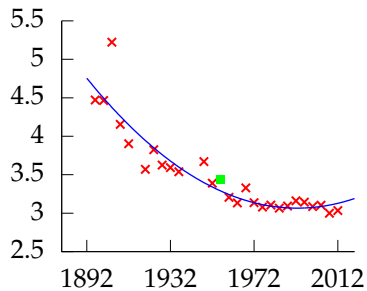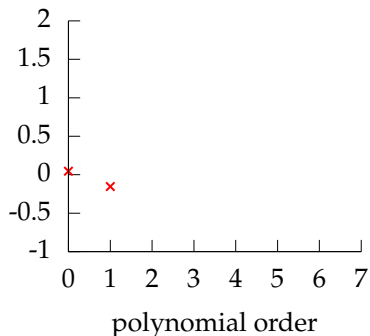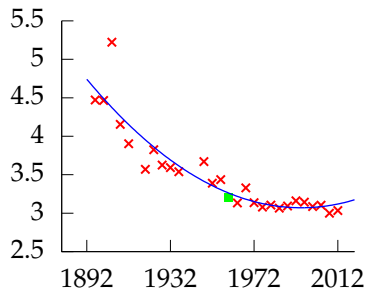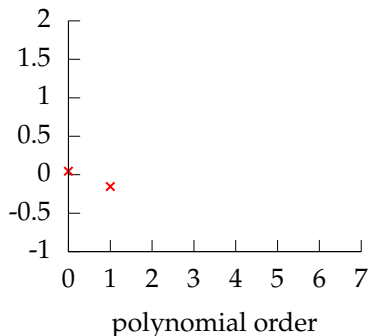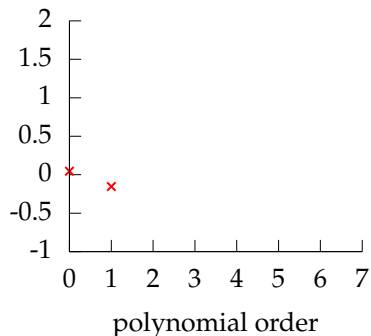
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Polynomial order 2, training error -28.403, leave one out error 0.34669.

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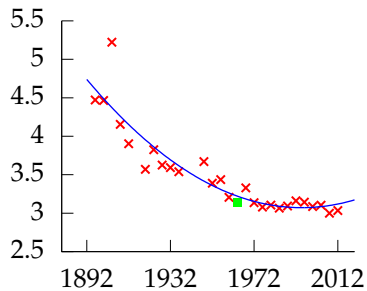Polynomial order 2, training error -28.403, leave one out error 0.34669.
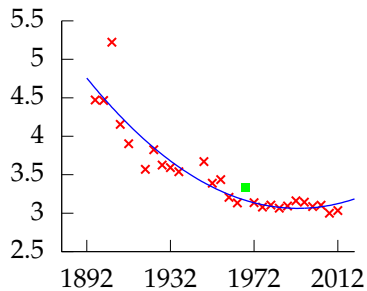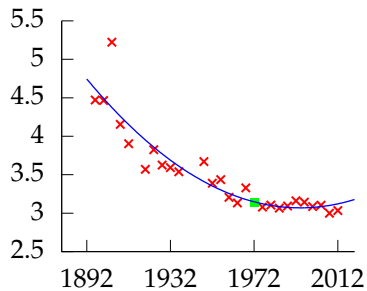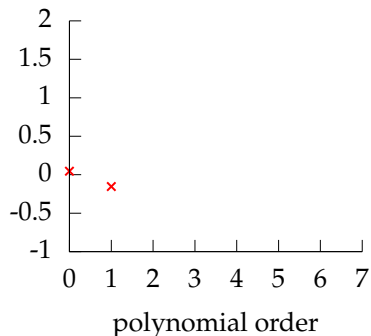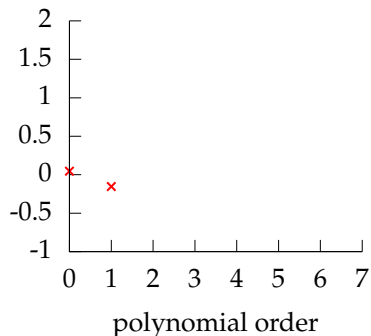
Polynomial order 2, training error -28.403, leave one out error 0.34669.

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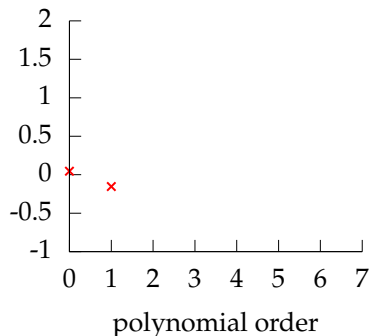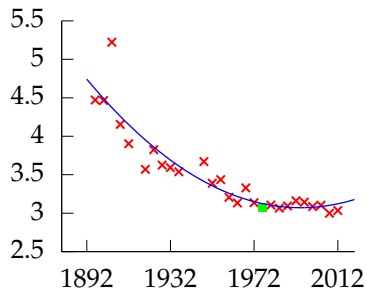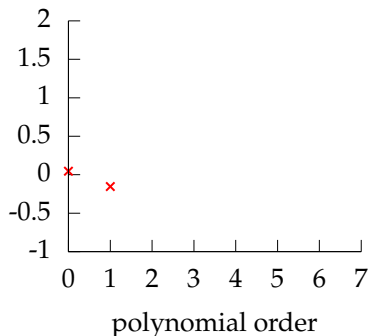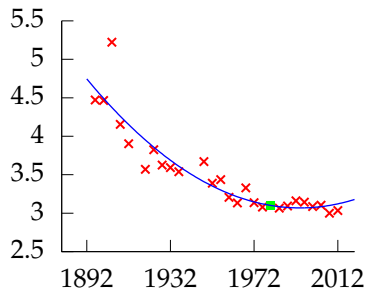
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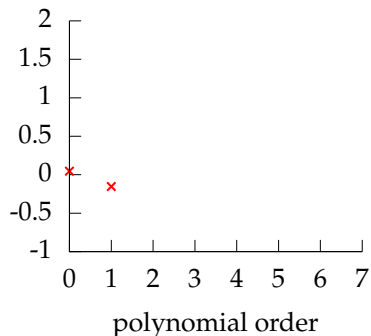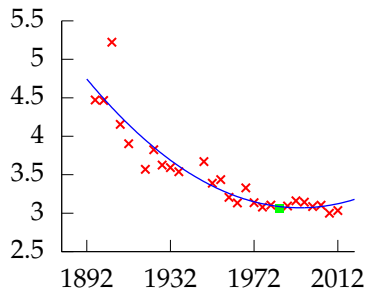
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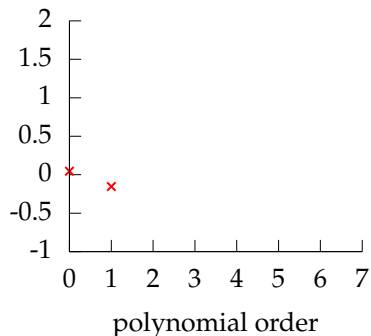
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Polynomial order 2, training error -28.403, leave one out error 0.34669.

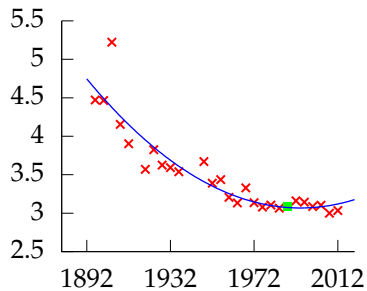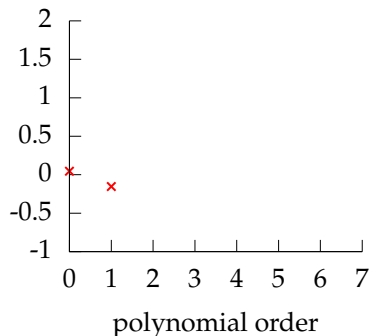Polynomial order 2, training error -28.403, leave one out error 0.34669.
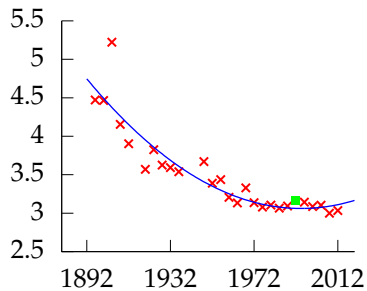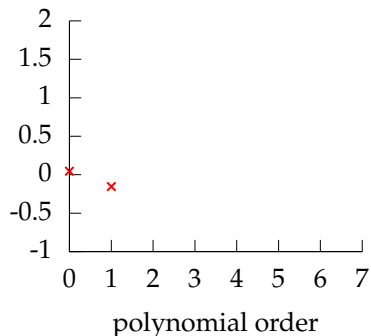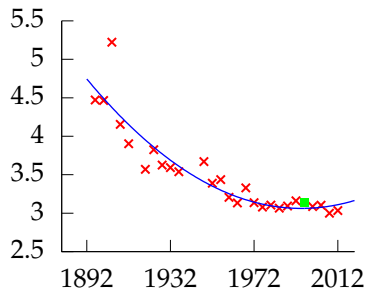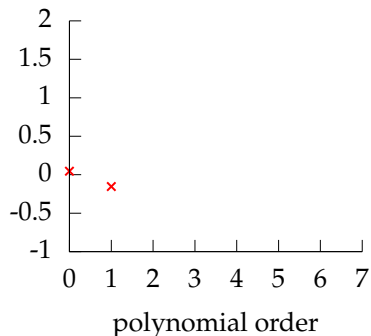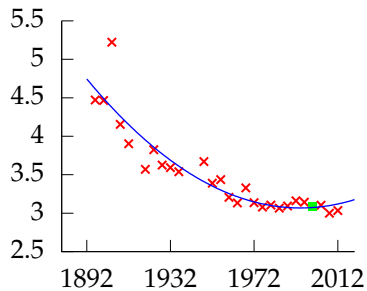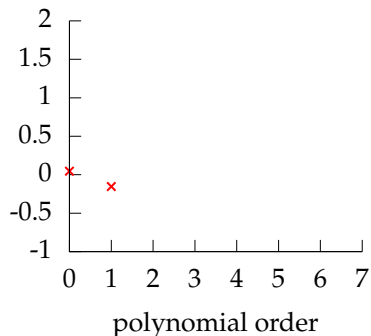
Leave One Out Error

Polynomial order 2, training error -28.403, leave one out error 0.34669.
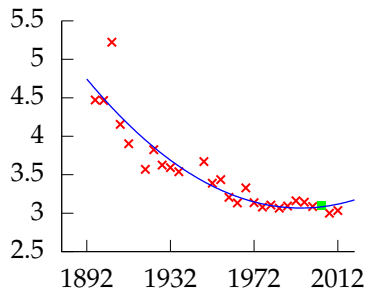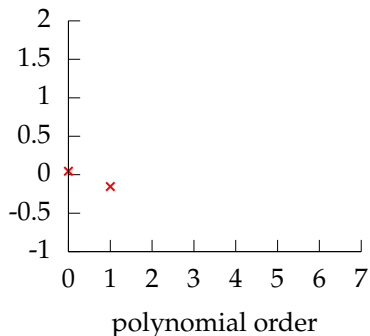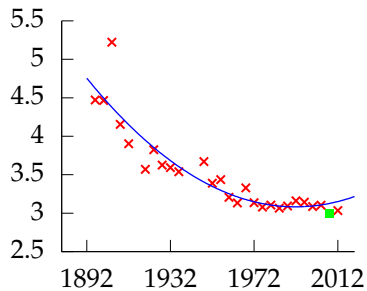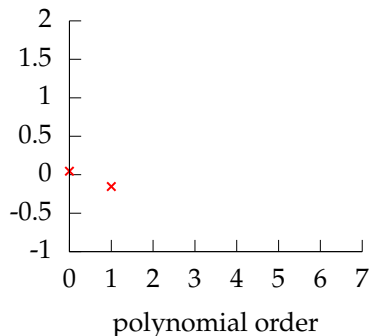
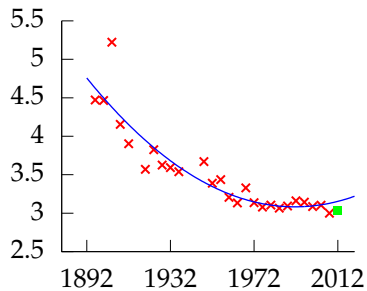# Leave One Out Error

Polynomial order 2, training error -28.403, leave one out error 0.34669.

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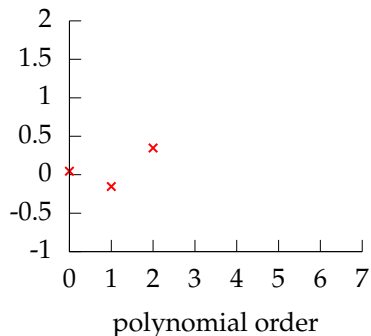Polynomial order 2, training error -28.403, leave one out error 0.34669.
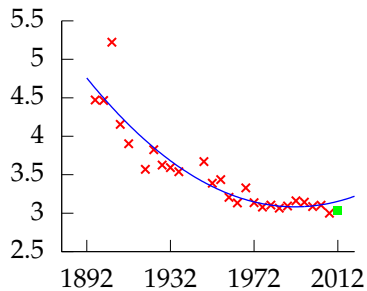
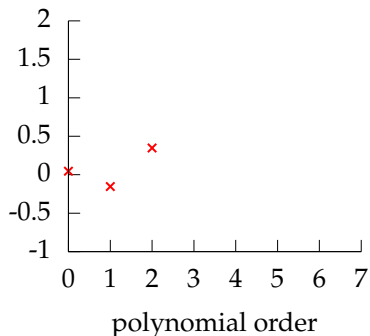Polynomial order 2, training error -28.403, leave one out error 0.34669.

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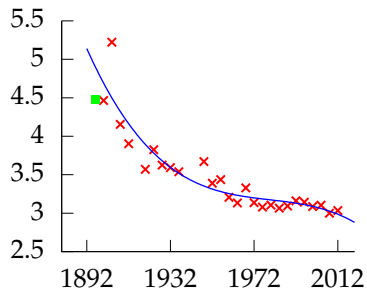Polynomial order 2, training error -28.403, leave one out error 0.34669.
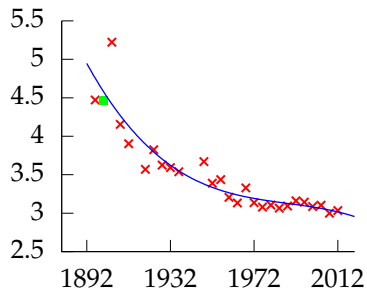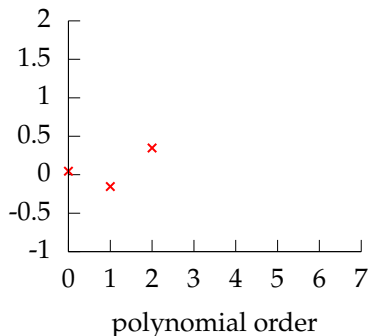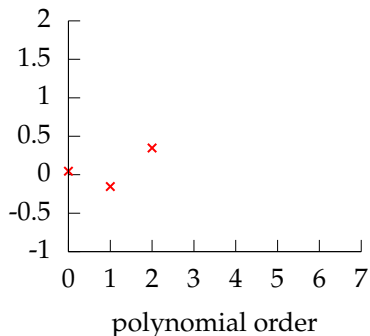
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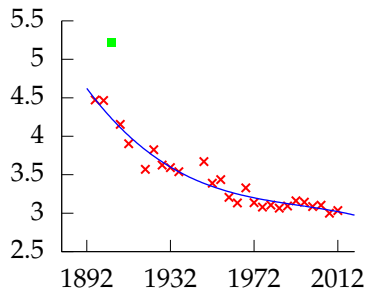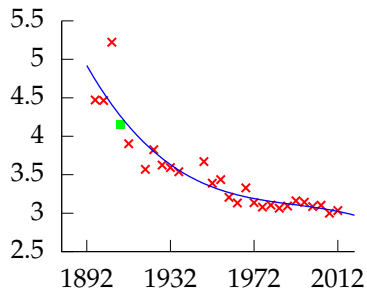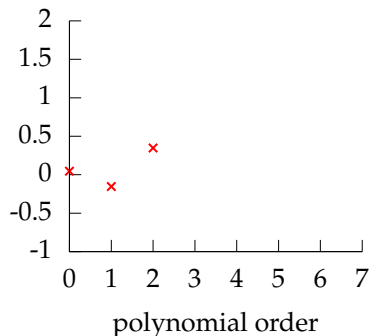Polynomial order 2, training error -28.403, leave one out error 0.34669.

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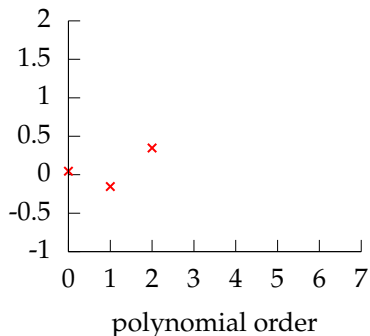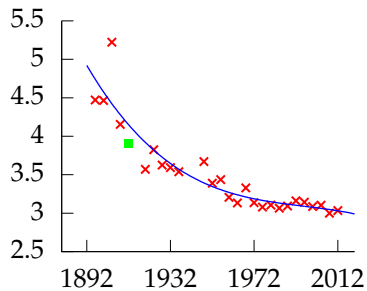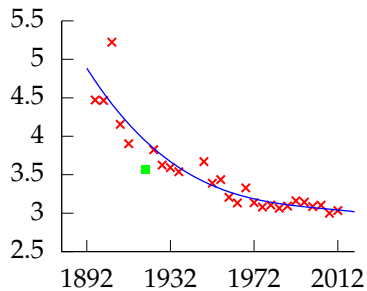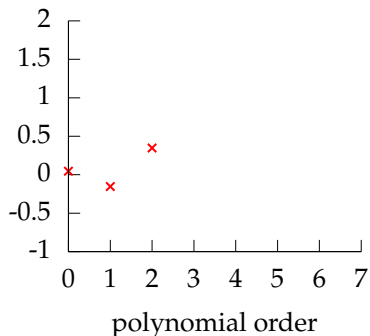
Leave One Out Error

Polynomial order 2, training error -28.403, leave one out error 0.34669.

Leave One Out Error

Polynomial order 3, training error -29.223, leave one out error 0.51621.

Leave One Out Error

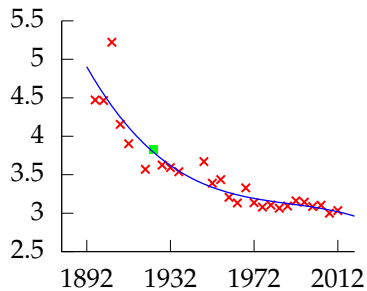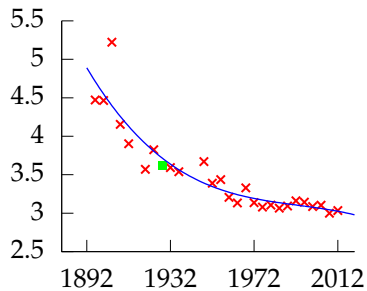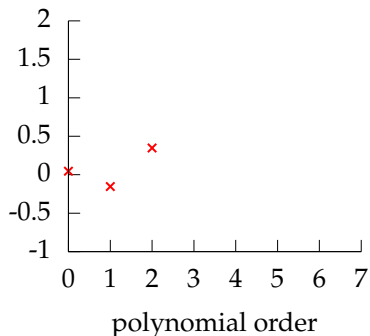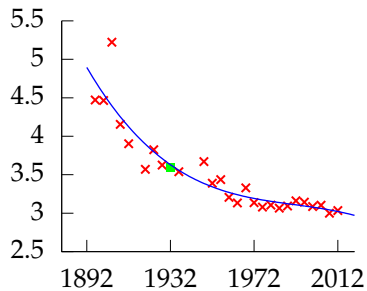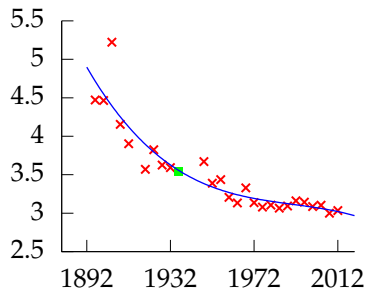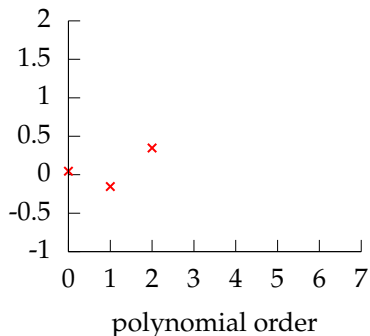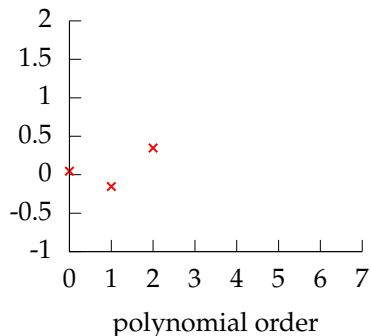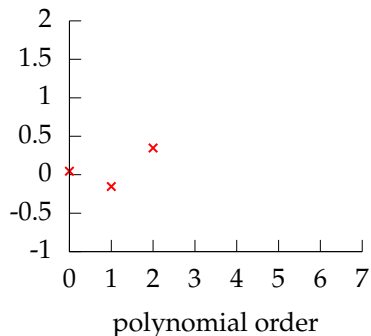Polynomial order 3, training error -29.223, leave one out error 0.51621.
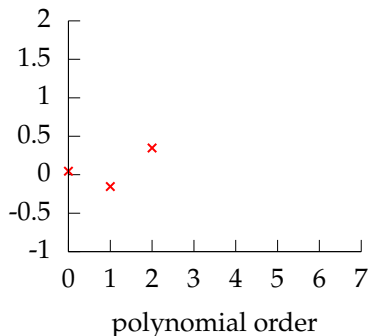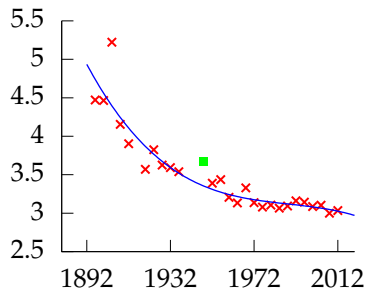
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Polynomial order 3, training error -29.223, leave one out error 0.51621.
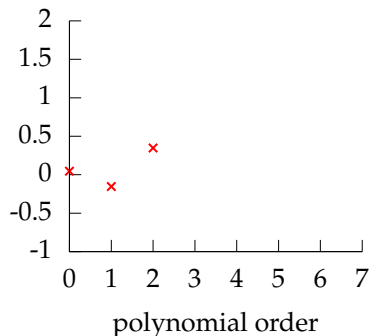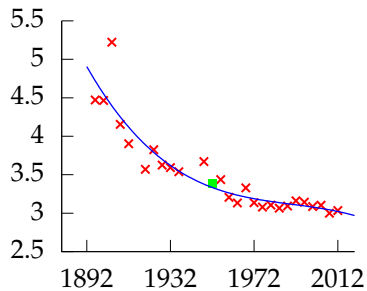
Leave One Out Error

Polynomial order 3, training error -29.223, leave one out error 0.51621.

Leave One Out Error
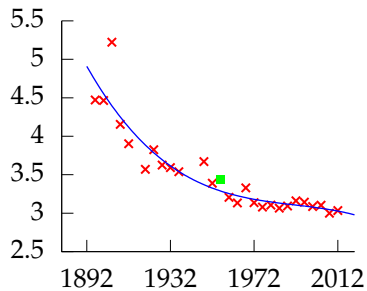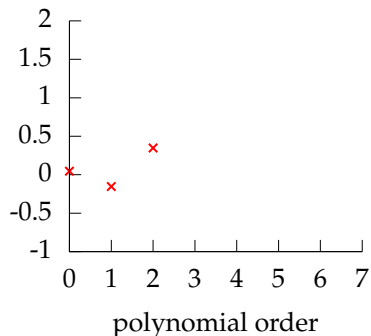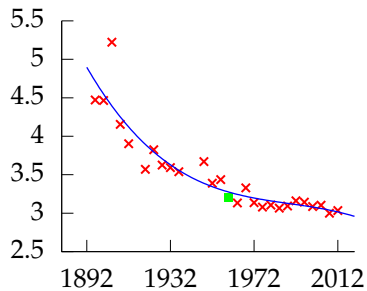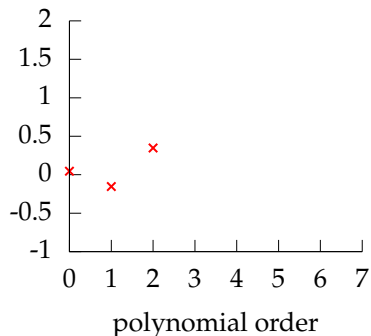

Polynomial order 3, training error -29.223, leave one out error 0.51621.

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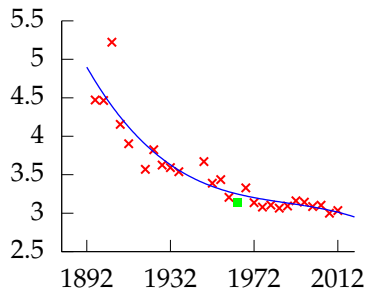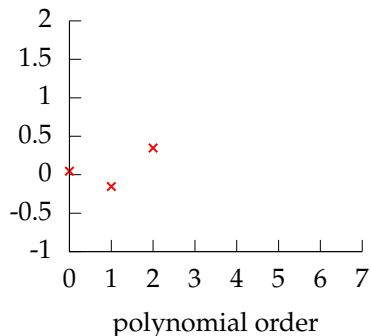Polynomial order 3, training error -29.223, leave one out error 0.51621.

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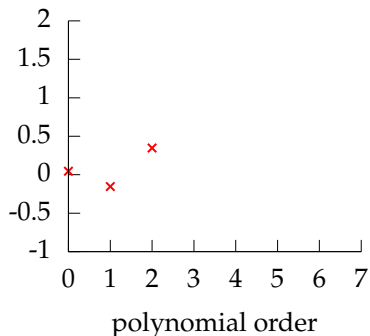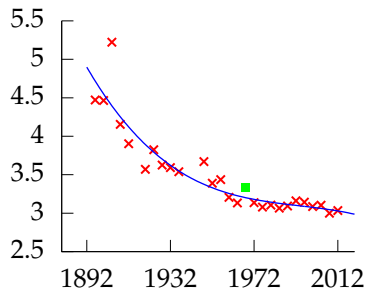Polynomial order 3, training error -29.223, leave one out error 0.51621.

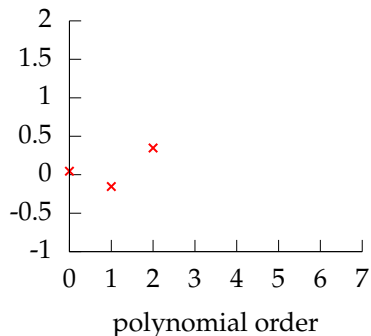Polynomial order 3, training error -29.223, leave one out error 0.51621.

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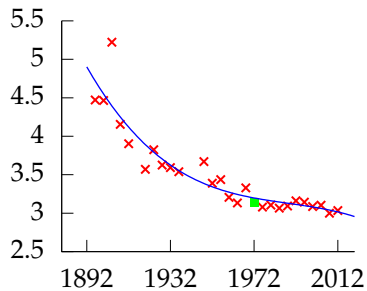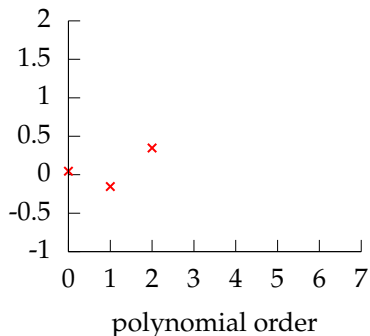
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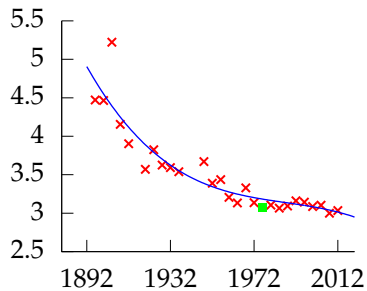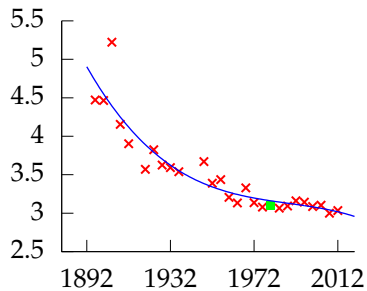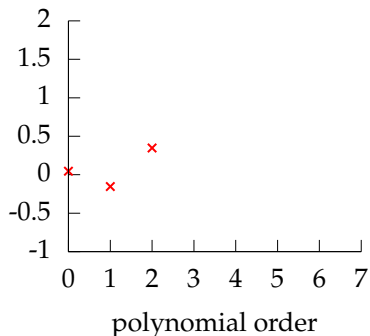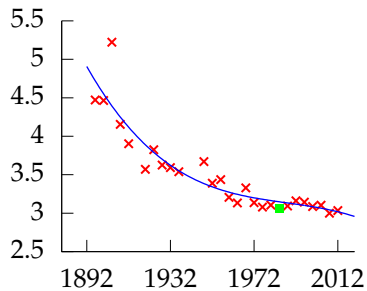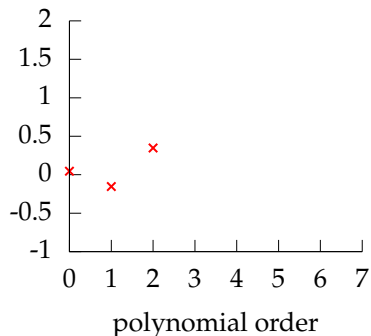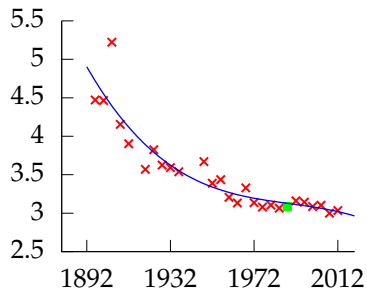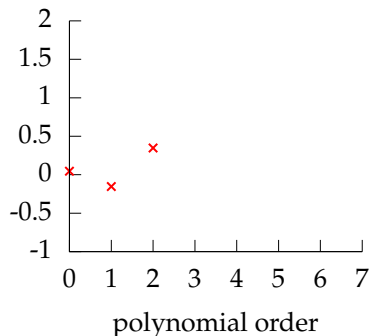Polynomial order 3, training error -29.223, leave one out error 0.51621.

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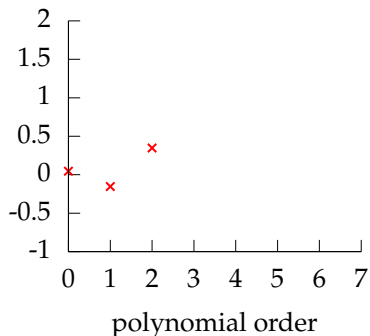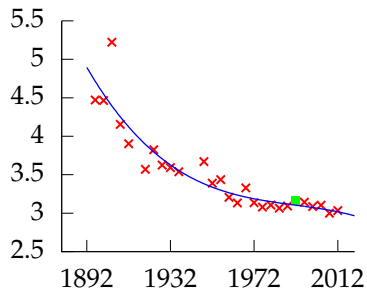

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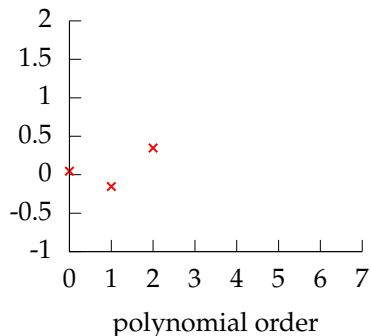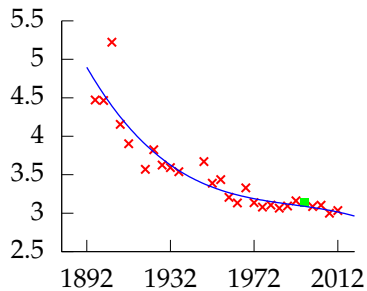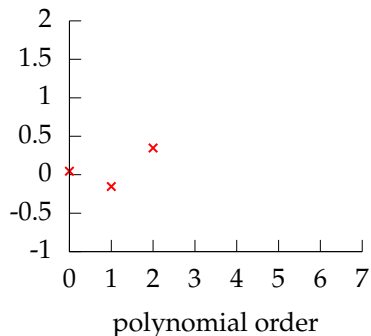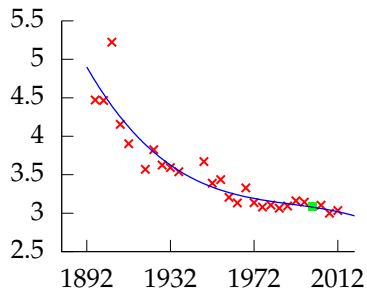
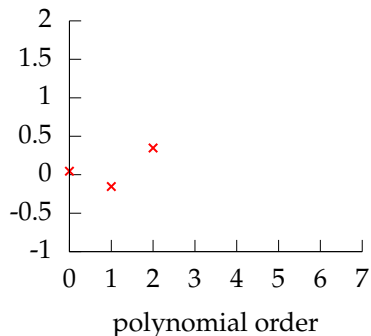Polynomial order 3, training error -29.223, leave one out error 0.51621.

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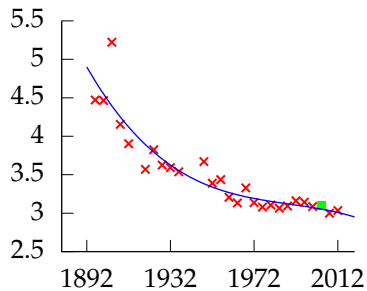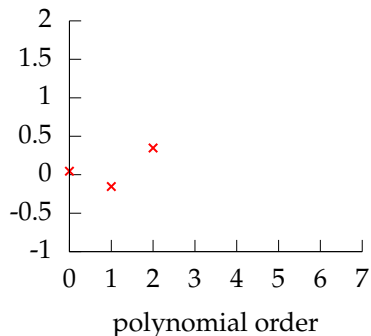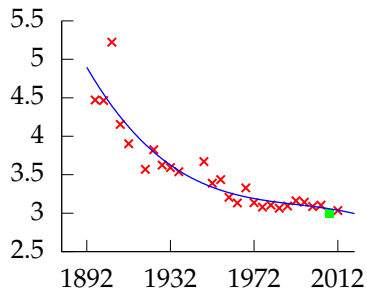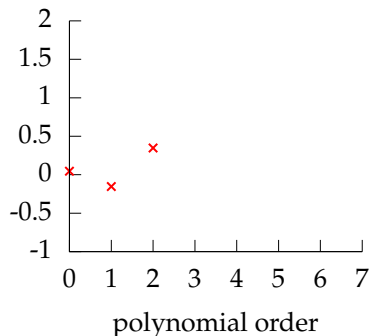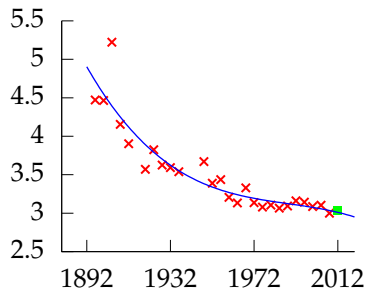
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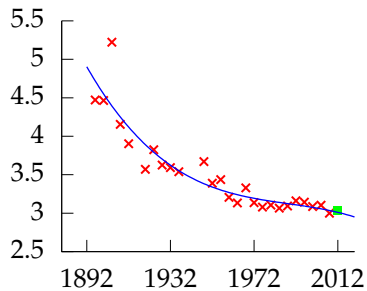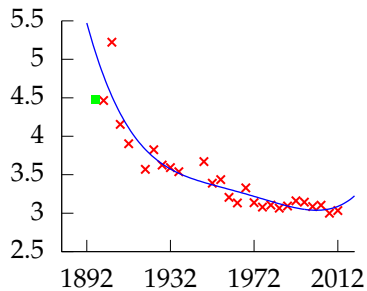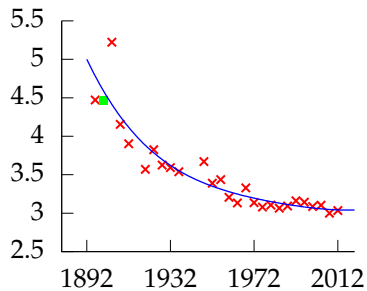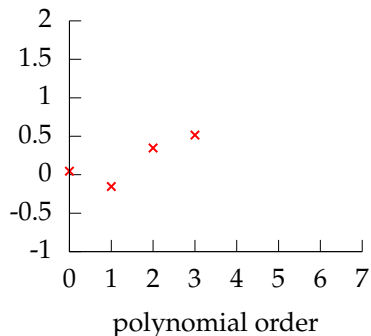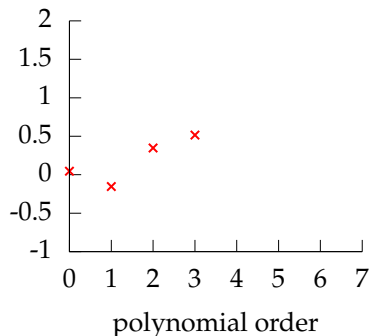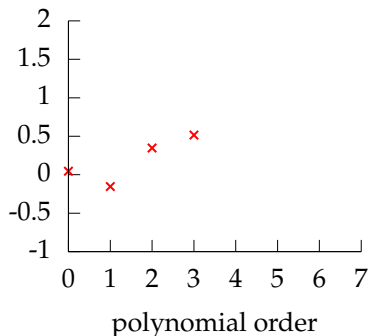Polynomial order 3, training error -29.223, leave one out error 0.51621.

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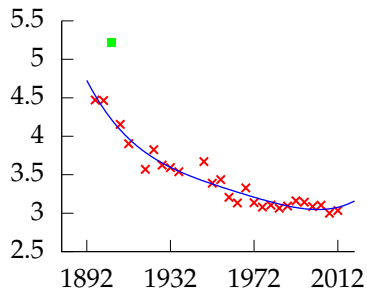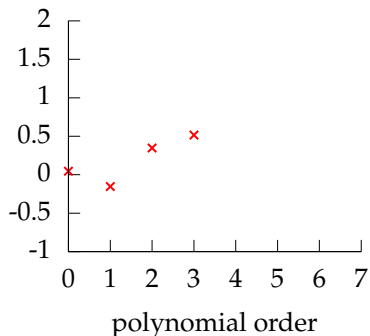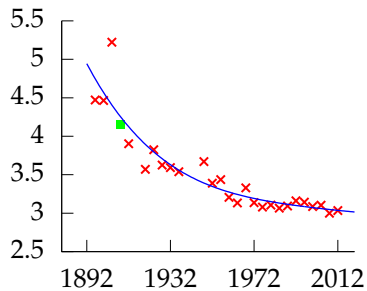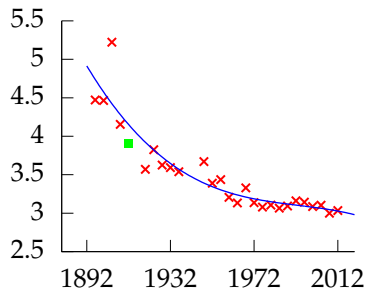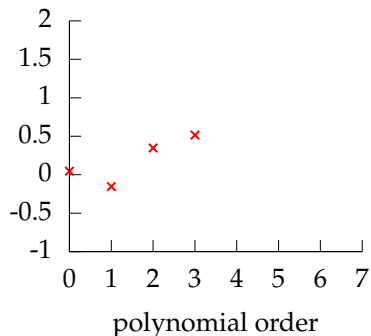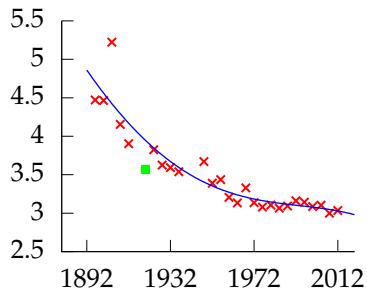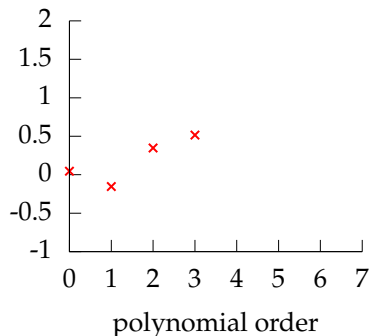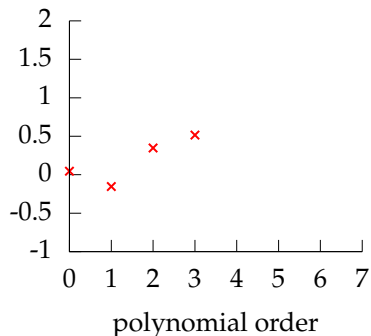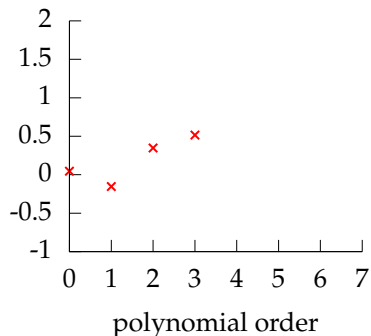
Leave One Out Error

Polynomial order 4, training error -29.324, leave one out error 0.84844.

Leave One Out Error

Polynomial order 4, training error -29.324, leave one out error 0.84844.
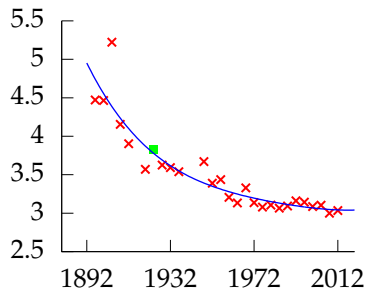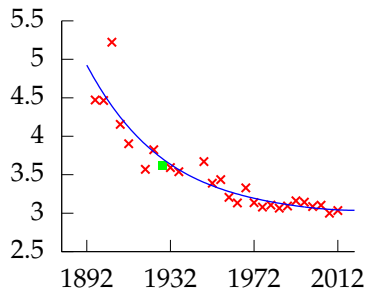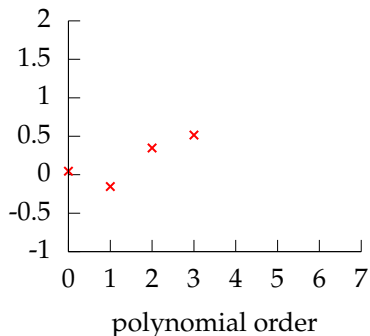
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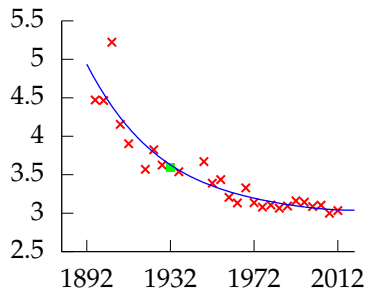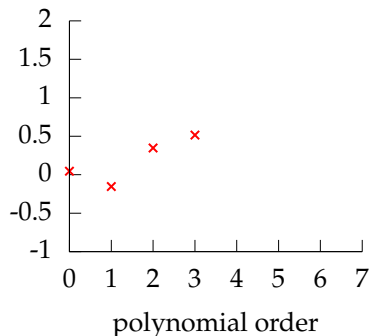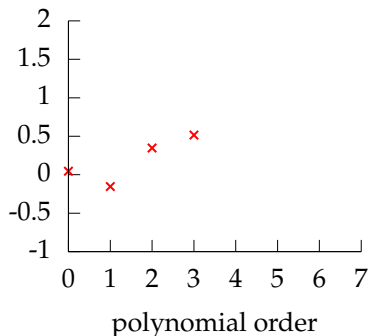

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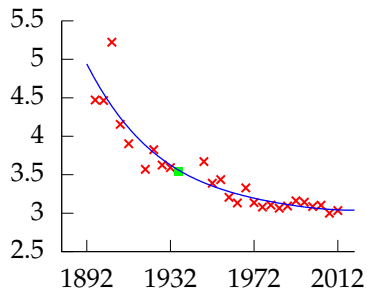Polynomial order 4, training error -29.324, leave one out error 0.84844.

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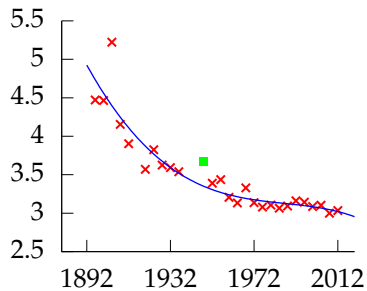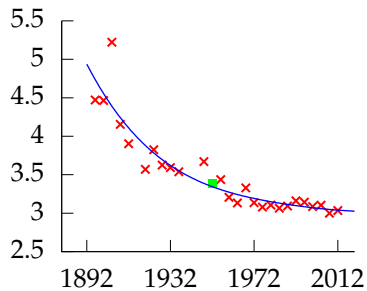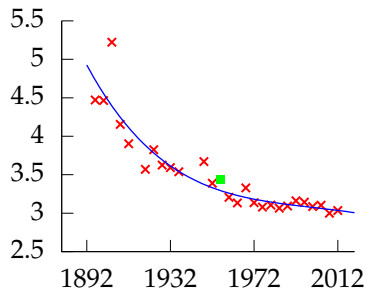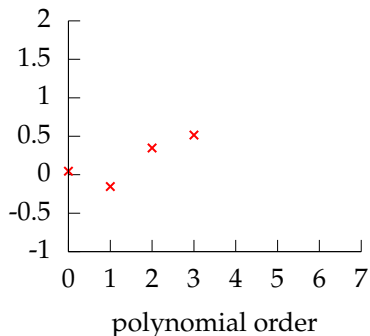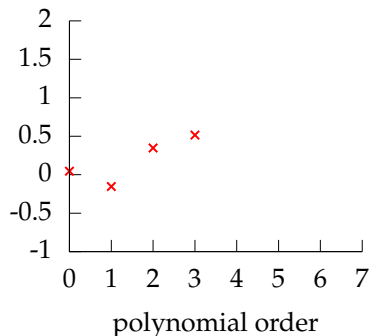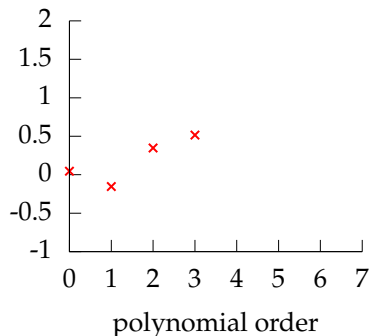Polynomial order 4, training error -29.324, leave one out error 0.84844.

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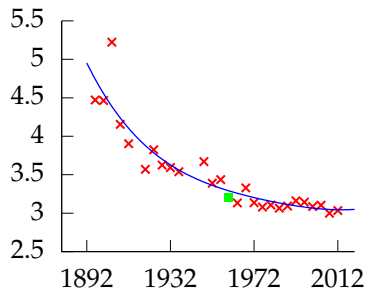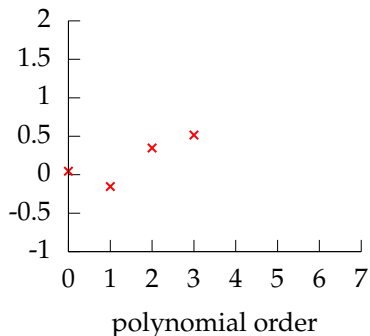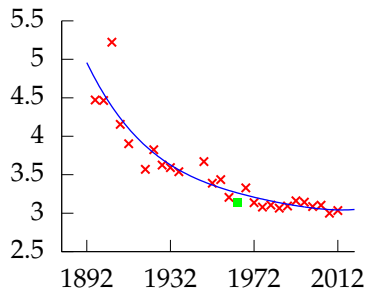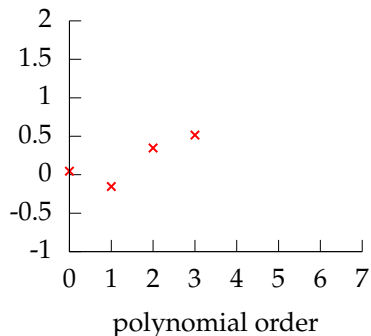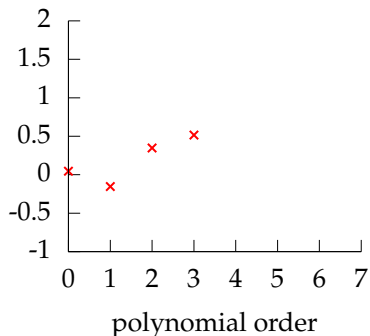Polynomial order 4, training error -29.324, leave one out error 0.84844.

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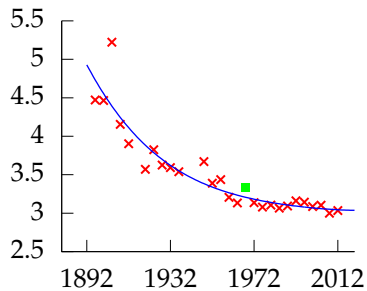Polynomial order 4, training error -29.324, leave one out error 0.84844.
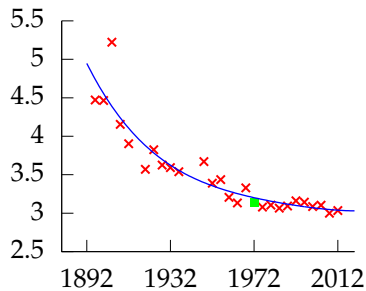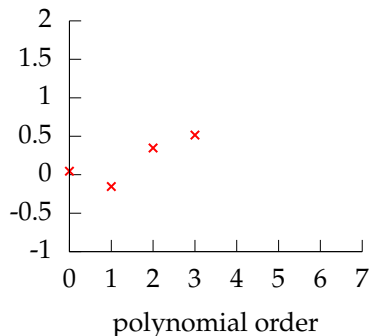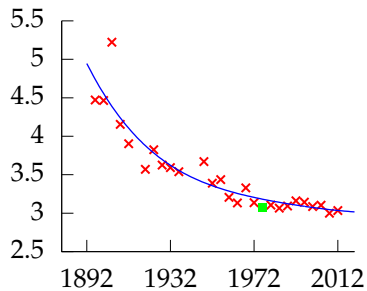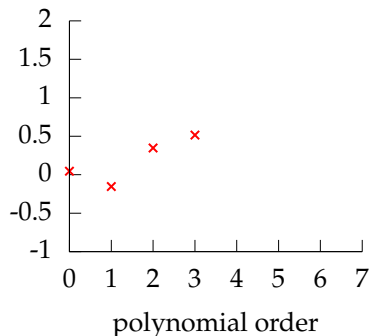
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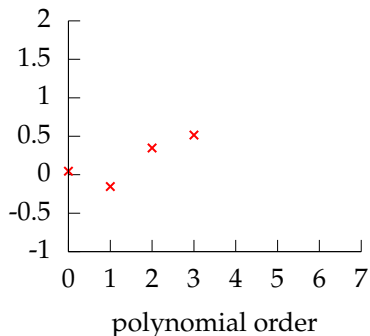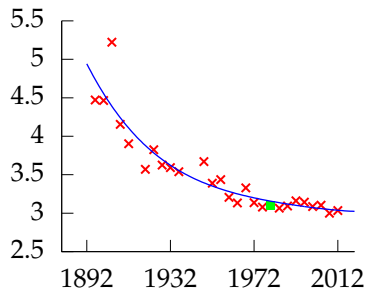
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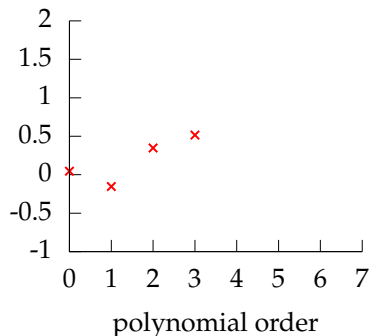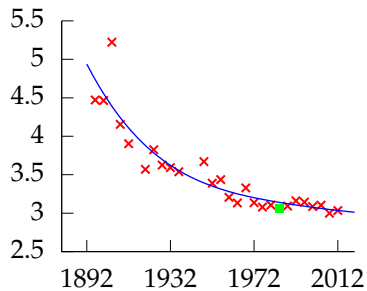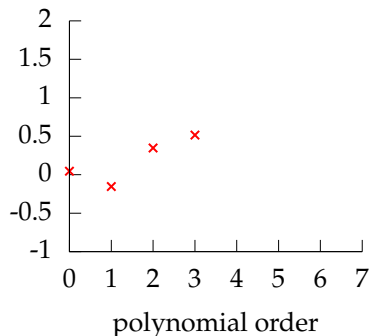# Leave One Out Error

Polynomial order 4, training error -29.324, leave one out error 0.84844.

Leave One Out Error

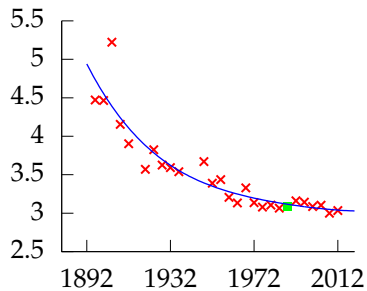Polynomial order 4, training error -29.324, leave one out error 0.84844.
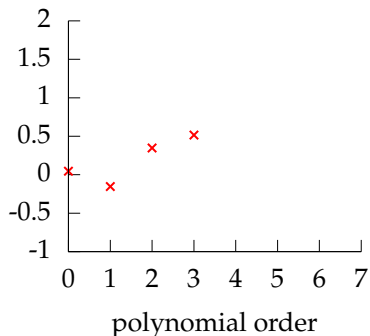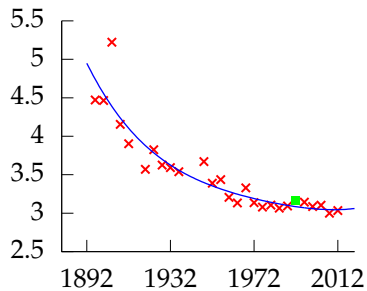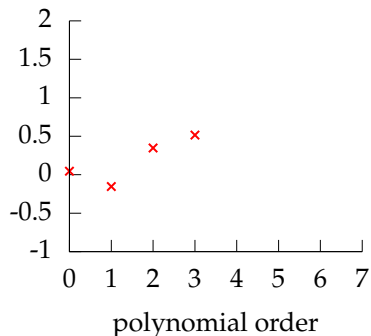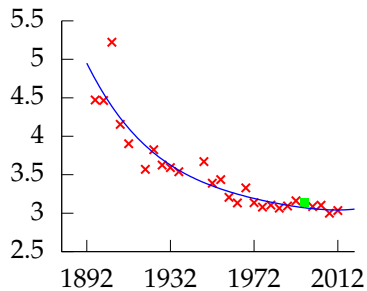
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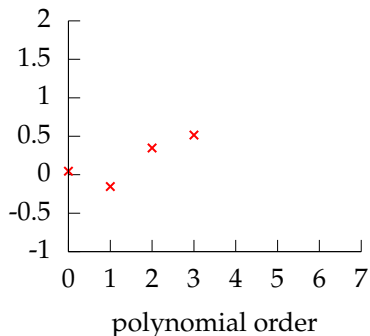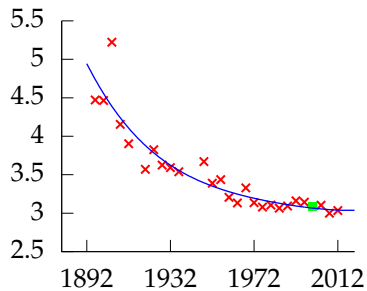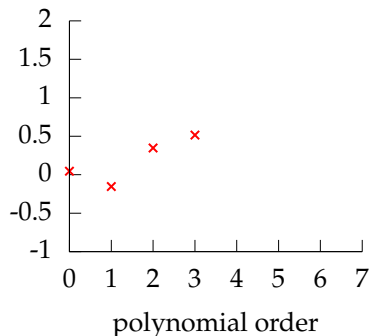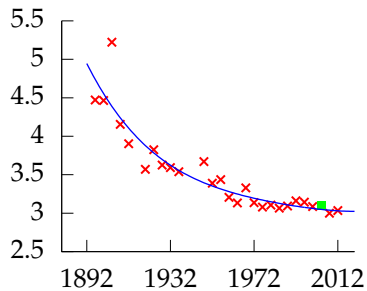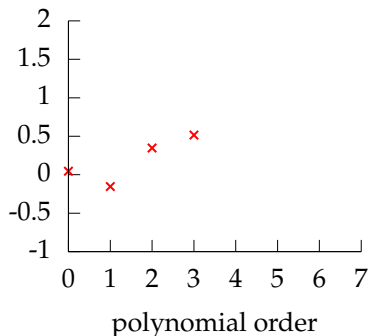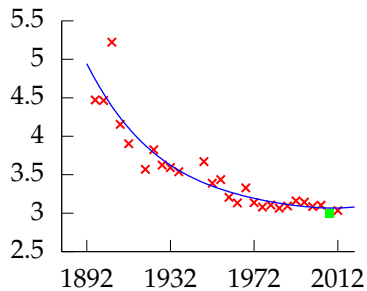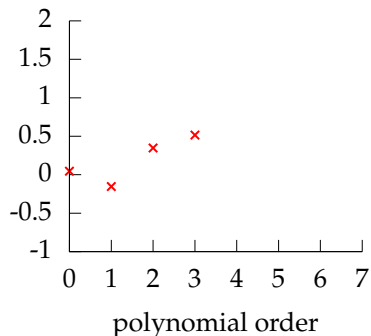Polynomial order 4, training error -29.324, leave one out error 0.84844.

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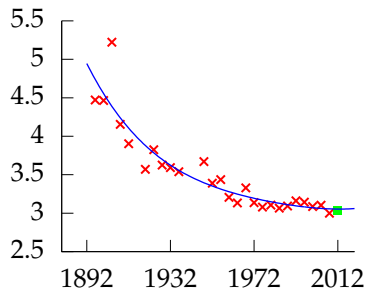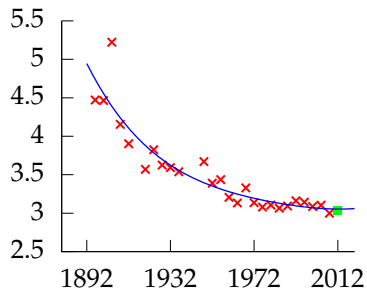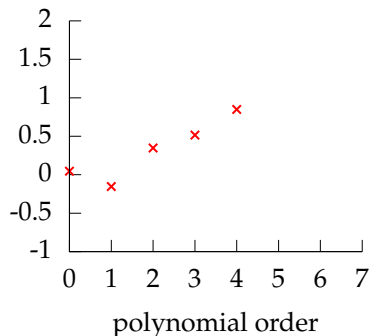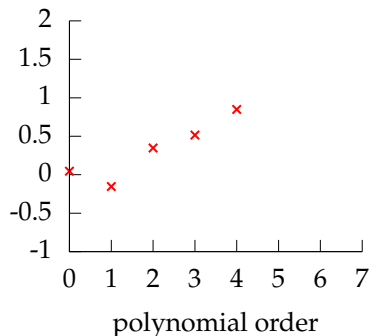
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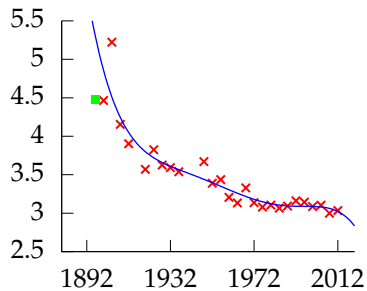Polynomial order 5, training error -29.524, leave one out error 1.48.

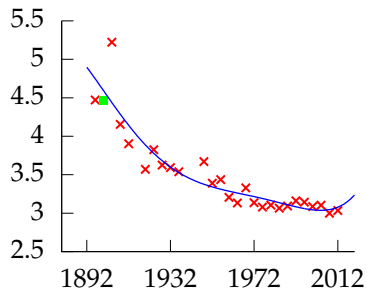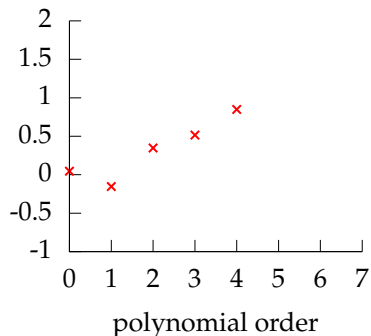Polynomial order 5, training error -29.524, leave one out error 1.48.

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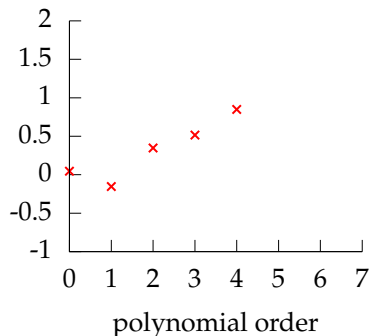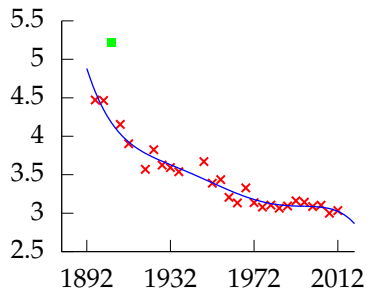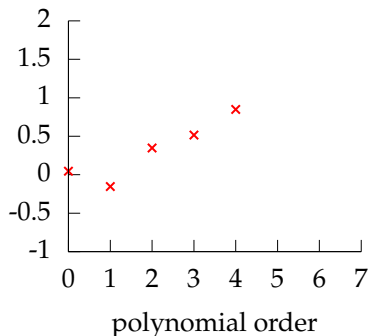
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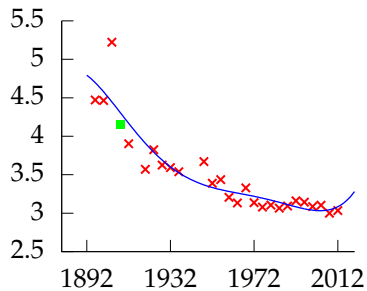

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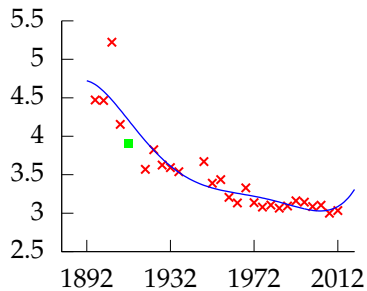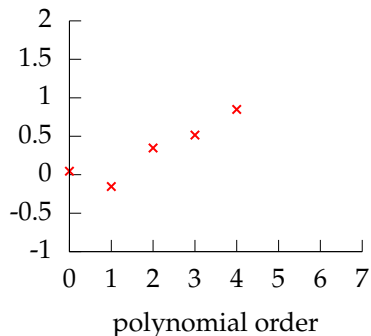
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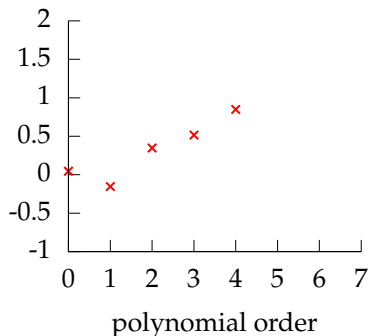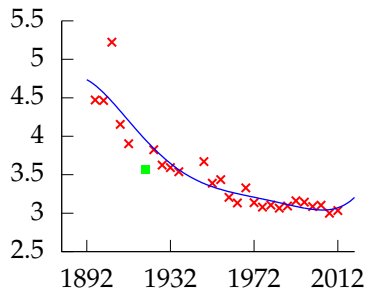

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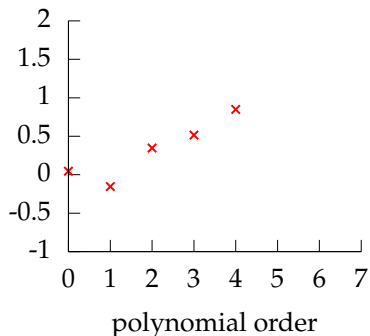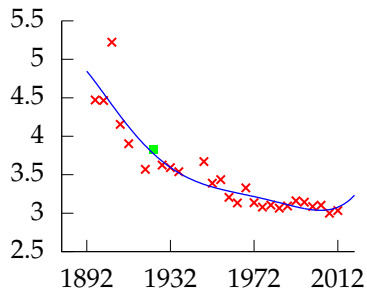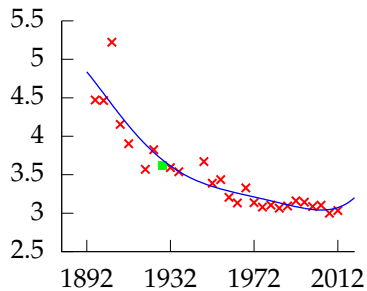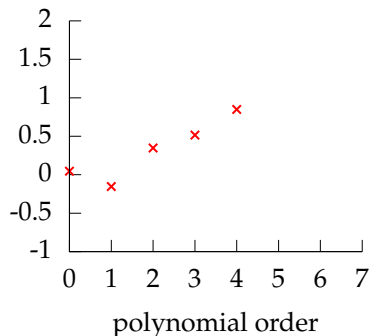

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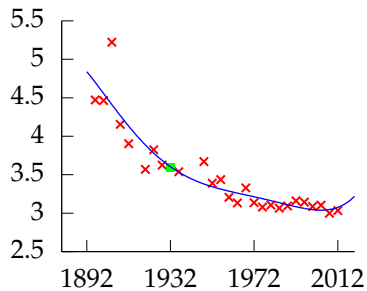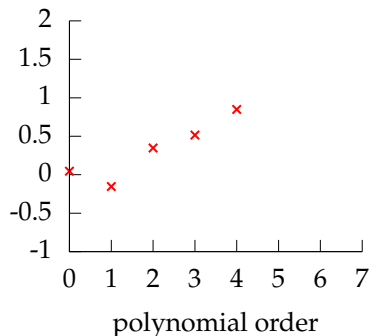1.48.

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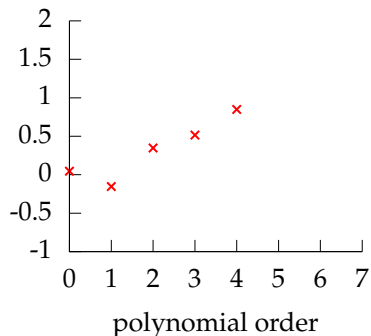Polynomial order 5, training error -29.524, leave one out error 1.48.

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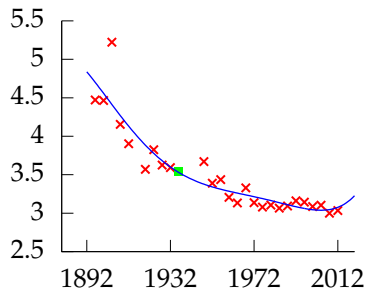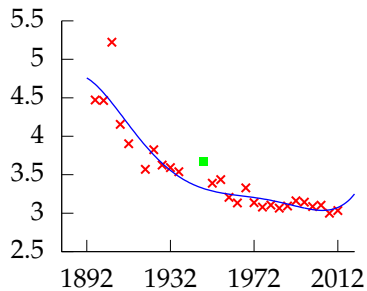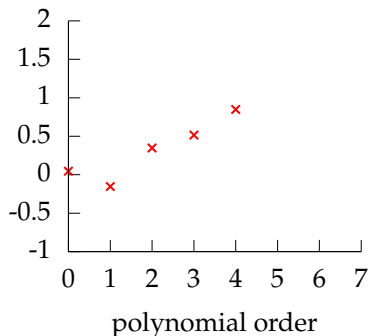
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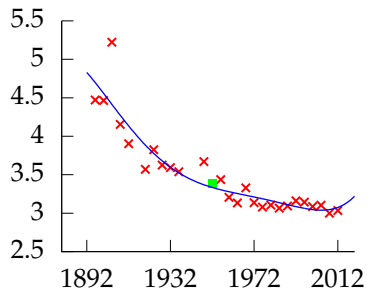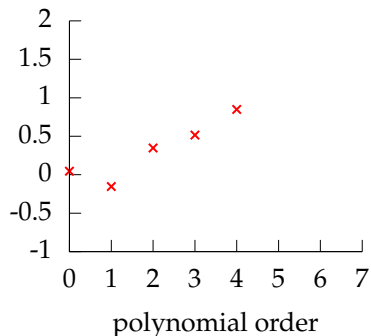Polynomial order 5, training error -29.524, leave one out error 1.48.

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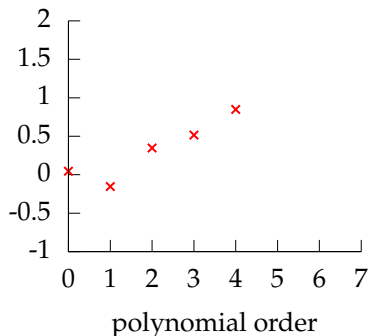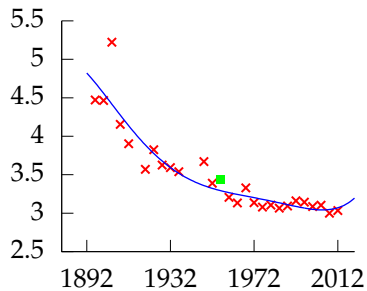
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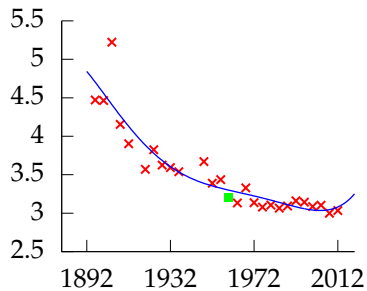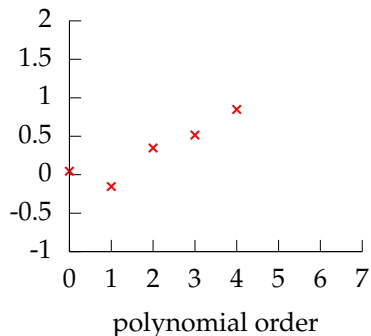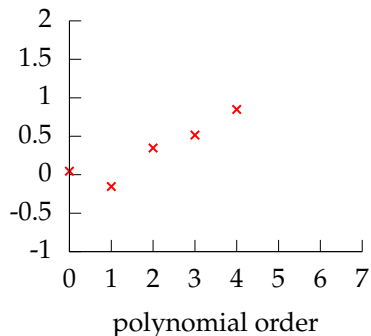
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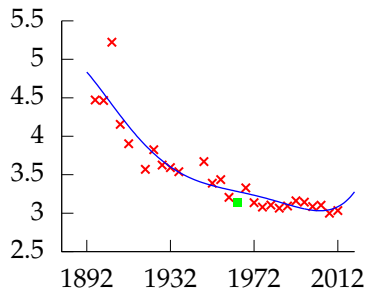

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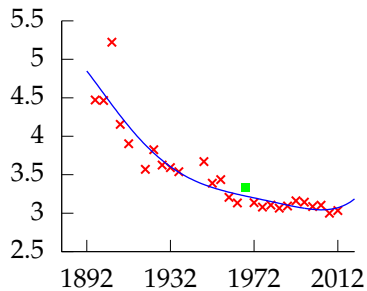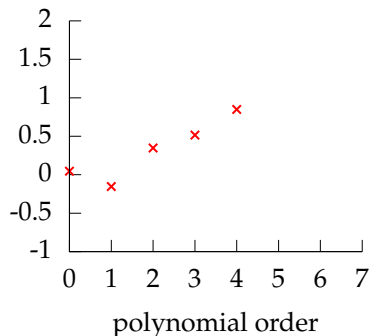

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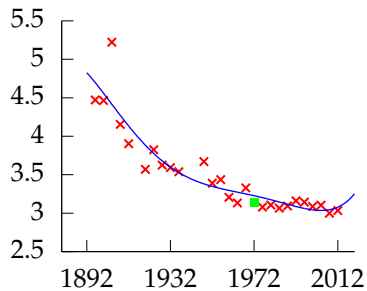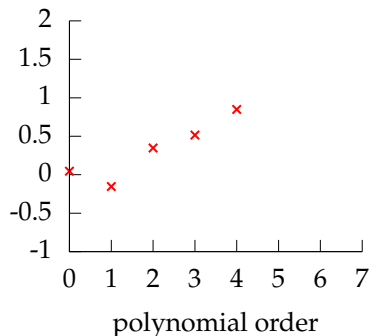
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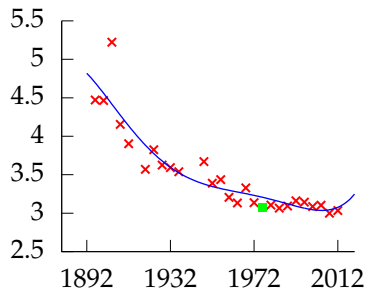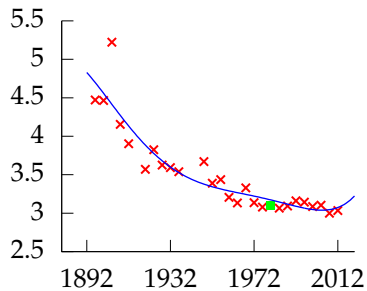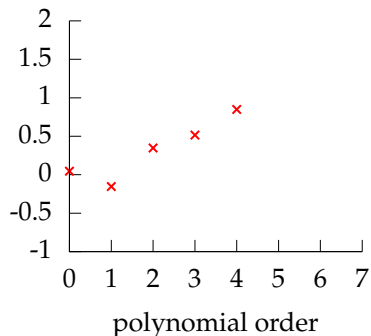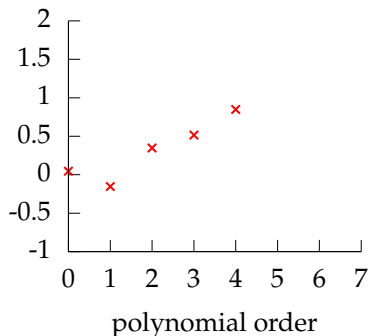
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Polynomial order 5, training error -29.524, leave one out error 1.48.

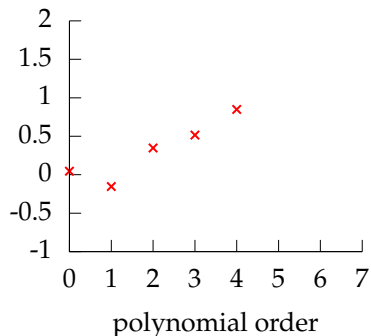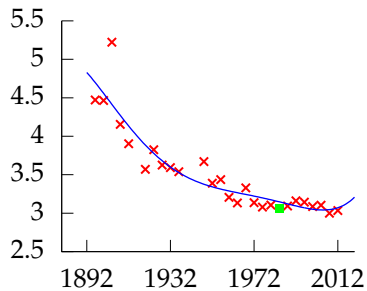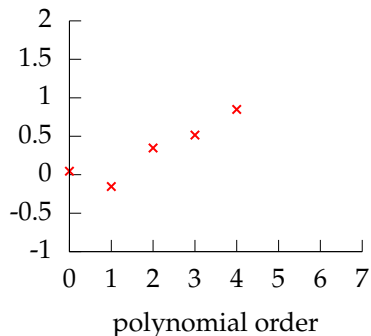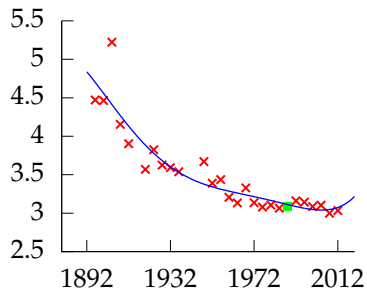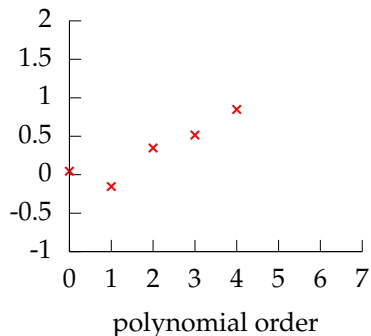Polynomial order 5, training error -29.524, leave one out error 1.48.

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Leave One Out Error

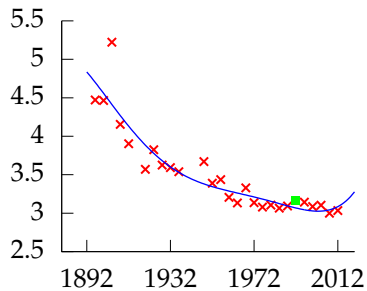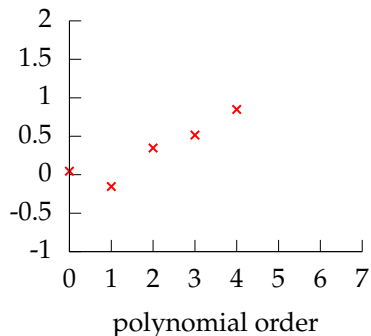Polynomial order 5, training error -29.524, leave one out error 1.48.

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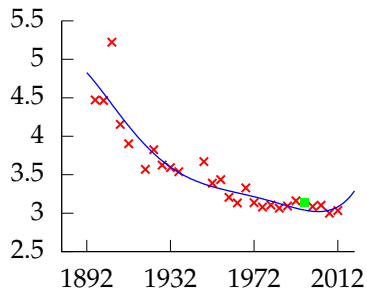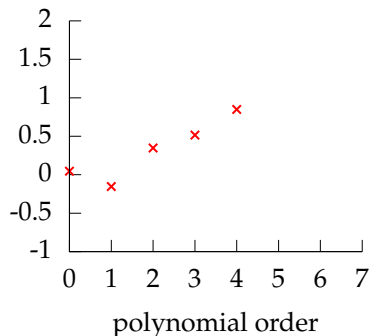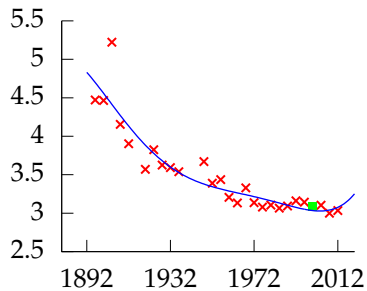
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Polynomial order 5, training error -29.524, leave one out error 1.48.

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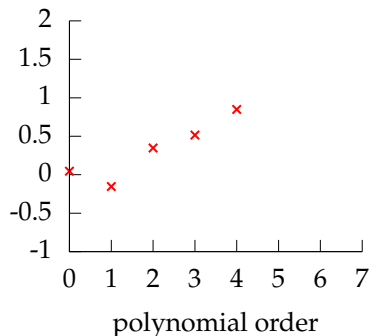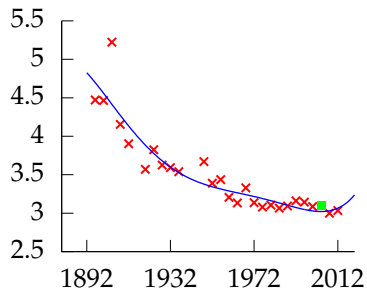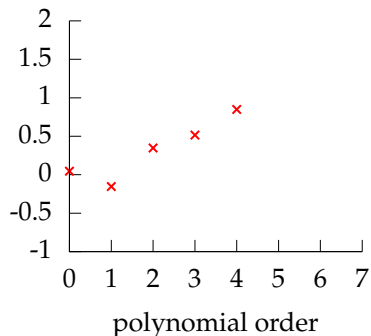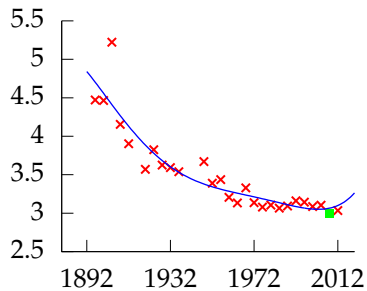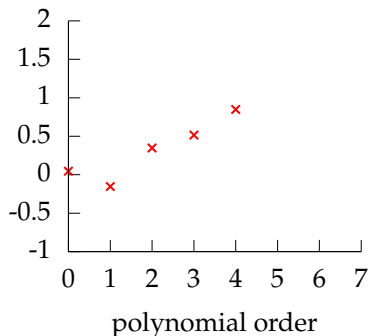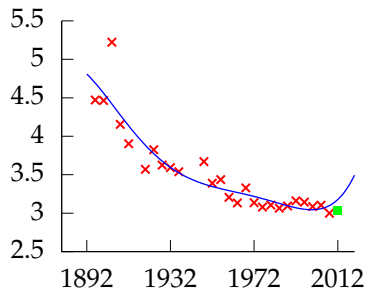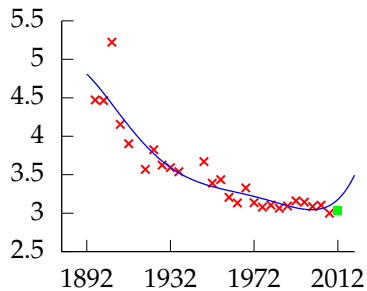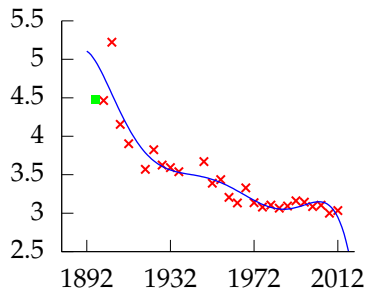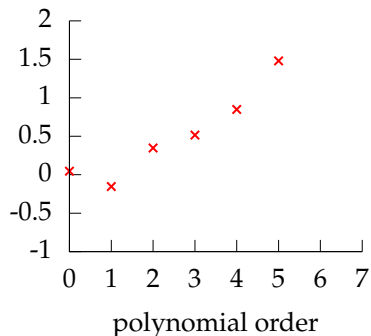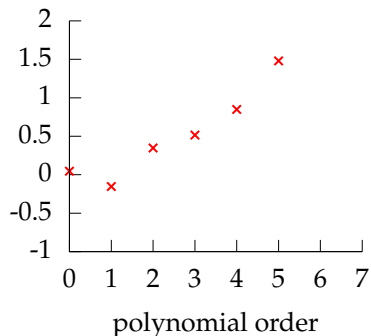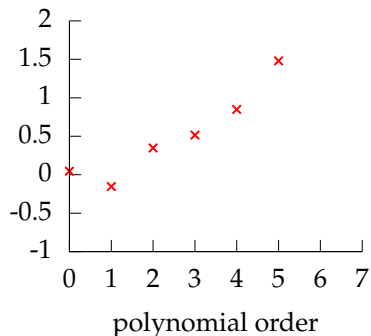
Polynomial order 6, training error -32.237, leave one out error 1.5047.

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Leave One Out Error

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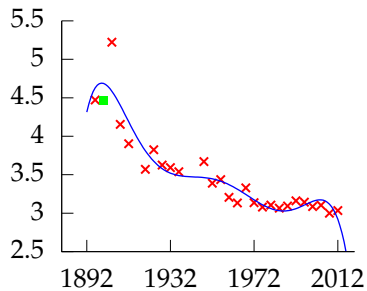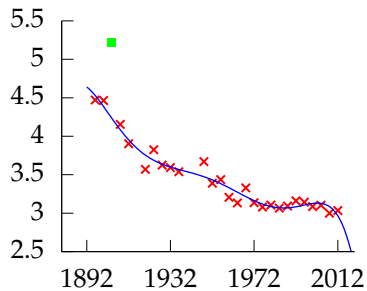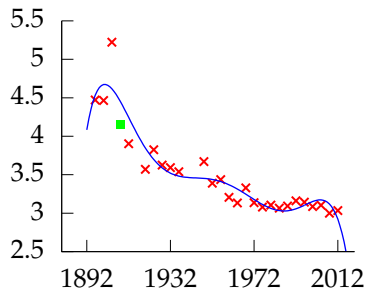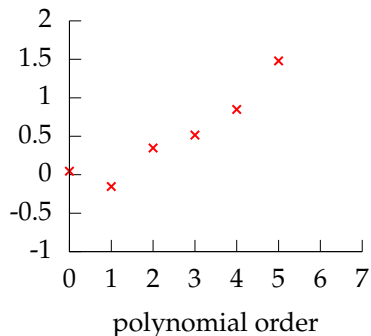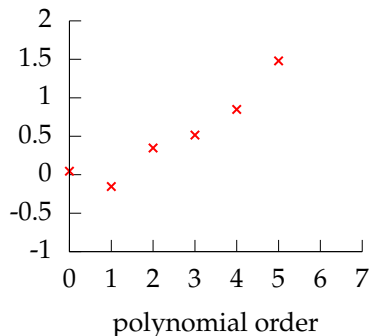
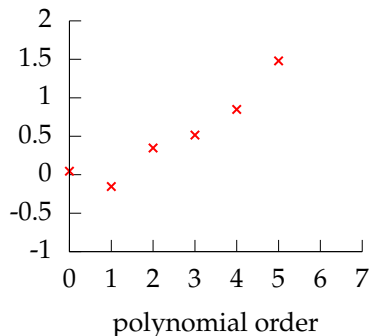Polynomial order 6, training error -32.237, leave one out error 1.5047.

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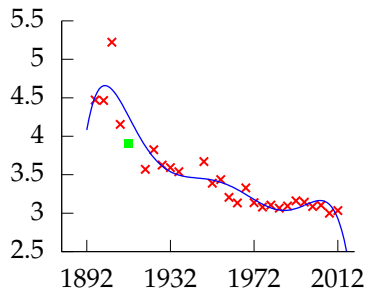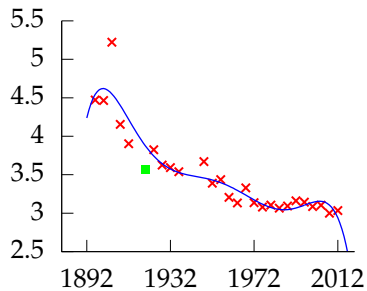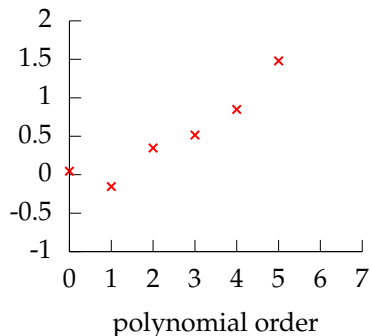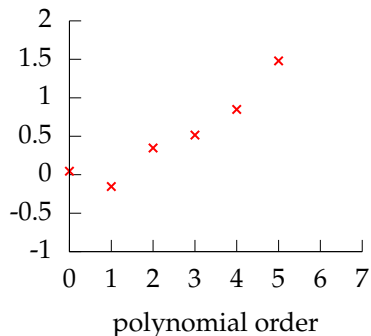
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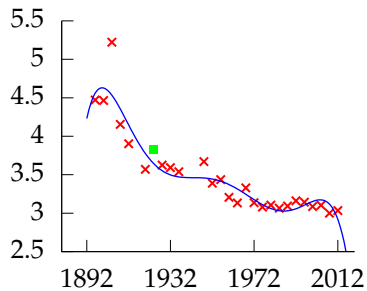Polynomial order 6, training error -32.237, leave one out error 1.5047.

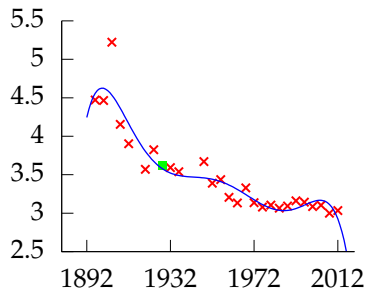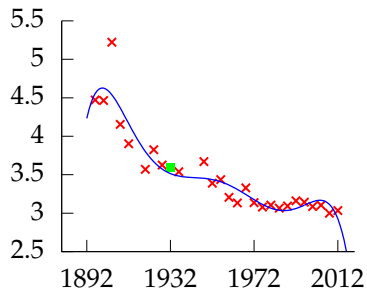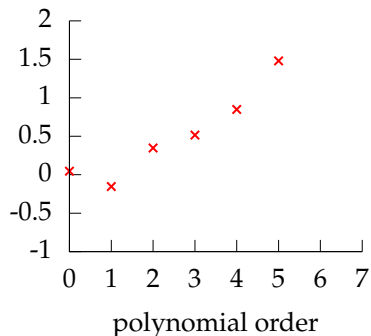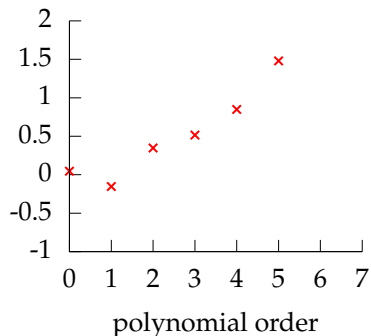Polynomial order 6, training error -32.237, leave one out error 1.5047.

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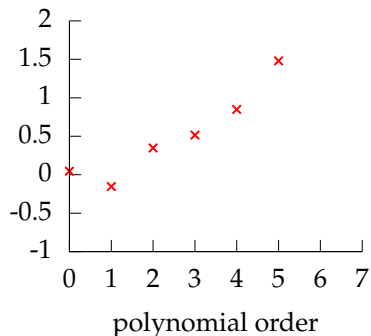
Leave One Out Error
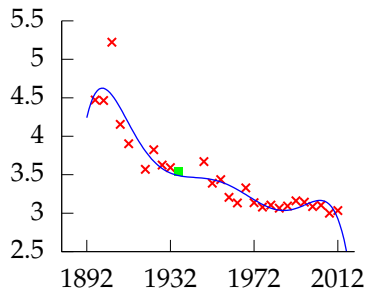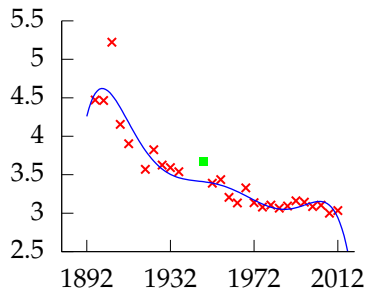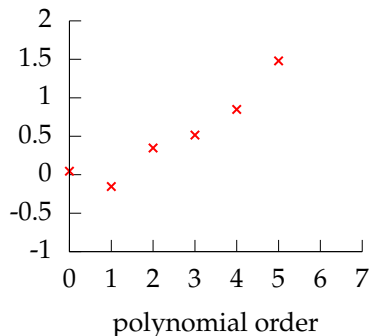

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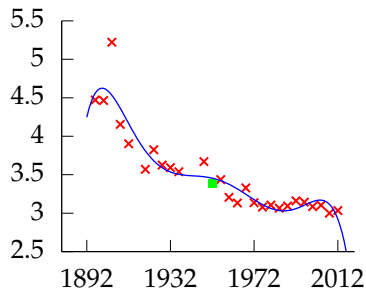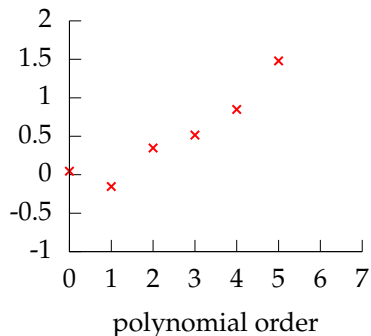

Polynomial order 6, training error -32.237, leave one out error 1.5047.
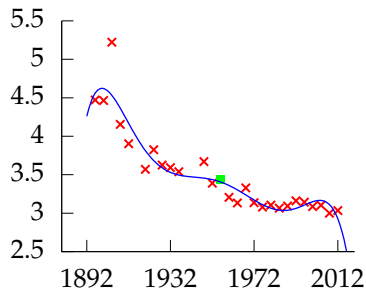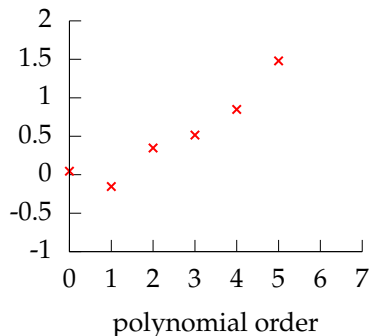
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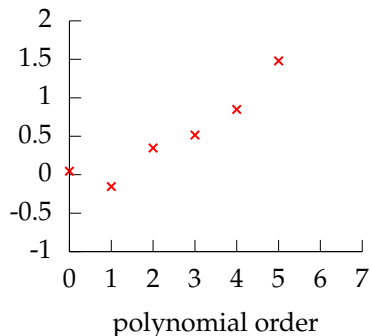Polynomial order 6, training error -32.237, leave one out error 1.5047.
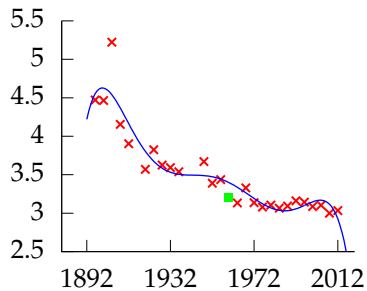
Leave One Out Error
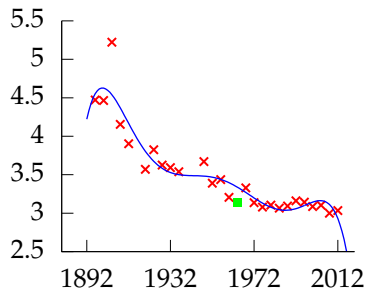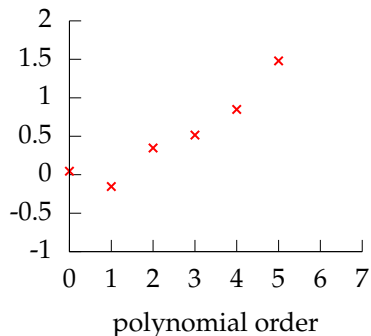

Polynomial order 6, training error -32.237, leave one out error 1.5047.

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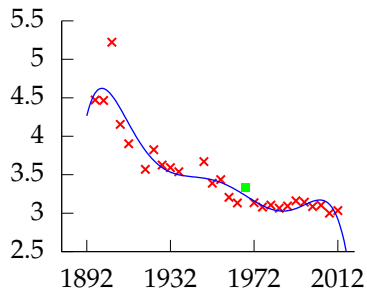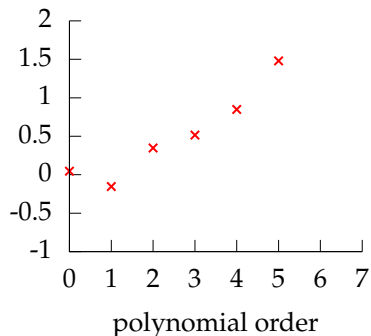

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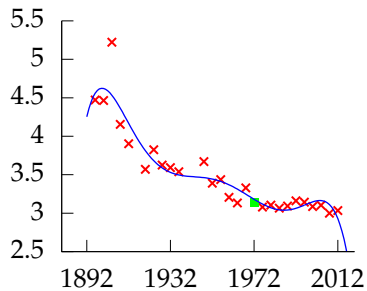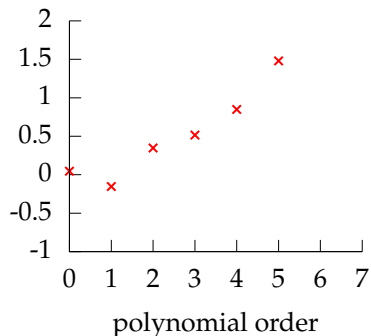

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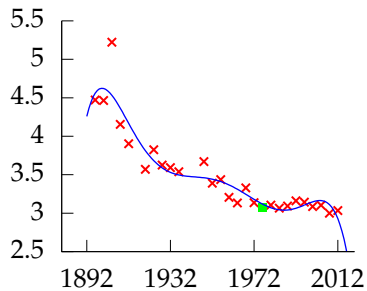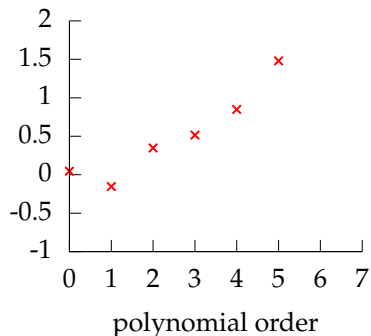

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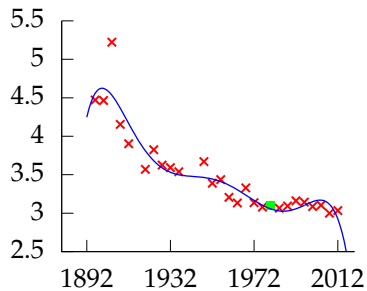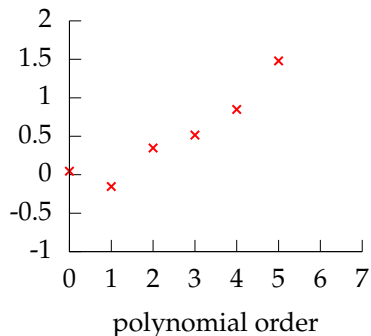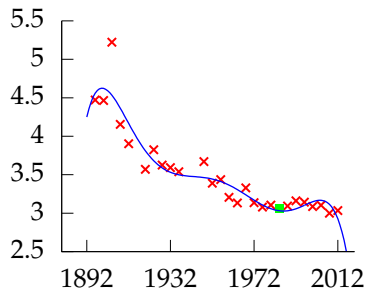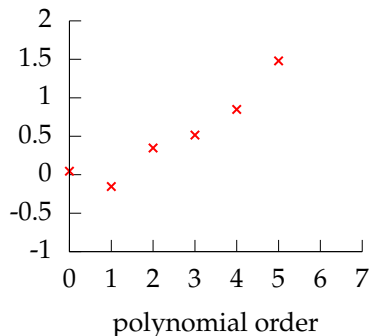# Leave One Out Error

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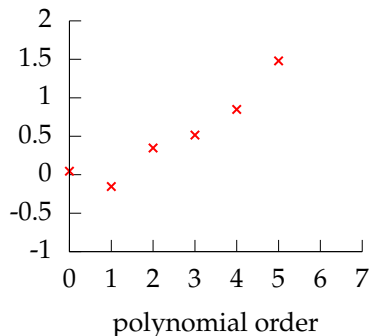
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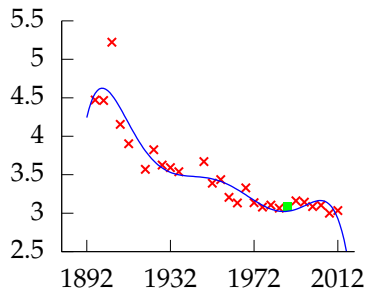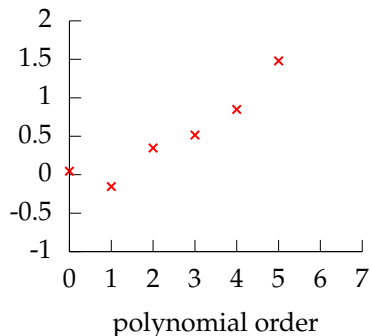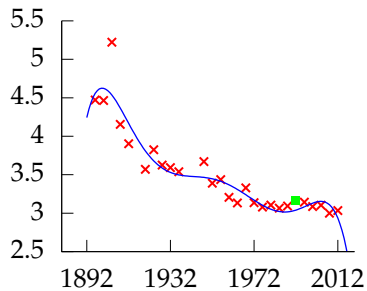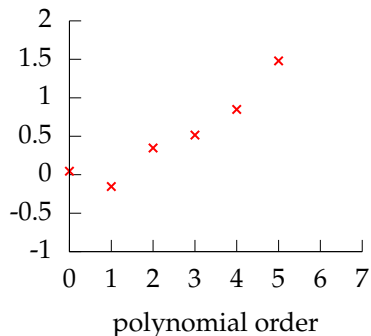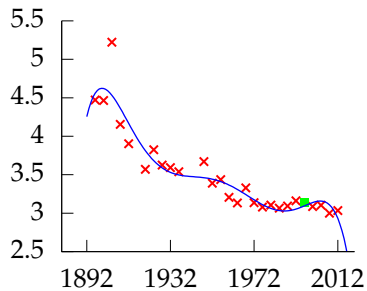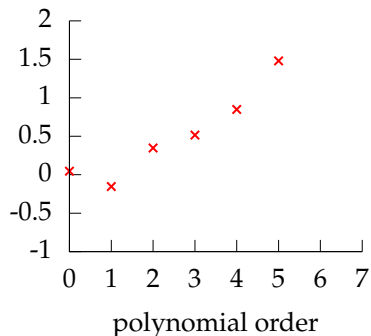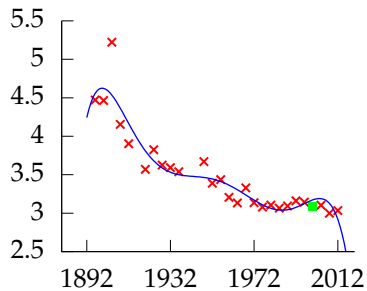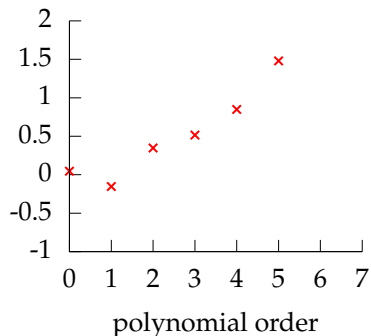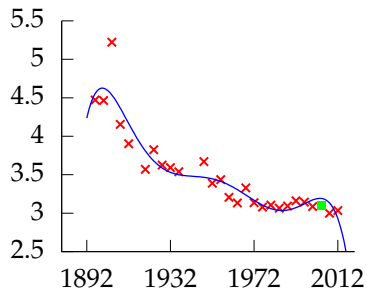
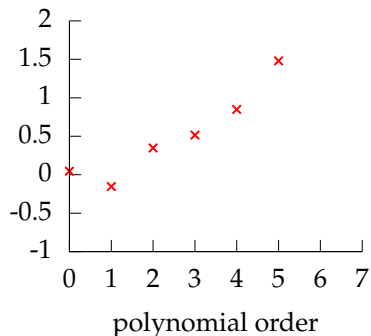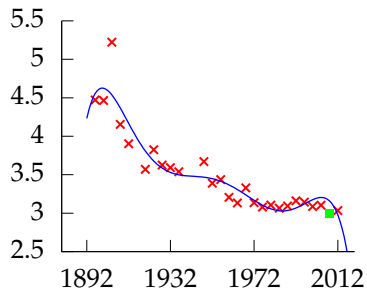Polynomial order 6, training error -32.237, leave one out error 1.5047.

k Fold Cross Validation

- 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 -3.2644, leave one out error 0.045811.

Cross Validation Error

Polynomial order 0, training error -3.2644, leave one out error 0.045811.

Cross Validation Error

Polynomial order 0, training error -3.2644, leave one out error 0.045811.
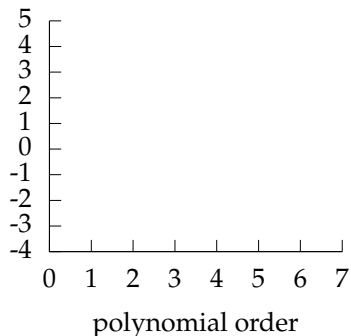
Cross Validation Error

Polynomial order 0, training error -3.2644, leave one out error 0.045811.

Cross Validation Error

Polynomial order 0, training error -3.2644, leave one out error 0.045811.

Cross Validation Error

Polynomial order 0, training error -3.2644, leave one out error 0.045811.

Cross Validation Error

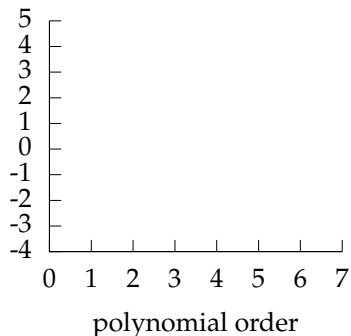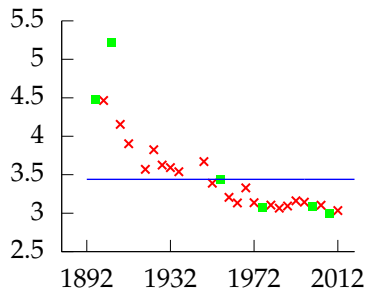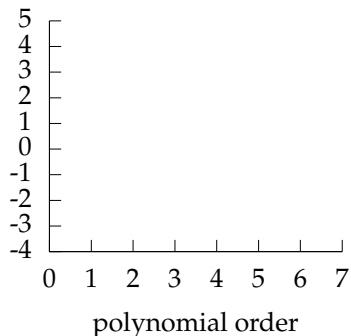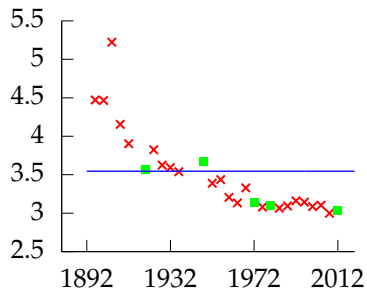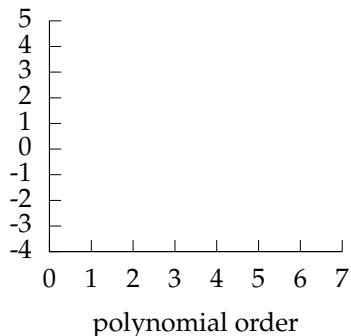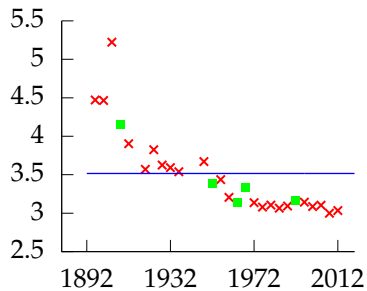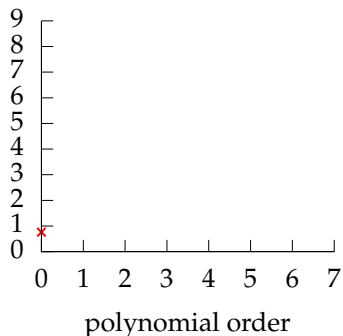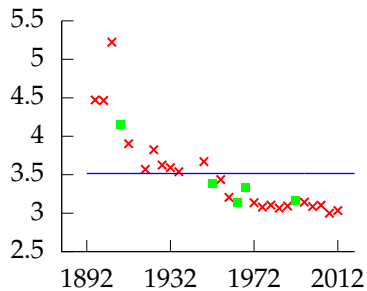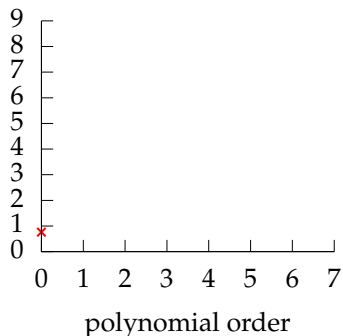Polynomial order 1, training error -18.873, leave one out error -0.15413.

Cross Validation Error

Polynomial order 1, training error -18.873, leave one out error -0.15413.

Cross Validation Error

Polynomial order 1, training error -18.873, leave one out error -0.15413.

Cross Validation Error

Polynomial order 1, training error -18.873, leave one out error -0.15413.

Cross Validation Error
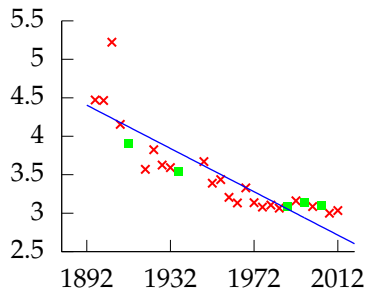

Polynomial order 1, training error -18.873, leave one out error -0.15413.
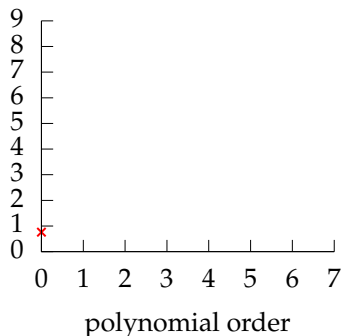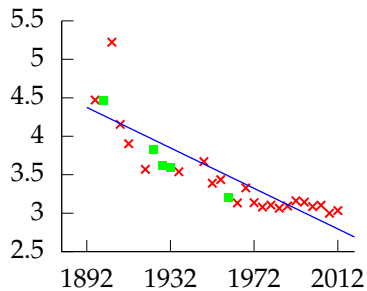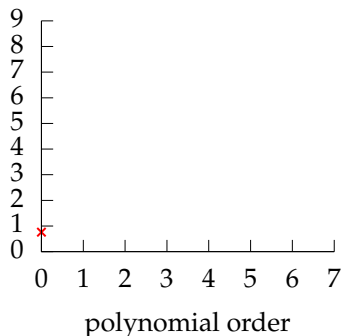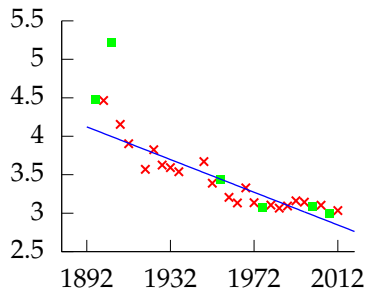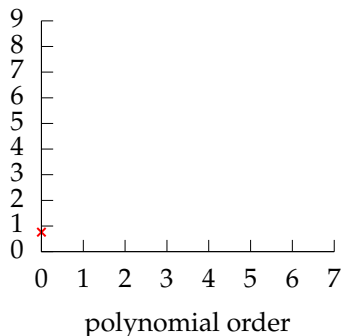
Cross Validation Error

Polynomial order 1, training error -18.873, leave one out error -0.15413.
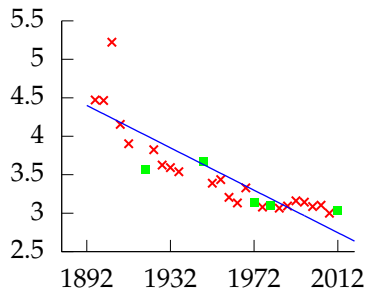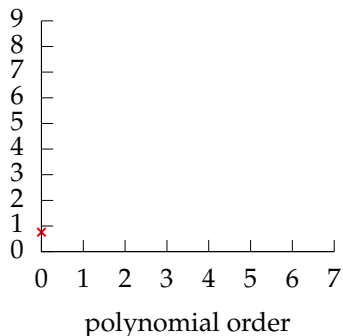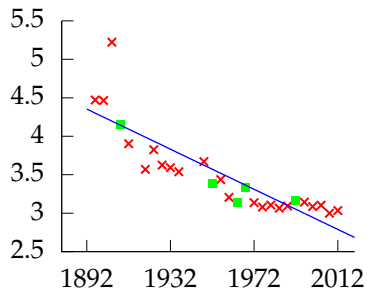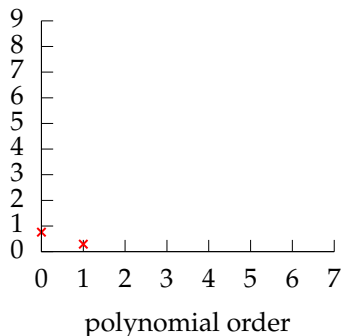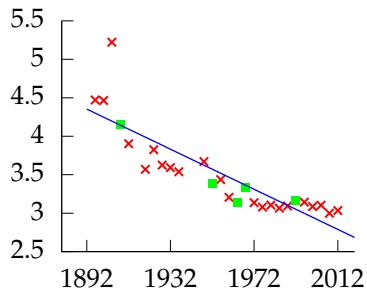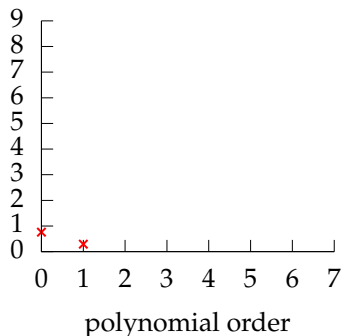
Cross Validation Error

Polynomial order 2, training error -25.177, leave one out error 0.34669.

Cross Validation Error

Polynomial order 2, training error -25.177, leave one out error 0.34669.

Cross Validation Error

Polynomial order 2, training error -25.177, leave one out error 0.34669.

Cross Validation Error

Polynomial order 2, training error -25.177, leave one out error 0.34669.
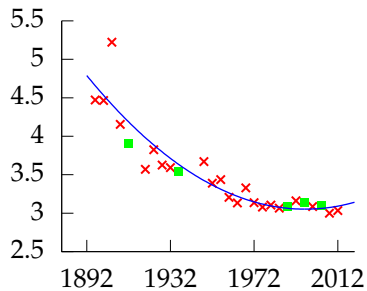
Cross Validation Error

Polynomial order 2, training error -25.177, leave one out error 0.34669.

Cross Validation Error

Polynomial order 2, training error -25.177, leave one out error 0.34669.

Cross Validation Error

Polynomial order 3, training error -25.777, leave one out error 0.51621.

Cross Validation Error

Polynomial order 3, training error -25.777, leave one out error 0.51621.
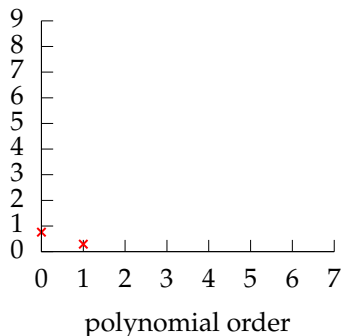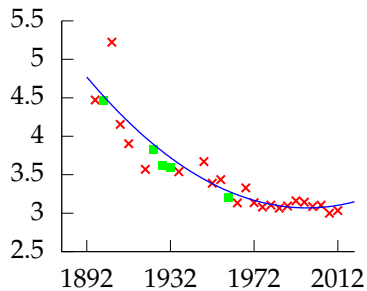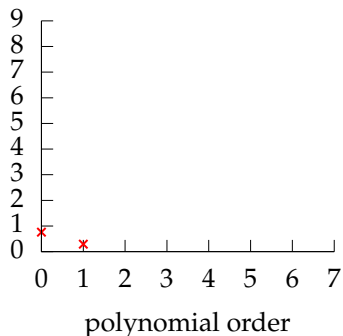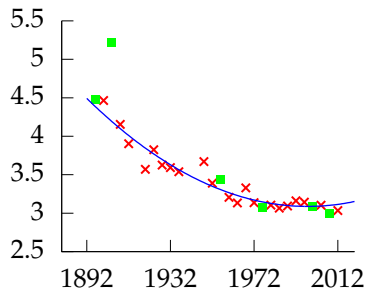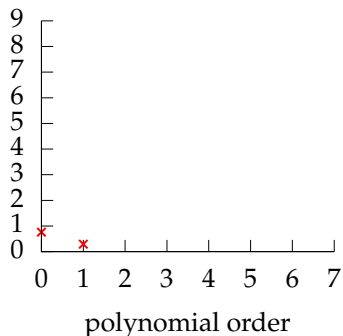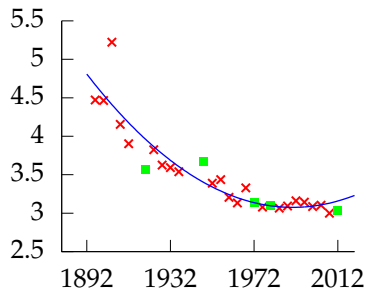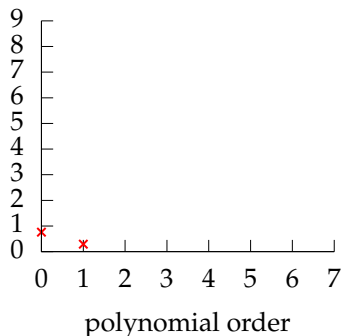
Cross Validation Error

Polynomial order 3, training error -25.777, leave one out error 0.51621.
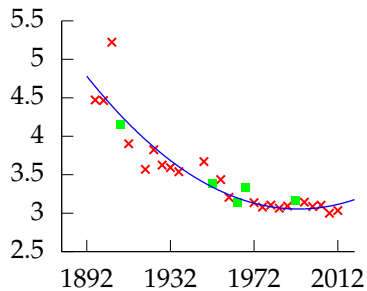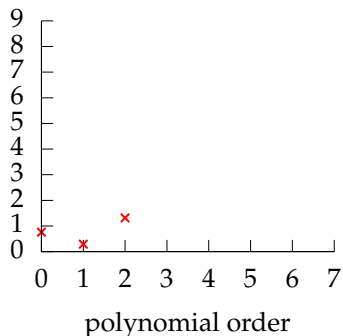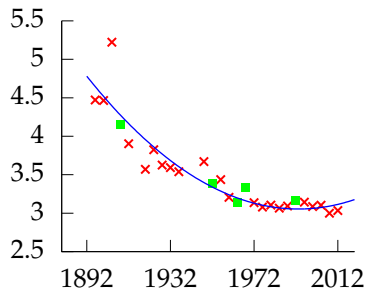
Cross Validation Error

Polynomial order 3, training error -25.777, leave one out error 0.51621.

Cross Validation Error

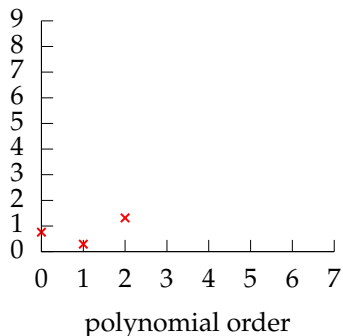Polynomial order 3, training error -25.777, leave one out error 0.51621.
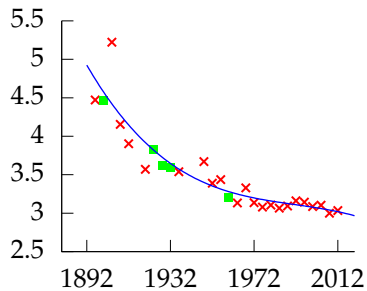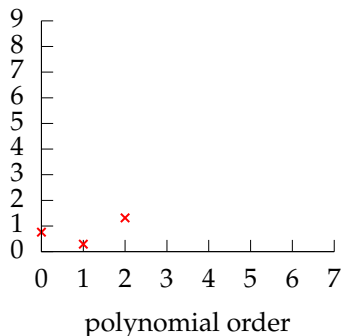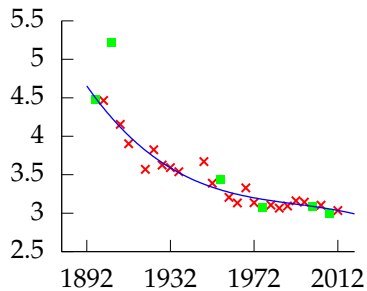
Cross Validation Error
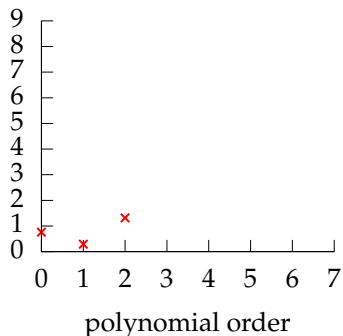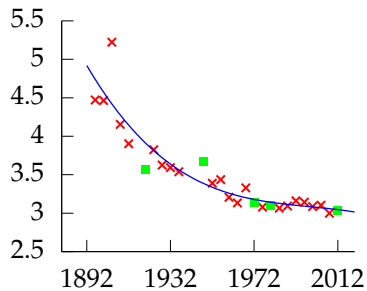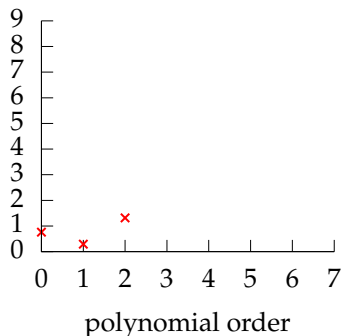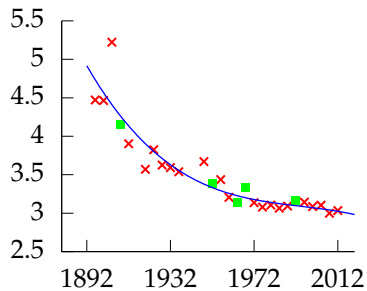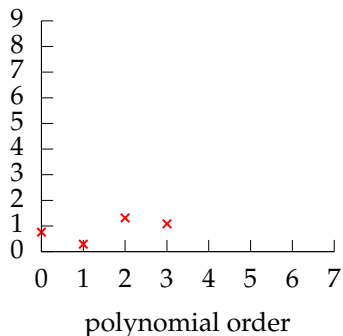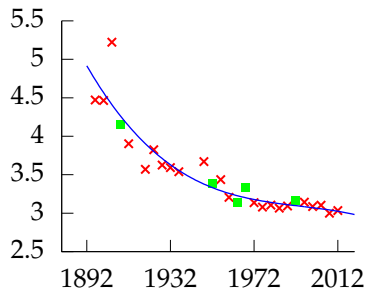

Polynomial order 3, training error -25.777, leave one out error 0.51621.

Cross Validation Error

Polynomial order 4, training error -26.048, leave one out error 0.84844.

Cross Validation Error

Polynomial order 4, training error -26.048, leave one out error 0.84844.

Cross Validation Error

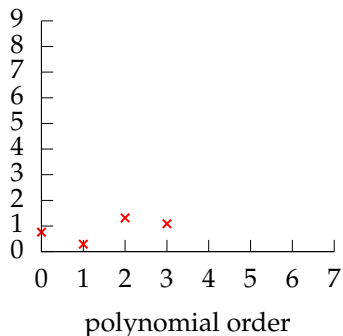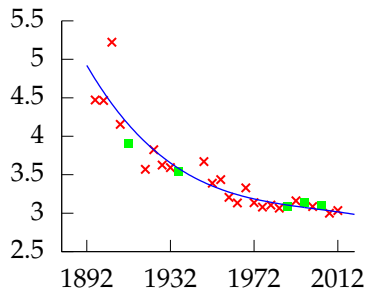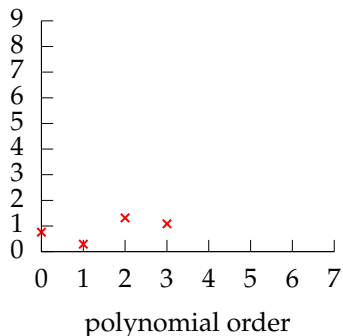Polynomial order 4, training error -26.048, leave one out error 0.84844.

Cross Validation Error

Polynomial order 4, training error -26.048, leave one out error 0.84844.

Cross Validation Error
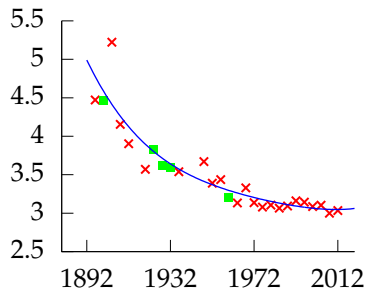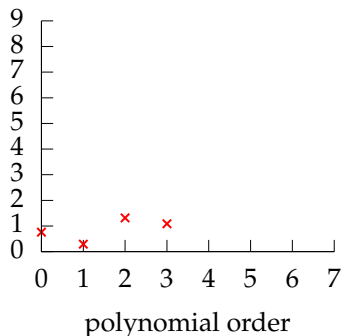

Polynomial order 4, training error -26.048, leave one out error 0.84844.

Cross Validation Error
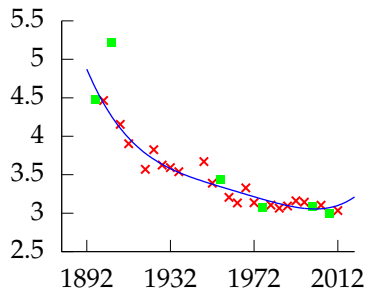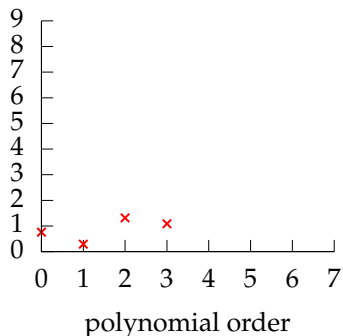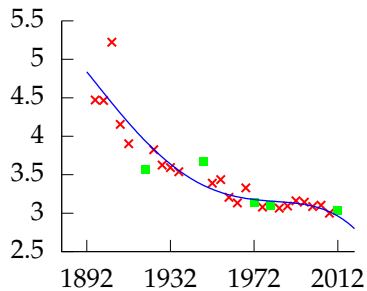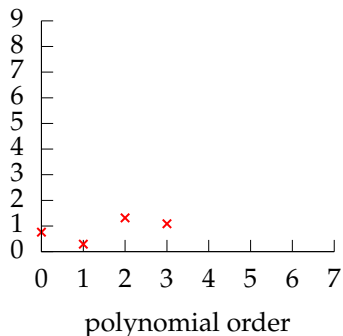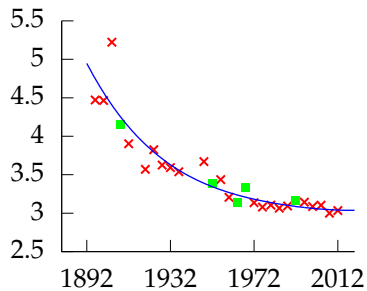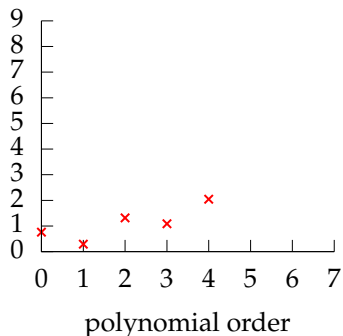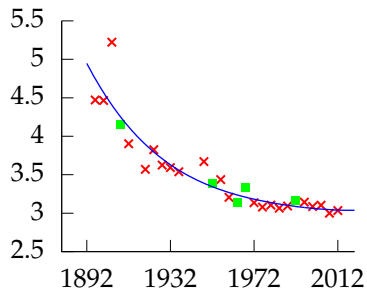

Polynomial order 4, training error -26.048, leave one out error 0.84844.

Cross Validation Error

Polynomial order 5, training error -26.892, leave one out error 1.48.

Cross Validation Error

Polynomial order 5, training error -26.892, leave one out error 1.48.

Cross Validation Error

Polynomial order 5, training error -26.892, leave one out error 1.48.

Cross Validation Error

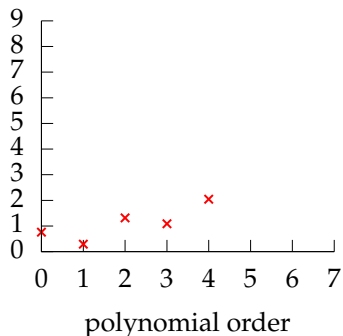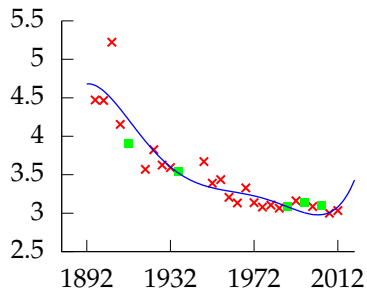

Polynomial order 5, training error -26.892, leave one out error 1.48.

Cross Validation Error

Polynomial order 5, training error -26.892, leave one out error 1.48.
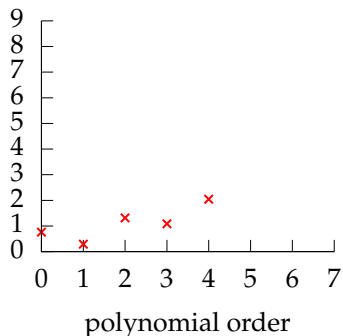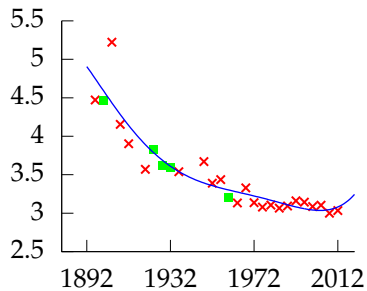
Cross Validation Error

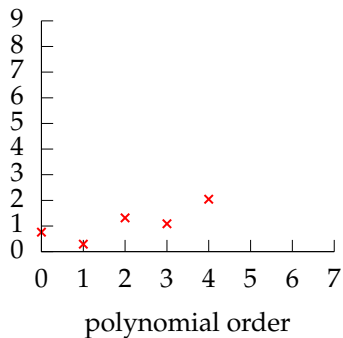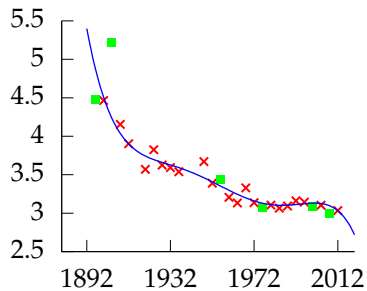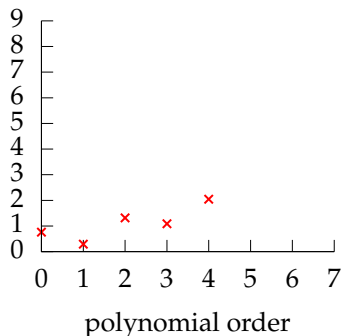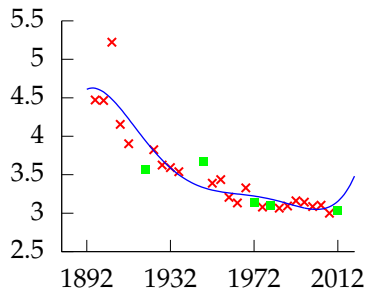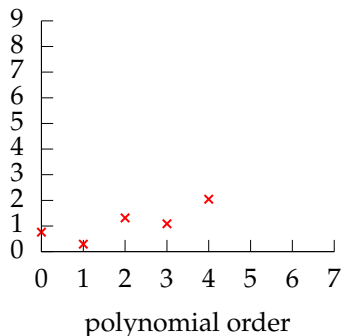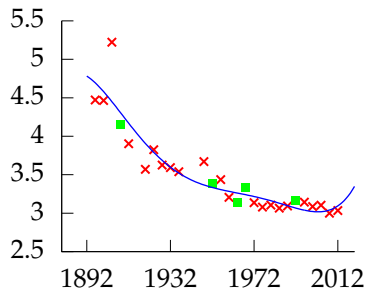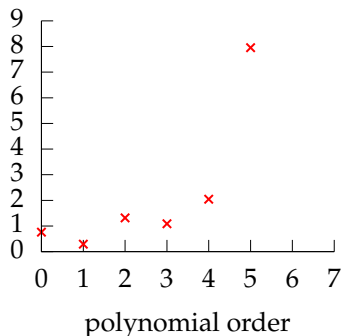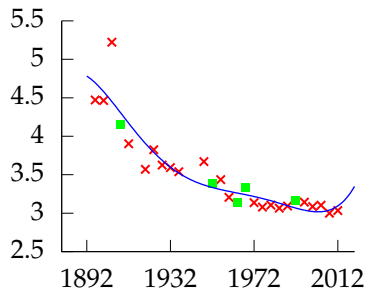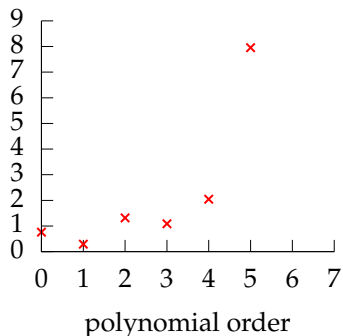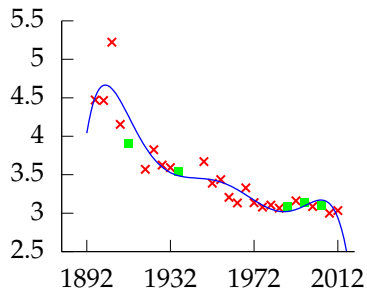Polynomial order 5, training error -26.892, leave one out error 1.48.

Cross Validation Error

Polynomial order 6, training error -29.395, leave one out error 1.5047.

Cross Validation Error

Polynomial order 6, training error -29.395, leave one out error 1.5047.

Cross Validation Error

Polynomial order 6, training error -29.395, leave one out error 1.5047.

Cross Validation Error

Polynomial order 6, training error -29.395, leave one out error 1.5047.
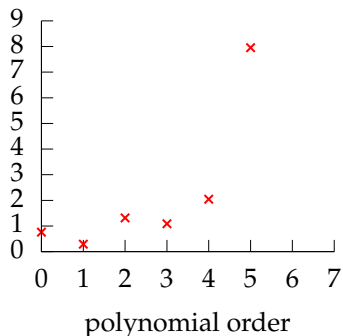
Cross Validation Error
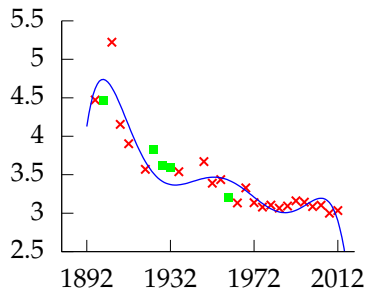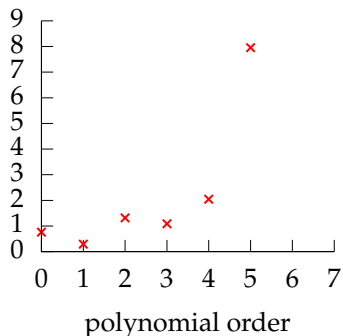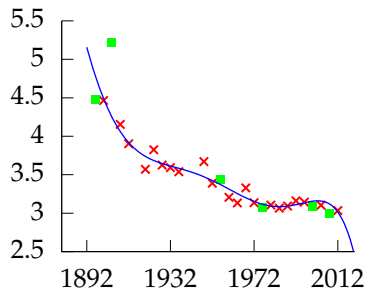

Polynomial order 6, training error -29.395, leave one out error 1.5047.
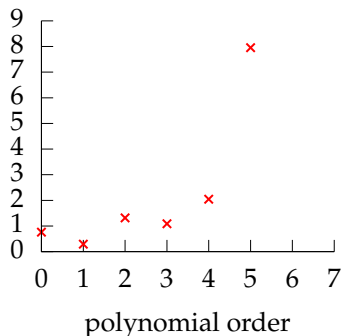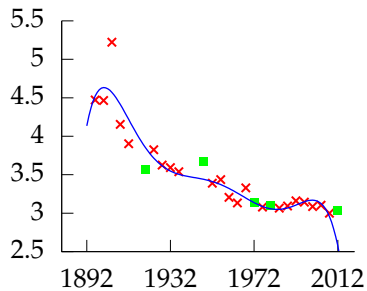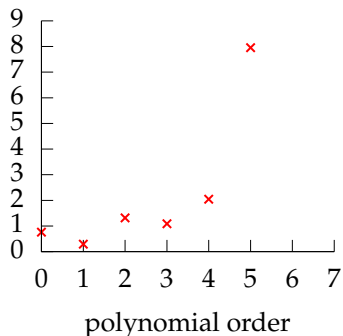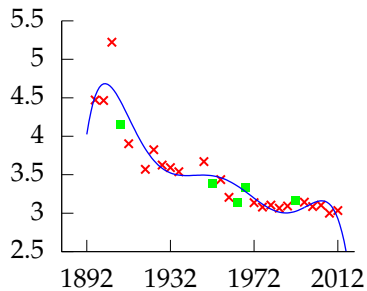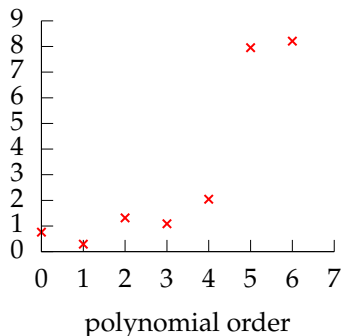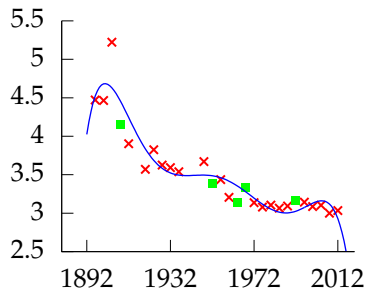
Cross Validation Error

Polynomial order 6, training error -29.395, leave one out error 1.5047.

- Section 1.5 of Rogers and Girolami.

Reading Summary

- Basis Functions (from last time)
  - Section 1.4 of Rogers and Girolami.
  - Chapter 1, pg 1-6 of Bishop.
  - Chapter 3, Section 3.1 of Bishop up to pg 143.
- Generalization
  - Section 1.5 of Rogers and Girolami.

References I

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