## Generalization

MLAI: Week 6

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Department of Computer Science Sheffield University

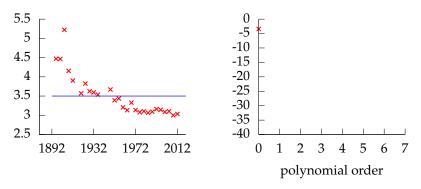
3rd November 2015

#### Review

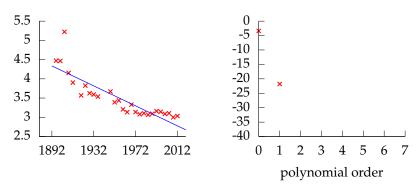
- ► Last time: Looked at univariate and multivariate linear regression.
- ► Showed how to maximize the likelihood of a multivariate model.
- ► Introduced basis functions to make the model non-linear.

## Outline

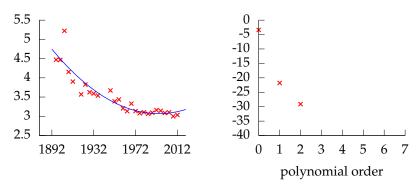
Generalization



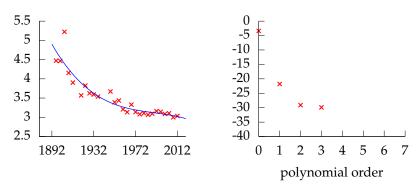
*Left*: fit to data, *Right*: model error. Polynomial order 0, model error -3.3989,  $\sigma^2 = 0.286$ ,  $\sigma = 0.535$ .



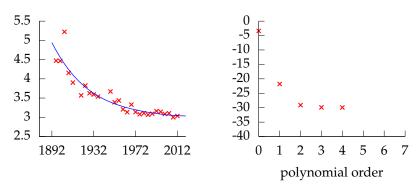
*Left*: fit to data, *Right*: model error. Polynomial order 1, model error -21.772,  $\sigma^2 = 0.0733$ ,  $\sigma = 0.271$ .



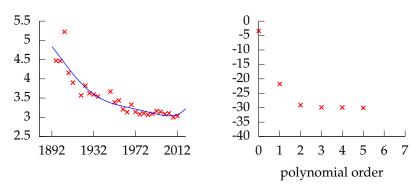
*Left*: fit to data, *Right*: model error. Polynomial order 2, model error -29.101,  $\sigma^2 = 0.0426$ ,  $\sigma = 0.206$ .



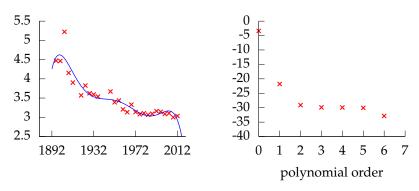
*Left*: fit to data, *Right*: model error. Polynomial order 3, model error -29.907,  $\sigma^2 = 0.0401$ ,  $\sigma = 0.200$ .



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



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



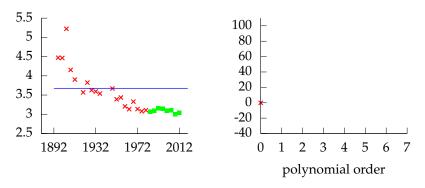
*Left*: fit to data, *Right*: model error. Polynomial order 6, model error -32.866,  $\sigma^2 = 0.0322$ ,  $\sigma = 0.180$ .

## Overfitting

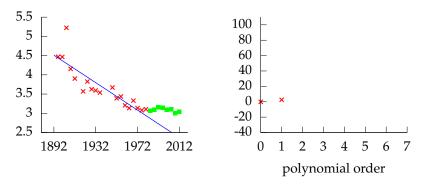
- ► Increase number of basis functions, we obtain a better 'fit' to the data.
- ► How will the model perform on previously unseen data?

## Training and Test Sets

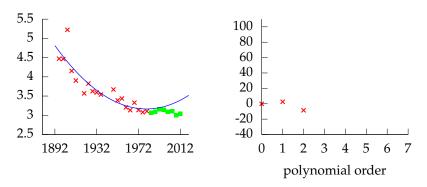
- We call the data used for fitting the model the 'training set'.
- ▶ Data not used for training, but when the model is applied 'in the field' is called the 'test data'.
- Challenge for generalization is to ensure a good performance on test data given only training data.



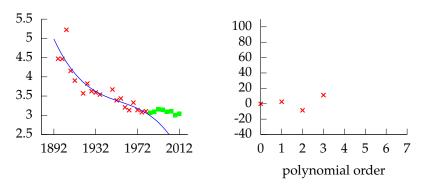
*Left*: fit to data, *Right*: model error. Polynomial order 0, training error -1.8774, validation error -0.13132,  $\sigma^2 = 0.302$ ,  $\sigma = 0.549$ .



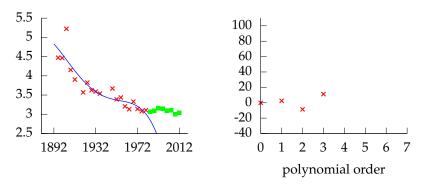
*Left*: fit to data, *Right*: model error. Polynomial order 1, training error -15.325, validation error 2.5863,  $\sigma^2 = 0.0733$ ,  $\sigma = 0.271$ .



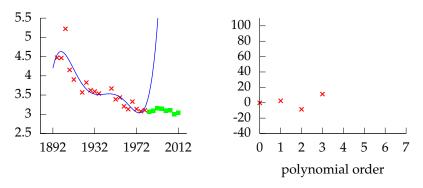
*Left*: fit to data, *Right*: model error. Polynomial order 2, training error -17.579, validation error -8.4831,  $\sigma^2 = 0.0578$ ,  $\sigma = 0.240$ .



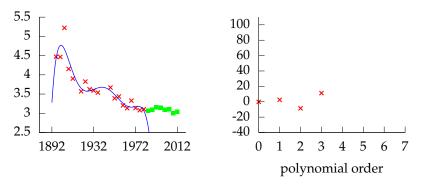
*Left*: fit to data, *Right*: model error. Polynomial order 3, training error -18.064, validation error 11.27,  $\sigma^2 = 0.0549$ ,  $\sigma = 0.234$ .



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

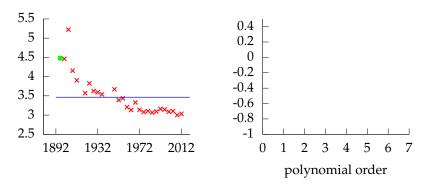


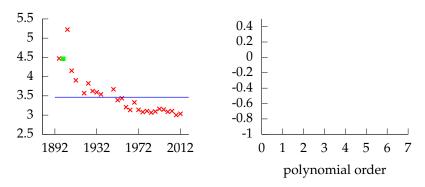
*Left*: fit to data, *Right*: model error. Polynomial order 5, training error -20.471, validation error 9898.1,  $\sigma^2 = 0.0426$ ,  $\sigma = 0.207$ .

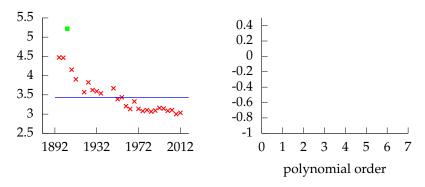


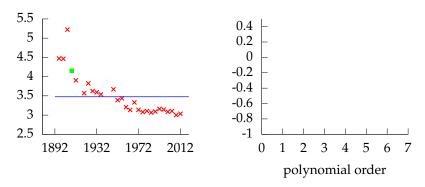
*Left*: fit to data, *Right*: model error. Polynomial order 6, training error -22.881, validation error 67775,  $\sigma^2 = 0.0331$ ,  $\sigma = 0.182$ .

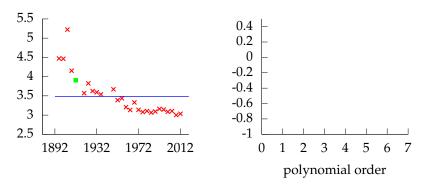
- ► Take training set and remove one point.
- ► Train on the remaining data.
- Compute the error on the point you removed (which wasn't in the training data).
- ▶ Do this for each point in the training set in turn.
- Average the resulting error. This is the leave one out error.

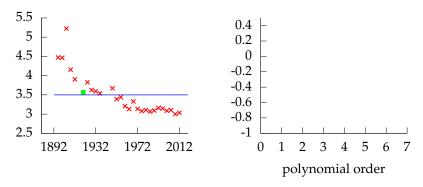




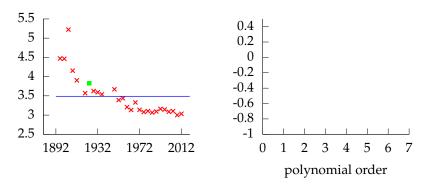


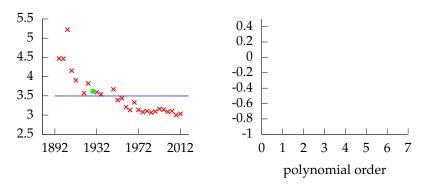


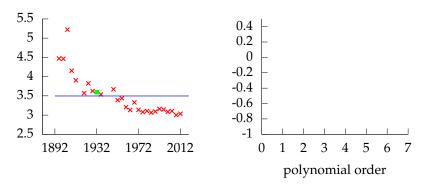


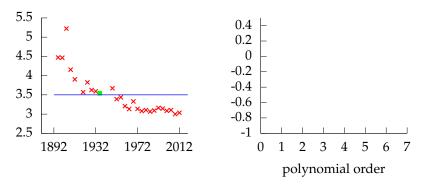


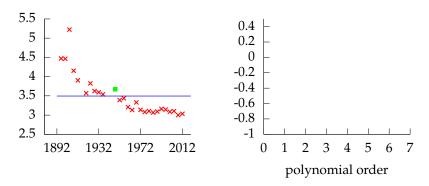
Polynomial order 0, training error -3.346, leave one out error 0.045811.

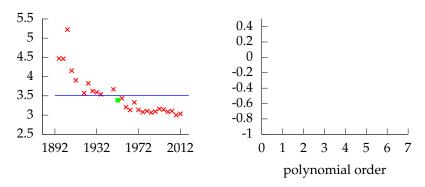


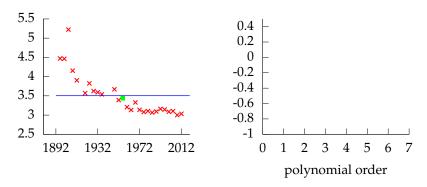


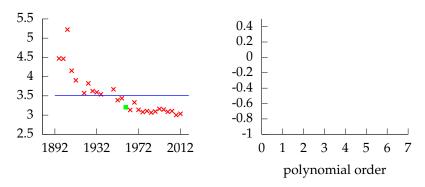


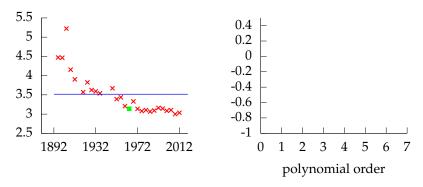


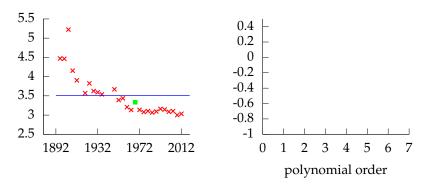


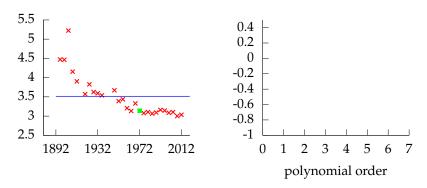


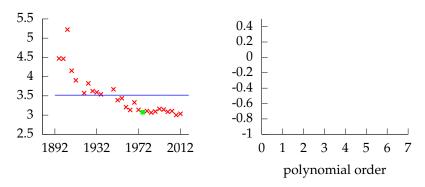


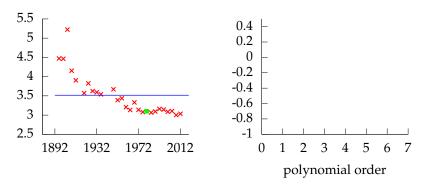


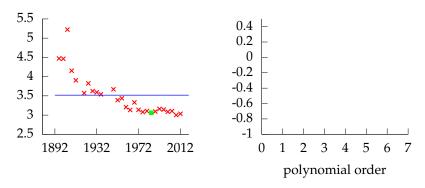


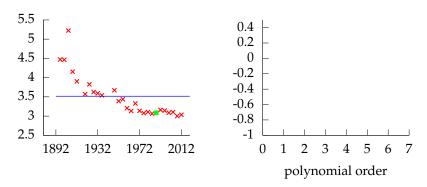




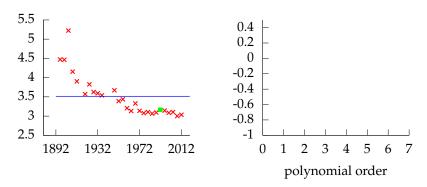




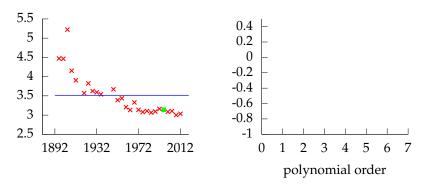


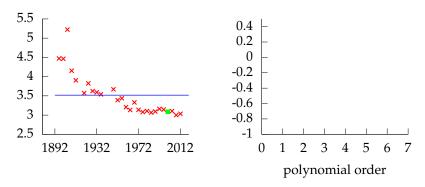


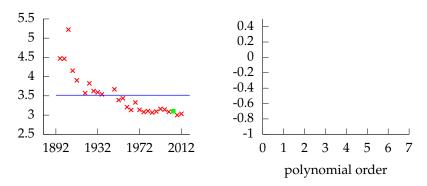
Polynomial order 0, training error -3.346, leave one out error 0.045811.

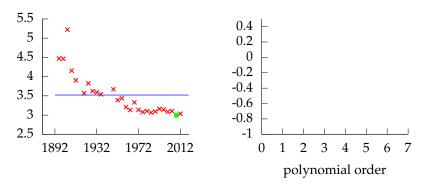


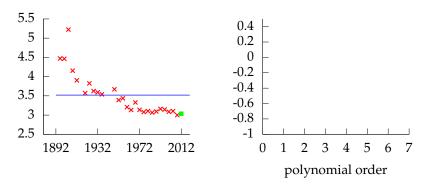
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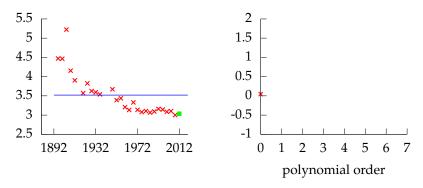


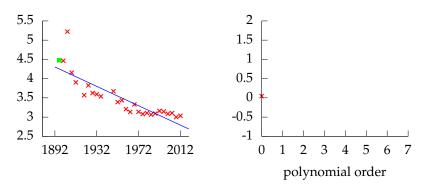




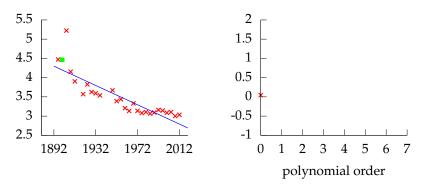




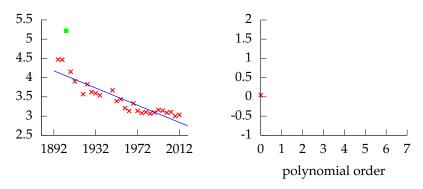




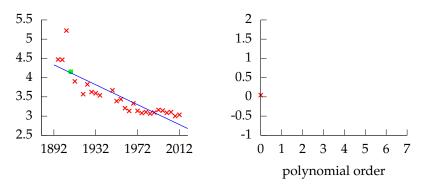
Polynomial order 1, training error -21.183, leave one out error -0.15413.



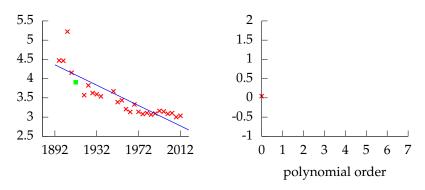
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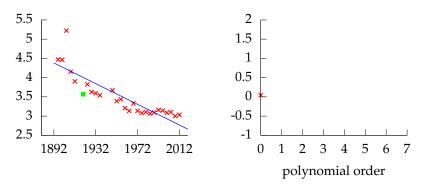
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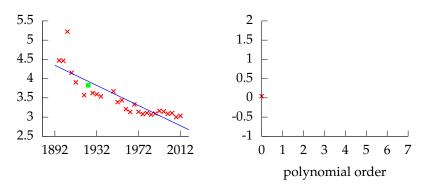
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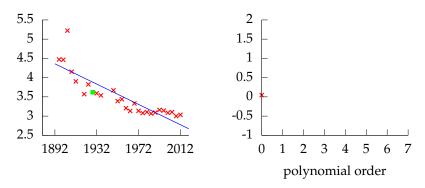
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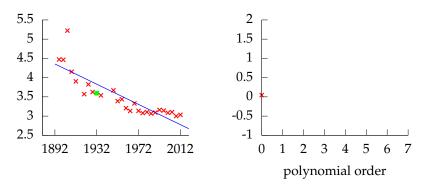
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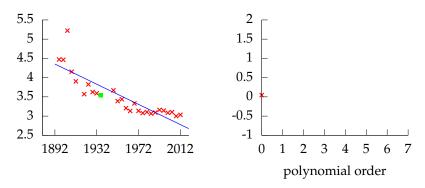
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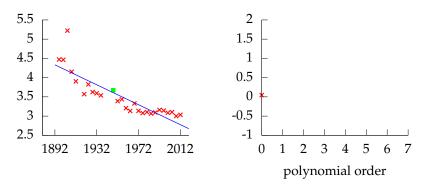
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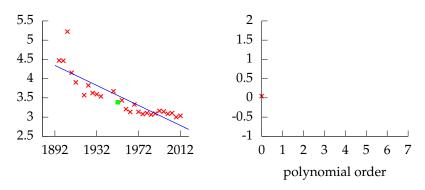
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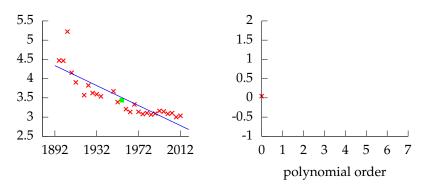
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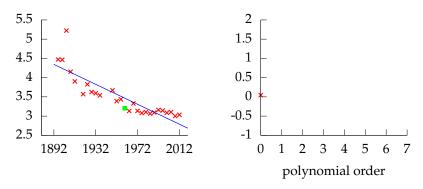
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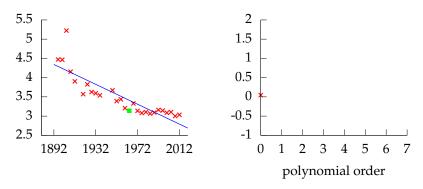
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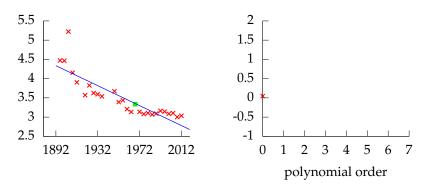
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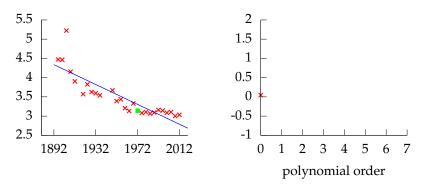
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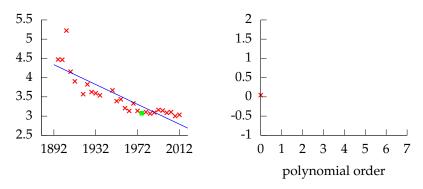
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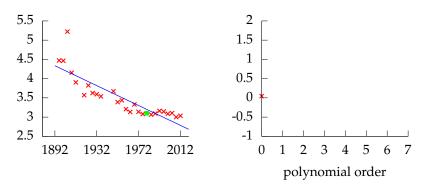
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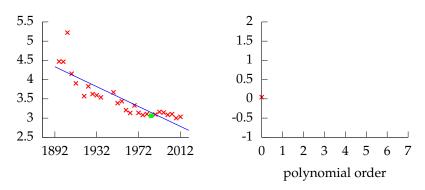
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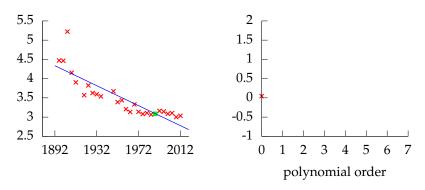
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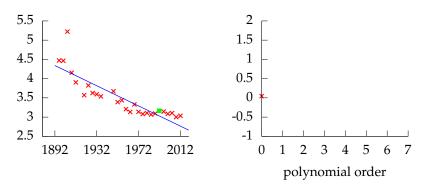
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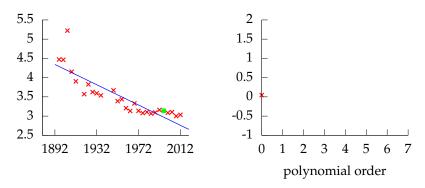
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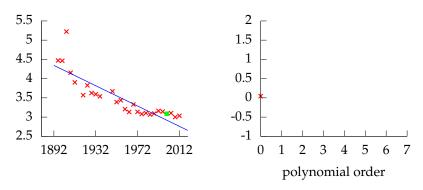
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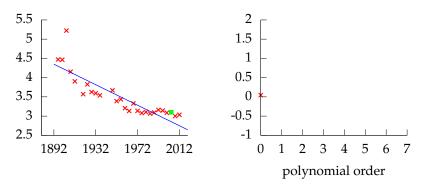
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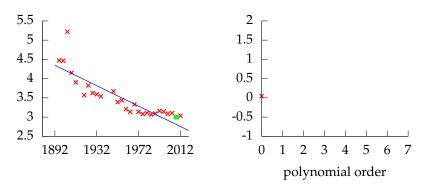
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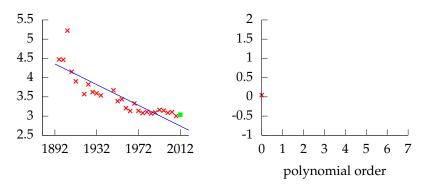
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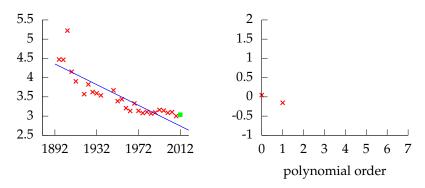
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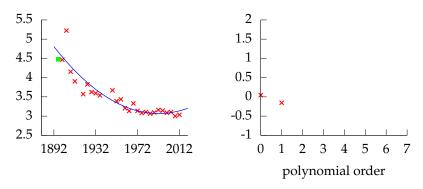
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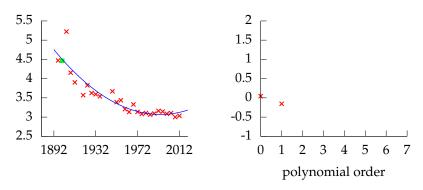


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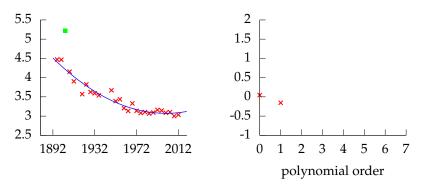


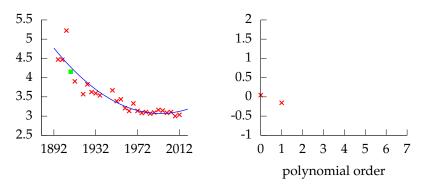
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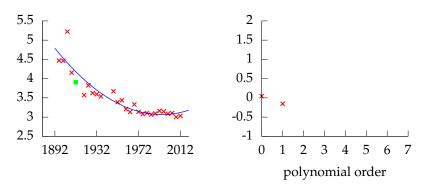




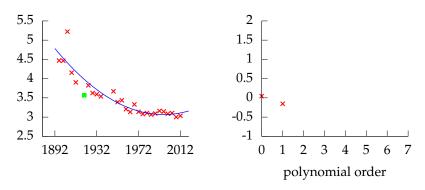
Polynomial order 2, training error -28.403, leave one out error 0.34669.



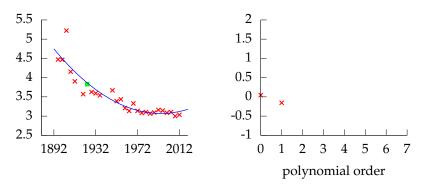


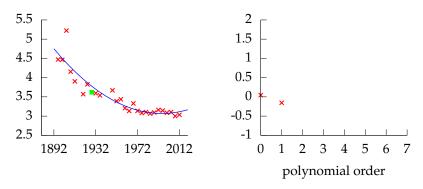


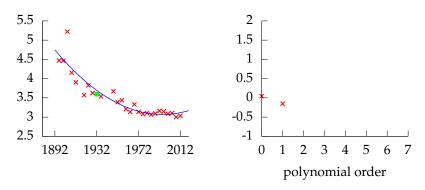
Polynomial order 2, training error -28.403, leave one out error 0.34669.



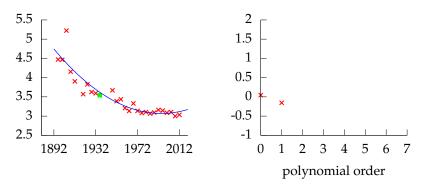
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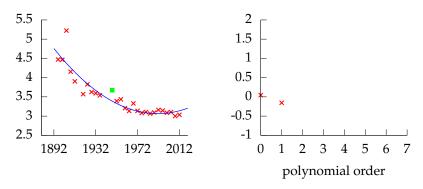


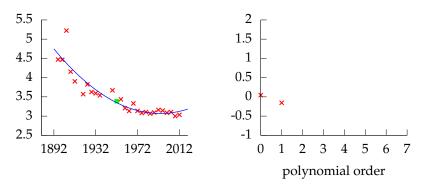


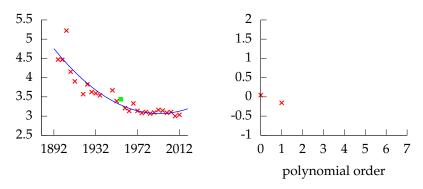


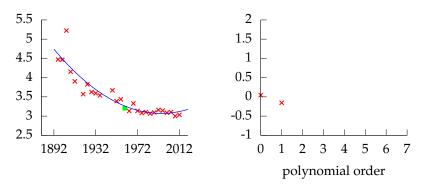
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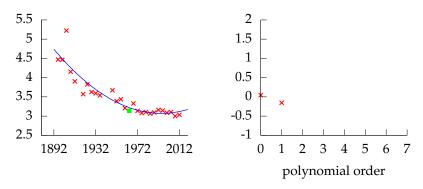


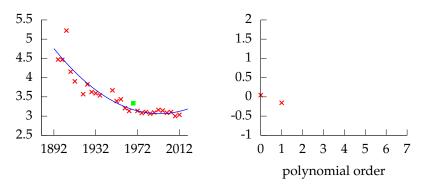


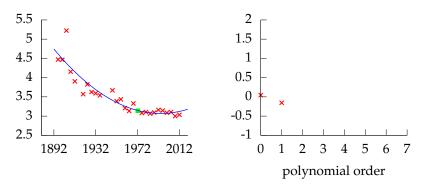


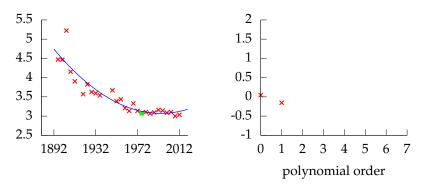


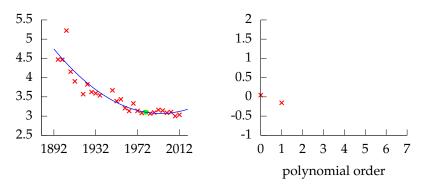


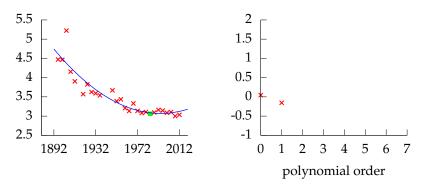


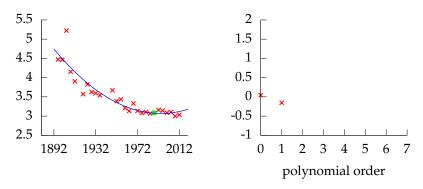


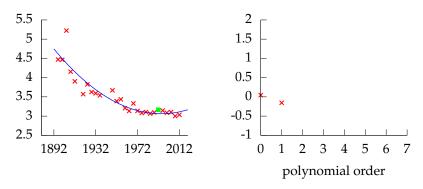


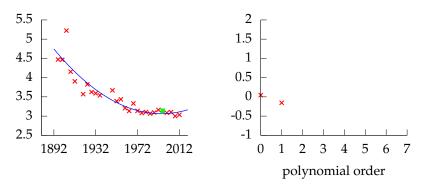


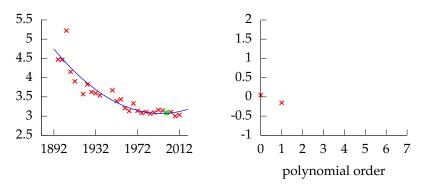


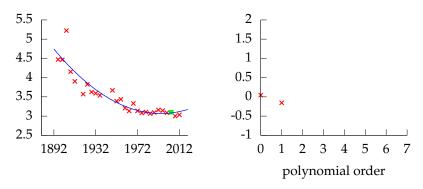


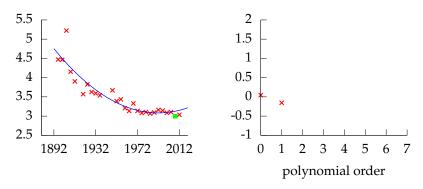


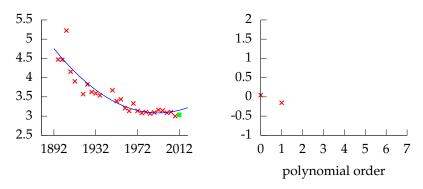


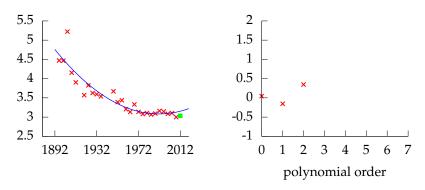




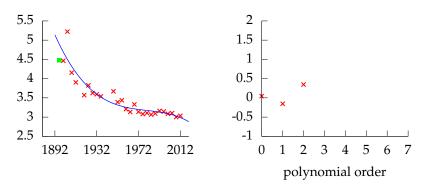




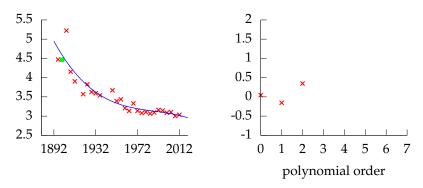




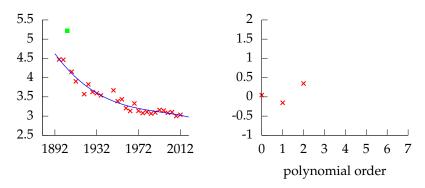
Polynomial order 2, training error -28.403, leave one out error 0.34669.



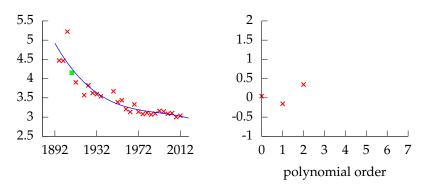
Polynomial order 3, training error -29.223, leave one out error 0.51621.



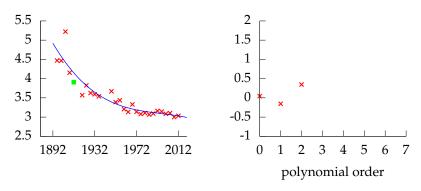
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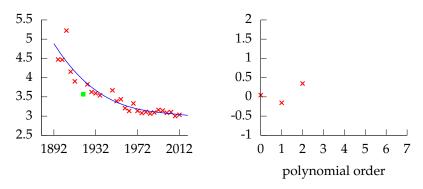
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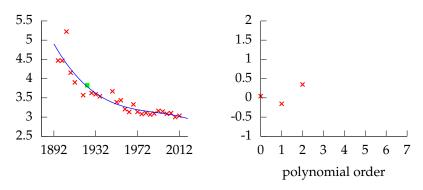
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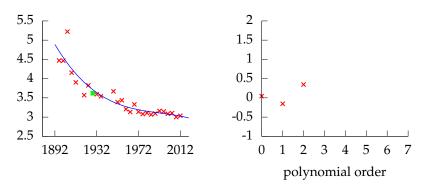
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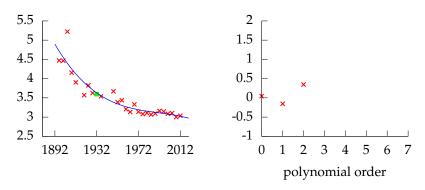
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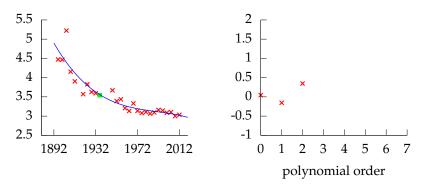
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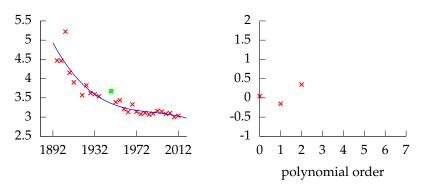
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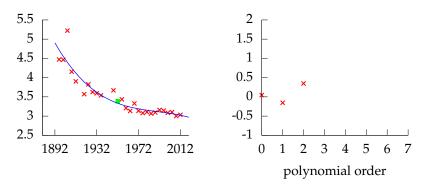
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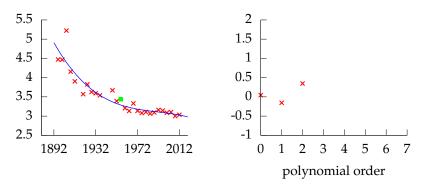
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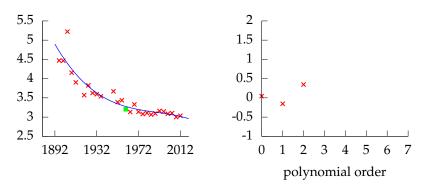
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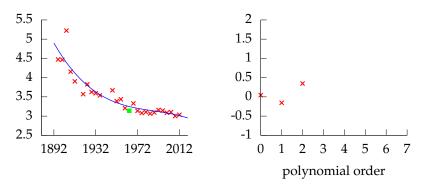
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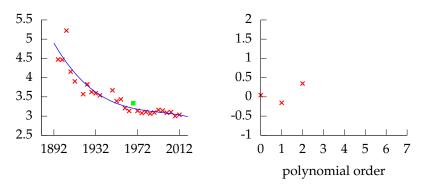
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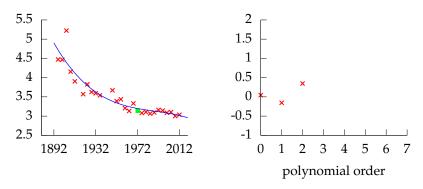
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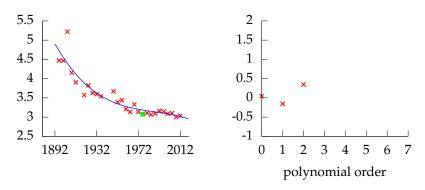
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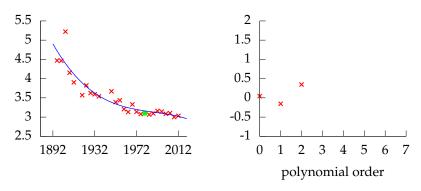
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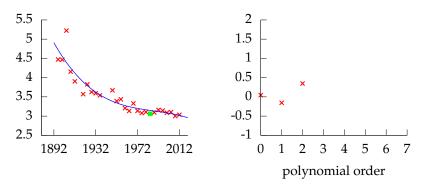
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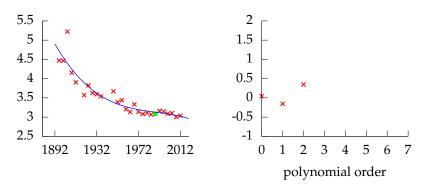
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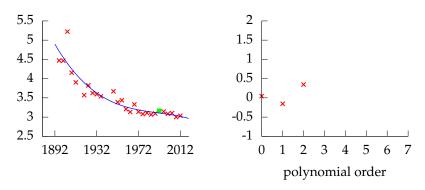
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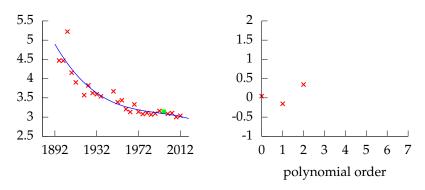
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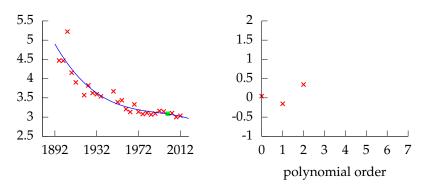
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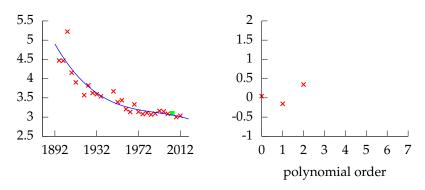
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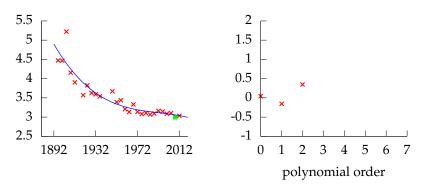
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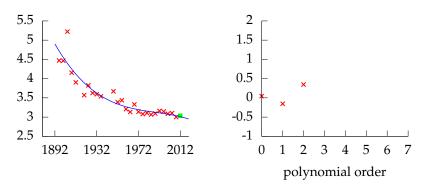
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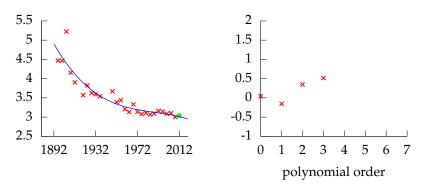
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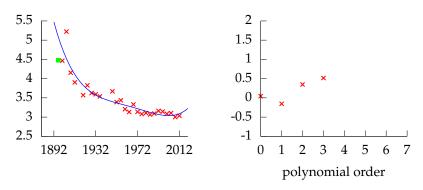
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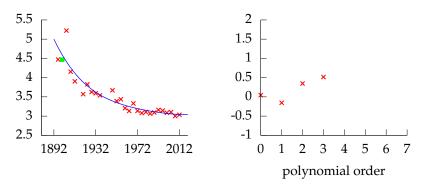
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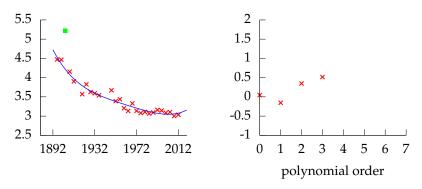
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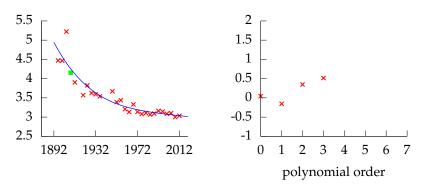
Polynomial order 4, training error -29.324, leave one out error 0.84844.



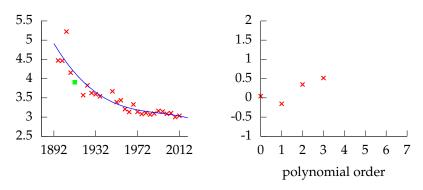
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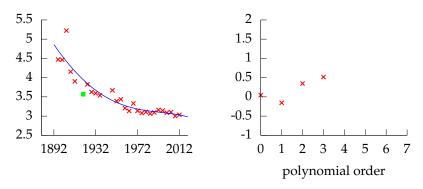
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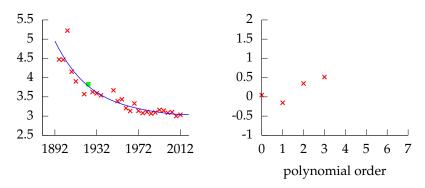
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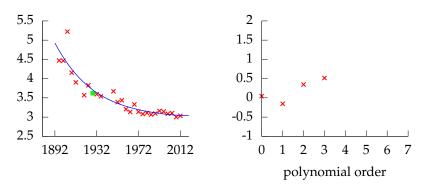
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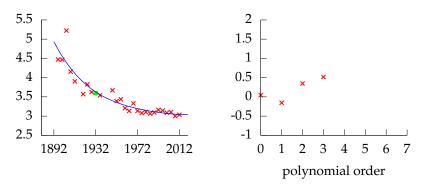
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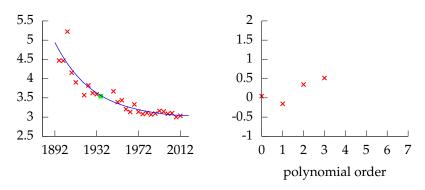
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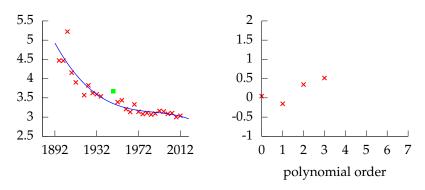
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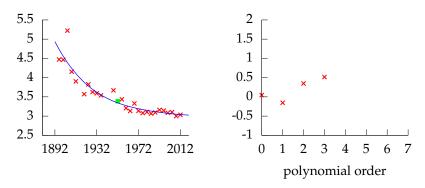
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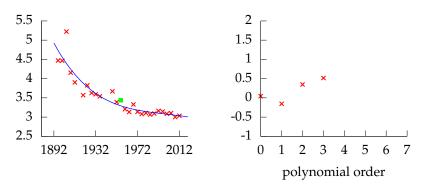
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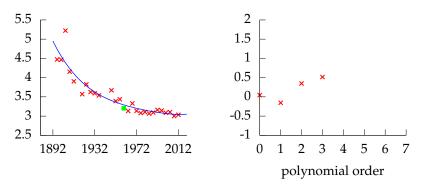
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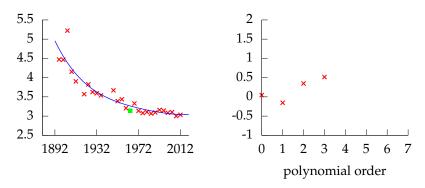
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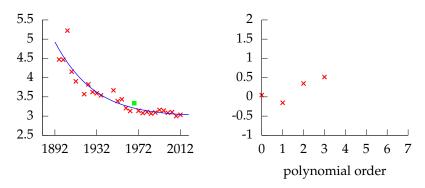
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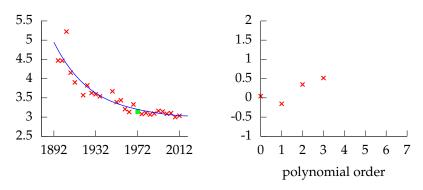
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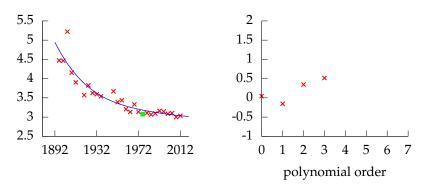
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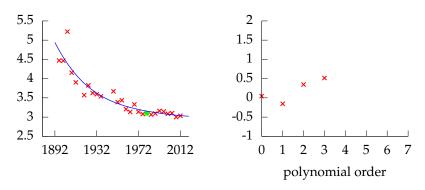
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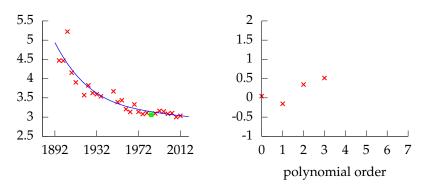
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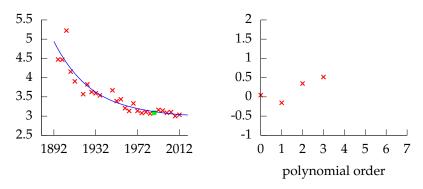
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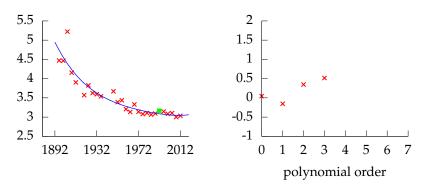
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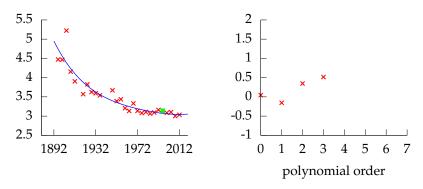
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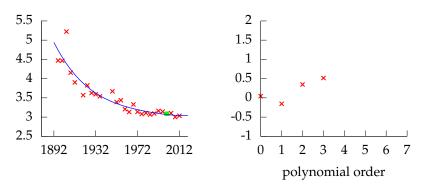
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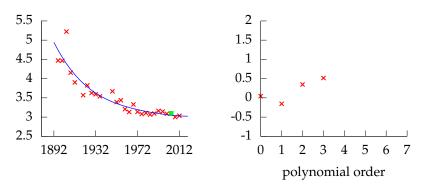
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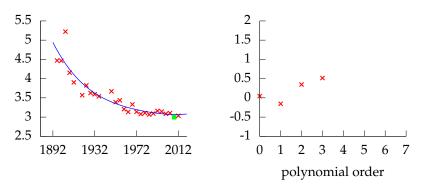
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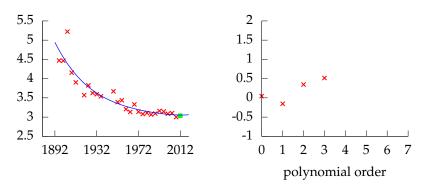
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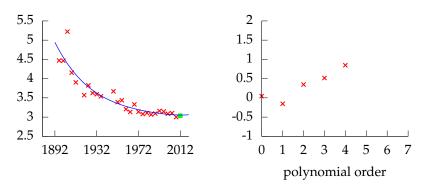
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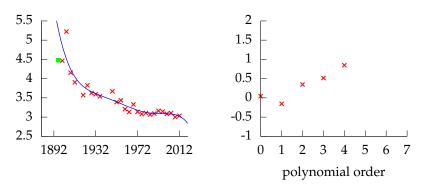
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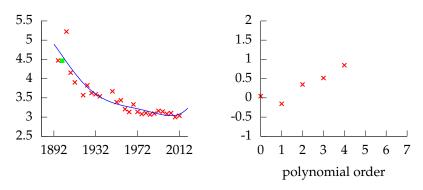
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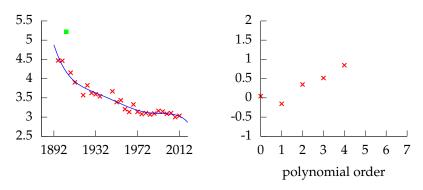
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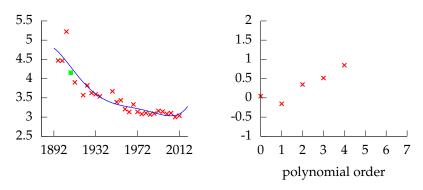
Polynomial order 5, training error -29.524, leave one out error 1.48.



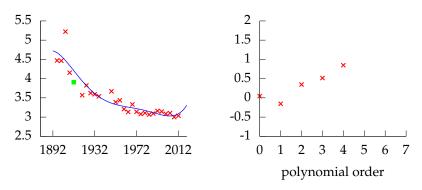
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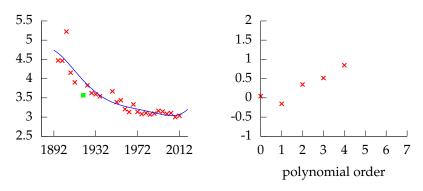
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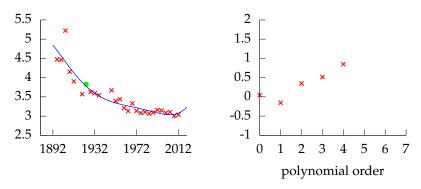
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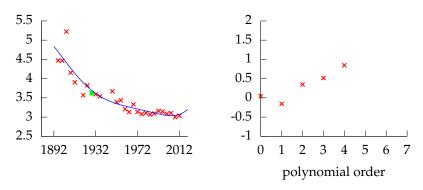
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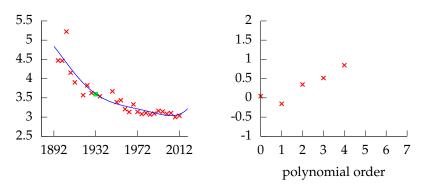
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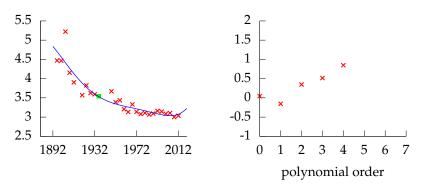
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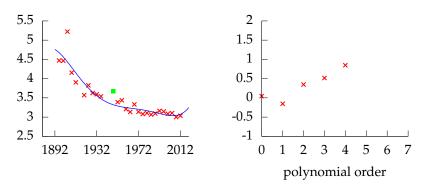
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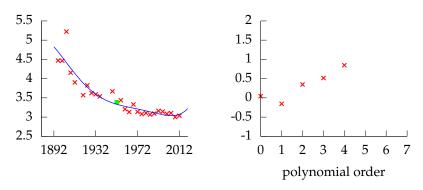
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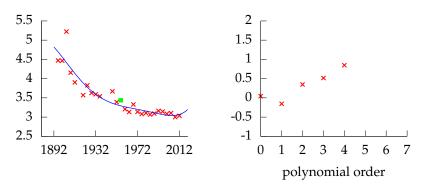
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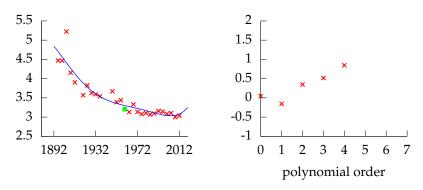
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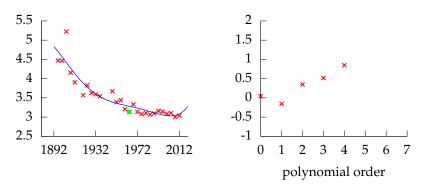
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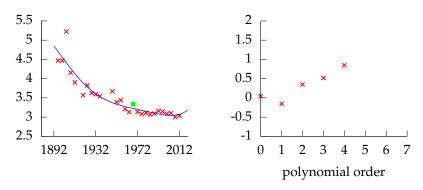
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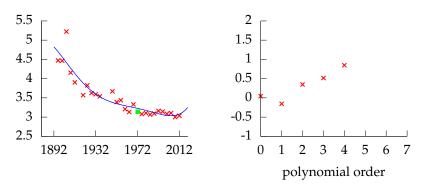
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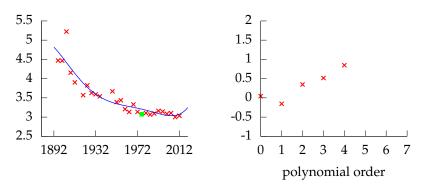
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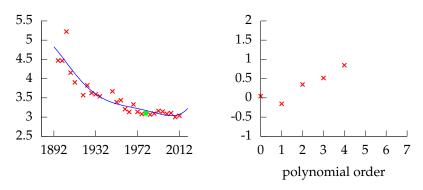
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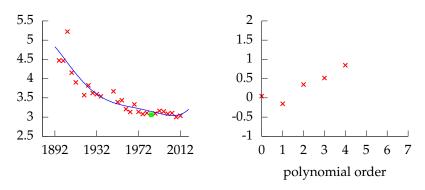
Polynomial order 5, training error -29.524, leave one out error 1.48.



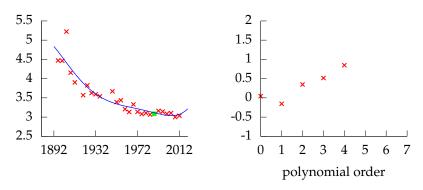
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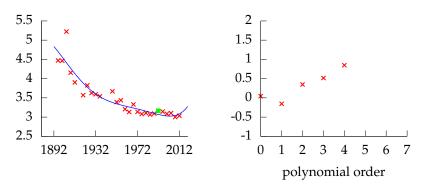
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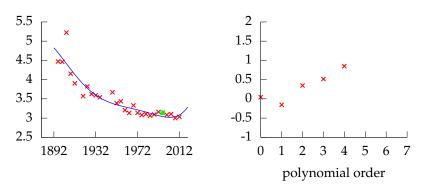
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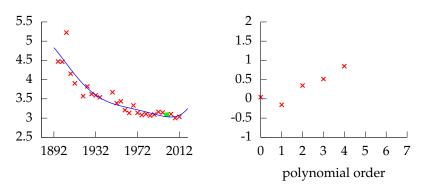
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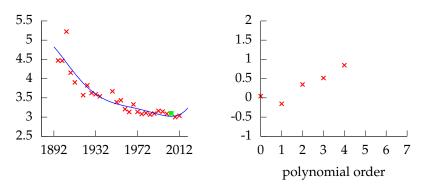
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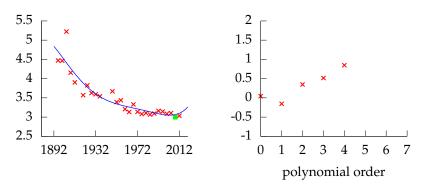
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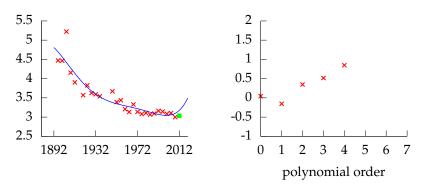
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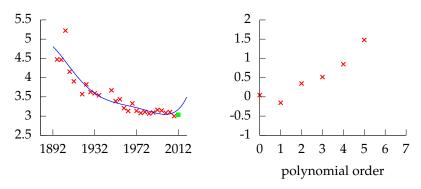
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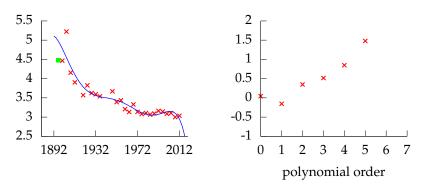
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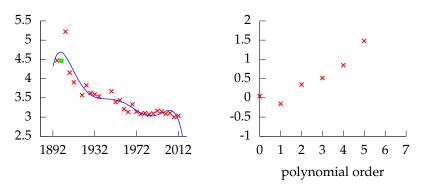
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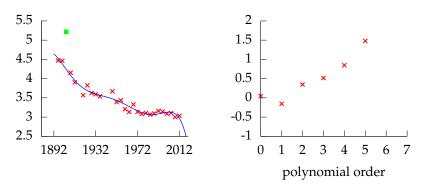
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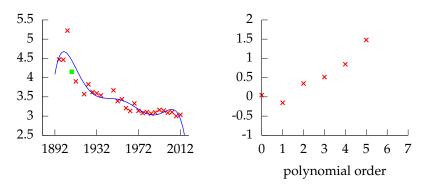
Polynomial order 6, training error -32.237, leave one out error 1.5047.



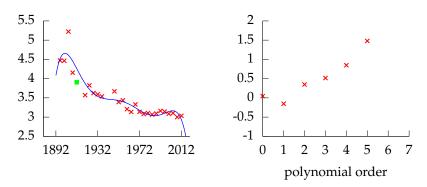
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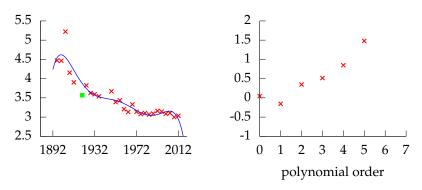
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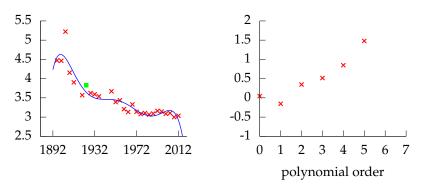
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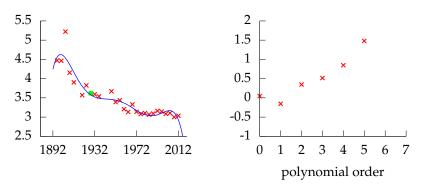
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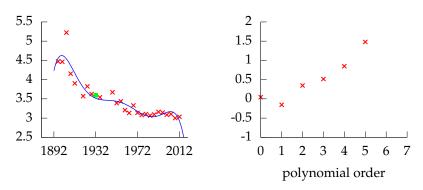
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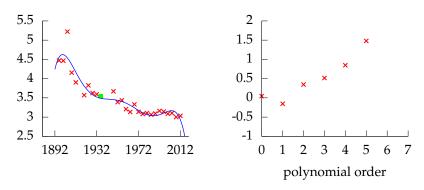
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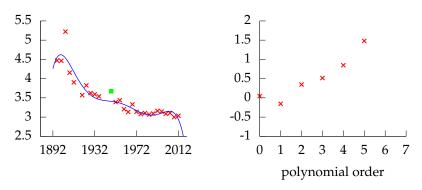
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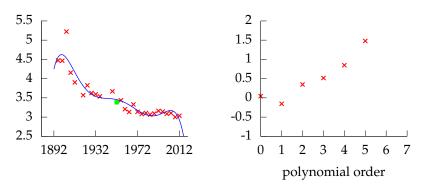
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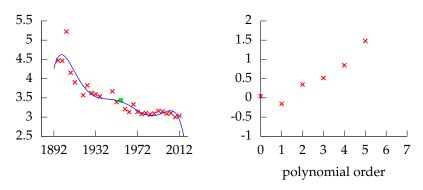
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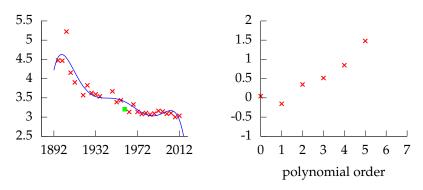
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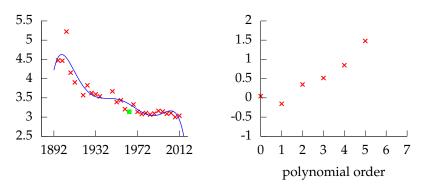
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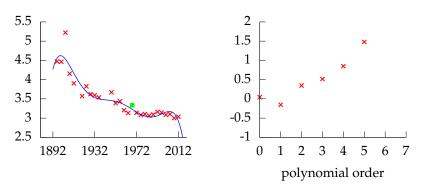
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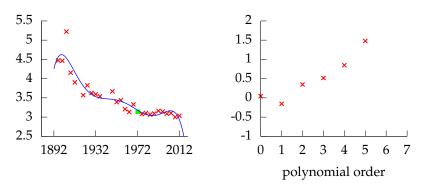
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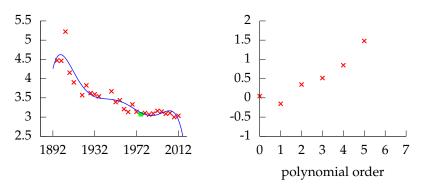
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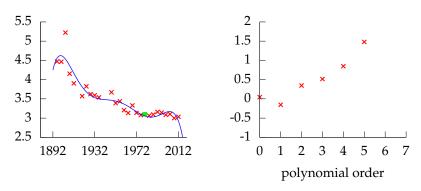
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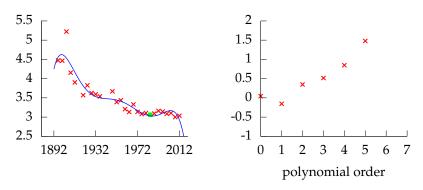
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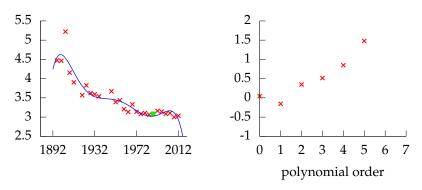
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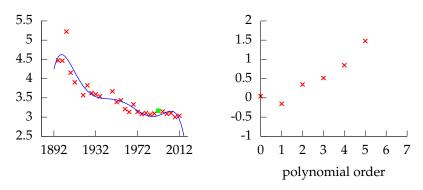
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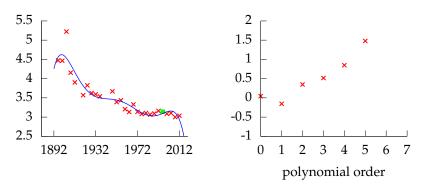
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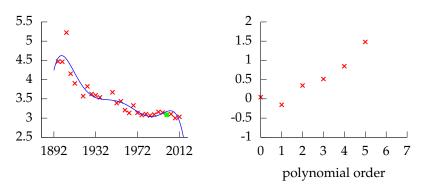
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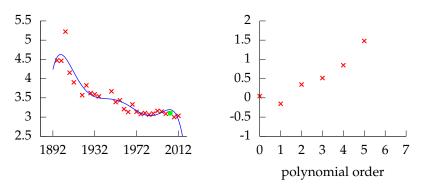
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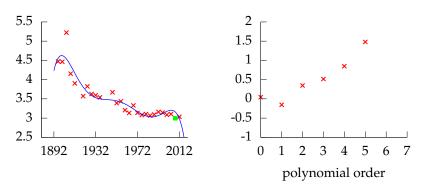
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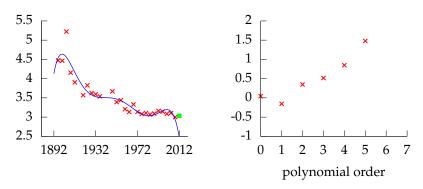
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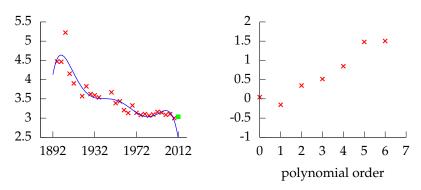
Polynomial order 6, training error -32.237, leave one out error 1.5047.



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



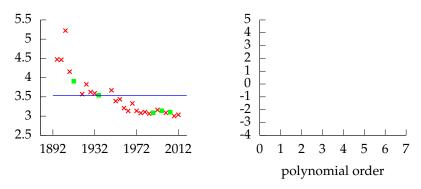
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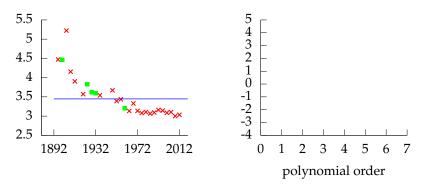


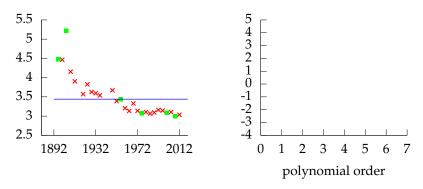
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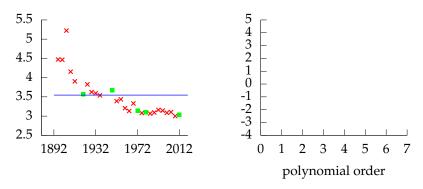
#### k Fold Cross Validation

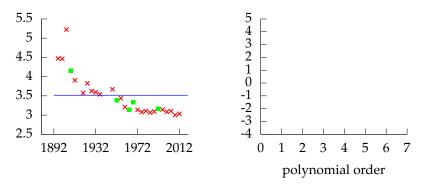
- Leave one out cross validation can be very time consuming!
- ► Need to train your algorithm *n* times.
- ► An alternative: *k* fold cross validation.

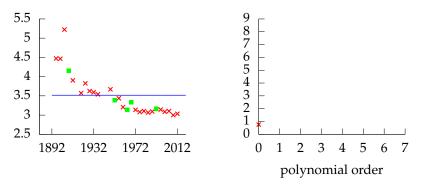


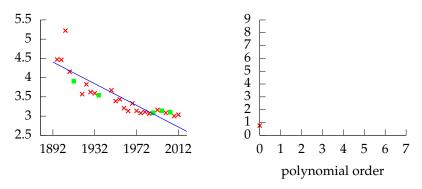




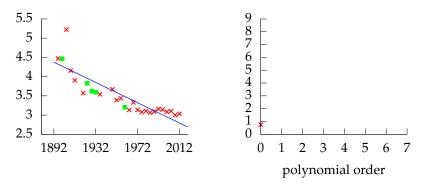




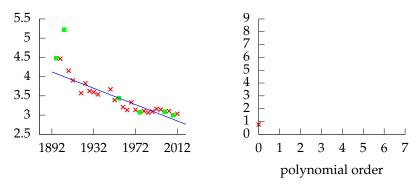




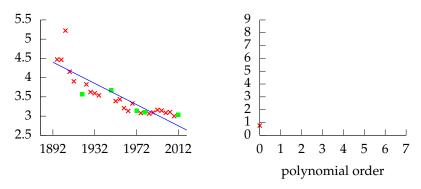
Polynomial order 1, training error -18.873, leave one out error -0.15413.



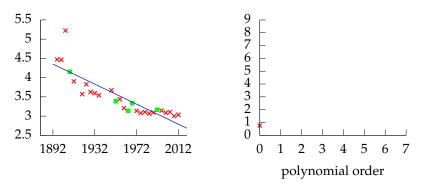
Polynomial order 1, training error -18.873, leave one out error -0.15413.



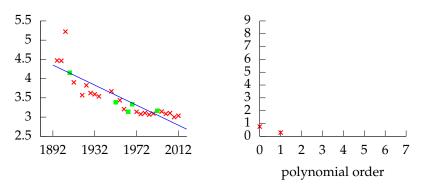
Polynomial order 1, training error -18.873, leave one out error -0.15413.



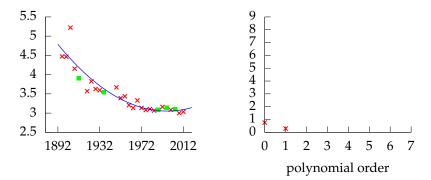
Polynomial order 1, training error -18.873, leave one out error -0.15413.



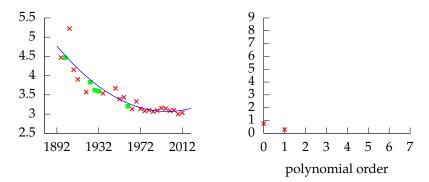
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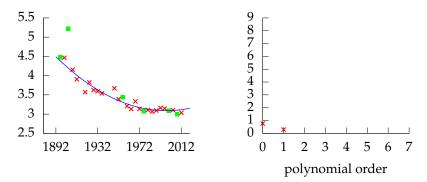
Polynomial order 1, training error -18.873, leave one out error -0.15413.



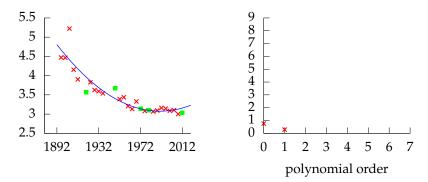
Polynomial order 2, training error -25.177, leave one out error 0.34669.



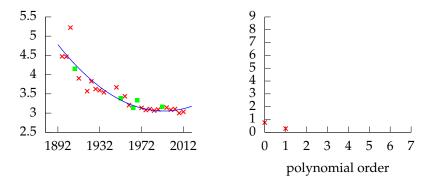
Polynomial order 2, training error -25.177, leave one out error 0.34669.



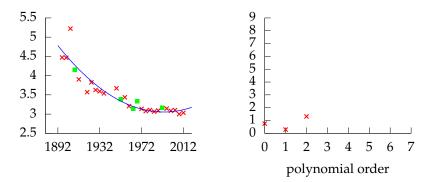
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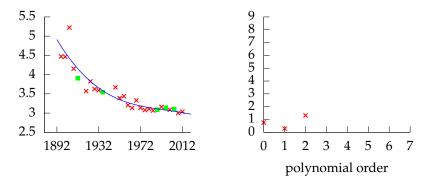
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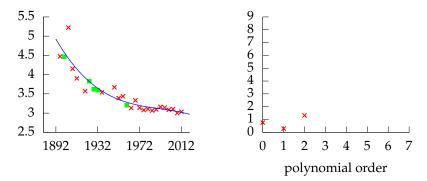
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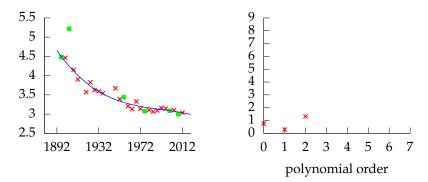
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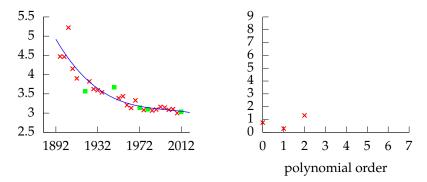
Polynomial order 3, training error -25.777, leave one out error 0.51621.



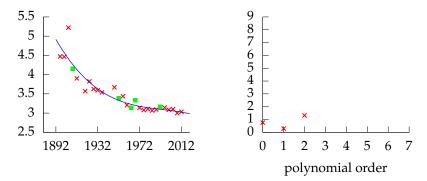
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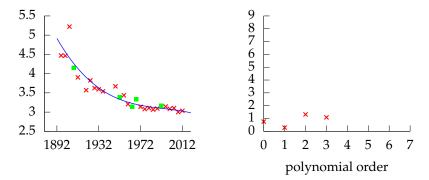
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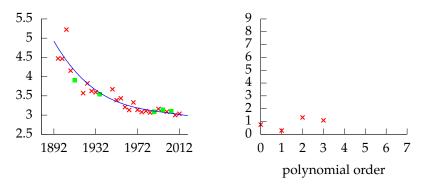
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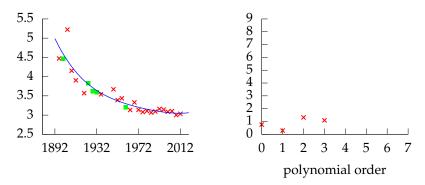
Polynomial order 3, training error -25.777, leave one out error 0.51621.



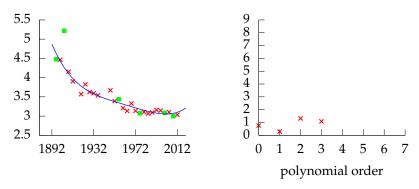
Polynomial order 3, training error -25.777, leave one out error 0.51621.



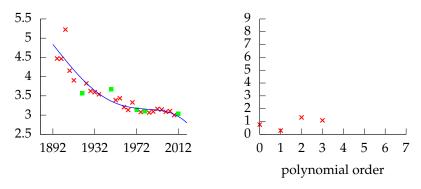
Polynomial order 4, training error -26.048, leave one out error 0.84844.



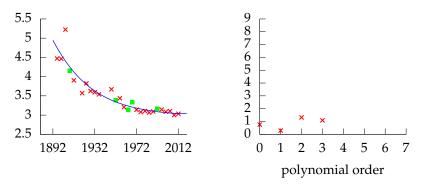
Polynomial order 4, training error -26.048, leave one out error 0.84844.



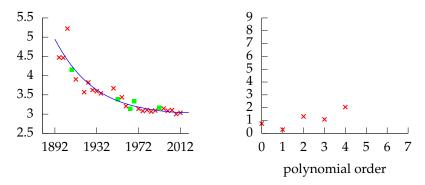
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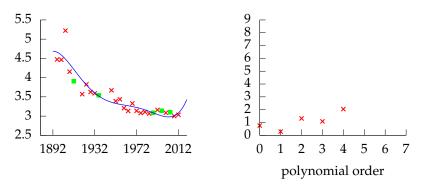
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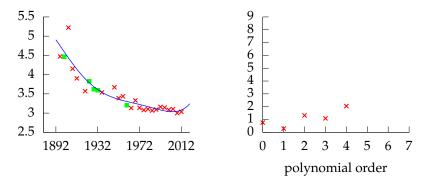
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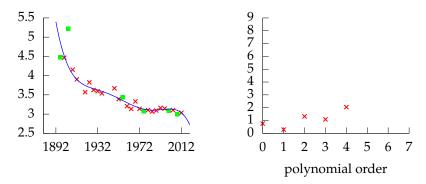
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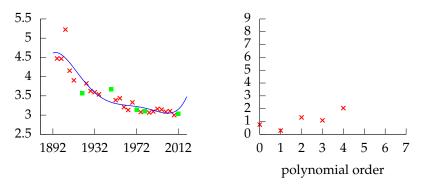
Polynomial order 5, training error -26.892, leave one out error 1.48.



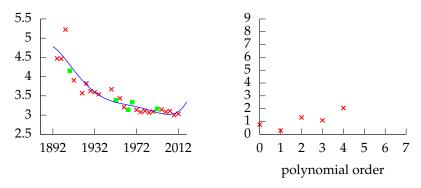
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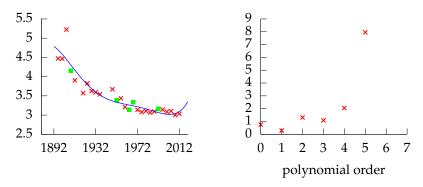
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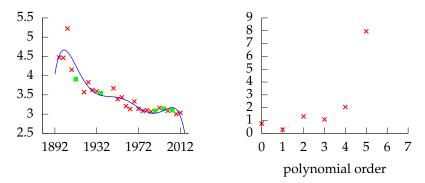
Polynomial order 5, training error -26.892, leave one out error 1.48.



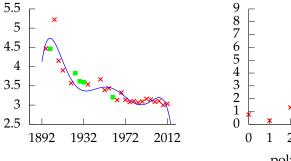
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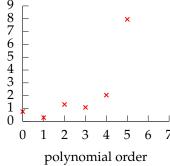


Polynomial order 5, training error -26.892, leave one out error 1.48.

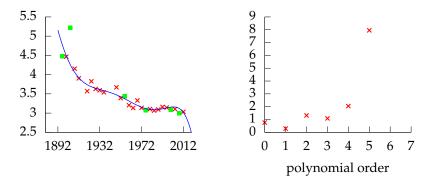


Polynomial order 6, training error -29.395, leave one out error 1.5047.

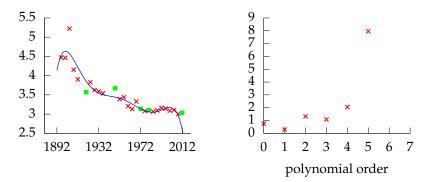




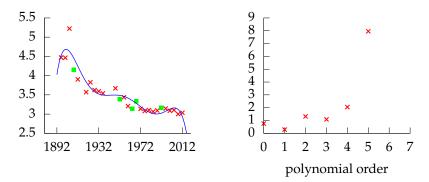
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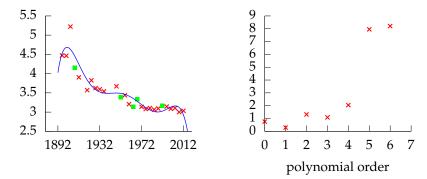
Polynomial order 6, training error -29.395, leave one out error 1.5047.



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



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



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

# Reading

► 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

- C. M. Bishop. *Pattern Recognition and Machine Learning*. Springer-Verlag, 2006. [Google Books].
- S. Rogers and M. Girolami. *A First Course in Machine Learning*. CRC Press, 2011. [Google Books].