Overfitting

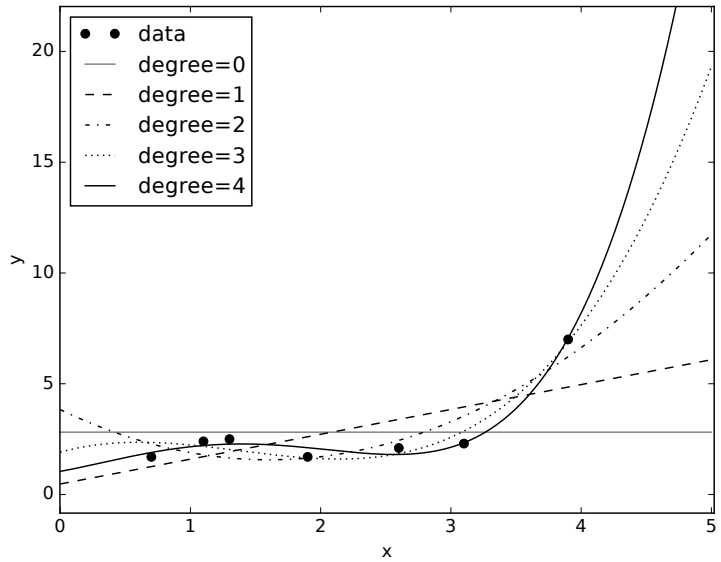
- Overfitting occurs when the learner finds regularities in the training set that do not occur in the world (or in the test set).
- Model tries to find signal in randomness.
- Often results in
  - more complex models than can be justified by the limited data.
  - overconfidence: more extreme probabilities than is justified.
- Fitting the training set better does not mean fitting the test set or better predictions of future cases

Example of Overfitting: Restaurant Ratings

- We have a web site where people rate restaurants with 1 to 5 stars.
- We want to report the most liked restaurant(s) — the one predicted to have the best future ratings.
- How can we determine the most liked restaurant?
- Are the restaurants with the highest average rating the most liked restaurants?
- Which restaurants have the highest average rating?
- Which restaurants have a rating of 5?
  - Only restaurants with few ratings have an average rating of 5.
  - Restaurants with few ratings but all high are unlikely to be as good as the ratings indicate.
- Ratings are a mix of quality and luck. Lots of data averages out luck.

Example of Overfitting: Model complexity

Polynomials of various degrees can be used to fit data:



- Can use standard linear regression with 1, x, x^2, x^3 ... as features. The maximum power with non-zero coefficient is the degree of the polynomial.
- Higher-degree polynomials can always(?) fit data better.
- What happens with extrapolation?
  How do polynomials of odd and even degrees differ?

Test set error

Test set error is caused by:

- Bias: error due to the algorithm finding an imperfect model. The bias can be divided into:
  - representation bias: the representation doesn't containing a hypothesis close to the ground truth
  - search bias: the algorithm doesn't search enough of the space of hypotheses to find the best hypothesis.
- Variance: error due to a lack of data.
  A fixed amount of data has a bias–variance trade-off:
  - a complicated model could be accurate, but there is not enough data to estimate it accurately
  - a simple may not be accurate, but you can estimate the parameters reasonably well given the data
- Noise: inherent error due to the data depending on features not modeled or the process generating the data is inherently stochastic.

Pseudocounts

- For many of the prediction measures, the optimal prediction on the training data is the mean.
- In the restaurant example, the mean rating wasn't a good measure (too extreme for restaurants with few ratings).
- A simple solution is to start with some pseudo-examples:
  - initially a restaurant is assumed to be average
  - As data comes in, the observed ratings are added to the pseudo-examples
  - Don't need to store pseudo-examples, just the sufficient statistics: pseudocounts.

Pseudocounts

- Suppose the examples are the values $v_1, \ldots, v_n$
- You want to make a prediction for the next v, written as $\widehat{v}$.
- When $n = 0$ – there is no data – use prediction a_0
- For the other cases, use

$$\widehat{v} = \frac{c * a_0 + \sum_i v_i}{c + n}$$

  where c is a nonnegative real-value constant.
- The value of c controls the relative importance of the initial hypothesis (the prior) and the data.
- a_0 and c can be estimated from other data (e.g., other restaurants)

A theoretical justification of pseudocounts is given in Chapter 10.

Regularization

"What can be done with fewer [assumptions] is done in vain with more."

William of Ockham (1285–1349)

- Prefer simpler hypotheses over more complex ones.
- Regularization: optimize fit-to-data plus a term that penalizes complexity
- Find a predictor $\widehat{Y}$ to minimize

$$\left(\sum_e loss(\widehat{Y}(e), Y(e))\right) + \lambda * regularizer(\widehat{Y})$$

  - $loss(\widehat{Y}(e), Y(e))$ is the loss of example e for predictor $\widehat{Y}$
  - $regularizer(\widehat{Y})$ is a penalty term that penalizes complexity.
  - The regularization parameter, λ, trades off fit-to-data and model simplicity

Regularization

- In decision tree learning, one complexity measure is the number of leaves in a decision tree.
- When building a decision tree, you could optimize the sum of a loss plus a function of the size of the decision tree, minimizing

$$\left(\sum_{e \in Es} loss(\widehat{Y}(e), Y(e))\right) + \gamma * |tree|$$

  where $|tree|$ is the number of leaves in a tree representation of $\widehat{Y}$.
- A single split on a leaf increases the number of leaves by 1.
- When greedily splitting, a single split is worthwhile if it reduces the sum of losses by γ.

L1 and L2 Regularization

Linear/logistic regression, minimize sum-of-squares:

$$\text{minimize } \mathit{Error}_E(\overline{w}) = \sum_{e \in E} \left(Y(e) - f(\sum_i w_i X_i(e)) \right)^2 .$$

L2 regularization (ridge regression):

$$\text{minimize } \sum_{e \in E} \left(Y(e) - f(\sum_i w_i X_i(e)) \right)^2 + \lambda \sum_i w_i^2$$

L1 regularization (lasso):

$$\text{minimize } \sum_{e \in E} \left(Y(e) - f(\sum_i w_i X_i(e)) \right)^2 + \lambda \sum_i |w_i|$$

λ is a parameter given a priori and/or learned.

SGD with L1 and L2 Regularization

- An $L2$ regularization is implemented in stochastic gradient descent by updating each weight w_i after a batch by:

$$w_i := w_i - \eta * \lambda * b/|Es| * w_i$$

where b is batch size.
The $m/|Es|$ is because the regularization is λ for the whole dataset, but the update occurs for each batch.

- An $L1$ regularizer can be implemented by updating each weight after a batch by:

$$w_i := sign(w_i) * max(0, |w_i| - \eta * \lambda * m/|Es|).$$

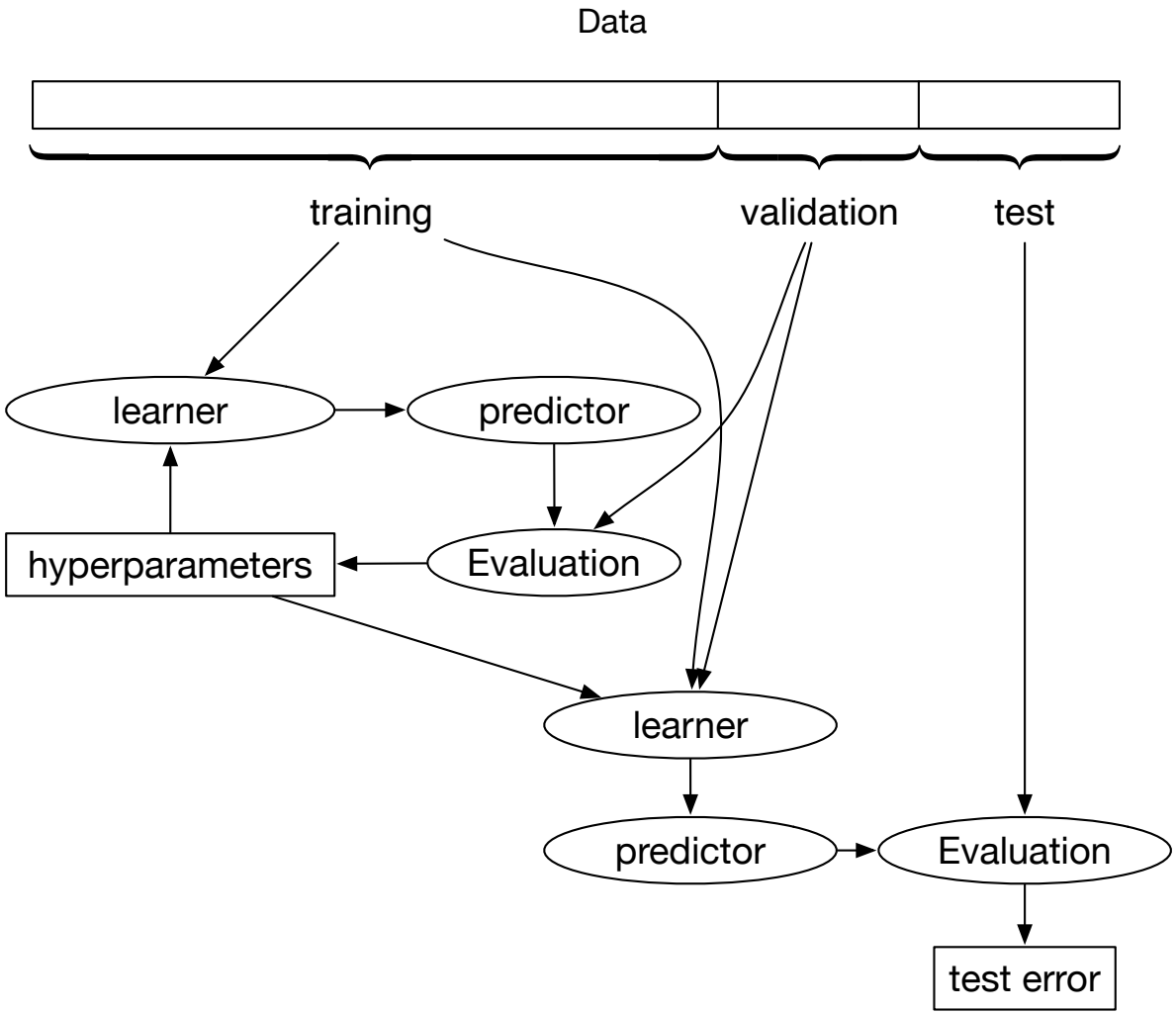
This is called iterative soft-thresholding

Cross Validation

- To evaluate an algorithms some of the data is used as *test data* (random data or latest in time). The test set *must not* be used for any part of training or choosing parameters.
- Idea: split the remaining data into:
  - training set
  - validation set
- A hyperparameter is a parameter used to define what is being optimized, or how it is optimized.
- Use the new training set to train on. Select the hyperparameters that work best on the validation set.

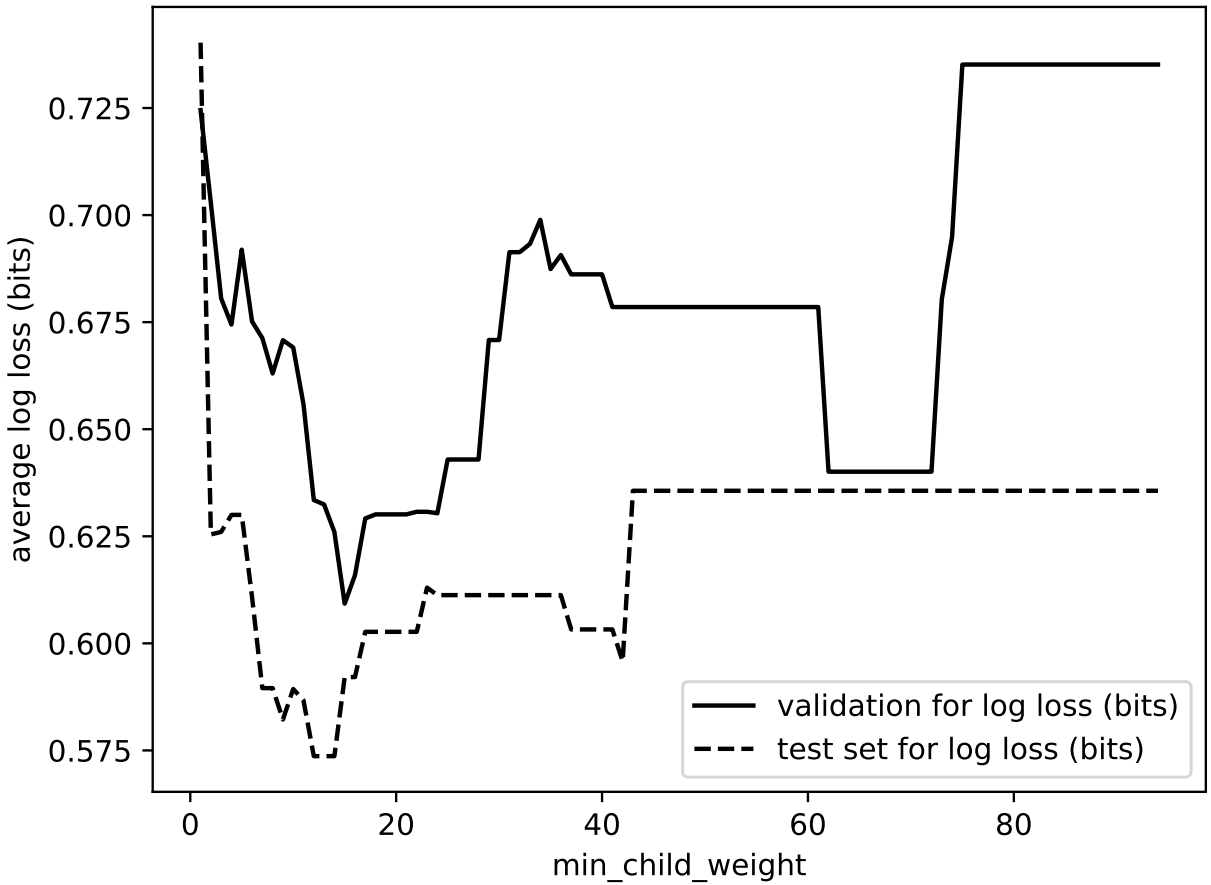
Cross Validation

Cross validation: use some of the non test set as a surrogate for test data:



Cross Validation

Cross validation assumptions: hyperparameter values that are best for validation examples will be best for test examples.



minimum number of examples that needs to be in a child for decision-tree learning.

k-Fold Cross Validation

- With limited data, either training data or validation data will be small (or both).
- How can we avoid overfitting to these small datasets?
- k-Fold Cross Validation:
  - partition non-test data Es into k folds, $E_1, \ldots E_k$ ($k = 10$ is common for 10-fold cross validation)
  - For i from 1 to k:
    train on $Es \setminus E_i$ evaluate on E_i
  - Select the hyperparameter settings with lowest average error on $E_1, \ldots E_k$
  - Train a model on Es with these settings
- If $k = 10$, during hyperparameter tuning, 90% of the training examples are used for training and 10% of the examples for validation.
  It does this 10 times, so each example is used once in a validation set.