15-830 – Machine Learning 4: Evaluation

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Evaluating algorithms

- How do we determine when an algorithm achieves "good" performance?
- How should we tune the parameters of the learning algorithms (regularization parameter, choice of feautres, parameters of kernel, etc?)
- How do we report the performance of learning algorithms?

- One possibility: just look at the loss function

$$J(\theta) = \sum_{i=1}^{m} \ell(\theta^T \phi(x_i), y_i)$$

- The problem: adding more features will *always* decrease the loss

- Example example: random outputs, random features, we can get zero loss for enough features

```
m = 500;
y = randn(m,1);
Phi = randn(m,m);
theta = (Phi' * Phi)  (Phi' * y);
norm(Phi*theta - y)^2

ans =
    2.3722e-22
```

- A better criterion: *training* and *testing* loss
  - **Training set:** $x_i \in \mathbb{R}^n, y_i \in \mathbb{R}, \;\; i = 1, \ldots, m$
  - **Testing set:** $x'_i \in \mathbb{R}^n, y'_i \in \mathbb{R}, \;\; i = 1, \ldots, m'$
- Find parameters by minimizing loss on the training set, but evaluate on the testing set

$$\text{Training:} \;\; \theta^\star = \arg\min_\theta \sum_{i=1}^{m} \ell(\theta^T \phi(x_i), y_i)$$

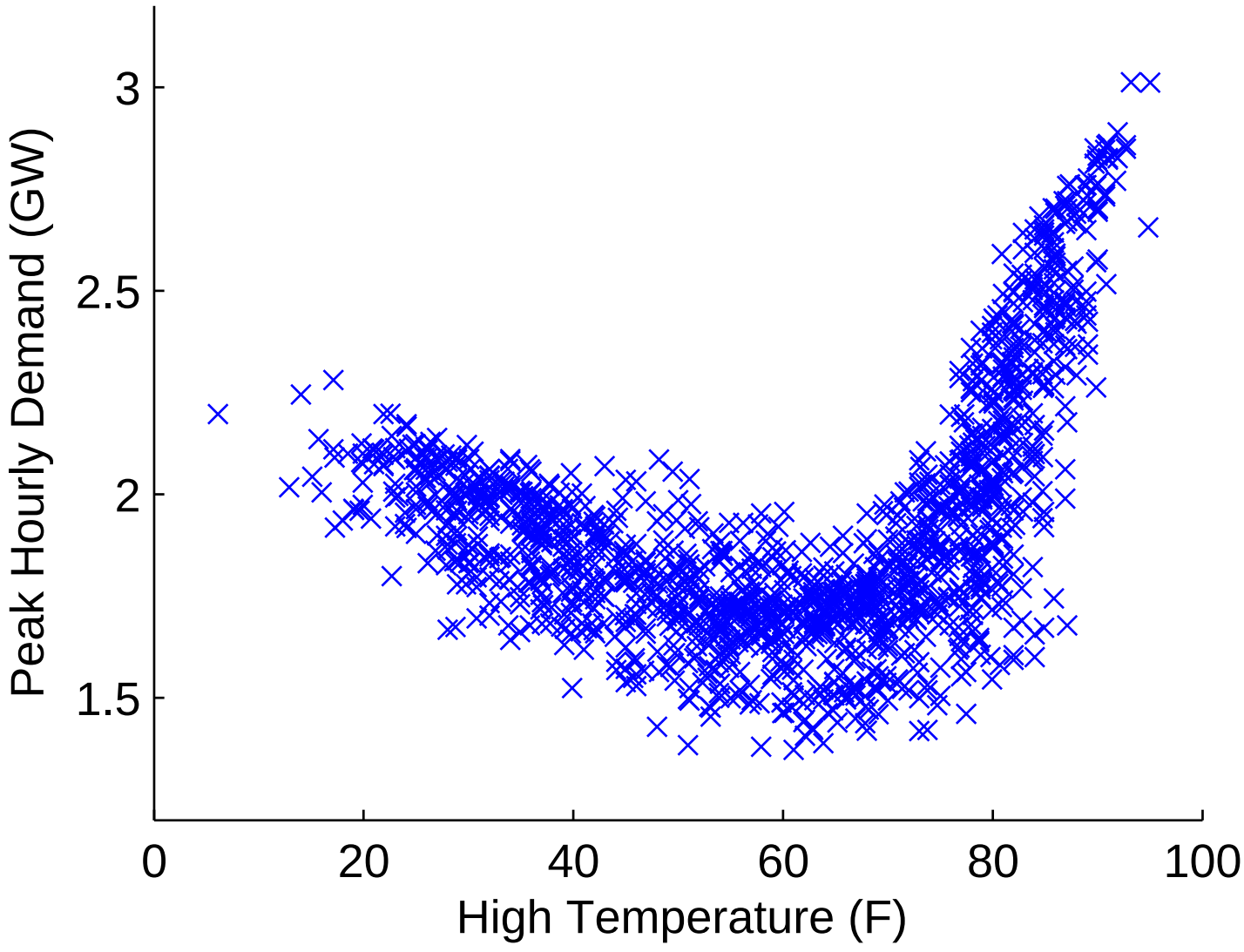
$$\text{Evaluation:} \;\; \text{Average Loss} = \frac{1}{m'} \ell((\theta^\star)^T \phi(x'_i), y'_i)$$

  - Performance on test set called *generalization* performance.

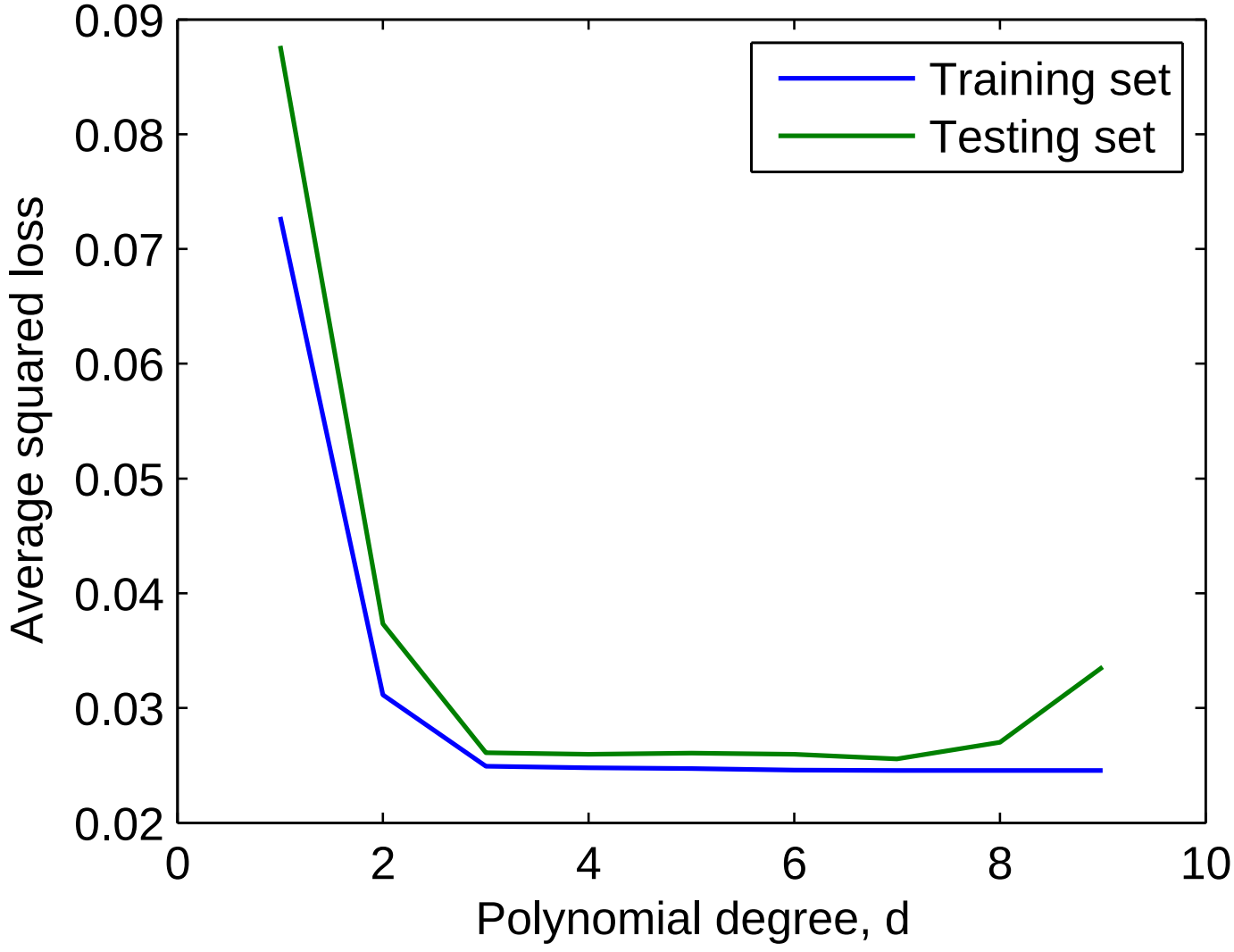
- Sometimes, there is a natural breakdown between training and testing data (e.g., train system on one year, test on the next)

- More common, simply device up the data: for example, use 70% for training, 30% for testing

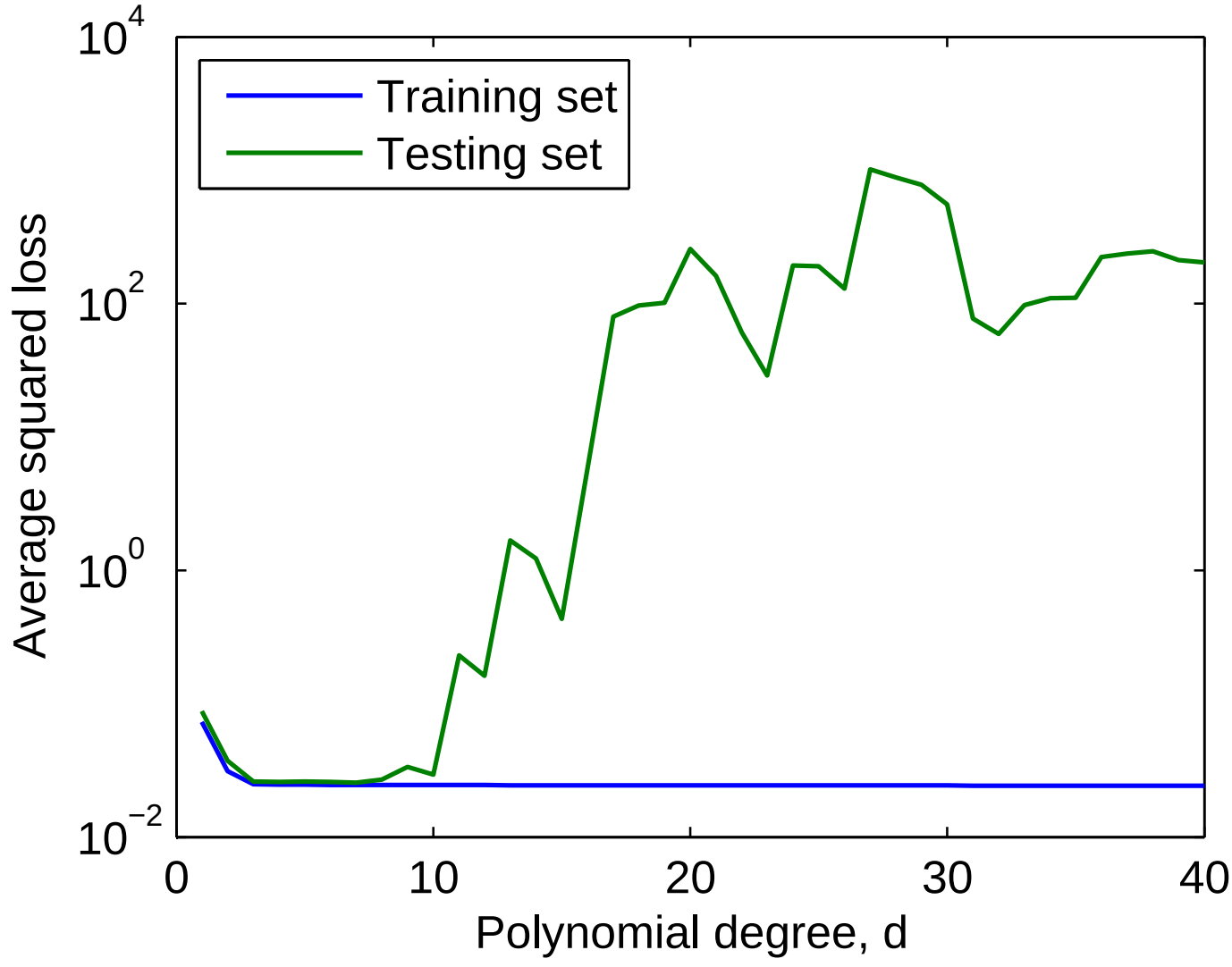
```
% Phi, y, m are all the data
 m_train = ceil(0.7*m);
 m_test = m - m_train;
 p = randperm(m);

 Phi_train = Phi(p(1:m_train),:);
 y_train = y(p(1:m_train));
 Phi_test = Phi(p(m_train+1:end),:);
 y_test = y(p(m_train+1:end));
```



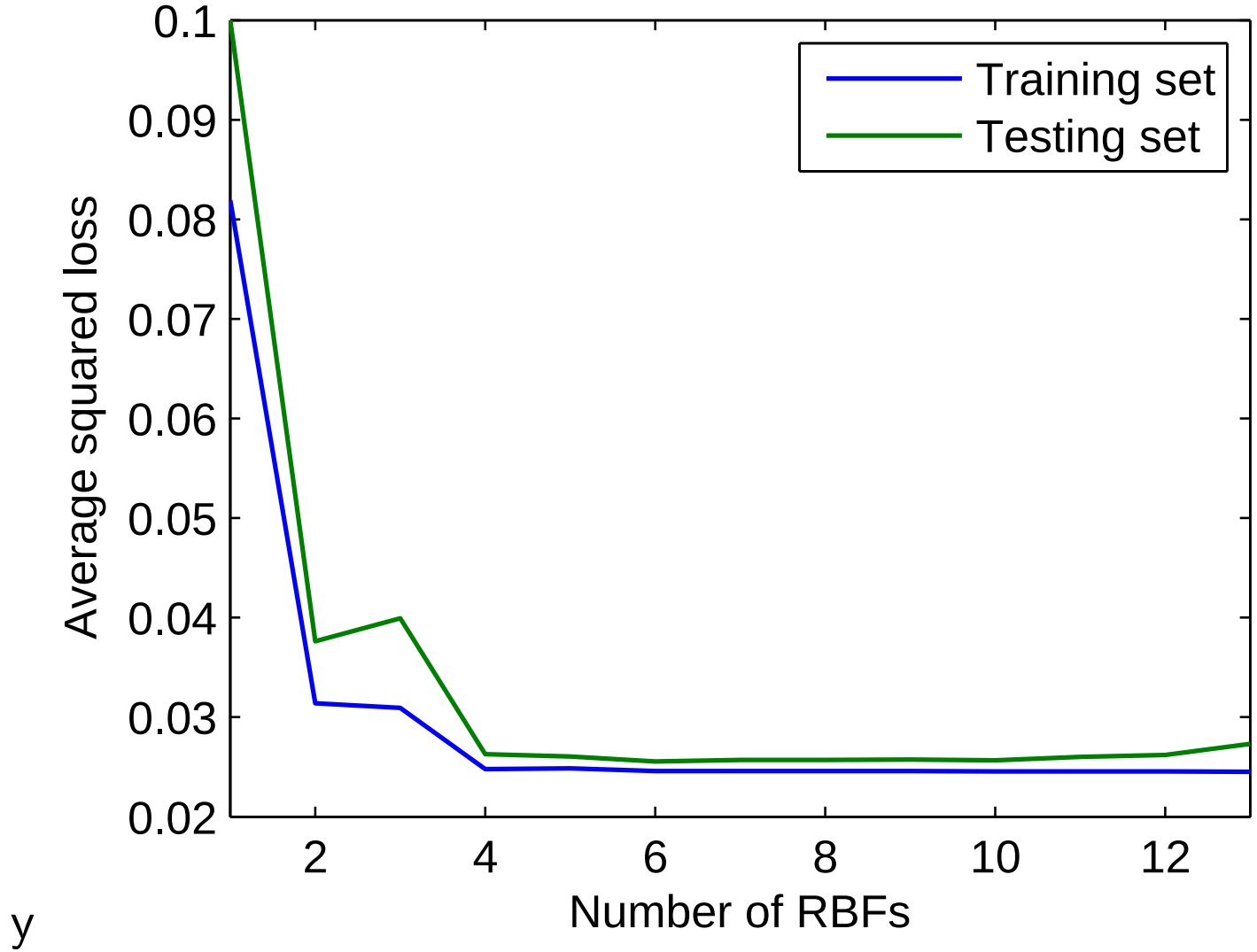
High temperature / peak demand observations



Testing loss versus degree of polynomial

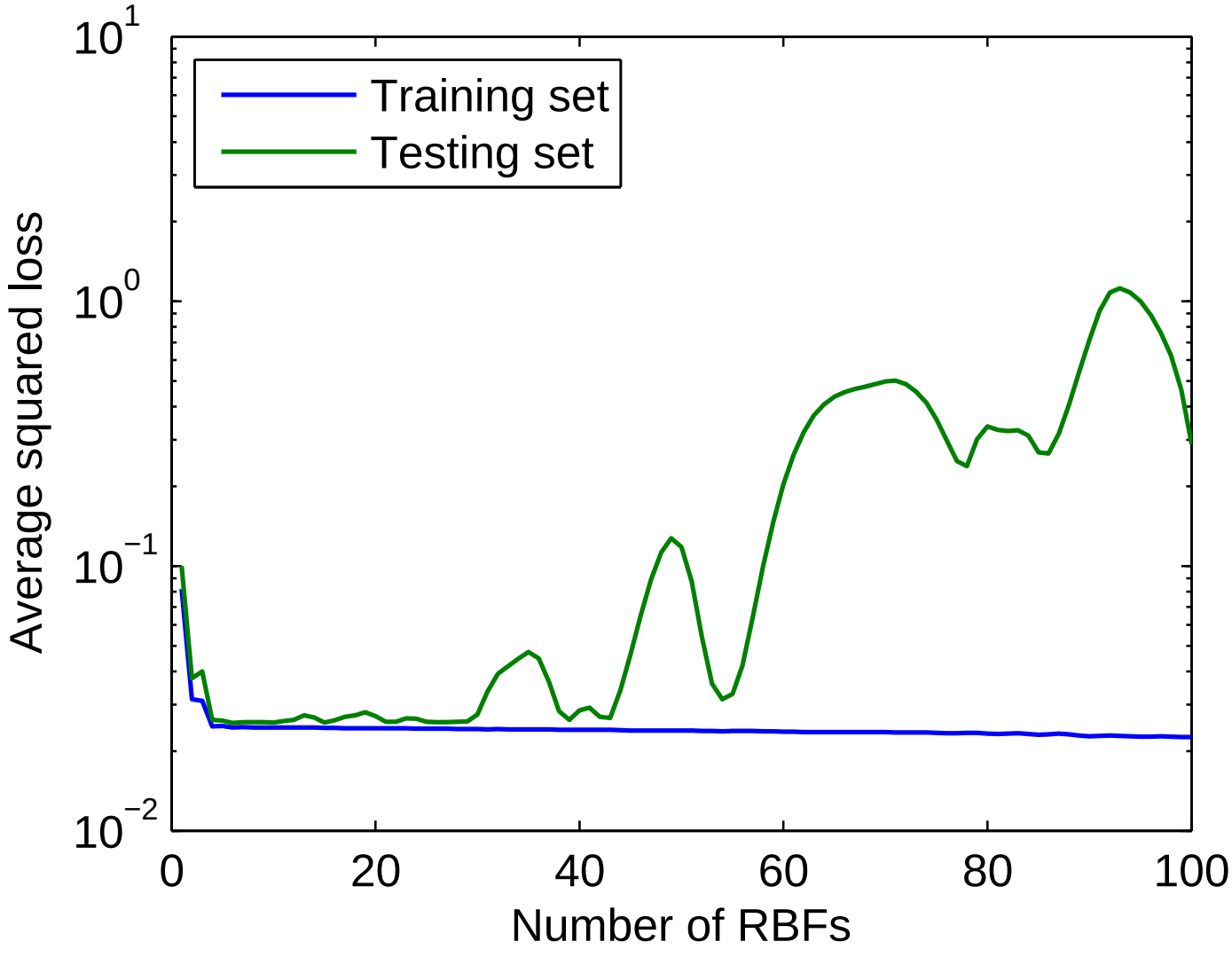


Testing loss (log-scale) versus degree of polynomial

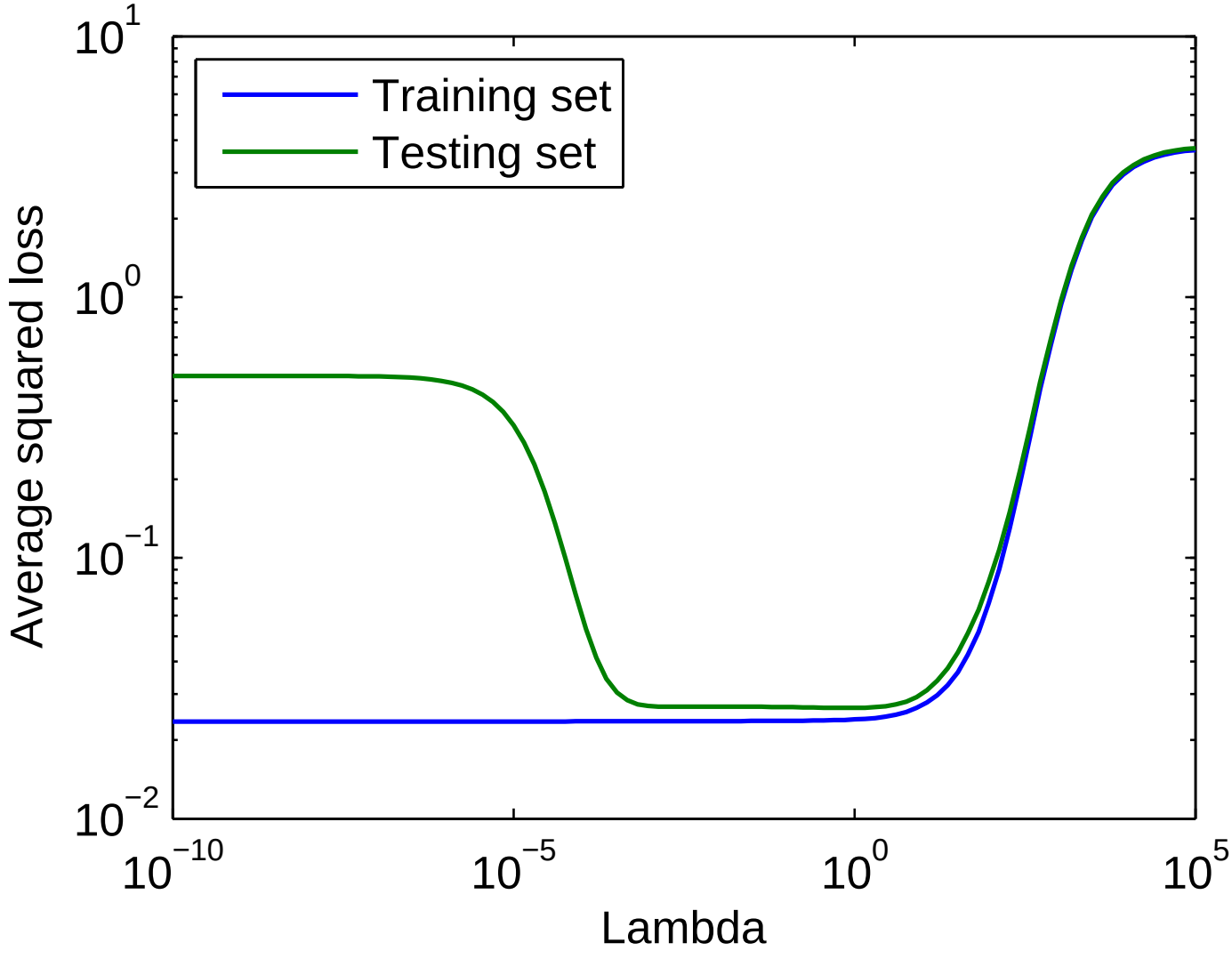


y

Testing loss versus number of RBF bases



Testing loss (log-scale) versus number of RBF bases



Testing loss (log-scale) versus regularization parameter (log-scale), for 70 RBF bases

Cross-validation

- A common mistake: split the data into training/testing sets, use testing set to find best performing features, regularization parameter, kernel parameters, etc (*hyperparameters*), then report the testing error for these best features

- This is not a valid method for evaluating error: the problem is that we effectively used the testing set to "train" the system

- What we need to do instead: break the training set itself into two sets (training and *cross-validation*) sets

- Cross-validation Procedure:
  1. Break all data into training/testing sets (e.g., 70%/30%)
  2. Break training set into training/cross-validation set (e.g., 70%/30% again)
  3. Choose hyperparameters using cross-validation set
  4. (Optional) Once we have selected hyperparameters, retrain using all the training set
  5. Evaluate performance on the testing set

- k-fold cross-validation: Split training set into k different "folds" (equally sized random subsets)
  - For each fold i, train on $k-1$ only folks, evaluate on held out fold i

- The extreme case, leave one out cross validation: folds are individual examples

Reporting Errors

- If we want to *report* performance of an algorithm, how do we do this?

- Reporting just test error doesn't give a sense of our "confidence" in the prediction
  - If we have a testing set of size 1000, doesn't this imply more confidence in result than a testing set of size 10?

  - What about variance in predictions? Are we getting some almost completely right and others very wrong?

- Setting: in our test set, we have a number of actual labels y_i', and predictions $\hat{y}_i'$ of our algorithm

- There are really two things we may care about:
  1. What is the *distribution* of our errors $y_i' - \hat{y}_i'$?

  2. If we want to report some average loss

$$\text{Average loss} = \frac{1}{m'} \sum_{i=1}^{m'} \ell(\hat{y}_i', \hat{y}_i)$$

  how *confident* are we in this value?

Some basic probability notation

- We'll use Z to denote a *random variable* (with distribution $\mathcal{D}$), and use $p(z)$ to denote the it's probability density

- Expected value, or mean:

$$\mu = \mathbf{E}[Z] = \int zp(z)dz$$

- Variance

$$\sigma^2 = \mathbf{E}[(Z - \mu)^2]$$

- If you haven't seen any of this notation before, there are a number of good reviews available

- Suppose we have m samples drawn from the probability distribution $\mathcal{D}$, written as $z_1, \ldots, z_m \sim \mathcal{D}$

- Then we can form *empirical estimates* of the mean and variance of the distribution

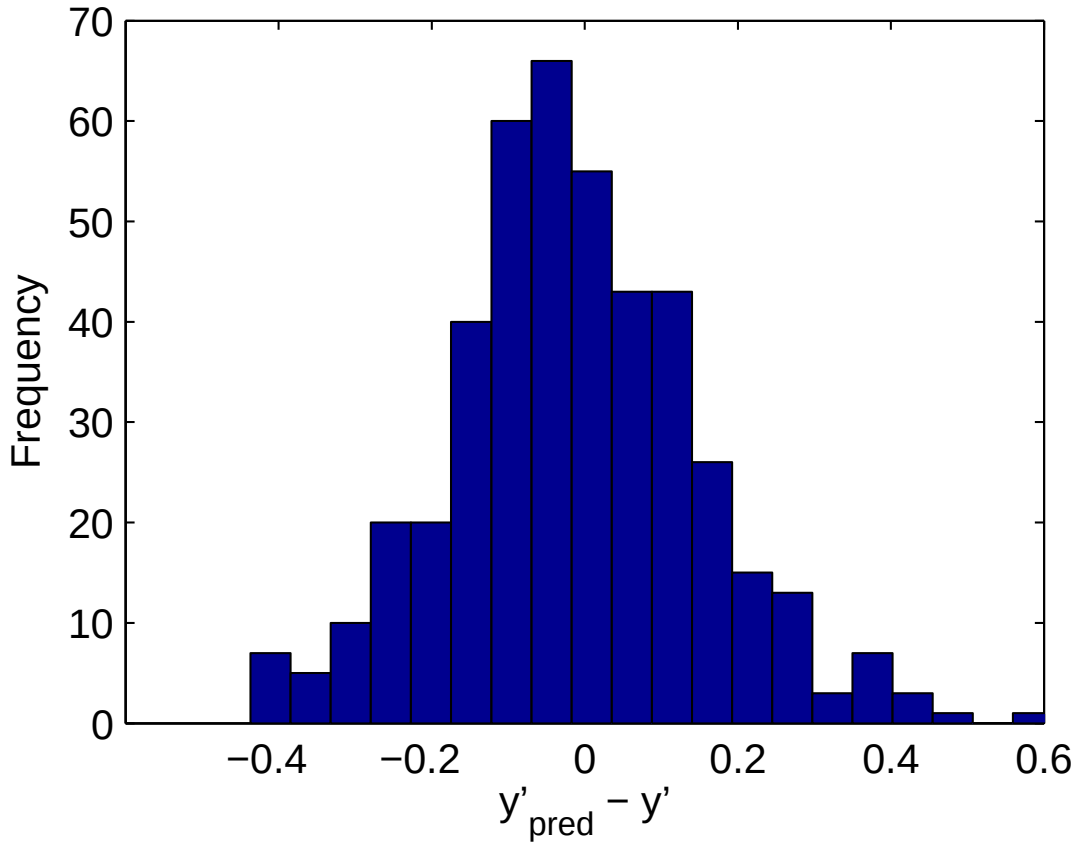
$$\hat{\mu} = \frac{1}{m} \sum_{i=1}^{m} z_i$$

$$\hat{\sigma}^2 = \frac{1}{m} \sum_{i=1}^{m} (z_i - \mu)^2 \approx \frac{1}{m} \sum_{i=1}^{m} (z_i - \hat{\mu})^2$$

[You may have seen variance estimates with a $\frac{1}{m-1}$ term instead; this is needed to make the estimator *unbiased*, but we'll typically deal with large m, so there isn't much difference]

Reporting errors

- As mentioned before, we might want to know about the distribution over our prediction errors $\hat{y}'_i - y'_i$



Histogram of errors $\hat{y}'_i - y'_i$

- Treat $\hat{y}'_i - y'_i$ as samples from a distribution

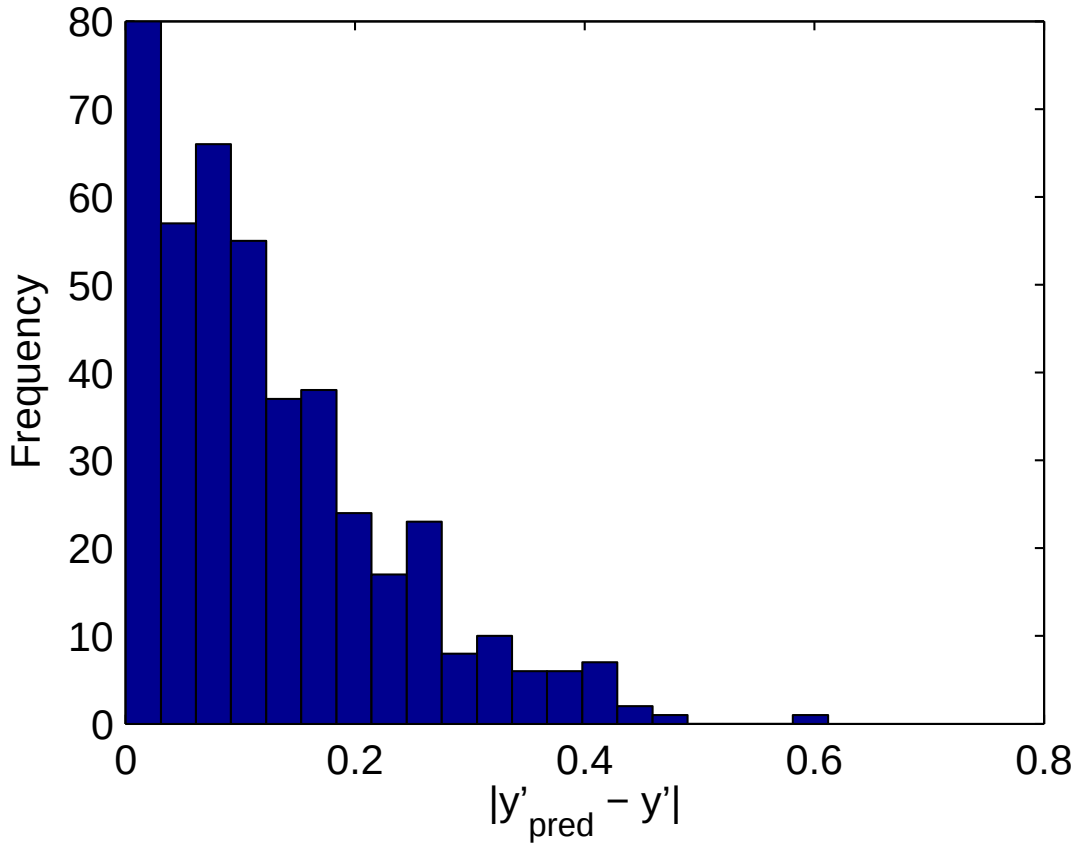
- Might want to know about the *mean* (also called *bias*), or *variance* of this distribution

- If we assume prediction errors are zero-mean Gaussian (but this is *not* always the case), then

$$\hat{\sigma}^2 = \frac{1}{m} \sum_{i=1}^{m} (\hat{y}'_i - y'_i)^2$$

  which is the mean squared error

- If we want to report some *average loss*, then we can treat $\ell(\hat{y}'_i, y'_i)$ (for any loss) as the random samples (the average loss is just the mean of these samples)



Histogram of losses $\ell(\hat{y}'_i, y'_i)$ for absolute loss

- How confident are we in our estimate of the mean (i.e., the average loss)?

- Here we'll exploit the *central limit theorem*: If $z_1, \ldots, z_m$ are (independent, identially distributed) samples from *any* distribution with mean μ and variance σ^2, then

$$\frac{1}{m}\sum_{i=1}^{m} z_i \to \mathcal{N}(\mu, \sigma^2/n)$$

  - I.e., the *mean* of any set of random variables is normally distributed

- For a normal distribution, 95% of the data falls within 1.96 standard deviations σ.

- This suggests a method for computing "confidence intervals" of our estimate of the average loss
  1. Form estimate of the mean:

$$\hat{\mu} = \frac{1}{m'} \sum_{i=1}^{m'} \ell(\hat{y}'_i, y_i)$$

  2. Form estimate of the variance:

$$\hat{\sigma}^2 = \frac{1}{m'} \sum_{i=1}^{m'} (\ell(\hat{y}'_i, y'_i) - \hat{\mu})^2$$

  3. With 95% confidence, the "true" mean lies within

$$\hat{\mu} \pm 1.96 \hat{\sigma} / \sqrt{m'}$$

- This procedure is technically *wrong* (we should be using the a different estimate of the variance, and a Student-t distribution instead of Gaussian), but it is close enough when m' is reasonably large, which is usually our setting

- Should report errors relative to some baseline (i.e., degree zero polynomial)

Degree	Test Error
0	0.2414 ± 0.0039
1	0.2407 ± 0.0027
2	0.1505 ± 0.0013
3	0.1255 ± 0.0009
4	0.1257 ± 0.0009
5	0.1267 ± 0.0009

- A better way of determining how algorithms compare: pairwise hypothesis testing