EECS 545: Machine Learning

Lecture 7. Regularization and model selection

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Outline

- ML, MAP
  - Maximum Likelihood
  - MAP
- Bias-Variance Tradeoff
- Model selection
  - Cross validation

MLE vs. MAP

- Maximum Likelihood Estimation (MLE)
  - Objective: Log-likelihood

    $\log P(D|\mathbf{w})$
  - Example: linear regression (w/o regularization)

- Maximum a Posteriori (MAP)
  - Objective: Log-likelihood + Log-Prior

    $\log P(D|\mathbf{w}) + \log P(\mathbf{w})$
  - Example: Regularized linear regression

Maximum Likelihood

- Objective function (to maximize): log-likelihood

$$\log \mathrm{P}(\mathbf{D} \mid \mathbf{w}) = \log \prod_{n=1}^{N} P(y^{(n)}|\phi(\mathbf{x}^{(n)}), \mathbf{w})$$

$$= \sum_{n=1}^{N} \log P(y^{(n)}|\phi(\mathbf{x}^{(n)}), \mathbf{w})$$

IID: Independent and Identically Distributed

- Example:
  - – Linear regression (without regularization)
  - – Logistic regression (without regularization)
- Problems: risk of overfitting

MAP

$$P(\mathbf{w}|D) = \frac{P(D|\mathbf{w})P(\mathbf{w})}{P(D)}$$
$$\propto P(D|\mathbf{w})P(\mathbf{w})$$

- Assumes prior distribution: $P(\mathbf{w})$
- Point estimate using Bayes rule:

$$\operatorname*{argmax}_{\mathbf{w}} P(\mathbf{w}|D) = \operatorname*{argmax}_{\mathbf{w}} P(D|\mathbf{w})P(\mathbf{w})$$

- Objective function (to maximize):

$$\log \mathrm{P}(\mathbf{D} \mid \mathbf{w})\mathrm{P}(\mathbf{w}) = \log \prod_{n=1}^{N} P(y^{(n)}|\phi(\mathbf{x}^{(n)}), \mathbf{w}) + \log \mathrm{P}(\mathbf{w})$$
$$= \sum_{n=1}^{N} \log P(y^{(n)}|\phi(\mathbf{x}^{(n)}), \mathbf{w}) + \log \mathrm{P}(\mathbf{w})$$

- Isotropic Gaussian (e.g., L2 norm) is a popular prior (regularizer):

$$P(\mathbf{w}) = N(0, \lambda^{-1}\mathbf{I})$$
$$\Leftrightarrow \log P(\mathbf{w}) = -\frac{\lambda}{2}\|\mathbf{w}\|^2 + const$$

- Example:
  - L2-regularized Linear regression
  - L2-regularized Logistic regression

Check: Gaussian Prior and L2 regularization

- Gaussian prior distribution for **w**

$$
\begin{aligned}
P(\mathbf{w}) &= \mathcal{N}(0, \lambda^{-1}\mathbf{I}) \\
&= const * \exp\left(-\frac{1}{2}\mathbf{w}^T(\lambda^{-1}I)^{-1}\mathbf{w}\right) \\
&= const * \exp\left(-\frac{\lambda}{2}\mathbf{w}^T\mathbf{w}\right)
\end{aligned}
$$

- Taking log

$$
\log P(\mathbf{w}) = const - \frac{\lambda}{2}\mathbf{w}^T\mathbf{w} = const - \frac{\lambda}{2}\|\mathbf{w}\|^2
$$

"Gaussian Prior" for **w** and L2 regularization are equivalent.

Solving Regularized Least Squares

- Consider the error function:

$$E_D(\mathbf{w}) + \lambda E_W(\mathbf{w})$$

Data term + Regularization term

- With the sum-of-squares error function and a quadratic regularizer, we get

Penalize large coefficient values

$$\widetilde{E}(\mathbf{w}) = \frac{1}{2}\sum_{n=1}^{N}(\mathbf{w}^T\phi(\mathbf{x}^{(n)}) - y^{(n)})^2 + \frac{\lambda}{2}||\mathbf{w}||^2$$

Remark: Here, we used $\beta = 1$ for simplicity.

λ is called the regularization coefficient.

- which is minimized by

$$\mathbf{w}_{ML} = (\lambda\mathbf{I} + \Phi^T\Phi)^{-1}\Phi^T\mathbf{y}$$

Derivation

Objective function

$$\widetilde{E}(\mathbf{w}) = \frac{1}{2}\sum_{n=1}^{N}(\mathbf{w}^T\phi(\mathbf{x}^{(n)}) - y^{(n)})^2 + \frac{\lambda}{2}||\mathbf{w}||^2$$

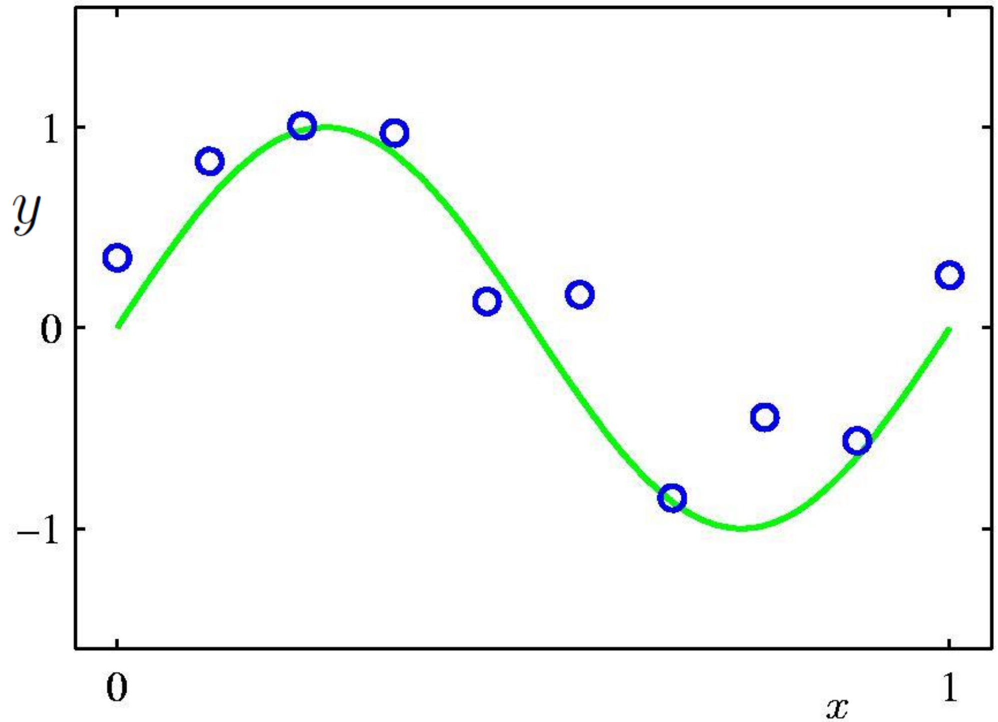
$$= \frac{1}{2}\mathbf{w}^T\Phi^T\Phi\mathbf{w} - \mathbf{w}^T\Phi^T\mathbf{y} + \frac{1}{2}\mathbf{y}^T\mathbf{y} + \frac{\lambda}{2}\mathbf{w}^T\mathbf{w}$$

Compute gradient and set it zero:

$$\begin{aligned}
\nabla_{\mathbf{w}}\widetilde{E}(\mathbf{w}) &= \nabla_{\mathbf{w}}[\frac{1}{2}\mathbf{w}^T\Phi^T\Phi\mathbf{w} - \mathbf{w}^T\Phi^T\mathbf{y} + \frac{1}{2}\mathbf{y}^T\mathbf{y} + \frac{\lambda}{2}\mathbf{w}^T\mathbf{w}] \\
&= \Phi^T\Phi\mathbf{w} - \Phi^T\mathbf{y} + \lambda\mathbf{w} \\
&= (\lambda\mathbf{I} + \Phi^T\Phi)\mathbf{w} - \Phi^T\mathbf{y} \\
&= 0
\end{aligned}$$

Therefore, we get: $\mathbf{w}_{ML} = (\lambda\mathbf{I} + \Phi^T\Phi)^{-1}\Phi^T\mathbf{y}$

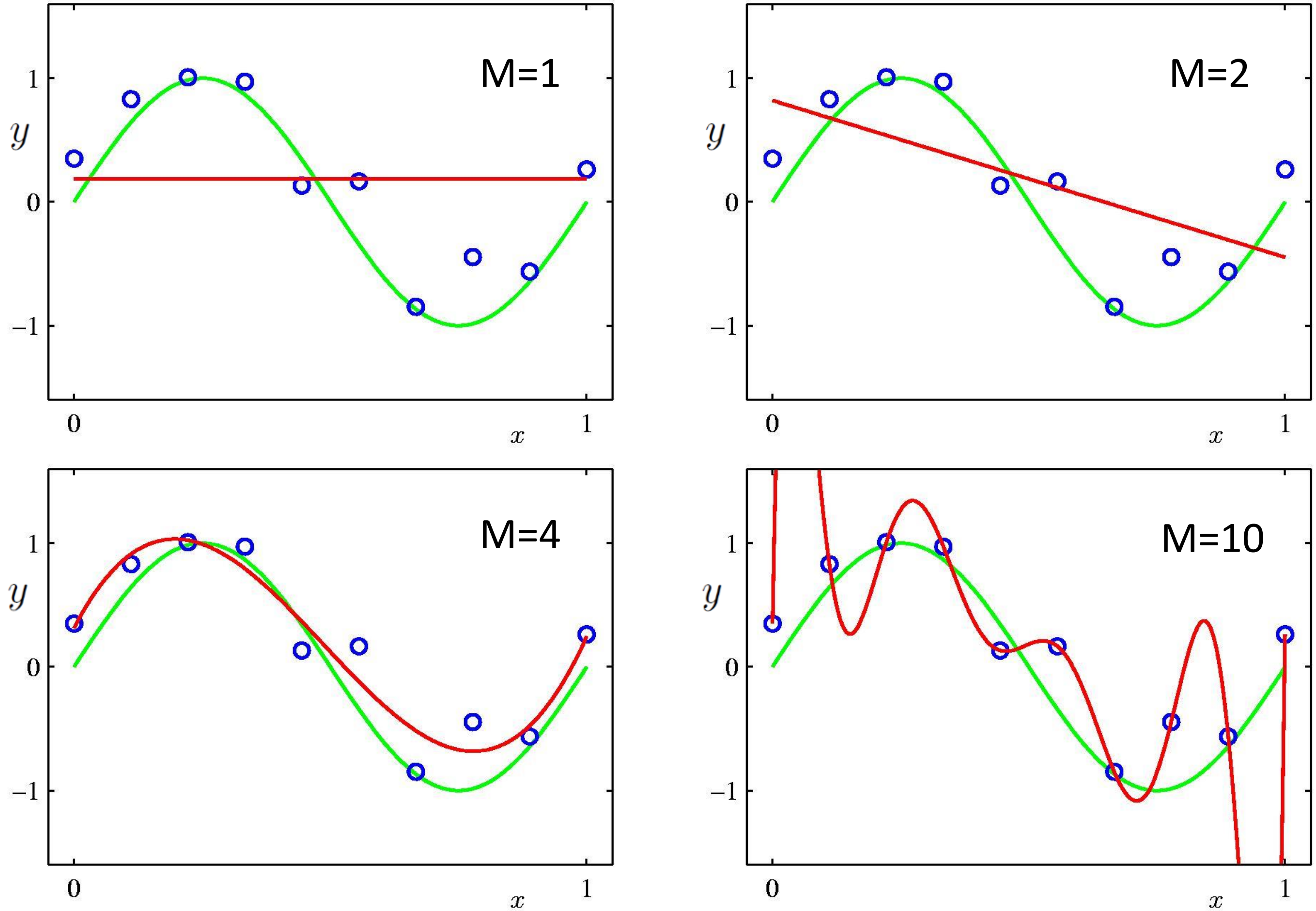
Revisiting Polynomial Curve Fitting



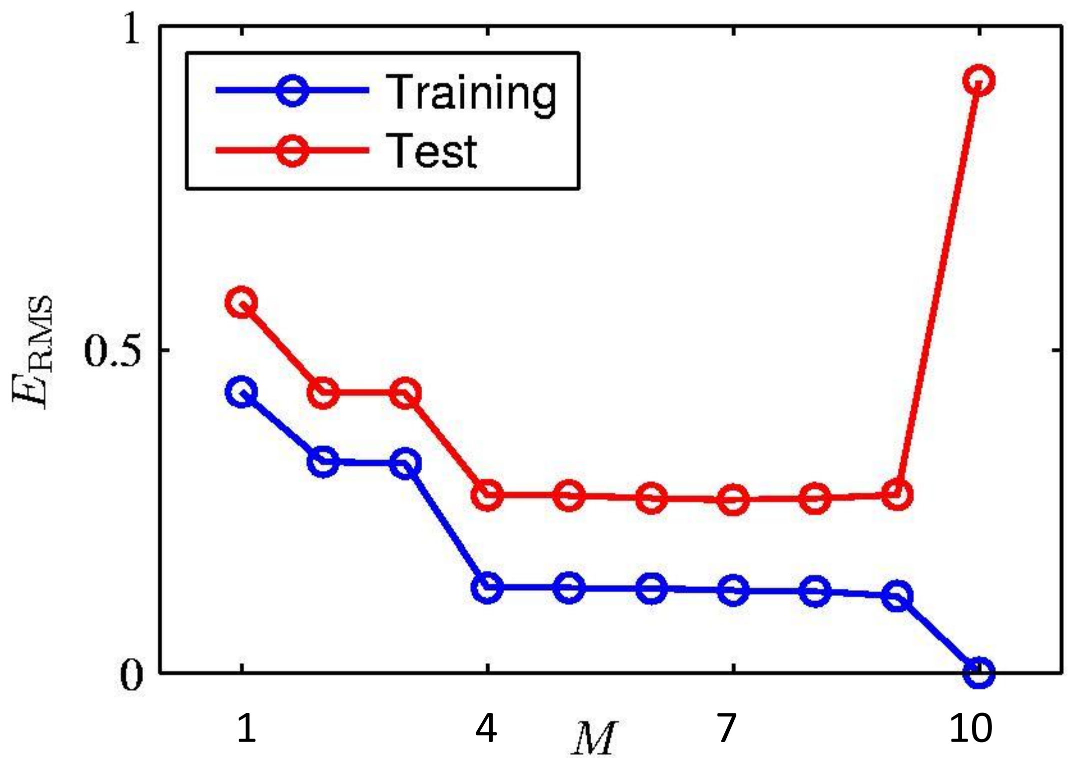
$$h(x, \mathbf{w}) = w_0 + w_1 x + w_2 x^2 + \ldots + w_{M-1} x^{M-1} = \sum_{j=0}^{M-1} w_j x^j$$

Maximum Likelihood (in Linear Regression)

- Choosing the right complexity is important
  - Watch out for underfitting/overfitting

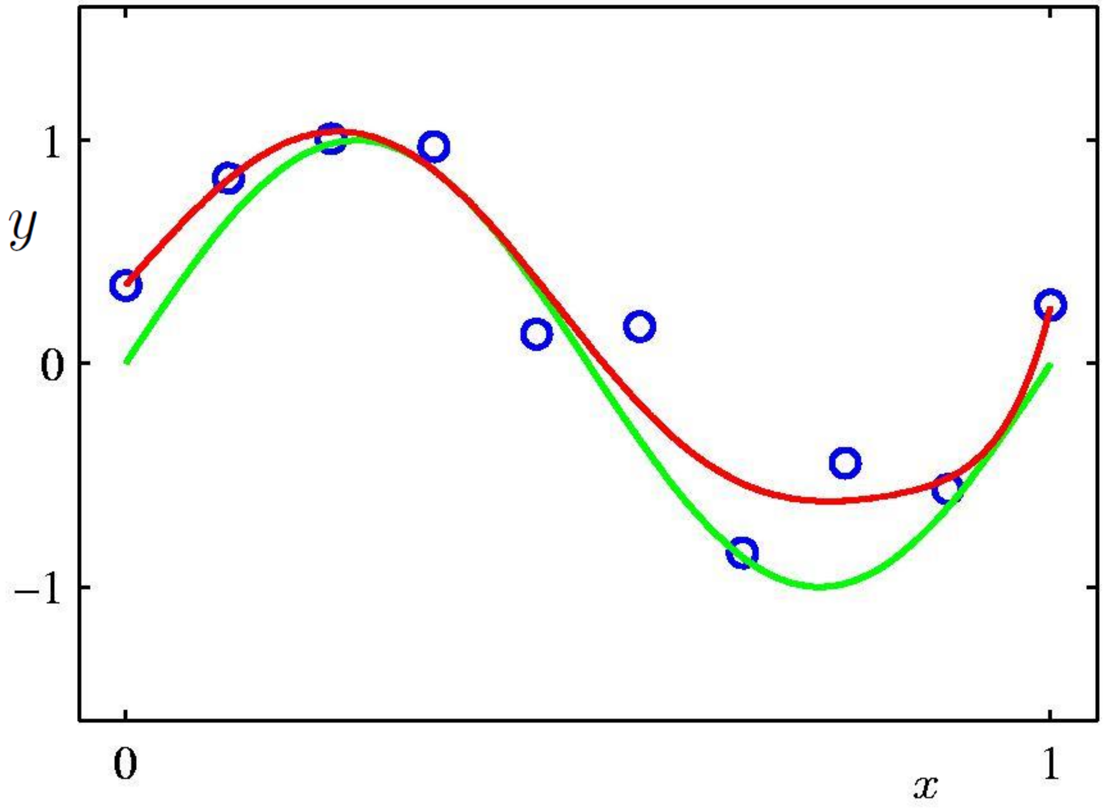


Underfitting vs. overfitting

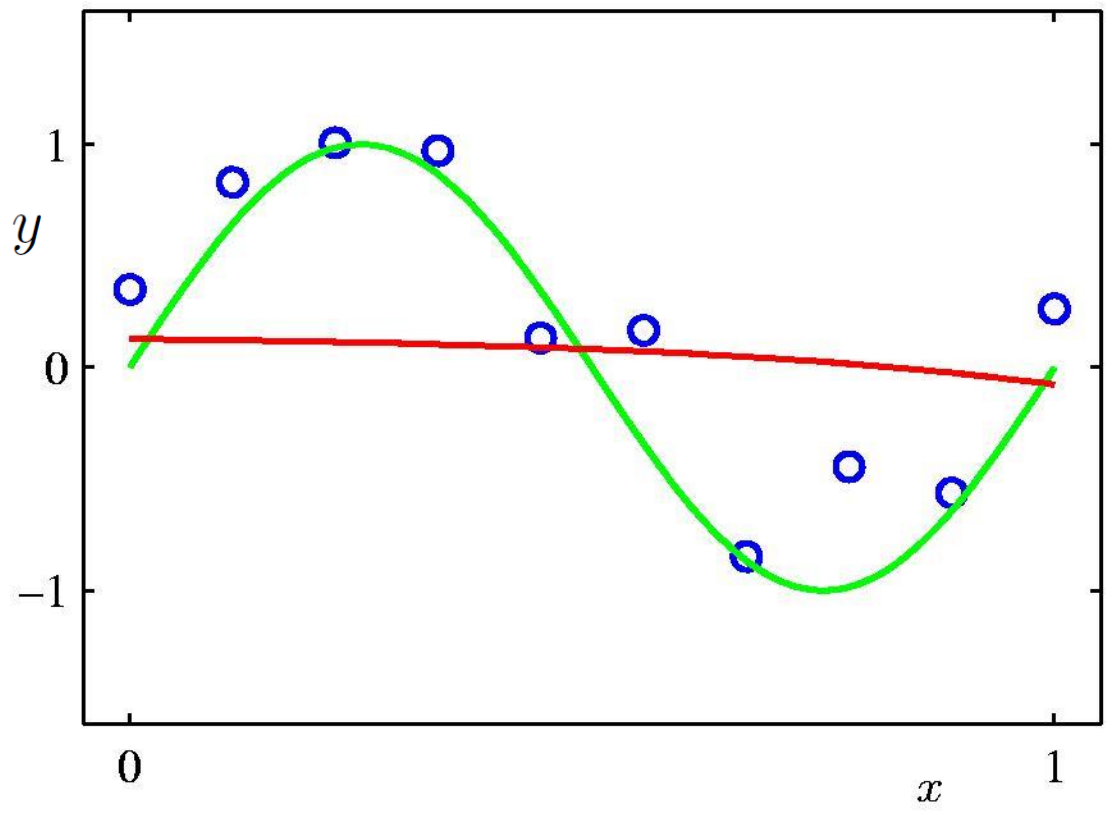


Root-Mean-Square (RMS) Error: $E_{\mathrm{RMS}} = \sqrt{2E(\mathbf{w}^{\star})/N}$

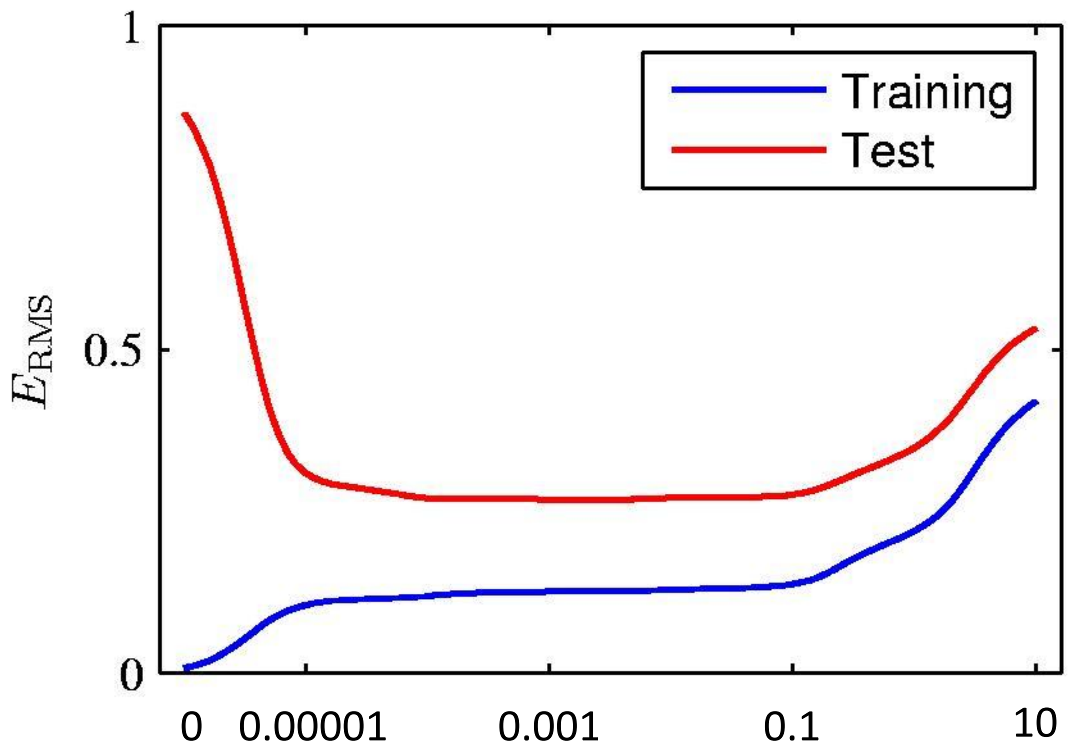
L2 Regularization: $\lambda = 0.001$



L2 Regularization: $\lambda = 10$



L2 Regularization: E_{RMS} vs. $\ln \lambda$



λ (in log scale)

$$E_{\mathrm{RMS}} = \sqrt{2E(\mathbf{w}^\star)/N}$$

Larger regualrization

NOTE: For simplicity of presentation, we divided the data into training set and test set. However, it's **not** legitimate to find the optimal hyperparameter based on the test set. We will talk about legitimate ways of doing this when we cover model selection and cross-validation.

Polynomial Coefficients

	λ=0	λ=0.001	λ=10
$w_0^\star$	0.35	0.35	0.13
$w_1^\star$	232.37	4.74	-0.05
$w_2^\star$	-5321.83	-0.77	-0.06
$w_3^\star$	48568.31	-31.97	-0.05
$w_4^\star$	-231639.30	-3.89	-0.03
$w_5^\star$	640042.26	55.28	-0.02
$w_6^\star$	-1061800.52	41.32	-0.01
$w_7^\star$	1042400.18	-45.95	-0.00
$w_8^\star$	-557682.99	-91.53	0.00
$w_9^\star$	125201.43	72.68	0.01

Summary: L2 regularized linear regression

- Simple modification of linear regression
- L2 regularization controls the tradeoff between "fitting error" and "complexity".
  - Small L2 regularization results in complex models (but with risk of overfitting)
  - Large L2 regularization results in simple models (but with risk of underfitting).

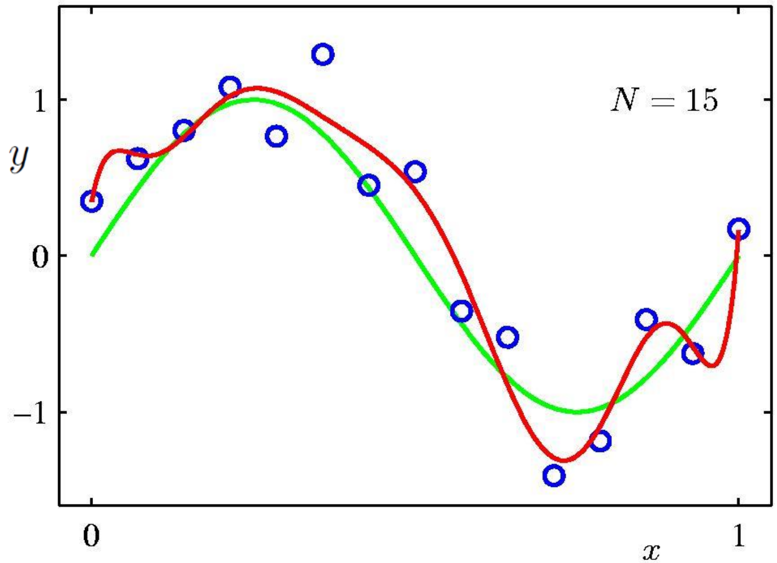
- It is important to find an optimal regularization that balances between the two.

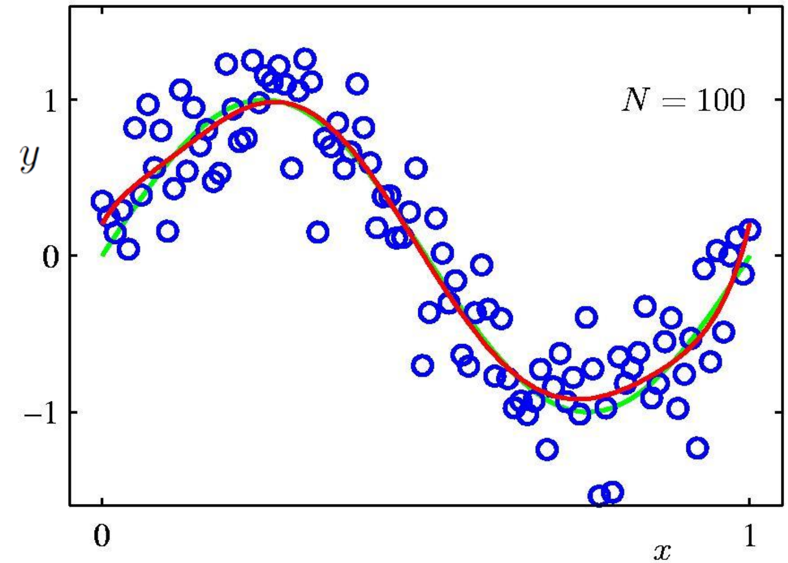
How can we avoid overfitting?

- More training data
  - Always helps
- Regularization (e.g., MAP)
  - Penalize complex models

Recap: More training data

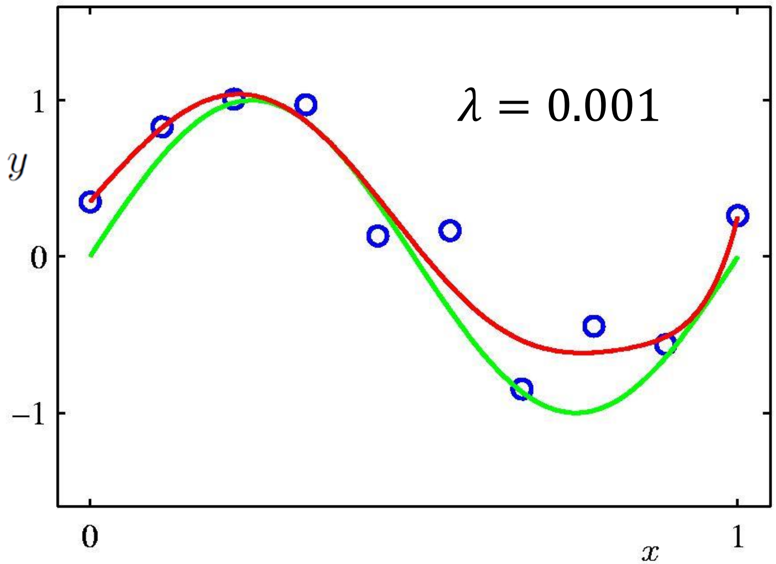
- Even complicated models can benefit (avoid overfitting) by having large amount of data
  - Example: 9^{th} order polynomial

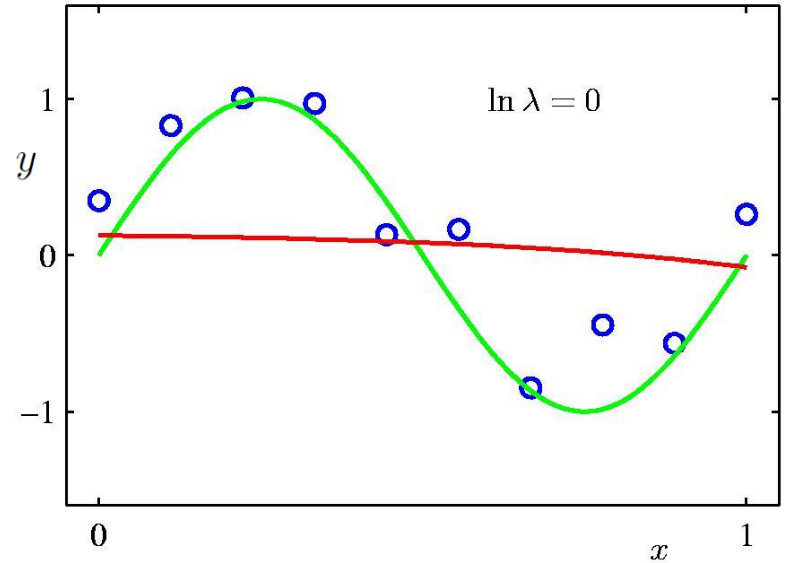




Recap: Regularization

- Regularization can implicitly control the complexity of models
  - Example: 9th order polynomial
  - Choosing right level of regularization is important





$$E_D(\mathbf{w}) + \lambda E_W(\mathbf{w})$$

Data term + Regularization term

$$\widetilde{E}(\mathbf{w}) = \frac{1}{2}\sum_{n=1}^{N}(\mathbf{w}^T\phi(\mathbf{x}^{(n)}) - y^{(n)})^2 + \frac{\lambda}{2}||\mathbf{w}||^2$$

Quiz: https://bit.ly/2OqFAQV

Quiz

1. If you have a small amount of training data, and if your learning algorithm uses complex features, your learning algorithm may
   a) Overfit
   b) Underfit
2. If you have a sufficient amount of training data, and if your learning algorithm uses too simple features, your learning algorithm may
   a) Overfit
   b) Underfit

Quiz

3. Increasing the **training** data size generally improves the **training** performance

   a) True

   b) False

4. Increasing the **training** data size generally improves the **testing** performance

   a) True

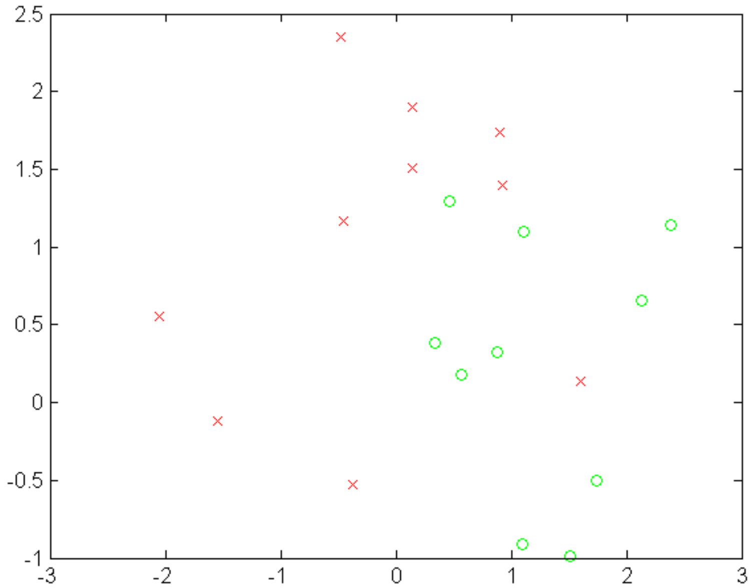
   b) False

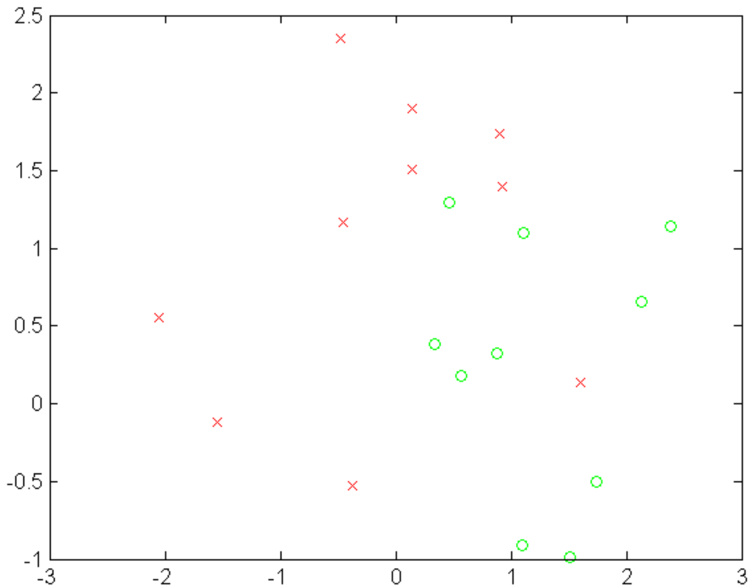
Quiz

5. For training a classifier with the 2d data below, which features would you use? Why?

   a) Linear (i.e., feature = (x1,x2))

   b) Nonlinear (e.g., polynomial, Gaussian, etc.)



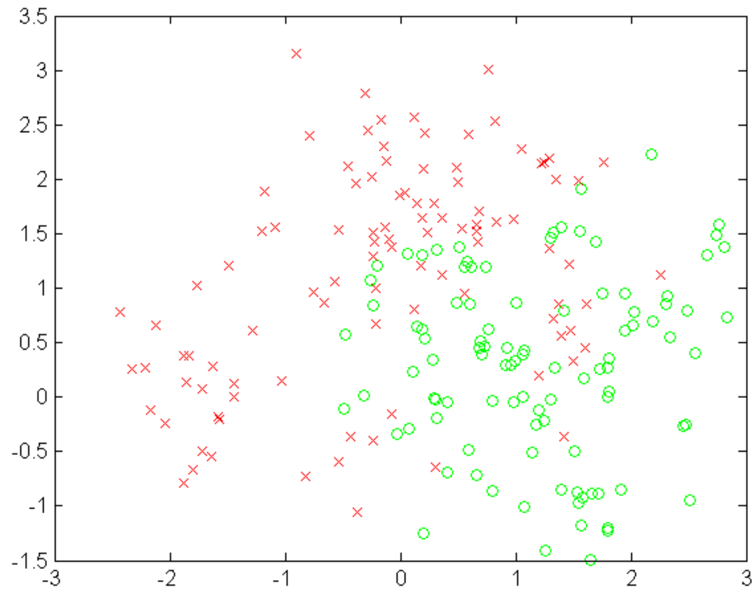


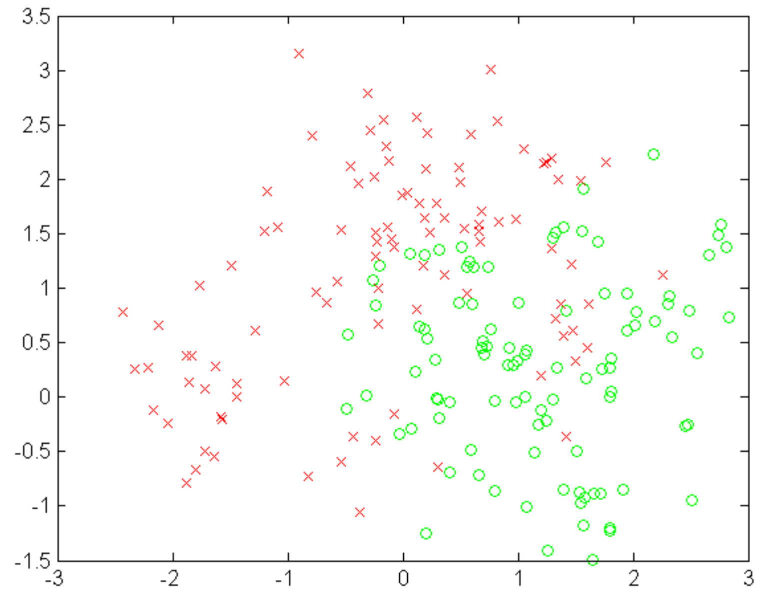
Quiz

6. For training a classifier with the 2d data below, which features would you use? Why?

   a) Linear (i.e., feature = (x1,x2))

   b) Nonlinear (e.g., polynomial, Gaussian, etc.)





Variance-Bias Tradeoff

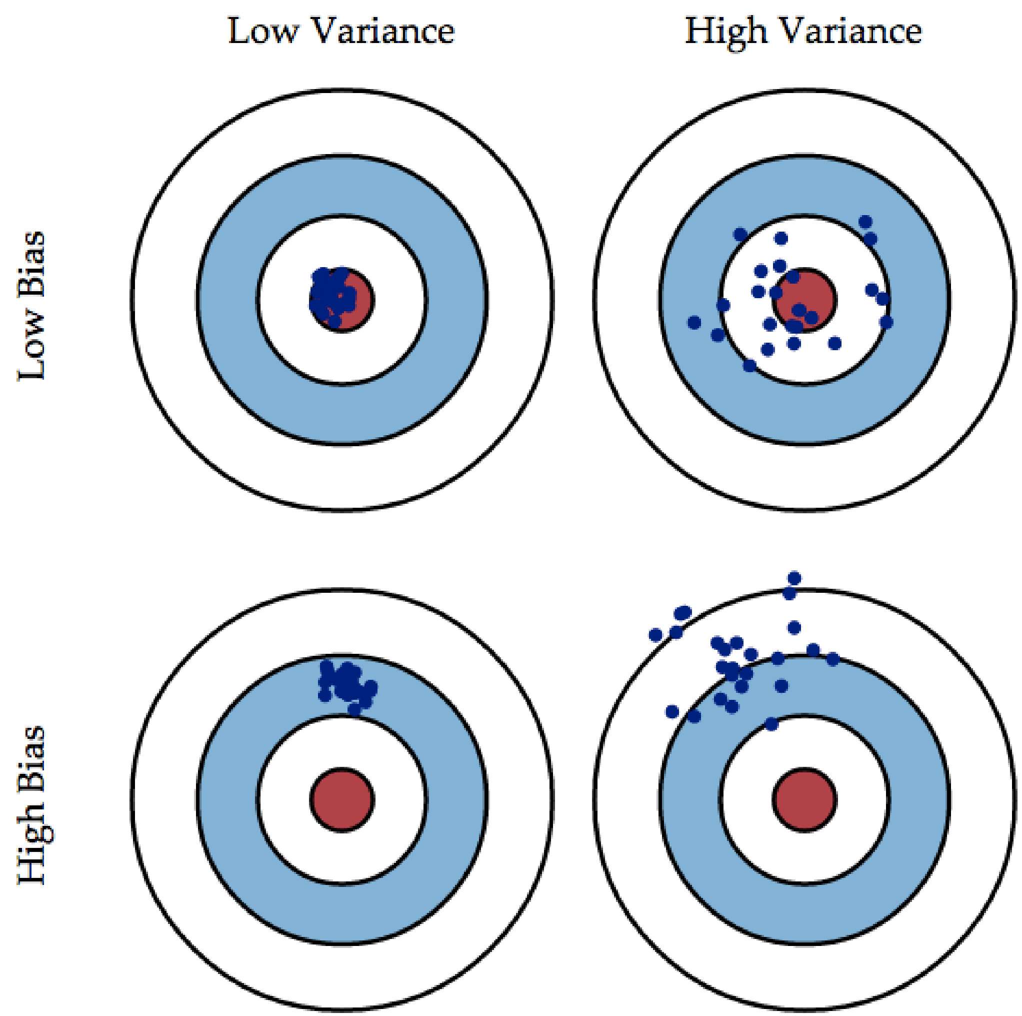
The Bias-Variance Decomposition

- Setting:
  - Given a distribution of $P(\mathbf{x}, y)$
  - Sample training data

$$D_{train} = \{(\mathbf{x}^{(n)}, y^{(n)}) : n = 1, ..., N\} \sim P(\mathbf{x}, y)$$

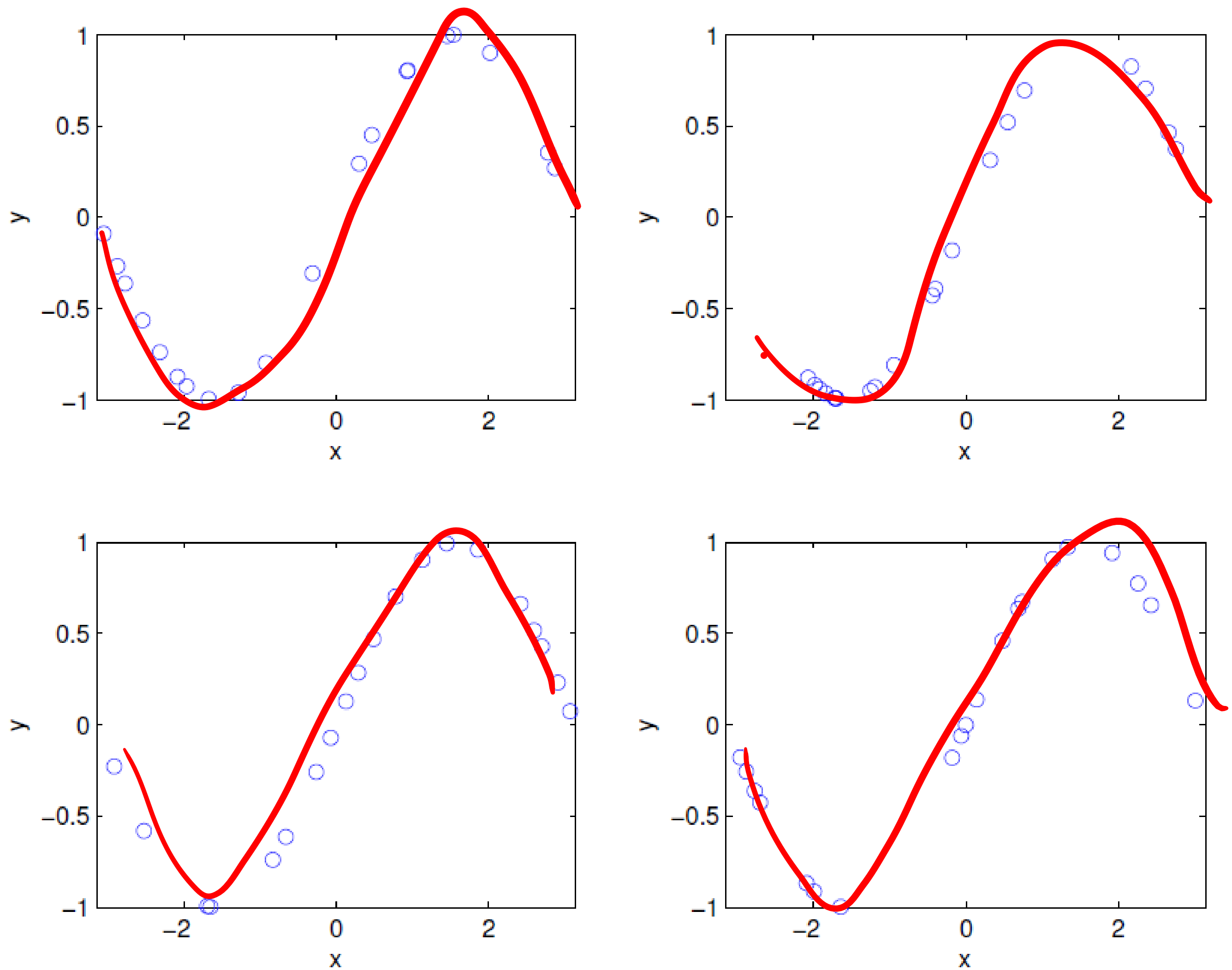
  - Train a learning algorithm on D
- Depending on samples, learning algorithm can still give different results (MLE, MAP, etc.)
- Goal: We want to learn a model with
  - Small bias (i.e., how well a model fits the data on average?)
  - Small variance (i.e., how stable a model is wrt data samples?)

Bias and Variance



The Bias-Variance Decomposition

- Example: samples from the sinusoidal function y=sin(x)



The Bias-Variance Decomposition

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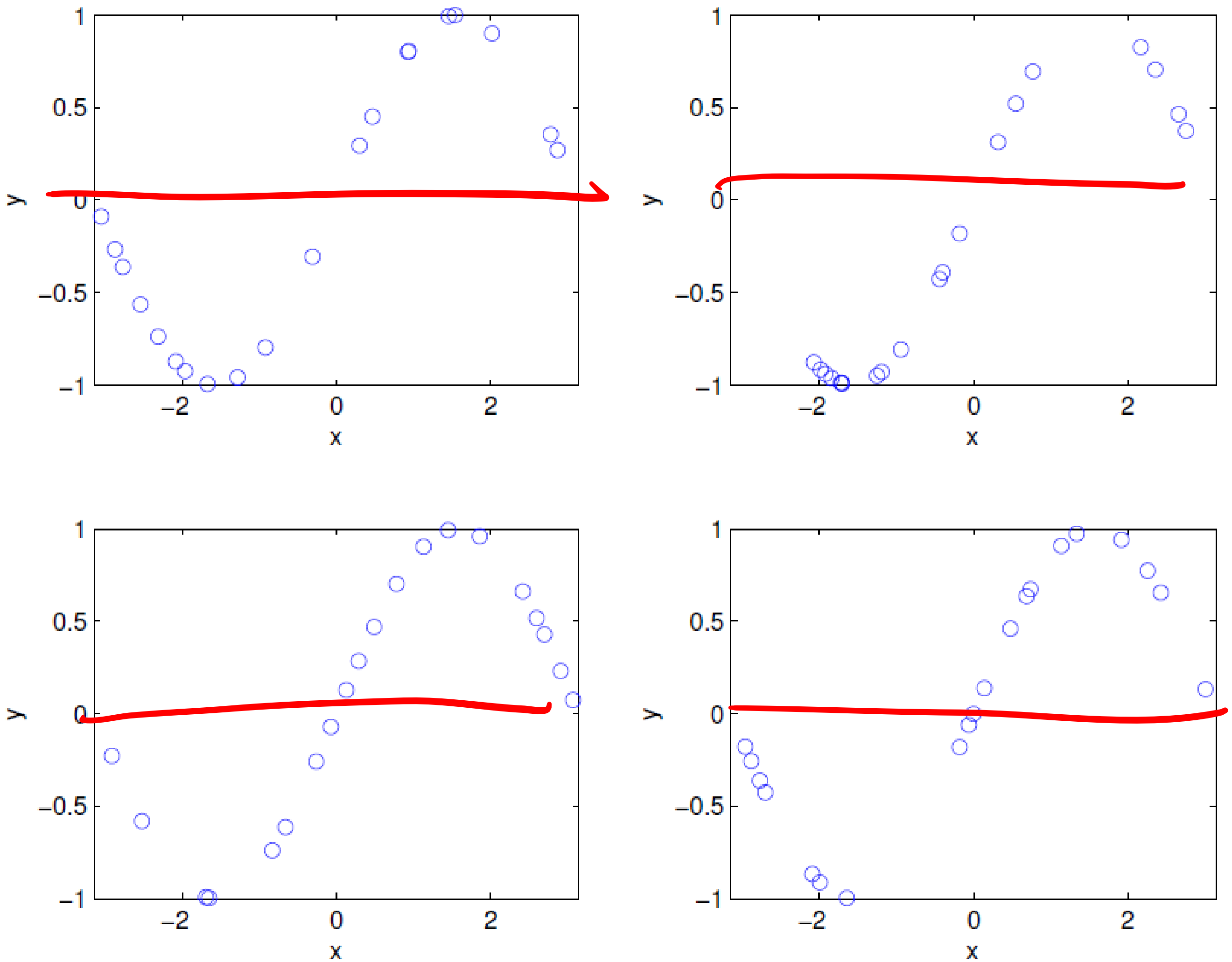

The Bias-Variance Decomposition

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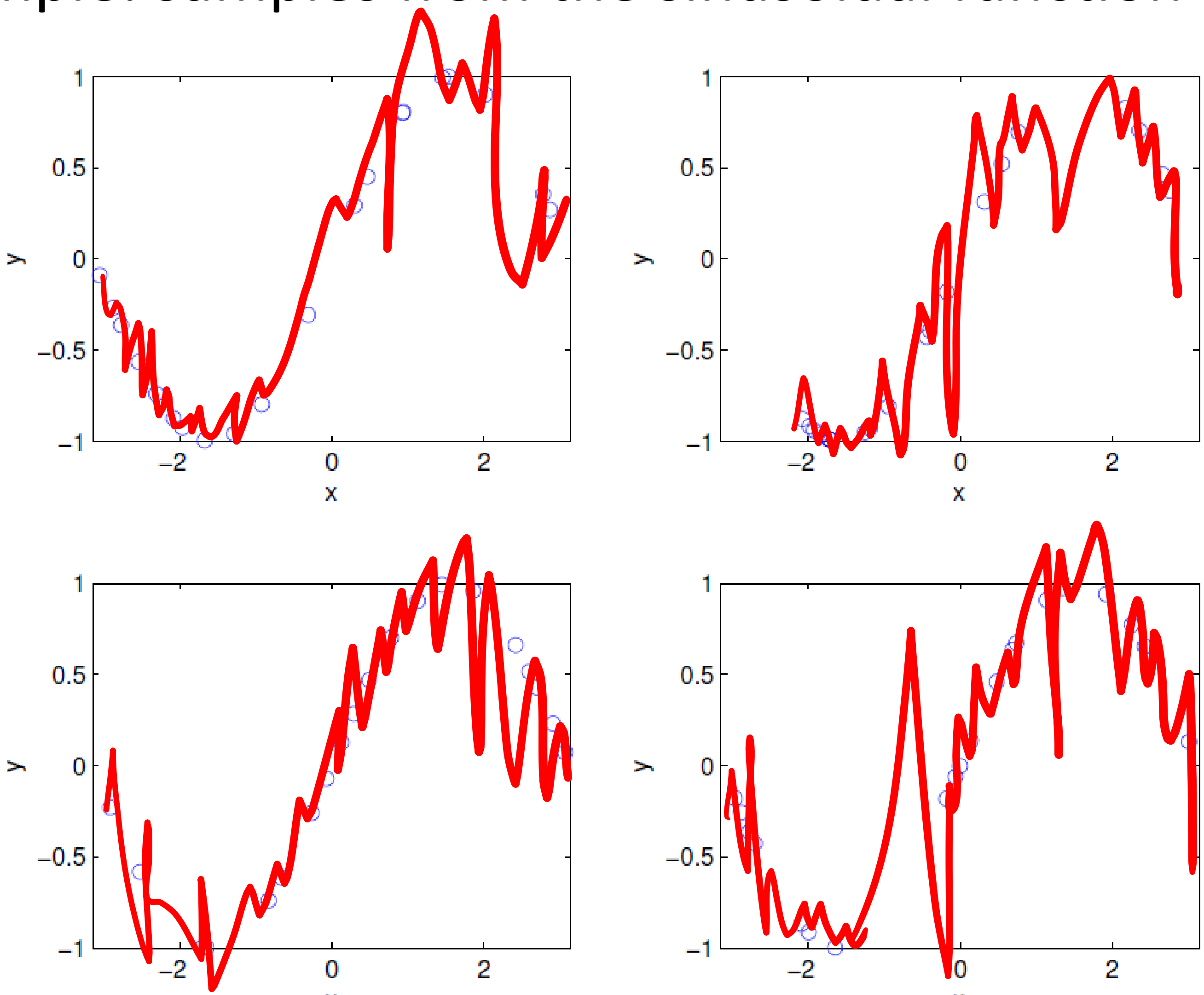


The Bias-Variance Decomposition*

- Expected squared loss:

$$\mathbb{E}[L] = \int\int \{h(\mathbf{x}) - y\}^2 p(\mathbf{x}, y) d\mathbf{x} dy$$

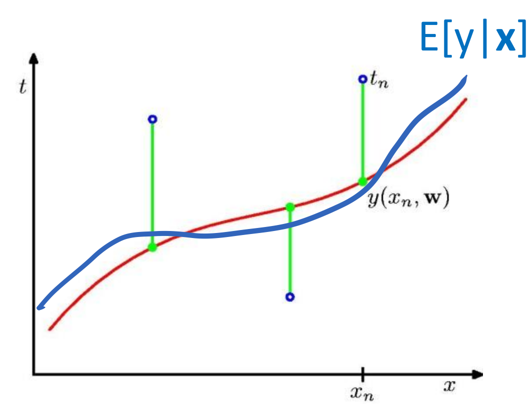
$$\mathbb{E}[L] = \int \{h(\mathbf{x}) - \mathbb{E}[y|\mathbf{x}]\}^2 p(\mathbf{x}) d\mathbf{x} + \int\int \{\mathbb{E}[y|\mathbf{x}] - y\}^2 p(\mathbf{x}, y) d\mathbf{x} dy$$

  – where

$$\mathbb{E}[y|\mathbf{x}] = \int y p(y|\mathbf{x}) dy$$

- The second term corresponds to the noise inherent in the random variable y.

- What about the first term?



The Bias-Variance Decomposition

- Suppose we were given multiple data sets, each of size N. Any particular data set (sampled from a distribution), D, will give a particular function h(x;D). We then have

$$\mathbb{E}_D[\{h(\mathbf{x};D) - y\}^2]$$

$$= \underbrace{\left(\mathbb{E}_D[h(\mathbf{x};D)] - y\right)^2}_{(\text{bias})^2} + \underbrace{\mathbb{E}_D\left[\{h(\mathbf{x};D) - \mathbb{E}_D[h(\mathbf{x};D)]\}^2\right]}_{\text{variance}}$$

The Bias-Variance Decomposition

- Expected loss

$$\mathbb{E}[L] = \int\int \{h(\mathbf{x}) - y\}^2 p(\mathbf{x}, y) d\mathbf{x} dy$$

$$\text{expected loss} = (\text{bias})^2 + \text{variance} + \text{noise}$$

- where

$$\mathbb{E}[y|\mathbf{x}] = \int y p(y|\mathbf{x}) dy$$

$$\begin{aligned} (\text{bias})^2 &= \\ \text{variance} &= \\ \text{noise} &= \end{aligned}$$

The Bias-Variance Decomposition

- Expected loss

$$\mathbb{E}[L] = \int\int \{h(\mathbf{x}) - y\}^2 p(\mathbf{x}, y) d\mathbf{x} dy$$

$$\text{expected loss} = (\text{bias})^2 + \text{variance} + \text{noise}$$

- where

$$\mathbb{E}[y|\mathbf{x}] = \int y p(y|\mathbf{x}) dy$$

$$\begin{aligned}
(\text{bias})^2 &= \int \{\mathbb{E}_D[h(\mathbf{x}; D)] - \mathbb{E}[y|\mathbf{x}]\}^2 p(\mathbf{x}) d\mathbf{x} \\
\text{variance} &= \int \mathbb{E}_D\left[\{h(\mathbf{x}; D) - \mathbb{E}_D[h(\mathbf{x}; D)]\}^2\right] p(\mathbf{x}) d\mathbf{x} \\
\text{noise} &= \int\int \{\mathbb{E}[y|\mathbf{x}] - y\}^2 p(\mathbf{x}, y) d\mathbf{x} dy
\end{aligned}$$

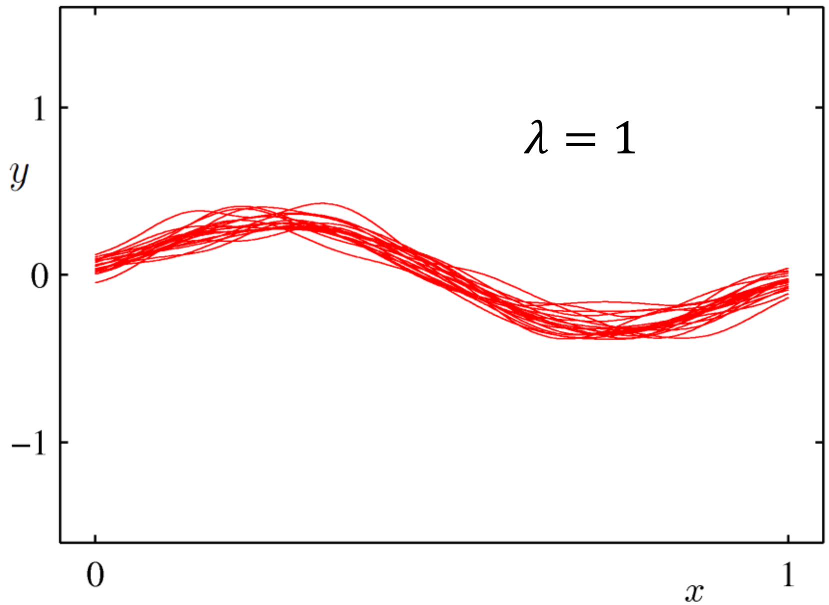
Proof: Details

D: training data; x: test example; y: label of x

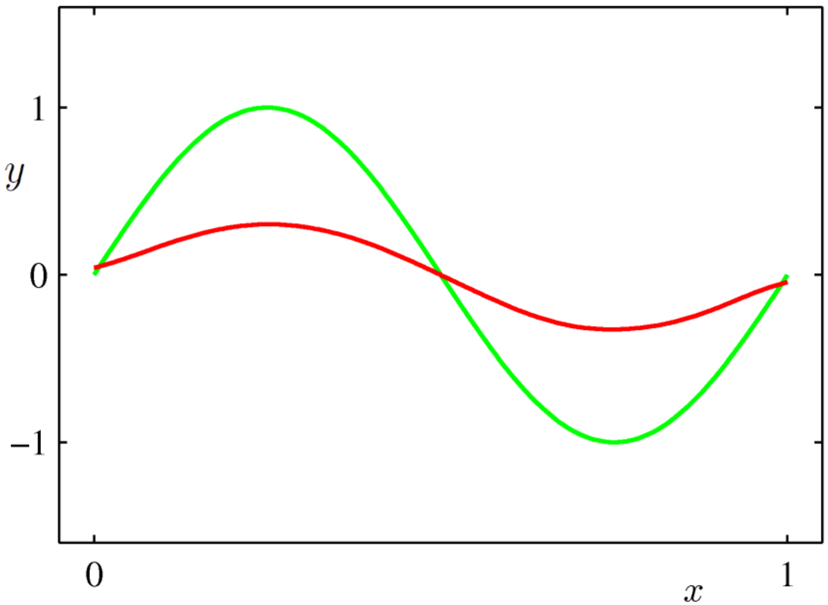
$$
\begin{aligned}
\mathbb{E}[L] &= \mathbb{E}_{\mathbf{x},y,D}\left[(h(\mathbf{x};D)-y)^2\right] \\
&= \mathbb{E}_{\mathbf{x},y,D}\left[(h(\mathbf{x};D)-\mathbb{E}[y|\mathbf{x}])^2\right] + \mathbb{E}_{\mathbf{x},y,D}\left[(y-\mathbb{E}[y|\mathbf{x}])^2\right] \\
&= \mathbb{E}_{\mathbf{x},D}\left[(h(\mathbf{x};D)-\mathbb{E}[y|\mathbf{x}])^2\right] + const \\
&= \mathbb{E}_{\mathbf{x}}\left[\mathbb{E}_D\left[(h(\mathbf{x};D)-\mathbb{E}[y|\mathbf{x}])^2\right]\right] + const \\
&= \mathbb{E}_{\mathbf{x}}\left[\mathbb{E}_D\left[(h(\mathbf{x};D)-\mathbb{E}_D[h(\mathbf{x};D)]+\mathbb{E}_D[h(\mathbf{x};D)]-\mathbb{E}[y|\mathbf{x}])^2\right]\right] + const \\
&= \mathbb{E}_{\mathbf{x}}\left[\mathbb{E}_D\left[\{h(\mathbf{x};D)-\mathbb{E}_D[h(\mathbf{x};D)]\}^2\right]\right] \\
&\quad +2\mathbb{E}_{\mathbf{x}}\left[\mathbb{E}_D\left[\{h(\mathbf{x};D)-\mathbb{E}_D[h(\mathbf{x};D)]\}\{\mathbb{E}_D[h(\mathbf{x};D)]-\mathbb{E}[y|\mathbf{x}]\}\right]\right] \\
&\quad +\mathbb{E}_{\mathbf{x}}\left[\{\mathbb{E}_D[h(\mathbf{x};D)]-\mathbb{E}[y|\mathbf{x}]\}^2\right] + const \\
&= \underbrace{\mathbb{E}_{\mathbf{x}}\left[\mathbb{E}_D\left[\{h(\mathbf{x};D)-\mathbb{E}_D[h(\mathbf{x};D)]\}^2\right]\right]}_{\text{Variance}} + \underbrace{\mathbb{E}_{\mathbf{x}}\left[\{\mathbb{E}_D[h(\mathbf{x};D)]-\mathbb{E}[y|\mathbf{x}]\}^2\right]}_{\text{Bias}} + const
\end{aligned}
$$

Example: regularized linear regression

- Example: 25 data sets from the sinusoidal, varying the degree of regularization, λ.



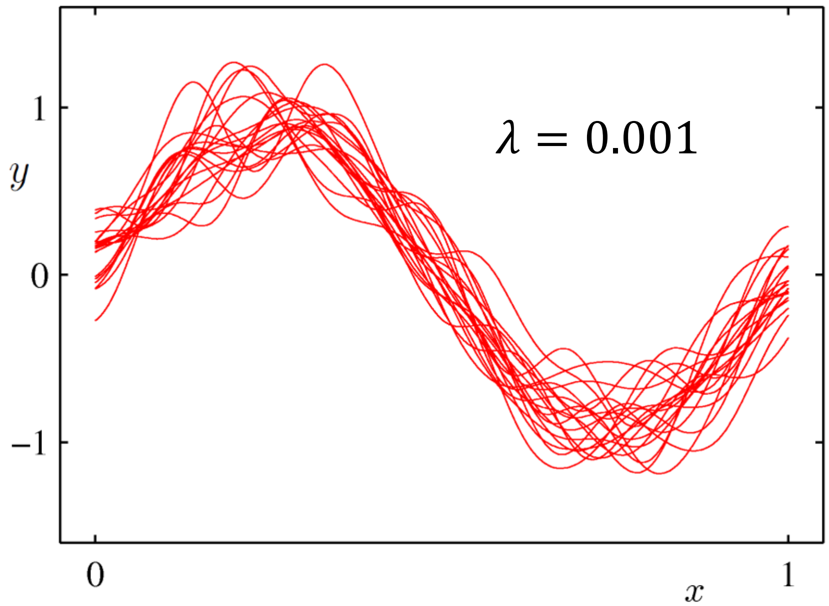
Samples of $h(\mathbf{x}; D)$



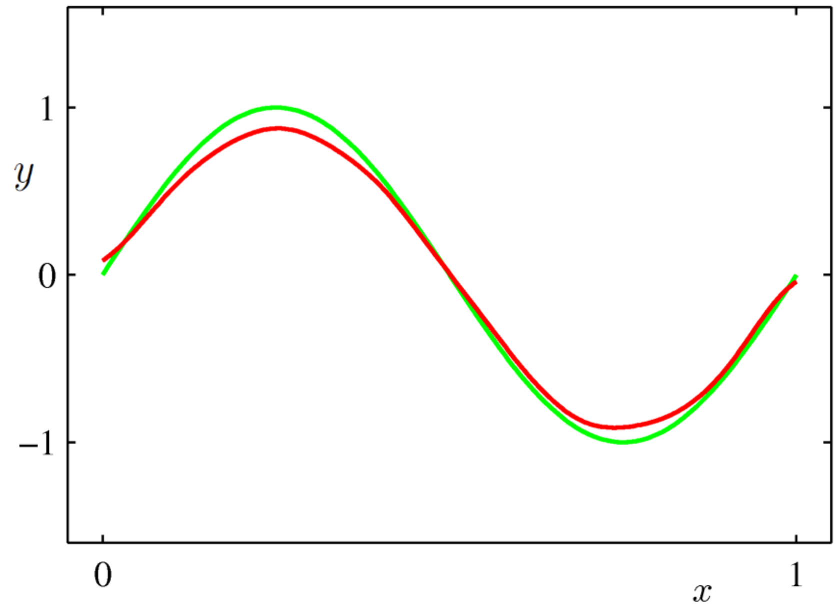
$\mathbb{E}_D[h(\mathbf{x}; D)]$ vs $\mathbb{E}[y|\mathbf{x}]$ = $\mathbb{E}_D[y|\mathbf{x}]$

Example: regularized linear regression

- Example: 25 data sets from the sinusoidal, varying the degree of regularization, λ.



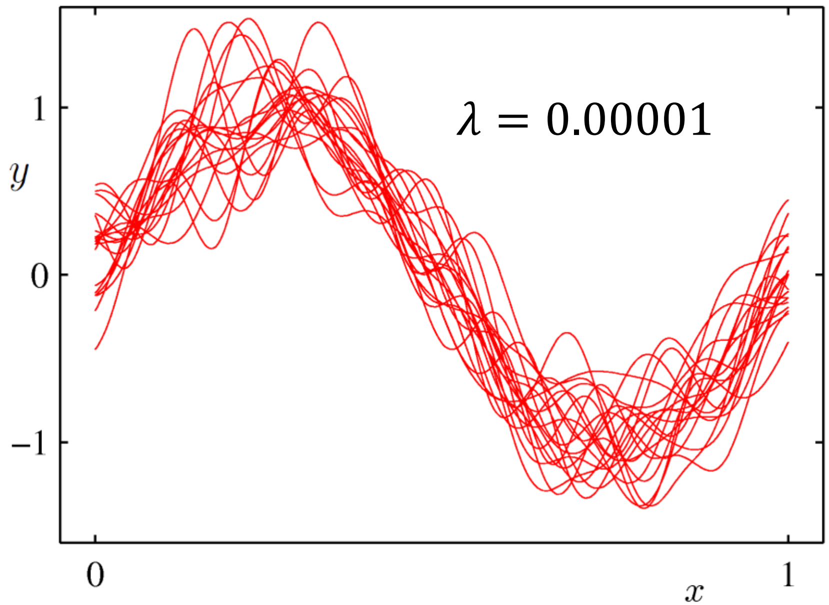
Samples of $h(\mathbf{x}; D)$



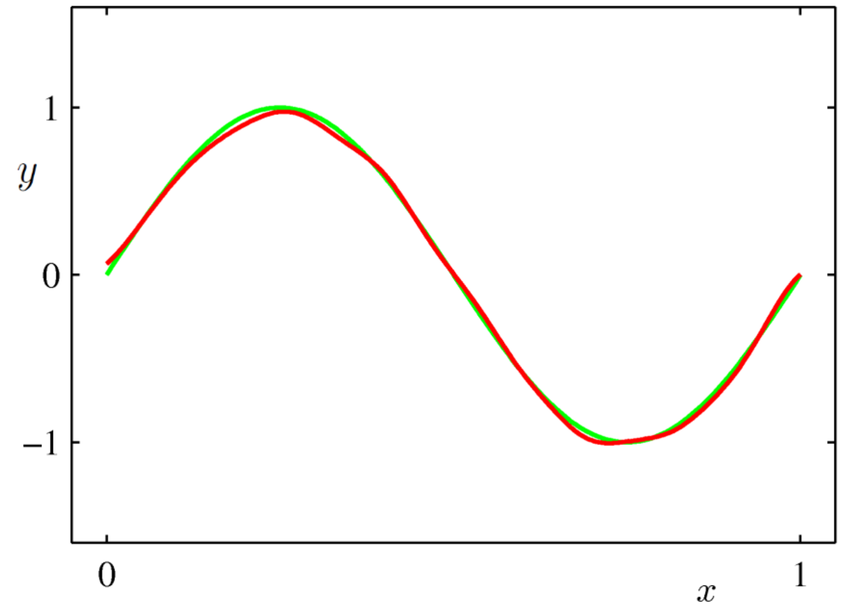
$\mathbb{E}_D[h(\mathbf{x}; D)]$ vs $\mathbb{E}[y|\mathbf{x}]$ = $\mathbb{E}_D[y|\mathbf{x}]$

Example: regularized linear regression

- Example: 25 data sets from the sinusoidal, varying the degree of regularization, λ.



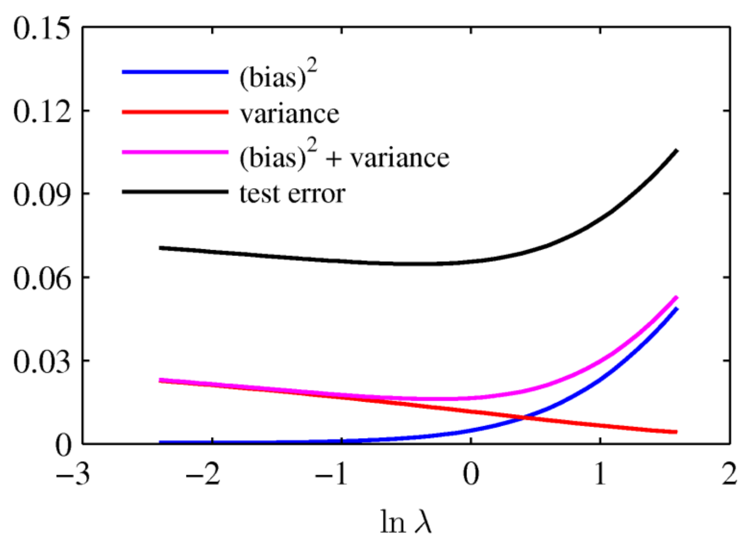
Samples of $h(\mathbf{x}; D)$



$\mathbb{E}_D[h(\mathbf{x}; D)]$ vs $\mathbb{E}[y|\mathbf{x}]$ = $\mathbb{E}_D[y|\mathbf{x}]$

The Bias-Variance Trade-off

- An over-regularized model (large λ) will have a high bias and low variance.
- An under-regularized model (small λ) will have a high variance and low bias.
- It is important to find a good balance between the two.
  - typically done by cross validation (will be covered later)



Quiz: https://bit.ly/31mn2Xb

Quiz

1. Overfitting is characterized by
   a) High variance and low bias
   b) High variance and high bias
   c) Low variance and low bias
   d) Low variance and high bias

2. Underfitting is characterized by
   a) High variance and low bias
   b) High variance and high bias
   c) Low variance and low bias
   d) Low variance and high bias

Model Selection

Choosing right models

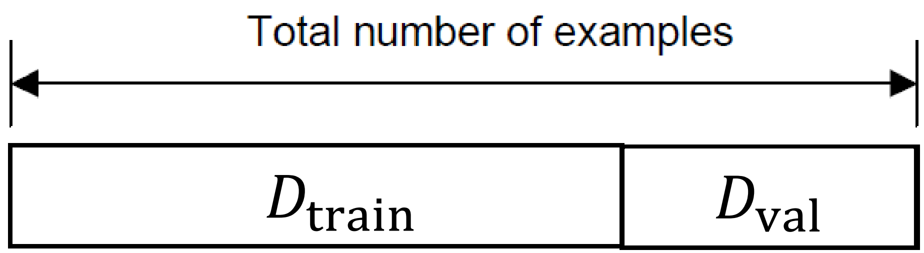
- For polynomial curve fitting (least squares), which value of M should we choose?
- For regularized least squares, which λ value should we choose?
- For regularized logistic regression, which λ value should we choose?
- Generally, given a set of models, $M = \{M_1, M_2, \dots, M_d\}$, how can we choose optimal M_{i*}?
  - Model:
    - Class (or set) of hypothesis: learning algorithm, hyperparameters, etc.
    - Fixed during training
  - Parameter:
    - Aka, hypothesis: (e.g., **w** for logistic regression/linear regression)
    - Can be trained based on data.

Simple Idea (that doesn't work)

- Given Data D
- Train each model M_i on D, to get a hypothesis h_i (for model i)
- Pick the hypothesis with the smallest training error
  - Problematic: this leads to overfitting..

Cross validation

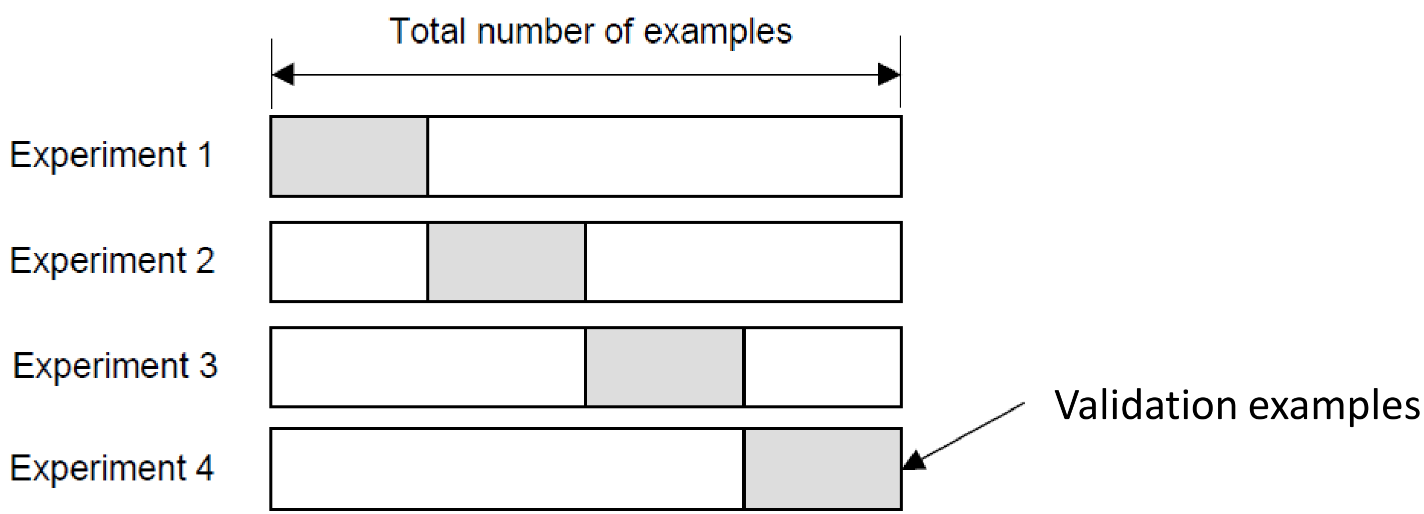
- Hold-out cross validation
  - 1. Randomly split D into D_{train} (say, 70% of the data) and D_{val} (the remaining 30%).
    - Here, D_{val} is called the hold-out validation set.



  - 2. Train each model M_i on D_{train} only, to get some hypothesis h_i.
  - 3. Select and output the hypothesis h_i that had the smallest error on the hold out validation set.
- Disadvantage:
  - Waste 30% of the data (less training examples available).
  - Some data are used only for training, others only for validation.

K-fold Cross validation

- Create a K-fold partition of the dataset
  - For each of K experiments, use K-1 folds for training and the remaining one for validating



- The true error is estimated as the average error rate

K fold Cross validation

- 1. Randomly split D into K disjoint subsets of N/K training examples each.
  - Lets call these subsets $D_1, \ldots, D_K$.
- 2. For each model M_i, we evaluate it as follows:
  - For k = 1, . . . , K (repeat for each fold)
    - Train the model M_i on $D_1 \cup \cdots \cup D_{k-1} \cup D_{k+1} \cup \cdots \cup D_K$ (i.e., train on all the data except D_k) to get some hypothesis $h_i(k)$.
    - Test the hypothesis $h_i(k)$ on D_k , to get error (or loss) $\epsilon_i(k)$.
    - The estimated generalization error of model M_i is then calculated as the average of the $\epsilon_i(k)$'s (over k).

$$\hat{\epsilon}_i = \frac{1}{K} \sum_k \epsilon_i(k)$$

- 3. Pick the model M_{i^*} with the lowest estimated generalization error $\hat{\epsilon}_{i^*}$, and retrain that model M_{i^*} on the entire training set S.
  - The resulting hypothesis is then output as our final answer.

K fold Cross validation

- Special case: K=N
  - Called, Leave-one-out cross validation (LOO CV)
  - Expensive, but wastes least amount of training data for cross validation.

- Which K value should we use?
  - For large data, then K=3 could be enough.
  - For small amount of data, you may need LOOCV to utilize as many training examples as possible.
  - Popular choice of K = 10, 5

Three way data splits

- If model selection and true error estimates are to be computed simultaneously, the data needs to be divided into three disjoint sets

- **Training set**: a set of examples used for learning: to fit the parameters of the classifier
  – Used for training parameters (w in logistic regression) given a fixed hyperparameters
- **Validation set**: a set of examples used to tune the hyperparameters of a classifier
  – we would use the validation set to find the "optimal" hyperparameters
  – E.g., l2 regularization parameter for L2 logistic regression
- **Test set**: a set of examples used only to assess the performance of a fully-trained classifier
  – After assessing the final model with the test set, **YOU MUST NOT** further tune the model
  – i.e., test set must be used only for evaluation, **NOT** for "tuning" your models & hyperparameters.

Procedure outline

1. Divide the available data into training, validation and test set
2. Select a model (and hyperparameters)
3. Train the model using the training set
4. Evaluate the model using the validation set
5. Repeat steps 2 through 4 using different models (and hyperparameters)
6. Select the best model (and hyperparameter) and train it using data from the training and validation set
7. Assess this final model using the test set

Procedure Illustration