Learning Theory & Regularization

Shan-Hung Wu
shwu@cs.nthu.edu.tw

Department of Computer Science,
National Tsing Hua University, Taiwan

Machine Learning

Outline

1. **Learning Theory**
2. **Point Estimation: Bias and Variance**
   - Consistency*
3. **Decomposing Generalization Error**
4. **Regularization**
   - Weight Decay
   - Validation

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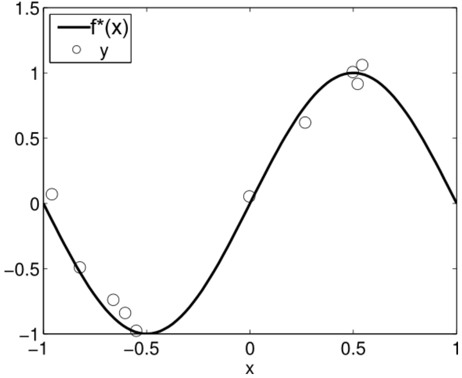
Which Polynomial Degree Is Better? I

- Given a training set $\mathbb{X} = \{(\boldsymbol{x}^{(i)}, \boldsymbol{y}^{(i)})\}_{i=1}^{N}$ i.i.d. sampled from of $\mathrm{P}(\mathrm{x}, \mathrm{y})$
- Assume $\mathrm{P}(\mathrm{x}, \mathrm{y}) = \mathrm{P}(\mathrm{y} \,|\, \mathrm{x})\mathrm{P}(\mathrm{x})$, where
  - $\mathrm{P}(\mathrm{x}) \sim \mathrm{Uniform}(-1, 1)$
  - $\mathrm{y} = \sin(\pi \mathrm{x}) + \varepsilon$, $\varepsilon \sim \mathcal{N}(0, \sigma^2)$



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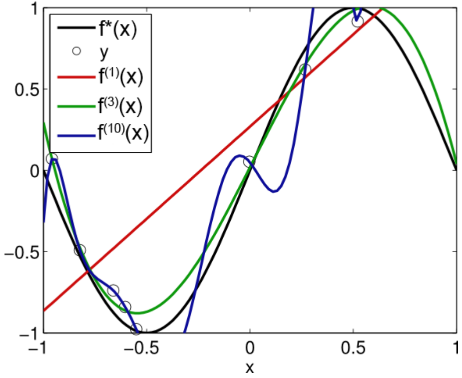
- Consider 3 unregularized polynomial regressors of degrees $P = 1$, 3, and 10



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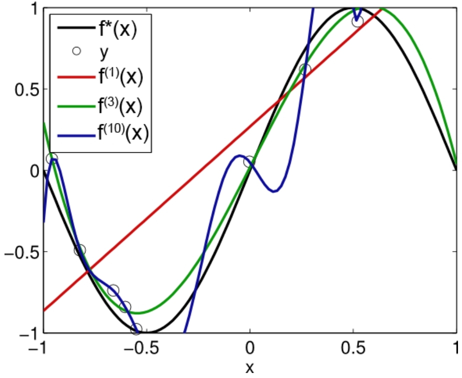

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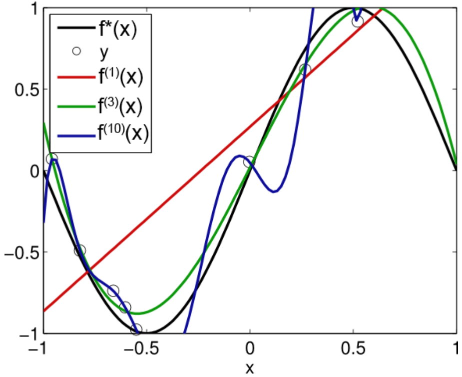

- Which one would you pick? Probably not $P = 1$ nor $P = 10$
- Note that $P = 10$ has ***zero*** training error
    - Any N points can be perfectly fitted by a polynomial of degree $N - 1$

Empirical Error vs. Generalization Error

- In ML, we usually "learn" a function by minimizing the ***empirical error/risk*** defined over a training set of size N:

$$C_N(\boldsymbol{w}) \text{ or } C_N[f] = \frac{1}{N}\sum_{i=1}^{N}\text{loss}\left(f(\boldsymbol{x}^{(i)};\boldsymbol{w}),\boldsymbol{y}^{(i)}\right)$$

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- Does a low $C_N[f]$ implies low $C[f]$? No, as $P = 10$ indicates

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- No machine learning algorithm is better than any other universally
- The goal of ML is ***not*** to seek a universally good learning algorithm
- Instead, a good algorithm that performs well on data drawn from a ***particular*** P we care about

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$$C[f_N] = \int \text{loss}(f_N(\boldsymbol{x};\boldsymbol{w}), y)\, d\text{P}(\boldsymbol{x}, y)?$$

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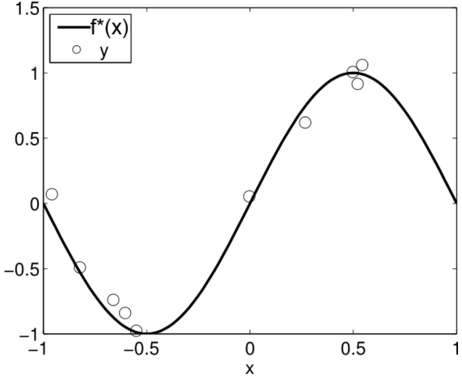
- Bounding methods
- Decomposition methods

Bounding Methods I

- $\min_f C[f] = C[f^*]$ is called the ***Bayes error***
  - Larger than 0 when there is randomness in $\mathrm{P}(\mathrm{y}\,|\,\mathrm{x})$
  - E.g., in our regression problem: $y = f^*(\boldsymbol{x};\boldsymbol{w}) + \varepsilon$, $\varepsilon \sim \mathcal{N}(0, \sigma^2)$



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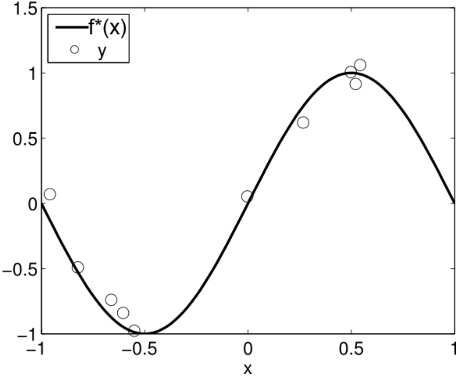

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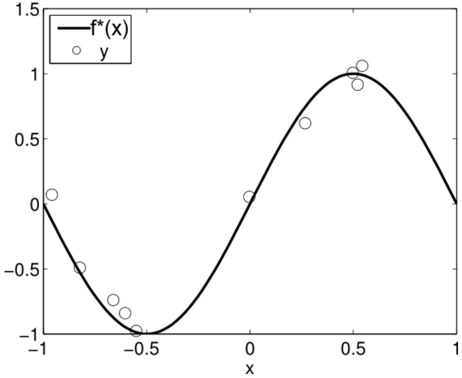

- So, our target is to make $C[f_N]$ as close to $C[f^*]$ as possible

Bounding Methods II

- Let $\mathscr{E} = C[f_N] - C[f^*]$ be the ***excess error***
- We have
$$\mathscr{E} = \underbrace{C[f^*_{\mathbb{F}}] - C[f^*]}_{\mathscr{E}_{\text{app}}} + \underbrace{C[f_N] - C[f^*_{\mathbb{F}}]}_{\mathscr{E}_{\text{est}}}$$

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Bounding Methods III

- Bounds of $\mathscr{E}_{\text{est}}$ for, e.g., binary classifiers [1, 2, 3]:

$$\mathscr{E}_{\text{est}} = O\left[\left(\frac{\text{Complexity}(\mathbb{F})\log N}{N}\right)^{\alpha}\right], \alpha \in \left[\frac{1}{2}, 1\right], \text{ with high probability}$$

- So, to reduce $\mathscr{E}_{\text{est}}$, we should either have
  - ***Simpler model*** (e.g., smaller polynomial degree P), or
  - Larger training set

Model Complexity, Overfit, and Underfit

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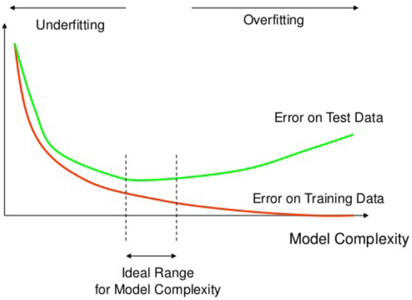

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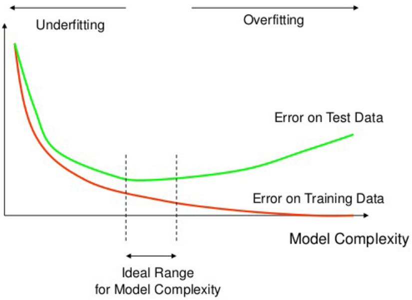

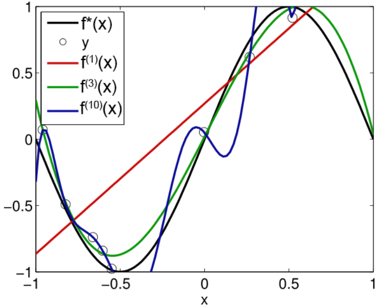

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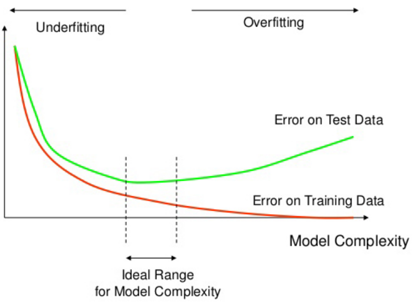

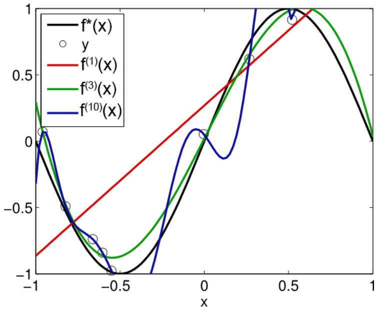

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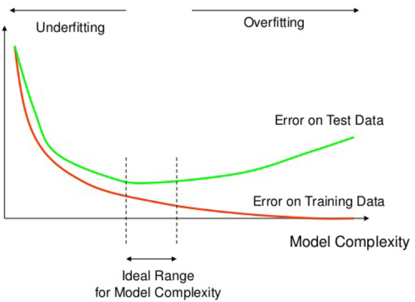

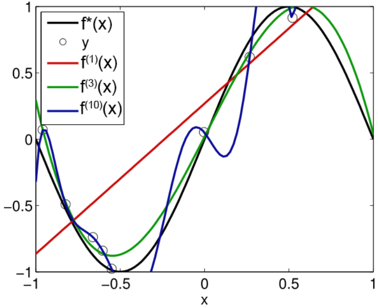

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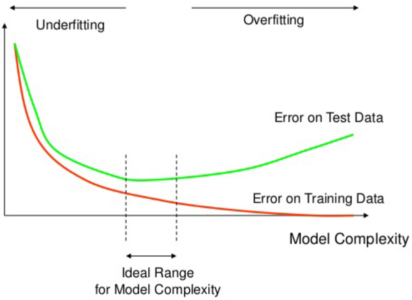

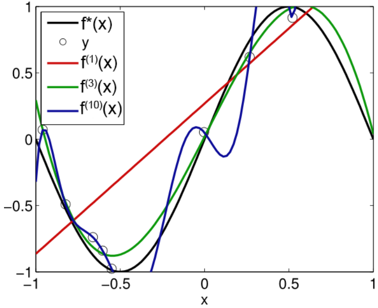

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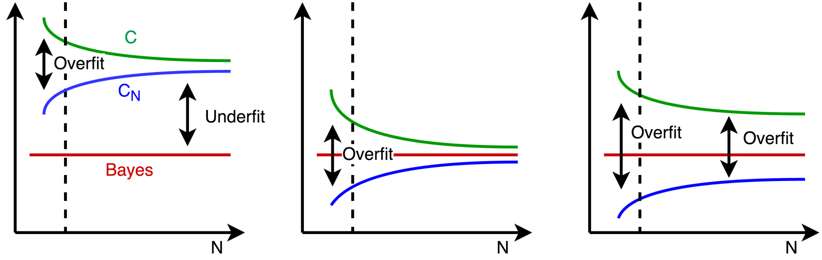

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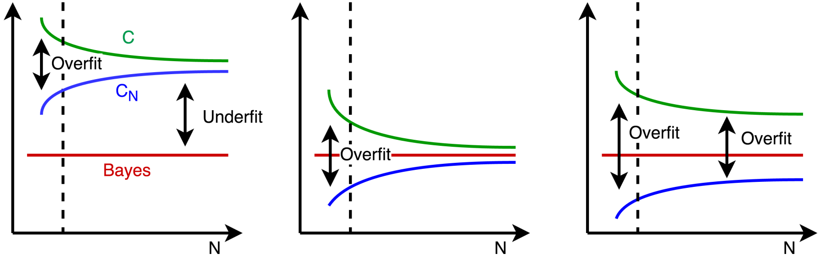
- Too small N results in overfit regardless of model complexity



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- Require knowledge about the ***point estimation***

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- How good are these estimators?

Bias & Variance

- ***Bias*** of an estimator:

$$\text{bias}(\hat{\theta}_n) = \text{E}_{\mathbb{X}}(\hat{\theta}_n) - \theta$$

  - Here, the expectation is defined over ***all possible $\mathbb{X}$'s of size n***, i.e., $\text{E}_{\mathbb{X}}(\hat{\theta}_n) = \int \hat{\theta}_n d\text{P}(\mathbb{X})$
- We call a statistic ***unbiased estimator*** iff it has zero bias

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Variance of $\hat{\mu}_{\mathrm{X}}$

$$\mathrm{Var}_{\mathbb{X}}(\hat{\mu}) \quad = \mathrm{E}_{\mathbb{X}}[(\hat{\mu} - \mathrm{E}_{\mathbb{X}}[\hat{\mu}])^2] = \mathrm{E}[\hat{\mu}^2 - 2\hat{\mu}\mu + \mu^2] = \mathrm{E}[\hat{\mu}^2] - \mu^2$$

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- The variance of $\hat{\mu}_{\mathrm{x}}$ diminishes as $n \to \infty$

Unbiased Estimator of $\sigma_{\mathbf{x}}$

- Is $\hat{\sigma}_{\mathrm{x}} = \frac{1}{n}\sum_i (x^{(i)} - \hat{\mu}_{\mathrm{x}})^2$ and an unbiased estimator of σ_{x}?

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&= \mathrm{Var}_{\mathbb{X}}(\hat{\theta}_n) + \mathrm{bias}(\hat{\theta}_n)^2
\end{aligned}$$

- MSE of an unbiased estimator is its variance

Outline

1. Learning Theory
2. Point Estimation: Bias and Variance
   - Consistency*
3. Decomposing Generalization Error
4. Regularization
   - Weight Decay
   - Validation

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- Strong consistent iff "converge almost surely"

Law of Large Numbers

Theorem (Weak Law of Large Numbers)

The sample mean $\hat{\mu}_{\mathrm{x}} = \frac{1}{n}\sum_i x^{(i)}$ *is a consistent estimator of* μ_{x}*, i.e.,* $\lim_{n\to\infty} \Pr(|\hat{\mu}_{\mathrm{x},n} - \mu_{\mathrm{x}}| < \varepsilon) = 1$ *for any* $\varepsilon > 0$*.*

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Theorem (Strong Law of Large Numbers)

In addition, $\hat{\mu}_{\mathrm{x}}$ *is a strong consistent estimator:* $\Pr(\lim_{n\to\infty} \hat{\mu}_{\mathrm{x},n} = \mu_{\mathrm{x}}) = 1$*.*

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$$\begin{aligned} \mathrm{E}_{\mathbb{X}}\left(C[f_N]\right) &= \mathrm{E}_{\mathbb{X}}\left[\int \mathrm{loss}(f_N(\boldsymbol{x}) - y) d\mathrm{P}(\boldsymbol{x}, y)\right] \\ &= \mathrm{E}_{\mathbb{X},\mathbf{x},\mathrm{y}}\left[\mathrm{loss}(f_N(\mathbf{x}) - \mathrm{y})\right] \\ &= \mathrm{E}_{\mathbf{x}}\left(\mathrm{E}_{\mathbb{X},\mathrm{y}}\left[\mathrm{loss}(f_N(\boldsymbol{x}) - \mathrm{y}) | \mathbf{x} = \boldsymbol{x}\right]\right) \end{aligned}$$

- There's a simple decomposition of $\mathrm{E}_{\mathbb{X},\mathrm{y}}\left[\mathrm{loss}(f_N(\boldsymbol{x}) - \mathrm{y}) | \boldsymbol{x}\right]$ for linear/polynomial regression

Example: Linear/Polynomial Regression

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Bias-Variance Tradeoff I

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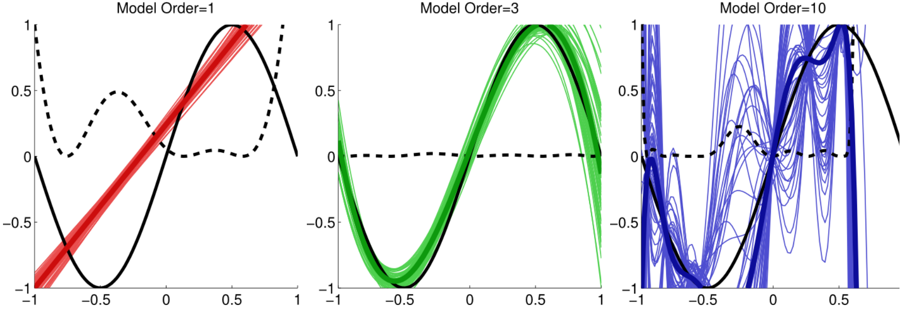
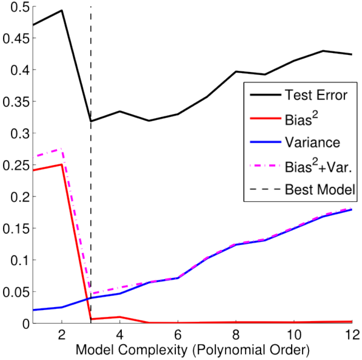
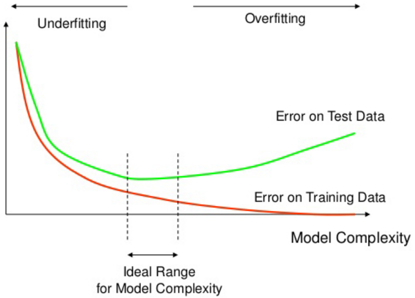
- The first term cannot be avoided when $\mathrm{P}(\mathrm{y}|\mathbf{x})$ is stochastic
- ***Model complexity*** controls the tradeoff between variance and bias
- E.g., polynomial regressors (dotted line = average training error):



Bias-Variance Tradeoff II

- Provides another way to understand the generalization/testing error





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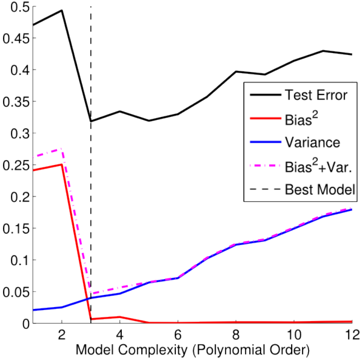

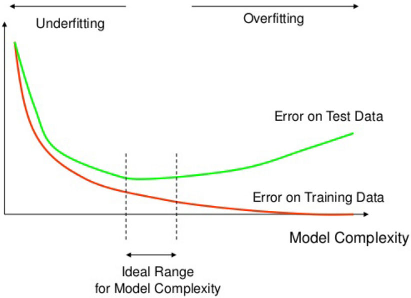

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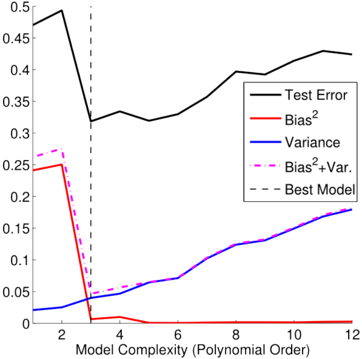

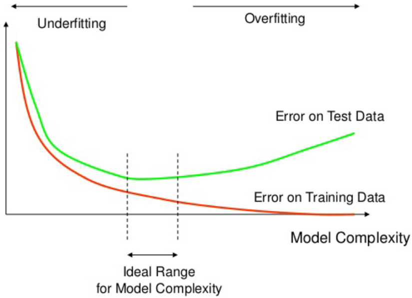

Outline

1 Learning Theory

2 Point Estimation: Bias and Variance
- Consistency*

3 Decomposing Generalization Error

4 Regularization
- Weight Decay
- Validation

Regularization

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- Regularization in the cost function: ***weight decay***
- Regularization during the training process: ***validation***

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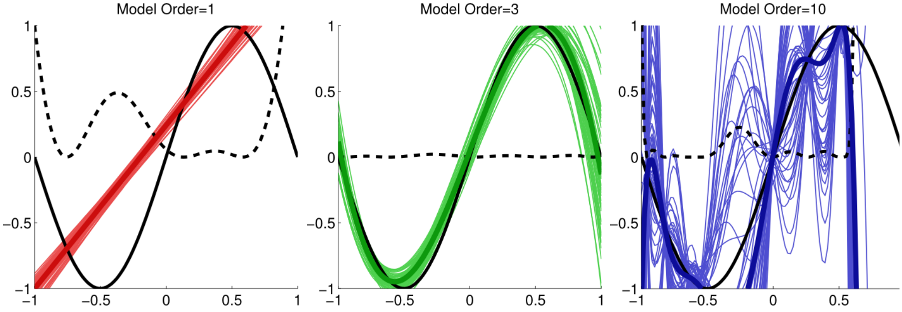
- Idea: to add a term in the cost function that panelizes complex functions
- So, with sufficiently complex $\mathbb{F}$:
  - Minimizing the empirical error term reduces bias
  - Minimizing the penalty term reduces variance



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- Can be penalized
- But which $\boldsymbol{w}$ implies a complex model?

Weight Decay

- In practice, $\boldsymbol{w} = \mathbf{0}$ is usually the "simplest" function
  - E.g, in binary classification for labels $\{-1, 1\}$, a perceptron with $\boldsymbol{w} = \mathbf{0}$ means random guessing

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$$\arg\min_{\boldsymbol{w},b} \frac{1}{2}\|\boldsymbol{y} - (\boldsymbol{X}\boldsymbol{w} - b\mathbf{1})\|^2 \text{ subject to } \|\boldsymbol{w}\|^2 \leq T$$

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- What does a larger α means? We prefer a more simple function

Flat Regressors

$$\arg\min_{\boldsymbol{w},b} \frac{1}{2}\left(\|\boldsymbol{y} - (\boldsymbol{X}\boldsymbol{w} - b\mathbf{1})\|^2 + \alpha\|\boldsymbol{w}\|^2\right)$$

- The bias b is ***not*** regularized, why?

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  - Remember R^2 (coefficient of determination)?
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- However, the label y's may not be standardized to have zero mean
- This explains why we prefer a "flat" hyperplane in the previous lecture
- We have discussed how to solve the Ridge regression problem

Sparse Weight Decay

- Alternatively we can minimizes the ***L^1-norm*** in weight decay
- E.g., ***LASSO*** (least absolute shrinkage and selection operator):

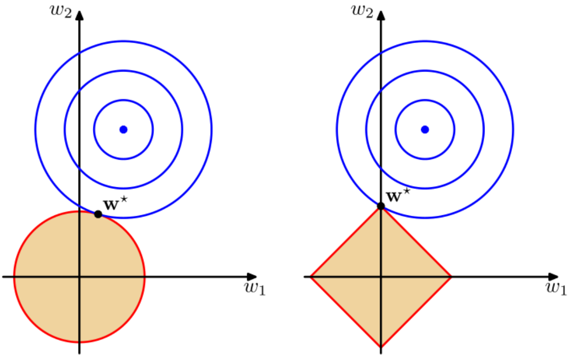
$$\arg\min_{\boldsymbol{w},b} \frac{1}{2N} \|\boldsymbol{y} - (\boldsymbol{X}\boldsymbol{w} - b\mathbf{1})\|^2 + \alpha \|\boldsymbol{w}\|_1$$

  for some constant $\alpha > 0$
- Usually results in ***sparse*** $\boldsymbol{w}$ that has many zero attributes
- Why?

Sparsity

$$\arg\min_{\boldsymbol{w},b} \frac{1}{2N} \|\boldsymbol{y} - (\boldsymbol{X}\boldsymbol{w} - b\mathbf{1})\|^2 + \alpha\|\boldsymbol{w}\|_1$$

- The surface of the cost function is the sum of SSE (blue contours) and 1-norm (red contours)
- Optimal point locates on some axes



Elastic Net**

- LASSO can be used as a feature selection technique
  - The sparse $\boldsymbol{w}$ selects explanatory variables that are most correlated to the target variable

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  - The sparse $\boldsymbol{w}$ selects explanatory variables that are most correlated to the target variable
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  for some constant $\beta \in (0,1)$
- Still gives a sparse $\boldsymbol{w}$
- Highly correlated variables will have similar values in $\boldsymbol{w}$

Outline

1 Learning Theory

2 Point Estimation: Bias and Variance
- Consistency*

3 Decomposing Generalization Error

4 Regularization
- Weight Decay
- Validation

Tuning Hyperparameters

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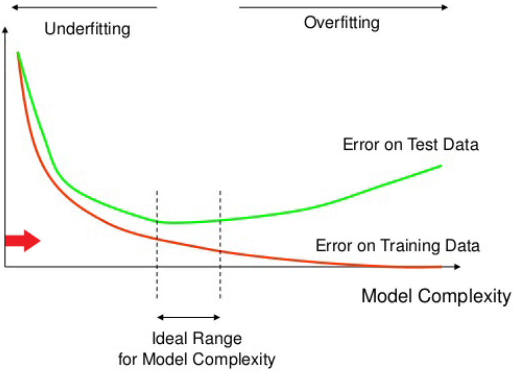
- How to set appropriate values?
- Train a model many times with different hyperparameters, and choose the function with best generalizability
- Very time consuming, can we have heuristics to speed up the process?

Structured Risk Minimization

- Consider again the Occam's razor
- ***Structured risk minimization***: start from the simplest model, gradually increase its complexity, and stop when overfitting



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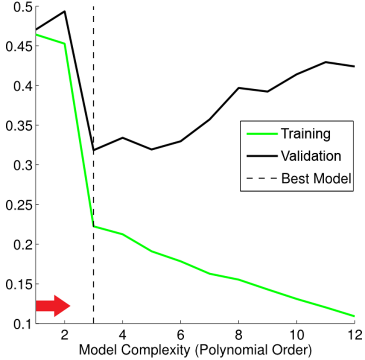
- Fix? Split a ***validation set*** from the training set and use it for hyperparameter selection



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Reference II

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