Learning Theory & Regularization

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Machine Learning

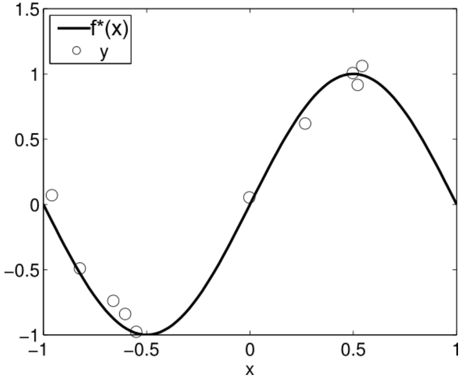
Outline

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

Outline

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
  - $\mathrm{P}(\mathrm{x}) \sim \mathrm{Uniform}(-1, 1)$
  - $\mathrm{P}(\mathrm{y} \,|\, \mathrm{x}) = \sin(\pi \mathrm{x}) + \varepsilon$, $\varepsilon \sim \mathcal{N}(0, \sigma^2)$



Which Polynomial Degree Is Better? II

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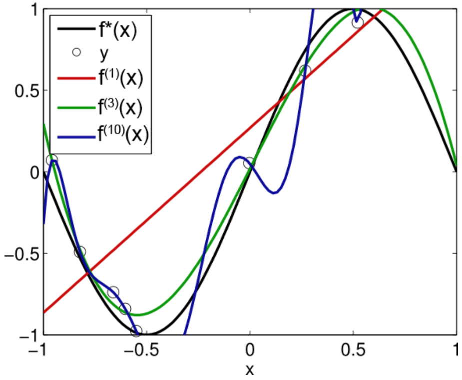

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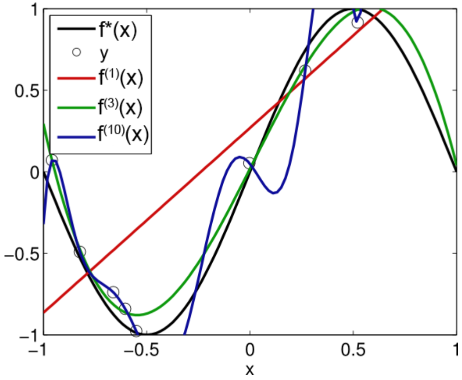

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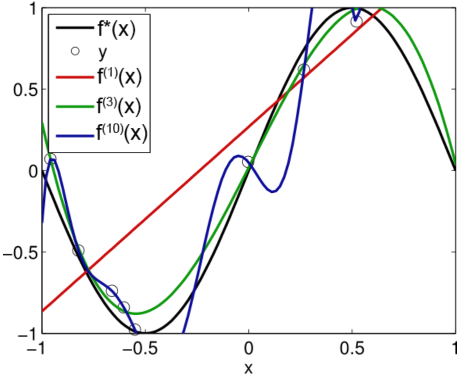

- Which one would you pick? Probably not $P = 1$ nor $P = 10$
- Note that $P = 10$ has ***zero*** training error
  - Any N points can be perfectly fitted by a polynomial of degree $N - 1$

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:

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

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

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Averaged over all possible data generating distributions, every classification algorithm has the same error rate when classifying unseen points.

- 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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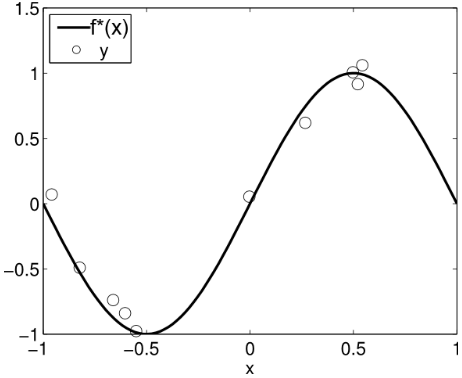
- Bounding methods
- Decomposition methods

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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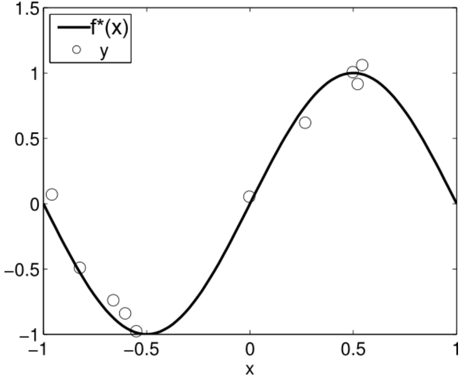

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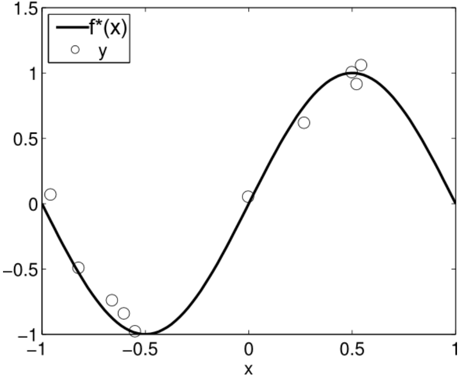

- So, our target is to make $C[f_N]$ as close to $C[f^*]$ as possible

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- Let $\mathscr{E} = C[f_N] - C[f^*]$ be the ***excess error***
- We have

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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

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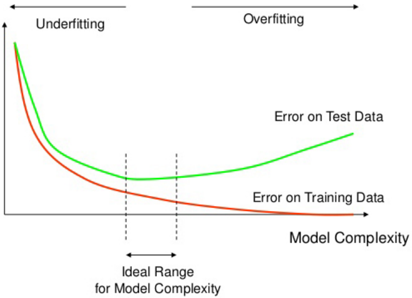

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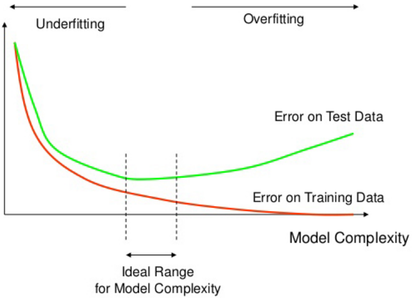

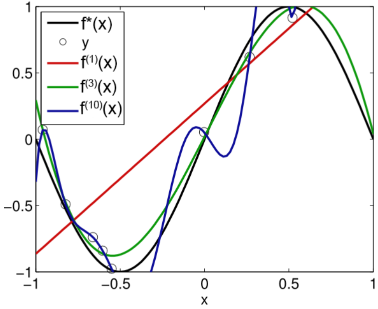

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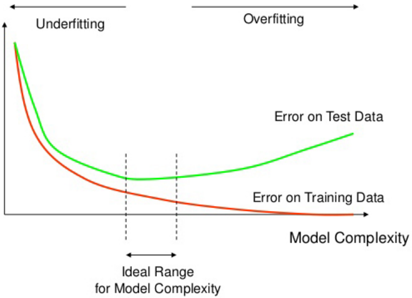

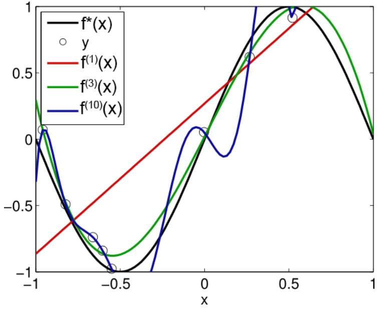

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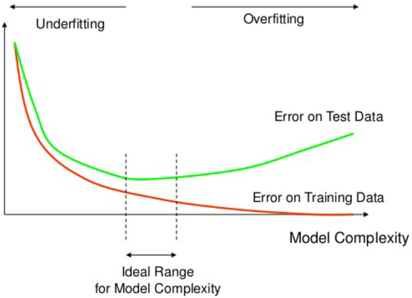

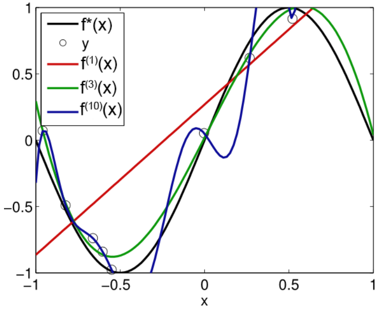

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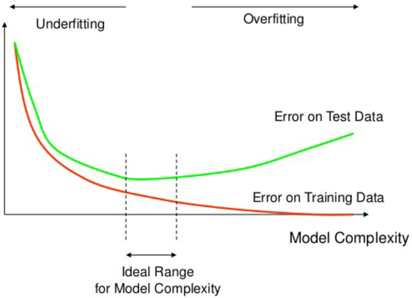

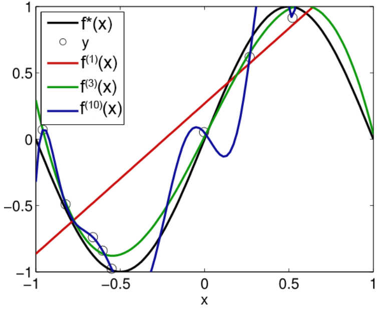

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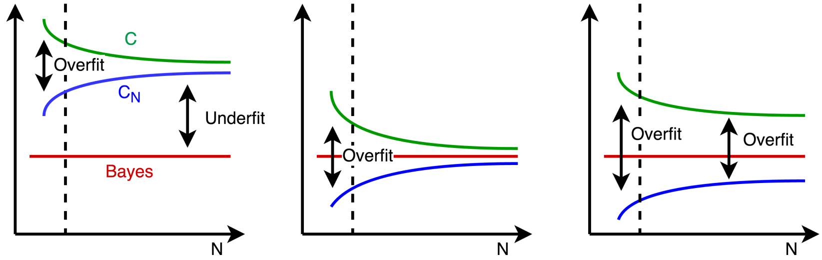

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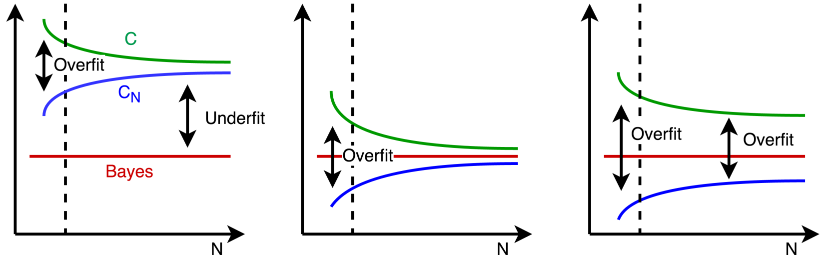
- Too small N results in overfit regardless of model complexity



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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:

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

  - Here, the expectation is defined over ***all possible $\mathbb{X}$'s of size n***, i.e., $\mathrm{E}_{\mathbb{X}}(\hat{\theta}_n) = \int \hat{\theta}_n d\mathrm{P}(\mathbb{X})$
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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 $\sigma_{\mathbf{x}}$

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Mean Square Error

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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

Consistency

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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:* $\Pr(\lim_{n\to\infty}\hat{\mu}_{\mathrm{x},n} = \mu_{\mathrm{x}}) = 1$.

Outline

Expected Generalization Error

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- How to decompose the generalization error $C[f_N]$?

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\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

- In linear/polynomial regression, we have
  - $\mathrm{loss}(\cdot) = (\cdot)^2$ a squared loss
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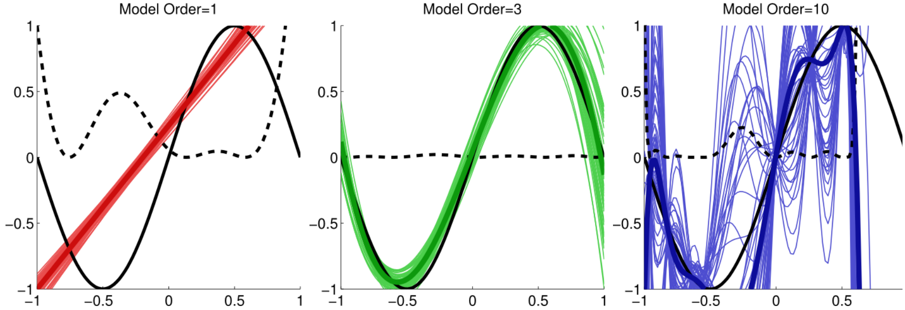
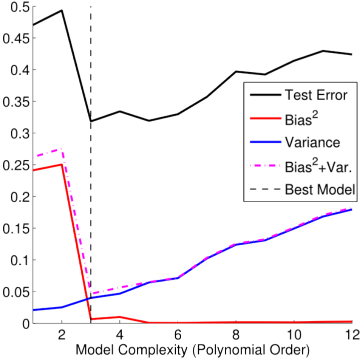
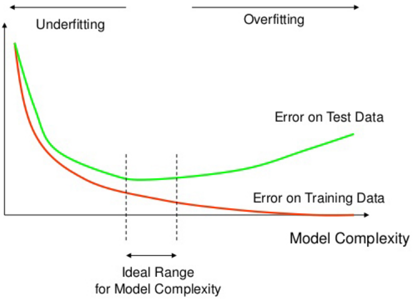
- ***Model complexity*** controls the tradeoff between variance and bias
- E.g., polynomial regressors (dotted line = average training error):



Bias-Variance Tradeoff II

- Provides another way to understand the generalization/testing error





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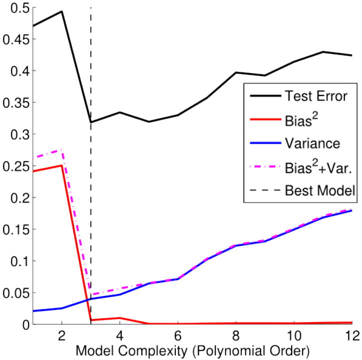

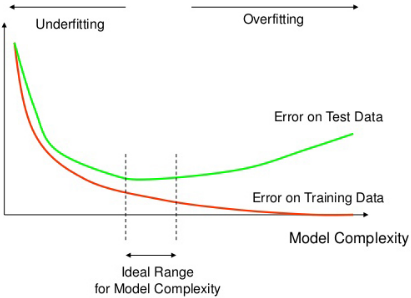

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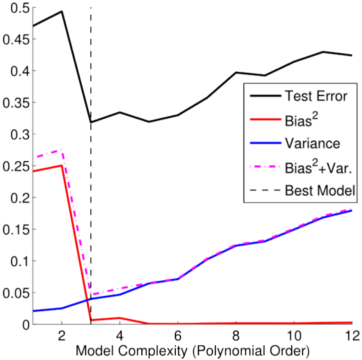

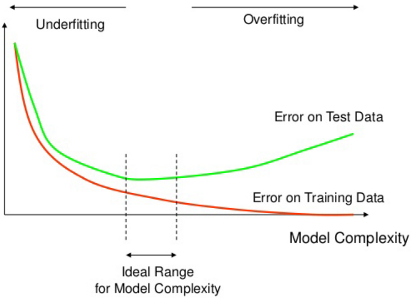

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- Regularization during the training process: ***validation***

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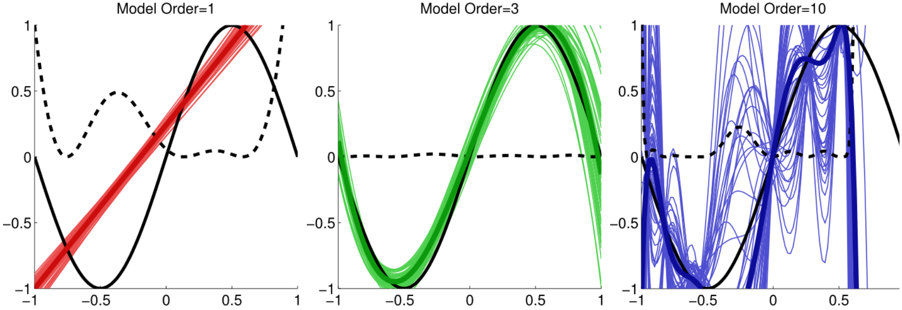
Panelizing Complex Functions

- *Occam's razor*: among equal-performing models, the simplest one should be selected
- 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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- But which $\boldsymbol{w}$ implies a complex model?

Weight Decay

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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):

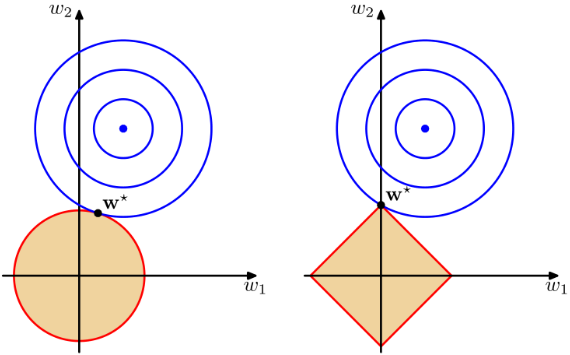
$$\arg\min_{\boldsymbol{w},b} \frac{1}{2N} \|\boldsymbol{y} - (\boldsymbol{X}\boldsymbol{w} - b\mathbf{1})\|^2 + \alpha\|\boldsymbol{w}\|_1$$

  for some constant $\alpha > 0$
- Usually results in ***sparse 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



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for some constant $\beta \in (0,1)$

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     - Important in some applications, e.g., gene selection problems
- ***Elastic net*** combines Ridge and LASSO:

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

  for some constant $\beta \in (0,1)$
- Still gives a sparse $\boldsymbol{w}$
- Highly correlated variables will have similar values in $\boldsymbol{w}$

Outline

Tuning Hyperparameters

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  - Degree P in polynomial regression
  - Coefficient α of the weight decay term in the cost function of Ridge and LASSO, etc.

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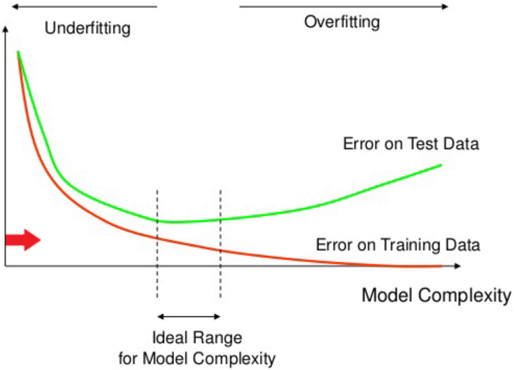
- How to set appropriate values?
- Train a model many times with different hyperparameters, and choose the function with best generalizability
- Very time consuming, can we have heuristics to speed up the process?

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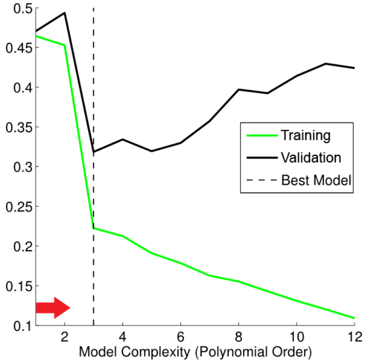
- Fix? Split a ***validation set*** from the training set and use it for hyperparameter selection



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