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Statistical Methods in AI (CSE/ECE 471)

Lecture-15: Bias-Variance, Model Selection, Regularization

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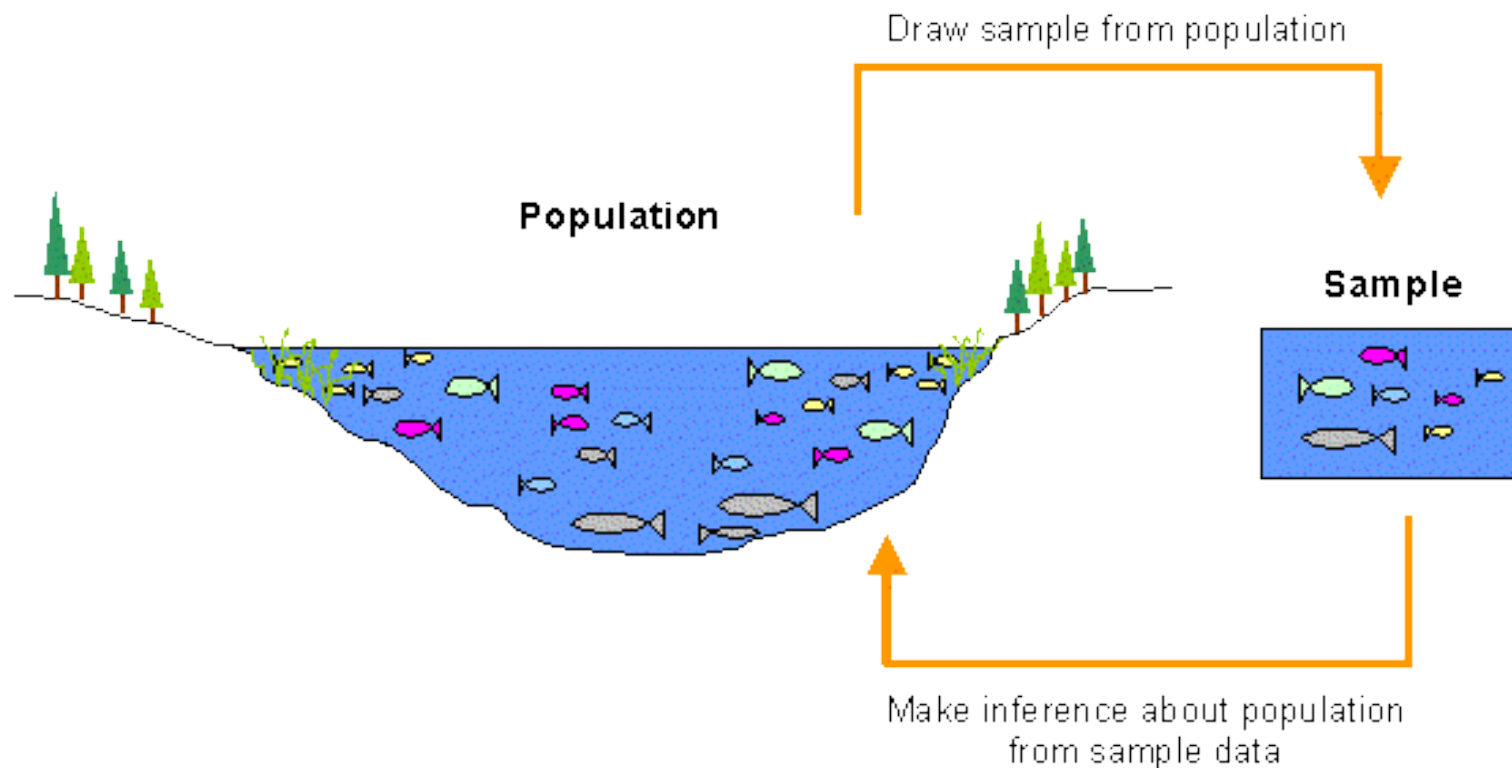
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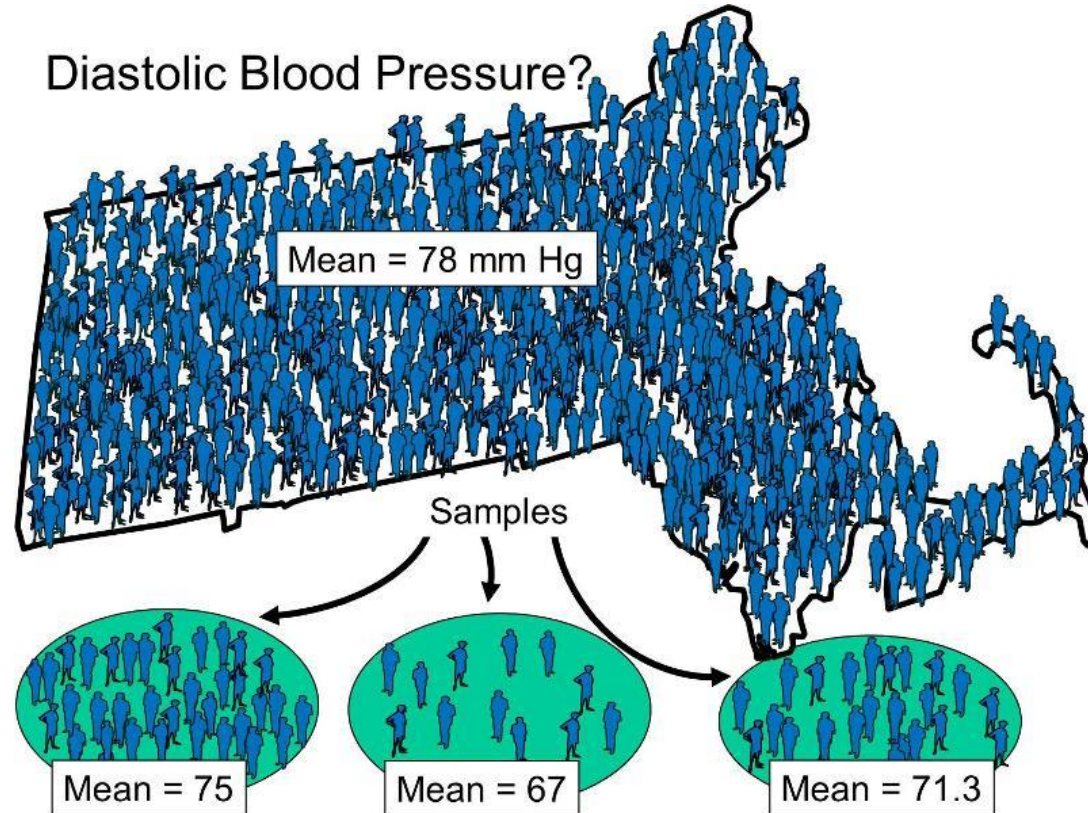
- ML workflow
 - Gather data
 - Select model (based on task)
 - Measure performance [using validation/test data]
 - Deploy model

- ML workflow
 - Gather data [“Data bias”]
 - Select model (based on task) [“Model bias”]
 - Measure performance [using validation/test data]
 - Deploy model

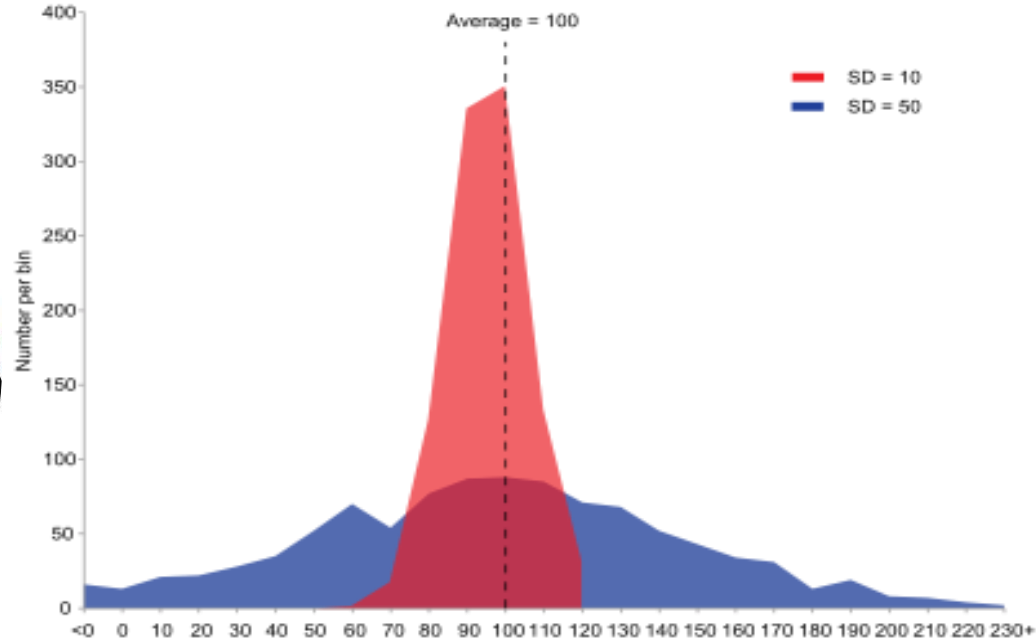
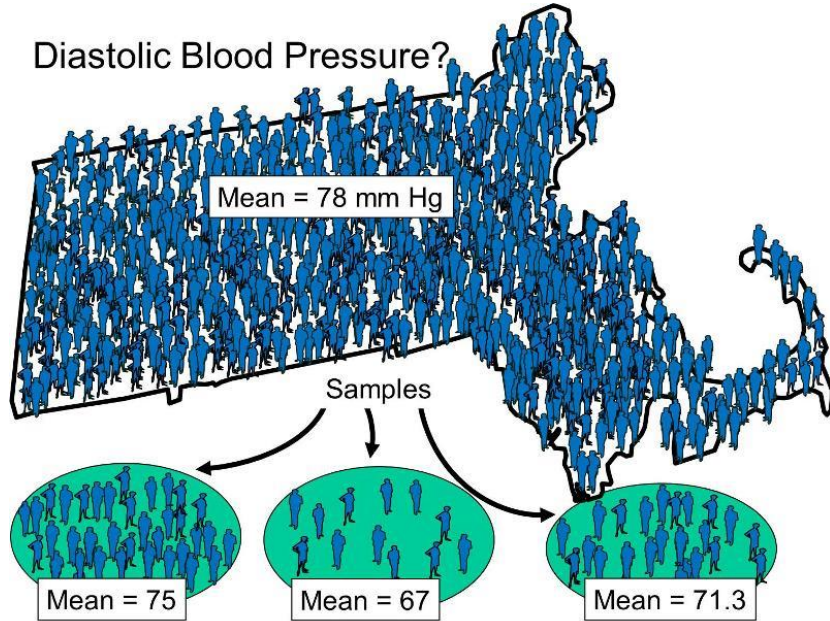
Sample vs Population



Statistics: Sample vs Population



Statistics: Sample vs Population



- A good model should generalize well

Data Collection Bias

- We place a huge amount of blind faith in the quality of datasets when training ML models.
- Quality
 - Coverage
 - Representative of Population
 - Label coverage
 - Noise
 - Input
 - Output [label noise]

Data Representation Bias

- Input representation
- Output representation

Model Bias

- Which ‘type’ of model ?
- Within the model ‘type’
 - Model-specific choices

Recall: Statistics 101

- Let X be a random variable with possible values $x_i, i = 1 \dots n$ and with probability distribution $P(X)$
- The *expected value* or *mean* of X is:

$$E[X] = \sum_{i=1}^n x_i P(x_i)$$

- If X is continuous, roughly speaking, the sum is replaced by an integral, and the distribution by a density function
- The *variance* of X is:

$$\begin{aligned} \text{Var}[X] &= E[(X - E(X))^2] \\ &= E[X^2] - (E[X])^2 \end{aligned}$$

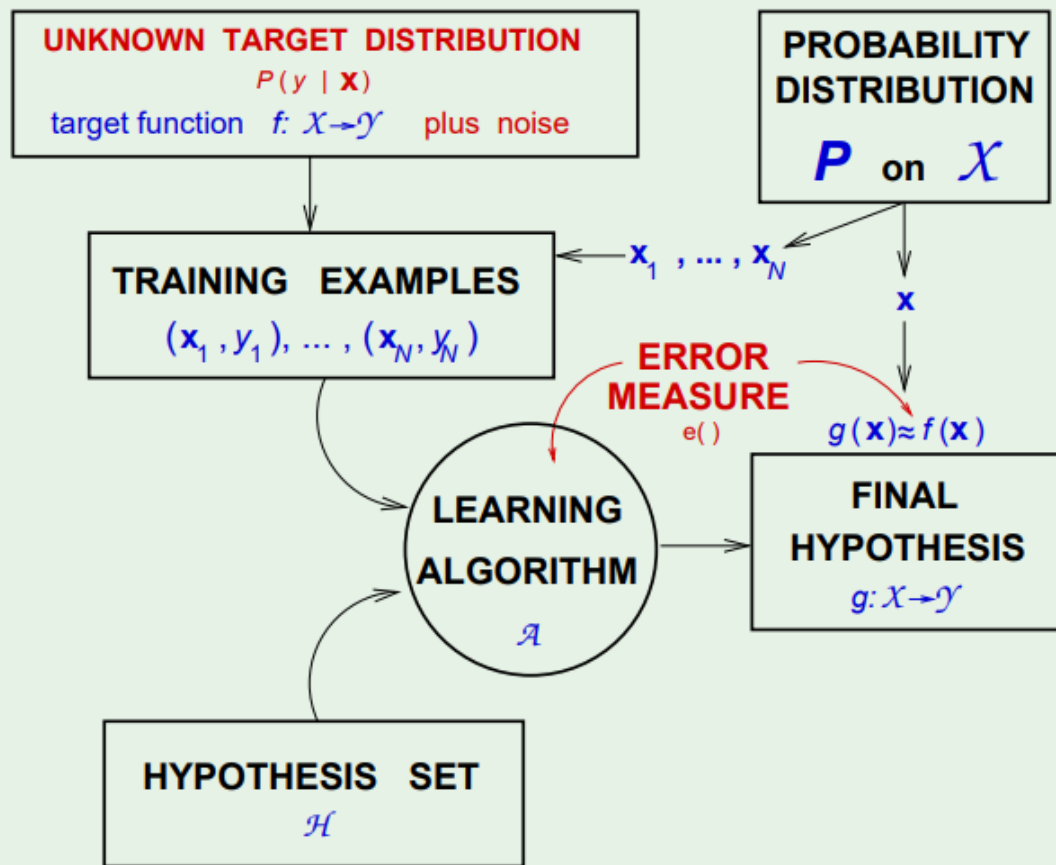
The variance lemma

$$\begin{aligned} Var[X] &= E[(X - E[X])^2] \\ &= \sum_{i=1}^n (x_i - E[X])^2 P(x_i) \\ &= \sum_{i=1}^n (x_i^2 - 2x_i E[X] + (E[X])^2) P(x_i) \\ &= \sum_{i=1}^n x_i^2 P(x_i) - 2E[X] \sum_{i=1}^n x_i P(x_i) + (E[X])^2 \sum_{i=1}^n P(x_i) \\ &= E[X^2] - 2E[X]E[X] + (E[X])^2 \cdot 1 \\ &= E[X^2] - (E[X])^2 \end{aligned}$$

We will use the form:

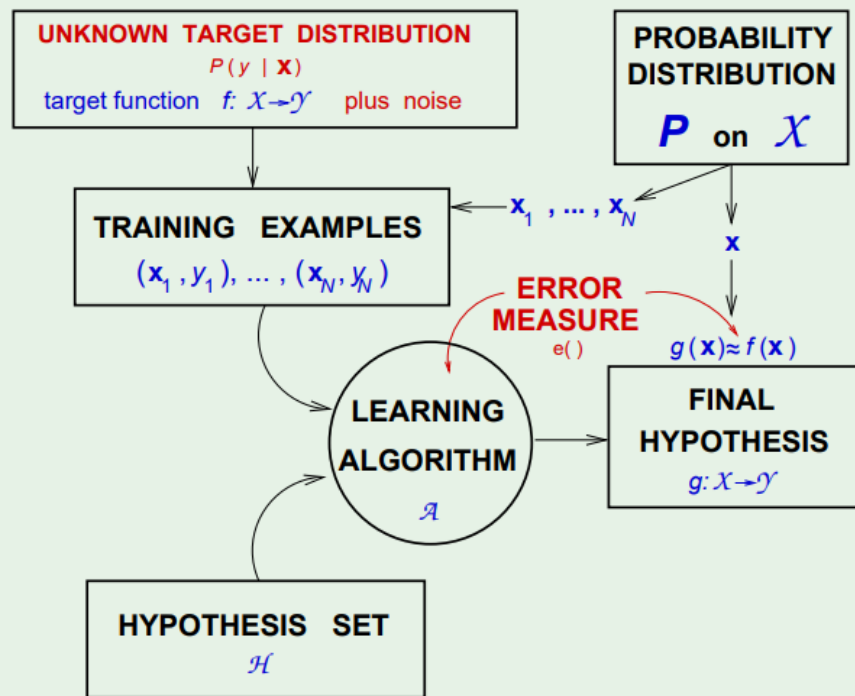
$$E[X^2] = (E[X])^2 + Var[X]$$

The learning diagram - including noisy target



Bias-Variance analysis

The learning diagram - including noisy target



1. How well \mathcal{H} can approximate f

2. How well we can zoom in on a good $h \in \mathcal{H}$

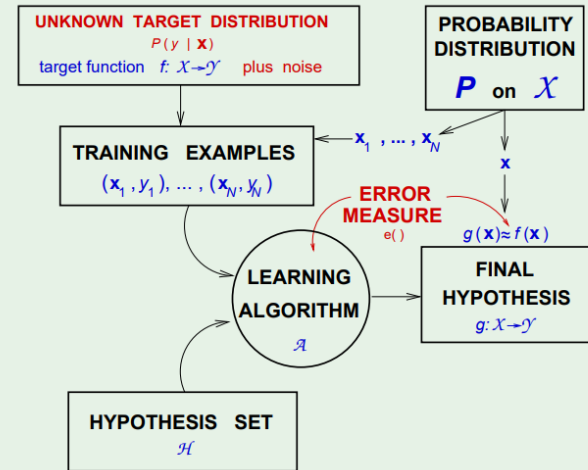
Applies to **real-valued targets** and uses **squared error**

$$E_{\text{out}}(g^{(\mathcal{D})}) = \left(g^{(\mathcal{D})}(\mathbf{x}) - f(\mathbf{x})\right)^2$$

$$E_{\text{out}}(g^{(\mathcal{D})}) = \mathbb{E}_{\mathbf{x}} \left[(g^{(\mathcal{D})}(\mathbf{x}) - f(\mathbf{x}))^2 \right]$$

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The learning diagram - including noisy target



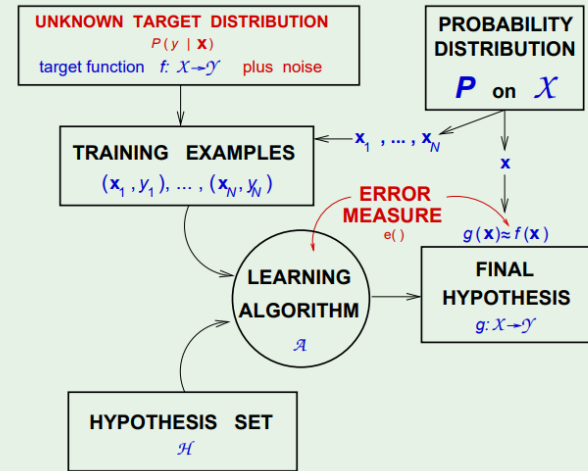
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$$\mathbb{E}_{\mathcal{D}} [E_{\text{out}}(g^{(\mathcal{D})})] = \mathbb{E}_{\mathcal{D}} \left[\mathbb{E}_{\mathbf{x}} \left[(g^{(\mathcal{D})}(\mathbf{x}) - f(\mathbf{x}))^2 \right] \right]$$

$$= \mathbb{E}_{\mathbf{x}} \left[\mathbb{E}_{\mathcal{D}} \left[(g^{(\mathcal{D})}(\mathbf{x}) - f(\mathbf{x}))^2 \right] \right]$$

The learning diagram - including noisy target



Bias-Variance analysis

$$\mathbb{E}_{\mathcal{D}} \left[(g^{(\mathcal{D})}(\mathbf{x}) - f(\mathbf{x}))^2 \right]$$

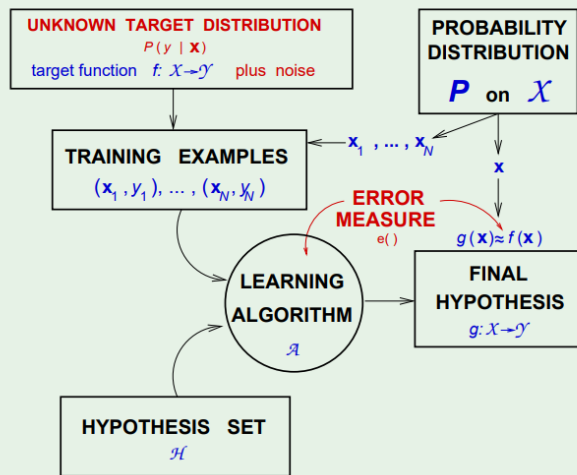
we define the 'average' hypothesis $\bar{g}(\mathbf{x})$:

$$\bar{g}(\mathbf{x}) = \mathbb{E}_{\mathcal{D}} \left[g^{(\mathcal{D})}(\mathbf{x}) \right]$$

Imagine many data sets $\mathcal{D}_1, \mathcal{D}_2, \dots, \mathcal{D}_K$

$$\bar{g}(\mathbf{x}) \approx \frac{1}{K} \sum_{k=1}^K g^{(\mathcal{D}_k)}(\mathbf{x})$$

The learning diagram - including noisy target



Bias-Variance analysis

$$\mathbb{E}_{\mathcal{D}} \left[(g^{(\mathcal{D})}(\mathbf{x}) - f(\mathbf{x}))^2 \right] = \underbrace{\mathbb{E}_{\mathcal{D}} \left[(g^{(\mathcal{D})}(\mathbf{x}) - \bar{g}(\mathbf{x}))^2 \right]}_{\text{var}(\mathbf{x})} + \underbrace{(\bar{g}(\mathbf{x}) - f(\mathbf{x}))^2}_{\text{bias}(\mathbf{x})}$$

$$\mathbb{E}_{\mathcal{D}} [E_{\text{out}}(g^{(\mathcal{D})})] = \mathbb{E}_{\mathbf{x}} \left[\mathbb{E}_{\mathcal{D}} \left[(g^{(\mathcal{D})}(\mathbf{x}) - f(\mathbf{x}))^2 \right] \right]$$

$$= \mathbb{E}_{\mathbf{x}} [\text{bias}(\mathbf{x}) + \text{var}(\mathbf{x})]$$

$$= \text{bias} + \text{var}$$

Bias-Variance analysis

$$\mathbb{E}_{\mathcal{D}} \left[(g^{(\mathcal{D})}(\mathbf{x}) - f(\mathbf{x}))^2 \right] = \underbrace{\mathbb{E}_{\mathcal{D}} \left[(g^{(\mathcal{D})}(\mathbf{x}) - \bar{g}(\mathbf{x}))^2 \right]}_{\text{var}(\mathbf{x})} + \underbrace{(\bar{g}(\mathbf{x}) - f(\mathbf{x}))^2}_{\text{bias}(\mathbf{x})}$$

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$$= \text{bias} + \text{var}$$

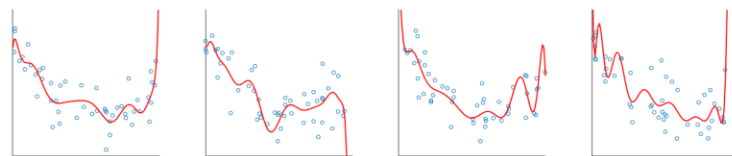
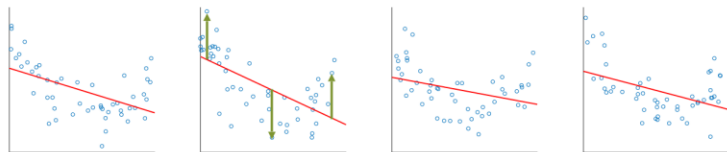
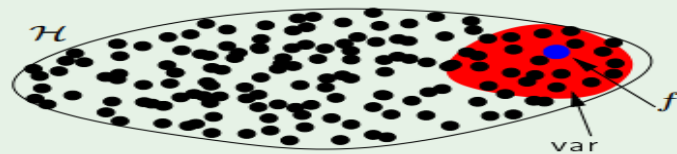
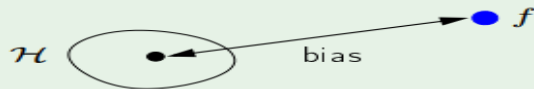
$$\mathbb{E}_{\mathcal{D}} \left[\left(g^{(\mathcal{D})}(\mathbf{x}) - f(\mathbf{x}) \right)^2 \right] = \underbrace{\mathbb{E}_{\mathcal{D}} \left[\left(g^{(\mathcal{D})}(\mathbf{x}) - \bar{g}(\mathbf{x}) \right)^2 \right]}_{\text{var}(\mathbf{x})} + \underbrace{\left(\bar{g}(\mathbf{x}) - f(\mathbf{x}) \right)^2}_{\text{bias}(\mathbf{x})}$$

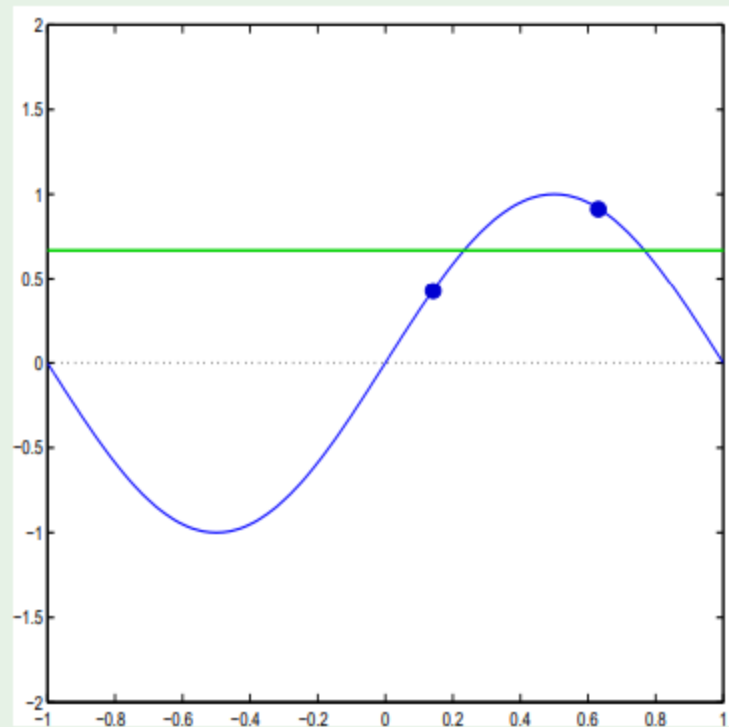
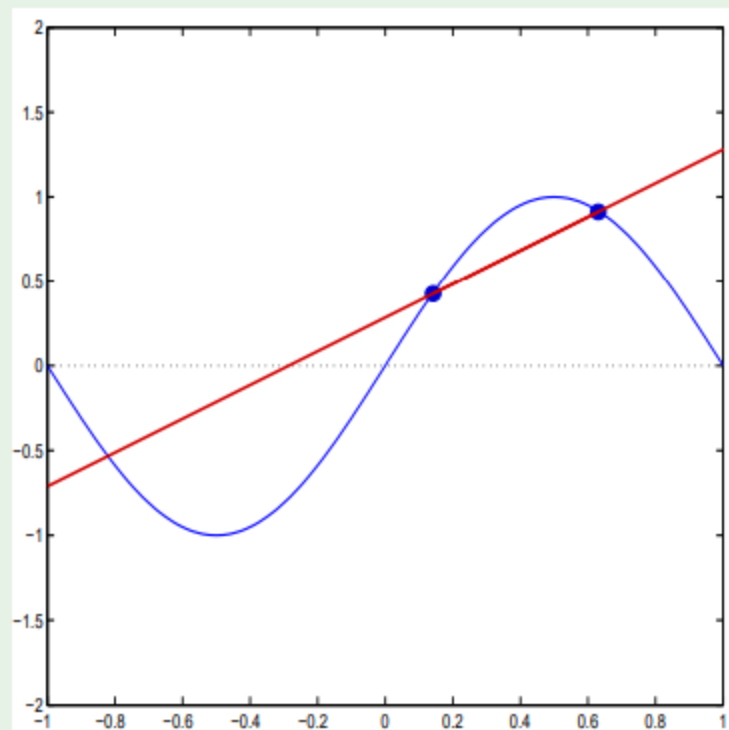
$$\mathbb{E}_{\mathbf{x}}[\text{bias}(\mathbf{x}) + \text{var}(\mathbf{x})]$$

The tradeoff

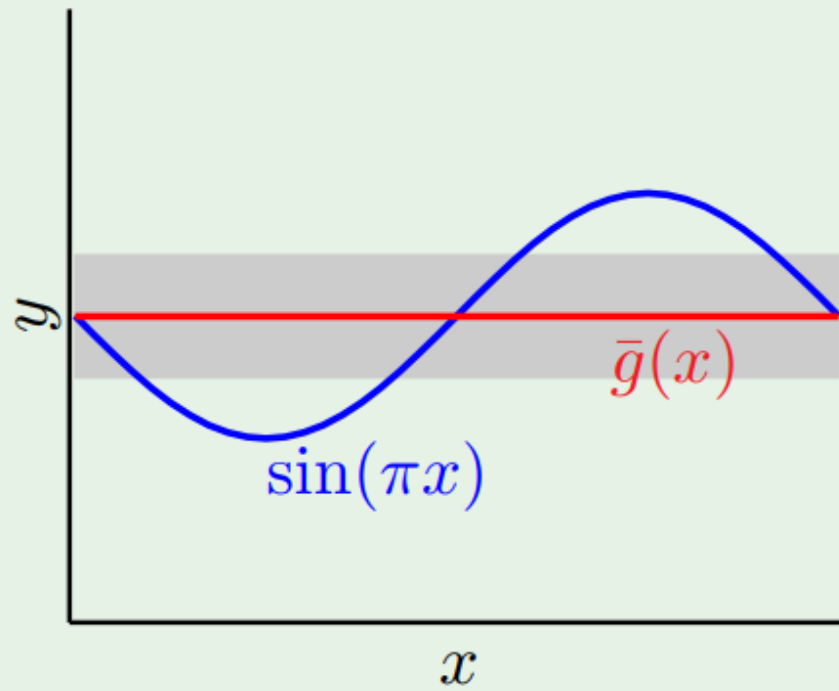
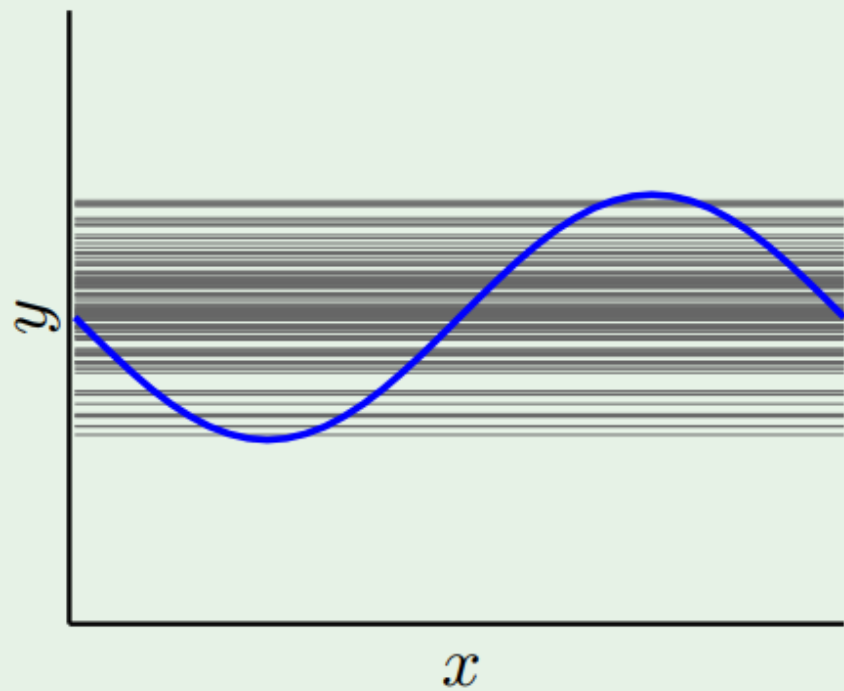
$$\text{bias} = \mathbb{E}_{\mathbf{x}} \left[\left(\bar{g}(\mathbf{x}) - f(\mathbf{x}) \right)^2 \right]$$

$$\text{var} = \mathbb{E}_{\mathbf{x}} \left[\mathbb{E}_{\mathcal{D}} \left[\left(g^{(\mathcal{D})}(\mathbf{x}) - \bar{g}(\mathbf{x}) \right)^2 \right] \right]$$

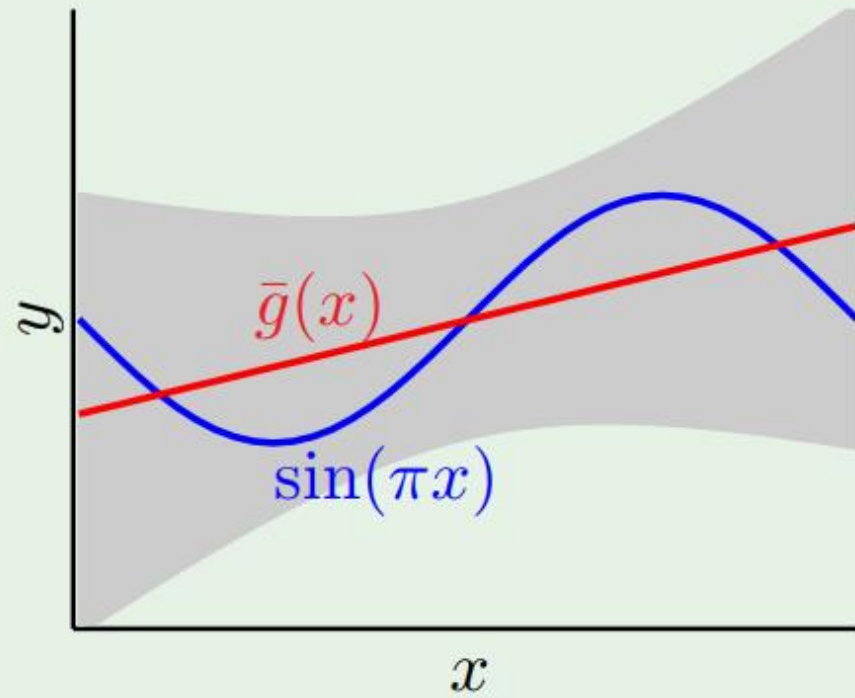
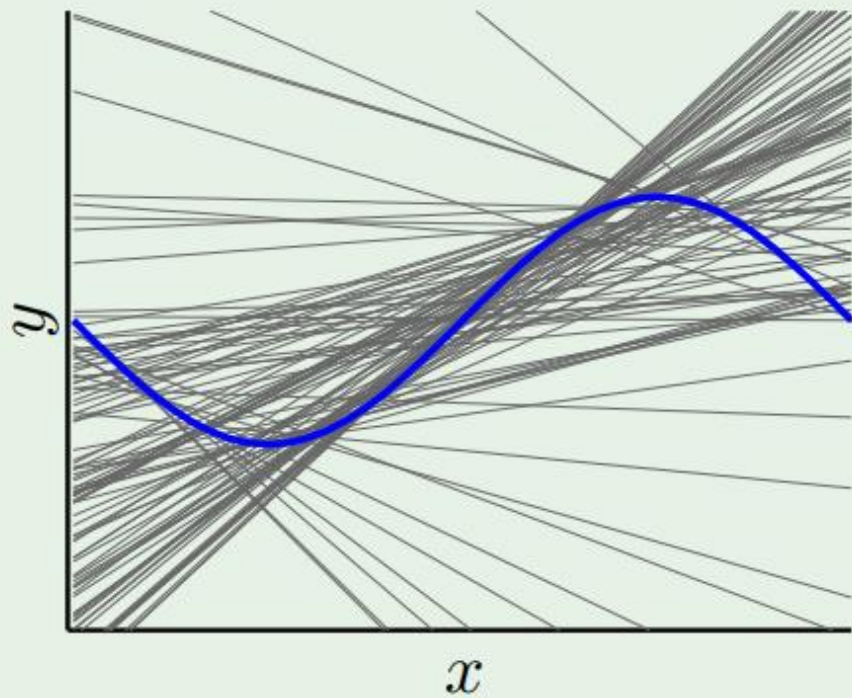


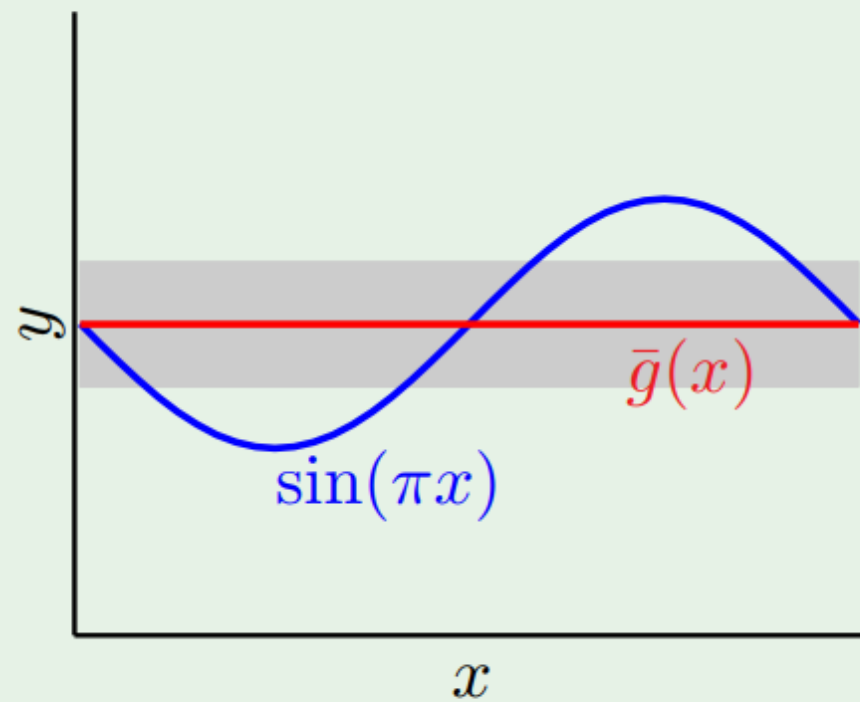
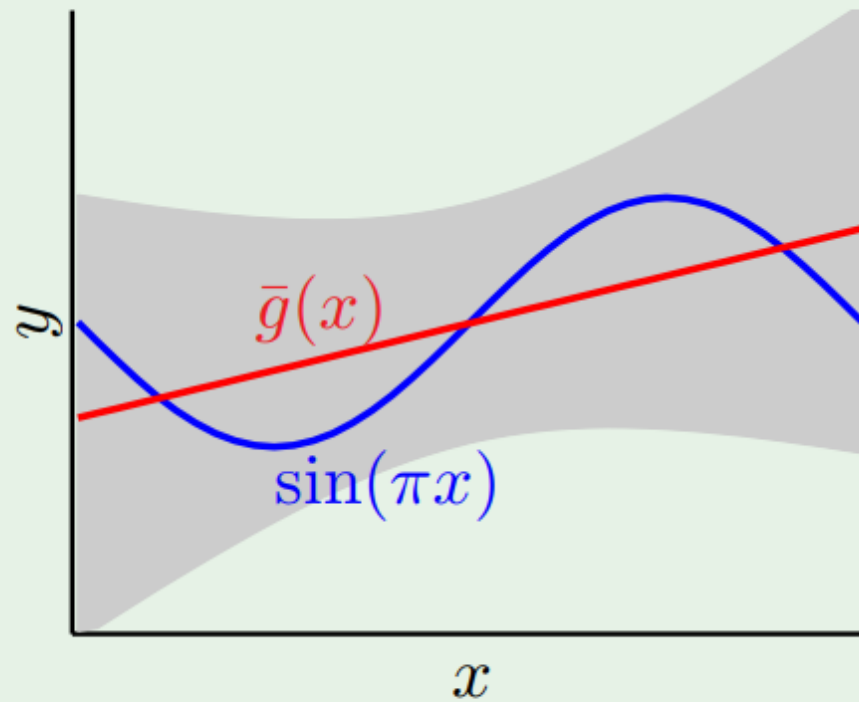
\mathcal{H}_0  \mathcal{H}_1 

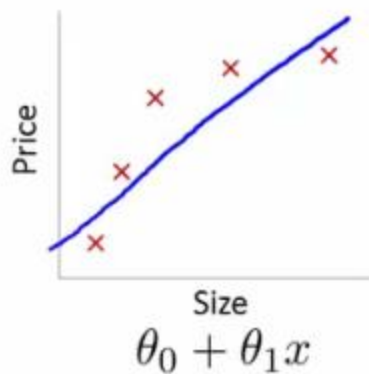
Bias and variance - \mathcal{H}_0



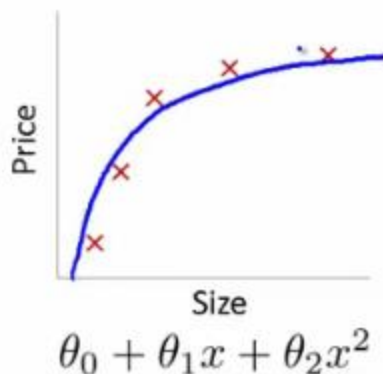
Bias and variance - \mathcal{H}_1



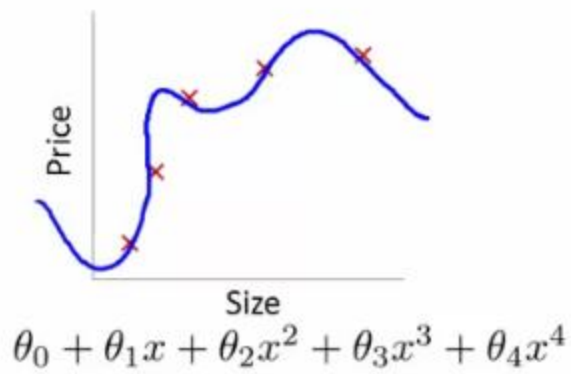
\mathcal{H}_0 bias = **0.50**var = **0.25** \mathcal{H}_1 bias = **0.21**var = **1.69**



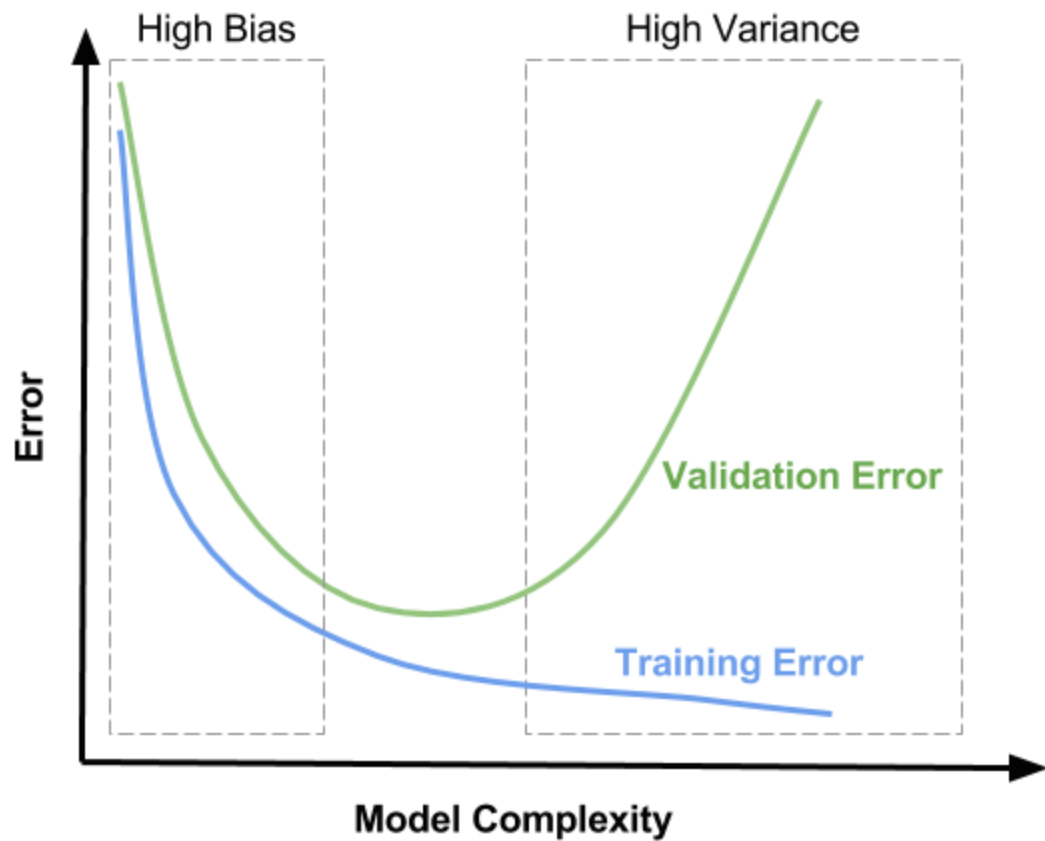
High bias
(underfit)



"Just right"



High variance
(overfit)



- Bias-Variance decomposition provides insight into model complexity issue
- Limited practical value since it is based on ensembles of data sets
 - In practice there is only a single observed data set
 - If there are many training samples then combine them
 - which would reduce over-fitting for a given model complexity

Regularization

- Remember the intuition: complicated hypotheses lead to overfitting
- Idea: change the error function to *penalize hypothesis complexity*:

$$J(\mathbf{w}) = J_D(\mathbf{w}) + \lambda J_{pen}(\mathbf{w})$$

This is called *regularization* in machine learning and *shrinkage* in statistics

- λ is called *regularization coefficient* and controls how much we value fitting the data well, vs. a simple hypothesis

Regularization for linear models

- A squared penalty on the weights would make the math work nicely in our case:

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

- This is also known as *L_2 regularization*, or *weight decay* in neural networks
- By re-grouping terms, we get:

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

- Optimal solution (obtained by solving $\nabla_{\mathbf{w}}J_D(\mathbf{w}) = 0$)

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

What L_2 regularization does

$$\arg \min_{\mathbf{w}} \frac{1}{2}(\Phi \mathbf{w} - \mathbf{y})^T(\Phi \mathbf{w} - \mathbf{y}) + \frac{\lambda}{2} \mathbf{w}^T \mathbf{w} = (\Phi^T \Phi + \lambda I)^{-1} \Phi^T \mathbf{y}$$

- If $\lambda = 0$, the solution is the same as in regular least-squares linear regression
- If $\lambda \rightarrow \infty$, the solution $\mathbf{w} \rightarrow 0$
- Positive λ will cause the magnitude of the weights to be smaller than in the usual linear solution
- This is also called *ridge regression*, and it is a special case of Tikhonov regularization
- A different view of regularization: we want to optimize the error while keeping the L_2 norm of the weights, $\mathbf{w}^T \mathbf{w}$, bounded.

L_2 Regularization for linear models revisited

- Optimization problem: minimize error while keeping norm of the weights bounded

$$\begin{aligned} \min_{\mathbf{w}} J_D(\mathbf{w}) &= \min_{\mathbf{w}} (\Phi \mathbf{w} - \mathbf{y})^T (\Phi \mathbf{w} - \mathbf{y}) \\ \text{such that } \mathbf{w}^T \mathbf{w} &\leq \eta \end{aligned}$$

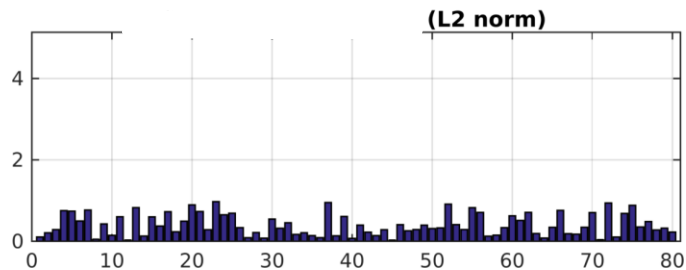
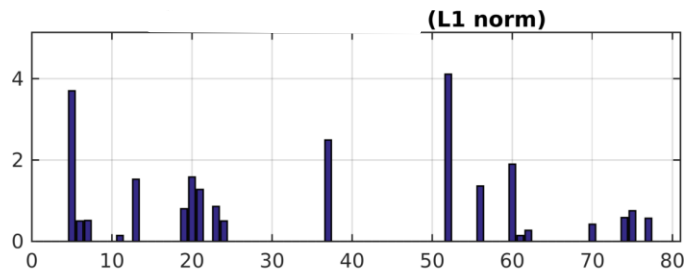
- The Lagrangian is:

$$L(\mathbf{w}, \lambda) = J_D(\mathbf{w}) - \lambda(\eta - \mathbf{w}^T \mathbf{w}) = (\Phi \mathbf{w} - \mathbf{y})^T (\Phi \mathbf{w} - \mathbf{y}) + \lambda \mathbf{w}^T \mathbf{w} - \lambda \eta$$

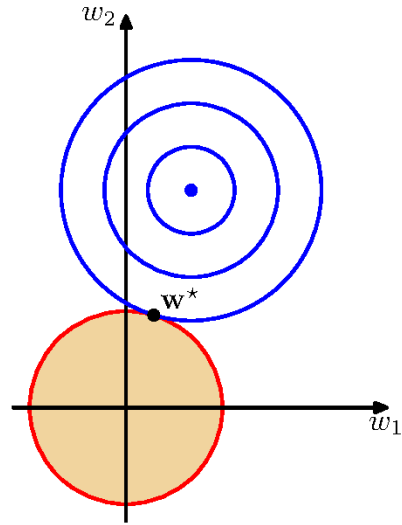
- For a fixed λ , and $\eta = \lambda^{-1}$, the best \mathbf{w} is the same as obtained by weight decay

Pros and cons of L_2 regularization

- If λ is at a “good” value, regularization helps to avoid overfitting
- Choosing λ may be hard: cross-validation is often used
- If there are irrelevant features in the input (i.e. features that do not affect the output), L_2 will give them small, but non-zero weights.
- Ideally, irrelevant input should have weights exactly equal to 0.



Visualizing regularization (2 parameters)



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

L_1 Regularization for linear models

- Instead of requiring the L_2 norm of the weight vector to be bounded, make the requirement on the L_1 norm:

$$\min_{\mathbf{w}} J_D(\mathbf{w}) = \min_{\mathbf{w}} (\Phi \mathbf{w} - \mathbf{y})^T (\Phi \mathbf{w} - \mathbf{y})$$

such that $\sum_{i=1}^n |w_i| \leq \eta$

- This yields an algorithm called Lasso (Tibshirani, 1996)

Solving L_1 regularization

- The optimization problem is a quadratic program
- There is one constraint for each possible sign of the weights (2^n constraints for n weights)
- For example, with two weights:

$$\min_{w_1, w_2} \sum_{j=1}^m (y_j - w_1 x_1 - w_2 x_2)^2$$

$$\text{such that } w_1 + w_2 \leq \eta$$

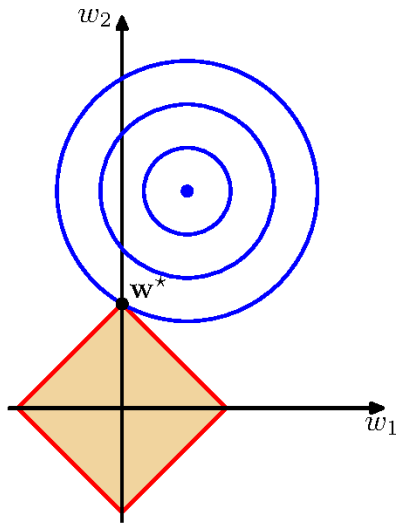
$$w_1 - w_2 \leq \eta$$

$$-w_1 + w_2 \leq \eta$$

$$-w_1 - w_2 \leq \eta$$

- Solving this program directly can be done for problems with a small number of inputs

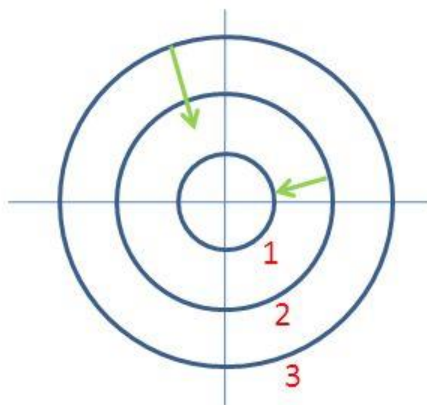
Visualizing L_1 regularization



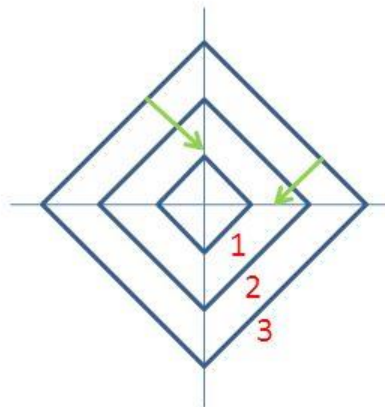
- If λ is big enough, the circle is very likely to intersect the diamond at one of the corners
- This makes L_1 regularization much more likely to make some weights *exactly* 0

A nice property of L_1

- Gradients of L_2 - and L_1 -norm



Negative gradient of L_2 -norm
always points directly toward 0

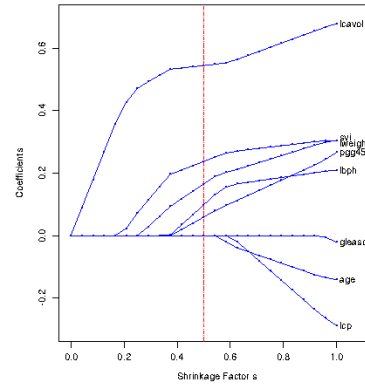
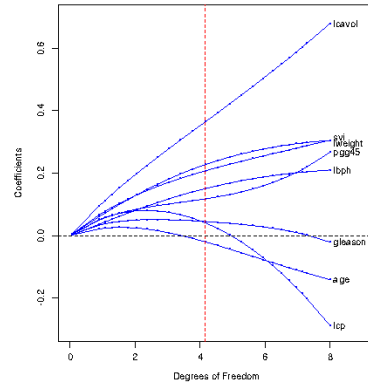


“Negative gradient” of L_1 -norm
(direction of steepest descent)
points toward coordinate axes

Pros and cons of L_1 regularization

- If there are irrelevant input features, Lasso is likely to make their weights 0, while L_2 is likely to just make all weights small
- Lasso is biased towards providing *sparse solutions* in general
- Lasso optimization is computationally more expensive than L_2
- More efficient solution methods have to be used for large numbers of inputs (e.g. least-angle regression, 2003).
- L_1 methods of various types are very popular

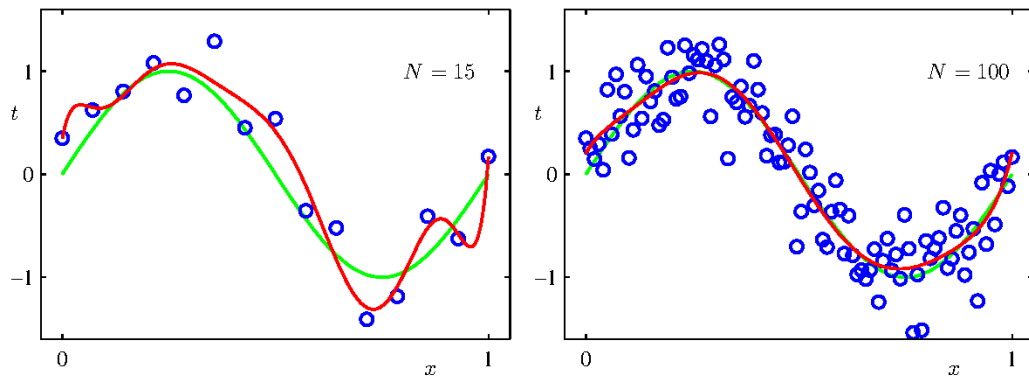
Example of L1 vs L2 effect



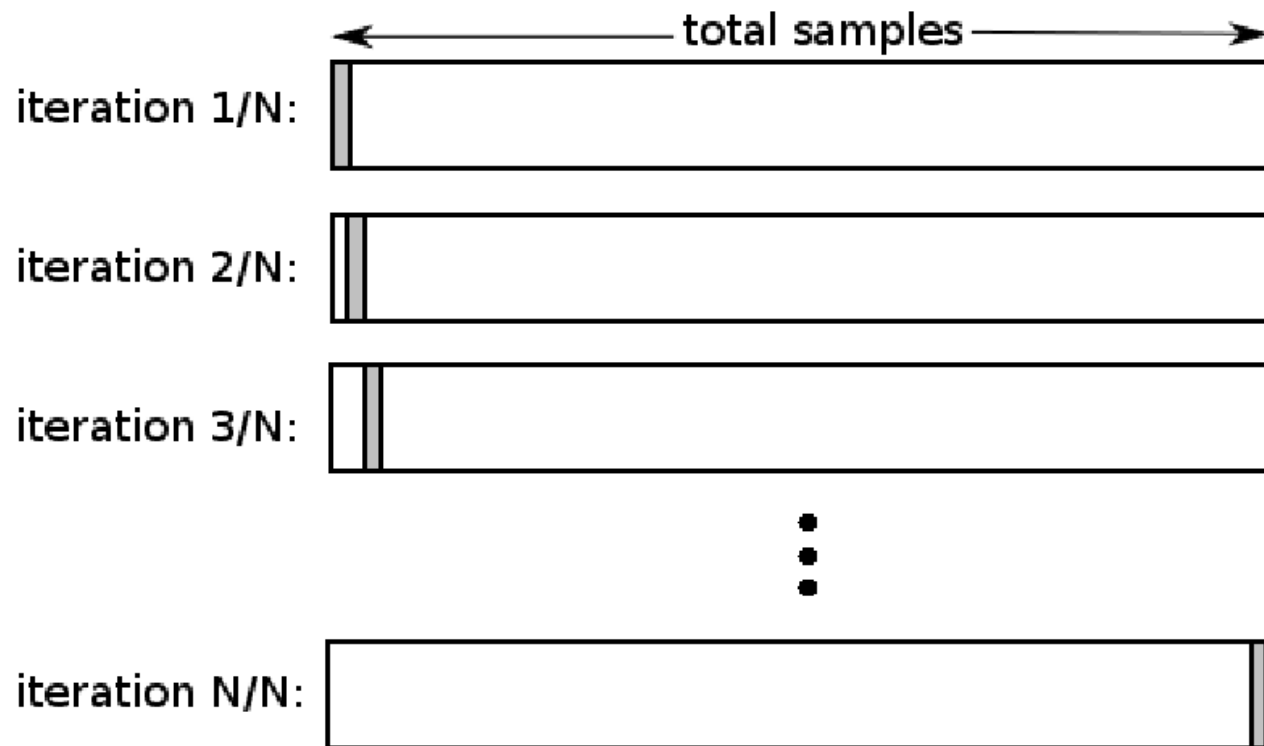
- Note the sparsity in the coefficients induced by L_1
- Lasso is an efficient way of performing the L_1 optimization

More on overfitting

- Overfitting depends on the amount of data, relative to the complexity of the hypothesis
- With more data, we can explore more complex hypotheses spaces, and still find a good solution

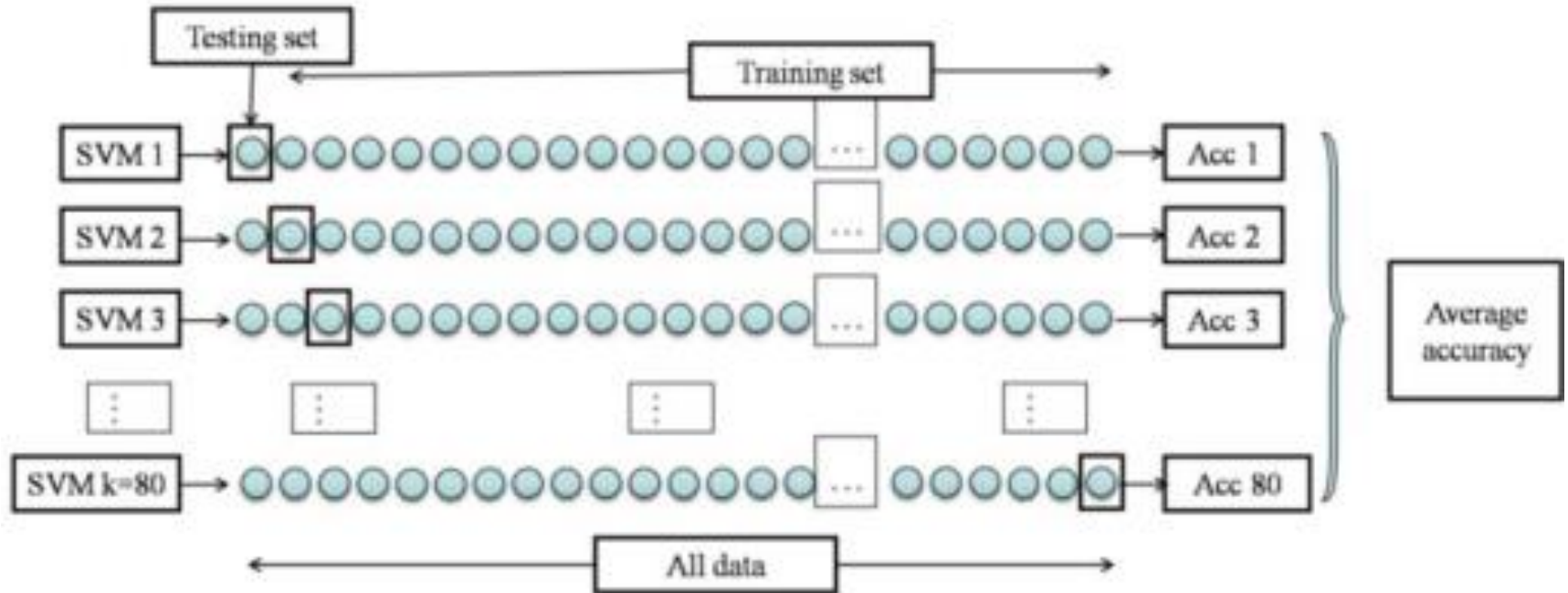


Leave One Out Cross Validation



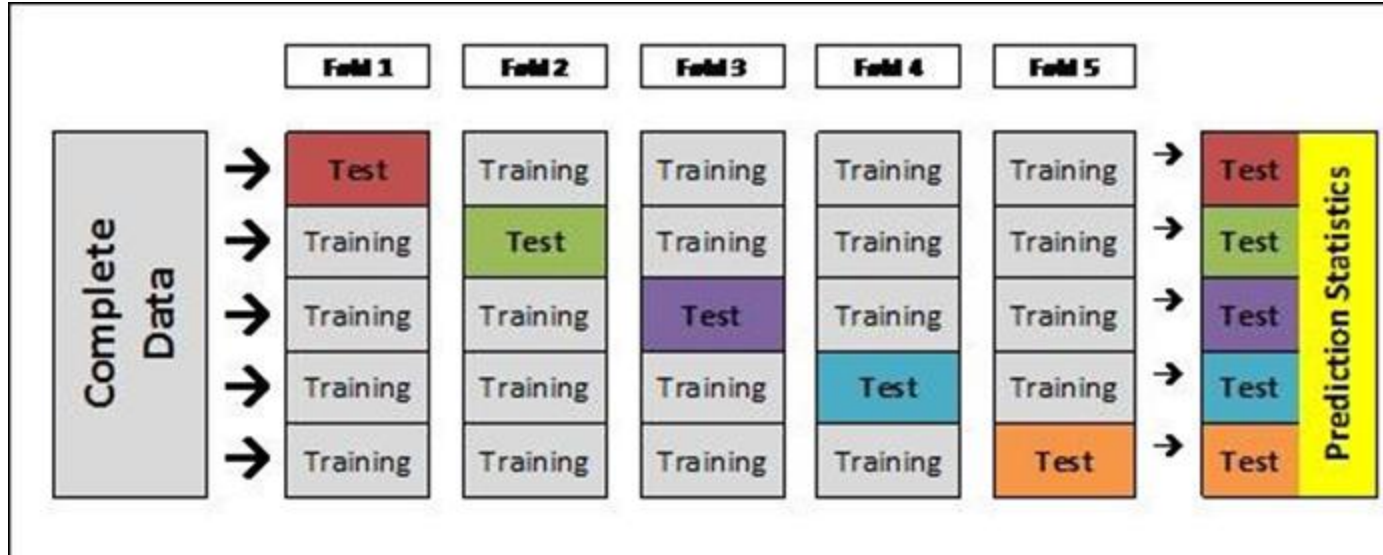
Leave One Out Cross Validation

High variance



K-fold Cross Validation

Fold → bias



Assess model's bias-variance characteristics using k-fold Cross Validation?

- With k -fold CV , you get k different estimates of your model's error- $e_1, e_2, e_3, \dots, e_k$
- $\text{Mean}(\text{errors}) \sim 0 \rightarrow \text{low bias}$
- $\text{Variance}(\text{errors}) \sim 0 \rightarrow \text{low variance}$