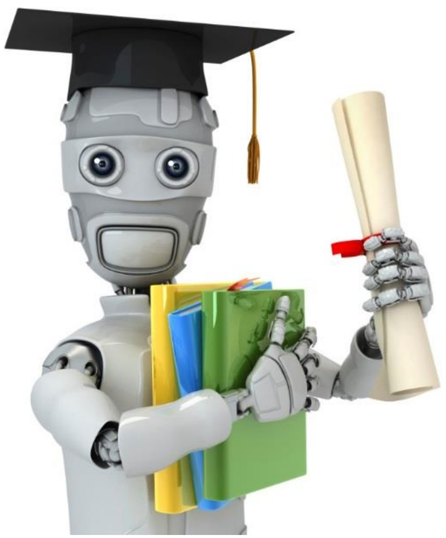


模型选择与正则化 (Model Selection & Regularization)

Machine Learning

梁毅雄

yxliang@csu.edu.cn

Some materials from Andrew Ng, Zico Kolter, Hung-yi Lee
and others

偏差与方差(Bias and Variance)

假设用某个函数$h(x)$去近似真实函数$y(x)$，其偏差和方差分别为

$$bias(h(x)) = E[h(x) - y(x)]$$

$$var(h(x)) = E\{h(x) - E[h(x)]\}^2 = E[h(x)^2] - E[h(x)]^2$$

Large Bias

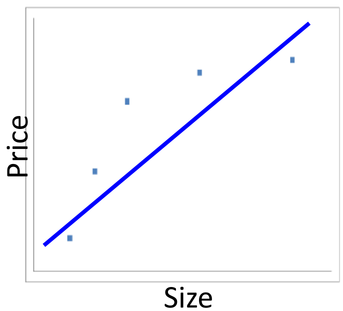
Small Variance

Small Bias

Large Variance

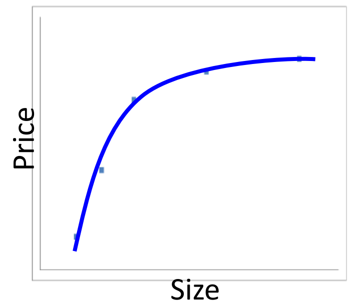
过拟合问题

例子: 线性回归 (房屋价格)



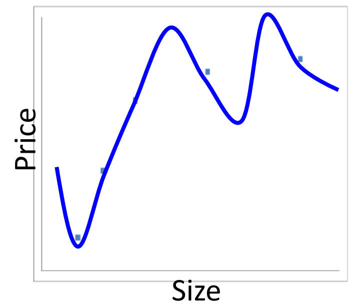
$\theta_0 + \theta_1 x$

Underfitting: Large bias



$\theta_0 + \theta_1 x + \theta_2 x^2$

Good fitting



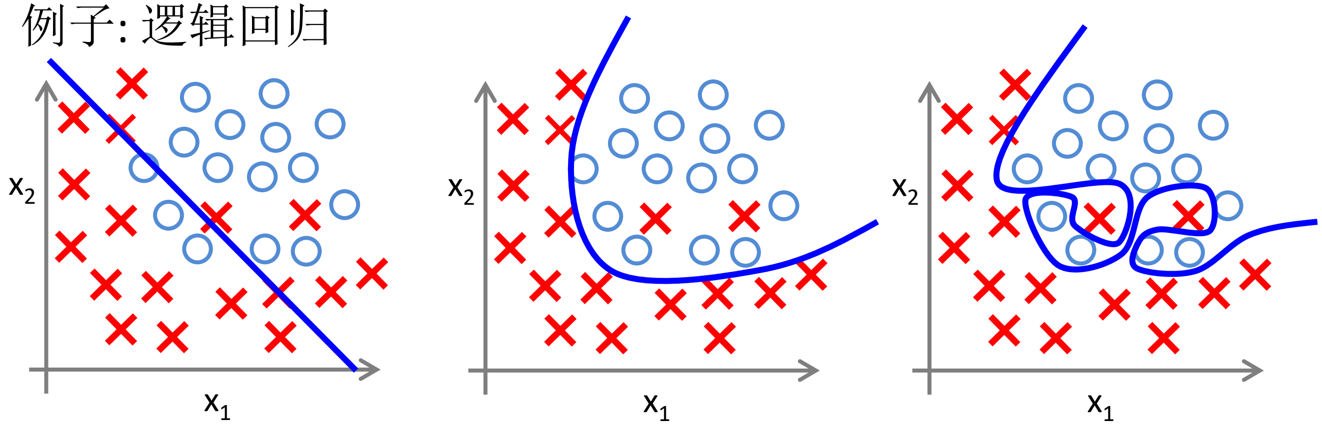
$\theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3 + \theta_4 x^4$

Overfitting: Large Variance

过拟合: 如果多项式阶数较大, 训练得到的模型对于训练集能正确拟合$J(\theta) = \frac{1}{2m}\sum_{i=1}^{m}\left[(h_\theta(x^{(i)}) - y^{(i)}\right]^2 \approx 0$, 但是对于新的样本预测效果却不好.

过拟合问题

例子: 逻辑回归



$h_\theta(x) = g(\theta_0 + \theta_1 x_1 + \theta_2 x_2)$

(g = sigmoid function)

Underfitting: Large bias

$g(\theta_0 + \theta_1 x_1 + \theta_2 x_2$
$+\theta_3 x_1^2 + \theta_4 x_2^2$
$+\theta_5 x_1 x_2)$

Good fitting

$g(\theta_0 + \theta_1 x_1 + \theta_2 x_1^2$
$+\theta_3 x_1^2 x_2 + \theta_4 x_1^2 x_2^2$
$+\theta_5 x_1^2 x_2^3 + \theta_6 x_1^3 x_2 + \dots)$

Overfitting: Large Variance

过拟合: 如果多项式阶数较大, 训练得到的模型对于训练集能正确分类($J(\theta) = -\frac{1}{2m}\left[\sum_{i=1}^{m} y^{(i)} \log h_\theta(x^{(i)}) + (1-y^{(i)}) \log(1-h_\theta(x^{(i)}))\right] \approx 0$), 但是对于新的样本预测效果却不好.

过拟合问题

- 实际应用中容易出现过拟合（模型足够复杂）
- 问题1：如何判断是否出现了过拟合或者欠拟合问题？（诊断）
- 问题2：如何解决过拟合或者欠拟合问题？

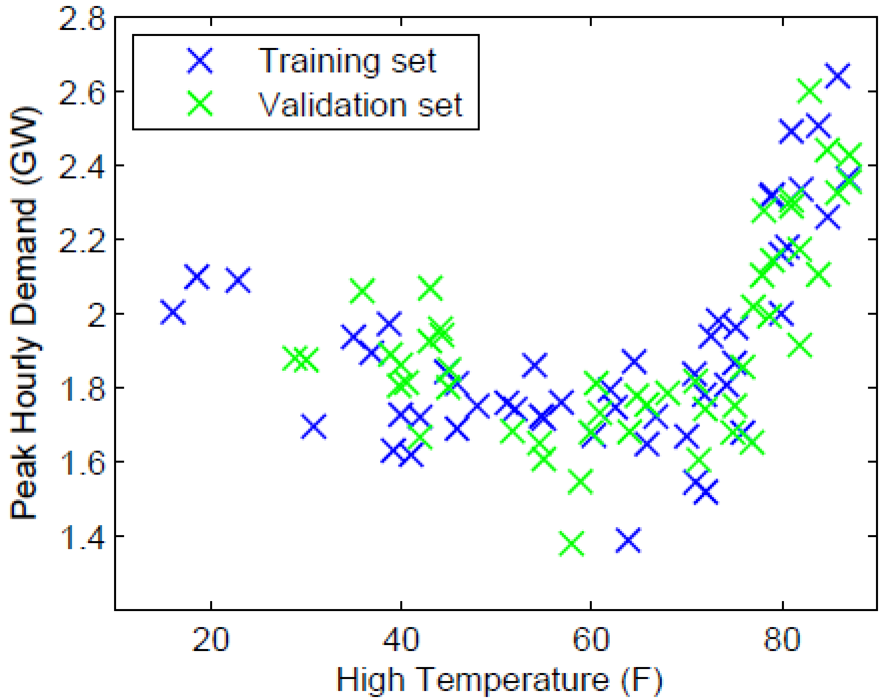
（开处方治疗）

模型选择

$$\theta^* = \arg\min_{\theta} \frac{1}{m} \sum_{i=1}^{m} \ell(h_\theta(x^{(i)}), y^{(i)})$$

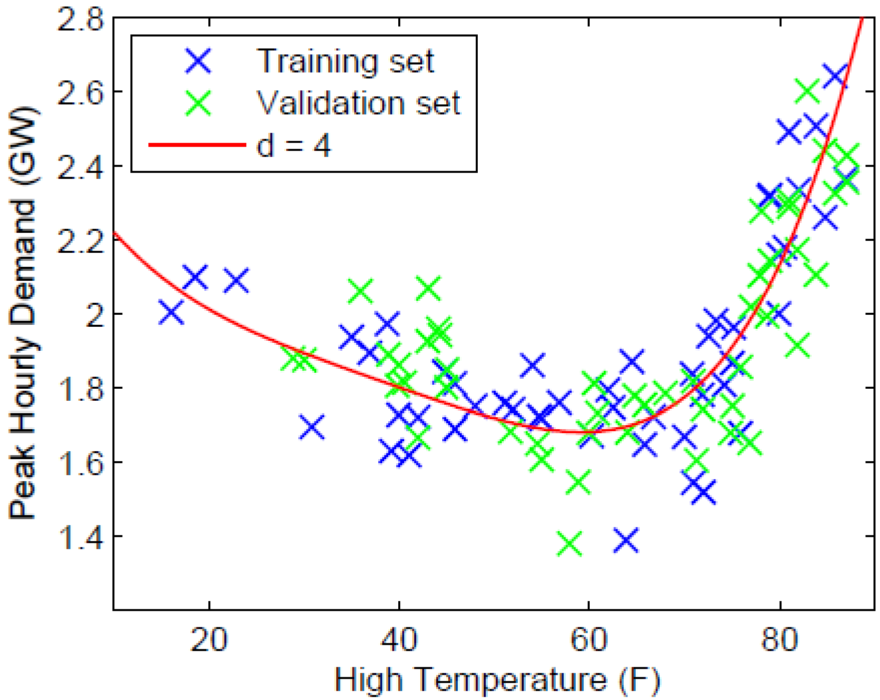
- 最小化训练集上的损失(损失错误)
- 一般而言，模型越复杂（如多项式阶数越高或特征越多），训练得到的模型经验错误越低，但却更容易出现过拟合
- 选择哪个模型更合适？
- 把训练集随机分成两部分：用于训练参数的训练集和用于模型选择的验证集(Validation Set)

模型选择



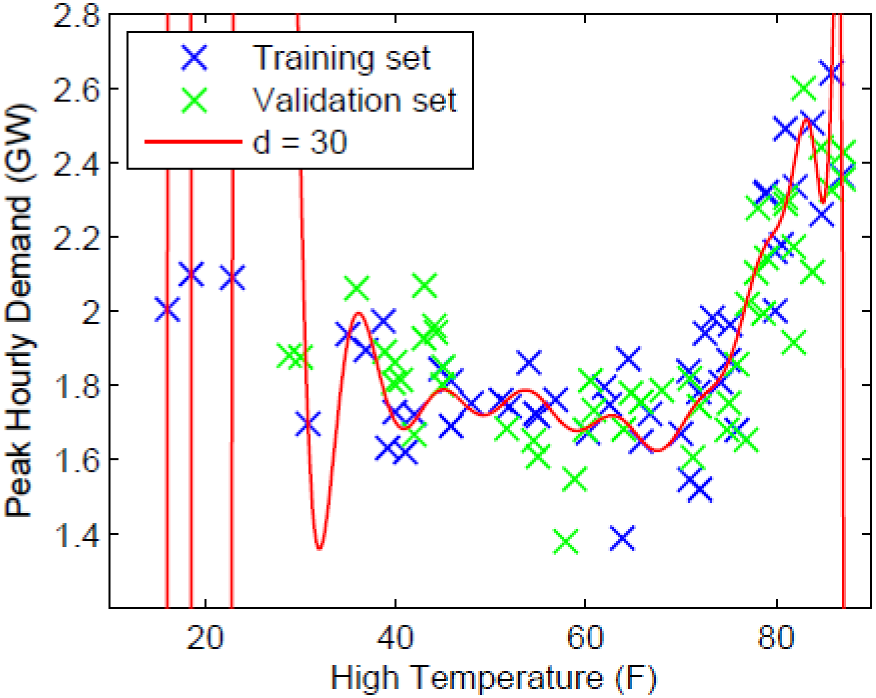
Training set and validation set

模型选择



Training set and validation set, fourth degree polynomial

模型选择

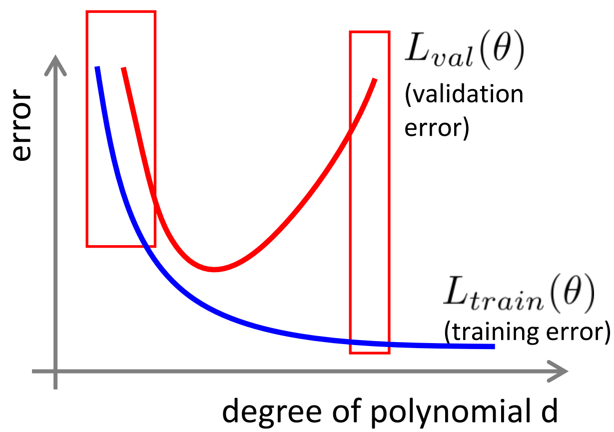


Training set and validation set, 30th degree polynomial

诊断偏差和方差

训练误差: $L_{train}(\theta) = \frac{1}{2m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})^2$

验证误差: $L_{val}(\theta) = \frac{1}{2m_{val}}\sum_{i=1}^{m_{val}}(h_\theta(x_{val}^{(i)}) - y_{val}^{(i)})^2$



偏差大(underfit):

训练误差：大

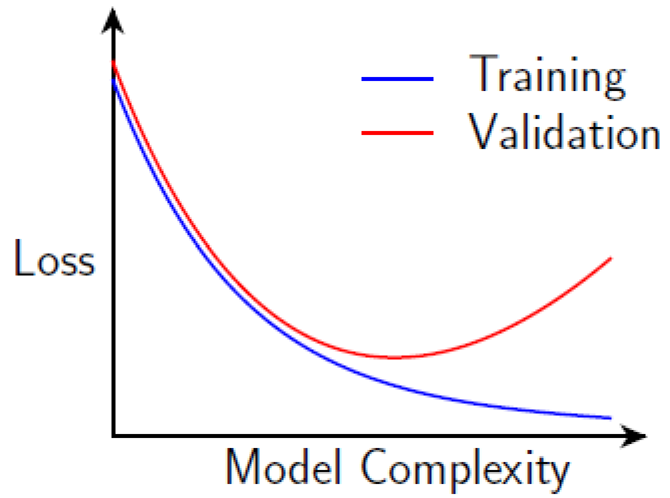
训练误差与验证误差差别较小

方差大(overfit):

训练误差：小

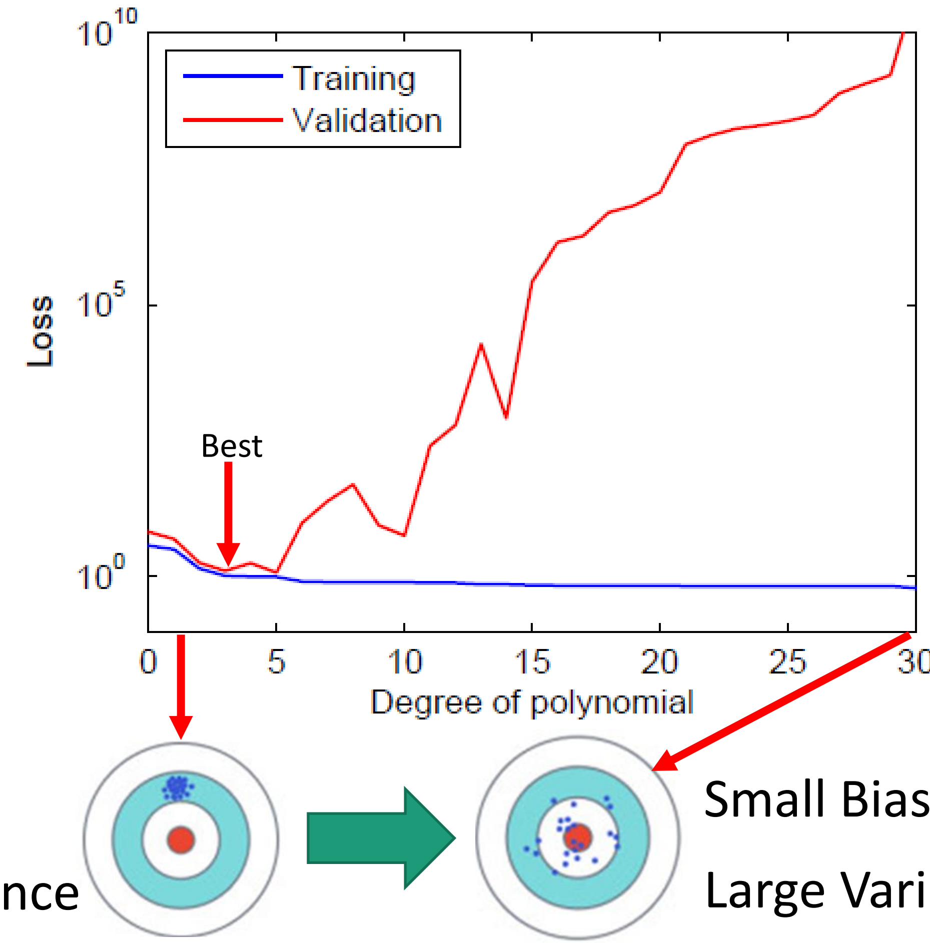
验证误差远大于训练误差

模型选择



- There is usually a trade-off between bias and variance.
- Select a model that balances two kinds of error to minimize total error

模型选择



Large Bias

Small Variance

Small Bias

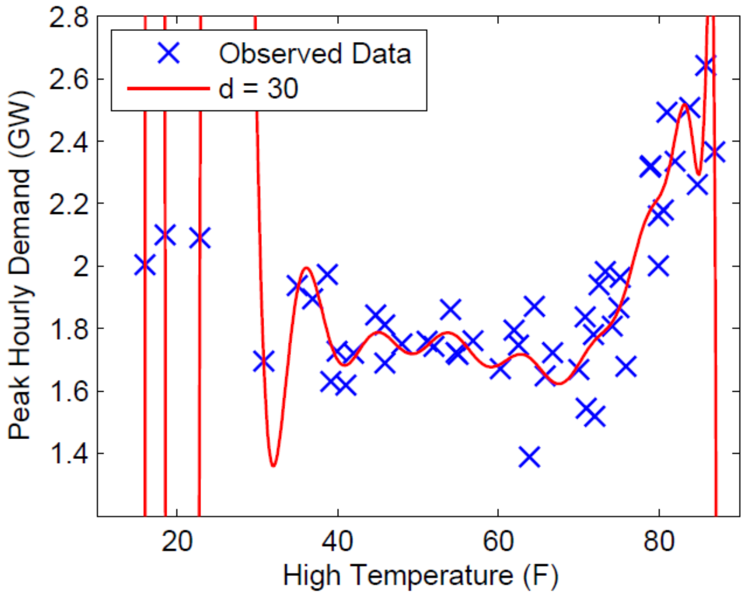
Large Variance

解决欠拟合和过拟合问题

- 欠拟合(Large Bias)：增加模型的复杂度
  - 收集新的特征
  - 增加多项式组合特征
  - … $(x_1^2, x_2^2, x_1x_2,\text{etc})$
- 过拟合(Large Variance)
  - 增加数据（Very effective, but not always practical）
  - 降低模型的复杂度
    - 减少特征（人为的选择一些特征，特征选择）
    - 正则化(Regularization)：非常有效的方法，可大幅度降低方差(增加偏差)
    - …

正则化线性回归

- Regularized Linear Regression
  - Intuition: A 30^{th} degree polynomial that passes exactly through many of the data points requires very large entries in θ
  - We can directly prevent large entries in θ by penalizing the magnitude of its entries



$$\min_{\theta} J(\theta)$$

λ : 正则化参数（因子）

$$J(\theta) = \frac{1}{2m}\left[\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})^2 + \lambda \sum_{j=1}^{n} \theta_j^2\right]$$

思考：正则化参数λ 的取值范围？

正则化线性回归

$$J(\theta) = \frac{1}{2m}\left[\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})^2 + \lambda\sum_{j=1}^{n}\theta_j^2\right]$$

$$J(\theta) = L(\theta) + \lambda R(\theta)$$

$$L(\theta) = \frac{1}{2m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})^2$$

$$\min_\theta J(\theta)$$

思考：若λ 的值足够大，如 $\lambda = 10^{10}$，下面正确的是：

A. Algorithm works fine
B. Algorithm fails to eliminate overfitting
C. Algorithm results in underfitting
D. Algorithm results in overfitting
E. Gradient descent will fail to converge

正则化线性回归

$$J(\theta) = \frac{1}{2m}\left[\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})^2 + \lambda\sum_{j=1}^{n}\theta_j^2\right]$$

$$\min_\theta J(\theta)$$

Gradient descent

Repeat $\{$

$$\theta_0 := \theta_0 - \alpha\frac{1}{m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})x_0^{(i)}$$

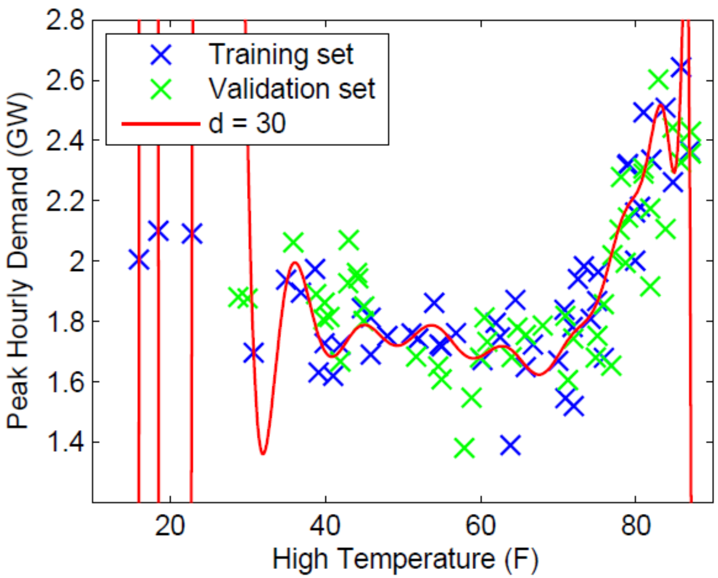
$$\theta_j := \theta_j - \alpha \quad \frac{1}{m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})x_j^{(i)}$$

$$(j = \cancel{0}, 1, 2, 3, \ldots, n)$$

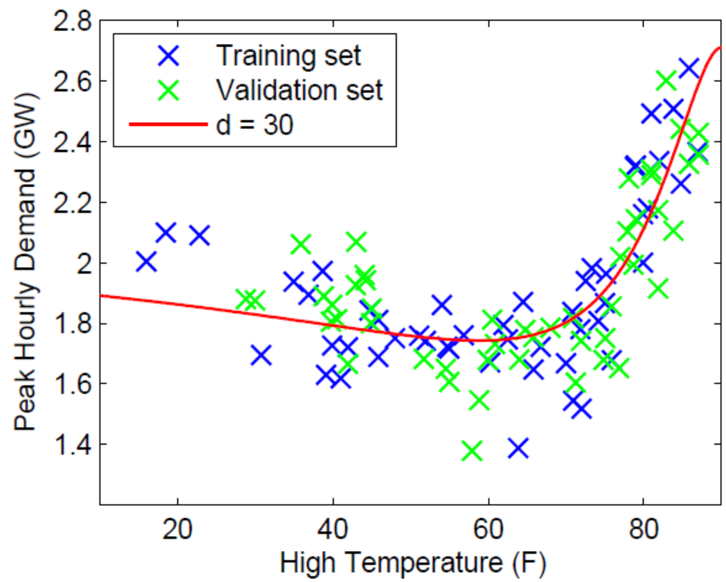
$\}$

$$\theta_j := \theta_j(1 - \alpha\frac{\lambda}{m}) - \alpha\frac{1}{m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})x_j^{(i)}$$

正则化线性回归



Degree 30 polynomial, with $\lambda = 0$ (unregularized)



Degree 30 polynomial, with $\lambda = 1$

正则化线性回归

- 如何选择正则化参数λ？

Model: $h_\theta(x) = \theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3 + \theta_4 x^4$

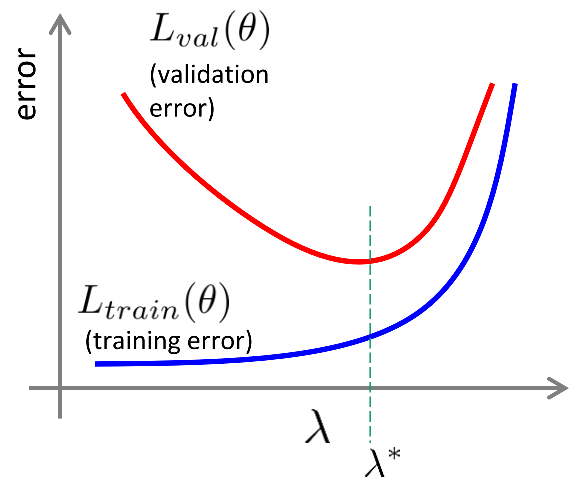
$$J(\theta) = \frac{1}{2m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})^2 + \frac{\lambda}{2m}\sum_{j=1}^{m}\theta_j^2$$

$$L(\theta) = \frac{1}{2m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})^2$$

1. Try $\lambda = 0$
2. Try $\lambda = 0.01$
3. Try $\lambda = 0.02$
4. Try $\lambda = 0.04$
5. Try $\lambda = 0.08$

$\vdots$

12. Try $\lambda = 10$



正则化线性回归: Normal equation

$$\min_\theta J(\theta) \qquad J(\theta) = \frac{1}{2m}\left[\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})^2 + \lambda\sum_{j=1}^{n}\theta_j^2\right]$$

$$X = \begin{bmatrix} (x^{(1)})^T \\ \vdots \\ (x^{(m)})^T \end{bmatrix} \qquad y = \begin{bmatrix} y^{(1)} \\ \vdots \\ y^{(m)} \end{bmatrix}$$

$$\theta = (X^TX)^{-1}X^Ty \quad \Rightarrow \quad \theta = \boxed{\left(X^TX + \lambda\begin{bmatrix} 0 & & & & \\ & 1 & & & \\ & & 1 & & \\ & & & \ddots & \\ & & & & 1 \end{bmatrix}\right)}^{-1} X^Ty$$

正则化Logistic回归

$$J(\theta) = \left[-\frac{1}{m} \sum_{i=1}^{m} y^{(i)} \log \left(h_\theta(x^{(i)}) + (1 - y^{(i)}) \log 1 - h_\theta(x^{(i)}) \right) \right] + \frac{\lambda}{2m} \sum_{j=1}^{n} \theta_j^2$$

Gradient descent

Repeat $\{$

$$\theta_0 := \theta_0 - \alpha \frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) x_0^{(i)}$$

$$\theta_j := \theta_j - \alpha \quad \frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) x_j^{(i)}$$

$$(j = \cancel{0}, 1, 2, 3, \ldots, n)$$

$\}$

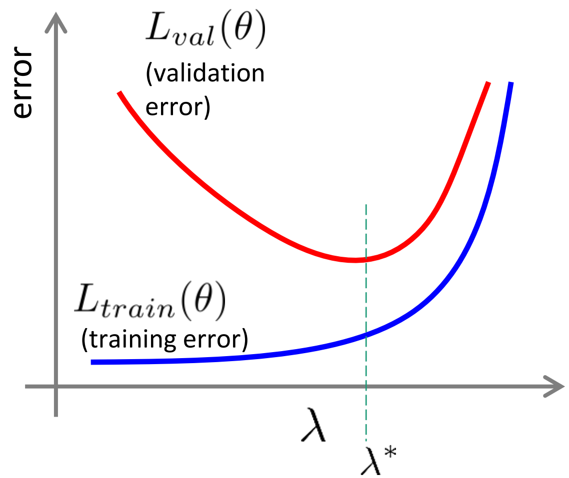
$$\theta_j := \theta_j (1 - \alpha \frac{\lambda}{m}) - \alpha \frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) x_j^{(i)}$$

正则化Logistic回归

$$J(\theta) = \left[-\frac{1}{m}\sum_{i=1}^{m} y^{(i)} \log\left(h_\theta(x^{(i)}) + (1-y^{(i)}) \log 1 - h_\theta(x^{(i)})\right)\right] + \frac{\lambda}{2m}\sum_{j=1}^{n}\theta_j^2$$

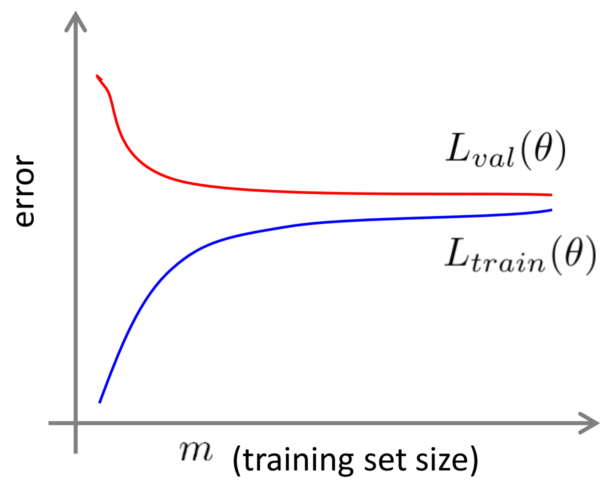
$$J(\theta) = L(\theta) + \lambda R(\theta)$$

$$L(\theta) = \left[-\frac{1}{m}\sum_{i=1}^{m} y^{(i)} \log\left(h_\theta(x^{(i)}) + (1-y^{(i)}) \log 1 - h_\theta(x^{(i)})\right)\right]$$

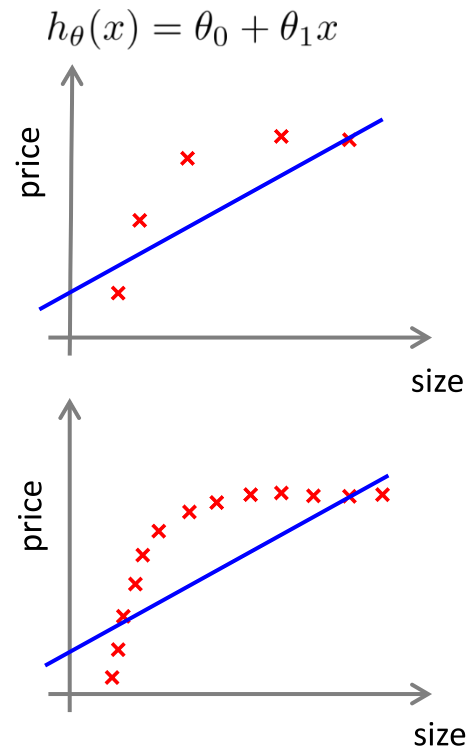


思考：是否可以选择其他的$L_{val}(\theta)$？

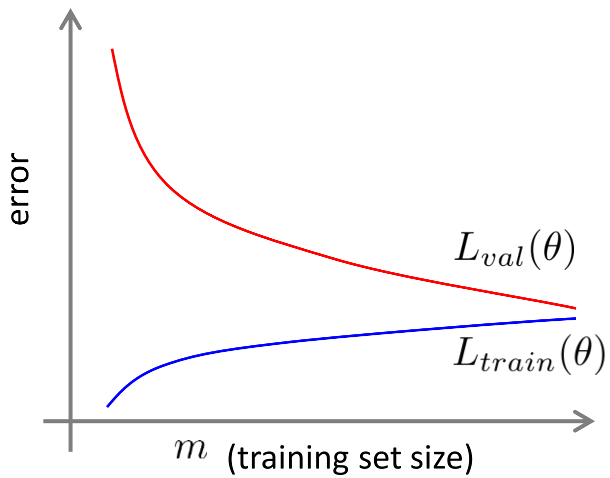
学习曲线

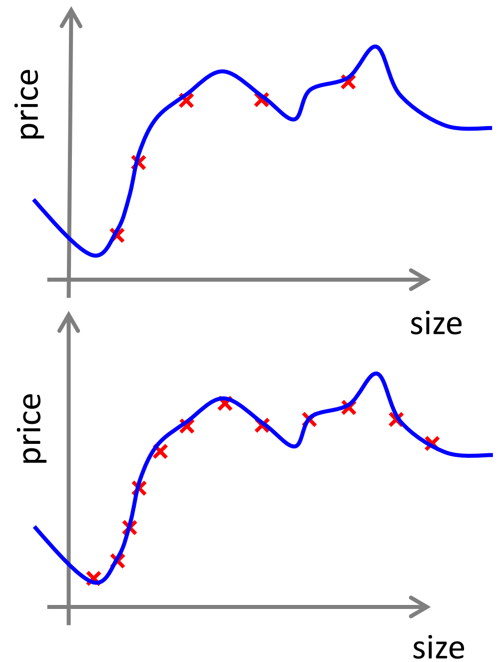


If a learning algorithm is suffering from high bias, getting more training data will not (by itself) help much.



学习曲线





If a learning algorithm is suffering from high variance, getting more training data is likely to help.

思考：

假设已经训练好了用于预测房价的正则化线性回归模型，但是，当在新的数据上进行测试时出现了很严重预测错误。下一步该怎么做呢?

- 获得更多的训练数据？
- 尝试较小的特征集？
- 尝试其他附加特征？
- 尝试加入多项式组合特征？
- 尝试减少正则化参数λ？
- 尝试增加正则化参数λ？

模型性能评估

- 我们用训练集优化参数

$$\theta^* = \arg\min_{\theta} \frac{1}{m} \sum_{i=1}^{m} \ell(h_\theta(x^{(i)}), y^{(i)})$$

- 用验证集选择模型

- 但我们真正关心的是模型在新的测试数据上的性能

模型性能评估

Dataset:

Size	Price
2104	400
1600	330
2400	369
1416	232
3000	540
1985	300
1534	315
1427	199
1380	212
1494	243

随机选取

$$(x^{(1)}, y^{(1)})$$
$$(x^{(2)}, y^{(2)})$$
$$\vdots$$
$$(x^{(m)}, y^{(m)})$$

Training Set

$$(x_{val}^{(1)}, y_{val}^{(1)})$$
$$(x_{val}^{(2)}, y_{val}^{(2)})$$
$$\vdots$$
$$(x_{val}^{(m_{val})}, y_{val}^{(m_{val})})$$

Validation Set (Development set)

$$(x_{test}^{(1)}, y_{test}^{(1)})$$
$$(x_{test}^{(2)}, y_{test}^{(2)})$$
$$\vdots$$
$$(x_{test}^{(m_{test})}, y_{test}^{(m_{test})})$$

Testing Set

模型性能评估

- 训练集：训练参数
- 验证集(开发集， Development set)：用于调参(如正则化参数、多项式阶数等)、特征选择以及other decisions regarding the learning algorithm
- 测试集: 仅仅用于性能评估，not to make any decisions about regarding what learning algorithm or parameters to use.

模型性能评估

- 验证集和测试集的选择：
  - Choose validation and test sets to reflect data you expect to get in the future and want to do well on.
  - 验证集和测试集应具有同分布

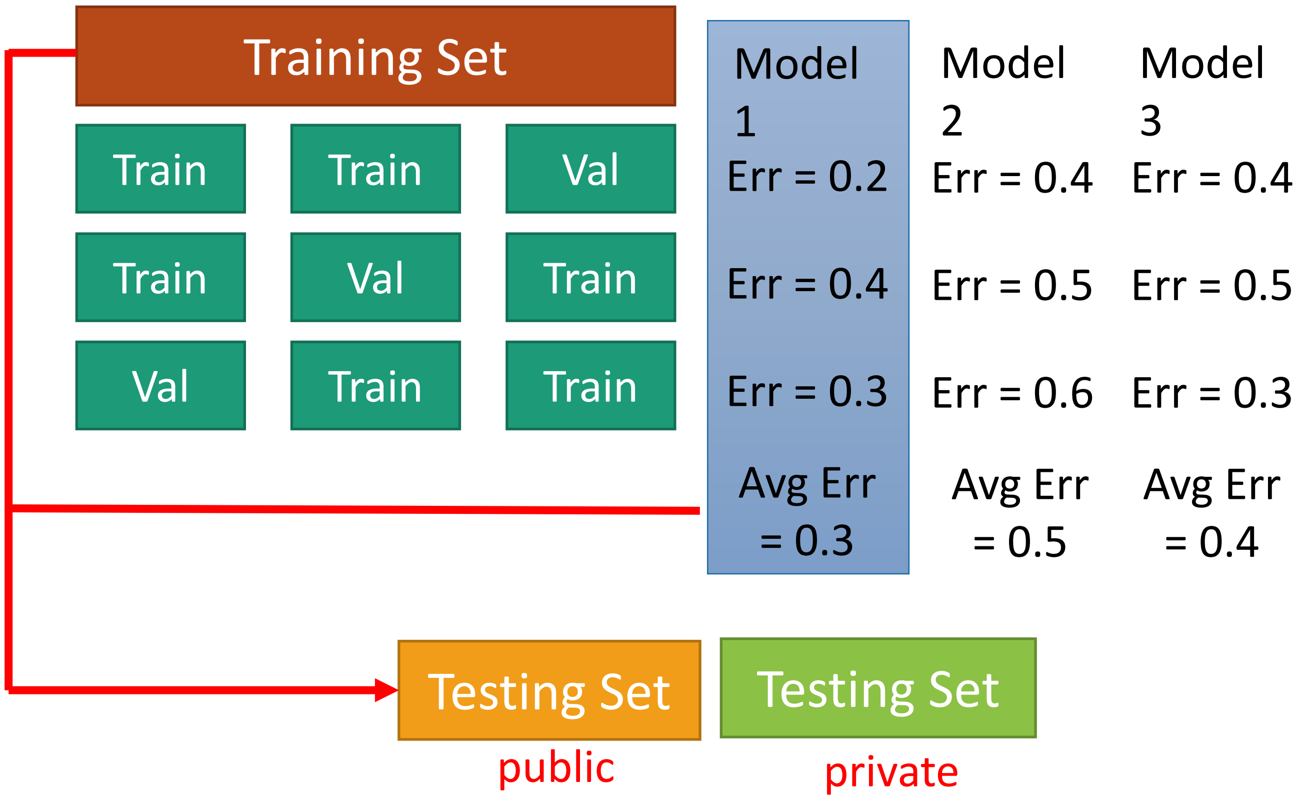
    思考：假设验证集和测试集具有同分布，若算法在验证集上效果较好但在测试集上性能很差，下一步该怎么办？

  - 验证集和测试集的大小
    - 验证集：1,000 to 10,000 examples are common；Should be large enough
    - 测试集：中小规模数据情况下一般取30%；大数据情况下，large enough
    - No need to have excessively large validation/test beyond what is needed to evaluate the performance of your algorithms

模型性能评估

- 交叉验证（*k*-fold Cross Validation）：
  - 数据集规模较小情况下采用
  - 把数据随机划分为k等份，每次用其中的$(k - 1)$份做训练，剩下的做验证
  - 计算平均误差（和方差）

k-fold Cross Validation



Thanks!

Any questions?