第6章 线性回归

根据已知训练数据学习/训练,选择合适的模型h(X),代价函数越小,h函数越逼近实际目标函数。

$$\min_{\beta} \quad J(\beta) = \frac{1}{2m} \sum_{i=1}^{m} (h_{\beta}(X_i) - Y_i)^2$$



找全局最优解

回归

- 指研究一组随机变量(Y1, Y2, …, Yi)和另一组(X1, X2, …, Xk)变量之间关系的统计分析方法。回归分析是一种数学模型。
- 是监督学习的一个重要问题,用于预测输入变量和输出变量之间的关系。
- 回归模型是表示输入变量到输出变量之间映射的函数。
- 回归问题等价于函数拟合:使用一条函数曲线使 其很好地拟合已知函数,且很好地预测未知数据。

回归应用

• 预测空气指数PM2.5

f (过去的PM2.5信息) = 明天的PM2.5值

• 股票预测

f (



) = 股票走势等

• 自动驾驶

f (



) = 方向盘角度、油门刹车幅度

• 推荐系统

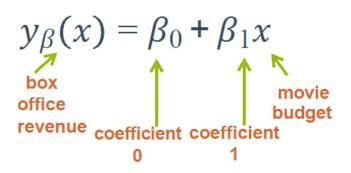
f (用户A 商品B) = 购买可能性值

- 线性回归(linear regression)是利用数理统计中的回归分析,来确定两个或两个以上变量间相互依赖的定量关系的一种统计分析方法,运用十分广泛。
- 机器学习中,线性回归假设特征和目标变量之间 满足线性关系,根据给定的训练数据建立一个线 性模型,并用此模型进行预测。



$$y_{\beta}(x) = \beta_0 + \beta_1 x$$



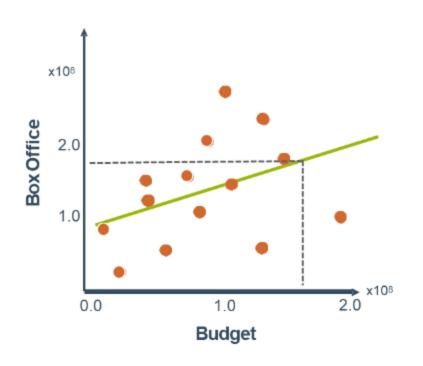




$$y_{\beta}(x) = \beta_0 + \beta_1 x$$

 β_0 = 80 million, β_1 = 0.6

使用线性回归预测

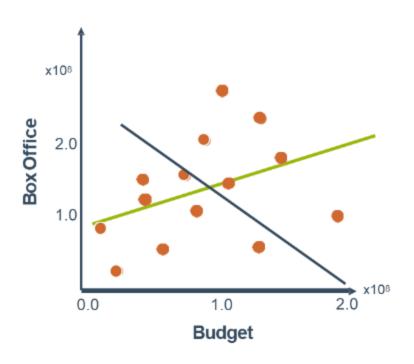


$$y_{\beta}(x) = \beta_0 + \beta_1 x$$

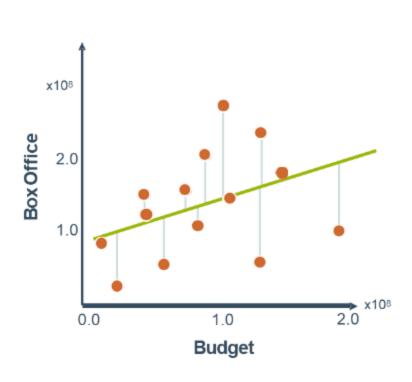
 β_0 = 80 million, β_1 = 0.6

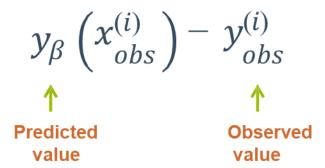
给定1.6亿的预算,预测票房收益为1.75亿

哪个模型拟合得更好?

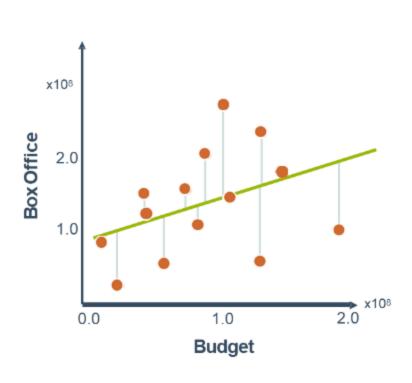


计算残差



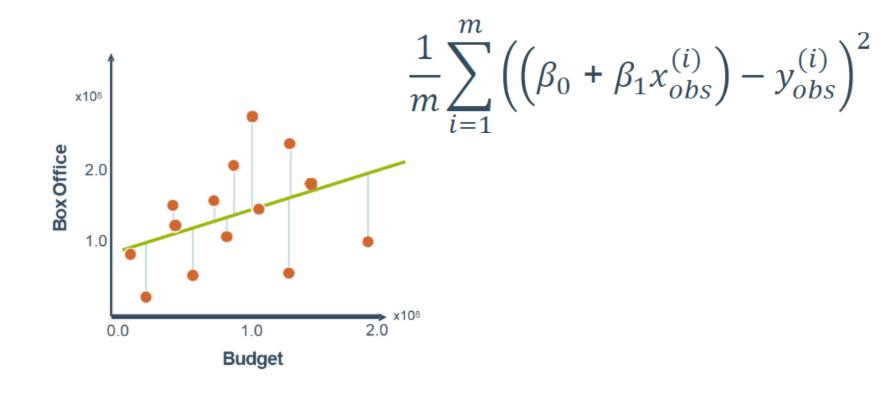


计算残差

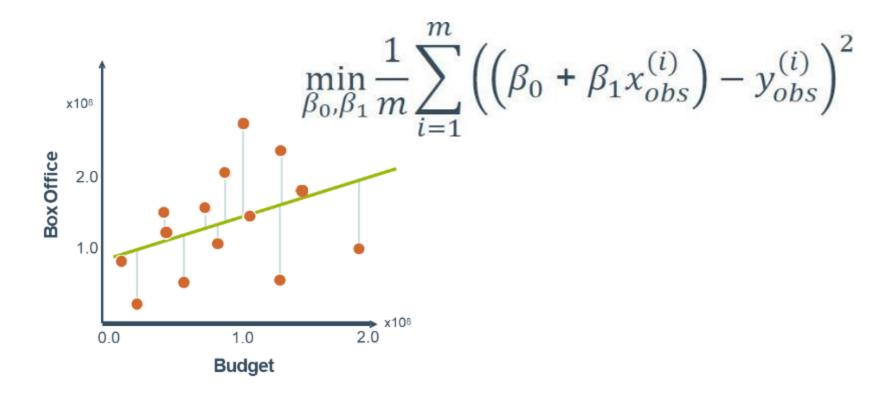


$$(\beta_0 + \beta_1 x_{obs}^{(i)}) - y_{obs}^{(i)}$$

均方误差(Mean Squared Error, MSE)



最小均方误差



其他评价指标

平均绝对误差(Mean Absolute Error, MAE):

$$\frac{1}{m} \sum_{i=1}^{m} \left| y_{\beta}(x^{(i)}) - y_{obs}^{(i)} \right|$$

均方根误差(Root Mean Squared Error, RMSE):

$$\sqrt{\frac{1}{m} \sum_{i=1}^{m} (y_{\beta}(x^{(i)}) - y_{obs}^{(i)})^2}$$

MAE is the easiest to understand, because it's the average error.

MSE is more popular than MAE, because MSE "punishes" larger errors.

RMSE is even more popular than MSE, because RMSE is interpretable in the "y" units.

其他评价指标

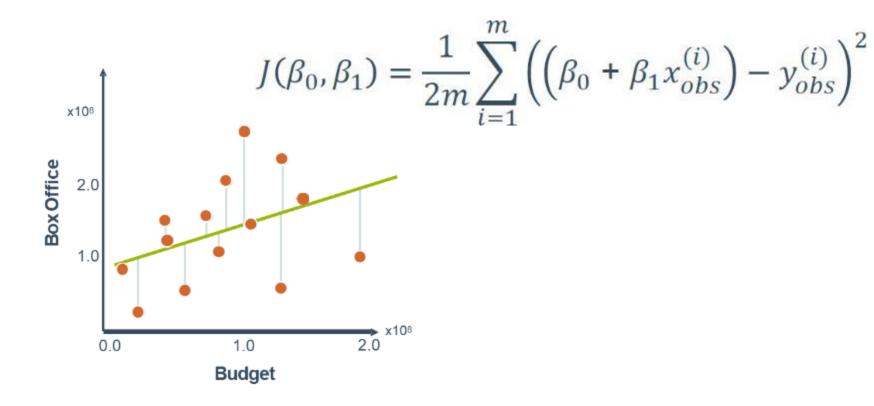
残差平方和(SSE):
$$\sum_{i=1}^m \left(y_\beta(x^{(i)}) - y_{obs}^{(i)} \right)^2$$

总离差平方和(TSS):
$$\sum_{i=1}^{m} \left(\overline{y_{obs}} - y_{obs}^{(i)} \right)^2$$

决定系数(R2):

$$1 - \frac{SSE}{TSS}$$

代价函数



最小二乘法

$$y_{\beta}(x) = \beta_0 + \beta_1 x$$

$$\widehat{\beta_1} = \frac{\sum_{i=1}^n (x_i - \overline{x})(y_i - \overline{y})}{\sum_{i=1}^n (x_i - \overline{x})^2}$$

$$\widehat{\beta_0} = \overline{y} - \widehat{\beta_1} \overline{x}$$

最小二乘法

	工资	额度
1	4000	20000
2	5000	30000
3	8000	50000
4	10000	70000
5	12000	60000
6	15000	?

- (1) 求贷款额度 y 关于月收入 x 的线性回归方程;
- (2)利用(1)中的回归方程,预测张三(月工资15000)的贷款额度。

最小二乘法

某地区2007年至2013年农村居民家庭人均纯收入 y (单位: 千元)的数据如下表:

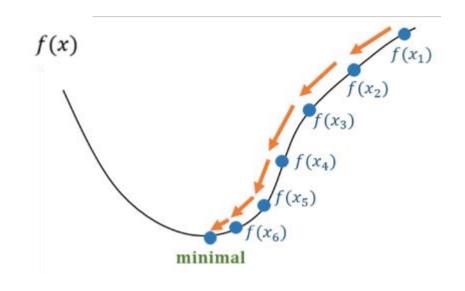
年份	2007	2008	2009	2010	2011	2012	2013
年份代 号 x	1	2	3	4	5	6	7
人均收 入 y	2.9	3.3	3.6	4.4	4.8	5.2	5.9

- (1) 求 y 关于 x 的线性回归方程;
- (2)利用(1)中的回归方程,预测该地区2015年农村居民家庭人均纯收入。

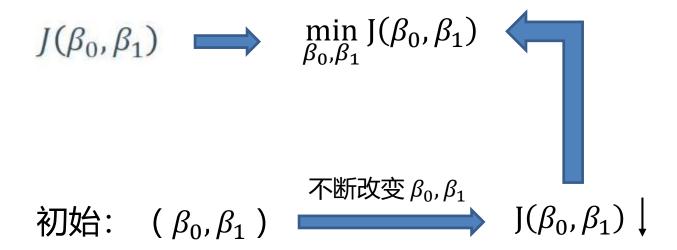
$$y_{\beta}(x) = \beta_0 + \beta_1 x$$

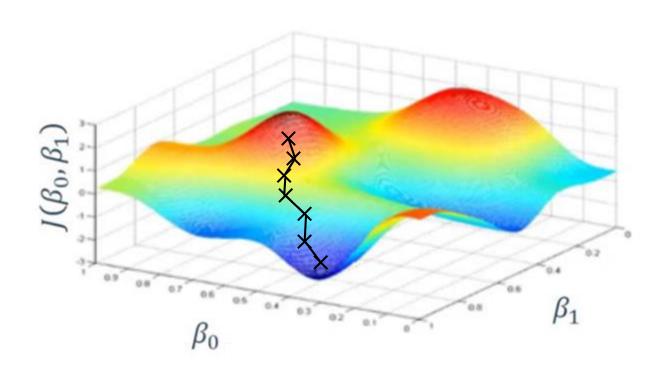
$$J(\beta_0, \beta_1) = \frac{1}{2m} \sum_{i=1}^{m} \left(\left(\beta_0 + \beta_1 x_{obs}^{(i)} \right) - y_{obs}^{(i)} \right)^2$$

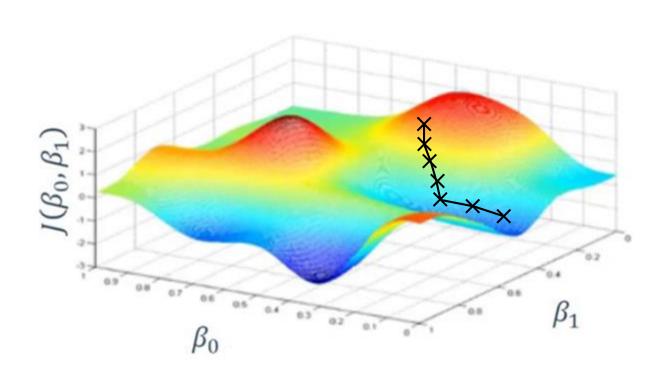
一种常用的一阶优化方法。该 算法从任一点开始,沿该点**梯 度**的反方向运动一段距离,再 沿新位置的梯度反方向运行一 段距离,如此迭代,解一直朝 下坡最陡的方向运动,希望能 运动到函数的全局最小点。



$$J(\beta_0, \beta_1) = \frac{1}{2m} \sum_{i=1}^{m} \left(\left(\beta_0 + \beta_1 x_{obs}^{(i)} \right) - y_{obs}^{(i)} \right)^2$$







数学定义:

$$\beta_i := \beta_i - \alpha \frac{\partial}{\partial \beta_i} J(\beta_0, \beta_1), i=0,1 \longrightarrow$$
 不断迭代直到收敛

正确过程: 同时更新

$$temp0 := \beta_0 - \alpha \frac{\partial}{\partial \beta_0} J(\beta_0, \beta_1)$$

temp1 :=
$$\beta_1 - \alpha \frac{\partial}{\partial \beta_1} J(\beta_0, \beta_1)$$

$$\beta_0 \coloneqq \text{temp0}$$

$$\beta_1 := \text{temp1}$$

偏导数项意义:

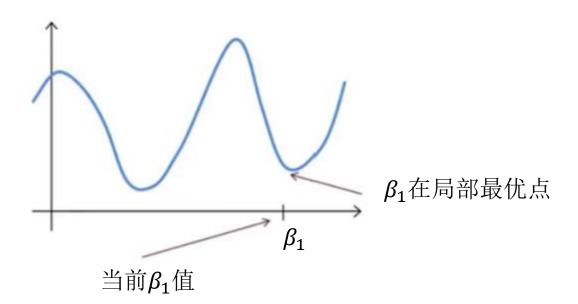
学习速率α:

$$\beta_i := \beta_i - \alpha \frac{\partial}{\partial \beta_i} J(\beta_0, \beta_1), \quad i=0,1$$

取值大小影响收敛速度

局部最低点:

$$\beta_1 := \beta_1 - \alpha \frac{\partial}{\partial \beta_1} J(\beta_1)$$



接近局部最优点时,梯度下降法会自动减小步长,所有没必要另外减小α。

线性回归模型:

$$h_{\beta}(x) = \beta_0 + \beta_1 x$$

$$J(\beta_0, \beta_1) = \frac{1}{2m} \sum_{i=1}^{m} \left(h_{\beta}(x^{(i)}) - y^{(i)} \right)^2$$

$$\beta_i := \beta_i - \alpha \frac{\partial}{\partial \beta_i} J(\beta_0, \beta_1), \quad i=0,1$$

$$\min_{\beta_0,\beta_1} J(\beta_0,\beta_1)$$

线性回归模型:

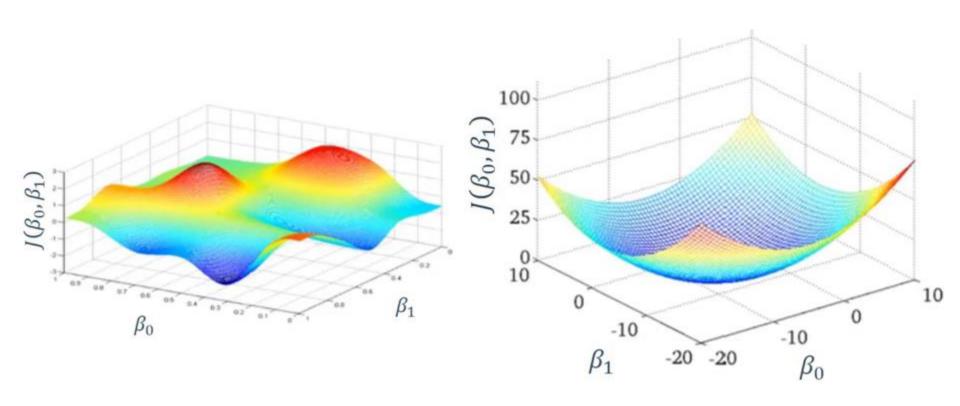
$$\frac{\partial}{\partial \beta_i} J(\beta_0, \beta_1) = ?$$

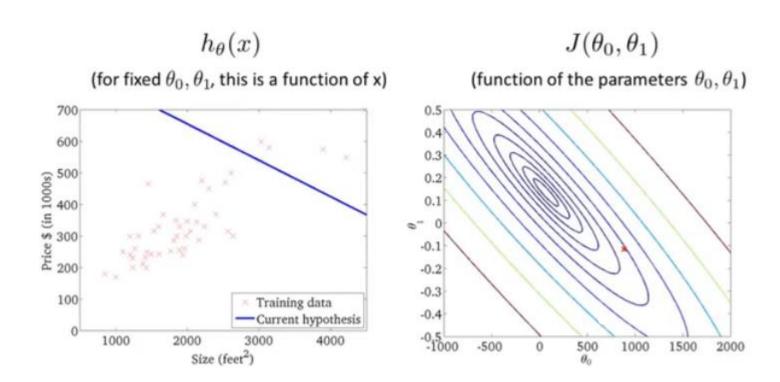
梯度下降算法:

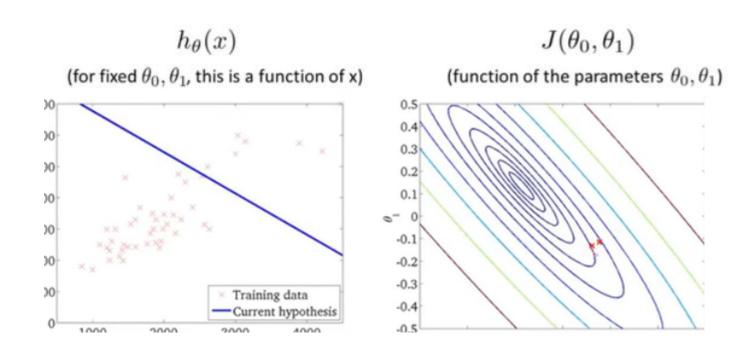
Repeat until convergence {

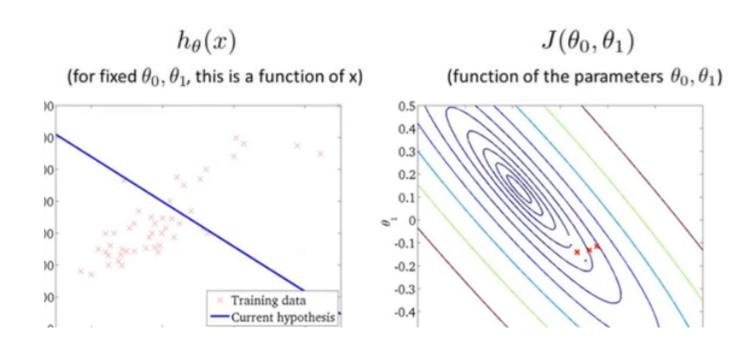
$$\beta_{0} := \beta_{0} - \alpha \frac{1}{m} \sum_{i=1}^{m} (h_{\beta}(x^{(i)}) - y^{(i)})$$

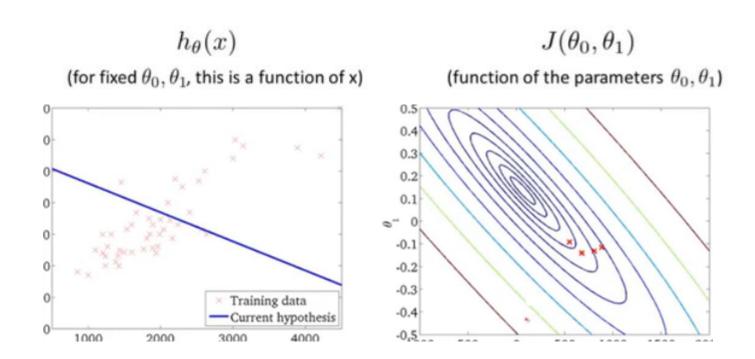
$$\beta_{1} := \beta_{1} - \alpha \frac{1}{m} \sum_{i=1}^{m} (h_{\beta}(x^{(i)}) - y^{(i)}) \cdot x^{(i)}$$
}

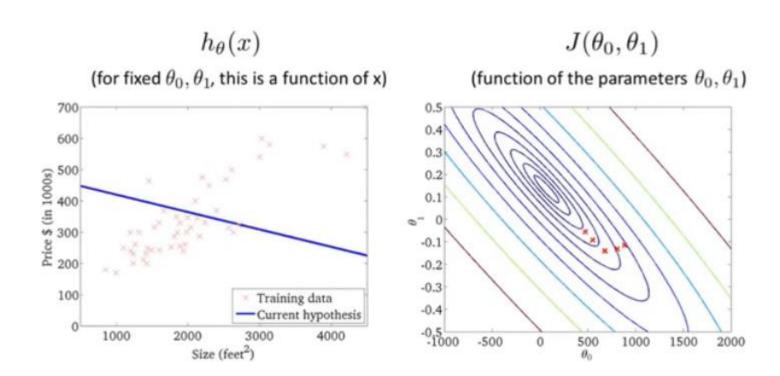


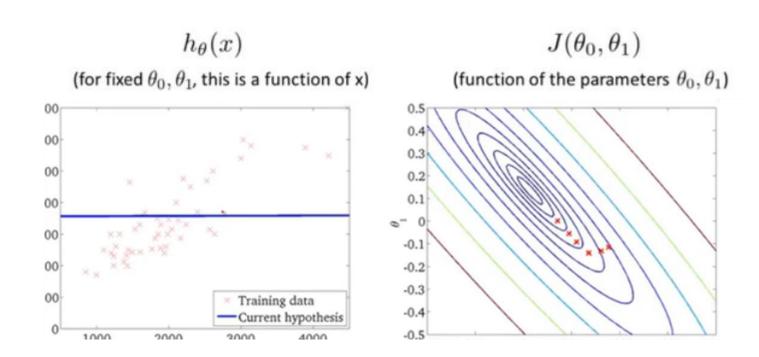


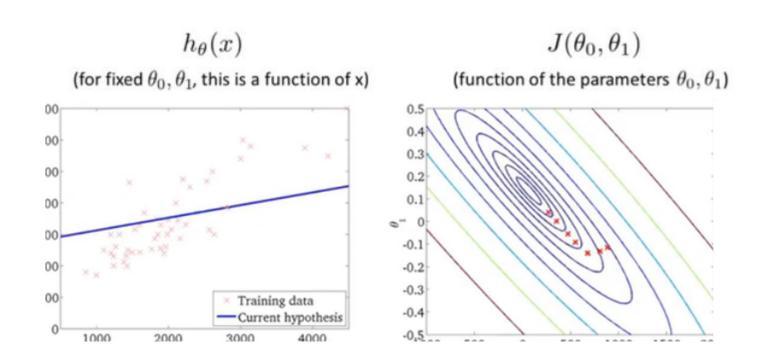


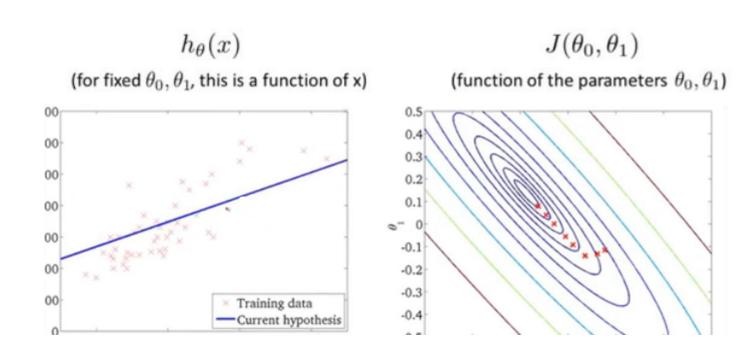


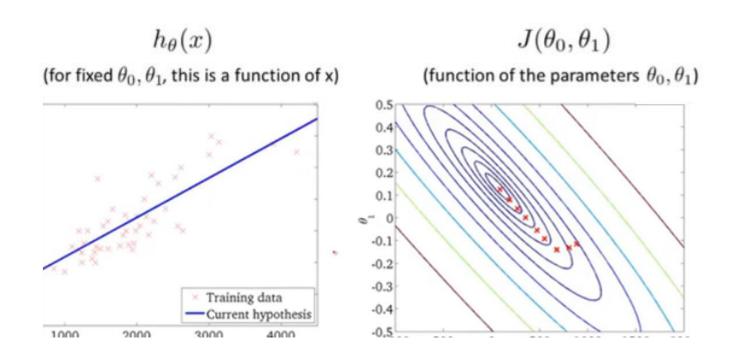












• 通过增加多项式特征来捕捉更高阶的数据特征

$$y_{\beta}(x) = \beta_0 + \beta_1 x + \beta_2 x^2$$



- 通过增加多项式特征来捕 捉更高阶的数据特征
- "线性回归"意味着特征间的线性组合

$$y_{\beta}(x) = \beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3$$



- 通过增加多项式特征来捕 捉更高阶的数据特征
- "线性回归"意味着特征间的线性组合

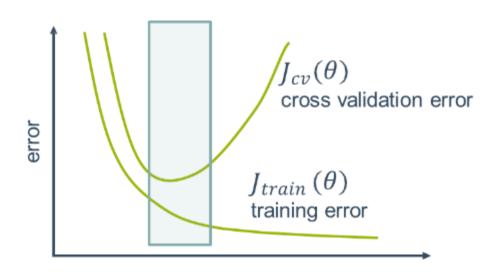
$$y_{\beta}(x) = \beta_0 + \beta_1 \log(x)$$



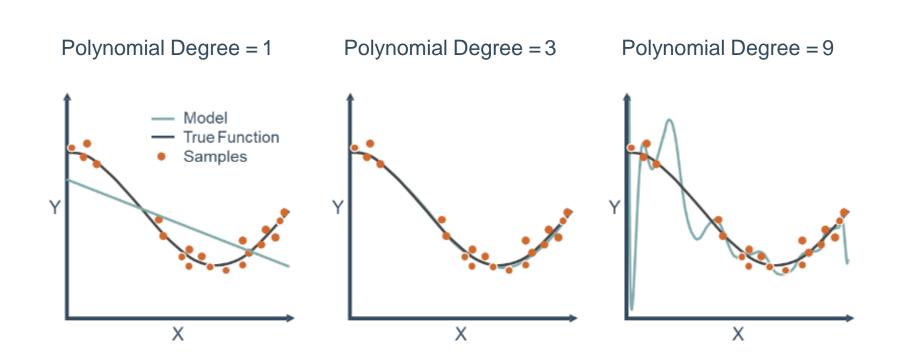
• 可以选择变量间的交互项: $y_{\beta}(x) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_1 x_2$

• 如何选择正确的函数形式: 检查每个变量与结果之间的关系

模型复杂度与误差

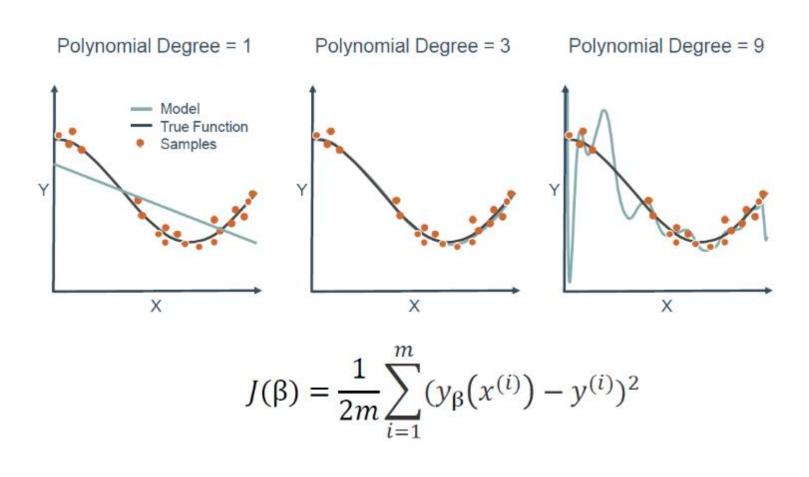


防止欠拟合与过拟合

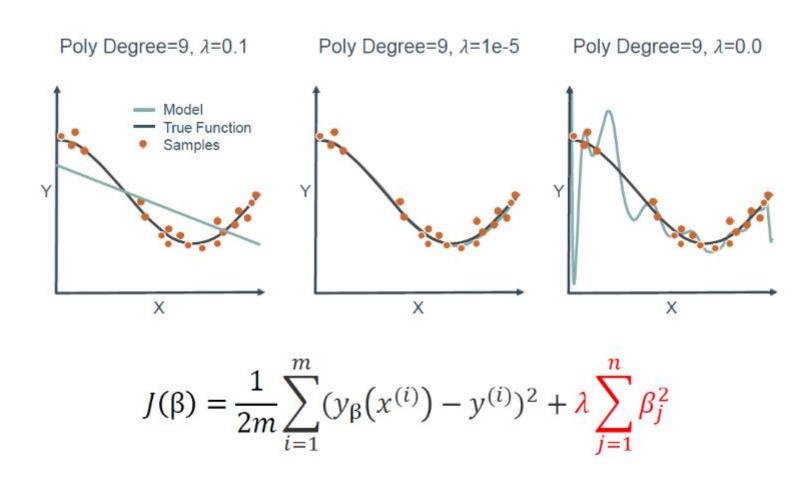


如何用一个9次多项式拟合数据,并防止过拟合?

防止欠拟合与过拟合



正则化(regularization)

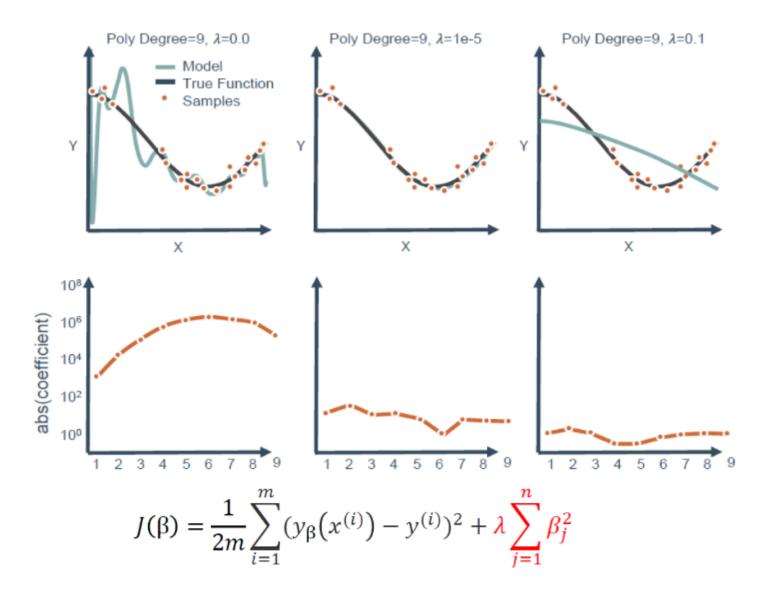


岭回归(Ridge Regression)(L2)

$$J(\beta) = \frac{1}{2m} \sum_{i=1}^{m} (y_{\beta}(x^{(i)}) - y^{(i)})^{2} + \lambda \sum_{j=1}^{n} \beta_{j}^{2}$$

- 惩罚项收缩了所有系数的大小
- 越大的系数被惩罚得越多,因为惩罚的是平方

岭回归对模型参数的效果

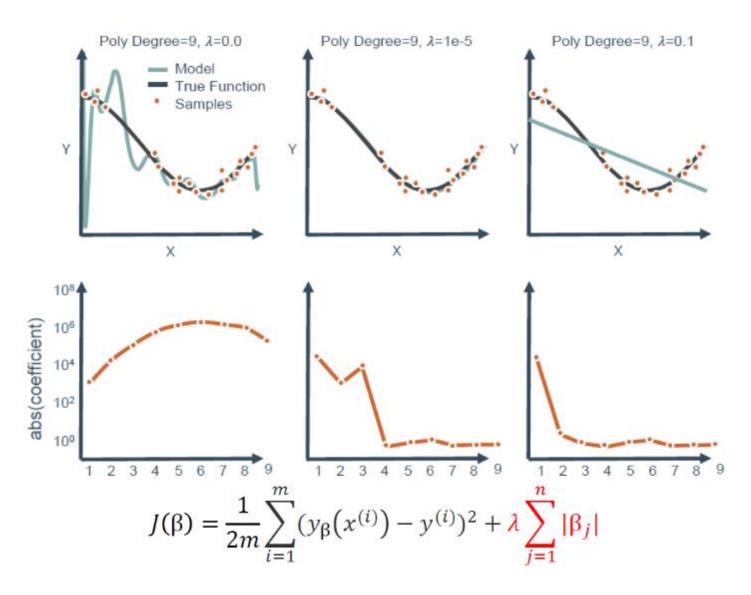


套索回归(Lasso Regression)(L1)

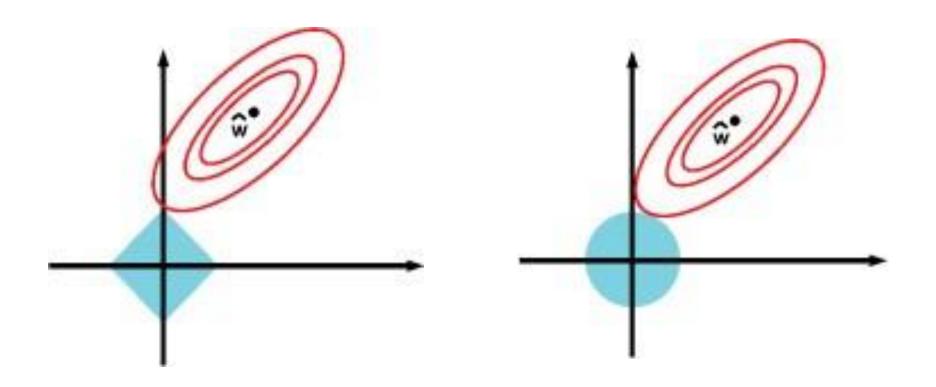
$$J(\beta) = \frac{1}{2m} \sum_{i=1}^{m} (y_{\beta}(x^{(i)}) - y^{(i)})^{2} + \lambda \sum_{j=1}^{n} |\beta_{j}|$$

- 惩罚项有选择地收缩了某些系数
- 可以被用来做特征选择
- 比岭回归收敛速度慢

套索回归对模型参数的效果



L1与L2正则化



ElasticNet正则化

$$J(\beta) = \frac{1}{2m} \sum_{i=1}^{m} (y_{\beta}(x^{(i)}) - y^{(i)})^{2} + \lambda_{1} \sum_{j=1}^{n} |\beta_{j}| + \lambda_{2} \sum_{j=1}^{n} \beta_{j}^{2}$$

- 岭回归和套索回归的综合,用以平衡稀疏和平滑两个问题
- 需要调节额外的参数,来分配L1和L2正则化惩罚 项的比例

超参数及其优化

• 正则化系数(λ_1 和 λ_2)是 根据经验决定的

使用测试数据调节 λ?

	Date	Title	Budget	DomesticTotalGross	Director		Rating	Runtime
a	2013-11-22	The Hurger Games: Calohing Fire	190000000	424909047	Francis Lawrence		PG-13	149
1	2013-05-03	Iron Mar 3	200000000	409013394	Share Black		PG-13	122
2	2013-11-22	Frozen	150000000	400738009	Chris Bucklennifer Lee		PG	103
а	2013-07-03	Despicable We 2	76000000	368061265	Plane CoffinChris Renaud		PG :	98
4	2013-08-16	Man of Steel	225000000	291045518	Zack Snyder		PG-13	143
6	2013-10-04	Brisity	11 /-1	NVI. LIT		Cuaron	PG-13	91
6	2010-06-21	Monaders University	II 2 4	数据		unkan	G	107
7	2013-12-13	The Hobbit The Desc	11-73	\ <i>></i> \\\		cisson	PG-13	181
a	2010-05-04	Fast & Purious 6				n i	PG-13	130
9	2013-03-08	Oz The Great and Powerful	215000000	234911825	Sam Raimi		PG	127
10	2013-05-16	Star Their Into Dareness	190000000	228778881	J.J. Abrims		PG-13	123
11	2013-11-06	That: The Dark World	170000000	200302140	Alan Taylor		PG-13	120
12	2013-05-21	Works War Z	190000000	202399711	Marc Forster		PG-13	118
10	2013-03-22	The Groods	122200000	100100400	Part Par	MiccoChris Sanders	PG	98
14	2013 65 28	The Heat	1d 2 _1	数据		9:	R	117
15	2013-08-07	WWhathe Millers	沙区	文义 17占		Marshall Treatur	n .	110
16	2013-12-13	American Hustle				Russell	R	133
17	2013-05-10	The Great Calaby	1105000000	144846470	Berto	ernanei	PG-13	141

超参数及其优化

• 正则化系数(λ_1 和 λ_2)是 根据经验决定的

测试数据集来调节1 和12

使用测试数据集调节 λ?



超参数及其优化

- 正则化系数($λ_1$ 和 $λ_2$)是
 根据经验决定的
- 想让模型泛化---不要使用 测试数据集来调节 λ_1 和 λ_2
- 划分出另一个数据集来调节超参数---验证集 (validation set)

用交叉验证来调节λ



——李宏毅2020机器学习深度学习



Step 1: Model

$$y = b + w \cdot x_{cp}$$

A set of function



$$f_1, f_2 \cdots$$

f(



w and b are parameters (can be any value)

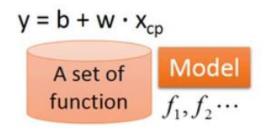
$$f_1$$
: y = 10.0 + 9.0 · x_{cp}

$$f_2$$
: y = 9.8 + 9.2 · x_{cp}

$$f_3$$
: y = -0.8 - 1.2 · x_{cp}

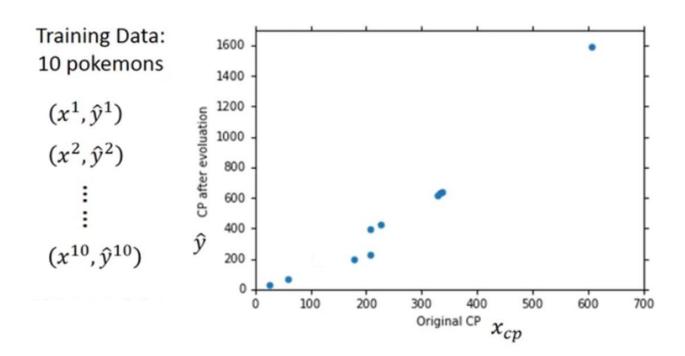
••••

Linear model: $y = b + \sum w_i x_i$

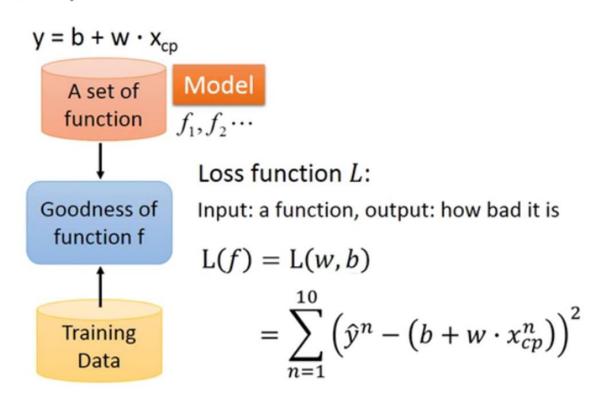


Training Data

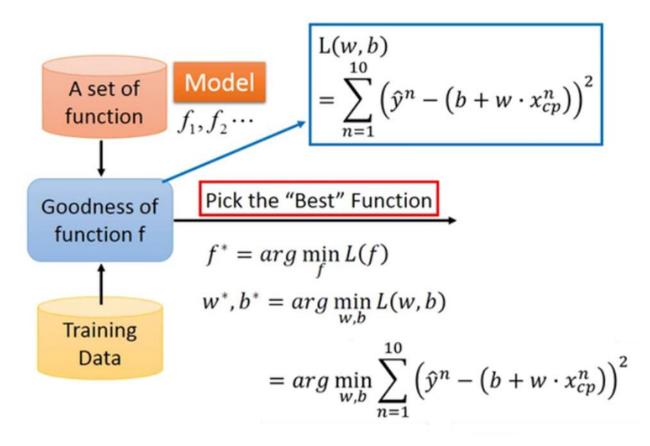


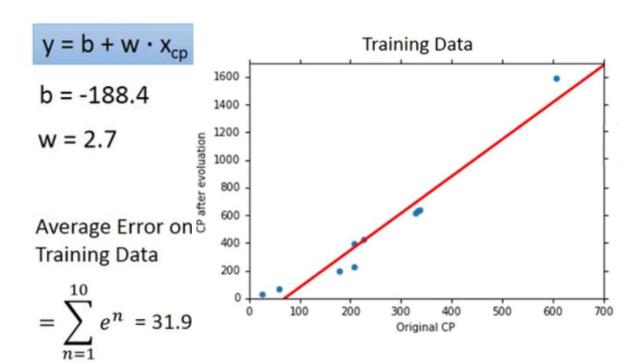


Step 2: Goodness of Function



Step 3: Best Function

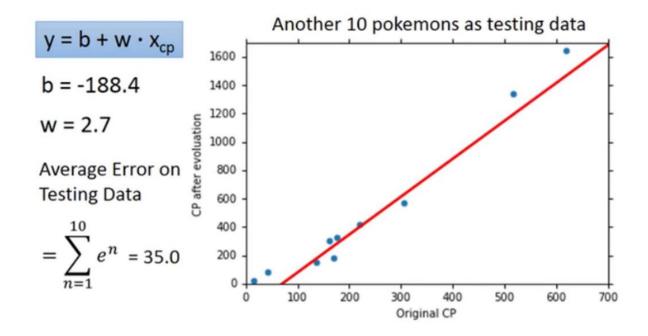




How's the results?

- Generalization

What we really care about is the error on new data (testing data)



Selecting another Model

$$y = b + w_1 \cdot x_{cp} + w_2 \cdot (x_{cp})^2$$

Best Function

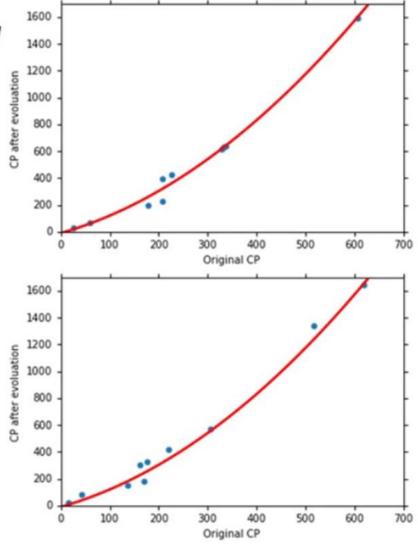
b = -10.3

 $W_1 = 1.0, W_2 = 2.7 \times 10^{-3}$

Average Error = 15.4

Testing:

Average Error = 18.4



Selecting another Model

$$y = b + w_1 \cdot x_{cp} + w_2 \cdot (x_{cp})^2 + w_3 \cdot (x_{cp})^3$$

Best Function

$$b = 6.4, w_1 = 0.66$$

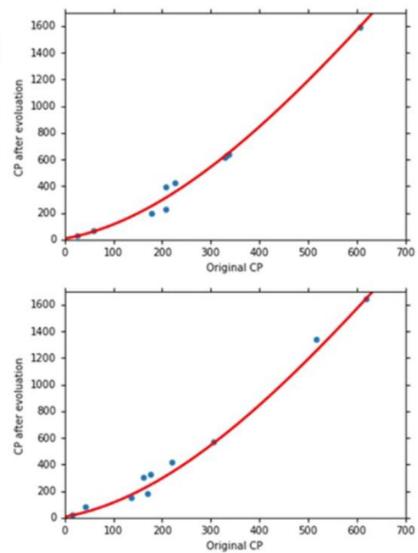
$$W_2 = 4.3 \times 10^{-3}$$

$$W_3 = -1.8 \times 10^{-6}$$

Average Error = 15.3

Testing:

Average Error = 18.1



Selecting another Model

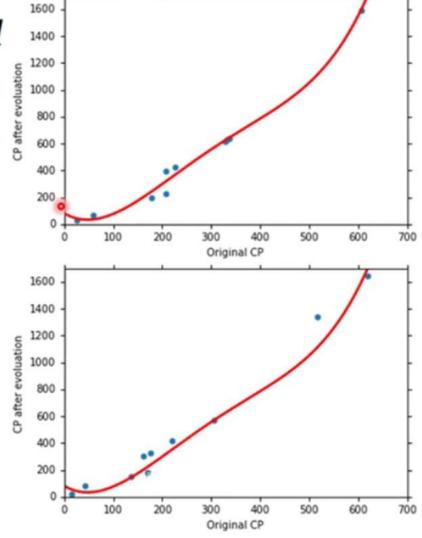
$$y = b + w_1 \cdot x_{cp} + w_2 \cdot (x_{cp})^2 + w_3 \cdot (x_{cp})^3 + w_4 \cdot (x_{cp})^4$$

Best Function

Average Error = 14.9

Testing:

Average Error = 28.8



Selecting another Model

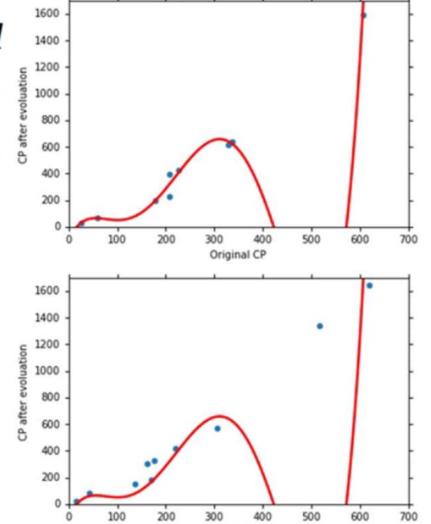
$$y = b + w_1 \cdot x_{cp} + w_2 \cdot (x_{cp})^2 + w_3 \cdot (x_{cp})^3 + w_4 \cdot (x_{cp})^4 + w_5 \cdot (x_{cp})^5$$

Best Function

Average Error = 12.8

Testing:

Average Error = 232.1



Original CP

Model Selection

1.
$$y = b + w \cdot x_{cp}$$

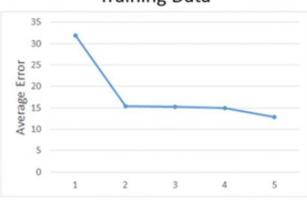
2.
$$y = b + w_1 \cdot x_{cp} + w_2 \cdot (x_{cp})^2$$

3.
$$y = b + w_1 \cdot x_{cp} + w_2 \cdot (x_{cp})^2 + w_3 \cdot (x_{cp})^3$$

4.
$$y = b + w_1 \cdot x_{cp} + w_2 \cdot (x_{cp})^2 + w_3 \cdot (x_{cp})^3 + w_4 \cdot (x_{cp})^4$$

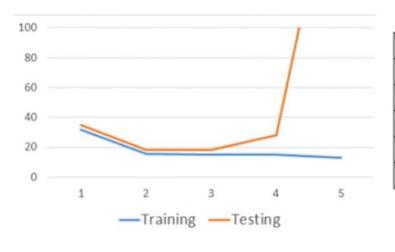
$$y = b + w_1 \cdot x_{cp} + w_2 \cdot (x_{cp})^2$$
5.
$$+ w_3 \cdot (x_{cp})^3 + w_4 \cdot (x_{cp})^4 + w_5 \cdot (x_{cp})^5$$

Training Data



A more complex model yields lower error on training data.

Model Selection



	Training	Testing
1	31.9	35.0
2	15.4	18.4
3	15.3	18.1
4	14.9	28.2
5	12.8	232.1

Model Selection



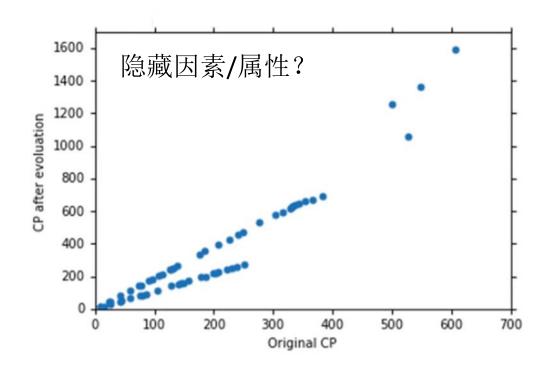
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Model Selection

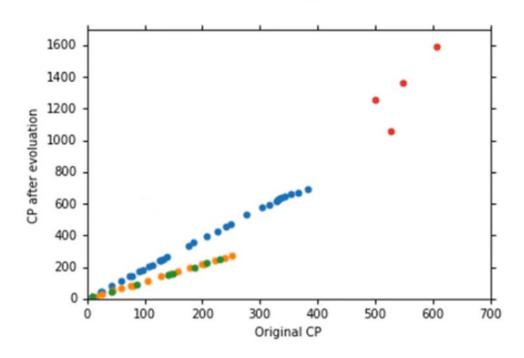


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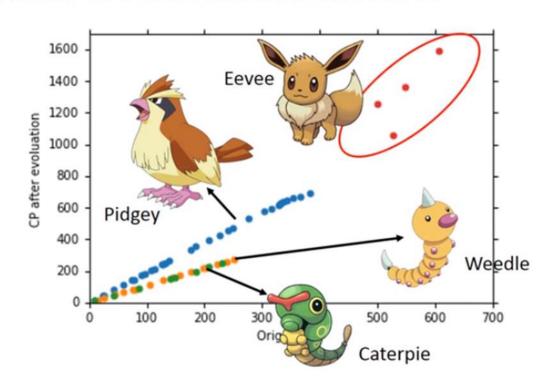
Let's collect more data (60只)



What are the hidden factors?



What are the hidden factors?



Back to step 1: Redesign the Model

 $x_s = \text{species of } x$



 $y = b_1 + w_1 \cdot x_{cp}$ If $x_s = Pidgey$:

 $y = b_2 + w_2 \cdot x_{cp}$ If x_s = Weedle:

 $y = b_3 + w_3 \cdot x_{cp}$ If x_s = Caterpie:

 $y = b_4 + w_4 \cdot x_{cp}$ If x_s = Eevee:



Back to step 1: Redesign the Model

$$y = b_1 \cdot \delta(x_s = \text{Pidgey})$$

 $+w_1 \cdot \delta(x_s = \text{Pidgey})x_{cp}$
 $+b_2 \cdot \delta(x_s = \text{Weedle})$
 $+w_2 \cdot \delta(x_s = \text{Weedle})x_{cp}$
 $+b_3 \cdot \delta(x_s = \text{Caterpie})$
 $+w_3 \cdot \delta(x_s = \text{Caterpie})x_{cp}$
 $+b_4 \cdot \delta(x_s = \text{Eevee})$
 $+w_4 \cdot \delta(x_s = \text{Eevee})x_{cp}$

$$y = b + \sum w_i x_i$$

Linear model?

$$\delta(x_s = \text{Pidgey})$$

$$\begin{cases} = 1 & \text{If } x_s = \text{Pidgey} \\ = 0 & \text{otherwise} \end{cases}$$
If $x_s = \text{Pidgey}$

Back to step 1: Redesign the Model

$$y = b_1 \cdot \boxed{1}$$

$$+w_1 \cdot \boxed{1}$$

$$+b_2 \cdot 0$$

$$+w_2 \cdot 0$$

$$+b_3 \cdot 0$$

$$+w_3 \cdot 0$$

$$+b_4 \cdot 0$$

$$+w_4 \cdot 0$$

$$y = b + \sum w_i x_i$$

Linear model?

$$\delta(x_s = Pidgey)$$

$$\begin{cases} =1 & \text{If } x_s = \text{Pidgey} \\ =0 & \text{otherwise} \end{cases}$$

If
$$x_s = \text{Pidgey}$$

$$y = b_1 + w_1 \cdot x_{cp}$$

Back to step 1: Redesign the Model

$$y = b_1 \cdot \delta(x_s = \text{Pidgey})$$

 $+w_1 \cdot \delta(x_s = \text{Pidgey})x_{cp}$
 $+b_2 \cdot \delta(x_s = \text{Weedle})$
 $+w_2 \cdot \delta(x_s = \text{Weedle})x_{cp}$
 $+b_3 \cdot \delta(x_s = \text{Caterpie})$
 $+w_3 \cdot \delta(x_s = \text{Caterpie})x_{cp}$
 $+b_4 \cdot \delta(x_s = \text{Eevee})$
 $+w_4 \cdot \delta(x_s = \text{Eevee})x_{cp}$

$$y = b + \sum w_i x_i$$

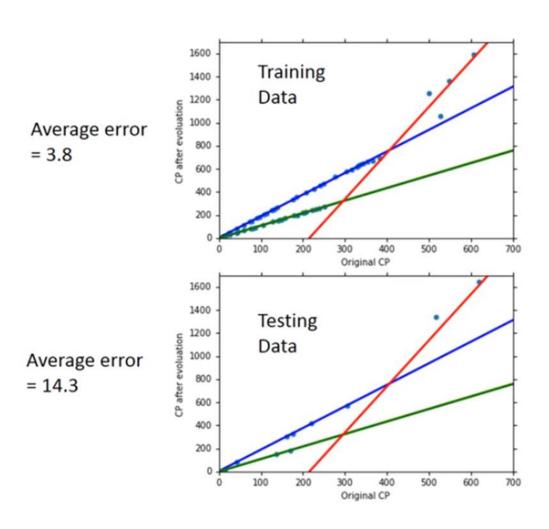
Linear model?

$$\delta(x_S = \text{Pidgey})$$

$$\begin{cases} =1 & \text{If } x_S = \text{Pidgey} \\ =0 & \text{otherwise} \end{cases}$$

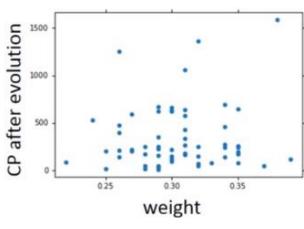
If
$$x_s = Pidgey$$

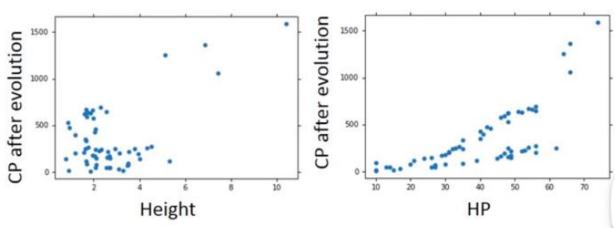
$$y = b_1 + w_1 \cdot x_{cp}$$



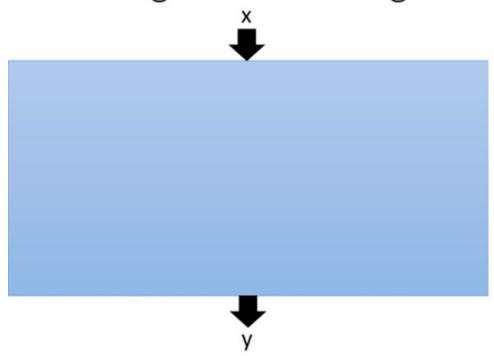


Are there any other hidden factors?





Back to step 1: Redesign the Model Again



Back to step 1: Redesign the Model Again



If
$$x_s = \text{Pidgey}$$
: $y' = b_1 + w_1 \cdot x_{cp} + w_5 \cdot (x_{cp})^2$

If
$$x_s = \text{Weedle}$$
: $y' = b_2 + w_2 \cdot x_{cp} + w_6 \cdot (x_{cp})^2$ Training Error

If
$$x_s = \text{Caterpie}$$
: $y' = b_3 + w_4 \cdot x_{cp} + w_7 \cdot (x_{cp})^2 = 1.9$

If
$$x_s = \text{Eevee}$$
: $y' = b_4 + w_4 \cdot x_{cp} + w_8 \cdot (x_{cp})^2$

$$y = y' + w_9 \cdot x_{hp} + w_{10} \cdot (x_{hp})^2$$

$$+w_{11} \cdot x_h + w_{12} \cdot (x_h)^2 + w_{13} \cdot x_w + w_{14} \cdot (x_w)^2$$

Testing Error = 102.3

Overfitting!



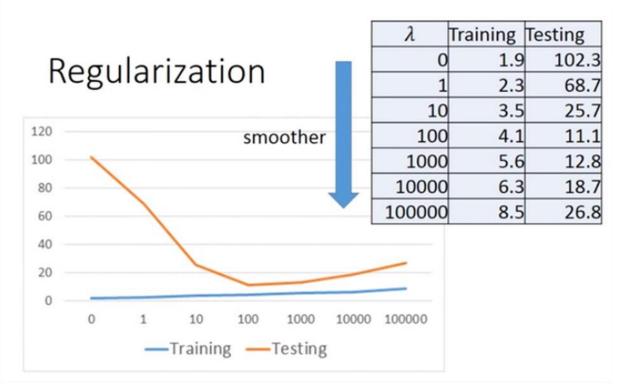
Back to step 2: Regularization

$$y = b + \sum w_i x_i$$
 The functions with smaller w_i are better
$$L = \sum_n \left(\hat{y}^n - \left(b + \sum w_i x_i \right) \right)^2 + \lambda \sum_i (w_i)^2$$

Why smooth functions are preferred?
$$y = b + \sum w_i x_i + w_i \Delta x_i + \Delta x_i$$

If some noises corrupt input x, when testing

A smoother function has less influence.



- \triangleright Training error: larger λ , considering the training error less
- ➤ We prefer smooth function, but don't be too smooth.