迴歸問題

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迴歸問題有哪些？

- 利用月收入來核定信用卡額度
- 利用坪數、房間數來預測房價
- 利用每日最高氣溫來預測飲料店的冰紅茶銷量
- ...etc.

大家都在尋找 $\boldsymbol{f}$

$$y = f(x)$$

- 但沒有人知道 $\boldsymbol{f}$ 到底為何、是否存在？我們只能假設：

$$\hat{y} = h(x)$$

當 $\hat{y}$ 與 y 之間的差異愈小，我們更有自信地說 h 跟 f 愈相似

- 成本函數

$$\text{minimize:}\frac{1}{2m}\sum_{i=1}^{m}(\hat{y}_i - y_i)^2$$

將 $\boldsymbol{h}$ 表示得更完整：只有一個觀測值的時候

$$h(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \ldots + \theta_n x_n$$

- 假如我們令 $x_0 = 1$，就可以將式子廣義地表示為：

$$\hat{y} = h(x) = \begin{bmatrix} \theta_0 & \theta_1 & \ldots & \theta_n \end{bmatrix} \begin{bmatrix} x_0 \\ x_1 \\ . \\ . \\ . \\ x_n \end{bmatrix} = \theta^T x$$

將 $\boldsymbol{h}$ 表示得更完整：有 **m+1** 個觀測值的時候

$$\hat{y} = h(X) = \begin{bmatrix} x_{00}, x_{01}, \ldots, x_{0n} \\ x_{10}, x_{11}, \ldots, x_{1n} \\ . \\ . \\ . \\ x_{m0}, x_{m1}, \ldots, x_{mn} \end{bmatrix} \begin{bmatrix} \theta_0 \\ \theta_1 \\ . \\ . \\ . \\ \theta_n \end{bmatrix} = X\theta$$

迴歸問題與房屋價格資料

House Prices: Advanced Regression Techniques

https://www.kaggle.com/c/house-prices-advanced-regression-techniques

In [1]:

```
import pandas as pd

train_url = "https://storage.googleapis.com/kaggle_datasets/House-Prices-Advanced-Regression-Techni
ques/train.csv"
test_url = "https://storage.googleapis.com/kaggle_datasets/House-Prices-Advanced-Regression-Techniq
ues/test.csv"
labeled = pd.read_csv(train_url)
test = pd.read_csv(test_url)
print(labeled.shape)
print(test.shape)
```

```
(1460, 81)
(1459, 80)
```

In [2]:
```
labeled.head()
```

Out[2]:

	Id	MSSubClass	MSZoning	LotFrontage	LotArea	Street	Alley	LotShap
0	1	60	RL	65.0	8450	Pave	NaN	Reg
1	2	20	RL	80.0	9600	Pave	NaN	Reg
2	3	60	RL	68.0	11250	Pave	NaN	IR1
3	4	70	RL	60.0	9550	Pave	NaN	IR1
4	5	60	RL	84.0	14260	Pave	NaN	IR1

5 rows × 81 columns

In [3]:

```
test.head()
```

Out[3]:

	Id	MSSubClass	MSZoning	LotFrontage	LotArea	Street	Alley	LotS
0	1461	20	RH	80.0	11622	Pave	NaN	Reg
1	1462	20	RL	81.0	14267	Pave	NaN	IR1
2	1463	60	RL	74.0	13830	Pave	NaN	IR1
3	1464	60	RL	78.0	9978	Pave	NaN	IR1
4	1465	120	RL	43.0	5005	Pave	NaN	IR1

5 rows × 80 columns

什麼是標籤資料（labeled data）？

- 機器學習中的 E(Experience) 要素
- 可進一步再切割為訓練與驗證樣本

什麼是訓練（train）樣本？

- 由標籤資料切割出來
  - 通常分出 70% 作為訓練樣本
- 訓練樣本用來建立 $h(x)$

什麼是驗證（validation）樣本？

- 由標籤資料切割出來
  - 通常分出 30% 作為驗證樣本
- 驗證樣本投入 $h(x)$ 產出預測值 $\hat{y}$
- 比對驗證樣本的 y 與 $\hat{y}$ 來評估 $h(x)$ 的績效（performance）

什麼是測試（test）樣本？

- 測試樣本是沒有標籤的資料
- 將測試樣本投入 $\boldsymbol{h(x)}$ 能夠建立預測值 $\hat{\boldsymbol{y}}$
- 利用 $\hat{\boldsymbol{y}}$ 做出預測並應用在正式環境中
- 僅能以實驗在事後量測績效

如何切割訓練與驗證樣本？

- 隨機排序標籤資料的觀測值（Random shuffle）
- 再利用索引值分割（Subset）

隨堂練習：自己來切割訓練、驗證樣本

```python
def my_train_test_split(train, test_size=0.3, random_state=123)
    # ...
```

往後請 sklearn 來切割

In [4]:
```
# 切割訓練與驗證樣本
from sklearn.model_selection import train_test_split

train_df, validation_df = train_test_split(labeled, test_size=0.3, random_state=123)
print(labeled.shape)
print(train_df.shape)
print(validation_df.shape)
```

```
(1460, 81)
(1022, 81)
(438, 81)
```

將訓練與驗證樣本描繪出來

- 挑一個變數來預測 SalePrice
- 利用 Correlation Matrix 來找一個變數

In [5]:
```python
labeled.corr()["SalePrice"].abs().sort_values(ascending=False)[:10]
```

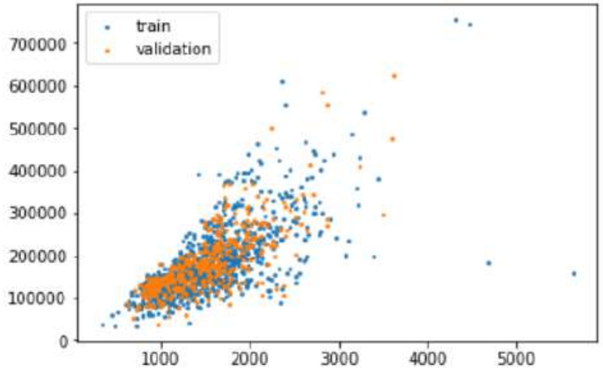
Out[5]:
```
SalePrice       1.000000
OverallQual     0.790982
GrLivArea       0.708624
GarageCars      0.640409
GarageArea      0.623431
TotalBsmtSF     0.613581
1stFlrSF        0.605852
FullBath        0.560664
TotRmsAbvGrd    0.533723
YearBuilt       0.522897
Name: SalePrice, dtype: float64
```

In [6]:
```
import matplotlib.pyplot as plt

plt.scatter(train_df["GrLivArea"], train_df["SalePrice"], label='train', s=3)
plt.scatter(validation_df["GrLivArea"], validation_df["SalePrice"], label='validation', s=3)
plt.legend()
```

Out[6]: <matplotlib.legend.Legend at 0x1a1c8d07f0>

In [7]:

```
plt.show()
```

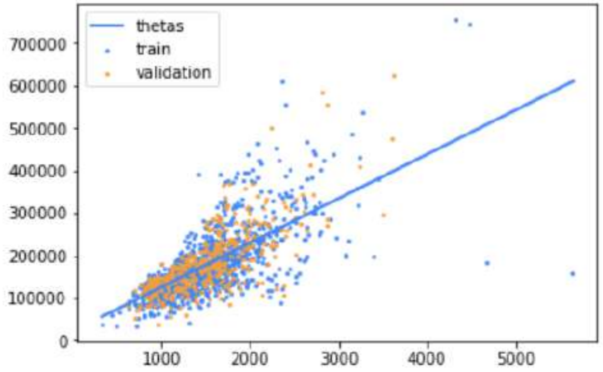


train
validation
700000
600000
500000
400000
300000
200000
100000
0
1000
2000
3000
4000
5000

任務

- 找到一組θ讓成本函數最小化

In [9]:
```
plt.show()
```



thetas
train
validation
700000
600000
500000
400000
300000
200000
100000
0
1000
2000
3000
4000
5000

完成任務的方法

- Normal Equation
- Gradient Descent

Normal Equation

In [10]:
```
train_df[["GrLivArea", "SalePrice"]].head()
```

Out[10]:

	GrLivArea	SalePrice
376	914	148000
250	1306	76500
228	912	125000
40	1324	160000
428	1208	195400

In [11]:

```
train_df[["GrLivArea", "SalePrice"]].tail()
```

Out[11]:

	GrLivArea	SalePrice
1041	1632	173000
1122	960	112000
1346	2156	262500
1406	768	133000
1389	1218	131000

線性聯立方程組

$$
\begin{aligned}
\theta_0 + 914\theta_1 &= 148000 \\
&\cdots \\
\theta_0 + 1218\theta_1 &= 131000
\end{aligned}
$$

以向量與矩陣表示

$$X = \begin{bmatrix} 1 & 914 \\ \dots & \dots \\ 1 & 1218 \end{bmatrix}, \quad \theta = \begin{bmatrix} \theta_0 \\ \theta_1 \end{bmatrix}, \quad \text{and} \quad y = \begin{bmatrix} 148000 \\ \dots \\ 131000 \end{bmatrix}$$

如果 $\boldsymbol{X}^T\boldsymbol{X}$ 可逆

$$
\begin{aligned}
X\theta &= y \\
\theta &= (X^TX)^{-1}X^Ty
\end{aligned}
$$

獲得 $\boldsymbol{\theta}$ 的推導過程源自於成本函數的最小化

$$\text{minimize:}\frac{1}{2m}\sum_{i=1}^{m}(\hat{y}_i - y_i)^2$$

$$\text{minimize:}J(\theta) = \frac{1}{2m}(X\theta - y)^T(X\theta - y)$$

$$\text{minimize:}J(\theta) = \frac{1}{2m}[(X\theta)^T - y^T)(X\theta - y)]$$

$$\text{minimize:}J(\theta) = \frac{1}{2m}[(X\theta)^T X\theta - (X\theta)^T y - y^T(X\theta) + y^T y]$$

$$\text{minimize:}J(\theta) = \frac{1}{2m}[\theta^T X^T X\theta - 2(X\theta)^T y + y^T y]$$

$$\frac{\partial J}{\partial \theta} = \frac{1}{2m}[2X^T X\theta - 2X^T y] = 0$$

$$X^T X\theta = X^T y$$

$$\theta = (X^T X)^{-1} X^T y$$

In [12]:
```python
X_train = train_df["GrLivArea"].values.reshape(-1, 1)
X_train
```

Out[12]:
```
array([[ 914],
       [1306],
       [ 912],
       ...,
       [2156],
       [ 768],
       [1218]])
```

In [13]:

```
y_train = train_df["SalePrice"].values.reshape(-1, 1)
y_train
```

Out[13]:

```
array([[148000],
       [ 76500],
       [125000],
       ...,
       [262500],
       [133000],
       [131000]])
```

In [14]:
```
m = X_train.shape[0]
ones_col = np.ones((m, 1), dtype=int)
X_train = np.concatenate((ones_col, X_train), axis=1)
X_train
```

Out[14]:
```
array([[   1,  914],
       [   1, 1306],
       [   1,  912],
       ...,
       [   1, 2156],
       [   1,  768],
       [   1, 1218]])
```

In [15]:

```
LHS = np.dot(np.transpose(X_train), X_train)
RHS = np.dot(np.transpose(X_train), y_train)
```

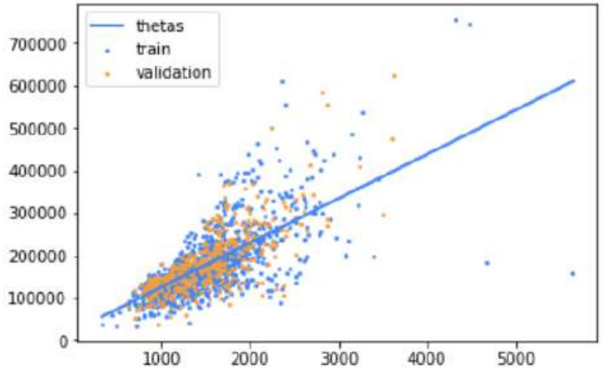
In [16]:

```
thetas = np.dot(np.linalg.inv(LHS), RHS)
theta_0 = thetas[0, 0]
theta_1 = thetas[1, 0]
print("讓成本函數最小的 Theta")
print("Theta_0:{:.4f}, Theta_1:{:.4f}".format(theta_0, theta_1))
```

```
讓成本函數最小的 Theta
Theta_0:21905.1315, Theta_1:104.0985
```

隨堂練習：求得 $\boldsymbol{\theta}$ 後將 $\boldsymbol{y} = \boldsymbol{\theta_0} + \boldsymbol{\theta_1 x}$ 畫出

In [18]:
```
plt.show()
```



Gradient Descent

$h(x)$:

$$h(x) = \theta_0 + \theta_1 x_1$$

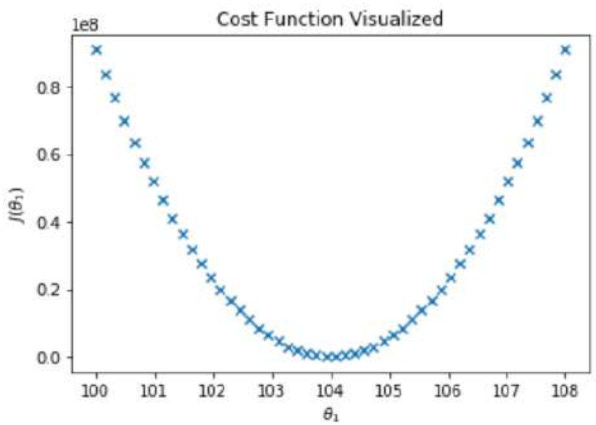
先簡化成只有 $\boldsymbol{\theta_1}$：

$$h(x) = \theta_1 x_1$$

在 $\mathbf{100} < \boldsymbol{\theta_1} < \mathbf{110}$ 之間打點來計算成本函數 $\boldsymbol{J(\theta_1)}$

In [20]:

```
plt.show()
```



假如我們的運氣不好，在一個沒有包含 $\boldsymbol{\theta}_1$ 的區間尋找怎麼辦？

透過很聰明的方式：Gradient Descent

每組 θ 所得的成本函數偏微分取得斜率，利用這個斜率逐步取得局部最佳解。

$$\text{minimize:} J(\theta) = \frac{1}{2m}[\theta^T X^T X\theta - 2(X\theta)^T y + y^T y]$$

$$\frac{\partial J}{\partial \theta} = \frac{1}{2m}[2X^T X\theta - 2X^T y] = 0$$

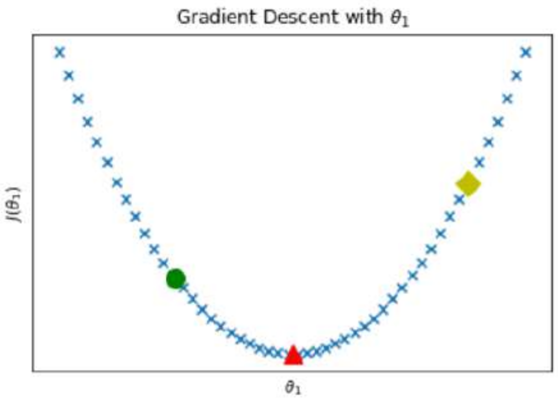
$$\theta := \theta - \alpha \frac{\partial}{\partial \theta} J(\theta)$$

$$\theta := \theta - \alpha \frac{1}{m}(X^T X\theta - X^T y)$$

$$\theta := \theta - \alpha \frac{1}{m}[X^T (X\theta - y)]$$

In [22]:

```
plt.show()
```

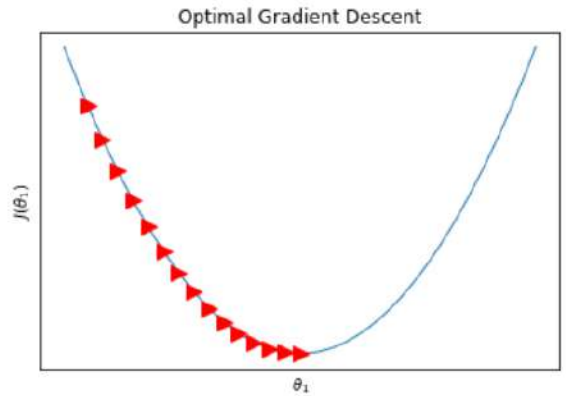


如何做修正

- θ_1 位於綠圓點，$\frac{\partial}{\partial\theta_1}J(\theta_1)$ 為負值，所以 θ_1 會向右邊修正
- θ_1 位於黃方塊，$\frac{\partial}{\partial\theta_1}J(\theta_1)$ 為正值，所以 θ_1 會向左邊修正
- θ_1 位於紅三角，$\frac{\partial}{\partial\theta_1}J(\theta_1)$ 為零，θ_1 收斂

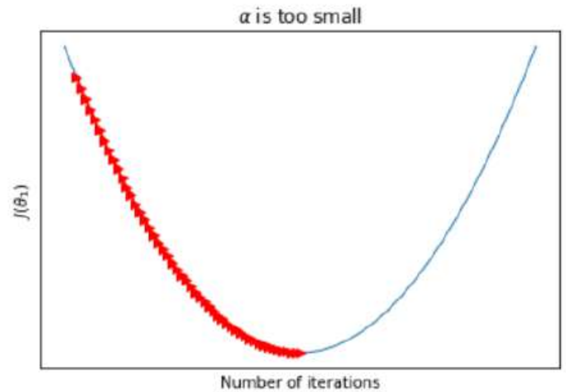
$\boldsymbol{\theta_1}$ 修正的速度與 $\boldsymbol{\alpha}$ 相關，$\boldsymbol{\alpha}$ 稱為學習速率

In [24]:
```
plt.show()
```

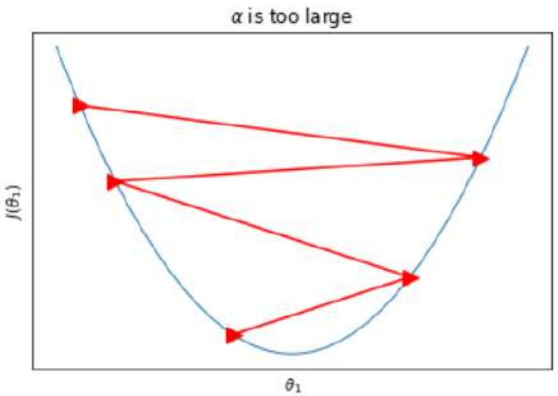


In [26]:

```
plt.show()
```



In [28]:
```
plt.show()
```



怎麼挑選學習速率

- 如果學習速率夠小，成本函數每一次都會下降
- 學習速率太小，收斂的速度太慢
- 學習速率太大，可能會無法收斂

In [29]:

```
import numpy as np

def compute_cost(X, y, thetas = np.array([0, 0]).reshape(2, 1)):
    m = y.shape[0]
    h = X.dot(thetas)
    J = 1/(2*m)*np.sum(np.square(h-y))

    return(J)
```

In [30]:

```python
def gradient_descent(X, y, alpha=0.01, num_iters=1500):
    thetas = np.array([0, 0]).reshape(2, 1)
    m = y.shape[0]
    J_history = np.zeros(num_iters)

    for num_iter in range(num_iters):
        h = X.dot(thetas)
        loss = h - y
        gradient = X.T.dot(loss) / m
        thetas = thetas - alpha * gradient
        J_history[num_iter] = compute_cost(X, y, thetas=thetas)
    return thetas, J_history
```

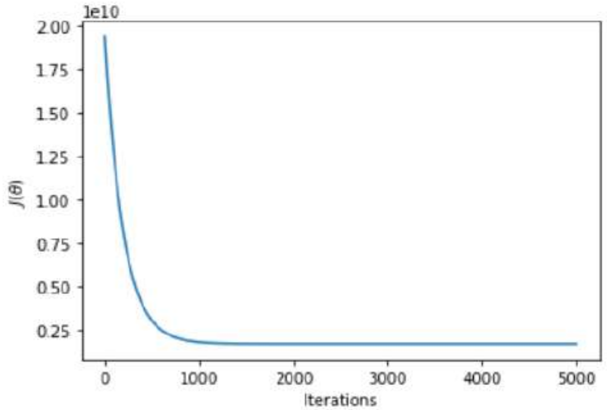
In [31]:
```python
import numpy as np

X_train = train_df["GrLivArea"].values.reshape(-1, 1)
m = X_train.shape[0]
ones_col = np.ones((m, 1))
X_train = np.concatenate((ones_col, X_train), axis=1)
y_train = train_df["SalePrice"].values.reshape(-1, 1)

thetas, cost_J = gradient_descent(X_train, y_train, alpha=0.000000001, num_iters=5000)
theta_0 = thetas[0, 0]
theta_1 = thetas[1, 0]
print("讓成本函數最小的 Thetas")
print("Theta_0:{:.4f}, Theta_1:{:.4f}".format(theta_0, theta_1))
plt.plot(cost_J)
plt.ylabel(r"$J(\theta)$")
plt.xlabel('Iterations')
```

```
讓成本函數最小的 Thetas
Theta_0:0.0806, Theta_1:116.9090
```

Out[31]:
```
<matplotlib.text.Text at 0x1a10db6240>
```

In [32]:

```
plt.show()
```



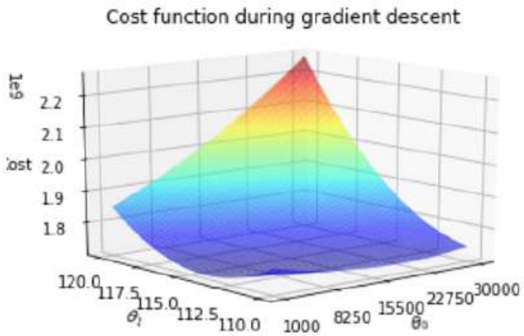
如何將梯度遞減利用視覺化呈現觀察

- 利用mpl_toolkits.mplot3d模組的Axes3D

In [33]:
```
from mpl_toolkits.mplot3d import Axes3D

def surface_plot(theta0_range, theta1_range, X, y):
    theta0_start, theta0_end = theta0_range
    theta1_start, theta1_end = theta1_range
    length = 50
    theta0_arr = np.linspace(theta0_start, theta0_end, length).reshape(-1, 1)
    theta1_arr = np.linspace(theta1_start, theta1_end, length).reshape(-1, 1)
    thetas_arr = np.concatenate([theta0_arr, theta1_arr], axis=1)
    Z = np.zeros((length, length))
    for i in range(length):
        for j in range(length):
            theta_0 = theta0_arr[i]
            theta_1 = theta1_arr[j]
            thetas_arr = np.array([theta_0, theta_1]).reshape(-1, 1)
            Z[i, j] = compute_cost(X, y, thetas=thetas_arr)
    xx, yy = np.meshgrid(theta0_arr, theta1_arr)
    fig = plt.figure()
    ax = fig.add_subplot(111, projection='3d')
    ax.plot_surface(xx, yy, Z, alpha=0.6, cmap=plt.cm.jet)
    ax.set_zlabel('Cost')
    ax.set_zlim(Z.min(),Z.max())
    ax.view_init(elev=15, azim=230)
    ax.set_xticks(np.linspace(theta0_start, theta0_end, 5))
    ax.set_yticks(np.linspace(theta1_start, theta1_end, 5))
    ax.set_xlabel(r'$\theta_0$')
    ax.set_ylabel(r'$\theta_1$')
    ax.set_title("Cost function during gradient descent")
    plt.show()
```

In [34]:

```
surface_plot((1000, 30000), (110, 120), X_train, y_train)
```



$\boldsymbol{\theta_0}$ 與 $\boldsymbol{\theta_1}$ 的坡度差距太大

利用標準化（Normalization）來應對

- MinMax scaler:

$$X_{scaled} = \frac{X - X_{min}}{X_{max} - X_{min}}$$

- Standard scaler:

$$X_{scaled} = \frac{X - \mu_X}{\sigma_X}$$

In [35]:

```
# 自己做 Standard scaler 標準化
X_train_gd = train_df["GrLivArea"].values.reshape(-1, 1)
mu_X = X_train_gd.mean()
sigma_X = X_train_gd.std()
X_train_scaled = (X_train_gd - mu_X)/sigma_X
print(X_train_scaled)
```

```
[[-1.12253923]
 [-0.3949409 ]
 [-1.12625147]
 ...,
 [ 1.18275955]
 [-1.39353249]
 [-0.5582793 ]]
```

In [36]:

```python
# 請 sklearn 做 Standard scaler 標準化
from sklearn.preprocessing import StandardScaler

ss = StandardScaler()
X_train_scaled = ss.fit_transform(X_train_gd.astype(float))
y_train_scaled = ss.fit_transform(y_train.astype(float))
print(X_train_scaled)
```

```
[[-1.12253923]
 [-0.3949409 ]
 [-1.12625147]
 ...,
 [ 1.18275955]
 [-1.39353249]
 [-0.5582793 ]]
```

In [37]:

```
ones = np.ones(X_train_scaled.shape[0]).reshape(-1, 1)
X_train_scaled = np.concatenate([ones, X_train_scaled], axis=1)
X_train_scaled
```

Out[37]:

```
array([[ 1.        , -1.12253923],
       [ 1.        , -0.3949409 ],
       [ 1.        , -1.12625147],
       ...,
       [ 1.        ,  1.18275955],
       [ 1.        , -1.39353249],
       [ 1.        , -0.5582793 ]])
```

In [38]:

```python
thetas, cost_J = gradient_descent(X_train_scaled, y_train_scaled)
print("讓成本函數最小的 Thetas")
print(thetas)
plt.plot(cost_J)
plt.ylabel(r"$J(\theta)$")
plt.xlabel('Iterations')
```

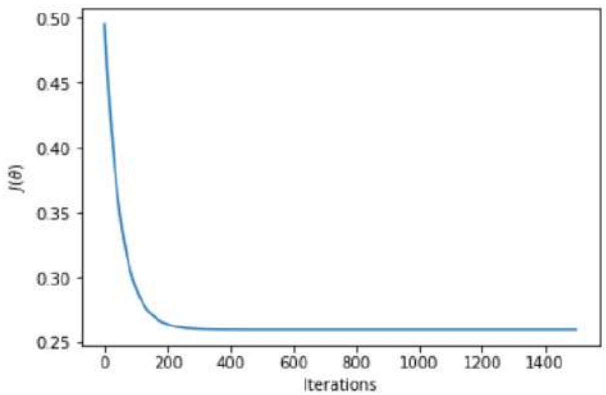
```
讓成本函數最小的 Thetas
[[ -2.76947415e-17]
 [  6.93103700e-01]]
```

Out[38]:

```
<matplotlib.text.Text at 0x1a1eb9f0b8>
```

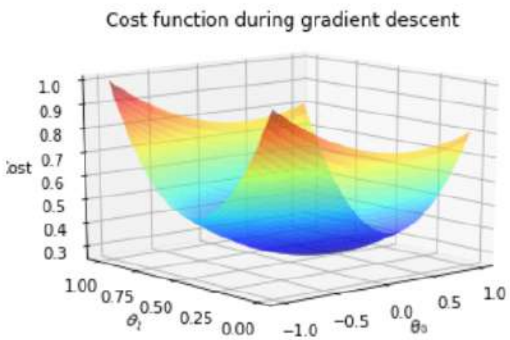
In [39]:

```
plt.show()
```



In [40]:

```
surface_plot((-1, 1), (0, 1), X_train_scaled, y_train_scaled)
```



更適合觀察梯度的圖形

https://plot.ly/python/3d-surface-plots/

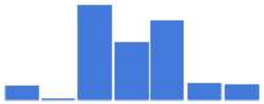
In [41]:

```
import plotly.plotly as py
import plotly.graph_objs as go

def get_surface_Z(theta0_range, theta1_range, X, y):
    theta0_start, theta0_end = theta0_range
    theta1_start, theta1_end = theta1_range
    length = 50
    theta0_arr = np.linspace(theta0_start, theta0_end, length).reshape(-1, 1)
    theta1_arr = np.linspace(theta1_start, theta1_end, length).reshape(-1, 1)
    thetas_arr = np.concatenate([theta0_arr, theta1_arr], axis=1)
    Z = np.zeros((length, length))
    for i in range(length):
        for j in range(length):
            theta_0 = theta0_arr[i]
            theta_1 = theta1_arr[j]
            thetas_arr = np.array([theta_0, theta_1]).reshape(-1, 1)
            Z[i, j] = compute_cost(X, y, thetas=thetas_arr)
    return Z

Z = get_surface_Z((-5, 5), (-5, 5), X_train_scaled, y_train_scaled)
py.sign_in('tonykuoyj', '6doG9IEHGW1QT7uD9vY8') # Use your own plotly Username / API Key
data = [go.Surface(z=Z)]
layout = go.Layout(
  title='Cost function during gradient descent',
  scene=dict(
      xaxis = dict(title='theta_0'),
      yaxis = dict(title="theta_1"),
      zaxis = dict(title="J(theta)")
  )
)
fig = go.Figure(data=data, layout=layout)
```

In [42]:

```
py.iplot(fig, filename='gd-3d-surface')
```

Out[42]:



EDIT CHART

標準化後如何回推 $\boldsymbol{\theta}$

$$y = \theta_0 + \theta_1 x_1$$

$$\frac{y - \mu_y}{\sigma_y} = \theta_0' + \frac{x_1 - \mu_{x_1}}{\sigma_{x_1}} \theta_1'$$

$$y = \mu_y + \sigma_y \theta_0' + \frac{\sigma_y}{\sigma_{x_1}} (x_1 - \mu_{x_1}) \theta_1'$$

$$y = \mu_y + \sigma_y \theta_0' - \frac{\sigma_y \mu_{x_1}}{\sigma_{x_1}} \theta_1' + \frac{\sigma_y}{\sigma_{x_1}} \theta_1' x_1$$

$$\theta_0 = \mu_y + \sigma_y \theta_0' - \frac{\sigma_y \mu_{x_1}}{\sigma_{x_1}} \theta_1'$$

$$\theta_1 = \frac{\sigma_y}{\sigma_{x_1}} \theta_1'$$

隨堂練習：請回推 $\boldsymbol{\theta}$

Phew...

- 總算完成了兩種找到 θ 的方式！
- 這是不能忽略的學習步驟，但並不是實作上要採用的

有哪些模組可以幫我們找到 $\boldsymbol{\theta}$

- statsmodel
- scikit-learn
- TensorFlow

我們建議使用 Scikit-Learn

- 比 StatsModel 完整
- TensorFlow 是自成一格的框架

In [43]:

```python
from sklearn.linear_model import LinearRegression

X_train = train_df["GrLivArea"].values.reshape(-1, 1)
y_train = train_df["SalePrice"].values.reshape(-1, 1)
X_valid = validation_df["GrLivArea"].values.reshape(-1, 1)
y_valid = validation_df["SalePrice"].values.reshape(-1, 1)
reg = LinearRegression()
reg.fit(X_train, y_train)
```

Out[43]:

```
LinearRegression(copy_X=True, fit_intercept=True, n_jobs=1, normalize=False)
```

評估迴歸模型的指標

- MSE（愈低愈好）

$$MSE = \frac{1}{m}\sum_{i=1}^{m}(\hat{y}_i - y_i)^2$$

In [44]:
```
# 自己算
train_MSE= np.mean((y_train - reg.predict(X_train))**2)
validation_MSE= np.mean((y_valid - reg.predict(X_valid))**2)
print("Computation:")
print("Training MSE: {:.4f}".format(train_MSE))
print("Validation MSE: {:.4f}".format(validation_MSE))
```

```
Computation:
Training MSE: 3402166887.1990
Validation MSE: 2541490406.3163
```

請 sklearn 幫我們算

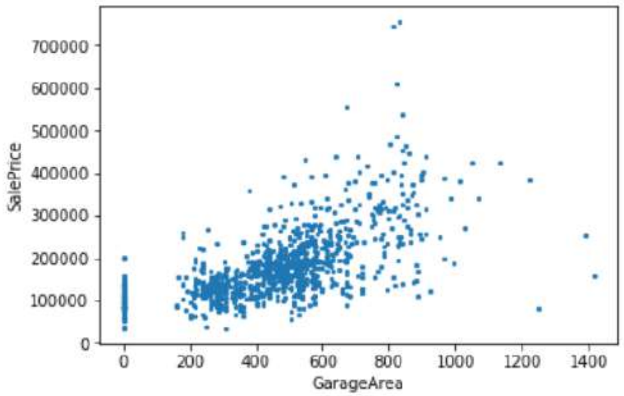
In [45]:
```
# sklearn.metrics
from sklearn.metrics import mean_squared_error

print("\nFrom sklearn.metrics:")
print("Training MSE: {:.4f}".format(mean_squared_error(y_train, reg.predict(X_train))))
print("Validation MSE: {:.4f}".format(mean_squared_error(y_valid, reg.predict(X_valid))))
```

```
From sklearn.metrics:
Training MSE: 3402166887.1990
Validation MSE: 2541490406.3163
```

隨堂練習：挑兩個變數來預測 SalePrice

- 試試看GrLivArea與GarageArea

In [47]:
```
plt.show()
```



In [51]:
```
print('Thetas from sklearn:\ntheta_0: {:.4f}\ntheta_1: {:.4f}\ntheta_2: {:.4f}'.format(theta_0_sk
l, theta_1_skl, theta_2_skl))
```

```
Thetas from sklearn:
theta_0: -4600.3771
theta_1: 77.7825
theta_2: 142.7484
```

In [53]:

```
print("Computation:")
print("Training MSE: {:.4f}".format(train_MSE))
print("Validation MSE: {:.4f}".format(validation_MSE))

# sklearn.metrics
print("\nFrom sklearn.metrics:")
print("Training MSE: {:.4f}".format(mean_squared_error(y_train, regressor_skl.predict(X_train))))
print("Validation MSE: {:.4f}".format(mean_squared_error(y_validation, regressor_skl.predict(X_vali
dation))))
```

```
Computation:
Training MSE: 2682062423.1890
Validation MSE: 1930533819.9319

From sklearn.metrics:
Training MSE: 2682062423.1890
Validation MSE: 1930533819.9319
```

In [54]:

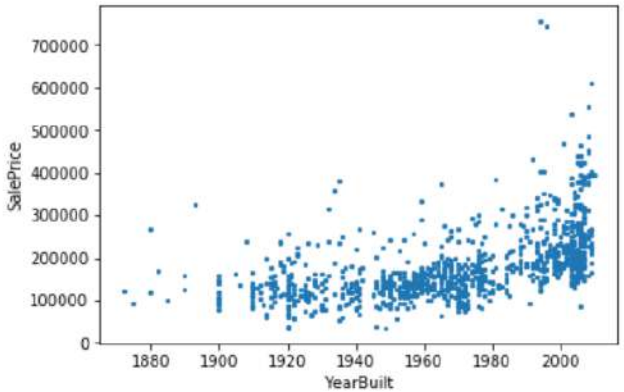
```
import matplotlib.pyplot as plt

train_df.plot.scatter("YearBuilt", "SalePrice", s=5)
```

Out[54]:

```
<matplotlib.axes._subplots.AxesSubplot at 0x1a1fed6710>
```

In [55]:

```
plt.show()
```



$$y_i = \theta_0 + \theta_1 x_i + \theta_2 x_i^2 + \ldots + \theta_d x_i^d$$

In [56]:

```
# 訓練樣本
y_train = train_df["SalePrice"].values.reshape(-1, 1)
X_train = train_df["YearBuilt"].values.reshape(-1, 1)
print(y_train.shape)
print(X_train.shape)
```

```
(1022, 1)
(1022, 1)
```

In [57]:

```
# 驗證樣本
y_validation = validation_df["SalePrice"].values.reshape(-1, 1)
X_validation = validation_df["YearBuilt"].values.reshape(-1, 1)
print(y_validation.shape)
print(X_validation.shape)
```

```
(438, 1)
(438, 1)
```

使用 PolynomialFeatures(d) 與 fit_transform() 建立 X

In [58]:
```
from sklearn.preprocessing import PolynomialFeatures

PolynomialFeatures(3).fit_transform(X_train)[0, :]
```

Out[58]:
```
array([  1.00000000e+00,   1.99600000e+03,   3.98401600e+06,
         7.95209594e+09])
```

In [59]:
```
X_train[0, :]
```

Out[59]:
```
array([1996])
```

In [60]:

```
def make_features(train_set, validation_set, degrees):
    train_dict = {}
    validation_dict = {}
    for d in degrees:
        train_dict[d] = PolynomialFeatures(d).fit_transform(train_set.reshape(-1, 1))
        validation_dict[d] = PolynomialFeatures(d).fit_transform(validation_set.reshape(-1, 1))
    return train_dict, validation_dict
```

In [61]:

```
degrees = range(11)
train_dict, validation_dict = make_features(X_train, X_validation, degrees)
```

隨堂練習：將不同次方項的 validation error(MSE) 算出來，並找出 error 最小的 degree

```python
def get_best_degree():
    # ...
```

In [63]:

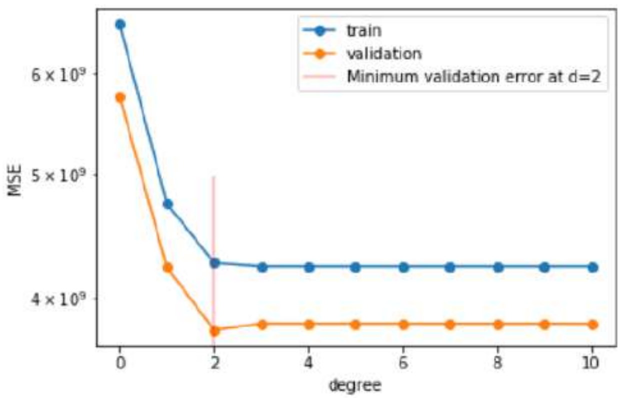
```
best_degree, error_validation, error_train = get_best_degree()

print("Validation Error:\n")
print(error_validation)
print("\nError 最低的次方是 {}".format(best_degree))
```

```
Validation Error:

[  5.74773085e+09   4.22306392e+09   3.76996972e+09   3.81499577e+09
   3.81482104e+09   3.81463312e+09   3.81443382e+09   3.81422447e+09
   3.81400642e+09   3.81378108e+09   3.81354988e+09]

Error 最低的次方是 2
```

In [64]:

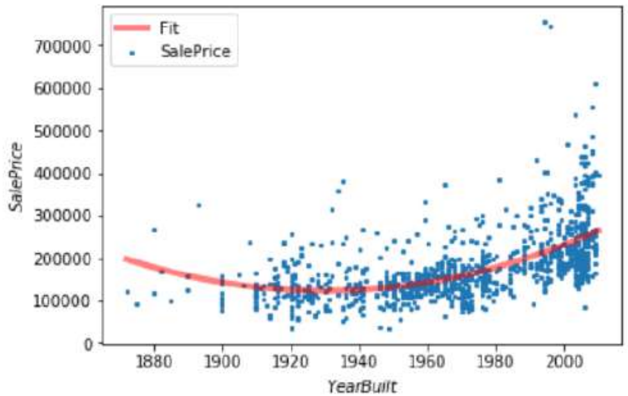
```
plt.plot(degrees, error_train, marker='o', label='train')
plt.plot(degrees, error_validation, marker='o', label='validation')
plt.axvline(best_degree, 0, 0.5, color='r', label="Minimum validation error at d={}".format(best_de
gree), alpha=0.3)
plt.ylabel('MSE')
plt.xlabel('degree')
plt.legend(loc='upper right')
plt.yscale("log")
```

In [65]:
```
plt.show()
```



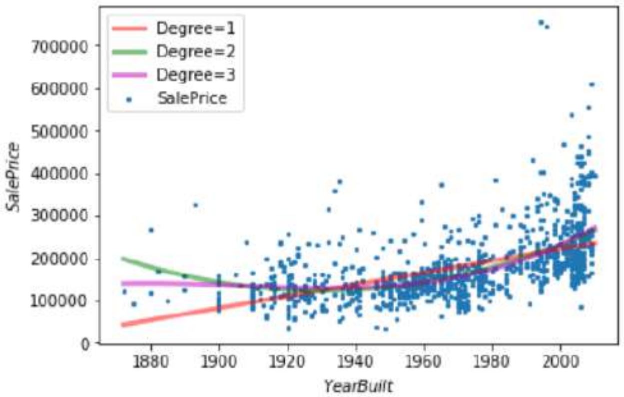
In [66]:
```
def get_plot():
    d = 2
    X_train = train_dict[d]
    X_validation = validation_dict[d]
    regressor = linear_model.LinearRegression()
    # fitting
    regressor.fit(X_train, y_train)
    prediction_on_training = regressor.predict(X_train)
    prediction_on_validation = regressor.predict(X_validation)
    x_arr = np.linspace(train_df["YearBuilt"].min(), train_df["YearBuilt"].max(), num=1000)
    x_arr_poly = PolynomialFeatures(d).fit_transform(x_arr.reshape(-1, 1))
    y_arr = regressor.predict(x_arr_poly)
    # plotting
    plt.scatter(train_df["YearBuilt"], train_df["SalePrice"], s=5)
    plt.plot(x_arr, y_arr, 'r-', alpha=0.5, label = "Fit", linewidth=4)
    plt.xlabel('$YearBuilt$');
    plt.ylabel('$SalePrice$')
    plt.legend(loc="upper left")
    plt.show()
```

In [67]:
```
get_plot()
```



隨堂練習：在上圖加入 d=1 與 d=3 的線

In [69]:
```
get_plot()
```



在不設定 random_state 參數的情況下切割訓練與驗證樣本

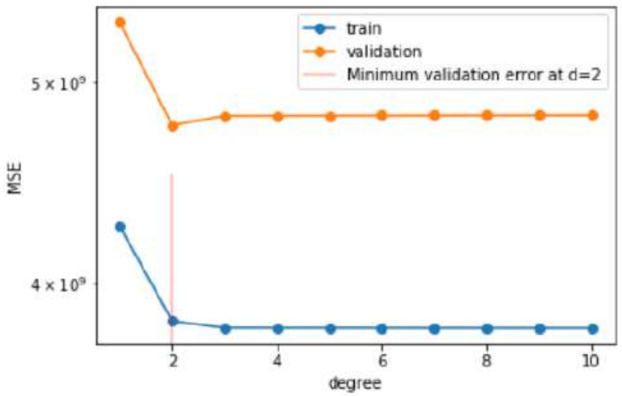
In [70]:

```python
import numpy as np
import pandas as pd
from sklearn.model_selection import train_test_split
from sklearn.preprocessing import PolynomialFeatures
from sklearn.linear_model import LinearRegression
from sklearn.metrics import mean_squared_error

# 切割訓練與驗證樣本
train_url = "https://storage.googleapis.com/kaggle_datasets/House-Prices-Advanced-Regression-Techniques/train.csv"
labeled = pd.read_csv(train_url)
train_df, validation_df = train_test_split(labeled, test_size=0.3)
y_train = train_df["SalePrice"].values.reshape(-1, 1)
X_train = train_df["YearBuilt"].values.reshape(-1, 1)
y_validation = validation_df["SalePrice"].values.reshape(-1, 1)
X_validation = validation_df["YearBuilt"].values.reshape(-1, 1)

degrees = range(1, 11)
error_train = np.empty(len(degrees))
error_validation = np.empty(len(degrees))
for d in degrees:
    X_train_poly = PolynomialFeatures(d).fit_transform(X_train)
    X_validation_poly = PolynomialFeatures(d).fit_transform(X_validation)
    regressor = LinearRegression()
    regressor.fit(X_train_poly, y_train)
    prediction_on_training = regressor.predict(X_train_poly)
    prediction_on_validation = regressor.predict(X_validation_poly)
    #calculate mean squared error
    error_train[d - 1] = mean_squared_error(y_train, prediction_on_training)
    error_validation[d - 1] = mean_squared_error(y_validation, prediction_on_validation)

best_degree = np.argmin(error_validation) + 1
print("Validation Error:\n")
print(error_validation)
```

In [71]:

```
import matplotlib.pyplot as plt

plt.plot(degrees, error_train, marker='o', label='train')
plt.plot(degrees, error_validation, marker='o', label='validation')
plt.axvline(best_degree, 0, 0.5, color='r', label="Minimum validation error at d={}".format(best_de
gree), alpha=0.3)
plt.ylabel('MSE')
plt.xlabel('degree')
plt.legend(loc='upper right')
plt.yscale("log")
```

In [72]:
```
plt.show()
```



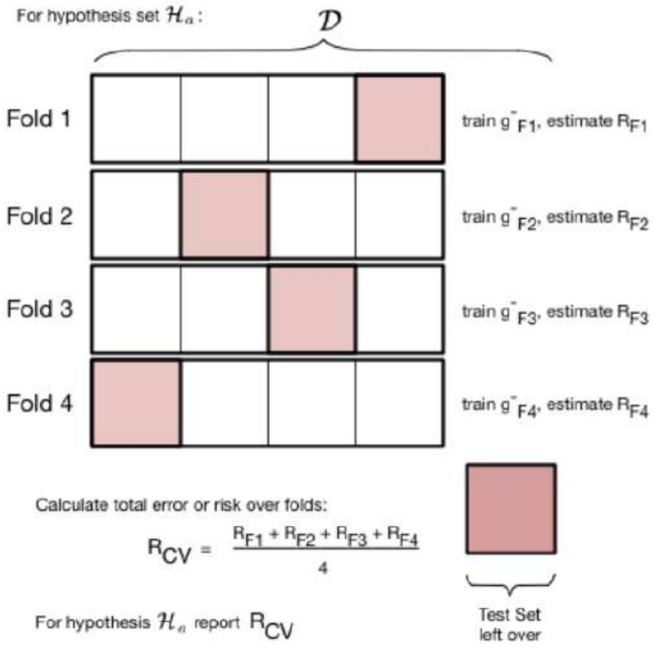
重複執行前面的程式碼

- 發現驗證資料的 error_validation 與 best_degree 每次都不一樣，這是什麼緣故？

隨機的 train_test_split()

- 憑藉單次隨機給予模型的訓練、驗證樣本就決定 best_degree 與 MSE 有些大意
- 我們需要一個機制來因應這樣的隨機性

交叉驗證示意圖



Source: CS109 Data Science

交叉驗證的步驟

1. 將 labeled data 切分為 n_folds
2. 將 n_folds - 1 作為訓練樣本，剩餘的一個 fold 作為驗證樣本
3. 將所有 folds 所求得的 MSE 平均
4. 選擇評估最佳的設定再應用至測試樣本

In [73]:

```
from sklearn.model_selection import KFold

n_folds = 4
labeled_data_m = labeled.shape[0]
kfold = KFold(n_folds)
```

In [74]:
```python
list(kfold.split(range(labeled_data_m)))[0]
```

Out[74]:
```
(array([ 365,  366,  367, ..., 1457, 1458, 1459]),
 array([  0,   1,   2,   3,   4,   5,   6,   7,   8,   9,  10,  11,  12,
         13,  14,  15,  16,  17,  18,  19,  20,  21,  22,  23,  24,  25,
         26,  27,  28,  29,  30,  31,  32,  33,  34,  35,  36,  37,  38,
         39,  40,  41,  42,  43,  44,  45,  46,  47,  48,  49,  50,  51,
         52,  53,  54,  55,  56,  57,  58,  59,  60,  61,  62,  63,  64,
         65,  66,  67,  68,  69,  70,  71,  72,  73,  74,  75,  76,  77,
         78,  79,  80,  81,  82,  83,  84,  85,  86,  87,  88,  89,  90,
         91,  92,  93,  94,  95,  96,  97,  98,  99, 100, 101, 102, 103,
        104, 105, 106, 107, 108, 109, 110, 111, 112, 113, 114, 115, 116,
        117, 118, 119, 120, 121, 122, 123, 124, 125, 126, 127, 128, 129,
        130, 131, 132, 133, 134, 135, 136, 137, 138, 139, 140, 141, 142,
        143, 144, 145, 146, 147, 148, 149, 150, 151, 152, 153, 154, 155,
        156, 157, 158, 159, 160, 161, 162, 163, 164, 165, 166, 167, 168,
        169, 170, 171, 172, 173, 174, 175, 176, 177, 178, 179, 180, 181,
        182, 183, 184, 185, 186, 187, 188, 189, 190, 191, 192, 193, 194,
        195, 196, 197, 198, 199, 200, 201, 202, 203, 204, 205, 206, 207,
        208, 209, 210, 211, 212, 213, 214, 215, 216, 217, 218, 219, 220,
        221, 222, 223, 224, 225, 226, 227, 228, 229, 230, 231, 232, 233,
        234, 235, 236, 237, 238, 239, 240, 241, 242, 243, 244, 245, 246,
        247, 248, 249, 250, 251, 252, 253, 254, 255, 256, 257, 258, 259,
        260, 261, 262, 263, 264, 265, 266, 267, 268, 269, 270, 271, 272,
        273, 274, 275, 276, 277, 278, 279, 280, 281, 282, 283, 284, 285,
        286, 287, 288, 289, 290, 291, 292, 293, 294, 295, 296, 297, 298,
        299, 300, 301, 302, 303, 304, 305, 306, 307, 308, 309, 310, 311,
        312, 313, 314, 315, 316, 317, 318, 319, 320, 321, 322, 323, 324,
        325, 326, 327, 328, 329, 330, 331, 332, 333, 334, 335, 336, 337,
        338, 339, 340, 341, 342, 343, 344, 345, 346, 347, 348, 349, 350,
        351, 352, 353, 354, 355, 356, 357, 358, 359, 360, 361, 362, 363, 364]))
```

這樣有什麼問題？

In [75]:
```
kfold = KFold(n_folds, shuffle=True)
list(kfold.split(range(labeled_data_m)))[0]
```

Out[75]:
```
(array([   0,    3,    4, ..., 1456, 1458, 1459]),
 array([   1,    2,    5,    8,    9,   11,   15,   23,   24,   25,   26,
          27,   28,   29,   36,   43,   56,   57,   59,   60,   61,   62,
          70,   77,   78,   79,   80,   83,   87,   88,   94,  100,  104,
         111,  117,  121,  126,  138,  143,  148,  149,  153,  158,  159,
         165,  166,  167,  173,  175,  179,  184,  187,  189,  190,  195,
         197,  198,  203,  204,  214,  215,  216,  218,  223,  225,  226,
         228,  231,  239,  244,  249,  250,  264,  265,  273,  274,  276,
         290,  297,  300,  301,  303,  307,  315,  323,  325,  331,  333,
         336,  339,  351,  353,  354,  358,  361,  364,  367,  368,  377,
         380,  388,  389,  393,  403,  404,  407,  408,  411,  415,  416,
         423,  427,  429,  430,  432,  437,  440,  445,  447,  449,  452,
         453,  456,  459,  460,  461,  464,  465,  467,  468,  471,  478,
         492,  496,  506,  507,  510,  512,  513,  514,  517,  522,  526,
         528,  536,  538,  542,  544,  552,  554,  566,  573,  579,  581,
         585,  587,  588,  594,  597,  598,  609,  610,  613,  616,  620,
         621,  622,  627,  643,  652,  657,  663,  664,  671,  687,  697,
         700,  701,  703,  711,  713,  717,  719,  738,  748,  755,  767,
         774,  779,  783,  786,  789,  790,  795,  796,  800,  801,  803,
         804,  806,  813,  817,  829,  831,  833,  836,  844,  846,  850,
         854,  855,  861,  864,  868,  874,  878,  879,  883,  890,  896,
         902,  903,  904,  908,  910,  920,  927,  928,  933,  935,  941,
         943,  947,  948,  950,  951,  956,  959,  968,  972,  974,  975,
         977,  981,  986,  989, 1000, 1004, 1005, 1006, 1012, 1014, 1015,
        1020, 1022, 1031, 1035, 1036, 1037, 1040, 1045, 1046, 1056, 1057,
        1058, 1061, 1062, 1068, 1071, 1083, 1089, 1098, 1106, 1107, 1108,
        1109, 1111, 1123, 1127, 1136, 1139, 1142, 1143, 1147, 1149, 1154,
        1159, 1162, 1172, 1175, 1179, 1180, 1184, 1187, 1196, 1200, 1205,
        1207, 1212, 1216, 1222, 1225, 1229, 1251, 1252, 1255, 1258, 1261,
        1263, 1267, 1274, 1280, 1282, 1285, 1286, 1289, 1290, 1294, 1296,
        1297, 1298, 1303, 1306, 1307, 1315, 1321, 1323, 1327, 1336, 1337,
```

In [76]:

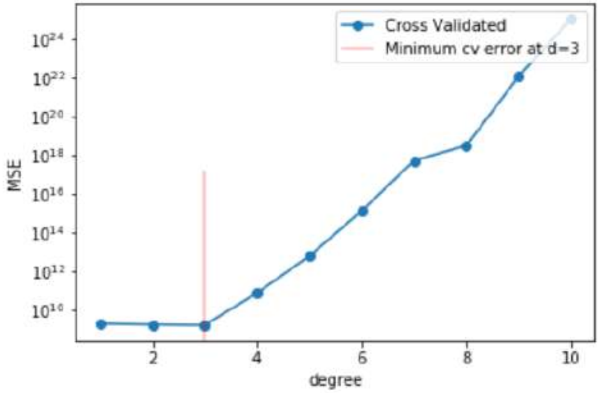
```
import numpy as np
import pandas as pd
from sklearn.model_selection import train_test_split
from sklearn.preprocessing import PolynomialFeatures
from sklearn.linear_model import LinearRegression
from sklearn.model_selection import cross_val_score

# 切割訓練與驗證樣本
train_url = "https://storage.googleapis.com/kaggle_datasets/House-Prices-Advanced-Regression-Techni
ques/train.csv"
labeled = pd.read_csv(train_url)
y = labeled["SalePrice"].values.reshape(-1, 1)
X = labeled[["GrLivArea", "YearBuilt", "GarageArea", "TotalBsmtSF"]].values

degrees = range(1, 11)
cv_error = np.empty(len(degrees))
for d in degrees:
    X_poly = PolynomialFeatures(d).fit_transform(X)
    regressor = LinearRegression()
    cv_score = cross_val_score(regressor, X_poly, y, scoring="neg_mean_squared_error")
    cv_error[d - 1] = cv_score.mean()

best_degree = np.argmin(np.absolute(cv_error)) + 1
print("CV Error:\n")
print(np.absolute(cv_error))
print("\nError 最低的次方是 {}".format(best_degree))
```

```
CV Error:

[  1.88924474e+09   1.69883010e+09   1.58725356e+09   7.34165929e+10
   6.06317865e+12   1.31150214e+15   5.22649401e+17   3.10338252e+18
   1.19258851e+22   1.08156495e+25]

Error 最低的次方是 3
```

In [77]:

```
plt.plot(degrees, np.absolute(cv_error), marker='o', label='Cross Validated')
plt.axvline(best_degree, 0, 0.5, color='r', label="Minimum cv error at d={}".format(best_degree), a
lpha=0.3)
plt.ylabel('MSE')
plt.xlabel('degree')
plt.legend(loc='upper right')
plt.yscale("log")
```

In [78]:
```
plt.show()
```



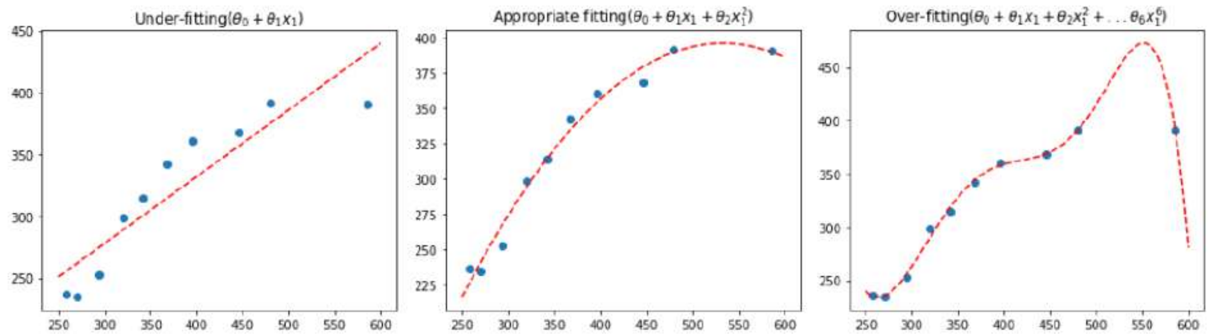
正規化 regularization

目前加入變數、納入次方項與交叉驗證已經很不錯

- 但有可能碰上什麼麻煩？

In [81]:

```
plt.show()
```



過度配適 Overfitting 的麻煩

Bias	Variance	Fitting
High	Low	Under-fitting
Medium	Medium	Appropriate fitting
Low	High	Over-fitting

如果我們採用了高的 degrees

- 想個辦法去平滑它：Ridge 方法（C 為一個常數）

$$\sum_{i=0}^{d} \theta_i^2 < C$$

- 在成本函數後面加入 $\lambda \sum_{i=0}^{d} \theta_i^2$ 來消弭 θ_i

$$J(\theta)_{Ridge} = \sum_{i=1}^{m} (\hat{y}_i - y_i)^2 + \lambda \sum_{i=0}^{d} \theta_i^2$$

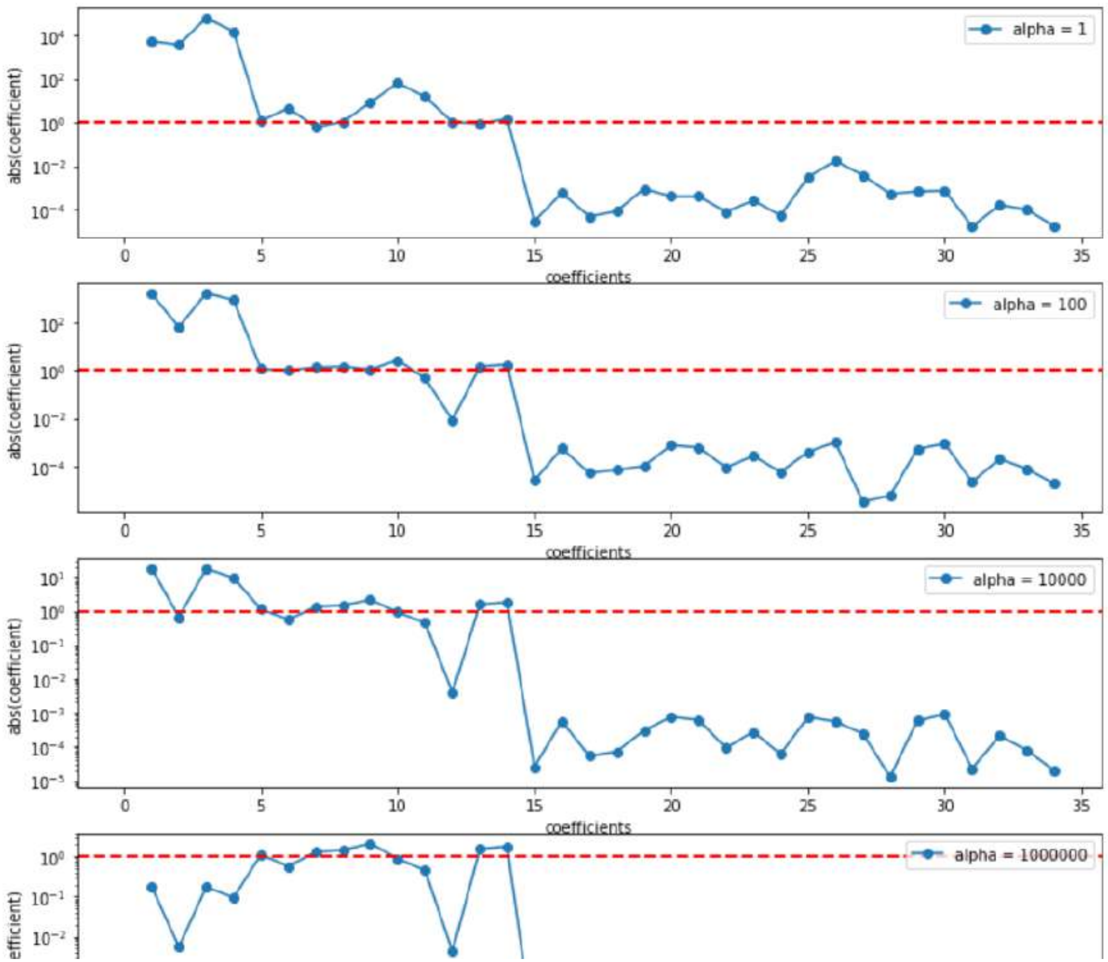
觀察 $\boldsymbol{\lambda}$ 上升，$\boldsymbol{\theta}_i$ 是否顯著地降低

In [82]:

```python
import numpy as np
import pandas as pd
from sklearn.model_selection import train_test_split
from sklearn.preprocessing import PolynomialFeatures
from sklearn.linear_model import Ridge
from sklearn.model_selection import cross_val_score

# 切割訓練與驗證樣本
train_url = "https://storage.googleapis.com/kaggle_datasets/House-Prices-Advanced-Regression-Techni
ques/train.csv"
labeled = pd.read_csv(train_url)
train, validation = train_test_split(labeled, test_size=0.3)
y_train = train["SalePrice"].values.reshape(-1, 1)
X_train = train[["GrLivArea", "YearBuilt", "GarageArea", "TotalBsmtSF"]].values

fig, axes = plt.subplots(5, 1, figsize=(12, 16))
d = 3
lambdas = [1, 10**2, 10**4, 10**6, 10**8]
for i in range(len(lambdas)):
    X_train_poly = PolynomialFeatures(d).fit_transform(X_train)
    ridge = Ridge(alpha=lambdas[i])
    ridge.fit(X_train_poly, y_train)
    thetas = ridge.coef_.ravel()
    print("lambda: {}, thetas:".format(lambdas[i]))
    print(thetas)
    axes[i].semilogy(np.abs(thetas), marker='o', label="alpha = {}".format((lambdas[i])))
    axes[i].axhline(y=1, linestyle="dashed", linewidth=2, color="r")
    axes[i].set_ylabel('abs(coefficient)')
    axes[i].set_xlabel('coefficients')
    axes[i].legend(loc='upper right')
```

```
lambda: 1, thetas:
[  0.00000000e+00   5.26714855e+03   3.65037385e+03   6.03334599e+04
   1.45543490e+04  -1.15925636e+00  -4.44291406e+00   6.10256364e-01
```

In [83]:
```
plt.show()
```



那我們又該如何找到合適的 $\boldsymbol{\lambda}$ 呢？

網格搜尋 GridSearch

GridSearchCV() 函數

- 能夠幫助我們挑選 **Hyper Parameters**
- 整合了交叉驗證

```
from sklearn.model_selection import GridSearchCV

regressor = Ridge()
parameters = {"alpha": [1, 10, 10**2, 10**3, 10**4, 10**5]}
gridclassifier=GridSearchCV(regressor, param_grid=parameters, cv=4, scoring="neg_mean_squared_erro
r")
```

In [84]:

```
from sklearn.model_selection import GridSearchCV

def cv_optimize_ridge(X, y, n_folds=4):
    regressor = Ridge()
    parameters = {"alpha": [1, 10, 10**2, 10**3, 10**4, 10**5]}
    gs = GridSearchCV(regressor, param_grid=parameters, cv=n_folds, scoring="neg_mean_squared_erro
r")
    gs.fit(X, y)
    return gs
```

In [85]:

```
fit_model = cv_optimize_ridge(X_train, y_train, n_folds=4)
```

In [86]:

```
print(fit_model.best_estimator_)
print(fit_model.best_params_)
print(fit_model.best_score_)
```

```
Ridge(alpha=1, copy_X=True, fit_intercept=True, max_iter=None,
   normalize=False, random_state=None, solver='auto', tol=0.001)
{'alpha': 1}
-2118861006.65
```

In [87]:

```
best_alpha = fit_model.best_params_['alpha']
regressor = Ridge(alpha=best_alpha).fit(X_train,y_train)
```