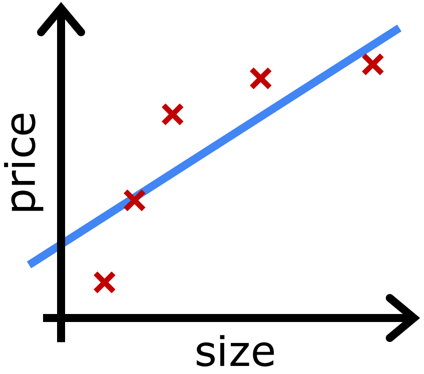
Regularization to Reduce Overfitting

The Problem of Overfitting

Regression example

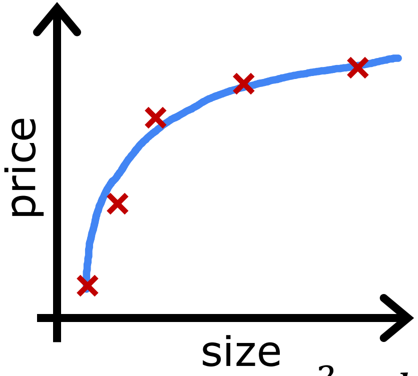


$w_1x + b$

underfit

- Does not fit the training set well

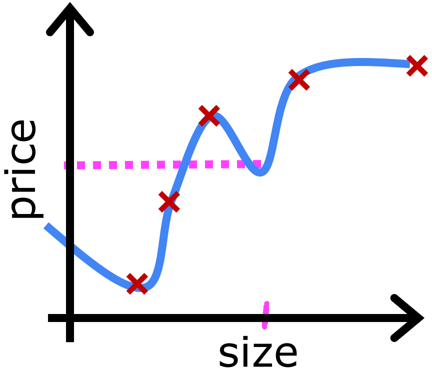
high bias



$w_1x + w_2x^2 + b$

- Fits training set pretty well

generalization



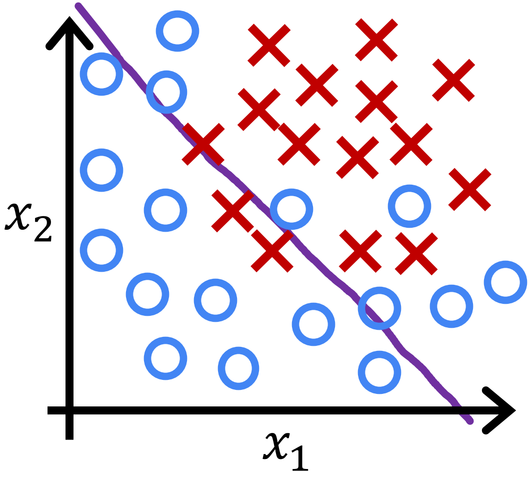
$w_1x + w_2x^2 + w_3x^3 + w_4x^4 + b$

overfit

- Fits the training set extremely well

high variance

Classification

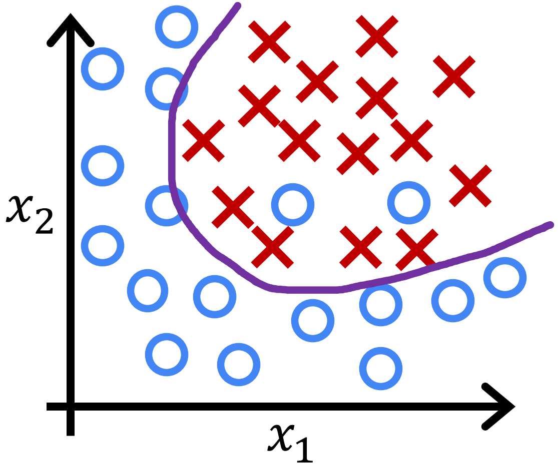


$z = w_1x_1 + w_2x_2 + b$

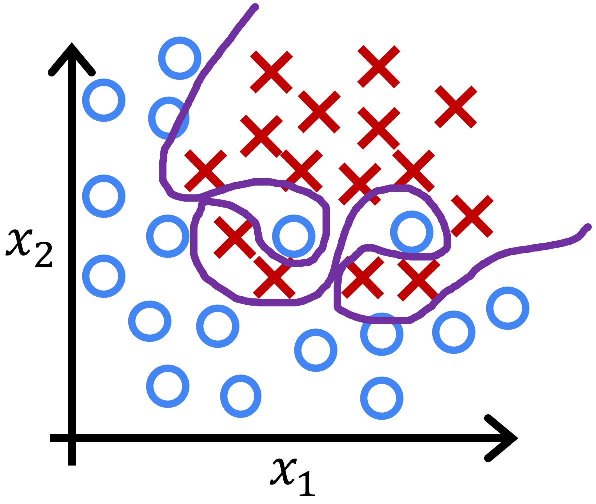
$f_{\vec{w},b}(\vec{x}) = g(z)$

g is the sigmoid function

underfit high bias



$z = w_1x_1 + w_2x_2$
$+w_3x_1^2 + w_4x_2^2$
$+w_5x_1x_2 + b$



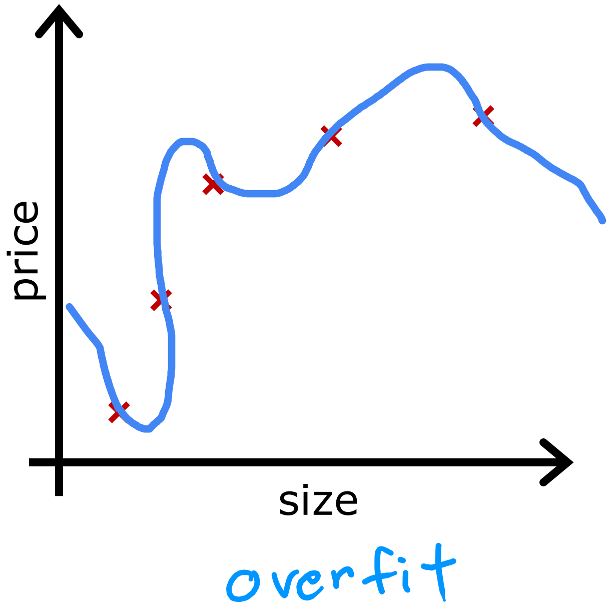
$z = w_1x_1 + w_2x_2$
$+w_3x_1^2x_2 + w_4x_1^2x_2^2$
$+w_5x_1^2x_2^3 + w_6x_1^3x_2$
$+ \cdots + b$

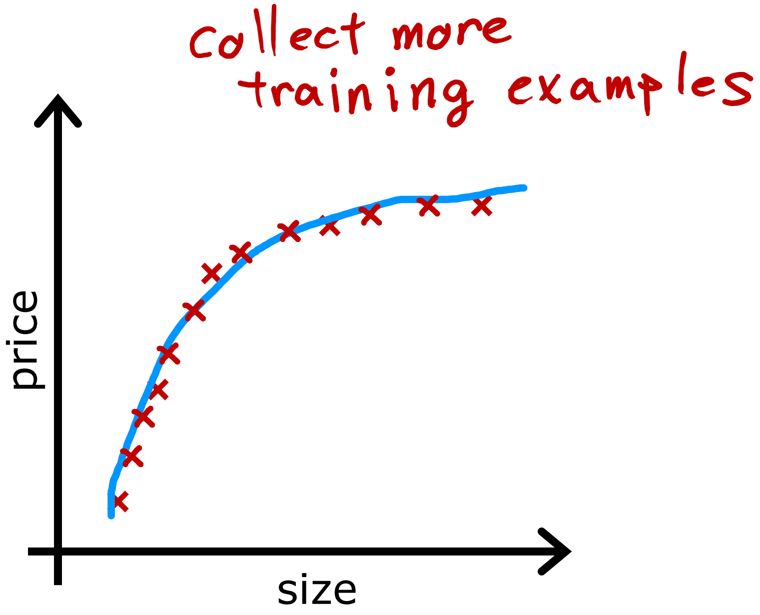
overfit

Regularization to Reduce Overfitting

Addressing Overfitting

Collect more training examples





Select features to include/exclude

size	bedrooms	floors	age	avg income	...	distance to coffee shop	price
x_1	x_2	x_3	x_4	x_5		x_{100}	y

all features

+

insufficient data

↓

overfit

selected features

size
bedrooms
age
just right

feature selection

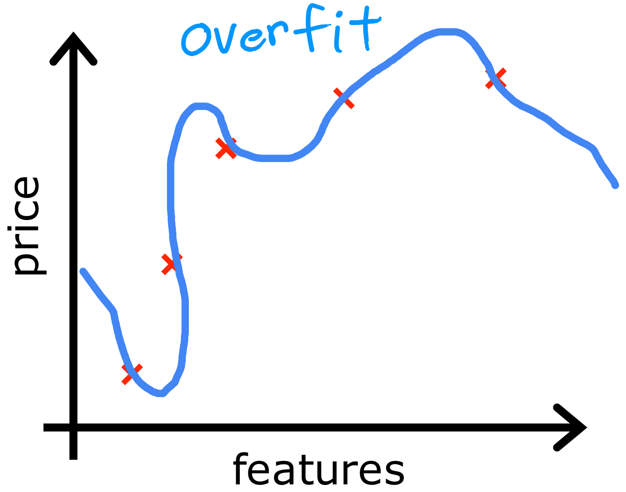
disadvantage

↓

useful features could be lost

Regularization

Reduce the size of parameters w_j

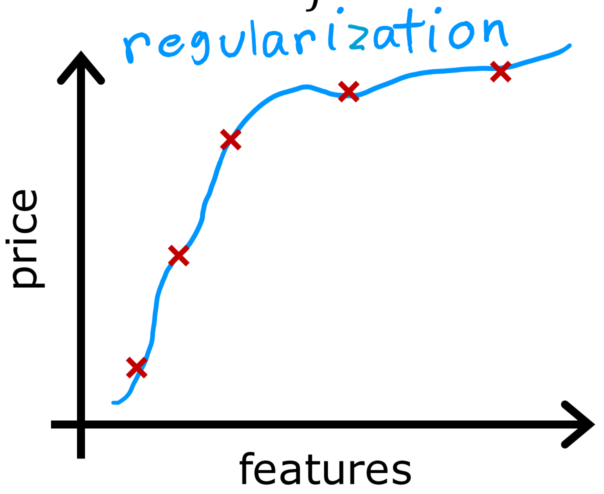


$$f(x) = 28x - 385x^2 + 39x^3 - \cancel{174}x^4 + 10$$

0

large values for w_j

eliminate feature



$$f(x) = 13x - 0.23x^2 + 0.000014x^3 - 0.0001\,x^4 + 10$$

small values for w_j

Addressing overfitting

Options

1. Collect more data

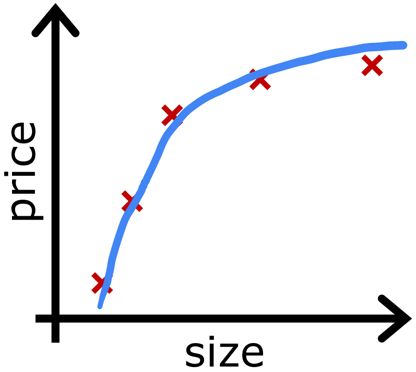
2. Select features
   – Feature selection

3. Reduce size of parameters
   – “Regularization”

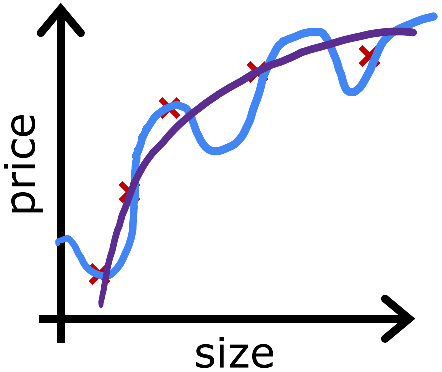
Regularization to Reduce Overfitting

Cost Function with Regularization

Intuition



$w_1x + w_2x^2 + b$



$w_1x + w_2x^2 + w_3x^3 + w_4x^4 + b$

≈0 ≈0

make w_3, w_4 really small (≈ 0)

$$\min_{\vec{w},b} \frac{1}{2m}\sum_{i=1}^{m}\left(f_{\vec{w},b}\left(\vec{x}^{(i)}\right) - y^{(i)}\right)^2 + 1000\, w_3^2 + 1000\, w_4^2$$

0.001 0.002

Regularization

small values $w_1, w_2, \cdots, w_n, b$

simpler model $w_3 \approx 0$

less likely to overfit $w_4 \approx 0$

size	bedrooms	floors	age	avg income	...	distance to coffee shop	price
x_1	x_2	x_3	x_4	x_5		x_{100}	y

n features

$n = 100$

$w_1, w_1, w_2, \cdots, w_{100}, b$

regularization term

$$J(\vec{w}, b) = \frac{1}{2m}\left[\sum_{i=1}^{m}\left(f_{\vec{w},b}\left(\vec{x}^{(i)}\right) - y^{(i)}\right)^2 + \frac{\lambda}{2m}\sum_{j=1}^{n} w_j^2\right]$$

"lambda"

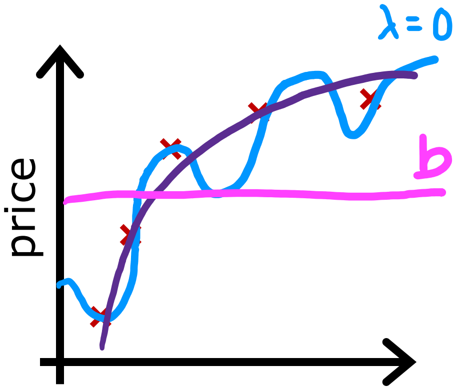
regularization parameter

Regularization

mean squared error / regularization term

$$\min_{\vec{w},b} J(\vec{w},b) = \min_{\vec{w},b}\left[\frac{1}{2m}\sum_{i=1}^{m}\left(f_{\vec{w},b}(\vec{x}^{(i)}) - y^{(i)}\right)^2 + \frac{\lambda}{2m}\sum_{j=1}^{n} w_j^2\right]$$

fit data → λ balances both goals ← Keep w_j small



choose $\lambda = 10^{10}$

$$f_{\vec{w},b}(\vec{x}) = w_1 x + w_2 x^2 + w_3 x^3 + w_4 x^4 + b$$

($w_1 \approx 0$, $w_2 \approx 0$, $w_3 \approx 0$, $w_4 \approx 0$)

$f(x) = b$

Choose λ

Regularization to Reduce Overfitting

Regularized Linear Regression

Regularized linear regression

$$\min_{\vec{w},b} J(\vec{w},b) = \min_{\vec{w},b}\left[\frac{1}{2m}\sum_{i=1}^{m}\left(f_{\vec{w},b}(\vec{x}^{(i)}) - y^{(i)}\right)^2 + \frac{\lambda}{2m}\sum_{j=1}^{n} w_j^2\right]$$

Gradient descent

repeat {

$$w_j = w_j - \alpha \frac{\partial}{\partial w_j} J(\vec{w},b) \qquad = \frac{1}{m}\sum_{i=1}^{m}\left(f_{\vec{w},b}(\vec{x}^{(i)}) - y^{(i)}\right) x_j^{(i)} + \frac{\lambda}{m} w_j$$

$j = 1, \ldots, n$

$$b = b - \alpha \frac{\partial}{\partial b} J(\vec{w},b) \qquad = \frac{1}{m}\sum_{i=1}^{m}\left(f_{\vec{w},b}(\vec{x}^{(i)}) - y^{(i)}\right)$$

} simultaneous update

Implementing gradient descent

repeat {

$$w_j = w_j - \alpha \left[\frac{1}{m} \sum_{i=1}^{m} \left[\left(f_{\vec{w},b}(\vec{x}^{(i)}) - y^{(i)} \right) x_j^{(i)} \right] + \frac{\lambda}{m} w_j \right]$$

$$b = b - \alpha \frac{1}{m} \sum_{i=1}^{m} \left(f_{\vec{w},b}(\vec{x}^{(i)}) - y^{(i)} \right)$$

} simultaneous update $j = 1 \ldots n$

$$w_j = 1 w_j - \alpha \frac{\lambda}{m} w_j - \alpha \frac{1}{m} \sum_{i=1}^{m} \left(f_{w,b}(\vec{x}^{(i)}) - y^{(i)} \right) x_j^{(i)}$$

$$w_j \left(1 - \alpha \frac{\lambda}{m} \right)$$

shrink w_j

usual update

$$\alpha \frac{\lambda}{m}$$

$$0.01 \frac{1}{50} = 0.0002$$

$$w_j (1 - 0.0002)$$

0.9998

How we get the derivative term (optional)

$$\frac{\partial}{\partial w_j} J(\vec{\mathrm{w}}, b) = \frac{\partial}{\partial w_j}\left[\frac{1}{2m}\sum_{i=1}^{m}\left(\underbrace{f(\vec{x}^{(i)})}_{\vec{w}\cdot\vec{x}^{(i)}+b} - y^{(i)}\right)^2 + \frac{\lambda}{2m}\sum_{j=1}^{n} w_j^2\right]$$

$$= \frac{1}{2m}\sum_{i=1}^{m}\left[\left(\vec{w}\cdot\vec{x}^{(i)} + b - y^{(i)}\right) 2 x_j^{(i)}\right] + \frac{\lambda}{2m} 2 w_j \quad \text{No } \sum_{j=1}^{n}$$

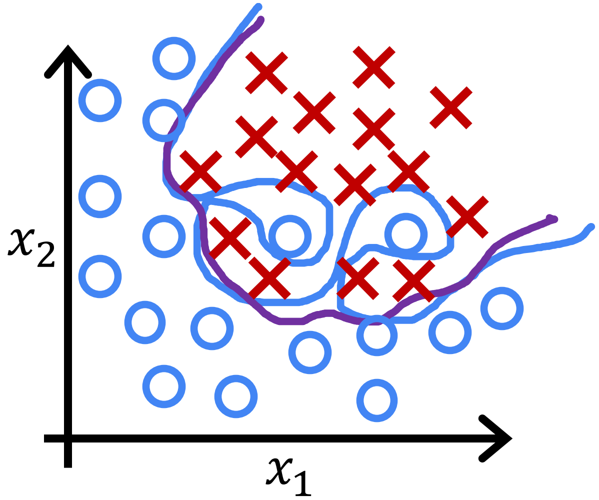
$$= \frac{1}{m}\sum_{i=1}^{m}\left[\left(\underbrace{\vec{w}\cdot\vec{x}^{(i)} + b}_{f(\vec{x})} - y^{(i)}\right) x_j^{(i)}\right] + \frac{\lambda}{m} w_j$$

$$= \frac{1}{m}\sum_{i=1}^{m}\left[\left(f_{\vec{\mathrm{w}},b}(\vec{\mathrm{x}}^{(i)}) - y^{(i)}\right)x_j^{(i)}\right] + \frac{\lambda}{m} w_j$$

Regularization to Reduce Overfitting

Regularized Logistic Regression

Regularized logistic regression



$$z = w_1 x_1 + w_2 x_2 + w_3 x_1^2 x_2 + w_4 x_1^2 x_2^2 + w_5 x_1^2 x_2^3 + \cdots + b$$

$$f_{\vec{w},b}(\vec{x}) = \frac{1}{1 + e^{-z}}$$

Cost function

$$J(\vec{w}, b) = -\frac{1}{m}\sum_{i=1}^{m}\left[y^{(i)}\log\left(f_{\vec{w},b}(\vec{x}^{(i)})\right) + (1 - y^{(i)})\log\left(1 - f_{\vec{w},b}(\vec{x}^{(i)})\right)\right] + \frac{\lambda}{2m}\sum_{j=1}^{n} w_j^2$$

$$\min_{\vec{w},b} J(\vec{w}, b) \rightarrow w_j \downarrow$$

Regularized logistic regression

$$J(\vec{\mathrm{w}},b) = -\frac{1}{m}\sum_{i=1}^{m}\left[y^{(i)}\log\left(f_{\vec{\mathrm{w}},b}(\vec{\mathrm{x}}^{(i)})\right) + (1-y^{(i)})\log\left(1-f_{\vec{\mathrm{w}},b}(\vec{\mathrm{x}}^{(i)})\right)\right] + \frac{\lambda}{2m}\sum_{j=1}^{n} w_j^2$$

$\min_{\vec{w},b}$

Gradient descent

repeat {

$$w_j = w_j - \alpha\frac{\partial}{\partial w_j}J(\vec{\mathrm{w}},b)$$

$j = 1 \ldots n$

$$b = b - \alpha\frac{\partial}{\partial b}J(\vec{\mathrm{w}},b)$$

}

Looks same as for linear regression!

$$= \frac{1}{m}\sum_{i=1}^{m}\left[\left(f_{\vec{\mathrm{w}},b}(\vec{\mathrm{x}}^{(i)}) - y^{(i)}\right)x_j^{(i)}\right] + \frac{\lambda}{m}w_j$$

$$= \frac{1}{m}\sum_{i=1}^{m}\left(f_{\vec{\mathrm{w}},b}(\vec{\mathrm{x}}^{(i)}) - y^{(i)}\right)$$

logistic regression