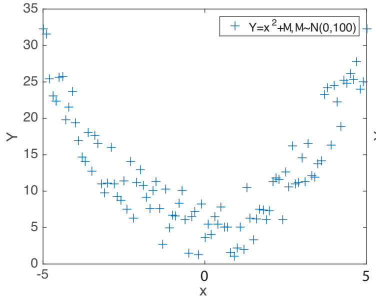
Overview

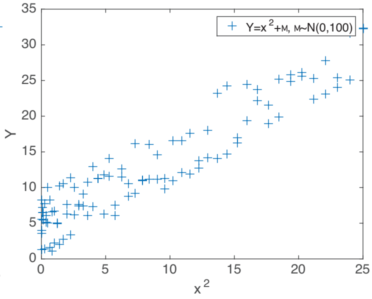
- Fitting nonlinear curves: choosing features
- Gradient Descent in Practice
- Closed-form Solution
- Regularisation and Model Selection

Fitting nonlinear curves: choosing features

Example:

- Hypothesis: $h_\theta(x) = \theta_0 + \theta_1 x^2$
- Define feature vector $\vec{z}$ with $z = x^2$. This new z can be computed given input x, so its known.
- Using this new feature vector our hypothesis can be rewritten as $h_\theta(z) = \theta_0 + \theta_1 z$, so can directly apply all the ideas we've just discussed.





Gradient Descent in Practice: Feature Scaling & Mean Normalisation

For better numerical behaviour:

- Try to make sure that features are on a similar scale, ideally every features lies approximately in range $-1 \leq x_j \leq 1$.
- Replace x_j with $x_j - \mu_j$ (where mean $\mu_j = \frac{1}{m}\sum_{i=1}^{n} x_j^{(i)}$) to make features have approximately zero mean (do not apply to $x_0 = 1$ though)

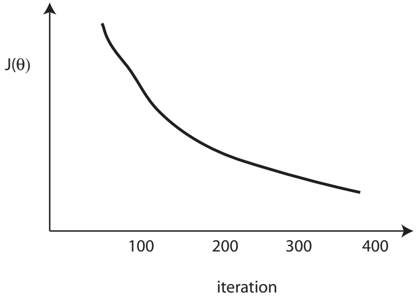
e.g.

- In advertising example TV budget values lie in range 0.7 to 296.4 with mean 147, so rescaling as $\frac{TV-147}{296}$ gives a feature with values in interval $-0.5 \leq x_1 \leq 0.5$
- In general can use $x_1 := \frac{x_1-\mu_1}{max(x_1)-min(x_1)}$ or $x_1 := \frac{x_1-\mu_1}{\sigma_1}$ (where standard deviation $\sigma_j = \sqrt{\frac{1}{m}\sum_{i=1}^{n}(x_j^{(i)} - \mu_j)^2}$)

Gradient Descent in Practice: Learning Rate

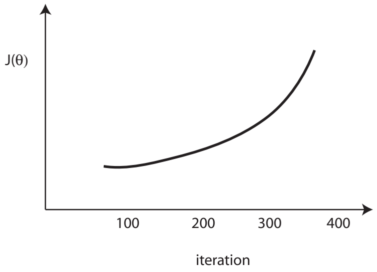
$\theta_j := \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta)$.

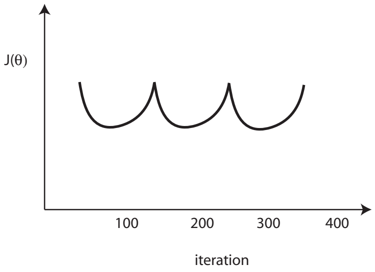
- "Debugging": How to make sure gradient descent is working correctly.
- How to choose learning rate α.



- $J(\theta)$ should decrease after every iteration
- Example stopping criterion: stop when decreases by less than 10^{-3}

Gradient Descent in Practice: Learning Rate





- Use smaller α
- But if α too small then can be slow to converge
- E.g. to choose α try 0.001,0.005,0.01,0.05,0.1

Gradient Descent in Practice: Learning Rate

There are also many automated approaches for adjusting α at each iteration. E.g. using **line search**:

-
  ```
  Repeat {
      Choose descent direction, e.g.
      for $j$=0 to $n$ $\{\delta_j := \frac{2}{m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})x_j^{(i)}\}$
      Select $\alpha$ that makes $J(\theta + \alpha\delta)$ smallest
      $\theta := \theta - \alpha\delta$
  }
  ```

But these involve greater computation cost than using a fixed α

Gradient Descent in Practice: Scalability

Batch Gradient Descent:

```
• Repeat {
      for $j$=0 to $n$ $\{tempj := \theta_j - \frac{2\alpha}{m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})x_j^{(i)}\}$
      for $j$=0 to $n$ $\{\theta_j := tempj\}$
  }
```

at each iteration (i) uses all m training data, (ii) updates all $n+1$ parameters. Common alternatives:

Co-ordinate Gradient Descent:

```
• $j = 0$
• Repeat {
      j:=(j+1)mod (n+1)
      $\theta_j := \theta_j - \frac{2\alpha}{m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})x_j^{(i)}$
  }
```

at each iteration only update a single parameter.

Stochastic Gradient Descent:

```
• Repeat {
  for $i$=1 to $m$ {
      for $j$=0 to $n$ {
          $tempj := \theta_j - \frac{2\alpha}{m}(h_\theta(x^{(i)}) - y^{(i)})x_j^{(i)}$
      }
      for $j$=0 to $n$ $\{\theta_j := tempj\}$
  }
  }
```

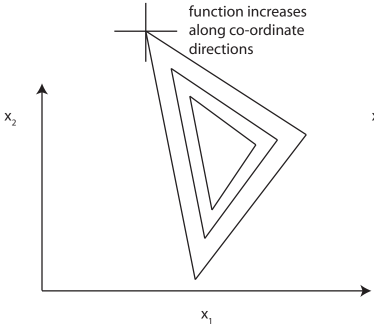
repeatedly runs through training set, each time updating the parameters with respect to a single training example.

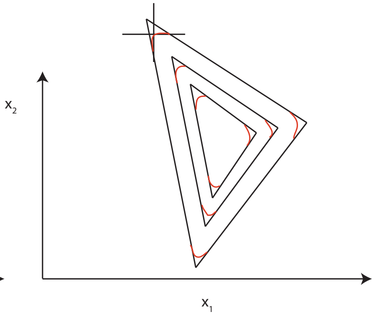
Gradient Descent in Practice: Scalability

Co-ordinate Gradient Descent:

```
• $j = 0$
• Repeat {
    j:=(j+1)mod (n+1)
    $\theta_j := \theta_j - \frac{2\alpha}{m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})x_j^{(i)}$
  }
```

At each iteration only update a single parameter θ_j. So long as update to θ_j causes $J(\theta)$ to decrease then we expect this algorithm to eventually minimise $J(\theta)$. We need some smoothness for this ...





Closed-form solution

We can find the θ that minimises $J(\theta)$ in closed form.

- Example: suppose we can one feature x_1 and one parameter θ_1
- Goal is to select θ_1 to minimise $J(\theta_1) = \sum_{i=1}^{m}(\theta_1 x_1^{(i)} - y^{(i)})^2$
- Compute derivative with respect to θ_1:

$$\frac{dJ}{d\theta_1} = \frac{1}{m}\sum_{i=1}^{m}(\theta_1 x_1^{(i)} - y^{(i)}))x_1^{(i)} = \frac{1}{m}\left(\theta_1 \sum_{i=1}^{m}(x_1^{(i)})^2 - \sum_{i=1}^{m} y^{(i)} x_1^{(i)}\right)$$

- Set derivative equal to 0 and solve for θ_1:

$$\theta_1 \sum_{i=1}^{m}(x_1^{(i)})^2 - \sum_{i=1}^{m} y^{(i)} x_1^{(i)} = 0$$

$$\text{i.e. } \theta_1 = \sum_{i=1}^{m} y^{(i)} x_1^{(i)} / \sum_{i=1}^{m}(x_1^{(i)})^2$$

Closed-form solution

$$\theta_1 = \sum_{i=1}^{m} y^{(i)} x_1^{(i)} / \sum_{i=1}^{m} (x_1^{(i)})^2$$

In vector-matrix notation:

$$\theta_1 = (X^T X)^{-1} X^T y$$

where $y = \begin{bmatrix} y^{(1)} \\ y^{(1)} \\ \vdots \\ y^{(m)} \end{bmatrix}, X = \begin{bmatrix} x_1^{(1)} \\ x_1^{(2)} \\ \vdots \\ x_1^{(m)} \end{bmatrix}$

Closed-form solution (optional)

With multiple features, the minimising vector θ is

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

where $y = \begin{bmatrix} y^{(1)} \\ y^{(1)} \\ \vdots \\ y^{(m)} \end{bmatrix}, X = \begin{bmatrix} 1 & x_1^{(1)} & x_2^{(1)} & \cdots & x_n^{(1)} \\ 1 & x_1^{(2)} & x_2^{(2)} & \cdots & x_n^{(2)} \\ \vdots & & & & \\ 1 & x_1^{(m)} & x_2^{(m)} & \cdots & x_n^{(m)} \end{bmatrix}$

- $(X^T X)^{-1}$ is the inverse of matrix $X^T X$
- It satisfies $(X^T X)^{-1}(X^T X)^{=} I$ where I is the identity matrix.

Comparison of Solution Approaches

m training examples, n features

Gradient Descent

- Need to choose α
- May need many iterations
- Works well even when n is large e.g. $n = 10^6$
- Stochastic gradient descent variant works well even when m is very large (big data)

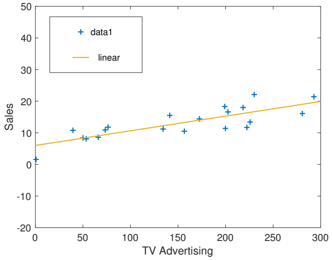
Closed-form Solution

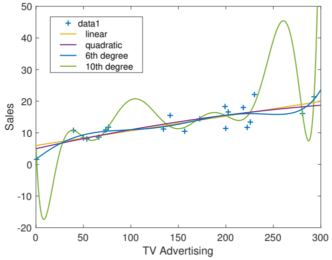
- No need to choose α
- Don't need to iterate
- Need to compute $(X^T X)^{-1}$, n by n matrix and $O(n^3)$ operation. Slow if n is large-ish e.g. ok up to about $n = 1000$.
- Matrix X is m by n so can be hard to work with if m is very large (big data)

Regularisation & Model Selection

Advertising example again. Thin out data by taking every 10th point. Try a few different hypothesis:

- $h_\theta(x) = \theta_0 + \theta_1 x$
- $h_\theta(x) = \theta_0 + \theta_1 x + \theta_2 x^2$
- $h_\theta(x) = \theta_0 + \theta_1 x + \theta_2 x^2 + \cdots + \theta_6 x^6$
- $h_\theta(x) = \theta_0 + \theta_1 x + \theta_2 x^2 + \cdots + \theta_{10} x^{10}$

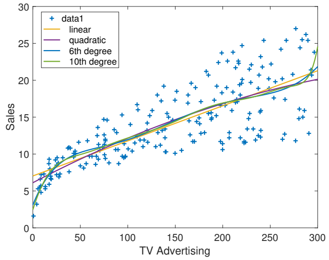


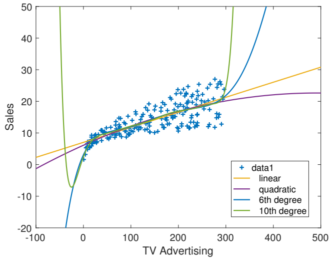


- As we add more parameters, we start to fit the “noise” in the training data, called **overfitting**.
- But of use too few parameters then will get a poor fit, **underfitting**.
- How to strike the right balance between these ? This is an example of the **bias-variance trade-off**.

Regularisation & Model Selection

More data can help, e.g. when don't thin out data:





- But even with more data, still our hypothesis doesn't generalise well i.e. doesn't predict well for data outside the training set.

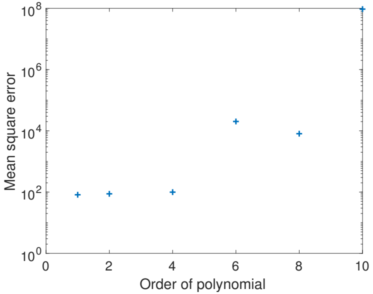
Model Selection

One tactic is to use **cross-validation** for **feature/model selection**.

- Draw **uniformly at random** and **with replacement** a set of $p < m$ points from the set of m training data, e.g. use $p = 0.7m$.
- For hypothesis of interest, find the parameter values θ that fit this set of p points and the corresponding minimum value of the square error $J(\theta) = \frac{1}{m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})^2$.
- Repeat to obtain multiple values of the square error $J(\theta)$, e.g. repeat 1000 times.
- Carry this out for each hypothesis of interest e.g. for different orders of polynomial

Model Selection

Advertising data again. Plot mean value of $J(\theta)$ obtained as the order q of the polynomial used in the hypothesis is varied from 1 to 10, $h_\theta(x) = \theta_0 + \theta_1 x + \theta_2 x^2 + \cdots + \theta_q x^q$



- Error is similar for all polynomials up to about 4, then increases rapidly. Linear fit ($q = 1$) thus seems reasonable.
- Note that since we have samples the training data, these values are themselves “noisy” (will change depending on the random sample used).

Regularisation

Another tool in our armoury is **regularisation** i.e. add constraints/penalties on the parameters θ. That is, change $J(\theta)$ to

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

where $R(\theta)$ is a penalty function. Two common regularisation penalties:

- Quadratic/L2 penalty: $R(\theta) = \theta^T\theta = \sum_{j=1}^{n}\theta_j^2$. Also called Tikhonov regularisation. Ridge regression. Encourages elements of θ to have small value.
- L1 penalty: $R(\theta) = \sum_{j=1}^{n}|\theta_j|$. LASSO regression. Encourages sparsity of solution i.e. few non-zero elements in θ.

Regularisation: Ridge Regression

Select θ to minimise

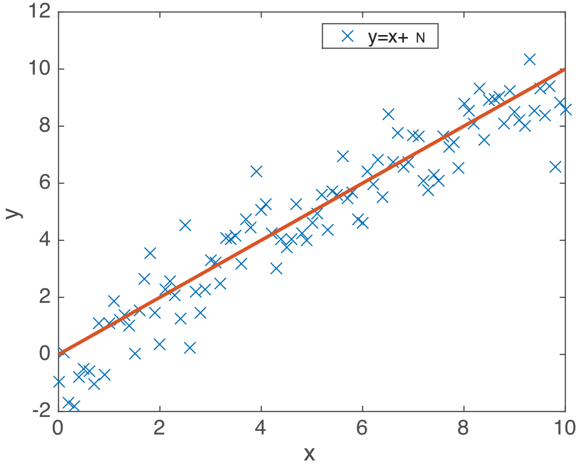
$$\frac{1}{m}\sum_{i=1}^{m}(h_\theta(x^{(i)})-y^{(i)})^2+\frac{1}{\lambda}\sum_{j=1}^{n}\theta_j^2$$

This is called **ridge regression**.

- When $\lambda \to 0$, then we are saying that we are certain $\theta = 0$.
- When λ is large we are saying that we know little about the value of θ prior to making the observations. The penalised estimate is then close to the non-penalised estimate.
- We can also use cross-validation to help choose λ

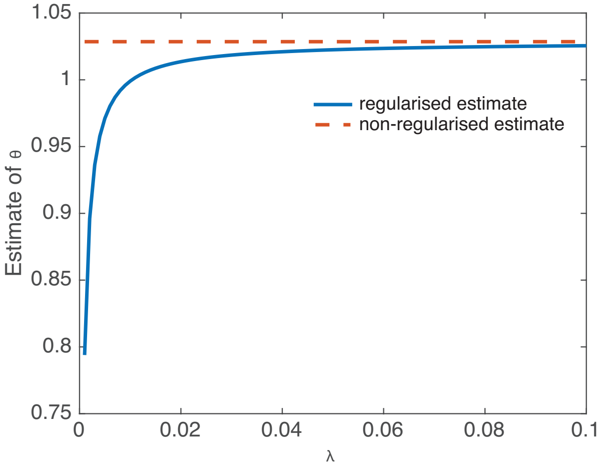
Regularisation: Ridge Regression

Example: training data is $y^{(i)} = x^{(i)} + N^{(i)}$, $i = 1, \ldots, m$ where $N^{(i)}$ is noise.



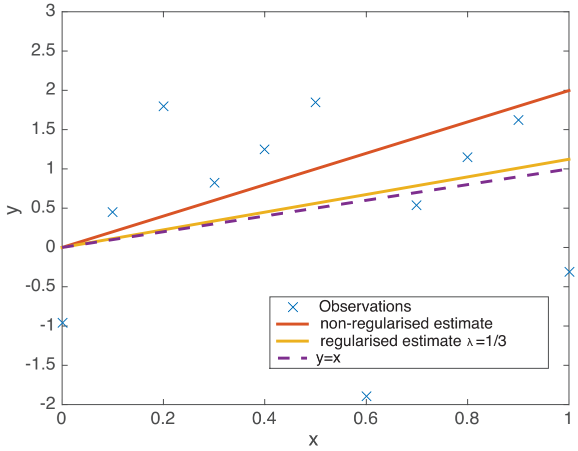
Regularisation: Ridge Regression

Impact of λ:



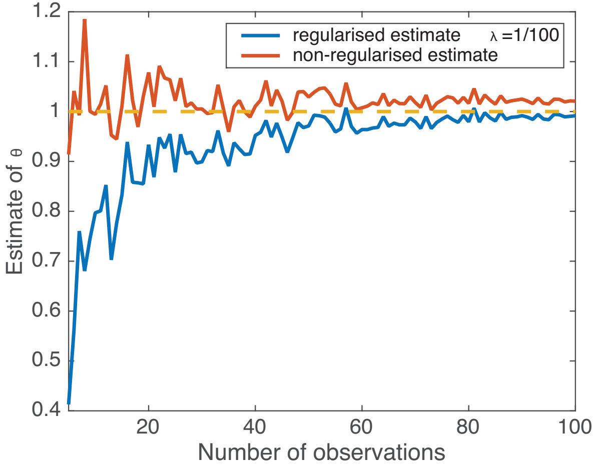
Regularisation

Regularisation really kicks in when we only have a small number of observations, yet still need to make a prediction. Our prior beliefs regarding whether θ is small or not are then especially important.



Regularisation

- But as number m of observations grows, other things being equal the impact of regularisation tends to decline.


regularised estimate
λ =1/100
non-regularised estimate
Estimate of θ
Number of observations