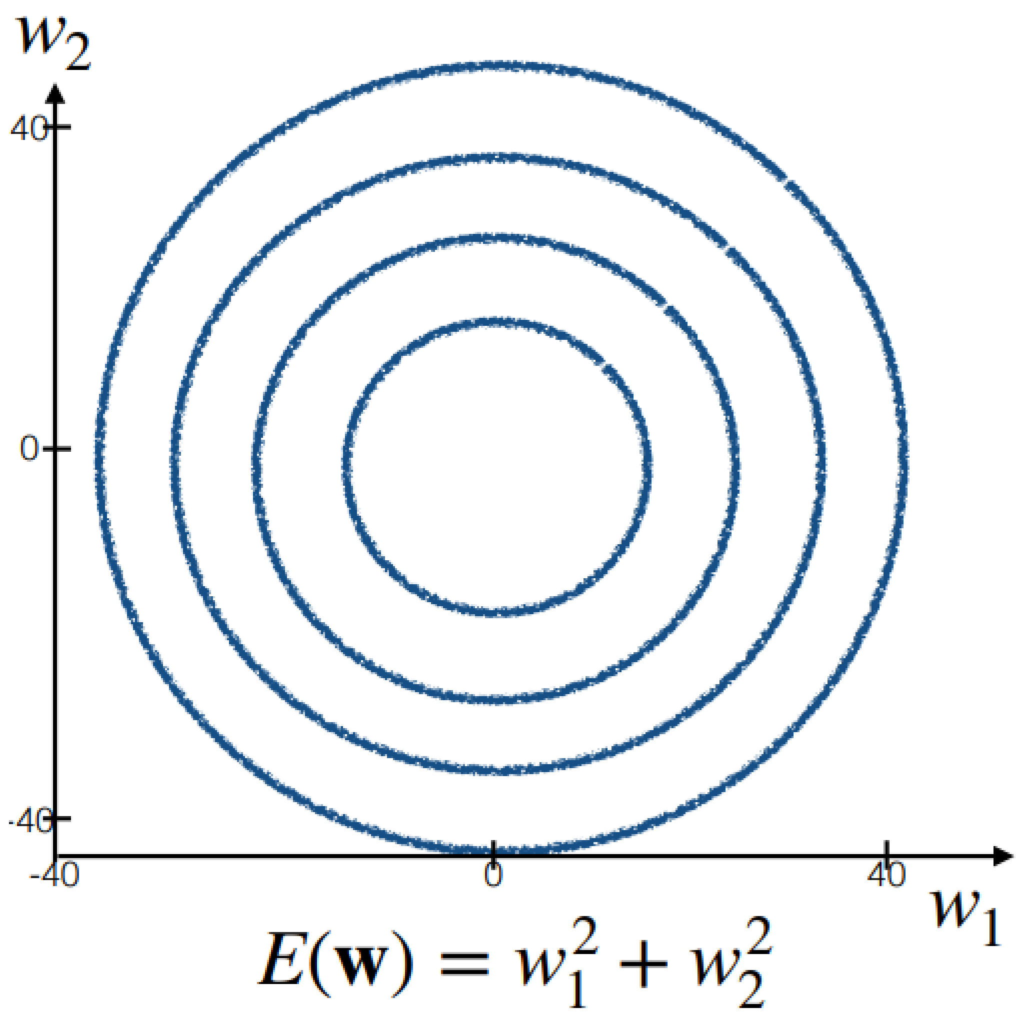
Week 2 Note

Gradient Descent

- Local Minima and Learning Rate
  - Gradient descent can get stuck in `local minima`
    - But this is not an issue in the case of **Logistic Regression** using **Cross-Entropy Loss**, because the function being optimised is `strictly convex`
  - **Too large** learning rate - The algorithm may **jump across** the optimum
  - **Too small** learning rate - It may take a **long time** to find the optimum
- Differential Curvature



$$E(\vec{w}) = w_1^2 + w_2^2 \text{ for example}$$

  - Contour plots(等高线图) of the loss function, where each line corresponds to points in the input space where the loss is the same

- Steepest descent forms a 90 degree angle with the line

$$E(\vec{w}) = w_1^2 + 4w_2^2$$

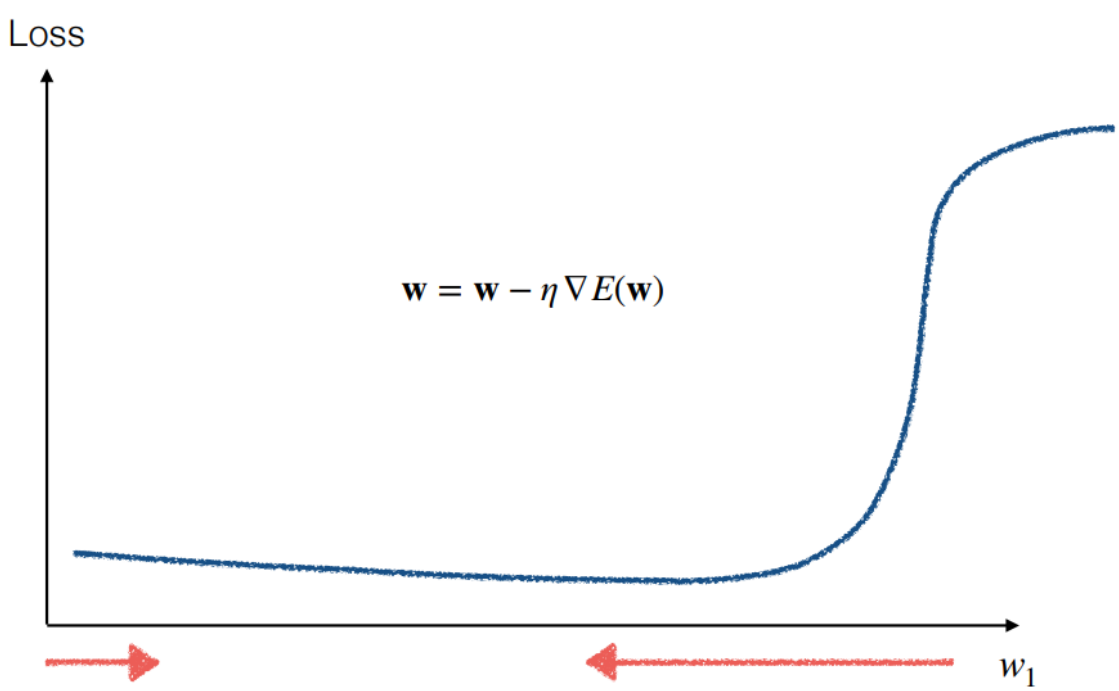
- In the elliptical bowl function, the gradients along the w_1 and w_2 axis have different magnitudes

> $\frac{\partial E}{\partial w_2} > \frac{\partial E}{\partial w_1}$ depending on the location

- The path of the steepest descent in most loss functions is only an instantaneous direction of best movement, and is not eh best direction in the longer term

- Standardisation
  - Different partial dervatives with respect to different weights can be a result of different input variables having different scales and variances affecting the loss function to different extents
  - Standardising input variables (e.g., by deducting the mean from each input variable and then dividing by the standard deviation) can help with this

- Difficult Topologies(可能存在的, GD非最优解的情况)



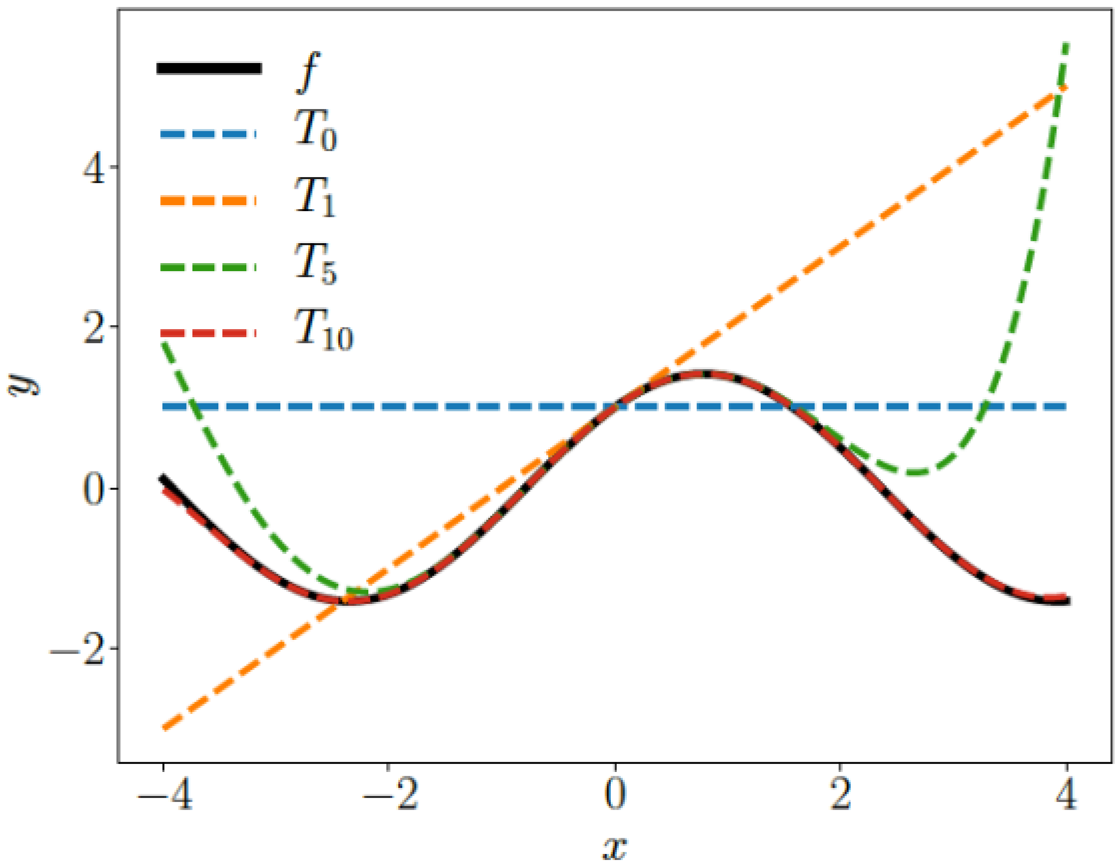
  - Smaller gradient, slow due to small steps
  - Big gradient, likely to overshoot

Newton-Raphson

$$w = w - \frac{E'(w)}{E''(w)}$$

> **Reduce** the size of the update if the curvature is high

- `Taylor Polynomial of degree` n can be used to approximate a function $E(w)$ at w_0:



$$f(x) = \sin(x) + \cos(x)$$

$$T_n(w) = \sum_{k=0}^{n} \frac{E^k(w_0)}{k!}(w - w_0)^k$$

where $E^{(k)}(w_0)$ is the k-th order derivative of E at w_0

> 在知道函数在w_0处的所有信息（即其值及其所有导数的值）的情况下，如何在该点附近近似函数的值

- `Taylor polynomial of degree 2` to approximate our loss function at w_0

$$\frac{d}{dw}(E(w_0) + (w - w_0)E'(w_0) + \frac{(w - w_0)^2}{w}E''(w_0)) = 0$$

this will lead to the following `weight update rule`:

$$w := w - \frac{E'(w)}{E''(w)}$$

Newton-Raphson Method: Multivariate Case

- The `Hessian matix`

$$\frac{\partial}{\partial x_i}(\frac{\partial f}{\partial x_i}) = \frac{\partial^2 f}{\partial x_i^2}, \frac{\partial}{\partial x_i}(\frac{\partial f}{\partial x_j}) = \frac{\partial^2 f}{\partial x_i \partial x_j}$$

$$H(f(\vec{x})) = H_f(\vec{x}) = \begin{bmatrix} \frac{\partial^2 f}{\partial x_0^2} & \frac{\partial^2 f}{\partial x_0 \partial x_1} & \cdots & \frac{\partial^2 f}{\partial x_0 \partial x_n} \\ \frac{\partial^2 f}{\partial x_1 \partial x_0} & \frac{\partial^2 f}{\partial x_1^2} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_d \partial x_1} & \frac{\partial^2 f}{\partial x_d \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_d^2} \end{bmatrix}$$

- Weight Update Rule
  - Univariate update rule:

$$w = w - \frac{E'(w)}{E''(w)}$$

  - Multivariate update rule:

$$\vec{w} = \vec{w} - H_E^{-1}(\vec{w}) \triangledown E(\vec{w})$$

  where $H_E^{-1}(\vec{w})$ is the inverse of the Hessian at the old $\vec{w}$ and $\triangledown E(\vec{w})$ is the gradient at the old w

- Logistic Regression - Iterative Reweighted Least Squares

$$\vec{w} = \vec{w} - H_E^{-1}(\vec{w}) \triangledown E(\vec{w})$$

$$H_E(\vec{w}) = \sum_{i=1}^{N} p(1|\vec{x}^{(i)}, \vec{w})(1 - p(1|\vec{x}^{(i)}, \vec{w}))\vec{x}^{(i)}\vec{x}^{(i)^T}$$

$$\triangledown_E(\vec{w}) = \sum_{i=1}^{N} (p(1|\vec{x}^{(i)}, \vec{w}) - y^{(i)})\vec{x}^{(i)}$$

Summary - Gradient Descent

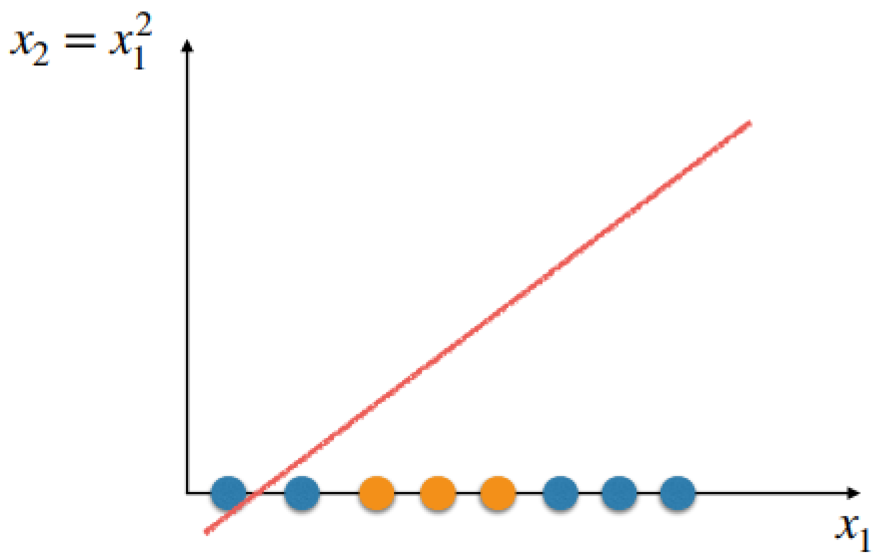
Gradient descent may require a large number of iterations depending on the shape of the loss function.

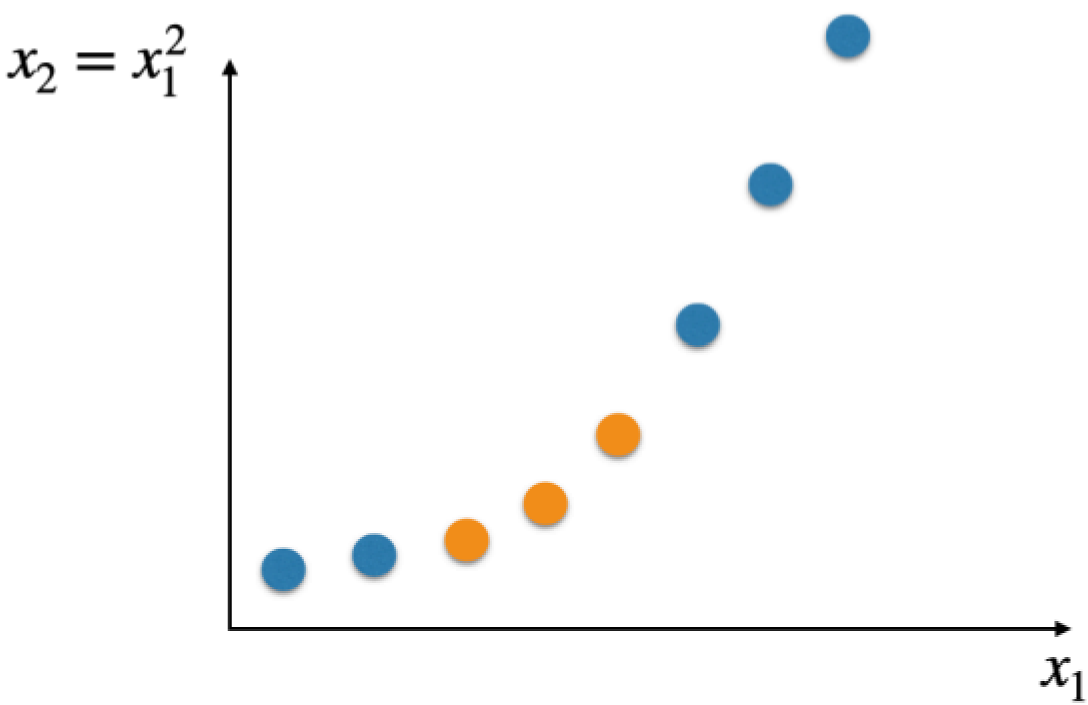
- Iterative Reweighted Least Squares / Newton-Raphson can be used in an attempt to reach the minimum with less steps.
- It does so by creating a quadratic approximation of the loss function and finding the minimum of this quadratic approximation.
- This results in making use of information about the curvature of the loss function to:
- avoid large steps in directions where the gradient is changing too much or
- increase the size of the steps in directions where the gradient is not changing much

> Norm - 向量的模长

Nonlinear Transformations

Higher dimensional embedding/feature space: $\underbrace{\phi(\vec{x})}_{\text{feature transform/basis expansion}} = \underbrace{(x_1, x_1^2)^T}_{\text{basis functions}}$





- Example for polynomial
  - of order 2and a problem with 1 input variables:

$$\vec{x} = (1, x_1) \rightarrow \phi(\vec{x}) = (1, x_1, x_1^2)^T$$

- of order 2 and a problem with 2 input variables:

$$\vec{x} = (1, x_1, x_2)^T \rightarrow \phi(\vec{x}) = (1, x_1, x_2, x_1^2, x_2^2, x_1 x_2)^T$$

> If we follow this idea, any decision boundary that is a polynomial of order p in $\vec{x}$ is linear in $\phi(\vec{x})$
>
> So, we can adopt linear models in the higher dimensional embedding formed by $\phi(\vec{x})$, to learn decision boundaries corresponding to polynomials of order p in x

Adopting Nonlinear Transformations in Logistic Regression

$$logit(p_1) = \vec{w}^T \phi(\vec{x})$$

$$p_1 = p(1|\phi(\vec{x}), \vec{w}) = \frac{e^{\vec{w}^T \phi(\vec{x})}}{1 + e^{\vec{w}^T \phi(\vec{x})}}$$

$$\text{Given } \; J = \{(\phi(\vec{x}^{(1)}, y^1), (\phi(\vec{x}^{(2)}, y^2), ..., (\phi(\vec{x}^{(N)}, y^N)\}, \arg\min_{\vec{w}} E(\vec{w})$$

$$E(\vec{w}) = -\sum_{i=1}^{N} y^i \ln p(1|\phi(\vec{x}^{(i)}, \vec{w}) + (1 - y^i) \ln(1 - p(1|\phi(\vec{x}^{(i)}, \vec{w}))$$

$$\nabla E(\vec{w}) = \sum_{i=1}^{N} (p(1|\phi(\vec{x}^{(i)}), \vec{w}) - y^i) \phi(\vec{x}^{(i)}$$

$$H_E(\vec{w}) = \sum_{i=1}^{N} p(1|\phi(\vec{x})^i, \vec{w})(1 - p(1|\phi(\vec{x}^{(i)}), \vec{w}))\phi(\vec{x}^{(i)})\phi(\vec{x}^{(i)})^T$$

1. Choose a nonlinear transformation.
2. Apply it to the training examples so that they have the format $(\phi(\vec{x}), y)$
3. Create a linear model $h'(\phi(\vec{x}))$ based on the transformed training examples
4. Determine the (nonlinear) model $h(\vec{x})$ by replacing $\phi_I(\vec{x})$ with the corresponding value that depends on $\vec{x}$

> - Advantages of Linear Models
>   - Linear models are often associated to relatively efficient learning algorithms
>   - They can be robust and have good generalisation properties
> - Caveats of Nonlinear Transforms
>   - The number of dimensions may become very high
>   - Choosing a nonlinear transformation that fits the training examples well does not necessarily mean that there will be good generalisation

Summary - Nonlinear Transformations

- We can create nonlinear transformations to obtain a higher dimensional embedding where our problems become linearly separable, even if they were not linearly separable in the original space
- We can then adopt our original logistic regression to create a linear decision boundary in this higher dimensional embedding
- This idea can is also applicable to other linear models