

QUESTION 4

ABHAY SHANKAR K: CS21BTECH11001 & KARTHEEK TAMMANA: CS21BTECH11028

(I) Knowing the maximum likelihood function,

$$p(\mathbf{t}|\mathbf{w}) = \prod_{n=1}^N y_n^{t_n} (1 - y_n)^{1-t_n}$$

we can obtain the cross-entropy error function by taking negative logarithm:

$$(1) \quad E(\mathbf{w}) = - \sum_{n=1}^N (t_n \ln y_n + (1 - t_n) \ln(1 - y_n))$$

Taking gradients of 1 with respect to \mathbf{w} , we have

- Gradient of the error:

$$\nabla E(\mathbf{w}) = \sum_{n=1}^N (y_n - t_n) \phi_n = \Phi^T (\mathbf{y} - \mathbf{t})$$

- The Hessian:

$$\nabla \nabla E(\mathbf{w}) = \sum_{n=1}^N y_n (1 - y_n) \phi_n \phi_n^T = \Phi^T \mathbf{R} \Phi$$

where \mathbf{R} is the diagonal matrix given by $R_{nn} = y_n(1 - y_n)$

- Update function:

$$(2) \quad \begin{aligned} \mathbf{w}^{(new)} &= \mathbf{w}^{(old)} - \mathbf{H}^{-1} \nabla E(\mathbf{w}) \\ \mathbf{w}^{(new)} &= \mathbf{w}^{(old)} - \mathbf{H}^{-1} \nabla E(\mathbf{w}) \\ &= \mathbf{w}^{(old)} - (\Phi^T \mathbf{R} \Phi)^{-1} \Phi^T (\mathbf{y} - \mathbf{t}) \\ &= (\Phi^T \mathbf{R} \Phi)^{-1} \left(\Phi^T \mathbf{R} \Phi \mathbf{w}^{(old)} - \Phi^T (\mathbf{y} - \mathbf{t}) \right) \\ &= (\Phi^T \mathbf{R} \Phi)^{-1} \Phi^T \mathbf{R} \mathbf{z} \end{aligned}$$

with

$$\mathbf{z} = \Phi \mathbf{w}^{(old)} - \mathbf{R}^{-1} (\mathbf{y} - \mathbf{t})$$

where Φ is the $N \times M$ design matrix, whose n 'th row is given by ϕ_n^T , and $y_n = \sigma(\mathbf{w}^T \phi_n)$.

The algorithm for update, implemented in python:

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import numpy as np
def update(w, Phi, t):
    y = np.array([sigmoid(p @ w) for p in Phi])
    R = np.diag(y * (1 - y))
    z = Phi @ w - np.linalg.inv(R) @ (y - t)
    return np.linalg.inv(Phi.T @ R @ Phi) @ Phi.T @ R @ z

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(II) • Modifying 2, we get

$$(\Phi^T \mathbf{R} \Phi) \mathbf{w} = \Phi^T \mathbf{R} \mathbf{z}$$

which is the normal equation for weighted least squares. Thus, the new weight vector $\mathbf{w}^{(new)}$ is the solution to the weighted least squares problem with \mathbf{z} and the weighing matrix \mathbf{R} .

- The weighing matrix R is not constant, but depends on the parameter vector \mathbf{w} .

Thus, we must apply the normal equations iteratively, each time using the new weight vector \mathbf{w} to compute a revised weighing matrix R . So, the algorithm is known as iterative reweighted least squares (IRLS).

(III) With the Hessian:

$$\mathbf{H} = \Phi^T \mathbf{R} \Phi$$

We know that a function is concave if it's Hessian is positive definite. Thus, it is sufficient to prove positive-definiteness of the Hessian.

Expanding $\mathbf{u}^T \mathbf{H} \mathbf{u}$, we can prove positive-definiteness

$$\begin{aligned}
 \mathbf{u}^T \mathbf{H} \mathbf{u} &= \mathbf{u}^T \Phi^T \mathbf{R} \Phi \mathbf{u} \\
 &= (\mathbf{u}^T \Phi^T) \mathbf{R} (\Phi \mathbf{u}) \\
 &= \sum_{n=1}^N u_n \phi_{\mathbf{n}}^T R_{nn} \phi_{\mathbf{n}} u \\
 &= \sum_{n=1}^N R_{nn} \|\phi_{\mathbf{n}}\|^2 (u_n)^2 \\
 &> 0
 \end{aligned}
 \tag{3}$$

We have used the fact that $R_{nn} > 0$ and $\mathbf{u} \neq 0$. Thus, the Hessian is positive-definite, and the function is concave-up with unique minimum.