

If there is a total of W weights and biases in the network, then \mathbf{w} and \mathbf{b} have length W and \mathbf{H} has dimensionality $W \times W$. From (7.3), the corresponding local approximation to the gradient is given by

$$\nabla E(\mathbf{w}) = \mathbf{b} + \mathbf{H}(\mathbf{w} - \hat{\mathbf{w}}). \quad (7.6)$$

For points \mathbf{w} that are sufficiently close to $\hat{\mathbf{w}}$, these expressions will give reasonable approximations for the error and its gradient.

Consider the particular case of a local quadratic approximation around a point \mathbf{w}^* that is a minimum of the error function. In this case there is no linear term, because $\nabla E = 0$ at \mathbf{w}^* , and (7.3) becomes

$$E(\mathbf{w}) = E(\mathbf{w}^*) + \frac{1}{2}(\mathbf{w} - \mathbf{w}^*)^T \mathbf{H}(\mathbf{w} - \mathbf{w}^*) \quad (7.7)$$

where the Hessian \mathbf{H} is evaluated at \mathbf{w}^* . To interpret this geometrically, consider the eigenvalue equation for the Hessian matrix:

$$\mathbf{H}\mathbf{u}_i = \lambda_i \mathbf{u}_i \quad (7.8)$$

Appendix A

where the eigenvectors \mathbf{u}_i form a complete orthonormal set so that

$$\mathbf{u}_i^T \mathbf{u}_j = \delta_{ij}. \quad (7.9)$$

We now expand $(\mathbf{w} - \mathbf{w}^*)$ as a linear combination of the eigenvectors in the form

$$\mathbf{w} - \mathbf{w}^* = \sum_i \alpha_i \mathbf{u}_i. \quad (7.10)$$

This can be regarded as a transformation of the coordinate system in which the origin is translated to the point \mathbf{w}^* and the axes are rotated to align with the eigenvectors through the orthogonal matrix whose columns are $\{\mathbf{u}_1, \dots, \mathbf{u}_W\}$. By substituting (7.10) into (7.7) and using (7.8) and (7.9), the error function can be written in the form

Appendix A

Exercise 7.1

$$E(\mathbf{w}) = E(\mathbf{w}^*) + \frac{1}{2} \sum_i \lambda_i \alpha_i^2. \quad (7.11)$$

Suppose we set all $\alpha_i = 0$ for $i \neq j$ and then vary α_j , corresponding to moving \mathbf{w} away from \mathbf{w}^* in the direction of \mathbf{u}_j . We see from (7.11) that the error function will increase if the corresponding eigenvalue λ_j is positive and will decrease if it is negative. If all eigenvalues are positive then \mathbf{w}^* corresponds to a local minimum of the error function, whereas if they are all negative then \mathbf{w}^* corresponds to a local maximum. If we have a mix of positive and negative eigenvalues then \mathbf{w}^* represents a saddle point.

A matrix \mathbf{H} is said to be *positive definite* if, and only if,

$$\mathbf{v}^T \mathbf{H} \mathbf{v} > 0, \quad \text{for all } \mathbf{v}. \quad (7.12)$$