CS 5785 – Modern Analytics – Lec. 4

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1 Newton-Raphson

As described at the end of last lecture, to maximize the log likelihood $\ell(\beta)$ we will make use of both its first and second order derivatives. Let's first review what we can do with just first order derivatives and then see what the second order derivatives have to offer. The sequence of panels in Fig. 1 from Wikipedia illustrates Newton's method for finding a root (zero crossing) of a function (shown in blue).

In our case we wish to solve the related problem of finding the maximum of a function. We will do this using both the first and second derivatives as shown in Fig. 2 for a 1D function. Instead of fitting a tangent line to the function to generate the next guess, we fit a local quadratic approximation, i.e., a function that has the same 1st and 2nd derivatives as the function in the neighborhood of a guess. In higher dimensions, as with our log likelihood $\ell(\beta)$ where $\beta \in \mathbb{R}^{p+1}$, the counterparts to the 1st and 2nd derivatives are the gradient and the Hessian, respectively.

As we saw in the last lecture, the gradient of the log likelihood is given by

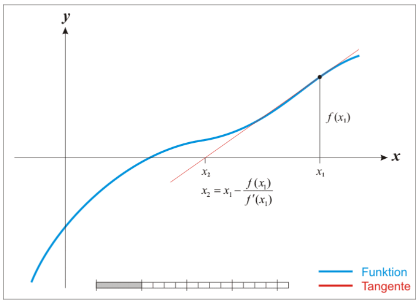
$$\frac{\partial \ell(\beta)}{\partial \beta} = \sum_{i=1}^{N} x_i(y_i - p(x_i;\beta)) \tag{1}$$

Note that the gradient is a length $p+1$ vector. We can see from this expression that the gradient can be expressed as a sum of feature vectors $x_i \in \mathbb{R}^{p+1}$, $i = 1, \ldots, N$, weighted by $y_i - p(x_i;\beta)$. We can interpret that weight as a signed error, since $p(x_i;\beta)$, the posterior probability, aims to approximate y_i.

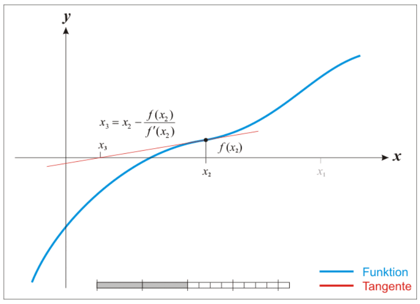
It is straightforward to show that the Hessian of $\ell(\beta)$, which is a $(p+1) \times (p+1)$ matrix, is given by

$$\frac{\partial^2 \ell(\beta)}{\partial \beta \partial \beta^\top} = -\sum_{i=1}^{N} x_i x_i^\top p(x_i;\beta)\,(1 - p(x_i;\beta))$$

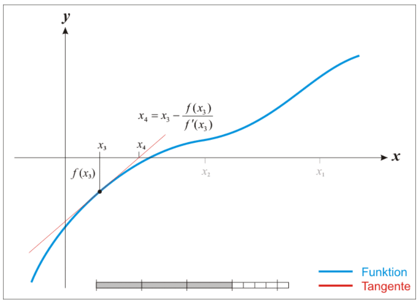
This matrix is a sum of terms of the form $x_i x_i^\top$ weighted by $p(x_i;\beta)(1-p(x_i;\beta))$ and it characterizes the curvature of the function we're trying to minimize. Each $x_i x_i^\top$ term is the *outer product* of x_i with itself, resulting in a symmetric matrix of size $(p+1) \times (p+1)$. We will see soon that this is closely related to how we compute the *covariance matrix* for $\{x_i\}_1^N$. The scalar weight $p(x_i;\beta)(1 - p(x_i;\beta))$ has a small value when $p(x_i;\beta)$ is close to y_i. If $p(x_i;\beta)$ is close to 1 then



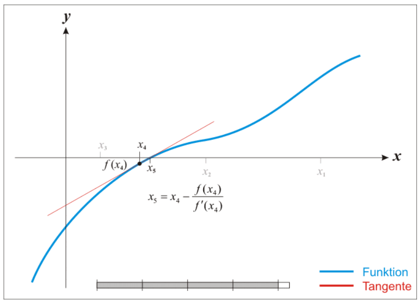
(a) Start with a guess x_1, find the tangent line using the first derivative, extrapolate to get next guess x_2.



(b) Repeat this process to get x_3, which as we can see overshoots in this case.



(c) Keep iterating



(d) until a sufficiently accurate value is reached.

Figure 1: Illustration of Newton's method for finding a root. (Wikipedia)

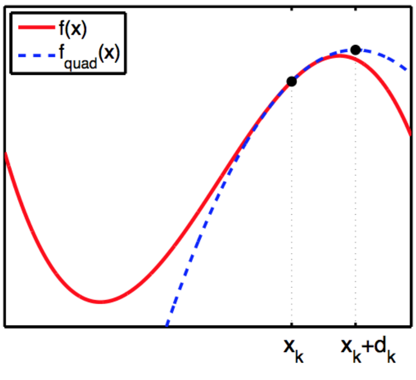


Figure 2: Finding a local maximum of a function $f(x)$ using a quadratic approximation. We start with a guess at x_k. Using both the 1st and 2nd order derivatives we fit a quadratic approximation to the function at that point. That function $f_{\text{quad}}(x)$, is equivalent to the 2nd order Taylor series approximation of $f(x)$ around x_k. We can easily solve for the maximum of this function and obtain the next guess for the maximum, $x_k + d_k$. We repeat this process until convergence. (Murphy)

$1 - p(x_i;\beta)$ is close to 0 and vice versa, which means that if the approximation is good at least one multiplier in the expression $p(x_i;\beta)(1 - p(x_i;\beta))$ is close to 0. As a result, the entire expression has a very low value far from the decision boundary. If $p(x_i;\beta)$ is a bad approximation of y_i there is a higher chance that the classification is incorrect and as such $p(x_i;\beta)$ is closer to 0.5, $1 - p(x_i;\beta)$ is also close to 0.5 making the entire expression close to 0.25. If we look back at the Hessian we can now see that the sum emphasizes x_is that we are less certain of their classification making the contribution to the Hessian larger when the choice of β results in a poor decision boundary.

1.1 Iterative Reweighted Least Squares (IRLS)

In IRLS we start by picking a random choice for β and apply a "Newton update" to get a better β. We continue taking Newton steps until we reach convergence. A Newton update is:

$$\beta^{new} = \beta^{old} - \left(\frac{\partial^2 \ell(\beta)}{\partial\beta\partial\beta^\top}\right)^{-1} \frac{\partial \ell(\beta)}{\partial\beta}$$

in which the derivatives are evaluated at $\beta = \beta^{old}$. If we put this in matrix notation we get:

$$\frac{\partial \ell(\beta)}{\partial\beta} = \mathbf{X}^\top(\mathbf{y} - \mathbf{p})$$

$$\frac{\partial^2 \ell(\beta)}{\partial\beta\partial\beta^\top} = -\mathbf{X}^\top\mathbf{W}\mathbf{X}$$

Where:

- $\mathbf{y}$ is a vector of all the y_is.
- $\mathbf{X} \in \mathbb{R}^{N\times(p+1)}$ is the matrix of all the feature vectors x_is.
- $\mathbf{p}$ is a vector of the $p(x_i;\beta)s$.
- $\mathbf{W} \in \mathbb{R}^{N\times N}$ is a diagonal weighting matrix containing the values of $p(x_i;\beta)(1 - p(x_i;\beta))$ on the diagonal.

When we write the Newton update using this notation we get:

$$\beta^{new} = \beta + (\mathbf{X}^\top\mathbf{W}\mathbf{X})^{-1}\mathbf{X}^\top(\mathbf{y} - \mathbf{p})$$

$$\Downarrow$$

(Multiply β by $(\mathbf{X}^\top\mathbf{W}\mathbf{X})^{-1}(\mathbf{X}^\top\mathbf{W}\mathbf{X})$ which is the same as not changing it)

$$\beta^{new} = (\mathbf{X}^\top\mathbf{W}\mathbf{X})^{-1}(\mathbf{X}^\top\mathbf{W}\mathbf{X})\beta + (\mathbf{X}^\top\mathbf{W}\mathbf{X})^{-1}\mathbf{X}^\top(\mathbf{y} - \mathbf{p})$$

$$\Downarrow$$

(Factor out $(\mathbf{X}^\top\mathbf{W}\mathbf{X})^{-1}\mathbf{X}^\top\mathbf{W}$)

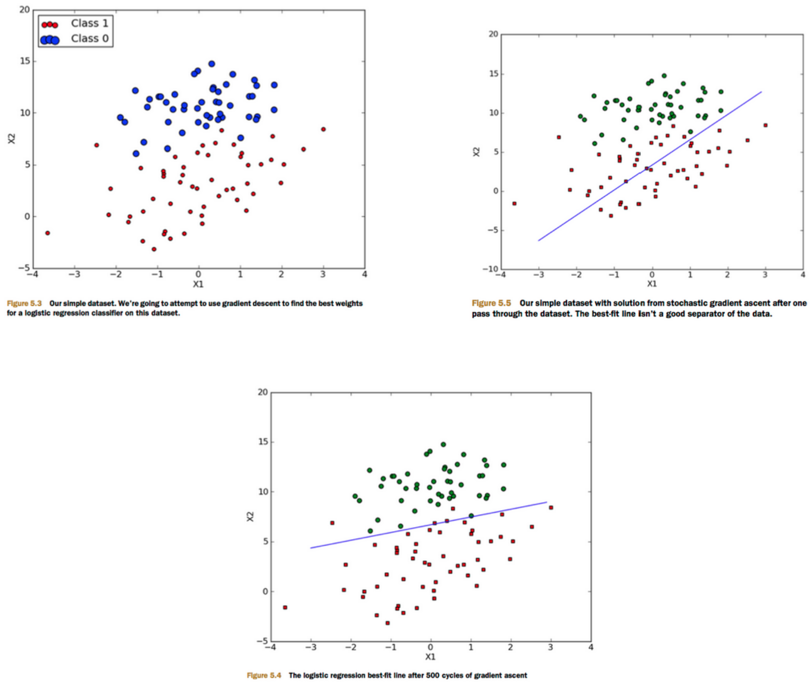


Figure 3: Logistic regression example (Harrington)

$$\beta^{new} = (\mathbf{X}^\top \mathbf{W}\mathbf{X})^{-1}\mathbf{X}^\top \mathbf{W}(\mathbf{X}\beta + \mathbf{W}^{-1}(\mathbf{y} - \mathbf{p}))$$

$$\Downarrow$$

$$\beta^{new} = (\mathbf{X}^\top \mathbf{W}\mathbf{X})^{-1}\mathbf{X}^\top \mathbf{W}\mathbf{z}$$

in which $\mathbf{z} = \mathbf{X}\beta + \mathbf{W}^{-1}(\mathbf{y} - \mathbf{p})$. We call $\mathbf{z}$ the *adjusted response*.
In every IRLS iteration we solve this equation with a new set of $\mathbf{p}$, $\mathbf{W}$ and $\mathbf{z}$. We get:

$$\beta^{new} \leftarrow \arg\min_\beta (\mathbf{z} - \mathbf{X}\beta)^\top \mathbf{W}(\mathbf{z} - \mathbf{X}\beta)$$

We iterate this step until convergence. This is named *Iteratively Reweighted Least Squares* since in every iteration it solves a weighted least squares problem.

One remaining question is, how do we initialize β? Starting with $\beta = 0$ is often OK. Another option is to use multiple randomized restarts to reduce the chances of getting stuck at a local maximum.

2 Online Learning

2.1 Stochastic Gradient Descent

IRLS is called a "batch" method since it has all the necessary data in advance, but that is not always possible or available. For example, the data could be too big to fit into memory. Online learning updates β every step based on

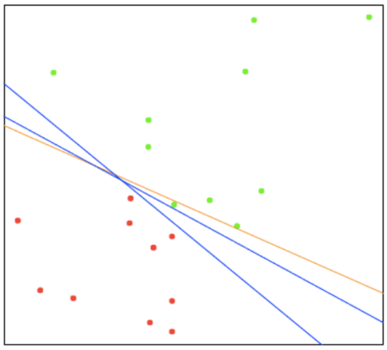


FIGURE 4.14. *A toy example with two classes separable by a hyperplane. The orange line is the least squares solution, which misclassifies one of the training points. Also shown are two blue separating hyperplanes found by the* perceptron learning algorithm *with different random starts.*

individual streamed instances, as opposed to IRLS that uses all the data in every step. *Stochastic Gradient Descent* (SGD) is an example of an online learning or streaming method that uses the following update step with *step size* or *learning rate* α:

$$\beta^{new} \leftarrow \beta^{old} - \alpha x_i (y_i - p(x_i; \beta))$$

Compared to the exact expression for the gradient in Eqn. (1), SGD updates β per data point rather than summing the gradient contributions over the entire data set. If the data point was classified correctly the boundary doesn't change, if not we use the update rule above to update it.

Technically that's perceptron learning; in this expression the update is proportional (including sign) to the discrepancy between the ground truth and the estimated posterior probability.

How do we choose the step size α? This is left as an exercise for the reader.

This algorithm is closely related to Rosenblatt's *Perceptron Learning Algorithm* (HTF §4.5.1), which is hard thresholded and doesn't maintain probability estimates. See an example here: `http://www.youtube.com/watch?v=vGwemZhPlsA` ("Perceptron Learning Rule"). The LMS algorithm of Widrow and Hoff is also an example of SGD. SGD are also used in training neural networks.

2.2 Thoughts on Separating Hyperplanes

As shown in HTF Fig. 4.14, given two classes that are linearly separable, there exists an infinite family of separating lines/planes/hyperplanes between the classes. The figure shows solutions found via perceptron learning with different initializations. Which solution is best? Our intuition suggests we should choose the line with the furthest perpendicular distance from the closest data points from each class, since this might prevent overfitting. How do we translate that into an algorithm? We will tackle this question later in the semester when we discuss *support vector machines*.

2.3 Kernels: a Preview

Note that so far we have just been using the input variables X in their raw form (apart from adding the 1 to the front). A whole new frontier of algorithms awaits us if we supplement x by squares and cross products of its variables like $x_1^2, x_2^2, x_1 x_2$, etc. This hints at the idea of a *kernel*, a mapping through which we can augment the representation by adding dimensionality. This is particularly useful when dealing with points that are not linearly separable, as in the XOR problem. We will discuss kernels later in the semester.