**8.58.** If we refer to AA, Aa and aa as categories 1, 2 and 3, then

$$p_1(\theta) = (1-\theta)^2$$
  

$$p_2(\theta) = 2\theta(1-\theta)$$
  

$$p_3(\theta) = \theta^2.$$

Note that  $p_1(\theta) + p_2(\theta) + p_3(\theta) = 1$  and all are legitimate probabilities  $(0 \le p_i(\theta) \le 1)$  provided  $0 \le \theta \le 1$ .

a) This is a multinomial sampling situation where the probabilities depend upon the unknown parameter  $\theta$ . If the observed frequencies for the categories are denoted  $x_1, x_2$  and  $x_3 (x_1 + x_2 + x_3 = n)$ , the log-likelihood is given by (see page 273)

$$l(\theta) = \log L(\theta) = \log n! - \sum_{i=1}^{m} \log x_i! + \sum_{i=1}^{m} x_i \log p_i(\theta).$$

Substituting in the above expressions for the probabilities  $p_i(\theta)$ , we obtain

$$l(\theta) = \log n! - \sum_{i=1}^{3} \log x_i! + x_1 \log((1-\theta)^2) + x_2 \log(2\theta(1-\theta)) + x_3 \log(\theta^2),$$

and, after a bit of simplification, this becomes

$$l(\theta) \propto (2x_1 + x_2)\log(1 - \theta) + (2x_3 + x_2)\log\theta.$$

Taking the derivative with respect to  $\theta$  yields

$$l'(\theta) = -\frac{2x_1 + x_2}{(1 - \theta)} + \frac{x_2 + 2x_3}{\theta}.$$

Setting  $l'(\theta)$  to zero, and solving for  $\theta$  gives

$$\theta = \frac{1}{2} \frac{x_2 + 2x_3}{x_1 + x_2 + x_3} = \frac{x_2 + 2x_3}{2n}$$

Because  $l''(\theta) < 0$  at this value of  $\theta$  (in fact, at all permitted values of  $\theta$ ), this root corresponds to a local maximum of the log-likelihood. But  $L(\theta) > 0$  for  $0 < \theta < 1$  and  $L(\theta) \to 0$  as  $\theta \to 0$  (provided  $x_2 > 0$  or  $x_3 > 0$ ) and as  $\theta \to 1$  (provided  $x_1 > 0$  or  $x_2 > 0$ ), so this is a global maximum; that is,

$$\hat{\theta}_{ML} = \frac{X_2 + 2X_3}{2n}.$$

Alternately, you could check that  $l'(\theta) > 0 \Leftrightarrow \theta < (x_2 + 2x_3)/2n$ , leading to the same conclusion.

Substituting in the observed values, the maximum likelihood estimate for this data set (the value of the ML estimator) becomes  $\hat{\theta}_{ML} = (68 + 2 \times 112)/(2 \times 190) \approx 0.768$ .

b) The asymptotic variance of  $\hat{\theta}_{ML}$  is given by  $1/nI(\theta)$ , where  $nI(\theta)$ , the Fisher Information for  $\theta$  in the sample, can be evaluated as

$$nI(\theta) = -E\left[\frac{\partial^2}{\partial\theta^2}\log L(\theta)\right]$$

The second derivative is given by

$$l''(\theta) = -\left(\frac{2x_1 + x_2}{(1 - \theta)^2} + \frac{x_2 + 2x_3}{\theta^2}\right)$$
  

$$\Rightarrow nI(\theta) = \frac{2EX_1 + EX_2}{(1 - \theta)^2} + \frac{EX_2 + 2EX_3}{\theta^2}$$

But each  $X_i$  is binomial with probability  $p_i(\theta)$ , so we have

$$EX_1 = n(1-\theta)^2$$
  

$$EX_2 = 2n\theta(1-\theta)$$
  

$$EX_3 = n\theta^2$$
  

$$\Rightarrow nI(\theta) = \frac{2n}{\theta(1-\theta)}.$$

Of course, the true value of  $\hat{\theta}$  is unknown, so we plug-in the value of  $\hat{\theta}_{ML} \cong 0.768$  to obtain the estimated asymptotic variance of  $\hat{Var}(\hat{\theta}_{ML}) = 1/nI(\hat{\theta}_{ML}) \approx 0.00047$ . Alternately, we have  $\hat{SE}(\hat{\theta}_{ML}) \cong \sqrt{0.00047} \cong 0.0216 \approx 0.022$ .

Note: As in problem 8.4, you can determine the exact expression for the variance of  $\hat{\theta}_{ML}$  using the properties of the multinomial distribution. You should check that you get exactly the same expression as above; that is,  $\operatorname{Var}(\hat{\theta}_{ML}) = \theta(1-\theta)/2n$ .

c) Recall that, for large values of n,  $\sqrt{nI(\theta)}(\hat{\theta}_{ML} - \theta)$  has approximately a standard normal distribution. Putting this another way, for large values of n,

$$\hat{\theta}_{ML} \approx N\left(\theta, SE^2(\hat{\theta}_{ML})\right),$$

where  $SE^2(\hat{\theta}_{ML}) = 1/nI(\theta)$ . So the form of the approximate  $1 - \alpha$  confidence interval (CI) for  $\theta$  is given by

$$\hat{\theta}_{ML} \pm z(\alpha/2) \hat{SE}^2(\hat{\theta}_{ML}),$$

where we plugged  $\hat{\theta}_{ML}$  into the expression for  $SE^2(\hat{\theta}_{ML})$  to obtain  $\hat{SE}^2(\hat{\theta}_{ML})$ . As  $z(0.01/2) \cong 2.58$ , the approximate 99% CI for  $\theta$  becomes  $0.768 \pm 2.58 \times 0.0216$ , or the interval  $(0.7126, 0.8243) \approx (0.71, 0.82)$ .

d) We generate bootstrap samples (of size n = 190) from a multinomial distribution with probabilities:

$$p_1 = (1 - \hat{\theta}_{ML})^2$$

$$p_2 = 2\hat{\theta}_{ML}(1 - \hat{\theta}_{ML})$$

$$p_3 = \hat{\theta}_{ML}^2$$

or 0.0536, 0.3559 and 0.5905, respectively. For each of these bootstrap samples, we calculate the MLE. Doing this B = 1000 times, and taking the standard deviation of these 1000 bootstrap MLE's gives  $\hat{SE}(\hat{\theta}_{ML}) \cong 0.02088 \approx 0.021$ , essentially the same value obtained for  $\hat{SE}(\hat{\theta}_{ML})$  in part b). Of course, you will get a slightly different answer because your bootstrap samples will be different (you would also get a different answer if you generated a different number of bootstrap samples) but your answer should be pretty close to the value obtained in part b) as long as you use a fairly large value of B (B > 200 say).

A piece of R code to do this is:

```
mlOuts <- rep(NA, 1000)
for (i in 1:1000){
    x <- rmultinom(1, 190, prob=c(0.0536, 0.3559, 0.5905))
    mlOuts[i] <- 0.5*(x[2]+2*x[3])/190)
}
sd(mlOuts)</pre>
```

e) Using the notation on page 284 of the text, we have  $\hat{\theta} = 0.768$ , and we use the bootstrap samples as in d) to generate estimates  $\theta^*$ . The distribution of  $\hat{\theta} - \theta$  is then approximated by the histogram of  $\theta^* - \hat{\theta}$  to obtain estimates of the desired quantiles of the distribution of  $\hat{\theta} - \theta$ . Carrying this out leads to an approximate 99% CI for  $\theta$  of (0.714, 0.827). This interval is very similar to the approximate 99% CI obtained in c).

A piece of R code to do this is:

```
mlDiffs <- rep(NA, 1000)
for (i in 1:1000){
    x <- rmultinom(1, 190, prob=c(0.0536, 0.3559, 0.5905))
    mlOuts <- 0.5*(x[2]+2*x[3])/190)
    mlDiffs[i] <- mlOuts - 0.768
}
0.768 - quantile(mlDiffs, c(0.005, 0.995))</pre>
```