Foundations
Statistics

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Exercise 4.4. [BIC for Gaussians]
(Source: Jaakkola.) The Bayesian information criterion (BIC) is a penalized log-likelihood function that can be used for model selection. It is defined as

$$BIC = log\, p(\mathcal{D}|\hat{\theta}_{ML}) - \frac{d}{2} log(N)$$

where d is the number of free parameters in the model and N is the number of samples. In this question, we will see how to use this to choose between a full covariance Gaussian and a Gaussian with a diagonal covariance. Obviously a full covariance Gaussian has higher likelihood, but it may not be "worth" the extra parameters if the improvement over a diagonal covariance matrix is too small. So we use the BIC score to choose the model.
We can write

$$log\, p(\mathcal{D}|\hat{\Sigma}, \hat{\mu}) = -\frac{N}{2} tr(\hat{\Sigma}^{-1}\hat{S}) - \frac{N}{2} log(|\hat{\Sigma}|)$$

$$\hat{S} = \frac{1}{N}\sum_{i=1}^{N}(x_i - \bar{x})(x_i - \bar{x})^T$$

where $\hat{S}$ is the scatter matrix (empirical covariance), the trace of a matrix is the sum of its diagonals, and we have used the trace trick.

a. Derive the BIC score for a Gaussian in D dimensions with full covariance matrix. Simplify your answer as much as possible, exploiting the form of the MLE. Be sure to specify the number of free parameters d.
b. Derive the BIC score for a Gaussian in D dimensions with a diagonal covariance matrix. Be sure to specify the number of free parameters d. Hint: for the digaonal case, the ML estimate of Σ is the same as $\hat{\Sigma}_{ML}$ except the off-diagonal terms are zero:

$$\hat{\Sigma}_{diag} = \text{diag}(\hat{\Sigma}_{ML}(1,1), ..., \hat{\Sigma}_{ML}(D,D))$$

Solution. a. The MLE for the covariance matrix is the empirical covariance matrix: $\hat{\Sigma}_{MLE} = \hat{S}$. The log likelihood becomes:

$$log\, p(\mathcal{D}|\hat{\Sigma}, \hat{\mu}) = -\frac{N}{2} tr(\hat{S}^{-1}\hat{S}) - \frac{N}{2} log(|\hat{S}|)$$

$$= -\frac{N}{2}tr(I) - \frac{N}{2}log(|\hat{S}|) = -\frac{N}{2}D - \frac{N}{2}log(|\hat{S}|)$$

The number of free parameters:

- for the symmetric covariance matrix = $\frac{D(D+1)}{2}$
- for the mean = D

Thus, the total number of free parameters:

$$d = \frac{D(D+1)}{2} + D$$

The BIC for a Gaussian with full covariance matrix:

$$BIC = log\, p(\mathcal{D}|\hat{\theta}_{ML}) - \frac{d}{2}log(N)$$

$$= -\frac{N}{2}D - \frac{N}{2}log(|\hat{S}|) - \frac{1}{2}(\frac{D(D+1)}{2} + D)\, log(N)$$

b. for a Gaussian with a diagonal covariance matrix

$$\hat{\Sigma}_{MLE} = \hat{\Sigma}_{diag} = \text{diag}(\hat{S}(1,1), ..., \hat{S}(D,D)).$$

The log likelihood becomes:

$$log\, p(\mathcal{D}|\hat{\Sigma}, \hat{\mu}) = -\frac{N}{2}tr(\hat{\Sigma}_{diag}^{-1}\hat{S}) - \frac{N}{2}log(|\hat{\Sigma}_{diag}|)$$

$$= -\frac{N}{2}\sum_{i=1}^{D}\frac{\hat{S}(i,i)}{\hat{\Sigma}_{diag}(i,i)} - \frac{N}{2}\sum_{i=1}^{D} log\, \hat{\Sigma}_{diag}(i,i) = -\frac{N}{2}D - \frac{N}{2}\sum_{i=1}^{D} log\, \hat{S}(i,i)$$

The number of free parameters:

- for the diagonal covariance matrix = D
- for the mean = D

Thus, the total number of free parameters:

$$d = 2D$$

The BIC for a Gaussian with full covariance matrix:

$$BIC = log\, p(\mathcal{D}|\hat{\theta}_{ML}) - \frac{d}{2}log(N)$$

$$= -\frac{N}{2}D - \frac{N}{2}\sum_{i=1}^{D} log\, \hat{S}(i,i) - D\, log(N)$$

□