Preliminary Identities

Proposition 1.1.1.

$$I = \int_{-\infty}^{\infty} u^{2k} e^{-\alpha u^2/2} du = \sqrt{2\pi}\alpha^{-(2k+1)/2} \prod_{j=1}^{k}(2j-1) \tag{1.1.1}$$

♦

Proof. Let $K(\alpha, u) = \exp(-\alpha u^2/2)$. Consider first the integral:

$$I_0 = \int_{-\infty}^{\infty} K(\alpha, u) du = \int_{-\infty}^{\infty} e^{-\alpha u^2/2} du.$$

Make the change of variables $\omega = \alpha u^2/2$, with differential:

$$d\omega = \alpha u du \implies du = 2^{-1/2}\alpha^{-1/2}\omega^{-1/2} d\omega.$$

Then, I_0 evaluates to:

$$I_0 = 2\int_{0}^{\infty} e^{-\omega} \cdot 2^{-1/2}\alpha^{-1/2}\omega^{-1/2} d\omega = 2^{1/2}\alpha^{-1/2} \int_{0}^{\infty} \omega^{1/2-1} e^{-\omega} d\omega = 2^{1/2}\alpha^{-1/2}\Gamma(1/2).$$

Overall, the integral of $K(\alpha, u)$ evaluates to:

$$I_0 = \sqrt{2\pi}\alpha^{-1/2}. \tag{1.1.2}$$

Next consider the partial of K wrt α:

$$\frac{\partial}{\partial \alpha} K(\alpha, u) = \frac{\partial}{\partial \alpha} e^{-\alpha u^2/2} = -\frac{u^2}{2} e^{-\alpha u^2/2} = -\frac{u^2}{2} K(\alpha, u).$$

The kth partial is:

$$\frac{\partial^k}{\partial \alpha^k} K(\alpha, u) = \frac{\partial^k}{\partial \alpha^k} e^{-\alpha u^2/2} = (-1)^k \frac{u^{2k}}{2^k} e^{-\alpha u^2/2} = (-1)^k \frac{u^{2k}}{2^k} K(\alpha, u).$$

Rearranging gives:

$$u^{2k} K(\alpha, u) = (-1)^k 2^k \frac{\partial^k}{\partial \alpha^k} K(\alpha, u).$$

Now integral is expressible as:

$$I = \int_{-\infty}^{\infty} u^{2k} K(\alpha, u) du = 2^k (-1)^k \frac{\partial^k}{\partial \alpha^k} \int_{-\infty}^{\infty} K(\alpha, u) du.$$

Applying (1.1.2):

$$I = 2^k(-1)^k \frac{\partial^k}{\partial \alpha^k} \sqrt{2\pi}\alpha^{-1/2} = 2^{k+1/2}(-1)^k \sqrt{\pi} \frac{\partial^k}{\partial \alpha^k} \alpha^{-1/2}.$$

Taking the derivatives in α:

$$\frac{\partial^k}{\partial\alpha^k}\alpha^{-1/2} = (-1)^k\frac{1}{2}\cdot\frac{3}{2}\cdots\frac{(2k-1)}{2}\alpha^{-(2k+1)/2} = \frac{(-1)^k}{2^k}\alpha^{-(2k+1)/2}\prod_{j=1}^{k}(2j-1)$$

Substituting the derivative into the expression for I:

$$I = 2^{k+1/2-k}(-1)^{2k}\sqrt{\pi}\alpha^{-(2k+1)/2}\prod_{j=1}^{k}(2j-1).$$

Simplifying gives the result. ■

Corollary 1.1.1.

$$\int_{-\infty}^{\infty} u^{2k+1}e^{-\alpha u^2/2}du = 0.$$

♣

Proof. The integral is expressible as:

$$I = 2^k(-1)^k\frac{\partial^k}{\partial\alpha^k}\int_{-\infty}^{\infty} ue^{-\alpha u^2/2}du = 0.$$

Here the integral evaluates to zero due to odd parity of the integrand about the origin. ■

Laplace Approximation

Result 1.2.1. Suppose $g(x)$ achieves a global minimum at $x^* \in (a, b)$, then for $n \to \infty$:

$$\int_a^b e^{-ng(x)}dx = e^{-ng(x^*)}\sqrt{\frac{2\pi}{n\ddot{g}(x^*)}}\left\{1 - \frac{1}{8n}\kappa_4 + \frac{5}{24n}\kappa_3^2 + \mathcal{O}(n^{-2})\right\}, \tag{1.2.3}$$

where:

$$\kappa_3 = \frac{g^{(3)}(x^*)}{\ddot{g}^{3/2}(x^*)}, \qquad \kappa_4 = \frac{g^{(4)}(x^*)}{\ddot{g}^2(x^*)}.$$

♣

Proof. Let $I = \int_a^b \exp\{-ng(x)\}dx$ denote the integral of interest. Take the Taylor expansion of $g(x)$ about x^*:

$$g(x) = g(x^*) + \frac{1}{2}\ddot{g}(x^*)(x - x^*)^2 + \sum_{k=3}^{\infty}\frac{g^{(k)}(x^*)}{k!}(x - x^*)^k.$$

Substituting the Taylor expansion into I:

$$I = e^{-ng(x^*)} \int_a^b e^{-n\ddot{g}(x^*)(x-x^*)^2/2} \exp\left\{ -n \sum_{k=3}^{\infty} \frac{g^{(k)}(x^*)}{k!}(x-x^*)^k \right\} dx.$$

Let $S_3(x)$ denote the series:

$$S_3(x) = -n \sum_{k=3}^{\infty} \frac{g^{(k)}(x^*)}{k!}(x-x^*)^k.$$

Take the Taylor expansion of the second exponential term:

$$\exp\{S_3(x)\} = \left\{ 1 + S_3(x) + \frac{1}{2}S_3(x)^2 + \cdots \right\},$$

then:

$$I = e^{-ng(x^*)} \int_a^b e^{-n\ddot{g}(x^*)(x-x^*)^2/2} \left\{ 1 + S_3(x) + \frac{1}{2}S_3(x)^2 + \cdots \right\} dx.$$

Make the change of variables $\omega = \sqrt{n\ddot{g}(x^*)}(x - x^*)$ with $d\omega = \sqrt{n\ddot{g}(x^*)}dx$:

$$I = \frac{e^{-ng(x^*)}}{\sqrt{n\ddot{g}(x^*)}} \int_{\sqrt{n\ddot{g}(x^*)}(a-x^*)}^{\sqrt{n\ddot{g}(x^*)}(b-x^*)} e^{-\omega^2/2} \left\{ 1 + S_3(\omega) + \frac{1}{2}S_3(\omega)^3 + \cdots \right\} d\omega,$$

where:

$$S_3(\omega) = -n \sum_{k=3}^{\infty} \frac{g^{(k)}(x^*)}{k!} \frac{\omega^k}{n^{k/2}\ddot{g}(x^*)^{k/2}} = -\sum_{k=3}^{\infty} \frac{g^{(k)}(x^*)}{k!} \frac{\omega^k}{n^{k/2-1}\ddot{g}(x^*)^{k/2}}$$

Expanding $\mathcal{O}(n^{-1})$ terms from $S_3(\omega)$:

$$I = \frac{e^{-ng(x^*)}}{\sqrt{n\ddot{g}(x^*)}} \int_{\sqrt{n\ddot{g}(x^*)}(a-x^*)}^{\sqrt{n\ddot{g}(x^*)}(b-x^*)} e^{-\omega^2/2} \left\{ 1 - \frac{g^{(4)}(x^*)\omega^4}{4!n\ddot{g}(x^*)^2} + \frac{1}{2}\left(\frac{g^{(3)}(x^*)\omega^3}{3!n^{1/2}\ddot{g}(x^*)^{3/2}} \right)^2 + \mathcal{O}(n^{-2}) \right\} d\omega,$$

where odd powers of ω are neglected, since these will integrate to zero. For $n \to \infty$, the bounds of integration may be approximated as infinite:

$$I \doteq \frac{e^{-ng(x^*)}}{\sqrt{n\ddot{g}(x^*)}} \int_{-\infty}^{\infty} e^{-\omega^2/2} \left\{ 1 - \frac{g^{(4)}(x^*)\omega^4}{4!n\ddot{g}(x^*)^2} + \frac{1}{2}\left(\frac{g^{(3)}(x^*)\omega^3}{3!n^{1/2}\ddot{g}(x^*)^{3/2}} \right)^2 + \mathcal{O}(n^{-2}) \right\} d\omega$$

Applying (1.1.1) to integrate the even powers of ω:

$$I = e^{-ng(x^*)} \sqrt{\frac{2\pi}{n\ddot{g}(x^*)}} \left\{ 1 - \frac{3g^{(4)}(x^*)}{4!n\ddot{g}(x^*)^2} + \frac{5 \cdot 3 \cdot g^{(3)}(x^*)^2}{2(3!)^2 n\ddot{g}(x^*)^3} + \mathcal{O}(n^{-2}) \right\}.$$

Simplifying coefficients gives the result. ■

Example 1.2.1 (Stirling's Approximation). Consider approximating $n!$ for $n \to \infty$. Express the factorial in terms of the Gamma function:

$$n! = \Gamma(n+1) = \int_0^\infty x^n e^{-x} dx = \int_0^\infty e^{n\ln(x) - x} dx.$$

Let $I = \int_0^\infty \exp\{n\ln(x) - x\}dx$. Make the change of variables $x = n\omega$, $dx = nd\omega$:

$$I = \int_0^\infty e^{n\ln(n\omega) - n\omega} nd\omega = n\int_0^\infty e^{n\ln(n) + n\ln(\omega) - n\omega} d\omega = n^{n+1}\int_0^\infty e^{-ng(\omega)} d\omega,$$

where $g(\omega) = \omega - \ln(\omega)$. The minimum of $g(\omega)$ occurs at $\dot{g}(\omega) = 1 - \omega^{-1} = 0$, or $\omega^* = 1$. Evaluating g and its derivatives at the critical point:

$$g(\omega^*) = 1, \qquad \ddot{g}(\omega^*) = 1, \qquad g^{(3)}(\omega^*) = -2, \qquad g^{(4)}(\omega^*) = 6.$$

Applying (1.2.3) gives:

$$I = n^{n+1}e^n\sqrt{\frac{2\pi}{n}}\left\{1 - \frac{1}{8n}\cdot\frac{6}{1} + \frac{5}{24n}\left(\frac{-2}{1}\right)^2 + \mathcal{O}(n^{-2})\right\}.$$

Simplifying coefficients gives:

$$n! = \Gamma(n+1) = \sqrt{2\pi}n^{n+1/2}e^n\left\{1 + \frac{1}{12n} + \mathcal{O}(n^{-2})\right\},$$

for $n \to \infty$. ♠

Example 1.2.2 (Multivariate Laplace Approximation). Consider approximation of the integral:

$$I = \int_{\mathbb{R}^p} e^{-ng(\boldsymbol{x})} d\boldsymbol{x},$$

where $g(\boldsymbol{x})$ achieves a global minimum at $\boldsymbol{x}^*$. Take the Taylor expansion of g about $\boldsymbol{x}^*$:

$$g(\boldsymbol{x}) = g(\boldsymbol{x}^*) + \frac{1}{2}(\boldsymbol{x} - \boldsymbol{x}^*)'\ddot{g}(\boldsymbol{x}^*)(\boldsymbol{x} - \boldsymbol{x}^*) + R(\boldsymbol{x}, \boldsymbol{x}^*).$$

Here $\ddot{g}(\boldsymbol{x})$ denotes the $p \times p$ Hessian:

$$\ddot{g}(\boldsymbol{x}) = \frac{\partial^2 g(\boldsymbol{x})}{\partial\boldsymbol{x}\partial\boldsymbol{x}'},$$

and the remainder $R(\boldsymbol{x}, \boldsymbol{x}^*) = \mathcal{O}(||\boldsymbol{x} - \boldsymbol{x}^*||^3)$.

Substituting the Taylor expansion into I:

$$\begin{aligned} I &= e^{-ng(\boldsymbol{x}^*)}\int e^{-(\boldsymbol{x}-\boldsymbol{x}^*)'n\ddot{g}(\boldsymbol{x}^*)(\boldsymbol{x}-\boldsymbol{x}^*)/2}e^{-nR}d\boldsymbol{x} \\ &= e^{-ng(\boldsymbol{x}^*)}\int e^{-(\boldsymbol{x}-\boldsymbol{x}^*)'n\ddot{g}(\boldsymbol{x}^*)(\boldsymbol{x}-\boldsymbol{x}^*)/2}\{1 + \mathcal{O}(nR)\}d\boldsymbol{x} \end{aligned}$$

Recall from multivariate normal distribution that:

$$\int e^{-(\boldsymbol{y}-\boldsymbol{\mu})'\boldsymbol{\Sigma}^{-1}(\boldsymbol{y}-\boldsymbol{\mu})/2} d\boldsymbol{y} = (2\pi)^{p/2} \det(\boldsymbol{\Sigma})^{1/2}.$$

Applied to integrate the leading term of I:

$$\int_{\mathbb{R}^p} e^{-ng(\boldsymbol{x})} d\boldsymbol{x} = (2\pi)^{p/2} e^{-ng(\boldsymbol{x}^*)} n^{-p/2} \det\left\{\ddot{g}(\boldsymbol{x}^*)\right\}^{-1/2} \left\{1 + \mathcal{O}(n||\boldsymbol{x} - \boldsymbol{x}^*||^3)\right\}, \tag{1.2.4}$$

for $n \to \infty$. ♠

Example 1.2.3 (BIC). Consider the marginal likelihood of the data $f(\boldsymbol{y})$ in a Bayesian model:

$$f(\boldsymbol{y}) = \int f(\boldsymbol{y}|\boldsymbol{\theta}) f(\boldsymbol{\theta}) d\boldsymbol{\theta} = \int e^{-ng(\boldsymbol{\theta})} d\boldsymbol{\theta},$$

where:

$$g(\boldsymbol{\theta}) = -\frac{1}{n} \ln f(\boldsymbol{y}|\boldsymbol{\theta}) - \frac{1}{n} f(\boldsymbol{\theta}).$$

Applying (1.2.4):

$$f(\boldsymbol{y}) \propto f(\boldsymbol{y}|\boldsymbol{\theta}^*) f(\boldsymbol{\theta}^*) n^{-p/2} \det\left\{\mathcal{J}_{\theta\theta'}(\boldsymbol{\theta}^*) + \mathcal{I}^0_{\theta\theta'}(\boldsymbol{\theta}^*)\right\}.$$

where:

$$\mathcal{J}_{\theta\theta'}(\boldsymbol{\theta}) = -\frac{1}{n} \frac{\partial^2 \ln f(\boldsymbol{y}|\boldsymbol{\theta})}{\partial\boldsymbol{\theta}\partial\boldsymbol{\theta}'}, \qquad \mathcal{I}^0_{\theta\theta'}(\boldsymbol{\theta}) = -\frac{1}{n} \frac{\partial^2 \ln f(\boldsymbol{\theta})}{\partial\boldsymbol{\theta}\partial\boldsymbol{\theta}'},$$

are the observed and prior information for $\boldsymbol{\theta}$, respectively. Taking the logarithm:

$$\ln f(\boldsymbol{y}) \propto \ln f(\boldsymbol{y}|\boldsymbol{\theta}^*) + \ln f(\boldsymbol{\theta}^*) - \frac{p}{2} \ln(n) + \ln\det\left\{\mathcal{J}_{\theta\theta'}(\boldsymbol{\theta}^*) + \mathcal{I}^0_{\theta\theta'}(\boldsymbol{\theta}^*)\right\}.$$

For increasing n, $\ln f(\boldsymbol{\theta}^*)$ and $\mathcal{I}^0_{\theta\theta'}$ are likely negligible, and $\mathcal{J}_{\theta\theta'}$ is expected to converge in probability to a constant. Hence the log marginal likelihood is roughly:

$$\ln f(\boldsymbol{y}) \approx \ln f(\boldsymbol{y}|\boldsymbol{\theta}^*) - \frac{p}{2} \ln(n).$$

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