Proof of Lemma 1

The proof is consolidated from Stein (1972), Stein (1981) and Liu (1994).

The first result is the univariate version of Stein's Identity (cf. Stein (1972) and Stein (1981)).

Let $\tilde{c}$ follow a standard normal distribution, $N(0,1)$, and $\phi(c)$ denote the standard normal density with the derivative satisfying $\phi'(c) = -c\phi(c)$. For any differentiable function $h:\mathbb{R}\to\mathbb{R}$ such that $\mathbf{E}[|h'(\tilde{c})|]<\infty$,

$$\begin{aligned}
\mathbf{E}[h'(\tilde{c})] &= \int_{-\infty}^{\infty} h'(c)\phi(c)\,dc \\
&= \int_{0}^{\infty} h'(c)\left[\int_{c}^{\infty} z\phi(z)\,dz\right]dc + \int_{-\infty}^{0} h'(c)\left[\int_{-\infty}^{c} -z\phi(z)\,dz\right]dc \\
&= \int_{0}^{\infty} z\phi(z)\left[\int_{0}^{z} h'(c)dc\right]dz - \int_{-\infty}^{0} z\phi(z)\left[\int_{z}^{0} h'(c)dc\right]dz \\
&= \left(\int_{0}^{\infty} + \int_{-\infty}^{0}\right)[z\phi(z)[h(z)-h(0)]]\,dz \\
&= \int_{-\infty}^{\infty} z\phi(z)\,h(z)dz \\
&= \mathbf{E}[\tilde{c}h(\tilde{c})],
\end{aligned}$$

where the third equality is justified by Fubini's Theorem. Note that since $\mathbf{E}[\tilde{c}]=0$ and $Var(\tilde{c})=1$, the equality proved above is essentially

$$Cov(\tilde{c}, h(\tilde{c})) = Var(\tilde{c})\mathbf{E}[h'(\tilde{c})]. \tag{EC.1}$$

Next, we present the generalization of the result to the multivariate case (cf. Stein (1981) and Liu (1994)).

Let $\tilde{\boldsymbol{z}} = (\tilde{z}_1,\dots,\tilde{z}_n)^T$, where $\tilde{z}_j$'s are independent and identically distributed standard normal random variables. From Equation (EC.1) it follows that for any function $\hat{h}:\mathbb{R}^n\to\mathbb{R}$ satisfying the same conditions as h in the Theorem,

$$\mathbf{E}\left[\tilde{z}_j\hat{h}(\tilde{\boldsymbol{z}})\middle|(\tilde{z}_1,\dots,\tilde{z}_{j-1},\tilde{z}_{j+1},\dots,\tilde{z}_n)\right] = \mathbf{E}\left[\frac{\partial\hat{h}(\tilde{\boldsymbol{z}})}{\partial z_j}\middle|(\tilde{z}_2,\dots,\tilde{z}_{j-1},\tilde{z}_{j+1},\dots,\tilde{z}_n)\right], \forall j=1,\dots,n.$$

Taking the expectation of both sides, we get

$$\mathbf{E}\left[\tilde{z}_1\hat{h}(\tilde{\boldsymbol{z}})\right] = \mathbf{E}\left[\frac{\partial\hat{h}(\tilde{\boldsymbol{z}})}{\partial z_1}\right].$$

Using a similar argument for the remaining random variables, we can show that

$$Cov\left(\tilde{\boldsymbol{z}}, \hat{h}\left(\tilde{\boldsymbol{z}}\right)\right) = \mathbf{E}\left[\nabla \hat{h}\left(\tilde{\boldsymbol{z}}\right)\right].$$

Note that the random vector $\tilde{\boldsymbol{c}}$ can be written as $\tilde{\boldsymbol{c}} = \Sigma^{1/2}\tilde{\boldsymbol{z}} + \boldsymbol{\mu}$. Consider $\hat{h}\left(\tilde{\boldsymbol{z}}\right) = h\left(\Sigma^{1/2}\tilde{\boldsymbol{z}} + \boldsymbol{\mu}\right)$, then $\nabla \hat{h}\left(\tilde{\boldsymbol{z}}\right) = \Sigma^{1/2}\nabla h\left(\tilde{\boldsymbol{c}}\right)$. Hence,

$$Cov\left(\tilde{\boldsymbol{c}}, h\left(\tilde{\boldsymbol{c}}\right)\right) = Cov\left(\Sigma^{1/2}\tilde{\boldsymbol{z}}, \hat{h}\left(\tilde{\boldsymbol{z}}\right)\right) = \Sigma^{1/2}\mathbf{E}\left[\nabla \hat{h}\left(\tilde{\boldsymbol{z}}\right)\right] = \Sigma\mathbf{E}\left[\nabla h\left(\tilde{\boldsymbol{c}}\right)\right].$$

References

Liu JS (1994) Siegel's formula via Stein's identities. *Statistics & Probability Letters.* 21: 247–251.

Stein CM (1972) A bound for the error in the normal approximation to the distribution of a sum of dependent random variables. *Proceedings of the Berkeley Symposium on Mathematical Statistics and Probability.* 2: 583–602.

Stein CM (1981) Estimation of the mean of a multivariate normal distribution. *The Annals of Statistics.* 9: 1135–1151.