

from the start as an expectation suggests that this p and f would be a natural choice of decomposition. However, the original specification of the problem may not be the optimal choice in terms of the number of samples required to obtain a given level of accuracy. Fortunately, the form of the optimal choice q^* can be derived easily. The optimal q^* corresponds to what is called optimal importance sampling.

Because of the identity shown in equation 17.8, any Monte Carlo estimator

$$\hat{s}_p = \frac{1}{n} \sum_{i=1, \mathbf{x}^{(i)} \sim p}^n f(\mathbf{x}^{(i)}) \quad (17.9)$$

can be transformed into an importance sampling estimator

$$\hat{s}_q = \frac{1}{n} \sum_{i=1, \mathbf{x}^{(i)} \sim q}^n \frac{p(\mathbf{x}^{(i)})f(\mathbf{x}^{(i)})}{q(\mathbf{x}^{(i)})}. \quad (17.10)$$

We see readily that the expected value of the estimator does not depend on q :

$$\mathbb{E}_q[\hat{s}_q] = \mathbb{E}_q[\hat{s}_p] = s. \quad (17.11)$$

However, the variance of an importance sampling estimator can be greatly sensitive to the choice of q . The variance is given by

$$\text{Var}[\hat{s}_q] = \text{Var}\left[\frac{p(\mathbf{x})f(\mathbf{x})}{q(\mathbf{x})}\right]/n. \quad (17.12)$$

The minimum variance occurs when q is

$$q^*(\mathbf{x}) = \frac{p(\mathbf{x})|f(\mathbf{x})|}{Z}, \quad (17.13)$$

where Z is the normalization constant, chosen so that $q^*(\mathbf{x})$ sums or integrates to 1 as appropriate. Better importance sampling distributions put more weight where the integrand is larger. In fact, when $f(\mathbf{x})$ does not change sign, $\text{Var}[\hat{s}_{q^*}] = 0$, meaning that *a single sample is sufficient* when the optimal distribution is used. Of course, this is only because the computation of q^* has essentially solved the original problem, so it is usually not practical to use this approach of drawing a single sample from the optimal distribution.

Any choice of sampling distribution q is valid (in the sense of yielding the correct expected value) and q^* is the optimal one (in the sense of yielding minimum variance). Sampling from q^* is usually infeasible, but other choices of q can be feasible while still reducing the variance somewhat.