Simple variance bounds with applications to Bayesian posteriors and intractable distributions

Fraser Daly, Fatemeh Ghaderinezhad, Christophe Ley[‡] and Yvik Swan[§]

November 11, 2019

Abstract Using coupling techniques based on Stein's method for probability approximation, we revisit classical variance bounding inequalities of Chernoff, Cacoullos, Chen and Klaassen. Taking advantage of modern coupling techniques allows us to establish novel variance bounds in settings where the underlying density function is unknown or intractable. Applications include bounds for asymptotically Gaussian random variables using zero-biased couplings, bounds for random variables which are New Better (Worse) than Used in Expectation, and analysis of the posterior in Bayesian statistics.

Key words and phrases: Stein kernel; Stein operator; prior density; stochastic ordering; variance bound.

MSC 2010 subject classification: 60E15; 26D10; 62F15

1 Introduction

Weighted Poincaré (or isoperimetric) inequalities, giving upper bounds on the variance of a function of a random variable, have a long and rich history, beginning with the work of Chernoff [6]. Chernoff proved that if X has a centred Gaussian distribution with variance σ^2 , then

$$\operatorname{Var}[g(X)] \le \sigma^2 \mathbb{E}[(g'(X))^2], \qquad (1.1)$$

for any absolutely continuous function $g : \mathbb{R} \to \mathbb{R}$ such that g(X) has finite variance. This inequality has since been generalized by many authors, including Cacoullos [2], Chen [4] and Klaassen [10]. To accompany these upper variance bounds, many of these authors

^{*}Department of Actuarial Mathematics and Statistics, Heriot-Watt University, Edinburgh EH14 4AS, UK. E-mail: f.daly@hw.ac.uk

[†]Department of Applied Mathematics, Computer Science and Statistics, Ghent University, Krijgslaan 281, S9, Campus Sterre, 9000 Gent, Belgium. E-mail: fatemeh.ghaderinezhad@ugent.be

[‡]Department of Applied Mathematics, Computer Science and Statistics, Ghent University, Krijgslaan 281, S9, Campus Sterre, 9000 Gent, Belgium. E-mail: christophe.ley@ugent.be

[§]Department of Mathematics, Université libre de Bruxelles, Boulevard du Triomphe, CP210, B-1050 Bruxelles

have also established corresponding lower bounds, in the form of generalized Cramér-Rao inequalities. In particular in the centred Gaussian case we have

$$\operatorname{Var}[g(X)] \ge \sigma^2 \mathbb{E}[g'(X)]^2, \tag{1.2}$$

see [2]. The above cited works represent early entries in what is now a vast literature; we refer to [7, 8] for recent overviews of this large body of work.

The purpose of the present article is to revisit these classical variance bounding inequalities in light of the coupling techniques at the heart of Stein's method for probability approximation (see, for example, [5] and [11] for recent introductions to Stein's method). These techniques allow us to establish upper and lower variance bounds in a variety of settings, including many in which the density of the underlying random variable is unknown or intractable. Making use, for example, of the zero-biased coupling allows us to establish explicit variance bounds for a wide range of situations in which the underlying random variable is known to be asymptotically Gaussian. In Sections 2–4 we will consider a variety of situations where bounds may be derived using this, and other, couplings. Before doing so, we use the remainder of this section to outline the general coupling techniques we employ from Stein's method, and how these can be used to establish upper and lower variance bounds in the spirit of Chernoff, Cacoullos, Chen and Klaassen.

Let W be a real random variable on some fixed probability space. Let γ be a realvalued function. We say that a pair of random variables (T_1, T_2) (living on the same probability space as W) form a Stein coupling for W with respect to γ if

$$\mathbb{E}\left[\gamma(W)\phi(W)\right] = \mathbb{E}\left[T_1\phi'(T_2)\right] \tag{1.3}$$

for all test functions $\phi \in C$ with $C \subset C^1(\mathbb{R})$ some appropriately chosen class of functions. Although the choice $C = C_0^{\infty}(\mathbb{R})$ is always allowed, it will generally be necessary to use C as wide as possible; this fact is often reflected in the literature wherein one rather makes use of the generic expression "where C is the class of functions for which expectations on both sides exist".

We begin by showing an elementary argument allowing us to use (1.3) to obtain tight upper variance bounds. To this end, suppose that γ is a strictly increasing, differentiable function with exactly one sign change. Then in particular it is invertible and $\gamma^{-1}(0)$ is well-defined. Let g be a real-valued differentiable function such that $\operatorname{Var}[g(W)]$ is finite. Following [12] we write

$$\begin{aligned} \operatorname{Var}[g(W)] &\leq \mathbb{E}\left[\left(g(W) - g(\gamma^{-1}(0))\right)^2\right] = \mathbb{E}\left[\left(\int_0^{\gamma(W)} \frac{g'(\gamma^{-1}(u))}{\gamma'(\gamma^{-1}(u))} \mathrm{d}u\right)^2\right] \\ &\leq \mathbb{E}\left[\gamma(W) \int_0^{\gamma(W)} \left(\frac{g'(\gamma^{-1}(u))}{\gamma'(\gamma^{-1}(u))}\right)^2 \mathrm{d}u\right],\end{aligned}$$

where the equality follows by differentiability of g and the subsequent inequality via Cauchy-Schwarz. Applying (1.3) as well as Leibnitz' rule for differentiating integrals we deduce the general upper variance bound

$$\operatorname{Var}[g(W)] \le \mathbb{E}\left[\frac{T_1}{\gamma'(T_2)} \left(g'(T_2)\right)^2\right],\tag{1.4}$$

which holds as soon as the function $x \mapsto \int_0^{\gamma(x)} \left(\frac{g'(\gamma^{-1}(u))}{\gamma'(\gamma^{-1}(u))}\right)^2 du$ belongs to the (so far unspecified) class C. Note that inequality (1.4) also holds if in (1.3) we replace the equality sign by an increasing inequality.

Identity (1.3) can also readily be combined with the Cauchy-Schwarz inequality to obtain lower variance bounds. To this end, consider a mean zero function γ (this is in any case necessary for relationships such as (1.3) to hold) for which $(\mathbb{E}[\gamma(W)g(W)])^2 = (\mathbb{E}[\gamma(W)(g(W) - \mathbb{E}[g(W)])])^2 \leq \mathbb{E}[\gamma(W)^2] \operatorname{Var}[g(W)]$. Then from (1.3) we deduce

$$\operatorname{Var}[g(W)] \ge \frac{\left(\mathbb{E}\left[T_1 g'(T_2)\right]\right)^2}{\operatorname{Var}\left[\gamma(W)\right]} \tag{1.5}$$

for all $g \in C$. As above, we note that inequality (1.5) also holds if in (1.3) we replace the equality sign by a decreasing inequality.

The rest of this paper is devoted to proposing situations wherein such couplings W, T_1 and T_2 occur naturally and may be used to establish upper and lower variance bounds. In Section 2 we use the framework of Stein kernels to express suitable couplings. Section 3 makes use of zero-biased couplings to derive variance bounds suitable for random variables which are asymptotically Gaussian. Finally, in Section 4 we consider random variables satisfying certain stochastic or convex ordering assumptions, which allow us to derive bounds sharper than we would otherwise obtain with our method. Some proofs and additional examples illustrating the results of Section 2 are deferred to the appendices.

2 Stein kernel and a bound of Cacoullos

Suppose that the target W has a differentiable density p with interval support. Following, for example, [3] and [7], we define the *Stein kernel* of W as the function τ satisfying

$$\operatorname{Cov}\left[W,\phi(W)\right] = \mathbb{E}\left[\tau(W)\phi'(W)\right] \tag{2.1}$$

for all functions ϕ such that either integral is defined. See [7] for an extensive discussion of this function. In the notation of Section 1, this means that we can take $\gamma(x) = x - \mathbb{E}[W]$, $T_1 = \tau(W)$ and $T_2 = W$ in (1.3). Note that $\mathbb{E}[\tau(W)] = \operatorname{Var}[W]$. Applying (1.4) and (1.5), we get for all $g \in L^2(W)$ that

$$\frac{\mathbb{E}\left[\tau(W)g'(W)\right]^2}{\operatorname{Var}\left[W\right]} \le \operatorname{Var}\left[g(W)\right] \le \mathbb{E}\left[\tau(W)\left(g'(W)\right)^2\right],\tag{2.2}$$

which is nothing but a restatement of classical bounds already available in [2].

Of course for (2.2) to be of use it remains to identify situations in which the Stein kernel has an agreeable form. We give several such situations.

Example 2.1. Following [13], it is easy to see that if $W = n^{-1/2} \sum_{i=1}^{n} X_i$, where the X_i are centred, independent random variables with Stein kernel $\tau_i(\cdot)$ and common variance σ^2 , then $\tau_W(w) = \frac{1}{n} \sum_{i=1}^{n} \mathbb{E}[\tau_i(X_i) | W = w]$ is a Stein kernel for W. If the X_i are copies of X_1 with kernel $\tau_1(\cdot)$, (2.2) becomes

$$\frac{\mathbb{E}\left[\tau_1(X_1)g'(W)\right]^2}{\sigma^2} \le \operatorname{Var}[g(W)] \le \mathbb{E}\left[\tau_1(X_1)(g'(W))^2\right]$$

If W and X_1 were independent, we could use $\mathbb{E}[\tau_1(X_1)] = \sigma^2$ to recover the Gaussian case stated in (1.1) and (1.2). Here we need to apply a limited development to make independence appear. Let $U \sim \text{Unif}[0,1]$ and recall the mean-value theorem g'(x+t) = $g'(x) + t\mathbb{E}[g''(x+Ut)]$. Let $W^{(1)} = W - n^{-1/2}X_1$. Then, by independence, if g is twice differentiable the lower bound becomes $\sigma^2\mathbb{E}[g'(W^{(1)})]^2 + \frac{C_1}{\sqrt{n}}$ where $C_1 = C_1(g,n)$ is given by $C_1 = 2\mathbb{E}[g'(W^{(1)})]\mathbb{E}[\tau_1(X_1)X_1g''(W^{(1)} + n^{-1/2}UX_1)] + n^{-1/2}/\sigma^2\mathbb{E}[\tau_1(X_1)X_1g''(W^{(1)} + n^{-1/2}UX_1)]^2$. Clearly $\lim_{n\to\infty} C_1(g,n)/\sqrt{n} = 0$ for all g. Similar considerations apply for the upper bound. Indeed, recall that for a twice differentiable function g we have

$$\left|g'(x+t)^2 - g'(x)^2\right| \le 2||g'g''|||t|, \qquad (2.3)$$

 $(where \|\cdot\| \text{ is the supremum norm}) \text{ so that we have } \mathbb{E}[\tau_1(X_1)(g'(W))^2] \le \sigma^2 \mathbb{E}[(g'(W^{(1)}))^2] + \frac{2}{\sqrt{n}} \|g'g''\|\sigma^2 \mathbb{E}[|X_1|] =: \sigma^2 \mathbb{E}[(g'(W^{(1)}))^2] + \frac{C_2}{\sqrt{n}}. Wrapping up,$

$$\sigma^{2} \mathbb{E}[(g'(W^{(1)}))]^{2} + \frac{C_{1}}{\sqrt{n}} \le \operatorname{Var}[g(W)] \le \sigma^{2} \mathbb{E}[(g'(W^{(1)}))^{2}] + \frac{C_{2}}{\sqrt{n}},$$

where the proximity with the corresponding inequalities for the Gaussian case are now made explicit.

Example 2.2 (Smoothing). Let Y be a real-valued random variable with $\mathbb{E}[Y] = \mu$. Note that we do not require Y to have a density function, and the bounds of this example apply if, for instance, Y is a discrete random variable. In order to allow us to derive variance bounds for Y using our approach, we smooth it by convolving it with independent Gaussian noise with small variance. We let $Z \sim \mathcal{N}(0, \epsilon^2)$ have a Gaussian distribution, independent of Y. Let φ_{ϵ} and Φ_{ϵ} be the density and distribution functions of Z, respectively, and define

$$\tau_{\epsilon}(x) = \epsilon^{2} + \frac{\mathbb{E}\left[(Y' - \mu)\bar{\Phi}_{\epsilon}(x - Y')\right]}{\mathbb{E}[\varphi_{\epsilon}(x - Y')]}, \qquad (2.4)$$

where $\overline{\Phi}_{\epsilon}(y) = 1 - \Phi_{\epsilon}(y)$ and Y' is an independent copy of Y. Then $\tau_{\epsilon}(x)$ is a Stein kernel for Y + Z (see Appendix A) and (2.2) applies to all differentiable functions $g : \mathbb{R} \to \mathbb{R}$ such that $\operatorname{Var}[g(Y + Z)]$ is finite. Moreover, the following hold:

(i). If the mapping $x \mapsto (g(x) - \mathbb{E}[g(Y+Z)])^2$ is convex, then

$$\operatorname{Var}[g(Y)] \leq \mathbb{E}\left[\tau_{\epsilon}(Y+Z)g'(Y+Z)^{2}\right] \,.$$

(ii). If the mapping $x \mapsto (g(x) - \mathbb{E}[g(Y)])^2$ is concave, then

$$\operatorname{Var}\left[g(Y)\right] \ge \frac{\mathbb{E}\left[\tau_{\epsilon}(Y+Z)g'(Y+Z)\right]^{2}}{\epsilon^{2} + \operatorname{Var}[Y]}$$

We defer the proofs of these claims to Appendix A.

Example 2.3 (Pearson family and application to posterior distributions). As is well known, the Pearson family has explicit Stein kernels given by Proposition B.1 recalled

in the Appendix. Such a result is particularly useful in the following situation inherited from Bayesian statistics. In a Bayesian setting, the initial distribution of the parameter of interest is some prior distribution with density $\pi_0(\theta)$; upon observing data points $\mathbf{x} =$ (x_1, \ldots, x_n) sampled independently with sampling distribution $\pi(\theta, \mathbf{x})$ we update from the prior to the posterior density given by $\pi_2(\theta) = \kappa_2(\mathbf{x})\pi(\theta, \mathbf{x})\pi_0(\theta)$. We use the notation Θ_0 to indicate the distribution of the parameter under the prior, Θ_2 its distribution under the posterior, and X a random variable following the same common distribution $\pi_1(\theta) =$ $\kappa_1(\mathbf{x})\pi(\theta, \mathbf{x})$, which corresponds to a posterior with flat (uninformative) prior. A popular choice of prior is that of a conjugate prior for which the mathematical properties of the posterior are the same as those of the sampling distribution; the impact of the data is then visible in the parameters of the posterior distribution who are updated. Restricting our attention to Pearson distributed families, we can apply Proposition B.1 and read variance bounds directly from the updated parameters. For instance:

• Gaussian data, inference on mean, Gaussian prior: If $X \sim \mathcal{N}(\theta, \sigma^2)$ with $\theta \in \mathbb{R}$ and fixed $\sigma > 0$, and $\Theta_0 \sim \mathcal{N}(\mu, \delta^2)$ with $\mu \in \mathbb{R}, \delta > 0$, then $\Theta_2 \sim \mathcal{N}\left(\frac{\sigma^2 \mu + n\delta^2 \bar{x}}{n\delta^2 + \sigma^2}, \frac{\sigma^2 \delta^2}{n\delta^2 + \sigma^2}\right)$, where $\bar{x} = \frac{1}{n} \sum_{i=1}^n x_i$. The Stein kernel for this Gaussian distribution is $\tau(\theta) = (\frac{n}{\sigma^2} + \frac{1}{\delta^2})^{-1}$. Consequently,

$$\mathbb{E}\left[g'(\Theta_2)\right]^2 \le \left(\frac{n}{\sigma^2} + \frac{1}{\delta^2}\right) \operatorname{Var}\left[g(\Theta_2)\right] \le \mathbb{E}\left[g'(\Theta_2)^2\right]$$

for all suitable g, all n and all values of the parameters.

• Gaussian data, inference on variance, Inverse Gamma prior: If $X \sim \mathcal{N}(\mu, \theta)$ with $\theta > 0$ and fixed $\mu \in \mathbb{R}$, and $\Theta_0 \sim \mathcal{IG}(\alpha, \beta)$ has an Inverse Gamma distribution with density

$$\theta \mapsto \frac{\beta^{\alpha}}{\Gamma(\alpha)} \theta^{-\alpha-1} \exp\left(-\frac{\beta}{\theta}\right), \ \alpha, \beta > 0,$$

then $\Theta_2 \sim \mathcal{IG}\left(\frac{n}{2} + \alpha, \frac{1}{2}\sum_{i=1}^n (x_i - \mu)^2 + \beta\right)$. The Stein kernel for this Inverse Gamma distribution is $\tau(\theta) = \frac{\theta^2}{\frac{n}{2} + \alpha - 1}$. Consequently, for all suitable g,

$$\frac{(\frac{n}{2} + \alpha - 2)}{(\frac{1}{2}\sum_{i=1}^{n}(x_i - \mu)^2 + \beta)^2} \mathbb{E}[\Theta_2^2 g'(\Theta_2)]^2 \le \operatorname{Var}[g(\Theta_2)] \le \frac{1}{\frac{n}{2} + \alpha - 1} \mathbb{E}[\Theta_2^2 g'(\Theta_2)^2].$$

• Binomial data, inference on proportion, Beta prior: If $X \sim Bin(n, \theta)$ with $\theta \in [0, 1]$, and $\Theta_0 \sim Beta(\alpha, \beta)$ with density

$$\theta \mapsto \frac{\theta^{\alpha-1}(1-\theta)^{\beta-1}}{\frac{\Gamma(\alpha)\Gamma(\beta)}{\Gamma(\alpha+\beta)}}, \ \alpha, \beta > 0,$$

then $\Theta_2 \sim Beta(x + \alpha, n - x + \beta)$, where x denotes the observed number of successes. The Stein kernel for this Beta distribution is $\tau(\theta) = \frac{\theta(1-\theta)}{n+\alpha+\beta}$. Consequently, for all suitable g,

$$\frac{(n+\alpha+\beta+1)}{(x+\alpha)(n-x+\beta)}\mathbb{E}[\Theta_2(1-\Theta_2)g'(\Theta_2)]^2 \le \operatorname{Var}[g(\Theta_2)] \le \frac{\mathbb{E}[\Theta_2(1-\Theta_2)g'(\Theta_2)^2]}{n+\alpha+\beta}.$$

Further examples are provided in Appendix B.

3 Variance bounds from zero-biased couplings

In this section, we suppose that the target W has mean zero, finite variance σ^2 , and can be coupled to some random variable W^* through

$$\mathbb{E}[W\phi(W)] = \sigma^2 \mathbb{E}[\phi'(W^*)] \tag{3.1}$$

for all functions $\phi : \mathbb{R} \to \mathbb{R}$. Such W^* always exists, and its law is unique. It has the *W*-zero-biased distribution; see, e.g., [5, Section 2.3.3] and references therein for more details. Note that W^* is a continuous random variable, regardless of whether *W* is discrete or continuous. Under (3.1), we immediately obtain

$$\sigma^{2} \mathbb{E}\left[g'(W^{\star})\right]^{2} \leq \operatorname{Var}[g(W)] \leq \sigma^{2} \mathbb{E}\left[g'(W^{\star})^{2}\right]$$
(3.2)

by using (1.4) and (1.5) with $\gamma(x) = x$, $T_1 = \sigma^2$ and $T_2 = W^*$ for all $g : \mathbb{R} \to \mathbb{R}$ for which $\operatorname{Var}[g(W)]$ is finite. Obviously it may be of interest to express (3.2) in terms of the original variable. Using (2.3), we obtain the following result.

Proposition 3.1. Let W have mean zero and finite variance σ^2 , and W^* have the W-zero biased distribution. Then

$$\operatorname{Var}[g(W)] \le \sigma^2 \mathbb{E}\left[g'(W)^2\right] + 2\sigma^2 \|g'g''\|\mathbb{E}|W^* - W|$$
(3.3)

for all twice differentiable functions $g : \mathbb{R} \mapsto \mathbb{R}$ for which $\operatorname{Var}[g(W)]$ exists.

It is classical that the Gaussian distribution is the unique fixed point of the zerobias transform, in the sense that $W \sim \mathcal{N}(0, \sigma^2)$ if and only if $W = W^*$. Hence $|W^* - W|$ gives information on the distributional proximity between the law $\mathcal{L}(W)$ of W and $\mathcal{N}(0, \sigma^2)$. Also, it is classical that the Gaussian is characterized by the fact that $\sigma^2 = \sup_g \operatorname{Var}[g(W)]/\mathbb{E}[g'(W)^2]$, see, e.g., [3]. Inequality (3.3) captures these two essential features of the Gaussian distribution.

Example 3.2. Let X_1, X_2, \ldots, X_n be independent mean zero random variables with finite variances $\mathbb{E}[X_i^2] = \sigma_i^2, i = 1, \ldots, n$. Set $W = X_1 + \cdots + X_n$ and $\mathbb{E}[W^2] = \sigma^2 = \sum_{i=1}^n \sigma_i^2$. Let I be a random index independent of all else such that $P(I = i) = \sigma_i^2/\sigma^2$ and let $W_i = W - X_i$. Finally let X_i^* be the zero-bias transform of X_i . Then $W^* - W = X_I - X_I^*$ (see Example 2.1 of [9]) so that the bound (3.3) becomes

$$\operatorname{Var}[g(W)] \le \sigma^2 \mathbb{E}[g'(W)^2] + 2 ||g'g''|| \sum_{i=1}^n \sigma_i^2 \mathbb{E}[|X_i - X_i^{\star}|].$$

If, furthermore, we suppose the summands to be independent copies of X such that $\sigma^2 = 1$ then

$$\operatorname{Var}[g(W)] \le \mathbb{E}[g'(W)^2] + 2\|g'g''\|\mathbb{E}[|X - X^*|].$$

To see how this plays out in practice, suppose that $X = (\xi - p)/\sqrt{npq}$ with ξ Bernoulli with success parameter p. Following [5, Corollary 4.1], we obtain $\mathbb{E}[|X - X^*|] = (p^2 + q^2)/(2\sqrt{npq})$ and

$$\operatorname{Var}[g(W)] \le \sigma^2 \mathbb{E}[g'(W)^2] + \|g'g''\| \frac{p^2 + q^2}{\sqrt{npq}}$$

Many other examples can be explicitly worked out along these lines.

Example 3.3. Let $(a_{i,j})_{i,j=1}^n$ be an array of real numbers and π a uniformly chosen permutation of $\{1, \ldots, n\}$. Let $W = \sum_{i=1}^n a_{i,\pi(i)}$. We further define

$$a_{\bullet\bullet} = \frac{1}{n^2} \sum_{i,j=1}^n a_{i,j} \,, \quad a_{i\bullet} = \frac{1}{n} \sum_{j=1}^n a_{i,j} \,, \quad and \quad a_{\bullet j} = \frac{1}{n} \sum_{i=1}^n a_{i,j} \,,$$

and note that $\mathbb{E}[W] = na_{\bullet \bullet}$ and

$$\operatorname{Var}[W] = \sigma^{2} = \frac{1}{n-1} \sum_{i,j=1}^{n} \left(a_{i,j} - a_{i\bullet} - a_{\bullet j} + a_{\bullet \bullet} \right)^{2} \,.$$

See, for example, [5, Section 4.4]. Letting $Z = \sigma^{-1}(W - na_{\bullet\bullet})$ and $C = \max_{1 \le i,j \le n} |a_{i,j} - a_{i\bullet} - a_{\bullet j} + a_{\bullet\bullet}|$, the proof of Theorem 6.1 of [5] shows that $\mathbb{E}|Z^* - Z| \le 8C\sigma^{-1}$ for some positive constant C, and so we have from (3.3) that

$$\operatorname{Var}[g(Z)] \leq \mathbb{E}\left[g'(Z)^2\right] + \frac{16C}{\sigma} \|g'g''\|,$$

for all twice differentiable g such that $\operatorname{Var}[g(Z)]$ is finite.

4 Variance bounds using stochastic ordering

We consider now some further applications in which we do not require explicit knowledge of the density of W in order to derive bounds on $\operatorname{Var}[g(W)]$ using our techniques. Unlike those examples in Section 3, the bounds we obtain here have the same form as in applications where we employ the exact expression for the underlying density, as in Section 2, without any additional 'remainder' terms. We may obtain such bounds under natural assumptions on the random variable W, which we express in terms of stochastic orderings; the price we pay is in some restriction on the class of functions g for which the bounds apply.

We begin by recalling the definitions of the orderings which we will use. For any random variables X and Y, we will say that X is stochastically smaller than Y (denoted $X \leq_{st} Y$) if $\mathbb{P}(X > t) \leq \mathbb{P}(Y > t)$ for all t. We will say that X is smaller than Y in the convex order (denoted $X \leq_{cx} Y$) if $\mathbb{E}[\phi(X)] \leq \mathbb{E}[\phi(Y)]$ for all convex functions ϕ for which the expectations exist. See [15] for background and many further details.

4.1 Zero-biased couplings and the convex order

Let W be a real-valued random variable with mean zero and variance σ^2 . Recall the definition (3.1) of W^* , the zero-biased version of W. We note that, from Lemma 2.1(ii) of [9], W^* is supported on the closed convex hull of the support of W and has density function given by

$$p_W^{\star}(w) = \frac{1}{\sigma^2} \mathbb{E}[WI(W > w)].$$
(4.1)

If we assume that $W^* \leq_{cx} W$, then we may write

$$\mathbb{E}[W\phi(W)] = \sigma^2 \mathbb{E}[\phi'(W^*)] \le \sigma^2 \mathbb{E}[\phi'(W)], \qquad (4.2)$$

for all differentiable functions ϕ such that ϕ' is convex. That is, (1.3) holds with the equality replaced by an inequality for all such ϕ , with the choices $\gamma(W) = W$, $T_1 = \sigma^2$, and $T_2 = W$.

Following the proof of (1.4), the inequality (4.2) is sufficient to obtain this upper bound on $\operatorname{Var}[g(W)]$. In proving this bound, we apply (4.2) with ϕ such that $\phi'(x) = g'(x)^2$; we must therefore assume that $g'(x)^2$ is convex in order to do this. We thus obtain the following bound.

Theorem 4.1. Let W have mean 0 and variance σ^2 , and assume that $W^* \leq_{cx} W$. For all differentiable $g : \mathbb{R} \mapsto \mathbb{R}$ such that $\operatorname{Var}[g(W)]$ exists and $g'(x)^2$ is convex,

$$\operatorname{Var}[g(W)] \le \sigma^2 \mathbb{E}[g'(W)^2].$$
(4.3)

Example 4.2. Let $W = X_1 + X_2 + \cdots + X_n$, where X_1, X_2, \ldots, X_n are independent, mean-zero random variables, with X_i supported on the set $\{-a_i, b_i\}$ for $a_i, b_i > 0$, for each $i = 1, \ldots, n$. That is, $\mathbb{P}(X_i = -a_i) = p_i = 1 - \mathbb{P}(X_i = b_i)$ for $1 \le i \le n$, where $p_i = b_i/(a_i + b_i)$ so that $\mathbb{E}[X_i] = 0$. Let $\sigma_i^2 = \operatorname{Var}(X_i)$ and $\sigma^2 = \sigma_1^2 + \cdots + \sigma_n^2$.

A straightforward calculation using (4.1) shows that, for each i = 1, ..., n, X_i^* is uniformly distributed on the interval $[-a_i, b_i]$. Hence, Theorem 3.A.44 of [15] gives that $X_i^* \leq_{cx} X_i$ for each i.

Let I be a random index, chosen independently of all else, with $\mathbb{P}(I=i) = \sigma_i^2/\sigma^2$, for $i = 1, \ldots, n$. Now, using Lemma 2.1(v) of [9], W^* is equal in distribution to $X_I^* + \sum_{j \neq I} X_j$, which is smaller than W in the convex order for each possible value of I by (3.A.46) of [15]. It then follows from Theorem 3.A.12(b) of [15] that $W^* \leq_{cx} W$, and hence our upper bound (4.3) applies.

4.2 Equilibrium couplings

Throughout this section, let W be a non-negative random variable with mean λ^{-1} . Following, for example, [14], we say that a random variable W^e has the equilibrium distribution with respect to W if

$$\mathbb{E}[\phi(W)] - \phi(0) = \lambda^{-1} \mathbb{E}[\phi'(W^e)], \qquad (4.4)$$

for all a.e. differentiable functions ϕ .

Remark 4.3. Note that this definition is motivated by the fact that W is Exponential if and only if W and W^e are equal in distribution. Applying the definition to the function $\phi_x(w) = (w - x)\mathbb{I}(w \ge x)$ and integrating by parts we obtain that $\mathbb{P}(W^e > x) = \lambda \int_x^\infty \mathbb{P}(W > y) \, dy$ for all $x \ge 0$.

In this section we consider random variables that are new better than used in expectation (NBUE) and new worse than used in expectation (NWUE). Recall that W is NBUE if $\lambda \int_x^\infty \mathbb{P}(W > s) \, ds \leq \mathbb{P}(W > x)$ for all $x \geq 0$, and that W is NWUE if this holds with the inequality reversed. These properties are well-known in reliability theory; see, for example, [15].

From this definition and the remark above, it is clear that W is NBUE if and only if $W^e \leq_{st} W$, and that W is NWUE if and only if $W \leq_{st} W^e$. For a random variable W which is either NBUE or NWUE, we employ this stochastic ordering in a similar way to the convex ordering we used in Section 4.1 above.

We begin by deriving an inequality analogous to (4.2). For a differentiable function ϕ , the definition of W^e gives that

$$\mathbb{E}[W\phi(W)] = \lambda^{-1}\mathbb{E}[\phi(W^e) + W^e\phi'(W^e)],$$

and hence

$$\mathbb{E}[(\lambda W - 1)\phi(W)] + \mathbb{E}[\phi(W)] = \mathbb{E}[W^e \phi'(W^e)] + \mathbb{E}[\phi(W^e)]$$

Thus, the inequality

$$\mathbb{E}[(\lambda W - 1)\phi(W)] \le \mathbb{E}[W\phi'(W)]$$
(4.5)

holds if and only if

$$\mathbb{E}[\phi(W^e) + W^e \phi'(W^e)] \le \mathbb{E}[\phi(W) + W \phi'(W)].$$

Therefore, inequality (4.5) holds if W is NBUE and $\phi(x) + x\phi'(x)$ is increasing in x. Alternatively, (4.5) also holds if W is NWUE and $\phi(x) + x\phi'(x)$ is decreasing in x. Analogously to the use of (4.2) in proving Theorem 4.1 above, an upper bound on $\operatorname{Var}[g(W)]$ therefore holds for some functions g under either of these assumptions; see Theorem 4.4 below for a precise statement.

Similarly, we may ask when the reversed inequality $\mathbb{E}[(\lambda W - 1)\phi(W)] \ge \mathbb{E}[W\phi'(W)]$ holds. By similar reasoning, this holds if either (i) W is NBUE and $\phi(x) + x\phi'(x)$ is decreasing in x, or (ii) W is NWUE and $\phi(x) + x\phi'(x)$ is increasing in x. Under either of these assumptions, we have a lower variance bound.

We have thus proved the following.

Theorem 4.4. Let W be a non-negative random variable with mean $\mathbb{E}[W] = \lambda^{-1}$.

- (a) For a differentiable function $g : \mathbb{R}^+ \to \mathbb{R}$ such that $\operatorname{Var}[g(W)]$ exists, let $\phi_g(x) = \int_0^{\lambda x 1} g'(\lambda^{-1}(u+1)) \, du$. Assume that either
 - (i) W is NBUE and $\phi_g(x) + x \phi'_g(x)$ is increasing in x; or
 - (ii) W is NWUE and $\phi_q(x) + x\phi'_q(x)$ is decreasing in x.

Then

$$\operatorname{Var}[g(W)] \le \frac{1}{\lambda} \mathbb{E}[Wg'(W)^2].$$

- (b) For a differentiable function $g : \mathbb{R}^+ \to \mathbb{R}$ such that $\operatorname{Var}[g(W)]$ exists, assume that either
 - (i) W is NBUE and g(x) + xg'(x) is decreasing in x; or
 - (ii) W is NWUE and g(x) + xg'(x) is increasing in x.

Then

$$\operatorname{Var}[g(W)] \ge \frac{(\mathbb{E}[Wg'(W)])^2}{\lambda^2 \operatorname{Var}[W]}$$

Example 4.5. Consider the random sum $W = \sum_{i=1}^{N} X_i$, where X, X_1, X_2, \ldots are independent and identically distributed, continuous, real-valued random variables and N is a counting random variable supported on the non-negative integers. Conditions are known under which W is NWUE. For example, [1] shows that if N is Geometric, then W is NWUE, regardless of the distribution of X. More generally, Corollary 2.1 of [17] establishes that if N satisfies

$$\sum_{k=0}^{\infty} \mathbb{P}(N > n + k + 1) \ge \mathbb{P}(N > n) \sum_{k=0}^{\infty} \mathbb{P}(N > k), \qquad (4.6)$$

for all n = 0, 1, ..., then W is NWUE. This includes, for example, the case where N is mixed Poisson with a mixing distribution that is itself NWUE; see Corollary 3.1 of [17]. Thus, under the condition (4.6), the bounds of the NWUE cases of Theorem 4.4 apply, with $\lambda^{-1} = \mathbb{E}[N]\mathbb{E}[X]$ and $\operatorname{Var}[W] = (\mathbb{E}[X])^2 \operatorname{Var}[N] + \mathbb{E}[N] \operatorname{Var}[X]$.

Acknowledgements

Part of this work was completed while FD and YS were attending the Workshop on New Directions in Stein's Method, held at the Institute for Mathematical Sciences, National University of Singapore in May 2015. We thank the IMS, and the organisers of that workshop, for their support and hospitality. FD also thanks the University of Liège for supporting a visit there. The research of FG and CL is supported by a BOF Starting Grant of Ghent University.

References

- M. Brown. Error bounds for exponential approximations of geometric convolutions. The Annals of Probability, 18(3):1388–1402, 1990.
- [2] T. Cacoullos. On upper and lower bounds for the variance of a function of a random variable. *The Annals of Probability*, 10(3):799–809, 1982.

- [3] T. Cacoullos, V. Papathanasiou, and S. A. Utev. Variational inequalities with examples and an application to the central limit theorem. *The Annals of Probability*, 22(3):1607–1618, 1994.
- [4] L. H. Y. Chen. An inequality for the multivariate normal distribution. Journal of Multivariate Analyis, 12:306–315, 1982.
- [5] L. H. Y. Chen, L. Goldstein, and Q.-M. Shao. Normal Approximation by Stein's Method. Probability and its Applications (New York). Springer, Heidelberg, 2011.
- [6] H. Chernoff. A note on an inequality involving the normal distribution. *The Annals of Probability*, 9(3):533–535, 1981.
- [7] M. Ernst, G. Reinert, and Y. Swan. First order covariance inequalities via Stein's method. Preprint. Available at arXiv:1906.08372, 2019.
- [8] M. Ernst, G. Reinert, and Y. Swan. On infinite covariance expansions. Preprint. Available at arXiv:1906.08376, 2019.
- [9] L. Goldstein and G. Reinert. Stein's method and the zero bias transformation with application to simple random sampling. *The Annals of Applied Probability*, 7(4):935– 952, 1997.
- [10] C. A. J. Klaassen. On an inequality of Chernoff. The Annals of Probability, 13(3):966– 974, 1985.
- [11] C. Ley, G. Reinert, and Y. Swan. Stein's method for comparison of univariate distributions. *Probability Surveys*, 14:1–52, 2017.
- [12] C. Ley and Y. Swan. Parametric Stein operators and variance bounds. Brazilian Journal of Probability and Statistics, 30:171–195, 2016.
- [13] I. Nourdin, G. Peccati, and Y. Swan. Integration by parts and representation of information functionals. *IEEE International Symposium on Information Theory (ISIT)*, pages 2217–2221, 2014.
- [14] E. Peköz and A. Röllin. New rates for exponential approximation and the theorems of Rényi and Yaglom. The Annals of Probability, 39(2):587–608, 2011.
- [15] M. Shaked and J. G. Shanthikumar. *Stochastic Orders*. Springer New York, 2007.
- [16] C. Stein. Approximate Computation of Expectations. Institute of Mathematical Statistics Lecture Notes—Monograph Series, 7. Institute of Mathematical Statistics, Hayward, CA, 1986.
- [17] G. E. Willmot, S. Drekic, and J. Cai. Equilibrium compound distributions and stop-loss moments. *Scandinavian Actuarial Journal*, 2005(1):6–24, 2005.

A Example 2.2: Proofs of claims

We begin by showing that $\tau_{\epsilon}(x)$, as defined in (2.4), is the Stein kernel of Y + Z. To see this, note that $\mathbb{P}(Y+Z \leq t) = \mathbb{E}[\Phi_{\epsilon}(t-Y)]$, so that Y+Z has density $p_{\epsilon}(t) = \mathbb{E}[\varphi_{\epsilon}(t-Y)]$. Hence, since Y + Z has expectation μ , its Stein kernel is given by

$$\frac{1}{p_{\epsilon}(x)} \int_{x}^{\infty} (y-\mu) p_{\epsilon}(y) \, dy = \frac{1}{p_{\epsilon}(x)} \int_{x}^{\infty} \int_{-\infty}^{\infty} (y-\mu) \varphi_{\epsilon}(y-t) \, dF(t) \, dy$$

where F is the distribution function of Y; see [3]. Applying Fubini's theorem, this is equal to

$$\frac{1}{p_{\epsilon}(x)} \int_{-\infty}^{\infty} \int_{x-t}^{\infty} (s+t-\mu)\varphi_{\epsilon}(s) \, ds \, dF(t) = \frac{1}{p_{\epsilon}(x)} \mathbb{E}\left[\epsilon^{2}\varphi_{\epsilon}(x-Y) + (Y-\mu)\bar{\Phi}_{\epsilon}(x-Y)\right] \,,$$

since $\int_{y}^{\infty} s\varphi_{\epsilon}(s) ds = \epsilon^{2} \varphi_{\epsilon}(y)$. This Stein kernel is easily seen to be equal to $\tau_{\epsilon}(x)$ given in (2.4).

Now, to prove claim (i), we firstly note that $Y \leq_{cx} Y + Z$ (see Theorem 3.A.34 of [15]), so that $\mathbb{E}[\phi(Y)] \leq \mathbb{E}[\phi(Y+Z)]$ for any convex function ϕ . Noting that the function $f(\alpha) = \mathbb{E}[(g(Y) - \alpha)^2]$ is minimized at $\alpha = \mathbb{E}[g(Y)]$, we have

$$\operatorname{Var}[g(Y)] = \mathbb{E}\left[\left(g(Y) - \mathbb{E}[g(Y)]\right)^2\right] \le \mathbb{E}\left[\left(g(Y) - \mathbb{E}[g(Y+Z)]\right)^2\right] \le \operatorname{Var}[g(Y+Z)]$$

where the final inequality follows from the assumption in (i) that the mapping $x \mapsto (g(x) - \mathbb{E}[g(Y+Z)])^2$ is convex. Applying the upper bound from (2.2) completes the proof of (i).

We use a similar argument for (ii). We have that

$$\operatorname{Var}[g(Y+Z)] \le \mathbb{E}[(g(Y+Z) - \mathbb{E}[g(Y)])^2] \le \mathbb{E}[(g(Y) - \mathbb{E}[g(Y)])^2],$$

where the final inequality uses the convex ordering between Y and Y + Z (from which $\mathbb{E}[\phi(Y+Z)] \leq \mathbb{E}[\phi(Y)]$ for any concave function ϕ) and the assumption that the mapping $x \mapsto (g(x) - \mathbb{E}[g(Y)])^2$ is concave. We now apply the lower bound from (2.2) to complete the proof of (ii).

B Example 2.3: Stein kernel and further applications

We start by recalling a result taken from [16, Equation (40), p. 65], which was used in Example 2.3.

Proposition B.1 (Pearson distribution). A random variable with mean μ and variance σ^2 is of Pearson type if and only if there exist $\delta_1, \delta_2, \delta_3 \in \mathbb{R}$, not all equal to 0, such that

$$\frac{p'(x)}{p(x)} = -\frac{(2\delta_1 + 1)(x - \mu) + \delta_2}{\delta_1(x - \mu)^2 + \delta_2(x - \mu) + \delta_3}$$

In this case, its Stein kernel is $\tau(x) = \delta_1(x-\mu)^2 + \delta_2(x-\mu) + \delta_3$.

To complement Example 2.3 and illustrate the scope of its application, we use the remainder of this appendix to present further examples along similar lines.

Example B.2 (Negative binomial data, inference on proportion, Beta prior). If $X \sim NB(r,\theta)$ has a negative binomial distribution with $\theta \in [0,1]$ and fixed $r \in \mathbb{N}$, and $\Theta_0 \sim Beta(\alpha,\beta)$ with $\alpha,\beta > 0$, then $\Theta_2 \sim Beta(\sum_{i=1}^n x_i + \alpha, nr + \beta)$. The Stein kernel for this Beta distribution is $\tau(\theta) = \frac{\theta(1-\theta)}{\sum_{i=1}^n x_i + nr + \alpha + \beta}$. Consequently,

$$\frac{\left(\sum_{i=1}^{n} x_i + nr + \alpha + \beta + 1\right)}{\left(\sum_{i=1}^{n} x_i + \alpha\right)(nr + \beta)} \mathbb{E}[\Theta_2(1 - \Theta_2)g'(\Theta_2)]^2 \le \operatorname{Var}[g(\Theta_2)] \le \frac{\mathbb{E}[\Theta_2(1 - \Theta_2)g'(\Theta_2)^2]}{\sum_{i=1}^{n} x_i + nr + \alpha + \beta}$$

Example B.3 (Weibull data, inference on scale, Inverse Gamma prior). If $X \sim Wei(k, \theta)$ has a Weibull distribution with $\theta > 0$ and fixed k > 0 (note that here we consider the Weibull density $x \mapsto \frac{kx^{k-1}}{\theta} \exp(-x^k/\theta), x > 0$), and $\Theta_0 \sim IG(\alpha, \beta)$ with $\alpha, \beta > 0$, then $\Theta_2 \sim IG(n + \alpha, \sum_{i=1}^n x_i^k + \beta)$. The Stein kernel for this Inverse Gamma distribution is $\tau(\theta) = \frac{\theta^2}{n+\alpha-1}$. Consequently,

$$\frac{n+\alpha-2}{(\sum_{i=1}^{n} x_i^k + \beta)^2} \mathbb{E}[\Theta_2^2 g'(\Theta_2)]^2 \le \operatorname{Var}[g(\Theta_2)] \le \frac{\mathbb{E}[\Theta_2^2 g'(\Theta_2)^2]}{n+\alpha-1}.$$

Example B.4 (Gamma data, inference on scale, Gamma prior). If $X \sim Gam(k, \theta)$ has a Gamma distribution with $\theta, k > 0$, and $\Theta_0 \sim Gam(\alpha, \beta)$ with $\alpha, \beta > 0$, then $\Theta_2 \sim Gam(nk + \alpha, \sum_{i=1}^n x_i + \beta)$. The Stein kernel for this Gamma distribution is $\tau(\theta) = \frac{\theta}{\sum_{i=1}^n x_i + \beta}$. Consequently,

$$\frac{\mathbb{E}[\Theta_2 g'(\Theta_2)]^2}{nk + \alpha} \le \operatorname{Var}[g(\Theta_2)] \le \frac{1}{\sum_{i=1}^n x_i + \beta} \mathbb{E}[\Theta_2 g'(\Theta_2)^2].$$

Example B.5 (Laplace data, inference on scale, inverse gamma prior). If $X \sim Lap(\mu, \theta)$ has a Laplace distribution with $\theta > 0$ and fixed $\mu \in \mathbb{R}$, and $\Theta_0 \sim IG(\alpha, \beta)$ with $\alpha, \beta > 0$, then $\Theta_2 \sim IG(n + \alpha, \sum_{i=1}^n |x_i - \mu| + \beta)$. The Stein kernel can readily be deduced from previous examples, and we get

$$\frac{n+\alpha-2}{(\sum_{i=1}^{n}|x_i-\mu|+\beta)^2}\mathbb{E}\left[\Theta_2^2 g'(\Theta_2)\right]^2 \le \operatorname{Var}[g(\Theta_2)] \le \frac{1}{n+\alpha-1}\mathbb{E}\left[\Theta_2^2 g'(\Theta_2)^2\right].$$

Example B.6 (Poisson data, inference on mean=scale, Gamma prior). If $X \sim Poi(\theta)$ has a Poisson distribution with $\theta > 0$, and $\Theta_0 \sim Gam(\alpha, \beta)$ with $\alpha, \beta > 0$, then $\Theta_2 \sim Gam(\sum_{i=1}^n x_i + \alpha, n + \beta)$. The Stein kernel can readily be deduced from previous examples, and we get

$$\frac{\mathbb{E}[\Theta_2 g'(\Theta_2)]^2}{\sum_{i=1}^n x_i + \alpha} \le \operatorname{Var}[g(\Theta_2)] \le \frac{1}{n+\beta} \mathbb{E}\left[\Theta_2 g'(\Theta_2)^2\right].$$

Example B.7 (Uniform data, inference on interval length, Pareto prior). If $X \sim U(0,\theta)$ has a Uniform distribution with $\theta > 0$, and $\Theta_0 \sim Par(\alpha, \beta)$ has a Pareto distribution with $\alpha, \beta > 0$ (as a reminder, the density of such a Pareto distribution is $\theta \mapsto \frac{\alpha\beta^{\alpha}}{\theta^{\alpha+1}} \mathbb{I}[\beta \leq \theta]$

where $\mathbb{I}[A]$ is the indicator function of the event A), then $\Theta_2 \sim Par(n + \alpha, \max(m(x), \beta))$ with $m(x) = \max(x_1, \ldots, x_n)$. The Stein kernel for this Pareto distribution is $\tau(\theta) = \frac{\max(m(x), \beta) - \theta}{n + \alpha - 1} \theta$. Consequently, we get

$$\frac{(n+\alpha-2)}{(n+\alpha)(\max(m(x),\beta))^2} \mathbb{E}\left[(\max(m(x),\beta)-\Theta_2)\Theta_2 g'(\Theta_2)\right]^2 \\ \leq \operatorname{Var}[g(\Theta_2)] \leq \frac{1}{n+\alpha-1} \mathbb{E}\left[(\max(m(x),\beta)-\Theta_2)\Theta_2 g'(\Theta_2)^2\right].$$