

## Uncertainty quantification via codimension one domain partitioning and a new concentration inequality

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In [LOO08], it was proposed that a concentration-of-measure inequality known as McDiarmid’s inequality [McD89] be used to provide upper bounds on the failure probability of a system of interest, the response of which depends on a collection of independent random inputs. McDiarmid’s inequality has the advantage of providing an upper bound in terms of only the mean response of the system, the failure threshold, and measures of system spread known as the McDiarmid subdiameters. A disadvantage of McDiarmid’s inequality is that it takes a global view of the response function: even if the response function exhibits large plateaus of success with only small, localized regions of failure, McDiarmid’s inequality is unable to use this to any advantage. We propose a partitioning algorithm that uses McDiarmid diameters to generate “good” sequences of partitions, on which McDiarmid’s inequality can be applied to each partition element, yielding arbitrarily tight upper bounds. We also investigate some new concentration-of-measure inequalities that arise if mean performance is known only through sampling.

Let  $F: \mathcal{X} := \mathcal{X}_1 \times \cdots \times \mathcal{X}_n \rightarrow \mathbb{R}$  be a response function of interest; the event  $[F \leq \theta]$  is considered to be a failure event. McDiarmid’s inequality bounds the failure probability uniformly in terms of the mean response and a measure of system variability known as the McDiarmid diameter:

$$\mathbb{P}[F \leq \theta] \leq \exp\left(-\frac{2(\mathbb{E}[F] - \theta)_+^2}{\mathcal{D}[F]^2}\right), \quad (1)$$

where the *McDiarmid subdiameters*  $\mathcal{D}_j[F]$  for  $j = 1, \dots, n$  are defined by

$$\mathcal{D}_j[F] := \sup \left\{ |F(x) - F(y)| \mid \begin{array}{l} x = (x_1, \dots, x_n), y = (y_1, \dots, y_n) \in \mathcal{X}, \\ x_k = y_k \in \mathcal{X}_k \text{ for every } k \neq j \end{array} \right\} \quad (2)$$

and the *McDiarmid diameter* is  $\mathcal{D}[F] := \left(\sum_{j=1}^n \mathcal{D}_j[F]^2\right)^{1/2}$ . The inequality (1) can be improved to take account of the local behaviour of  $F$  by partitioning the parameter space and using the conditional/restricted expected values and diameters: if  $\mathcal{P}$  is any partition of  $\mathcal{X}$  into pairwise-disjoint measurable rectangles, then it holds that

$$\mathbb{P}[F \leq \theta] = \sum_{A \in \mathcal{P}} \mathbb{P}(A) \mathbb{P}[F \leq \theta | A] \leq \sum_{A \in \mathcal{P}} \mathbb{P}(A) \exp\left(-\frac{2(\mathbb{E}[F|A] - \theta)_+^2}{\mathcal{D}[F|A]^2}\right). \quad (3)$$

The upper bound (3) is valid for any rectangular partition  $\mathcal{P}$ ; our interest lies in constructing  $\mathcal{P}$  such that the right-hand side is only a small overestimate of  $\mathbb{P}[F \leq \theta]$ . We propose a recursive partitioning algorithm that uses the local McDiarmid subdiameters as sensitivity indices:<sup>1</sup>

Given  $\mathcal{P}_m$  from the previous iteration of the algorithm, for each  $A \in \mathcal{P}_m$ : find the direction  $j$  such that  $\mathcal{D}_j[F|A]$  is maximal, then bisect  $A$  by a codimension 1 hyperplane normal to direction  $j$  through the centre of  $A$ ; include the two “child” sets in  $\mathcal{P}_{m+1}$ .

It is important to note that this algorithm avoids the curse of dimension that affects the naïve strategy of bisecting every box  $A$  in every coordinate direction at every iteration: the number of boxes at most doubles at each iteration, rather a  $2^n$ -fold increase. Furthermore, the same subdiameters  $\mathcal{D}_j[F|A]$  that are used to produce the upper bound (3) are used to select the coordinate direction of greatest parameter sensitivity and thereby refine the upper bound.

The algorithm described above satisfies a convergence theorem: if  $F$  is continuous, then this algorithm produces a sequence of partitions  $(\mathcal{P}_m)_{m \in \mathbb{N}}$  such that

$$\mathbb{P}[F \leq \theta] = \lim_{m \rightarrow \infty} \sum_{A \in \mathcal{P}_m} \mathbb{P}(A) \exp\left(-\frac{2(\mathbb{E}[F|A] - \theta)_+^2}{\mathcal{D}[F|A]^2}\right). \quad (4)$$

While it is to be expected that the order of convergence will depend on the regularity of  $F$ , piecewise-smooth examples investigated to date show that the overestimate associated to  $\mathcal{P}_m$  is approximately  $|\mathcal{P}_m|^{-1/2}$  times the overestimate associated to the global McDiarmid bound (1).

In many applications, the local means  $\mathbb{E}[F|A]$  in (3) are known only through sampling. The question of with what level of confidence we can conclude that

$$\mathbb{P}[F \leq \theta] \leq \sum_{A \in \mathcal{P}} \mathbb{P}(A) \exp\left(-\frac{2(\widehat{\mathbb{E}}[F|A] - \alpha(A) - \theta)_+^2}{\mathcal{D}[F|A]^2}\right), \quad (5)$$

for suitable “confidence shifts”  $\alpha(A) > 0$ , can be answered using the independent concentration of each of the empirical means  $\widehat{\mathbb{E}}[F|A]$  about the corresponding local mean  $\mathbb{E}[F|A]$ ; geometrically, this amounts to estimating the measure of a subset of  $\mathbb{R}^P$  by that of an orthant (a product of half-lines). However, given additional information on  $F$ , it is possible to apply new concentration-of-measure results to obtain greater confidence in a given empirically-derived upper bound for  $\mathbb{P}[F \leq \theta]$ ; the geometric analogue is estimation of the measure of a subset of  $\mathbb{R}^P$  by that of a half-space.

## References

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- [McD89] C. McDiarmid. On the method of bounded differences. In *Surveys in Combinatorics, 1989 (Norwich, 1989)*, volume 141 of *London Math. Soc. Lecture Note Ser.*, pages 148–188. Cambridge Univ. Press, Cambridge, 1989.

<sup>1</sup>There are variants of this algorithm in which the bisection is done through the barycentre of  $A$ , and in which only those  $A \in \mathcal{P}_m$  that are “non-trivial” (i.e.  $\inf_{x \in A} F(x) < \theta < \sup_{x \in A} F(x)$ ) are bisected.