Fully Parallel Hyperparameter Search: Reshaped Space-Filling

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Abstract

Space-filling designs such as scrambled-Hammersley, Latin Hypercube Sampling and Jittered Sampling have been proposed for fully parallel hyperparameter search, and were shown to be more effective than random or grid search. In this paper, we show that these designs only improve over random search by a constant factor. In contrast, we introduce a new approach based on reshaping the search distribution, which leads to substantial gains over random search, both theoretically and empirically. We propose two flavors of reshaping. First, when the distribution of the optimum is some known $P_0$, we propose Recentering, which uses as search distribution a modified version of $P_0$ tightened closer to the center of the domain, in a dimension-dependent and budget-dependent manner. Second, we show that in a wide range of experiments with $P_0$ unknown, using a proposed Cauchy transformation, which simultaneously has a heavier tail (for unbounded hyperparameters) and is closer to the boundaries (for bounded hyperparameters), leads to improved performances. Besides artificial experiments and simple real world tests on clustering or Salmon mappings, we check our proposed methods on expensive artificial intelligence tasks such as attend/infer/repeat, video next frame segmentation forecasting and progressive generative adversarial networks.

1 Introduction

One-shot optimization, a critical component of hyperparameter search, consists in approximating the minimum of a function $f$ by its minimum $\min(f(x_1), \ldots, f(x_n))$ over a finite subset $\{x_1, \ldots, x_n\}$ of points provided by a sampler. Space-filling designs such as Halton, Hammersley or Latin hypercube sampling, aim at distributing the points more diversely than independent random sampling. While their performance is well known for numerical integration [Koksma, 1942], their use for one-shot optimization is far less explored. It was pointed out how much random sampling is sometimes hard to outperform [Bergstra and Bengio, 2012]. [Bousquet et al., 2017] advocated low discrepancy sequences, in particular Scrambled Hammersley. We quantify the benefit of such approaches and, looking for more headroom, propose the concept of distribution reshaping, i.e. using a search distribution different from the prior distribution of the optimum.

Contributions. Stochastic dispersion has been identified [Bousquet et al., 2017] as a tool for measuring the performance of one-shot optimization methods. We prove in Section 3 stochastic dispersion bounds of various sampling methods. These bounds are actually close to those of random search, including in the case of a limited number of critical variables [Bousquet et al., 2017], i.e. the case in which part of the variables have a strong impact on the objective functions whereas others have a negligible impact. Given this limited headroom, we propose reshaping (Section 4), i.e. changing the search distribution, in two distinct flavors. First, even if the prior probability distribution of the optimum is known, we use a search distribution tightened closer to the center as the dimension increases or as the budget decreases (Section 4, recentering). Second (and possibly simultaneously, in spite of the apparent contradiction), we use Cauchy counterparts for searching closer to the boundaries (for bounded hyperparameters) or farther from the center (for unbounded hyperparameters). Experiments validate the approach (Section 5).
Table 1: Comparison between non-reshaped sampling methods for one shot optimization. Red boxed results are contributions of the paper. The sequences of samples are of size $n$ in dimension $d$. $C_d$ is a dim-dependent constant.

| Sequence | Discrepancy $^*$ | Incrementality | Randomized with PDF $> 0$ $^1$ | Stochastic dispersion $^2$ | Stochastic dispersion preserved by projection $^3$ |
|----------|------------------|----------------|-------------------------------|---------------------------|-----------------------------------------------|
| LHS      | $\Theta(\sqrt{d/n})$ [Doerr et al., 2018] | $2n$, optimal (see SM) | yes | $1/n^{1/d}$ (Prop. 1) | yes |
| Grid     | $1/n^{1/d}$ | no | no | $1/n^{1/d}$ (easy) | no (easy) |
| Jittered | $\sqrt{d \log n/n^{1/2+1/2d}}$ | $2n$, optimal (SM) | yes | $1/n^{1/d}$ (easy) | yes (easy) |
| Random   | $\log \log(n)^{2/\pi}$ [Kiefer, 1961] | +1 | yes | $1/n^{1/d}$ (easy) | yes (easy) |
| Halton   | $(1 + o(1)) \times C_d(\log n)^2/n$ | +1 | no | $1/n^{1/d} #\$ | yes but # different constant |
| Hammersley | $(1 + o(1))C_d \times (\log n)^{d-1}/n$ | not $n + k \log(n)^{d-1}$ | no | $1/n^{1/d} #\$ | yes but # different constant |
| Scrambled Halton | as Halton, better constant | +1 | no | $1/n^{1/d} #\$ | yes but # different constant |
| Scrambled Hammersley | as Hammersley, better constant | not $n + k \log(n)^{d-1}$ | no | $1/n^{1/d} #\$ | yes but # different constant |
| Sobol    | as Halton +1 | no | log(n)/$n^{1/d}$ | yes but diff. const. |
| Random -Shift LHS | as original LDS (up to dim-dependent factor) | as original LDS | yes | as original LDS (up to dim-dependent factor) |

$^1$ The discrepancy of a projection $\Pi(S)$ of a sequence $S$, when $\Pi$ is a projection to a subset of indices, is less or equal to the discrepancy of $S$. Therefore we do not discuss the stability of the sequence in terms of discrepancy of the projection to a subspace, contrarily to what we do for dispersion (for which significant differences can occur, between $S$ and $\Pi(S)$).

$^2$ "Randomized with PDF $> 0$" means that the sampling is randomized with a probability distribution function (averaged over the sample) strictly positive over all the domain.

$^3$ Optimal rate is $O(1/n^{1/d})$ [Sukharev, 1971]. $^*$ We consider subspaces parallel to axes, i.e. switching to a subset of indices. We request that the dependency in the dimension becomes the dimension of the subspace.

$^4$ The bound on the distance to the optimum is an immediate application of the discrepancy, and low discrepancy is preserved by switching to a subspace, hence this positive result.

$^5$ Constants depend on which variables are in the subspace - first hyperparameters are “more” uniform than independent random search e.g. in terms of dispersion, discrepancy, stochastic dispersion.

Space-filling vs reshaping: the two components of one-shot optimization. Let us distinguish two probability distributions: the prior probability distribution $P_0$ of the optimum, and the search probability distribution $P_s$ used in the one-shot optimization method in particular in high dimension. We show below that $P_s$ different from $P_0$ is theoretically and experimentally better, in particular in high dimension. While usual space-filling designs, compared to random search, relax the assumptions that samples are independently drawn according to $P_s$, we propose (inspired by [Rahnamayan and Wang, 2009, Rahnamayan et al., 2007]) reshaped versions using $P_s$ spikier than $P_0$ around the center. We provide in Table 1 an overview of theoretical results regarding space-filling designs without any reshaping component, i.e. $P_s = P_0$. Regarding reshaping, maybe surprisingly, even if the optimum is randomly drawn as a standard normal distribution in an artificial problem (e.g. we know a priori that the optimum $x^*$ is randomly drawn as a standard Gaussian and the objective function is $x \mapsto \|x - x^*\|^2$), the optimal search distribution is not a Gaussian (Theorem 1). This is the principle behind the addition of a middle point and, by extension, the principle of the Recentering reshaping (Section 4).

Cauchy reshaping, on the other hand, is justified by distinct considerations, such as compensating the corner avoidance properties of some space-filling designs, and by the risk of expert errors on the correct range of an hyperparameter.

2 Space-filling designs

As recapped in Table 1, we consider the following sampling strategies (space-filling designs), aimed at being “more uniform” than independent random search e.g. in terms of dispersion, discrepancy, stochastic dispersion.

- **Grid** picks up the middle of each of $k^d$ hypercubes covering the unit hypercube, with $k$ maximum such that $k^d \leq n$. We then sample $n - k^d$ additional random points uniformly in the domain.

- **Latin Hypercube Sampling (LHS)** [Eglajs and Audze, 1977, McKay et al., 1979] defines $\sigma_1, \ldots, \sigma_d$, random independent permutations of $\{0, \ldots, n\}$ and then for $0 \leq i \leq n$, the $i^{th}$ coordinate of the $i^{th}$ point of the sequence is given by $(x_i)_j = (\sigma_j(i) + r_{i,j})/(n + 1)$ where the $r_{i,j}$ are...
Table 2: Artificial objective functions from Nevergrad (see text) with $P_0$ known: for each combination (dimension, budget), we mention the method which had the best frequency of outperforming other methods in that setting. 7400 replicas per run. O refers to opposite and QO refers to quasiopposite. We see that overall the Recentering (Rctg) methods perform best, with a parameter $k$ scaling roughly as Eq. 1 (we can see QO as further reducing the constant). Overall the Rctg reshaping outperforms its ancestor the quasiopposite sampling [Rahnamayan and Wang, 2009]. RctgX.Y refers to $\lambda = X.Y$. MetaRctg refers to $\lambda$ chosen by Eq. 1; it turns out to be one of the best methods overall, performing close to the best for each budget/dimension in the present context of $P_0$ known. These experiments use the artificial Nevergrad oneshot experiments, for which the distribution of the optimum is a standardized multivariate normal distribution. In this context, Cauchy distributions do not help much. In bold the method that most often performed best.

| Dimension | Scr Halton | Scr Halton | Scr Halton | Scr Halton | Scr Halton | Scr Halton | Scr Halton | Scr Halton | Scr Halton | Scr Halton |
|-----------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|
| 30        | Rctg1.2 Scr Halton | Rctg1.2 Scr Halton | Rctg1.2 Scr Halton | Rctg1.2 Scr Halton | Rctg1.2 Scr Halton | Rctg1.2 Scr Halton | Rctg1.2 Scr Halton | Rctg1.2 Scr Halton | Rctg1.2 Scr Halton | Rctg1.2 Scr Halton |
| 100       | Scr Halton Plus Middle | Scr Halton Plus Middle | Scr Halton Plus Middle | Scr Halton Plus Middle | Scr Halton Plus Middle | Scr Halton Plus Middle | Scr Halton Plus Middle | Scr Halton Plus Middle | Scr Halton Plus Middle | Scr Halton Plus Middle |
| 300000    | 300000     | 300000     | 300000     | 300000     | 300000     | 300000     | 300000     | 300000     | 300000     | 300000     |
| 10000     | 100000     | 100000     | 100000     | 100000     | 100000     | 100000     | 100000     | 100000     | 100000     | 100000     |
| 300       | 300        | 300        | 300        | 300        | 300        | 300        | 300        | 300        | 300        | 300        |

Jittered sampling consists in splitting $\mathcal{D}$ into $n = k^d$ (assuming that such a $k$ exists) hypercubes of volume $1/k^d$ and drawing one random point uniformly in each of these hypercubes [Pausinger and Steinerberger, 2016]. Other forms of jittered sampling exist, e.g., with different number of points per axis.

Quasi-random (QR) are also called low discrepancy sequences, due to some good distribution properties in the domain. This is the case for Halton, Hammersley and Sobol sequences. Halton [Halton, 1960] defines the $j$th coordinate of the $i$th point of the sequence as $(x_i)_j = \text{radixInverse}(i, p_j)$ where: (1) $p_0, \ldots, p_{d-1}$ are coprime numbers. Typically, but not necessarily, $p_i$ is the $(i + 1)^{th}$ prime number. (2) $\text{radixInverse}(k, p) = \sum_{j \geq 0} a_j p^{-j}$ with $(a_j) \geq 0$ being the writing of $k$ in basis $p$, i.e., $k = \sum_{j \geq 0} a_j p^j$. Hammersley’s sequence is given by $(x_i)_j = \text{radixInverse}(i, p_{j-1})$ when $j > 0$ and $(x_i)_0 = \frac{i + \frac{1}{2}}{n}$, see [Hammersley, 1960]. Sobol’s sequence [Sobol, 1967] is another advanced quasi-random sequence.

Modifiers. We use various modifiers of our samplers: scrambling [Atanasov, 2004, Tuffin, 1998, Owen, 1995], applied to our Halton and Hammersley implementations, and generic modifications applicable to all samplers: random shift (adding a random vector in the unit hypercube and applying modulo 1) [Tuffin, 1996]. Other modifications are based on reshaping (Section 4).

Performance measure and proxies. We use the classical notions of simple regret, discrepancy (with respect to axis-parallel rectangles and the $L^n$ norm), dispersion and low-discrepancy sequences (i.e. sequences with discrepancy decreasing as $O(\log(n)^d/n)$). We refer to [Niederreiter, 1992] or the supplementary material (SM) for classical notions such as discrepancy and dispersion, and to [Bubeck et al., 2009] for an overview of the literature on simple regret. Discrepancy is well known as a good criterion also for one-shot optimization [Bergstra and Bengio, 2012, Bousquet et al., 2017]. Given a domain $\mathcal{D}$, the stochastic dispersion [Bousquet et al., 2017] of a random variable $X = (x_1, \ldots, x_n)$ in $\mathcal{D}^n$ is defined as $\text{sdisp}(X) = \sup_{x^* \in \mathcal{D}} \mathbb{E}_{X} \inf_{1 \leq i \leq n} \|x_i - x^*\|$. Critical vs useless variables. We distinguish cases in which there are $d'$ unknown variables (termed critical variables) with an impact on the objective function whereas $d - d'$ variables have no impact.
3 Theory: are space-filling designs all equal?

Table 1 shows bounds on the performance of various space-filling designs, including the very classical LHS, the top performing (in terms of discrepancy) Scrambled-Hammersley, and the robust jittered sampling. We show that they perform well but just up to a constant factor, compared to random search, even in the case of critical variables: this is the key reason for introducing reshaping in Section 4. For simplicity, we always consider $D = [0, 1]^d$ as the search domain and $n$ the number of points in the sequence. See SM for other results and detailed proofs.

3.1 Latin hypercube sampling (LHS):

stochastic dispersion

LHS [McKay et al., 1979, Eglajs and Audze, 1977] is particularly appreciated for building a surrogate model, e.g. in Efficient Global Optimization [Jones et al., 1998]. Due to its popularity, some variants have been developed to generate better LHS, based for example on the maximin distance criterion [Johnson et al., 1990], or for sliced LHS [Qian, 2012]. [Doerr et al., 2018, Schoonees et al., 2016] have established discrepancy properties of LHS, in particular for moderate budgets. We show that the stochastic dispersion of LHS is optimal, i.e., it decreases at the optimal rate $O(1/n^{1/d})$ (see Prop. 1). Importantly, LHS is entirely preserved by projection to any subspace - as opposed to low discrepancy sequences, for which only segments of initial variables keep the same constants in discrepancy or dispersion bounds.

Property 1. Consider $m \leq n$ two powers of 2 and $\alpha = m/n^{1-1/d}$. Then, the probability $P_{n,m}$ that LHS$(n)$ does not intersect $[0, m/n]^d$ is at most $\left(1 - \frac{\alpha^{d-1}}{n^{d-1}}\right)^{n^{1-1/d}}$.

As a by-product of this proposition, the SM shows (limited) incrementality properties of LHS. Property 1 has implications in terms of distance to an arbitrary $x$ in $[0, 1]$. The probability that $x$ has no neighbor at distance (for the maximum norm) $m/n$ is at least the probability that LHS$(n)$ has no point in the hypercube $[0, m/n]^d$.

$P_{n,m}$ is 0 if $d = 1$, and, if $d > 1$ and $m = \alpha n^{1-1/d}$, then $P_{n,m}$ converges to $\exp(-\alpha^d)$. In other words, the quantile $1 - \delta$ of the minimum distance to $x$ is $O(\sqrt{d} \log(1/\delta) d^{1/d}/n^{1/d})$ - the same as random search, up to the constant (next Section).

Dispersion of projected Jittered Sampling

In this section, we show that Jittered Sampling benefits from the same stochastic dispersion bounds as random search. We use $V_d$ the volume of $x \in \mathbb{R}^d; \|x\| \leq 1$. We first mention a known property of random search (details in next section), useful for proving Prop. 2.

Lemma 1 (Random search). Consider $x$ an arbitrary point in $[0, 1]^d$. Consider $x_1, \ldots, x_M$ a sequence generated by random search. Define $\epsilon = \min_i \|x_i - x\|$. Then,

$$\forall \delta, P\left(\epsilon > 2^{1+1/d} \log(1/\delta)^{1/d}/(MV_d)^{1/d}\right) \leq \delta.$$

Property 2 (Jittered sampling has optimal dispersion after projection on a subset of axes). Consider $x \in [0, 1]^d$. Consider jittered sampling with $n = k^d$ points. Consider its projection on the $d'$ first coordinates. Let $x_1, \ldots, x_n$ be these projected points. Define $\epsilon = \min_i \|x_i - x\|$. Then, with probability at least $1 - \delta, \epsilon \leq 2^{1+1/d^2} \log(1/\delta)^{1/d}/\left(MV_d n^{1/d}\right)$.

The quantile $1 - \delta$ of this minimum distance, up to constant factors, is therefore the same as for a LHS sample of cardinal $n$ or for a pure random sample, namely $O(\sqrt{d} \log(1/\delta)^{1/d}/n^{1/d})$.

4 Theory of reshaping: middle point & recentering

Interestingly, in the context of the initialization of differential evolution [Storn and Price, 1997], [Rahnamayan and Wang, 2009] proposed a sampling focusing on the middle. Their method consists in adding for each point $x$ in the domain $[-1, 1]^d$, a point $-r \times x$ for $r$ uniformly drawn in $[0, 1]$. This combines opposite sampling (which corresponds to arithmetic variables, also used for population-based optimization in [Teytaud et al., 2006]) and focus to the center (multiplication by a constant $< 1$): their method is termed quasiopposite sampling. Consider dimension $d$ and $x^*$ randomly normally distributed with unit variance in $\mathbb{R}^d$. Consider $x_1, \ldots, x_n$, independently randomly normally distributed with unit variance in $\mathbb{R}^d$. The median of $\|x^*\|^2$ is denoted $m_0$ and the median of $\min_i \|x_i - x^*\|^2$ is denoted $m_n$. We first note lemmas 2 and 3.

Lemma 2. $m_0$ is equivalent to $d$ as $d \rightarrow \infty$.

Lemma 3. $P(\|x_1 - x^*\|^2 \leq m_n) \geq \frac{1}{2\pi}$.

We now note that $\frac{1}{\sqrt{2\pi}}(x_1 - x^*)^2$ follows a $\chi^2$ distribution with $d$ degrees of freedom.

\footnote{Without loss of generality; we might consider a projection to $d'$ arbitrarily chosen coordinates.}
We will propose another related distribution, \( \| x - x^* \| \geq \theta \) for all objects.

**Lemma 4.** By Chernoff’s bound for the \( \chi^2 \) distribution, \( \mathbb{P}(\| x_1 - x^* \|^2 \leq d(1 + o(1))) \leq \left(1 + o(1)\right)^{n/2} \exp \left(\frac{d}{2}\right) \). 

**Theorem 1.** Consider \( n > 0 \). There exists \( d_0 \) such that for all \( d > d_0 \), if \( X \) is a random sample of \( n \) independent standard normal points in dimension \( d \), if \( x^* \) is a random independent normal point in dimension \( d \), then, unless \( n \geq \frac{1}{2} (1 + o(1)) \exp \left(\frac{1}{2}\right) d^{-d/2} \), the median of the minimum distance \( \min_{x \in X} \| x - x^* \| \) is greater than the median of the distance \( \| x^* - (0,\ldots,0) \| \).

As having \( n \) points equal to 0 is pointless, we can consider \( n - 1 \) standard independent normal points, plus a single middle point: this is our modification “plus middle point”. We will propose another related reshaping, namely tightening the distribution closer to the center: the Recentering method. Then we will see a distinct reshaping, namely switching to the Cauchy distribution.

**Recentering (Rctg for short) reshaping.** Consider optimization in \([0,1]^d\). Given a sample \( s \), and using \( g \) the cumulative distribution function of the standard Gaussian, the Rctg reshaping consists in concentrating the distribution towards \((0.5,\ldots,0.5)\): it considers \( \{c(s) \mid s \in S\} \) rather than \( S \), with \( c(s) = g(\lambda \times g^{-1}(s_1)),\ldots,g(\lambda \times g^{-1}(s_d)) \). \( \lambda = 0 \) sets all points to the middle of the unit hypercube. \( \lambda = 1 \) means no reshaping. **MetaRecentering.** Preliminary experimental results lead to the specification of MetaRctg, using the dimension and the budget for choosing the parameter \( k \) of the Recentering reshaping: MetaRctg uses Scrambled-Hammersley and Rctg reshaping with

\[
\lambda = \frac{1 + \log(\text{budget})}{4\log(\text{dimension})}. \tag{1}
\]

**Cauchy.** When using the Cauchy distribution, we get \( c(s) = g(\lambda \times C^{-1}(s_1)),\ldots,g(\lambda \times C^{-1}(s_d)) \) with \( C \) the Cauchy cumulative distribution function. **Extension to unbounded hyperparameters.** \( g(\cdot) \) can be removed from those equations when we consider sampling in \( \mathbb{R}^d \) rather than in \([0,1]^d\): we then get \( c(s) = \lambda \times g^{-1}(s_1),\ldots,\lambda \times g^{-1}(s_d) \) in the normal case. \( g \) can also be applied selectively on some variables and not on others when we have both bounded and unbounded hyperparameters.

## 5 Experiments

See SM for reproduction of all our artificial experiments with one-liners in the Nevergrad platform [Rapin and Teytaud, 2018], and for additional deep learning experiments with FzFz [Luc et al., 2018]. We first test our baselines in a classical setting with \( P_0 \) known and without any reshaping (Section 5.1.1). We then check that Recentering works in such a context of \( P_0 \) known (Section 5.1.2). Then we switch to \( P_0 \) unknown (Section 5.2). We first check the impact of Cauchy (Section 5.2.1). We then check Recentering and Cauchy simultaneously (Section 5.2.2 and 5.2.3). We conclude that Cauchy is vastly validated for unknown \( P_0 \) and that Recentering works if \( P_0 \) is known or if underlying data are properly rescaled (Table 3, as opposed to the wildly unscaled problems in Table 4).

### 5.1 When the prior \( P_0 \) is known

There are real world cases in which \( P_0 \) is known; typically when optimizations are repeated: maximum likelihood in item response theory repeated for estimating the parameters of many questions, ELO evaluation of many gamers from their records, hyperparametrization of cloud-based machine learning [Allaire, 2018], repeated optimization of industrial oven parameters [Cavazzuti et al., 2013] for distinct scope statements. Another important case is when the objective function is the worst outcome over a family of scenarios, to be approximated by a finite sample corresponding to ranges of independent exogeneous variables (dozens of annual weather parameters and financial parameters), as usually done in network expansion planning [Escobar et al., 2008, Li et al., 2016].

#### 5.1.1 One-shot numerical optimization of artificial test functions with \( P_0 \) known and \( P_s = P_0 \): the baselines

While we use mainly real-world experiments in the present paper, we draw the following conclusions from synthetic experiments with controlled \( P_0 \) and without reshaping, using classical objective functions from the
Table 3: Experiments on the Nevergrad real-world rescaled testbed. This experiment termed “oneshotscale-deralworld” corresponds to real-world test cases in which a reasonable effort for rescaling problems according to human expertise has been done; $P_0$ is not known, but an effort has been made for rescaling problems as far as easily possible. Dimension from 10 to 120, budget from 25 to 12800. There is no prior knowledge on the position of the optimum in this setting; MetaRctg did not perform bad overall but Cauchy variants dominate many cases, as well as rescaled versions which sample close to boundaries. Hmsley stands for Hammersley, Cchy for Cauchy, Rctg for Rctg. In bold the method performing best overall; MetaCauchyRctg performs well overall though other CauchyRctg often performed better - most often with a constant $< 1$, i.e. recentering, and most often with Cauchy (all samplers are tested in both flavors, normal and Cauchy) for high dimension, which validates both Recentering and Cauchy.

5.1.2 Experiments including a reshaped space-filling design: Recentering works

We present an experiment on objective functions Sphere, Rastrigin and Cigar, with 100% or 16.67% of critical variables (i.e. in the latter case we add 5 randomly positioned useless variables for each critical variable), with budget in 30, 100, 300, 1000, 3000, 10000, 30000, 100000, 300000, with 3, 25 or 100 critical variables. We compare Rctg reshaping with constant $k \in \{0.01, 0.1, 0.4, 0.55, 1.0, 1.2, 2.0\}$, the same Rctg reshaping plus opposite sampling or quasi-opposite sampling, on top of LHS; Scrambled-Halton, Scrambled-Hammersley or pure random sampling; we consider Gauss or Cauchy as conversions to $\mathbb{R}^d$. Given the choice regarding critical variables previously mentioned, we get dimension 3, 18, 25, 100, 150, 600. This is reproducible with a one-liner “oneshotcalais” in Nevergrad (see SM). Results are presented in Table 2 and validate Recentering, in particular in its Meta version (Eq. 1), as soon as $P_0$ is known. They also show that in such a context ($P_0$ perfectly known) Cauchy is not useful.

5.2 Cauchy-reshaping with $P_0$ unknown

5.2.1 No $P_0$: Cauchy for attend/infer/repeat

Previous results have validated Recentering (our first proposed reshaping) in the case of $P_0$ known. The sec-

| $P_0$ | $Q_0$ | 25 | 50 | 100 | 200 | 400 | 800 | 1600 | 3200 | 4000 | 6400 | 8000 | 12800 |
|--------|-------|----|----|-----|-----|-----|-----|------|------|------|------|------|-------|
| 10     | Scr Hmsley | Scr Hmsley | Scr Hmsley | Scr Hmsley | Scr Hmsley | Scr Hmsley | Scr Hmsley | Scr Hmsley | Scr Hmsley | Scr Hmsley | Scr Hmsley | Scr Hmsley | Scr Hmsley |
| 20     | Scr Hmsley | Scr Hmsley | Scr Hmsley | Scr Hmsley | Scr Hmsley | Scr Hmsley | Scr Hmsley | Scr Hmsley | Scr Hmsley | Scr Hmsley | Scr Hmsley | Scr Hmsley | Scr Hmsley |
| 30     | Rescale Scr Hmsley | Scr Hmsley | Scr Hmsley | Scr Hmsley | Scr Hmsley | Scr Hmsley | Scr Hmsley | Scr Hmsley | Scr Hmsley | Scr Hmsley | Scr Hmsley | Scr Hmsley | Scr Hmsley |
| 40     | Scr Hmsley | Scr Hmsley | Scr Hmsley | Scr Hmsley | Scr Hmsley | Scr Hmsley | Scr Hmsley | Scr Hmsley | Scr Hmsley | Scr Hmsley | Scr Hmsley | Scr Hmsley | Scr Hmsley |
| 60     | Rescale Scr Hmsley | Scr Hmsley | Scr Hmsley | Scr Hmsley | Scr Hmsley | Scr Hmsley | Scr Hmsley | Scr Hmsley | Scr Hmsley | Scr Hmsley | Scr Hmsley | Scr Hmsley | Scr Hmsley |
| 120    | Rescale Scr Hmsley | Scr Hmsley | Scr Hmsley | Scr Hmsley | Scr Hmsley | Scr Hmsley | Scr Hmsley | Scr Hmsley | Scr Hmsley | Scr Hmsley | Scr Hmsley | Scr Hmsley | Scr Hmsley |
Table 4: Counterpart of Table 3 with the experiment termed “oneshotscaledrealworld” in Nevergrad, which contains more problems including many for which no rescaling effort has been made. Cutrg does not make sense in this “totally unknown \( P_0 \)” setting, but we still see a lot of Cauchy counterparts or Rescaled versions, showing that focusing close to boundaries (for bounded hyperparameters) or on large values (for unbounded hyperparameters) makes sense. The contrast with Table 3 in which CauchyMetaCtrg and close variants such as CauchyCtrg with \( \lambda = 0.55 \) perform well suggest that scaling parameters and data is a good idea for generic methods to be effective.

| 25 | 60 | 100 | 200 | 400 | 800 | 1600 | 3200 | 6400 | 12800 |
|----|----|-----|-----|-----|-----|------|------|------|-------|
| Scr Halton Plus Middle Point | Rescale Scr Hmsly | Scr Hmsly | Rescale Scr Hmsly | Meta Ctrg | Scr Hmsly | Rescale Scr Hmsly | Scr Hmsly | Scr Hmsly | L H S | Scr Hmsly Plus Middle Point |
| 15 | Cchy Ser Hmsly | Cchy Ran- dom | Cchy Hmsly | Cchy LHS | Ctrg20 Ser Hmsly | Cchy Ser Hmsly | Cchy Ser Hmsly | Cchy Ctrg12 Ser Hmsly | Cchy Ser Hmsly | Cchy Ctrg12 Ser Hmsly |
| 20 | L H S Random | Random | Rescale Scr Hmsly | Rescale Scr Hmsly | Rescale Scr Hmsly | Rescale Scr Hmsly | Rescale Scr Hmsly | Rescale Scr Hmsly | Rescale Scr Hmsly | Mhdly Plus Middle Point |
| 30 | Cchy Ran- dom | Cchy LHS | Cchy Ran- dom | Cchy Hmsly | Cchy Ran- dom | Cchy Hmsly | Cchy Ran- dom | Cchy LHS | Cchy Ran- dom | Cchy LHS |
| 40 | Ctrg12 Scr Halton | Rescale Scr Hmsly | Rescale Scr Hmsly | Rescale Scr Hmsly | Rescale Scr Hmsly | O Random | Rescale Scr Hmsly | O Random | Rescale Scr Hmsly |
| 60 | Cchy LHS Cchy Ran- dom | Cchy LHS | Cchy Ran- dom | Cchy LHS | Cchy Ran- dom | Cchy LHS | Cchy Ran- dom | Cchy LHS | Cchy Ran- dom | Cchy LHS |
| 120 | Cchy LHS | Cchy LHS | Cchy Ran- dom | Cchy LHS | Cchy Ran- dom | Cchy LHS | Cchy Ran- dom | Cchy LHS | Cchy Ran- dom | Cchy LHS |
| 675 | Cchy Ctrg12 Scr Hmsly | Cchy Ctrg4 Scr Hmsly | Cchy Ctrg4 Scr Hmsly | Cchy Ctrg4 Scr Hmsly | Ctrg4 Ser Hmsly | O Ctrg20 Scr Halton | Cchy Scr Meta Cchy Ctrg |

5.2.2 Generative adversarial networks (GANs).

We use Pytorch GAN Zoo [Riviere, 2019] for progressive GANs [Karras et al., 2018], with a short 10 minutes training on a single GPU. We optimize 3 continuous hyperparameters, namely leakyness of ReLU units in \([1e - 2, 0.6]\), the discriminator \( \epsilon \) parameter in \([1e - 5, 1e - 1]\), and the base learning rate in \([1e - 5, 1e - 1]\). MetaCauchyRctg performed best (Fig. 2), in spite of the fact that it was designed just by adding Cauchy to MetaRctg which was designed on independent distinct artificial experiments in Tab. 2.

5.2.3 Nevergrad real world experiments without control of \( P_0 \)

Nevergrad provides a real world family of experiments, built on top of the MLDA testbed [Gallagher and Saleem, 2018], using Salmon mappings and clustering and others: these experiments are less expensive and fully reproducible (see SM). We run all our one-shot optimizers on it with 7400 repetitions. We then check for each budget/dimension which method performed best (Tab. 3): in this real-world context, in which assuming a standard deviation of 1 for the uncertainty over the optimum is risky, the Cauchy sampling with Rctg reshaping 0.55 performs quite well. It is sometimes outperformed by rescaled Scrambled-Hammersley, which takes care of pushing points to the frontier (each variable is rescaled so that the min and the max of each variable, over the sample, hit the boundaries). This means that the best methods frequently have samplings able to work far from the center (either heavy tail for Cauchy, or sample rescaled for matching the boundaries). The exact optimal constant \( \lambda \) does not always match the MetaRecentering scaling we have proposed (Eq. 1) but is clearly < 1. Though this...
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Figure 2: Experiments on progressive GANs [Karras et al., 2018, Riviere, 2019]. MetaCauchyRctg dominates. All Cauchy variants (full lines) perform well compared to normal ones (dashed). The “Meta” choice of the recentering constant (Eq. 1) seemingly performs well though without Cauchy and low budgets this was not that clear. X-axis = budget. Y-axis = opposite of inception score, the lower the better.

setting already does not really have a known $P_0$ (just a rough rescaling of underlying data), we switch to a more hardcore setting in Table 4: we consider the “oneshotunscaledrealworld” experiment in Nevergrad for a case in which no rescaling effort was made; we still get a quite good behavior of Cauchy or rescaled variants, but (consistently with intuition) Recentering does not make sense anymore.

6 Conclusion

Theoretical results. We showed that LHS and jittered sampling have, up to a constant factor, the same stochastic dispersion rate as random sampling (Sections 3.1 and 3.1), including when restricted to a subset of variables. Low-discrepancy sequences have good stochastic dispersion rates but their performance depends on the order of variables so that they are preserved for subsets of variables only up to a constant which depends on which variables are selected. Typically they are outperformed by LHS when there is a single randomly positioned critical variable. Overall, the benefit of sophisticated space-filling designs turn out to be moderate compared to random search or LHS, hence the motivation for alternative fully parallel hyperparameter search ideas such as reshaping. We then showed that adding a middle point helps in many high-dimensional cases (Section 4). This element inspired the design of search distributions different from the Gaussian one, such as Cauchy and/or reshaping as in Rctg methods (Section 4) - which provide substantial improvements.

Practical recommendations. Table 5 surveys our practical conclusions. Our experiments suggest to use MetaRctg (Scrambled-Hammersley + Rctg reshaping with $\lambda$ as in Eq. 1) when we have a prior on the probability distribution of the optimum (Tab. 2 and SM). Precisely, with a standard normal prior $P_0$ (use copulas, i.e. multidimensional cumulative distribution functions, for other probability distributions), use

$$x_{i,j} = Gcdf\left(\frac{1 + \log(n)}{4 \log(d)}Gcdf^{-1}(ScrH_{i,j})\right)$$

for searching in $[0,1]^d$ with budget $n$, where $ScrH_{i,j}$ is the $j^{th}$ coordinate of the $i^{th}$ point in the Scrambled Hammersley sequence. In many cases, however, we do not have such a prior on the position of the optimum: experts provide a correct range of values for most variables, but miss a few ones so that best values are extreme. Unfortunately, low-discrepancy methods are weak, by a dimension-dependent factor, for searching close to boundaries - this is known as the corner avoidance effect [Owen, 2006, Hartinger et al., 2005]. Therefore low-discrepancy methods can then perform worse than random, and Cauchy helps. A second suggestion is therefore to use Cauchy in real world cases: we got in Tabs 3 and 4 or for AIR (Fig. 1) or PytorchGAN-zoo (Fig. 2), i.e. all our real-world experiments, better performances with Cauchy. Last, for real-world problems, rescaling data and parameters and using CauchyMetaRctg looks good - with a

| Context                        | Recommendation               | XPs               |
|--------------------------------|------------------------------|-------------------|
| $P_0$ perfectly known          | MetaCtrng                   | Table 2           |
| $P_0$ approx. known (rescaled data, normalized params) | CchyMetaCtrng | Table 3, Fig. 2. |
| $P_0$ wildly unknown (avoid this!) | CchyMetaCtrng | Table 4, Fig. 1. |

Table 5: Practical recommendations.
minimum of standardization, we got good results for CauchyMetaRctg in Fig. 2 (just using human expertise for rescaling) and Tab. 3 (just based on standardizing underlying data, so no real known prior $P_0$). When a proper scaling is impossible, we still get good performance for Cauchy variables but $\lambda$ is impossible to guess so that the best method varies from one case to the other (Table 4) - Cauchy-LHS and Rescale-Sr-Hammersley being the most stable.

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