

APPENDIX

1 The AvgHExp3 Mean and Variance

According to [1], Exp3 uses the total estimated reward $\hat{S}_{t-1,i}$ to evaluate the reward of arms. Although $\hat{S}_{t-1,i}$ is an unbiased estimator, its variance is very high. To decrease variance, AvgHExp3 uses the average estimated reward \hat{S}'_{t-1,ω_i} to replace $\hat{S}_{t-1,i}$ according to Theorem 11.

Theorem 11 *The average estimated reward \hat{S}'_{t-1,ω_i} used by AvgHExp3 is an unbiased estimator, and its variance is $1/(t-1)^2$ of Exp3's, i.e., $D[\hat{S}'_{t-1,\omega_i}] = \frac{1}{(t-1)^2} D[\hat{S}_{t-1,i}]$.*

Proof. According to the definition of \hat{S}'_{t-1,ω_i} , i.e., $\hat{S}'_{t-1,\omega_i} = \frac{1}{t-1} \sum_{s=1}^{t-1} \hat{R}_{s,\omega_i}$, where \hat{R}_{s,ω_i} is the estimated reward of ω_i in iteration t . The expectation of \hat{S}'_{t-1,ω_i} is

$$E[\hat{S}'_{t-1,\omega_i}] = E\left[\frac{1}{t-1} \sum_{s=1}^{t-1} \hat{R}_{s,\omega_i}\right] = \frac{1}{t-1} \sum_{s=1}^{t-1} E[\hat{R}_{s,\omega_i}]. \quad (1)$$

Since \hat{R}_{s,ω_i} is an unbiased estimator [1], $E[\hat{R}_{s,\omega_i}] = R_{s,\omega_i}$. So $E[\hat{S}'_{t-1,\omega_i}] = \frac{1}{t-1} \sum_{s=1}^{t-1} R_{s,\omega_i}$, which means \hat{S}'_{t-1,ω_i} is an unbiased estimator of the average actual reward in the subspace ω_i .

The variance of \hat{S}'_{t-1,ω_i} is

$$\begin{aligned} D[\hat{S}'_{t-1,\omega_i}] &= E\left[\left(\hat{S}'_{t-1,\omega_i}\right)^2\right] - E^2[\hat{S}'_{t-1,\omega_i}] \\ &= E\left[\left(\frac{1}{t-1} \sum_{s=1}^{t-1} \hat{R}_{s,\omega_i}\right)^2\right] - \left(\frac{1}{t-1} \sum_{s=1}^{t-1} R_{s,\omega_i}\right)^2 \\ &= \frac{1}{(t-1)^2} \left(E\left[\left(\sum_{s=1}^{t-1} \hat{R}_{s,\omega_i}\right)^2\right] - \left(\sum_{s=1}^{t-1} R_{s,\omega_i}\right)^2\right) \\ &= \frac{1}{(t-1)^2} D[\hat{S}_{t-1,i}] \end{aligned} \quad (2)$$

The theorem shows that, compared with Exp3, AvgHExp3 that uses the average estimated reward can decrease the Exp3's variance as the number (t) of GVAE-ABGEP running iterations increases.

2 Optimal Value of Parameter α

The parameter $\alpha \in [0, +\infty]$ in AvgHExp3 significantly affects the probability distribution \mathcal{P}_t of selecting subspaces. If $\alpha = 0$, according to the importance weight equation,

$$P_{t,\omega_i} = \frac{e^{\alpha \hat{S}_{t-1,\omega_i}}}{\sum_{j=1}^k e^{\alpha \hat{S}_{t-1,\omega_j}}}. \quad (3)$$

$P_{t,\omega_i} = e^{\alpha \hat{S}_{t-1,\omega_i}} / \sum_{j=1}^k e^{\alpha \hat{S}_{t-1,\omega_j}} = e^{0 \hat{S}_{t-1,\omega_i}} / \sum_{j=1}^k e^{0 \hat{S}_{t-1,\omega_j}} = 1/k$. If α is large or even close to positive infinity, $P_{t,\omega_i} = e^{\alpha \hat{S}_{t-1,\omega_i}} / \sum_{j=1}^k e^{\alpha \hat{S}_{t-1,\omega_j}} = 1 / \sum_{j=1}^k e^{\alpha(\hat{S}_{t-1,\omega_j} - \hat{S}_{t-1,\omega_i})} \approx 0$ (except for the subspace ω_j with the best reward, $P_{t,\omega_j} \approx 1$). Therefore, if α is too large or small, excluding the subspace with $P_{t,\omega_i} \approx 1$, the probability of selecting each subspace will be the same, and AvgHExp3 loses its meaning. Moreover, GVAE-ABGEP will be close to classical GEPs.

From the perspective of balancing the subspace exploration and the subspace exploitation, the expected regret $R_n(\pi, r_t)$ of AvgHExp3 should be as small as possible. For determining α , we try to use α to limit the upper bound of $R_n(\pi, r_t)$ [1]. According to Theorem 21, the optimal value of parameter α is $\sqrt{\frac{\log k + n(n-1)}{2nk}}$.

Theorem 21 *For limiting the upper bound of the regret reward $R_n(\pi, r_t)$, the optimal value of α is $\sqrt{\frac{\log k + n(n-1)}{2nk}}$ when $\alpha \leq t$.*

Proof. The following proof is similar to the proof of Theorem 11.1 in [1]. However, the difference between Theorem 11.1 [1] and Theorem 21 is the estimated reward \hat{R} . The classical Exp3 [1] uses the total estimated reward while AvgHExp3 uses the average estimated reward.

For any subspace ω_i , the regret after the round n is

$$R_{n,\omega_i} = \sum_{t=\alpha}^{n+\alpha} R_{t,\omega_i} - E \left[\sum_{t=\alpha}^{n+\alpha} R_t \right]. \quad (4)$$

According to Equation 1 and the definition of \hat{S}'_{t-1,ω_i} , i.e., $\hat{S}'_{t-1,\omega_i} = \frac{1}{t-1} \sum_{s=1}^{t-1} \hat{R}_{s,\omega_i}$, $\sum_{t=\alpha}^{n+\alpha} R_{t,\omega_i} = E \left[\sum_{t=\alpha}^{n+\alpha} \hat{R}_{t,\omega_i} \right] = E \left[n \hat{S}'_{n,\omega_i} \right]$. Meanwhile, according to the definition of expectation, $E[R_t]$ is expanded into $E[R_t] = \sum_{i=1}^k P_{t,\omega_i} R_{t,\omega_i} = \sum_{i=1}^k P_{t,\omega_i} E[\hat{R}_{t,\omega_i}]$. So Equation 4 can be computed as the

follow equation.

$$\begin{aligned}
R_{n,\omega_i} &= \sum_{t=\alpha}^{n+\alpha} R_{t,\omega_i} - E \left[\sum_{t=\alpha}^{n+\alpha} R_t \right] \\
&= nE \left[\hat{S}'_{n,\omega_i} \right] - E \left[\sum_{t=\alpha}^{n+\alpha} \sum_{i=1}^k P_{t,\omega_i} E \left[\hat{R}_{t,\omega_i} \right] \right] \\
&= nE \left[\hat{S}'_{n,\omega_i} - \frac{1}{n} \sum_{t=\alpha}^{n+\alpha} \sum_{i=1}^k P_{t,\omega_i} \hat{R}_{t,\omega_i} \right]
\end{aligned} \tag{5}$$

For the following inequality

$$e^{\alpha \hat{S}'_{n,\omega_i}} \leq \sum_{j=1}^k e^{\alpha \hat{S}'_{n,\omega_j}}, \tag{6}$$

the right side of Equation 6 is expanded into the form of continuous multiplication in Inequality 7. Since $\hat{S}'_{0,\omega_j} = 0$ at the initialization of AvgHExp3, $e^{\alpha \hat{S}'_{0,\omega_j}} = 1$. So, Inequality 6 is finally transformed into Inequality 7.

$$\begin{aligned}
e^{\alpha \hat{S}'_{n,\omega_i}} &\leq \sum_{j=1}^k e^{\alpha \hat{S}'_{0,\omega_j}} \frac{\sum_{j=1}^k e^{\alpha \hat{S}'_{1,\omega_j}}}{\sum_{j=1}^k e^{\alpha \hat{S}'_{0,\omega_j}}} \cdots \frac{\sum_{j=1}^k e^{\alpha \hat{S}'_{n,\omega_j}}}{\sum_{j=1}^k e^{\alpha \hat{S}'_{n-1,\omega_j}}} \\
&\leq k \prod_{t=1}^n \frac{\sum_{j=1}^k e^{\alpha \hat{S}'_{t,\omega_j}}}{\sum_{j=1}^k e^{\alpha \hat{S}'_{t-1,\omega_j}}}
\end{aligned} \tag{7}$$

According to the definition of \hat{S}'_{t,ω_j} and Equation 3, the continuous multiplication term in Ineqation 7 can be simplified to

$$\begin{aligned}
\frac{\sum_{j=1}^k e^{\alpha \hat{S}'_{t,\omega_j}}}{\sum_{j=1}^k e^{\alpha \hat{S}'_{t-1,\omega_j}}} &= \sum_{j=1}^k \frac{e^{\alpha \frac{t-1}{t} \hat{S}'_{t-1,\omega_j}} \cdot e^{\alpha \frac{1}{t} \hat{R}_{t,\omega_j}}}{\sum_{j=1}^k e^{\alpha \hat{S}'_{t-1,\omega_j}}} \\
&\leq \sum_{j=1}^k \frac{e^{\alpha \hat{S}'_{t-1,\omega_j}} \cdot e^{\alpha \frac{1}{t} \hat{R}_{t,\omega_j}}}{\sum_{j=1}^k e^{\alpha \hat{S}'_{t-1,\omega_j}}} \\
&= \sum_{j=1}^k P_{t,\omega_j} e^{\frac{\alpha}{t} \hat{R}_{t,\omega_j}}
\end{aligned} \tag{8}$$

Since $e^x \leq n + \frac{1}{n}x + 2x^2$ when $x \leq 1$, and according to the following Equation

$$\hat{R}_{t,\omega_j} = 1 - \frac{r_{t,a_t}}{P_{t,\omega_j}} = 1 - \frac{\Pi \{a_t = i\} r_{t,a_t}}{P_{t,\omega_j}} \tag{9}$$

where $r_{t,a_t} \geq 0$, so $\frac{\alpha}{t} \hat{R}_{t,\omega_j} \leq 1$, the right side of Equation 8 can be bounded as

$$\sum_{j=1}^k P_{t,\omega_j} e^{\frac{\alpha}{t} \hat{R}_{t,\omega_j}} \leq n + \frac{1}{n} \sum_{j=1}^k P_{t,\omega_j} \frac{\alpha}{t} \hat{R}_{t,\omega_j} + 2 \sum_{j=1}^k P_{t,\omega_j} \frac{\alpha^2}{t^2} \hat{R}_{t,\omega_j}^2. \quad (10)$$

Since $1 + x \leq e^x$ when $x \in R$, Inequality 10 can be further rewritten as

$$\sum_{j=1}^k P_{t,\omega_j} e^{\frac{\alpha}{t} \hat{R}_{t,\omega_j}} \leq e^{n-1 + \frac{1}{n} \sum_{j=1}^k P_{t,\omega_j} \frac{\alpha}{t} \hat{R}_{t,\omega_j} + 2 \sum_{j=1}^k P_{t,\omega_j} \frac{\alpha^2}{t^2} \hat{R}_{t,\omega_j}^2} \quad (11)$$

Combining Inequality 7, Inequality 8 and Inequality 11,

$$\begin{aligned} e^{\alpha \hat{S}'_{n,\omega_i}} &\leq k e^{n(n-1) + \frac{1}{n} \alpha \sum_{t=1}^n \sum_{j=1}^k \frac{1}{t} P_{t,\omega_j} \hat{R}_{t,\omega_j} + 2 \alpha^2 \sum_{t=1}^n \sum_{j=1}^k \frac{1}{t^2} P_{t,\omega_j} \hat{R}_{t,\omega_j}^2} \\ &\leq k e^{n(n-1) + \frac{1}{n} \alpha \sum_{t=1}^n \sum_{j=1}^k P_{t,\omega_j} \hat{R}_{t,\omega_j} + 2 \alpha^2 \sum_{t=1}^n \sum_{j=1}^k P_{t,\omega_j} \hat{R}_{t,\omega_j}^2} \end{aligned} \quad (12)$$

Taking logarithm on both sides of Equation 12 and dividing by α ,

$$\hat{S}'_{n,\omega_i} - \frac{1}{n} \sum_{t=1}^n \sum_{j=1}^k P_{t,\omega_j} \hat{R}_{t,\omega_j} \leq \frac{\log k}{\alpha} + \frac{n(n-1)}{\alpha} + 2\alpha \sum_{t=1}^n \sum_{j=1}^k P_{t,\omega_j} \hat{R}_{t,\omega_j}^2 \quad (13)$$

According to $E \left[\sum_{t=1}^n \sum_{j=1}^k P_{t,\omega_j} \hat{R}_{t,\omega_j}^2 \right] \leq nk$ in [1], The expectation of Inequality 13 can be further modified as

$$E \left[\hat{S}_{n,\omega_i} - \frac{1}{n} \sum_{t=1}^n \sum_{j=1}^k P_{t,\omega_j} \hat{R}_{t,\omega_j} \right] \leq \frac{\log k}{\alpha} + \frac{n(n-1)}{\alpha} + 2\alpha nk \quad (14)$$

Combining Equation 5 and Inequality 14,

$$R_{n,\omega_i} \leq \frac{n \log k + n^2(n-1)}{\alpha} + 2\alpha n^2 k \quad (15)$$

According to the inequality $a + b \geq 2\sqrt{ab}$, the right side of Inequality 15 is

$$\frac{n \log k + n^2(n-1)}{\alpha} + 2\alpha n^2 k \geq 2\sqrt{2n^2 k (n \log k + n^2(n-1))}. \quad (16)$$

For limit the right side of Inequality 15,

$$\frac{n \log k + n^2(n-1)}{\alpha} = 2\alpha n^2 k. \quad (17)$$

So the optimal value of α is $\sqrt{\frac{\log k + n(n-1)}{2nk}}$.

3 More Experimental Details

Table 1: Symbolic Regression Benchmarks

number	name	formula	dataset
F1	Nguyen-4	$x^6 + x^5 + x^4 + x^3 + x^2 + x$	$U[-1, 1, 20]$
F2	Nguyen-3	$x^5 + x^4 + x^3 + x^2 + x$	$U[-1, 1, 20]$
F3	Nguyen-2	$x^4 + x^3 + x^2 + x$	$U[-1, 1, 20]$
F4	Nguyen-1	$x^3 + x^2 + x$	$U[-1, 1, 20]$
F5	Koza-3	$x^6 - 2x^4 + x^2$	$U[-1, 1, 20]$
F6	Koza-2	$x^5 - 2x^3 + x$	$U[-1, 1, 20]$
F7	Nguyen-5	$\sin(x^2) \cos(x) - 1$	$U[-1, 1, 20]$
F8	Nguyen-6	$\sin(x) + \sin(x + x^2)$	$U[-1, 1, 20]$
F9	Nguyen-7	$\ln(x + 1) + \ln(x^2 + 1)$	$U[0, 2, 20]$
F10	Keijzer-1	$0.3x \sin(2\pi x)$	$E[-1, 1, 0.1]$
F11	Vladislavleva-2	$e^{-x} x^3 (\cos x \sin x) (\cos x \sin^2 x - 1)$	$E[0.05, 10, 0.1]$
F12	Keijzer-8	\sqrt{x}	$U[0, 4, 20]$
F13	Nguyen-9	$\sin(x) + \sin(y^2)$	$U[0, 1, 20]$
F14	Nguyen-10	$2 \sin(x) \cos(y)$	$U[-1, 1, 100]$
F15	Keijzer-11	$xy + \sin((x - 1)(y - 1))$	$U[-3, 3, 100]$
F16	Korns-2	$\frac{1}{1+x^{-4}} + \frac{1}{1+y^{-4}}$	$E[-5, 5, 0.4]$
F17	Keijzer-12	$x^4 - x^3 + \frac{y^2}{2} - y$	$U[-3, 3, 20]$
F18	Vladislavleva-3	$e^{-x} x^3 (\cos x \sin x) (\cos x \sin^2 x - 1) (y - 5) x$	$E[0.05, 10, 0.1] \ y : E[0.05, 10.05, 2]$

Table 2: Parameters of Algorithms

Name	Parameter	Value
GEP	function set	$+, -, \times, \div, \sin, \cos, \ln(n), \exp$
	population size	100
	head length	10
	chromosome length	21
	max generations	1000
	crossover Rate	0.7
	mutation rate	0.1
SL-GEP	function set	$+, -, \times, \div, \sin, \cos, \ln(n), \exp$
	population size	100
	head length	10
	chromosome length	21
	max generations	1000
	number of ADFs	2
AB-GEP	head length of ADFs	3
	function set	$+, -, \times, \div, \sin, \cos, \ln(n), \exp$
	population size	100
	head length	10
	chromosome length	21
	max generations	1000
	crossover Rate	0.7
GVAE-ABGEP	mutation rate	0.1
	number of subspaces	[81,100]
	function set	$+, -, \times, \div, \sin, \cos, \ln(n), \exp$
	population size	100
	head length	10
	chromosome length	21
	max generations	1000
	crossover Rate	0.7
	mutation rate	0.1
	number of subspaces	[81,100]
	learning rate	$\sqrt{\frac{\log k + n(n-1)}{2nk}}$

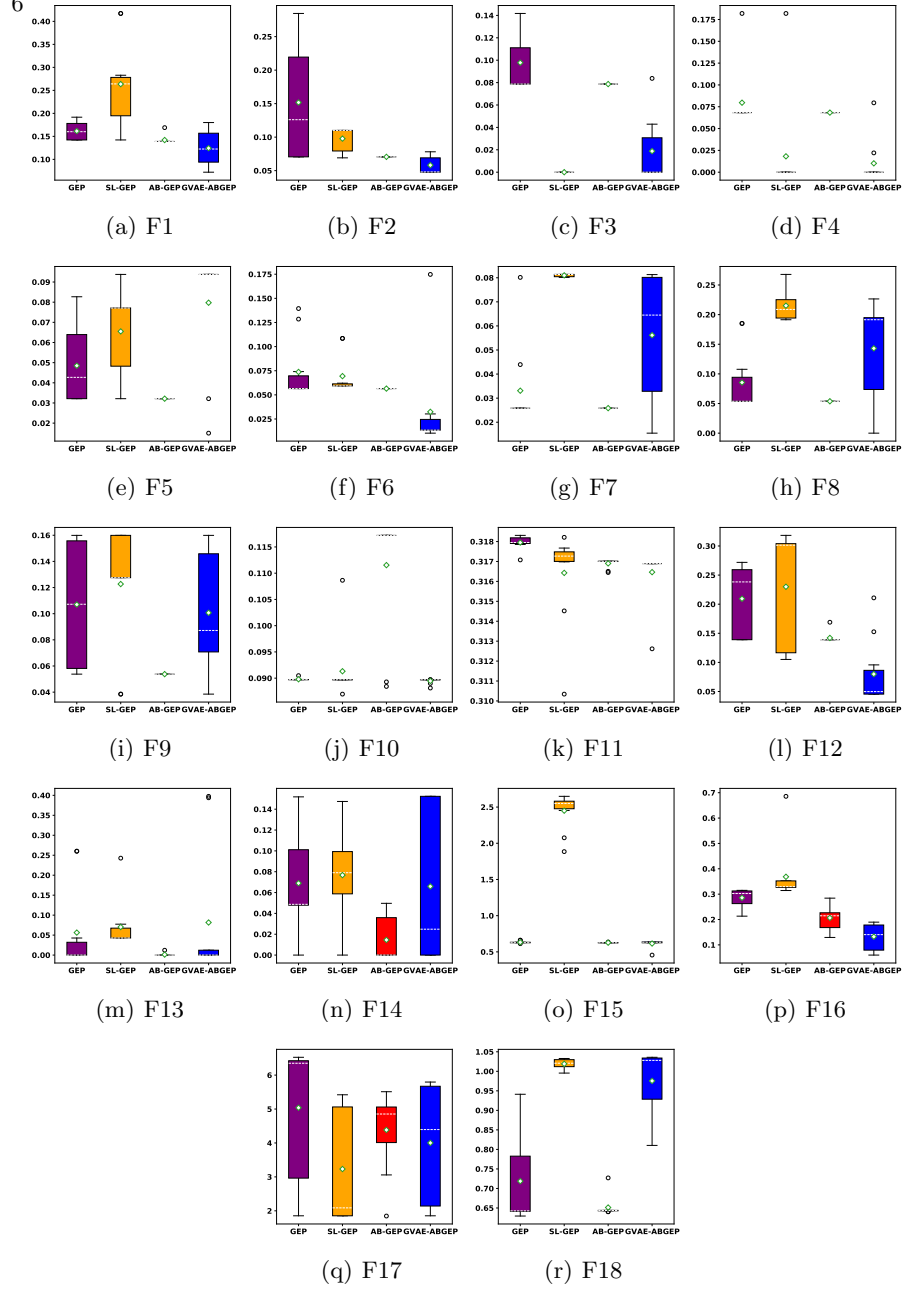


Fig. 1: Fitness comparison on all SRB benchmarks.

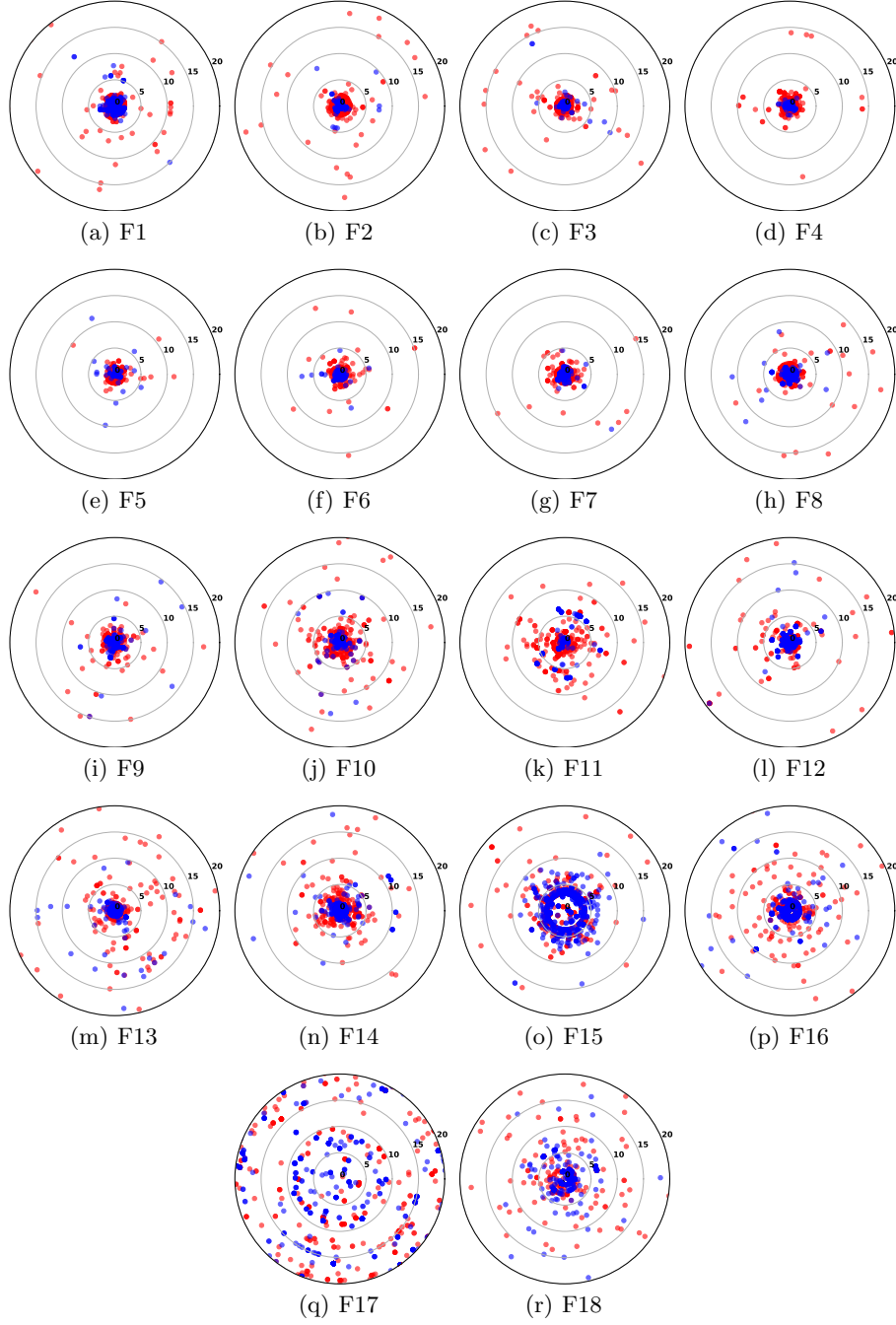


Fig. 2: Individual Fitness distribution on all SRB benchmarks. A blue (or red) point represents the fitness of a GVAE-ABGEP (or an AB-GEP) individual recorded every 100 generations.

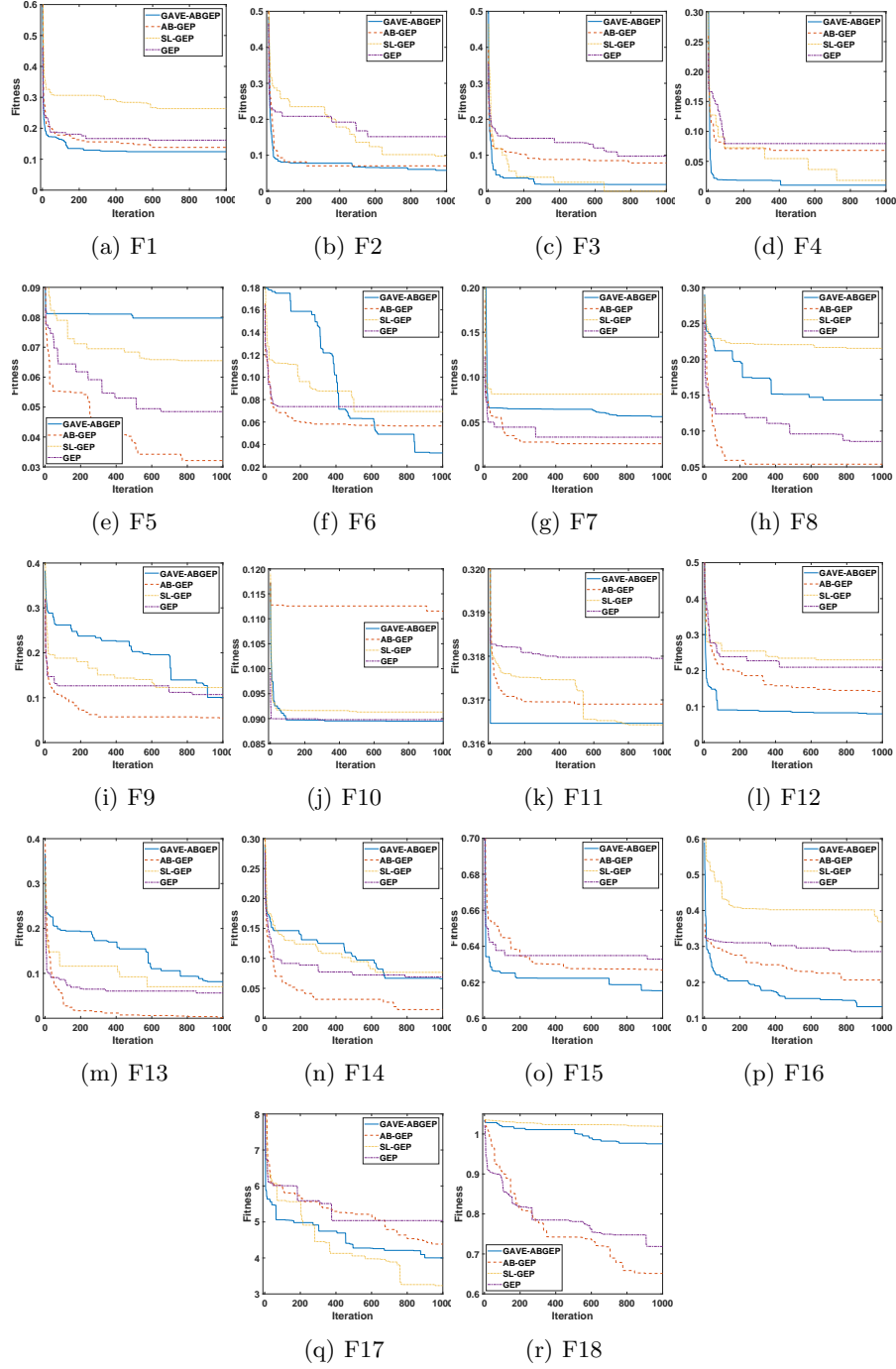


Fig. 3: Convergence comparison on all SRB benchmarks.

References

1. Lattimore, T., Szepesvári, C.: Bandit algorithms. Cambridge University Press (2020)