The First Mathematical Proof That Crossover Gives Super-Constant Performance Gains For the NSGA-II

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Abstract

Very recently, the first mathematical runtime analyses for the NSGA-II, the most common multi-objective evolutionary algorithm, have been conducted (Zheng, Liu, Doerr (AAAI 2022)). Continuing this research direction, we prove that the NSGA-II optimizes the OneJumpZeroJump benchmark asymptotically faster when crossover is employed. This is the first time such an advantage of crossover is proven for the NSGA-II. Our arguments can be transferred to single-objective optimization. They then prove that crossover can speed-up the $(\mu + 1)$ genetic algorithm in a different way and more pronounced than known before. Our experiments confirm the added value of crossover and show that the observed speed-ups are even larger than what our proofs can guarantee.

1 Introduction

The theory of randomized search heuristics [AD11] has greatly improved our understanding of heuristic search, in particular, via mathematical runtime analyses. Due to the complicated nature of the stochastic processes describing runs of these algorithms, mostly very simple, often synthetic, heuristics could be analyzed so far. Very recently, however, a runtime

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analysis was conducted [ZLD22] for the NSGA-II, the most common evolutionary multi-objective (EMO) algorithm [DPAM02] (47000 citations on Google scholar). This work was quickly followed up in different directions [ZD22, BQ22, DQ22]. The majority of these studies regards a simplified version of the NSGA-II that does not use crossover. Only in [BQ22] an NSGA-II with crossover is analyzed, but the runtime guarantees shown there were not better than those shown before for the mutation-only NSGA-II.

In this work, we conduct the first mathematical runtime analysis of the NSGA-II with crossover that proves runtime guarantees asymptotically stronger that those known for the NSGA-II without crossover. To this aim, we regard the OneJumpZeroJump benchmark [DZ21], which is a bi-objective version of the classic Jump benchmark intensively studied in the analysis of single-objective search heuristics. The mutation-based NSGA-II with population size $N$ (sufficiently large) computes the Pareto front of this problem in time $O(Nn^k)$, where $n$ is the length of the bit-string representation and $k$ is the jump size, a difficulty parameter of the problem [DQ22]. The authors say that they believe this bound to be tight, but prove a lower bound of $\Omega(n^k)$ only. That work includes preliminary experiments that show performance gains from crossover, but without proving them or giving additional insights on why they arise.

Our main result is that the NSGA-II using crossover with a constant rate solves this problem in expected time $O(N^2n^k/\Theta(k^k))$. This is faster than the previous bound and the $\Omega(n^k)$ lower bound when $k \geq c \log(N)/\log \log(N)$, where $c$ is a suitably large constant. The key to proving this performance advantage is a careful analysis of how the NSGA-II arrives at having substantially different solutions with same objective value in its population. This appears to be an advantage of the NSGA-II over algorithms previously analyzed mathematically such as the SEMO or global SEMO, where for each objective value at most one solution is kept in the population.

As a side result, we observe that our arguments for proving diversity in the population can also be used in single-objective optimization. This way we show that the $(\mu + 1)$ genetic algorithm (GA) – without additional diversity mechanisms or other adjustments favoring crossover – optimizes the jump function with encoding length $n$ and jump size $k$ in time $O(\mu^{k+1}n^k/\Theta(k^k))$. This result holds for all $n, k \geq 2$, and $\mu \geq 2$, the latter two possibly depending on $n$. For many parameter values, this compares favorably with the known $\Omega(n^k)$ runtime of the mutation-only analog of the $(\mu + 1)$ GA, the so-called $(\mu + 1)$ EA. Different from the previous analysis of the $(\mu + 1)$ GA on Jump in [DFK+18], our result shows super-constant speed-ups already for constant population sizes and our speed-ups increase with the problem difficulty $k$. In [DFK+18], speed-ups of at most a factor of $O(n)$ were shown regardless
of the size of $k$, and population sizes of roughly $\sqrt{n}$ were needed for the best results.

Our experimental results confirm the advantages of crossover for both the NSGA-II and the $(\mu + 1)$ GA. The advantages observed are even stronger than what our proofs guarantee. We note that it is not uncommon that mathematical runtime analyses cannot prove all advantages of an algorithm visible in experiments. In return, they give proven results and explanations on how the advantages arise.

Overall, our results give a strong mathematical justification for using the NSGA-II with crossover as proposed in the original work [DPAM02]. Our new analysis methods promise to be applicable also to other randomized search heuristics using crossover, as demonstrated briefly on the $(\mu + 1)$ GA.

2 Previous Works

Since this work conducts a mathematical runtime analysis of a classic, crossover-based EMO algorithm, let us briefly describe the state of the art in runtime analysis with respect to EMO algorithms and crossover.

Mathematical runtime analyses have a long history in the field of heuristic search [SH88, Bae93, Gut08, NW15, LO18, LOW19]. While often restricted to simple algorithms and problems, the mathematical nature of these works has led to many deep insights that could not have been obtained with empirical methods.

The mathematical runtime analysis of EMO algorithms was started in [LTZ02], [Gie03], and [Thi03]. As in the theory of single-objective heuristics, mostly simple synthetic algorithms were analyzed in that of multi-objective optimization. At the last AAAI conference, the first runtime analysis of the NSGA-II algorithm [DPAM02], the most common EMO algorithm in practice, was presented [ZLD22]. It proved that the NSGA-II with sufficiently large population size can find the Pareto front of the ONE_MIN_MAX and LOTZ benchmarks in the same asymptotic runtimes that were shown previously for the SEMO and GSEMO synthetic algorithms. This result is remarkable in that the NSGA-II has much more complex population dynamics than the (G)SEMO. In particular, it can lose desirable solutions due to the complex selection mechanism building on non-dominated sorting and crowding distance (and this was proven to happen consistently, e.g., when the population size is only equal to the size of the Pareto front [ZLD22]).

In [ZD22], it was proven that the NSGA-II with a smaller population size can still compute good approximations of the Pareto front. For this, however, a mild modification of the selection mechanism, proposed earlier [KD06], was
needed. In [DQ22], the first mathematical runtime analysis of the NSGA-II on a problem with multimodal objectives was conducted. Again, the NSGA-II was found to be as effective as the (G)SEMO algorithms when the population size was chosen suitably.

The three works just discussed consider the NSGA-II as proposed in the original work [DPAM02] except that they do not employ crossover. The only runtime analysis of the NSGA-II with crossover was conducted in [BQ22], namely on the COCZ, OneMinMax, and LOTZ benchmarks. However, the runtime guarantees shown there agree with the ones in [ZLD22], so no advantage of crossover was shown.

The question whether crossover, that is, generating new solutions from two existing ones, is useful or not, is as old as the area of genetic algorithms. Despite its importance, we are still far from having a satisfying answer. It is clear that at all times, the vast majority of evolutionary algorithms used in practice employ crossover. A solid scientific proof for the usefulness of crossover, however, is still missing.

For an example of one of many unsuccessful attempts to explain the power of crossover, we cite the building-block hypothesis (BBH) [Hol75], which states that crossover is effective because it allows to combine small profitable segments of different solutions. While very convincing on the intuitive level, a simple experimental analysis on a synthetic problem designed to perfectly fulfill the assumptions of the BBH raises some doubt. A simple randomized hill-climber was found to solve the proposed Royal Road problem around ten times faster than a comparably simple genetic algorithm using crossover [MFH92].

Theoretical approaches have been used as well to demonstrate the usefulness of crossover, but again mostly with limited success. We defer a discussion of the work on single-objective optimization to a later point of this work since our main focus is the use of crossover in multi-objective optimization. Here so far only three mathematical runtime analyses showing an advantage of crossover exist.

In [NT10], crossover was proven to be useful when solving multi-criteria versions of the all-pairs-shortest-path (APSP) problem. This work follows the ideas of the corresponding single-objective result [DHK12]. Both are somewhat problem-specific in the sense that the formulation of the APSP problem automatically leads to a very strong diversity mechanism, from which crossover substantially profits in both works.

In [QYZ13], a substantial advantage from crossover is shown, among others, for the classic COCZ problem. For this, however, a novel initialization is used which, for this problem, results in the initial and all subsequent pop-
ulations containing both the all-ones and the all-zeros string. It is clear that this strong diversity greatly helps crossover to become effective.

Both these works regard as baselines the SEMO and GSEMO algorithms, two synthetic algorithms proposed for theoretical analyses \cite{LTZ02, Gie03}. Given this and the particularities of the results, the diversity mechanism implicit in the APSP problem and the particular initialization in [QYZ13], it is not clear to what extent the insight that crossover is beneficial can be expected to generalize to the broader EMO field.

The third work showing an advantage of crossover in EMO optimization is [HZCH19]. Since it discusses a decomposition-based algorithm, it is very far from our work and we do not detail it further.

Crossover has been a topic of intensive research also in the theory of single-objective evolutionary computation. The works closest to ours regard the single-objective Jump benchmark, which looks like an ideal example for exploiting crossover. Surprisingly, it was much harder than expected to show that crossover is profitable here. The early analyses \cite{JW02, KST11} managed to show an advantage from crossover only with an unrealistically small crossover probability. Only in \cite{DFK18}, it was shown that a standard ($\mu + 1$) GA with standard parameters optimizes jump functions faster with crossover than without. Other examples proving advantages of crossover exist such as \cite{Sud05, LY11, DHK12, DDE15, DFK16}, but they appear specific to a particular problem or a particular algorithm.

3 Preliminaries

3.1 The NSGA-II Algorithm

In the interest of brevity, we only give a brief overview of the algorithm here and refer to \cite{DPAM02} for a more detailed description of the general algorithm and to \cite{ZLD22} for more details on the particular version of the NSGA-II we regard.

The NSGA-II uses two metrics to completely order any population, which are rank and crowding distance. The ranks are defined recursively based on the dominance relation. All non-dominated individuals have rank 1. Then, given that the individuals of ranks 1, \ldots, $k$ are defined, the individuals of rank $k + 1$ are those not dominated except by individuals of rank $k$ or smaller. This defines a partition of the population into sets $F_1$, $F_2$, \ldots such that $F_i$ contains all individuals with rank $i$. Clearly, individuals with lower ranks are preferred. The crowding distance, denoted by $\text{cDis}(x)$ for an individual $x$, is used to compare individuals of the same rank. To compute the crowding
distances of individuals of rank $i$ with respect to a given objective function $f_j$, we first sort the individuals in ascending order according to their $f_j$ objective values. The first and last individuals in the sorted list have infinite crowding distance. For the other individuals, their crowding distance is the difference between the objective values of its left and right neighbors in the sorted list, normalized by the difference of the minimum and maximum values. The final crowding distance of an individual is the sum of its crowding distances with respect to each objective function. Among individuals of the same rank, the ones with higher crowding distances are preferred.

The algorithm starts with a random initialization of a parent population of size $N$. At each iteration, $N$ children are generated from the parent population via a variation operator, and $N$ best individuals among the combined parent and children population survive to the next generation based on their ranks and, as a tie-breaker, the crowding distance (remaining ties are broken randomly). In each iteration, the critical rank $i^*$ is the rank such that if we take all individuals of ranks smaller than $i^*$, the total number of individuals will be less than or equal to $N$, but if we also take all individuals of rank $i^*$, the total number of individuals will be over $N$. Thus, all individuals of rank smaller than $i^*$ survive to the next generation, and for individuals of rank $i^*$, we take the individuals with the highest crowding distance, breaking ties randomly, so that in total exactly $N$ individuals are kept. In practice, the algorithm is run until some stopping criterion is met. In our mathematical analysis, we are interested in how long it takes until the full Pareto front is covered by the population if the algorithm is not stopped earlier. For that reason, we do not specify a termination criterion.

To create the offspring, the algorithm selects $N/2$ pairs of individuals from the parent population (possibly with repetition). For each pair, with probability 0.9, we generate two intermediate offspring via a 2-offspring uniform crossover (that is, for each position independently, with probability 0.5, the first child inherits the bit from the first parent, and otherwise from the second parent; the bits from the two parents that are not inherited by the first child make up the second child). Bit-wise mutation is then performed on these two intermediate offspring (that is, each bit is flipped independently with probability $\frac{1}{n}$). With the remaining 0.1 probability, this mutation is performed directly on the two parents.

Different methods can be employed to select the parents that are used to create the offspring population (that is, the aforementioned $N/2$ pairs). i) Fair selection: Each individual appears exactly once in a pair, apart from this, the pairing is random. ii) Uniform selection: Each pair consists of two random individuals. iii) $N$ independent binary tournaments: for $N$ times, uniformly at random sample 2 different parents and conduct a binary tournament between
the two, i.e., select the one with the lower rank, breaking ties by selecting the one with the larger crowding distance, breaking remaining ties randomly; form $N/2$ pairs from the winners randomly. iv) Two-permutation tournament scheme: Generate two random permutations $\pi_1$ and $\pi_2$ of $P_t$ and conduct a binary tournament between $\pi_j(2i - 1)$ and $\pi_j(2i)$ for all $i \in [1..N/2]$ and $j \in \{1, 2\}$. Form a pair from the two winners in each interval of length 4 in a permutation.

### 3.2 The $(\mu + 1)$ GA

The $(\mu + 1)$ GA maintains a population of $\mu$ individuals which are randomly initialized at the beginning of a run. In each generation, a new individual is created. With a constant probability $p_c$, it is created by selecting two parents from the population uniformly at random, crossing them over, and then applying mutation to the resulting offspring. With probability $1 - p_c$, a single individual is selected and only mutation is applied. At the end of the generation, the worst individual is removed from the population, with ties broken randomly.

Similarly to our analysis of the NSGA-II, in our analysis of the $(\mu + 1)$ GA, we consider applying uniform crossover with probability $p_c = 0.9$. Here crossover only produces one child where each bit has 50% chance coming from the first parent and 50% chance coming from the second. Bit-wise mutation of rate $\frac{1}{n}$ is employed.

### 3.3 Benchmark Problems

For $x \in \{0, 1\}^n$, let $|x|_0$ and $|x|_1$ denote the number of 0-bits and 1-bits in $x$, respectively. Let $k = \lceil 2..n/4 \rceil$. The function $\text{Jump}_{n,k} = f : \{0, 1\}^n \to \mathbb{R}$ was proposed by [DJW02]. It is defined by

$$f(x) = \begin{cases} 
k + |x|_1, & \text{if } |x|_1 \leq n - k \text{ or } x = 1^n, \\
n - |x|_1, & \text{else}, \end{cases}$$

for all $x \in \{0, 1\}^n$. The aim is to maximize $f$. It has a valley of low fitness around its optimum, which can be crossed only by flipping the $k$ correct bits, if no solutions of lower fitness are accepted.

The function $\text{OneJumpZeroJump}_{n,k} = (f_1, f_2) : \{0, 1\}^n \to \mathbb{R}^2$, proposed by [DZ21], is defined by

$$f_1(x) = \begin{cases} 
k + |x|_1, & \text{if } |x|_1 \leq n - k \text{ or } x = 1^n, \\
n - |x|_1, & \text{else}; \end{cases}$$

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\[ f_2(x) = \begin{cases} 
 k + |x|_0, & \text{if } |x|_0 \leq n - k \text{ or } x = 0^n, \\
 n - |x|_0, & \text{else;}
\end{cases} \]

for all \( x \in \{0,1\}^n \); here \( |x|_0 \) is the number of 0-bits in \( x \). The aim is to maximize both \( f_1 \) and \( f_2 \), two multimodal objectives. The first objective is the classical \( \text{Jump}_{n,k} \) function. The second objective is isomorphic to the first, with the roles of zeroes and ones exchanged.

According to Theorem 2 of [DZ21], the Pareto set of the benchmark is \( S^* = \{x \in \{0,1\}^n \mid |x|_1 = [k..n-k] \cup \{0, n\}\} \), and the Pareto front \( F^* = f(S^*) \) is \( \{(a,2k+n-a) \mid a \in [2k..n] \cup \{k, n+k\}\} \), making the size of the front \( n - 2k + 3 \). We define the inner part of the Pareto set by \( S^*_I = \{x \mid |x|_1 \in [k..n-k]\} \), and the inner part of the Pareto front by \( F^*_I = f(S^*_I) = \{(a,2k+n-a) \mid a \in [2k..n]\} \). [DQ22] showed that when using a population of size \( N \geq 4(n - 2k + 3) \) to optimize this benchmark, the NSGA-II algorithm never loses a Pareto-optimal solution value once found. Moreover, \( O(n^k) \) iterations are needed in expectation to find the full Pareto front (all Pareto optimal solution values).

## 4 Runtime Analysis of the NSGA-II with Crossover

In this section, we analyze the complexity of the NSGA-II algorithm with population size \( N = c(n - 2k + 3) \) for some \( c > 4 \). We consider all four different ways of selecting the parents for variation described in the previous section. For any generation \( t \) of a run of the algorithm, we use \( P_t \) to denote the parent population and \( R_t \) to denote the combined parent and offspring population. For individuals \( x \) and \( y \), we use \( H(x,y) \) to denote the Hamming distance between \( x \) and \( y \).

[DQ22] proved that the NSGA-II in an expected time (number of fitness evaluations) of \( O(Nn^k) \) covers the entire Pareto front of the \textit{OneJumpZeroJump} benchmark. This time mostly stems from the waiting times to generate the extremal points on the front, i.e., the all-zeroes string \( 0^n \) and the all-ones string \( 1^n \). Since individuals with lower fitness values are not kept in the population, these two extremal points can only be created from individuals with \( i \in [k..n - k] \) 1-bits. Crossing the fitness valley of length \( k \) happens for an individual with probability \( \Theta(n^{-k}) \), resulting in the \( O(Nn^k) \) runtime.

To profit from crossover, we exploit the fact that there can be diverse individuals at the outermost points of \( F^*_I \). For example if in a \( P_t \) there are two individuals \( x \) and \( y \) such that \( |x|_1 = |y|_1 = n-k \) and \( x \) and \( y \) are different, i.e., \( H(x,y) = 2d \) for \( d \geq 1 \), crossing them over creates an individual \( z \) such
that $|z|_1 = n - k + d$ with probability $\Theta(\frac{1}{n^2})$. Then mutating $z$ gives $1^n$ with probability $\Theta(\frac{1}{n^2})$. Therefore, the probability that $1^n$ is generated in iteration $t$ is $\Omega(\frac{n}{2n^2})$, making the waiting time smaller than $O(n^k)$. Following this idea, our analysis focuses on the runtime needed to create, maintain, and in the end, take advantage of such diversity at the outermost points of $F^*_i$.

First, some observations on the selection and survival probabilities of rank-1 individuals will help us argue that diversity can be created and maintained.

**Lemma 1.** Consider an iteration $t$ of the NSGA-II algorithm optimizing the $\text{ONEJUMPZEROJUMP}_n^k$ benchmark with population size $N = c(n - 2k + 3)$ for some $c > 4$. With any of the four selection methods, the probability that two rank-1 individuals $x, y \in P_t$ are both selected to mutate in iteration $t$ is $\Theta(1)$.

**Lemma 2.** Consider an iteration $t$ of the NSGA-II algorithm optimizing the $\text{ONEJUMPZEROJUMP}_n^k$ benchmark with population size $N = c(n - 2k + 3)$ for some $c > 4$ where $F^* \notin f(R_t)$. Suppose $x$ and $y$ are two rank-1 individuals in $R_t$. Then with probability at least $(\frac{c}{2c^2})^2$, we have $x, y \in P_{t+1}$.

Now, we give a Lemma on the runtime needed to create and maintain diversity at the outermost points of $F^*_i$. The idea is that in an iteration $t$, through mutation, an individual $x$ with $n - k$ 1-bits can generate an individual $y$ with the same number of 1-bits but different from $x$ (e.g., $H(x, y) = 2$), creating diversity among individuals with $n - k$ 1-bits. Then by Lemma 2, $x$ and $y$ survive to iteration $t + 1$ with a constant probability, where further diversity can be created in the same way. Accumulating diversity in $k$ iterations, we will have two individuals both with $n - k$ 1-bits and having a Hamming distance of $2^k$.

**Lemma 3.** Consider an iteration $t$ of the NSGA-II algorithm optimizing the $\text{ONEJUMPZEROJUMP}_n^k$ benchmark for $k = o(\sqrt{n})$ with population size $N = c(n - 2k + 3)$ for some $c > 4$. With any of the four parent selection methods, applying uniform crossover with probability 0.9 and bit-wise mutation, if there is $x \in P_t$ such that $|x|_1 = n - k$, then in another $O(\frac{K_n}{(k-1)!})$ iterations, for $K = (\frac{2c^2}{k-1})^2$, in expectation, the parent population will contain $x$ and $y$ such that $|x|_1 = |y|_1 = n - k$ and $H(x, y) = 2k$.

**Theorem 4.** Consider an iteration $t$ of the NSGA-II algorithm optimizing the $\text{ONEJUMPZEROJUMP}_n^k$ benchmark for $k = o(\sqrt{n})$ with population size $N = c(n - 2k + 3)$ for some $c > 4$. Suppose $1^n \notin P_t$. With any of the four
parent selection methods, applying uniform crossover with probability 0.9 and bit-wise mutation, if there is $x \in P_t$ such that $|x|_1 = n - k$, then in expectation the algorithm needs another $O\left(\frac{N^2(Cn)^k}{(k-1)!}\right)$ fitness evaluations, for $C = (\frac{4c}{c-4})^2$, to find $1^n$.

Note that the case for finding $0^n$ is symmetrical. Therefore, it takes $O\left(\frac{N(Cn)^k}{(k-1)!}\right)$ iterations to find both $1^n$ and $0^n$. To cover any other point on the front, since there is a 0.1 chance that crossover is not applied and since covered points remain covered, the $O(Nn \log n)$ time for covering the whole inner part of the Pareto front shown in [DQ22] remains valid (and is a lower order term compared to the time to generate the extremal points). In conclusion, in total, with uniform crossover happening at a constant probability, the number of iterations taken is $O\left(\frac{N(Cn)^k}{(k-1)!}\right)$.

Our analysis has revealed that the advantage of using crossover comes from the fact that now the algorithm does not need to flip all $k$ bits at once to cross the fitness valley. Still, $k$ bits need to be flipped for an individual $x$ with $n - k$ bits of 1 to create another individual with $n - k$ bits of 1 that is different enough from $x$ so that the two can produce $1^n$ by only crossover. This explains the $n^k$ term in the runtime proven. However, now these $k$ bits can be flipped one at a time in $k$ iterations, and this happens with probability larger than flipping them all at once since at each iteration the algorithm only needs to flip one bit from multiple available choices. This explains the $\frac{1}{(k-1)!}$ term in the proven runtime. We note that a disadvantage is that flipping one bit at a time means the diversity needed is created in $k$ iterations and in all these $k$ iterations, the diversity that has been created so far needs to be maintained, which is where the $C^k$ term in the runtime comes from. Another disadvantage is that in the end, creating the extremal point through only crossover requires pairing up two particular individuals, which happens with probability $\Theta(1/N)$ only. Therefore, crossover brings an asymptotic speed-up only when $(k-1)!$ outweighs $NC^k$, i.e., when $k \geq c \log(N)/\log \log(N)$ where $c$ is a suitably large constant. Our experiments, however, show that crossover is profitable already from $k = 2$ on.

5 Runtime Analysis of the $(\mu + 1)$ GA with crossover

[DFK+18] analyzed the runtime of the $(\mu + 1)$ GA optimizing the $\text{JUMP}_{n,k}$ function where uniform crossover and bit-wise mutation are used. Their proof requires complex analysis of the population dynamics, and shows improvement from crossover only when $\mu$ is large. In this section, we provide a simpler
analysis using the same insights made in the previous section, proving that crossover is helpful even when μ is Θ(1).

[DFK+18] proved that the expected time that the algorithm takes so that the entire population reaches the local optimum, i.e., all individuals have n − k bits of 1, is O(n√k(μ log μ + log n)). We now show that after the entire population reaches the local optimum, similarly to how crossover helps to speed up the NSGA-II, it can also decrease the waiting time to find the all-ones string with the (μ + 1) GA.

Lemma 5. Consider the (μ + 1) GA optimizing the Jump_{n,k} function, applying uniform crossover with probability 0.9 and bit-wise mutation. Suppose that in some iteration t the entire population is at the local optimum. Then in another O((10eμ+1)μk−1k n^k) iterations in expectation, the population contains x and y such that |x| = |y| = n − k and H(x, y) = 2k.

Theorem 6. Consider the (μ + 1) GA optimizing the Jump_{n,k} function, applying uniform crossover with probability 0.9 and bit-wise mutation. The number of iterations needed in expectation is O((40eμ(μ + 1))k−10e n^k (k−1)! + n√k(μ log μ + log n)).

The runtime proven in Theorem 6 is minimized when μ = Θ(1). Take μ = 2 for example. There the speed-up compared with the expected Θ(n^k) runtime of EAs without crossover is Ω((k−1)!), which is a real speed-up for k = ω(1). In [DFK+18], crossover is only shown to lead to speed up when μ is large. Specifically, for k = 2, the best speed-up is observed for μ = Θ(n/ log n) and for k ≥ 3, the best speed-up is observed for μ = Θ(n). For μ = Θ(1) however, no real speed-up can be inferred from [DFK+18]. Our arguments here demonstrate that crossover is helpful for the (μ + 1) GA even for a small population.

6 Experiments

To complement our theoretical results, we also experimentally evaluate some runs of the NSGA-II algorithm on the OneJumpZeroJump benchmark, and the (μ + 1) GA on the Jump benchmark.

6.1 NSGA-II optimizing OneJumpZeroJump

6.1.1 Settings

We implemented the algorithm as described in the preliminaries section in Python, and experimented with the following settings.
Table 1: Average runtime of the NSGA-II on the OneJumpZeroJump benchmark with $n = 50, 100$ and $k = 2$.

|                  | $p_c = 0$ | $p_c = 0.9$ |
|------------------|-----------|-------------|
| $n = 50, N = 2(n - 2k + 3)$ | 247,617   | 190,577     |
| $n = 50, N = 4(n - 2k + 3)$ | 416,284   | 147,921     |
| $n = 100, N = 2(n - 2k + 3)$ | 2,411,383 | 1,954,681   |
| $n = 100, N = 4(n - 2k + 3)$ | 3,858,084 | 1,322,046   |

- Problem size $n$: 50 and 100.
- Jump size $k$: 2.
- Population size $N$: $2(n - 2k + 3)$ and $4(n - 2k + 3)$. As in [DQ22], our mathematical guarantees apply only for $N \geq 4(n - 2k + 3)$, but already for $N = 2(n - 2k + 3)$ the algorithm succeeds empirically.
- Selection for variation: fair selection.
- Variation: with probability $p_c$, uniform crossover is applied followed by bit-wise mutation, otherwise only mutation is performed. Crossover probabilities $p_c = 0$ (no crossover) and $p_c = 0.9$.
- Number of independent repetitions per setting: 10. We will increase this number for the final version.

We note that [DQ22] already present some results on the runtime (for $k = 3$, $N/(2n - k + 3) = 2, 4, 8$, and $n = 20, 30, 40$). Therefore, we chose these settings to present new data points, in particular, for smaller $k$ and larger problem size.

6.1.2 Results

Table 1 contains the average number of fitness evaluations taken by the NSGA-II algorithm to cover the entire Pareto front of the OneJumpZeroJump$_{n,k}$ benchmark for $n \in \{50, 100\}$ and $k = 2$. For all results, a standard deviation between 50% to 80% of the mean was observed.

The data clearly supports our claim that crossover speeds up the NSGA-II on the OneJumpZeroJump benchmark (by a factor of between 1.2 and 2.9). The benefit of crossover is much more pronounced for the larger of the two population sizes. We suspect that this is because when the population becomes larger, there will be more individuals close to the outermost points.
of $F^*_i$. As a result, it is easier for the algorithm to reach and maintain diversity there, which as our analysis has suggested, is what makes crossover beneficial.

The runtimes for $k = 3$ (and smaller problem sizes) reported by [DQ22] showed speed-ups from crossover between a factor of 3.9 and 9. This fits to our mathematical analysis which showed more significant speed-ups for larger problem difficulties $k$.

To support our reasoning on how efficient crossover could be for different population sizes, we have also recorded for $n = 50$ the diversity among the individuals with $k$ and $n - k$ bits of 1 throughout the runs of the experiments. Specifically, for every $n^k/50$ iterations, we look at the individuals in the parent population with $k$ and $n - k$ bits of 1. Among all individuals with $k$ bits of 1, we calculate the Hamming distances between any two individuals, and record the maximum distance divided by 2. This number gives us an idea on how much a lucky crossover can decrease the waiting time of finding $0^n$, since as discussed in our analysis, pairing up two individuals with $k$ bits of 1 whose hamming distance is $2d$ means there is an $\Omega\left(\frac{1}{2^d n-k}\right)$ chance of creating the all-zeroes string. We do the same for the individuals with $n - k$ bits of 1. Note that the greatest this number can be is $k$. Since as shown in [DQ22], the runtime is dominated by the waiting time needed to find the all-ones and the all-zeroes strings after the inner part of the Pareto front has been covered, we are mostly interested in how the diversity develops in that phase. To this end, we discard data points recorded when the inner part of the Pareto front has not been fully covered, and those recorded after one of the extremal points has already been discovered. For one run of the experiment, we average the data points recorded for $k$ and $n - k$ bits of 1 together in the end. Finally we average the mean values obtained from the 10 repetitions. For $N = 2(n - 2k + 3)$, we have observed that the diversity measure is $0.76 \pm 0.62$, while for $N = 4(n - 2k + 3)$, it is $0.99 \pm 0.45$. This means indeed there is more diversity on the boundaries with a larger population, explaining why with $N = 4(n - 2k + 3)$ the speed-up from crossover is more than that with $N = 2(n - 2k + 3)$. We note that this does not mean that large population sizes are preferable since the higher cost of one iteration has to be taken into account. Due to the high runtimes, we do not have yet data allowing to answer this question conclusively, but preliminary experiments for $n = 50$ suggest that a population size of $N = 8(n - 2k + 3)$ already gives inferior results.

We note that the speed-up from crossover empirically is more profound than what we have shown theoretically. Though it is normal that mathematical runtime guarantees cannot capture the full strength of an algorithm, as a first attempt to understand where the discrepancy comes from we also recorded for each run how the all-ones string is generated (for the
case \( n = 100 \) and \( N = 2(n - 2k + 3) \). As a result, among the 10 runs that we have done, 9 times crossover has participated in the generation of \( 1^n \). Out of these 9 times, there are 5 times where crossover by itself has created \( 1^n \). However, for all of those 5 times, only one of the parents has \( n - k = 98 \) 1-bits, while the other parent has between 95 to 97 1-bits. Among all the runs, we have observed it only once that both of the parents have 98 bits of 1. This suggests that crossover also profits from diversity between individuals of different objective values, a fact not exploited in our runtime analysis.

6.2 The \((\mu + 1)\) GA Optimizing Jump

6.2.1 Settings
We implemented the algorithm as described in the preliminaries section in Python, and experimented with the following settings.

- Problem size \( n \): 100 and 1000.
- Jump size \( k \): 4.
- Population size \( \mu \): 2\(^i\) for \( i \in [0..9] \) for \( n = 100 \), and 2\(^i\) for \( i \in [5..11] \) for \( n = 1000 \).
- Variation operator: with 0.9 chance uniform crossover is applied followed by bit-wise mutation, and otherwise only bit-wise mutation is performed.
- Number of independent repetitions per setting: 10.

6.2.2 Runtime
Figure 1 gives the average number of fitness evaluations needed for the \((\mu + 1)\) GA to optimize Jump\(_{n,k}\) for \( n \in \{100, 1000\} \). The results confirm that crossover is beneficial for the \((\mu + 1)\) GA optimizing Jump as predicted from the runtime analyses in [DFK+18] and this work. The experimental results suggest that the best speed-up is observed for large population (128 for \( n = 100 \) and 512 for \( n = 1000 \)), different from our analysis. However, already smaller populations give significant speed-ups. For example, when \( n = 100 \) and \( k = 4 \), merely with \( \mu = 2 \), crossover is able to decrease the runtime from over \( (1/n)^k(1 - 1/n)^{n-k} \geq 10^8 \), the expected waiting time for a successful mutation, to \( 1.7 \times 10^7 \). With \( \mu = 4 \), the runtime is further decreased to \( 6.3 \times 10^6 \). These results suggest that the effects exploited in our analysis contribute measurably significantly to the advantages of crossover,
Figure 1: Average runtime of the \((\mu + 1)\) GA to optimize \(\text{JUMP}_{n,k}\) for \(n \in \{100,1000\}\) and \(k = 4\) using uniform crossover with probability 0.9.
in particular, when $\mu = \Theta(1)$ where the analysis in [DFK+18] could not show a speed-up.

7 Conclusions and Future Works

In this work, we conducted the first mathematical runtime analysis of the NSGA-II that shows a speed-up from crossover (on the ONEJUMPZEROJUMP benchmark), already for small population sizes (larger than four times the Pareto front, a number required already for previous runtime analyses of a mutation-only version of the NSGA-II). Interestingly, the proven gain from crossover increases with the difficulty parameter $k$ of the ONEJUMPZEROJUMP benchmark.

Our results are very different from previous runtime analyses of crossover-based algorithms. With no runtime analyses of MOEAs on the ONEJUMPZEROJUMP benchmark or comparable problems existing, the work closest to ours might be the runtime analysis of the $(\mu + 1)$ GA on the single-objective JUMP benchmark in [DFK+18]. There the best speed-ups were obtained from population sizes of order $\sqrt{n}$, and the speed-ups were at most a factor of $\Theta(n)$, regardless of how large the difficulty parameter $k$ was chosen.

This comparison suggests that our work has detected a novel way how crossover-based algorithms can leave local optima. As a side result, we show that our arguments can indeed be employed for the $(\mu + 1)$ GA, showing significant speed-ups there as well, again from small (constant) population sizes on and increasing significantly with the difficulty parameter $k$.

Our experimental results, similar to the ones in [DFK+18], confirm the proven advantages of crossover, but also show that crossover is much more powerful than what the mathematical proofs could distill. For the NSGA-II, for example, we observe considerable speed-ups already for the smallest possible value $k = 2$ of the difficulty parameter. Trying to explain these via proven results is clearly a great challenge for future research. One direction here could be to profit also from solutions that are further away from the target solution than the minimum distance. As our experiments have shown, such solutions often contribute to successful crossovers.

As a second direction for further research, we note that we did not prove any lower bounds, so we have not estimate on how far our runtime guarantees are from the truth. Clearly, proving lower bounds for a crossover-based algorithm is challenging as it requires a detailed understanding of the population dynamics and of the typical diversity observed in the population.
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8 Appendix

**Proof of Lemma 7.** We first show the probability that any single rank 1 individual is selected. The probability that any individual being selected with fair selection is 1. With uniform selection, the probability that any individual is selected is at least $1 - (1 - \frac{1}{N})^N \geq 1 - \frac{1}{e}$. Now consider using tournaments. Let $F_1$ be all the rank-1 individuals in the current parent population. Then by Corollary 6 of [DZ21], $|f(F_1)| \leq n - 2k + 3$. Let $F_1^*$ denote the number of individuals in $F_1$ with positive crowding distances. Then by Lemma 1 of [DQ22], $|F_1^*| \leq 4(n - 2k + 3)$. Suppose $x$ participates in a binary tournament. If the opponent of $x$ is not in $F_1^*$, which happens with probability at least $\frac{(c-4)(n-2k+3)}{c(n-2k+3)}$, then $x$ has at least $\frac{1}{2}$ chance of winning the tournament. With $N$ binary tournaments, the probability that $x$ participates in a particular binary tournament is $\frac{1}{N}$. So the probability that $x$ wins at least one of the $N$ independent tournaments is $1 - (1 - (1 - \frac{2}{N} \frac{c-4}{c})^N \geq 1 - e^{-\frac{c-4}{e}}$. With the two independent permutations, $x$ participates in two tournaments, so the probability that $x$ wins at least once is at least $2\frac{1}{2} \frac{c-4}{e} - (\frac{1}{2} \frac{c-4}{e})^2 = \frac{c-4}{e} - \frac{(c-4)^2}{4e^2}$.

Then, we can obtain the probability that two rank 1 individuals $x$ and $y$ of rank 1 are both selected. With fair selection, the probability that $x$ and $y$ are both selected is 1. With uniform selection, the probability that $x$ is selected is at least $1 - \frac{1}{e}$. Denote the number of times that $x$ is selected by $X$, then $\Pr[x \text{ selected} \land y \text{ selected}] = \sum_{i=1}^{N-1} \Pr[X = i] \Pr[y \text{ selected}|X = i] \geq \Pr[X = 1] \Pr[y \text{ selected}|X = 1] \geq N \frac{1}{N} (1 - \frac{1}{N})^{N-1} (1 - (1 - \frac{1}{N})^{N-1}) = \Theta(1)$.

With $N$ independent binary tournaments, given that $x$ is selected, if the opponent of $y$ in the binary tournament is not in $F_1^*$ and not $x$, then $y$ has at least $\frac{1}{2}$ chance of winning the tournament. So $\Pr[x \text{ selected} \land y \text{ selected}] \geq (1 - e^{-\frac{2(c-4)}{e}})(1 - \frac{1}{N} \Theta(\frac{c-4}{e}))^N = \Theta(1)$. Similarly, under the two permutation scheme, $\Pr[x \text{ selected} \land y \text{ selected}] \geq \Theta(\Theta(\frac{c-4}{e}) - \Theta((\frac{1}{2} \frac{c-4}{e})^2)) = \Theta(1)$. \hfill \Box

**Proof of 2.** First we prove that the probability that any one individual of rank 1 survives is $\frac{c-4}{2e}$. Let $F_1$ be all the rank-1 individuals in $R_t$. Since $x \in F_1$, if $|F_1| \leq N$, $x$ will survive to generation $t + 1$ with probability 1. So consider the case where rank 1 is the critical rank, i.e., the rank where some but not all individuals survive. Since the algorithm has not discovered the entire Pareto front, we have $|f(F_1)| < n - 2k + 3$. By Lemma 1 of [DQ22], there are at most $4|f(F_1)| < N$ individuals in $F_1$ with positive crowding distances. Therefore, if $x$ has a positive crowding distance, it will survive to generation $t + 1$ with probability 1. So consider the case where the crowding distance of $x$ is zero. Moreover, there are at least $N - 4|f(F_1)| > (c - 4)(n - 2k + 3)$
rank-1 individuals with zero crowding distance that survive to generation \( t + 1 \). Also, there are less than \( 2N = 2c(n-2k+3) \) individuals in \( R_t \) with rank 1 and zero crowding distance. Since all individuals of the critical rank and zero crowding distance are selected for survival uniformly at random, \( x \) survives to generation \( t + 1 \) with probability greater than \( \frac{(c-4)(n-2k+3)}{2c(n-2k+3)} = \frac{c-4}{2c} \).

The we prove that the probability that any pair of individuals \( x \) and \( y \) of rank 1 both survive is \( (\frac{c-4}{2c})^2 \) if both \( x \) and \( y \) have positive crowding distances, the probability that they both survive is 1 since there are at most \( N \) individuals in \( F_1 \) with positive crowding distances. Suppose, without loss of generality, that \( x \) has a positive crowding distance and \( y \) has zero crowding distance. The probability that both of them survive is \( \frac{c-4}{2c} \) since the probability of \( x \) surviving is 1 and that of \( y \) is \( \frac{c-4}{2c} \), and the two events are independent. Suppose both \( x \) and \( y \) have zero crowding distance, then one of them survives with probability greater than \( \frac{c-4}{2c} \). Given that one has survived, there are now \( N - 4|F(F_1)| - 1 \geq (c-4)(n-2k+3) \) spots left for rank-1 individuals with zero crowding distance to survive. So the probability that the other one also survives is still at least \( \frac{c-4}{2c} \). So the probability that both of them survive is at least \( (\frac{c-4}{2c})^2 \).

\( \square \)

**Proof of Lemma 3.** By the proof of Lemma 1, the probability that \( x \) is selected as a parent is \( \Theta(1) \). The probability that no crossover happens with \( x \) is 0.1. The probability that \( x \) generates some \( x_1 \) by bit-wise mutation such that \( |x_1|_1 = n-k \) and \( H(x,y) = 2 \) is \( k \frac{n-k}{n}(1 - \frac{1}{n})^{n-2} \geq \frac{1}{e} \frac{n-k}{n} \). By Lemma 2, the probability that both \( x \) and \( x_1 \) survive to generation \( t + 1 \) is at least \( (\frac{c-4}{2c})^2 \). Therefore, given that \( x \in P_t \), the probability that both \( x \) and \( x_1 \) are in \( P_{t+1} \) is \( \Omega((\frac{c-4}{2c})^2) \frac{n-k}{n} \). Similarly, given that \( x_1 \) is in \( P_{t+1} \), the probability that \( x_1 \) generates \( x_2 \) such that \( |x_2|_1 = n-k \) and \( H(x,y) = 4 \), and both \( x \) and \( x_2 \) survive to generation \( t + 2 \) is \( \Omega((\frac{c-4}{2c})^2) \frac{n-k}{n} \). Continuing this way, the probability that \( x \) and \( x_k \) exist in \( P_{t+k} \) where \( |x|_1 = |x_k|_1 = n-k \) and \( H(x,x_k) = 2k \) is \( \Omega((\frac{c-4}{2c})^{2k}) \frac{k!}{n^k} (\frac{n-k}{n})^{n-k} (\frac{n}{n^k})^{k+2} \Omega((\frac{c-4}{2c})^{2k}) \frac{k!}{n^k} \) for \( k = o(\sqrt{n}) \). Therefore, in expectation, if there is \( x \in P_t \) such that \( |x|_1 = n-k \), in \( O(k^{Kn^h}) = O\left(\frac{(Kn^h)^k}{(k-1)!}\right) \) iterations in expectation, for \( K = (\frac{2c}{c-4})^2 \), the parent population will contain \( x \) and \( x_k \) such that \( |x|_1 = |x_k|_1 = n-k \) and \( H(x,x_k) = 2k \). \( \square \)

**Proof of Theorem 4.** By Lemma 3, since there is \( x \in P_t \) such that \( |x|_1 = n-k \), in \( O(k^{Kn^h}) = O\left(\frac{(Kn^h)^k}{(k-1)!}\right) \) iterations, for \( K = (\frac{2c}{c-4})^2 \), the parent population will contain \( x \) and \( x_k \) such that \( |x|_1 = |x_k|_1 = n-k \) and \( H(x,x_k) = 2k \). We call this phase, i.e., producing a population containing such \( x \) and \( x_k \) from a population containing \( x \), the diversification phase.
Denote the generation that $x$ and $x_k$ first appear in the parent population by $t'$. By Lemma 1, the probability that they are both selected in generation $t'$ is $\Theta(1)$. The probability that they are then paired up is $\frac{1}{N}$, and the probability that crossover happens on this pair is 0.9. The probability that one of the intermediate children resulted from crossing $x$ and $x_k$ is the all-ones string is $\left(\frac{1}{2}\right)^{2k}$. The probability that after mutation the intermediate child remains the all-ones string is $(1 - \frac{1}{n})^n = \Theta(\frac{1}{c^2}) = \Theta(1)$. Therefore, the probability that $1^n$ is generated in generation $t'$ is $\Omega(\frac{1}{N})$.

By Lemma 1 of [DQ22], once there is an $x \in P_t$ such that $|x|_1 = n - k$, all the future populations will contain an individual with $n - k$ 1-bits. So if $1^n$ is not found in generation $t'$, we can repeat the argument from the beginning of the diversification phase. The expected number of such trials is $\Omega((\frac{1}{N})^{2k})^{-1} = O(N^{2k})$, and the expected length of one trial, i.e., one run of the diversification phase, is $O((\frac{K^n}{C_n})^{k})$ for $K = \frac{2c}{e}$ by Lemma 3.

Adding all up, once there is an $x \in P_t$ such that $|x|_1 = n - k$, in expectation, $O((\frac{K^n}{C_n})^{k} N^{2k}) = O(\frac{N^{2(n-k)}}{(k-1)!})$ iterations are needed, for $C = \frac{4c}{e^2}$, iterations are needed to find $1^n$, corresponding to $O(\frac{N^{2(n-k)}}{(k-1)!})$ fitness evaluations.

**Proof of** [DQ22] The probability that no crossover happens in iteration $t$ is 0.1. Denote the parent individual chosen in iteration $t$ by $x$. Since the entire population is at the local optimum, we have $|x|_1 = n - k$. Then with probability $\frac{k}{n} n - k (1 - \frac{1}{n})^{n-2} \geq \frac{k}{n} n - k \frac{n}{n} n - k$, the result of applying bit-wise mutation to $x$ is some $x_1$ such that $|x_1|_1 = n - k$ and $H(x, x_1) = 2$. Since all the individuals in $P_t$ and $x_1$ have the same fitness, the probability that neither $x$ nor $x_1$ is removed from the population at the end of iteration $t$ is $\frac{n-k}{n+1}$. Therefore, the probability that $x, x_1 \in P_{t+1}$ is at least $\frac{1}{e} \frac{k}{n} n - k \frac{n}{n} n - k +1$. Now consider iteration $t + 1$. The probability that no crossover happens in iteration $t + 1$ is 0.1, and the probability that $x_2$ is chosen for mutation is $\frac{1}{n}$. With probability $\frac{k-1}{n} n - k - 1 (1 - \frac{1}{n})^{n-2} \geq \frac{k-1}{n} n - k - 1 \frac{n}{n} n - k$, the child of $x_2$ is some $x_2$ such that $|x_2|_1 = n - k - 1$ and $H(x, x_2) = 4$. Again the probability that neither $x$ nor $x_2$ is removed from the population at the end of iteration $t + 1$ is $\frac{n-1}{n+1}$. Therefore, the probability that $x, x_2 \in P_{t+2}$ is at least $\frac{1}{e} \frac{k-1}{n} n - k - 1 \frac{n}{n} n - k +1$. Continuing this way, the probability that $x, x_k \in P_{t+k}$ such that $|x|_1 = |x|_k = n - k$ and $H(x, x_k) = 2k$ is at least $\frac{1}{n} (\frac{1}{e} \frac{n}{n} n - k - 1 \frac{n}{n} n - k - 1) = \Omega((\frac{1}{e} \frac{n}{n})^{k-1} k^{k-1} \frac{n}{n}^{k-1} (n-k)\cdots(n-2k+1)) = \Omega((\frac{1}{e} \frac{n}{n})^{k-1} k^{k-1} \frac{n}{n}^{k-1})$ for $k = o(\sqrt{n})$.

Once the algorithm enters the stage where the entire population is at the local optimum, the entire population will remain there until the all-ones string is found, since any newly-generated individuals with fitness levels lower than the local optimum will not be kept. So if the algorithm fails to find such $x$
Proof of Theorem 6. By Lemma 1 of [DFK+18], in expectation, in $O(n\sqrt{k}(\mu \log \mu + \log n))$ iterations, the entire population is at the local optimum. Then by Lemma 5, in another $O((10e^{\mu+1}/\mu-1)^k \mu^{k-1} n^k / (k-1)!)$ iterations in expectation, the population contains $x$ and $y$ such that $|x|_1 = |y|_1 = n - k$ and $H(x, y) = 2k$. We call the phase, i.e., producing a population containing such $x$ and $y$ from a population at the local optimum, the diversification phase.

Denote the generation that $x$ and $y$ first appear in the population by $t$. The probability that crossover happens in iteration $t$ is $0.9$. The probability that $x$ and $y$ are chosen in this iteration is $\frac{1}{\mu(\mu-1)}$. The probability that the result of applying crossover on $x$ and $y$ is the all-ones string is $(\frac{1}{2})^{2k}$, and the probability that no mutation happens on this intermediate child is $(1 - \frac{1}{n})^n = \Theta(\frac{1}{e})$. Therefore, the probability that the all-ones string is found in iteration $t$ is $\Theta(\frac{9}{10e \mu(\mu-1)} (\frac{1}{2})^k)$.

If the algorithm fails to find the all-ones string in iteration $t$, we can repeat the argument from the beginning of the diversification phase since the population remains at the local optimum. The expected number of such trials is $O(\frac{10e}{\mu}(\mu - 1)4^k)$ and the expected length of one trial is $O((10e^{\mu+1}/\mu-1)^k \mu^{k-1} n^k / (k-1)!)$ by Lemma 5. So after the entire population is at the local optimum, in expectation in another $O((40e\mu(\mu+1))^k (\frac{2}{\mu-1})^{k-1} 10e \frac{n^k}{(k-1)!})$ iterations, the all-ones string will be found. Adding all together, the algorithm needs in expectation $O((40e\mu(\mu+1))^k (\frac{2}{\mu-1})^{k-1} 10e \frac{n^k}{(k-1)!}) + n\sqrt{k}(\mu \log \mu + \log n))$ iterations to optimize the $\text{JUMP}_{n,k}$ function.