





Evolutionary Computation

Comparing Optimization Algorithms

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Outline

- 1. Introduction
- 2. Views on Performance and Time
- 3. Statistical Measures
- 4. Statistical Comparisons
- 5. Testing is Not Enough
- 6. Other Stuff
- 7. Summary





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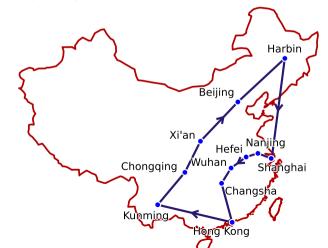
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- As a complement to this lesson, I suggest the report "Benchmarking in Optimization: Best Practice and Open Issues" on Arxiv.

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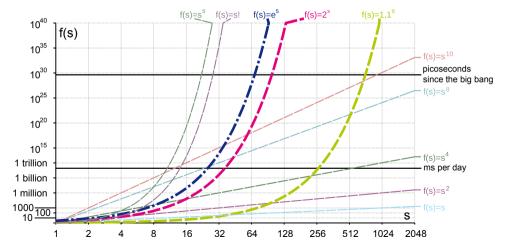


- In optimization, there exist exact and heuristic algorithms.
- Let's look at the classical Traveling Salesperson Problem (TSP).
 - Clearly, there is (at least) one shortest tour.
 - Theory proofs that the time to find this tour may grow exponentially with the number of cities we want to visit in the worst case.⁴⁻⁸

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very much / too (?) long

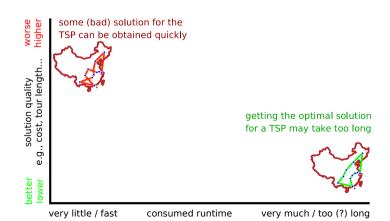
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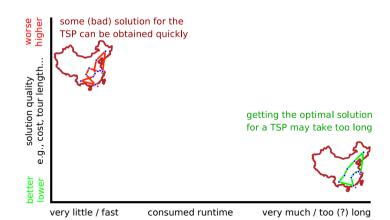
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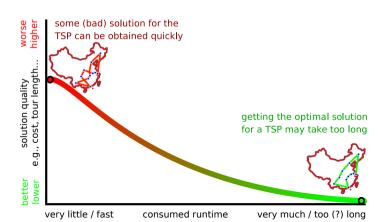
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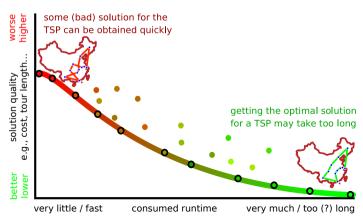
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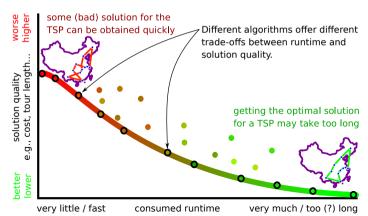
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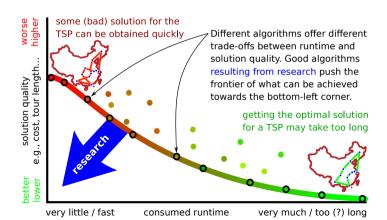
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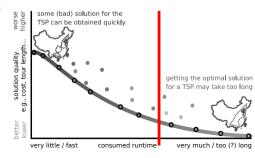
Views on Performance and Time



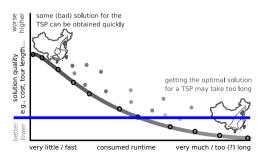
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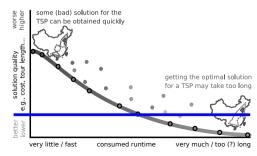
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What is Runtime?

• What actually is runtime?

Measure the (absolute) consumed runtime of the algorithm in ms.

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- ... for research they may be less interesting, while for a specific application they do matter.

Measure (count) the number of fully constructed and tested candidate solutions.

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- Relevant for comparing algorithms, but not so much for the practical application or comparing implementations.

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- I suggest to prefer FEs over generations if you want to count algorithm steps.

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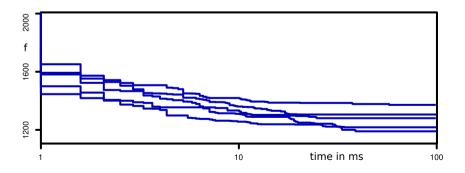
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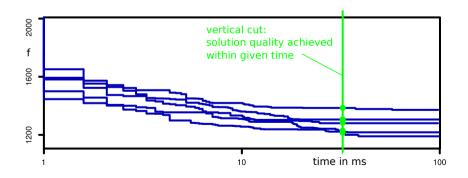
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Views on Performance

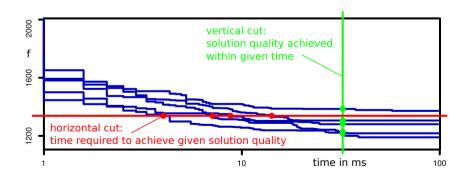
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- Which one is the "better" view on performance?
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- This question is still debated in research...

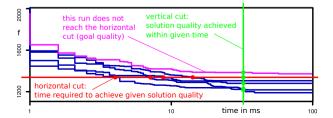
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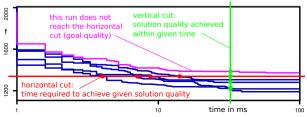
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- Sometimes problematic: What if one run does not reach the goal quality?
- Then, alternative measures need to be computed, such as the ERT^{14 15} or PAR2 and PAR10^{16 17}.



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- "How good is the tour for the TSP that we can find in 5 minutes with our algorithm?"
- Always well-defined, because vertical cuts can always be reached.

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- Maybe cast a net of several horizontal and vertical cuts, to get a better picture. . .

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 - 6. based on known results or well-accepted bounds

Statistical Measures



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 - ullet 1 run = 1 application of an optimization algorithm to a problem, runs are independent from all prior runs.

Problem Instances and Randomized Algorithms

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 - We always must use multiple different problem instances to get reliable results.
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# throws	number	f(1)	f(2)	f(3)	f(4)	f(5)	f(6)
1	5	0.0000	0.0000	0.0000	0.0000	1.0000	0.0000



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1	5	0.0000	0.0000	0.0000	0.0000	1.0000	0.0000
2	4	0.0000	0.0000	0.0000	0.5000	0.5000	0.0000



# throws	number	f(1)	f(2)	f(3)	f(4)	f(5)	f(6)
1	5	0.0000	0.0000	0.0000	0.0000	1.0000	0.0000
2	4	0.0000	0.0000	0.0000	0.5000	0.5000	0.0000
3	1	0.3333	0.0000	0.0000	0.3333	0.3333	0.0000



# throws	number	f(1)	f(2)	f(3)	f(4)	f(5)	f(6)
1	5	0.0000	0.0000	0.0000	0.0000	1.0000	0.0000
2	4	0.0000	0.0000	0.0000	0.5000	0.5000	0.0000
3	1	0.3333	0.0000	0.0000	0.3333	0.3333	0.0000
4	4	0.2500	0.0000	0.0000	0.5000	0.2500	0.0000



# throws	number	f(1)	f(2)	f(3)	f(4)	f(5)	f(6)
1	5	0.0000	0.0000	0.0000	0.0000	1.0000	0.0000
2	4	0.0000	0.0000	0.0000	0.5000	0.5000	0.0000
3	1	0.3333	0.0000	0.0000	0.3333	0.3333	0.0000
4	4	0.2500	0.0000	0.0000	0.5000	0.2500	0.0000
5	3	0.2000	0.0000	0.2000	0.4000	0.2000	0.0000



# throws	number	f(1)	f(2)	f(3)	f(4)	f(5)	f(6)
1	5	0.0000	0.0000	0.0000	0.0000	1.0000	0.0000
2	4	0.0000	0.0000	0.0000	0.5000	0.5000	0.0000
3	1	0.3333	0.0000	0.0000	0.3333	0.3333	0.0000
4	4	0.2500	0.0000	0.0000	0.5000	0.2500	0.0000
5	3	0.2000	0.0000	0.2000	0.4000	0.2000	0.0000
6	3	0.1667	0.0000	0.3333	0.3333	0.1667	0.0000



# throws	number	f(1)	f(2)	f(3)	f(4)	f(5)	f(6)
1	5	0.0000	0.0000	0.0000	0.0000	1.0000	0.0000
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3	1	0.3333	0.0000	0.0000	0.3333	0.3333	0.0000
4	4	0.2500	0.0000	0.0000	0.5000	0.2500	0.0000
5	3	0.2000	0.0000	0.2000	0.4000	0.2000	0.0000
6	3	0.1667	0.0000	0.3333	0.3333	0.1667	0.0000
7	2	0.1429	0.1429	0.2857	0.2857	0.1429	0.0000
8	1	0.2500	0.1250	0.2500	0.2500	0.1250	0.0000
9	4	0.2222	0.1111	0.2222	0.3333	0.1111	0.0000
10	2	0.2000	0.2000	0.2000	0.3000	0.1000	0.0000



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4	4	0.2500	0.0000	0.0000	0.5000	0.2500	0.0000
5	3	0.2000	0.0000	0.2000	0.4000	0.2000	0.0000
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8	1	0.2500	0.1250	0.2500	0.2500	0.1250	0.0000
9	4	0.2222	0.1111	0.2222	0.3333	0.1111	0.0000
10	2	0.2000	0.2000	0.2000	0.3000	0.1000	0.0000
11	6	0.1818	0.1818	0.1818	0.2727	0.0909	0.0909
12	3	0.1667	0.1667	0.2500	0.2500	0.0833	0.0833



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1	5	0.0000	0.0000	0.0000	0.0000	1.0000	0.0000
2	4	0.0000	0.0000	0.0000	0.5000	0.5000	0.0000
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12	3	0.1667	0.1667	0.2500	0.2500	0.0833	0.0833
100		0.1900	0.2100	0.1500	0.1600	0.1200	0.1700
1'000		0.1700	0.1670	0.1620	0.1670	0.1570	0.1770
10'000		0.1682	0.1699	0.1680	0.1661	0.1655	0.1623
100'000		0.1671	0.1649	0.1664	0.1676	0.1668	0.1672
1'000'000		0.1673	0.1663	0.1662	0.1673	0.1666	0.1664



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8	1	0.2500	0.1250	0.2500	0.2500	0.1250	0.0000
9	4	0.2222	0.1111	0.2222	0.3333	0.1111	0.0000
10	2	0.2000	0.2000	0.2000	0.3000	0.1000	0.0000
11	6	0.1818	0.1818	0.1818	0.2727	0.0909	0.0909
12	3	0.1667	0.1667	0.2500	0.2500	0.0833	0.0833
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1'000		0.1700	0.1670	0.1620	0.1670	0.1570	0.1770
10'000		0.1682	0.1699	0.1680	0.1661	0.1655	0.1623
100'000		0.1671	0.1649	0.1664	0.1676	0.1668	0.1672
1'000'000		0.1673	0.1663	0.1662	0.1673	0.1666	0.1664
10'000'000		0.1667	0.1667	0.1666	0.1668	0.1667	0.1665
100'000'000		0.1667	0.1666	0.1666	0.1667	0.1667	0.1667
1'000'000'000		0.1667	0.1667	0.1667	0.1667	0.1667	0.1667



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- We usually want to reduce this set of numbers to a single value which can give us an impression of what the "average outcome" (or result quality is).
- Three of the most common options for doing so, for estimating the "center" of a distribution, are to either compute the arithmetic mean, the median, or the geometric mean.

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$$mean(A) = \frac{1}{n} \sum_{i=0}^{n-1} a_i$$
 (1)

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$$A = (a_0, a_1, \dots, a_{n-1})$$
 where $a_{i-1} \le a_i \ \forall i \in 1 \dots (n-1)$.

$$\operatorname{med}(A) = \left\{ \begin{array}{ll} a_{\frac{n-1}{2}} & \text{if } n \text{ is odd} \\ \frac{1}{2} \left(a_{\frac{n}{2}-1} + a_{\frac{n}{2}} \right) & \text{otherwise} \end{array} \right. \quad \text{if } a_{i-1} \leq a_i \ \forall i \in 1 \dots (n-1)$$

$$n$$
 is odd

$$n$$
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if
$$a_{i-1} \leq a_i \ \forall i \in 1 \dots (n-1)$$

if
$$a$$

$$a_1 \le a_i \ \forall i \in 1 \dots (n-1)$$

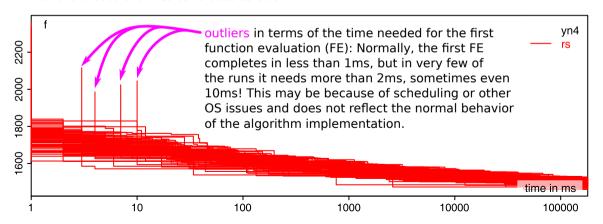
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Outliers

- For example, maybe the operating system was updating itself during a run of one of our algorithms and, thus, took away some of the computation budget.
- In my experiments here, there are sometimes outliers in the time that it takes to create and evaluate the first candidate solution.
- But outliers are actually important. So I say this right now. I will also say it again later.
 But I am afraid that you may tune out during the following example. So remember:
 Outliers are important. Anyway. . .

$$A = (1,3,4,4,4,5,6,6,6,6,7,7,9,9,9,10,11,12,14)$$

$$B = (1,3,4,4,4,5,6,6,6,6,7,7,9,9,9,10,11,12,10'008)$$

• Two sets of data samples A and B with $n_a=n_b=19$ values.

$$\begin{array}{lll} A & = & (1,3,4,4,4,5,6,6,6,6,7,7,9,9,9,10,11,12,14) \\ B & = & (1,3,4,4,4,5,6,6,6,6,7,7,9,9,9,10,11,12,10'008) \end{array}$$

We find that

$$A = (1,3,4,4,4,5,6,6,6,6,7,7,9,9,9,10,11,12,14)$$

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- We find that
 - $\operatorname{mean}(A) = \frac{1}{19} \sum_{i=0}^{18} a_i = \frac{133}{19} = 7$

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- We find that
 - $\operatorname{mean}(A) = \frac{1}{19} \sum_{i=0}^{18} a_i = \frac{133}{19} = 7$ and
 - mean(B) = $\frac{1}{19} \sum_{i=0}^{18} b_i = \frac{10'127}{19} = 553$

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 - $\bullet \mod(A) = a_9 = 6$

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 - $med(A) = a_9 = 6$ and
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- The median is not affected by the outliers.

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 - $med(A) = a_9 = 6$ and
 - $med(B) = b_9 = 6$.
- The median is not affected by the outliers.
- mean(B) = 553 is a value completely different from anything that actually occurs in B... it gives us a completely wrong impression.

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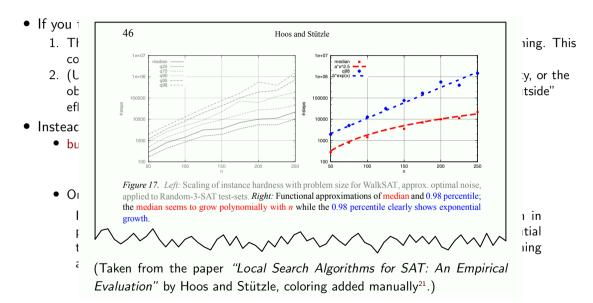
Imagine that: Your algorithm can actually solve the TSP or MaxSat problem in polynomial time on 90% of all instances... but on 10%, it needs exponential time.

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 - 1. The operating systems scheduling or other strange effects could mess with our timing. This could cause worse results. But usually this is already it.
 - 2. (Unless your objective function is noisy, e.g., if you measure some physical quantity, or the objective function involves randomized simulations, there are hardly any other "outside" effects that could mess up our results!)
- Instead, most likely there could be
 - bugs in our code!
 - Bugs in our code are the most important number one reason for outliers!
 - Yes, also in your code! (Btw: Please use unit tests.)
 - Or: bad (but rare) worst-case behaviors of our algorithm!

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 - Imagine that: Your algorithm can actually solve the TSP or MaxSat problem in polynomial time on 90% of all instances... but on 10%, it needs exponential time. If you just look at the median runtime, you may think you discovered something awesome. Actually, this is quite common...
- Thus, we may actually want that outliers influence our statistics. . .

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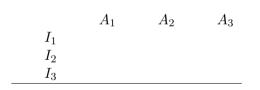
$$geom(A) = \exp\left(\frac{1}{n}\sum_{i=0}^{n-1}\log a_i\right) \tag{4}$$

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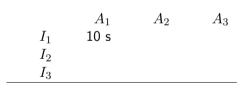
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I_1	10 s	20 s	40 s
I_2	20 s	40 s	10 s
I_3	40 s	10 s	20 s

- Often, our data is somehow normalized.
- We measure the required runtimes as follows:
- The arithmetic mean values are the same.

	A_1	A_2	A_3
I_1	10 s	20 s	40 s
I_2	20 s	40 s	10 s
I_3	40 s	10 s	20 s
mean:	23.33 s	23.33 s	23.33 s

- Often, our data is somehow normalized.
- The arithmetic mean and the median values are the same.

	A_1	A_2	A_3
I_1	10 s	20 s	40 s
I_2	20 s	40 s	10 s
I_3	40 s	10 s	20 s
mean:	23.33 s	23.33 s	23.33 s
med:	20.00 s	20.00 s	20.00 s

- Often, our data is somehow normalized.
- The arithmetic mean, the median, and the geometric mean values are the same.

	A_1	A_2	A_3
I_1	10 s	20 s	40 s
I_2	20 s	40 s	10 s
I_3	40 s	10 s	20 s
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med:	20.00 s	20.00 s	20.00 s
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- We can conclude that the three algorithms offer the same performance in average over these benchmark instances.

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I_3	40 s	10 s	20 s
mean:	23.33 s	23.33 s	23.33 s
med:	20.00 s	20.00 s	20.00 s
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- We can conclude that the three algorithms offer the same performance in average over these benchmark instances.
- But often the measured numbers "look messier" and are harder to compare at first glance.

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I_1	10 s	20 s	40 s
I_2	20 s	40 s	10 s
I_3	40 s	10 s	20 s
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- So often we want to normalize them by picking one algorithm as "standard" and dividing them by its measurements.

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I_3	40 s	10 s	20 s
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med:	20.00 s	20.00 s	20.00 s
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I_1	10 s	20 s	40 s
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I_1	10 s	20 s	40 s
I_2	20 s	40 s	10 s
I_3	40 s	10 s	20 s
mean:	23.33 s	23.33 s	23.33 s
med:	20.00 s	20.00 s	20.00 s
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- OK, so we get this table with normalized values, which allow us to make sense of the data at first glance.

	A_1	A_2	A_3		A_1	A_2	A_3
I_1	10 s	20 s	40 s	I_1	1.00	2.00	4.00
I_2	20 s	40 s	10 s	I_2	1.00	2.00	0.50
I_3	40 s	10 s	20 s	I_3	1.00	0.25	0.50
mean:	23.33 s	23.33 s	23.33 s				
med :	20.00 s	20.00 s	20.00 s				

20.00 s 20.00 s

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- If we now compute the arithmetic mean

	A_1	A_2	A_3			A_1	A_2	A_3
I_1	10 s	20 s	40 s		I_1	1.00	2.00	4.00
I_2	20 s	40 s	10 s		I_2	1.00	2.00	0.50
I_3	40 s	10 s	20 s		I_3	1.00	0.25	0.50
mean:	23.33 s	23.33 s	23.33 s	_	mean:	1.00	1.42	1.67
med:	20.00 s	20.00 s	20.00 s					
geom:	20.00 s	20.00 s	20.00 s					
geom:	20.00 s	20.00 s	20.00 s					

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- OK, so we get this table with normalized values, which allow us to make sense of the data at first glance.
- If we now compute the arithmetic mean, then A_1 is best

	A_1	A_2	A_3			A_1	A_2	A_3
I_1	10 s	20 s	40 s		I_1	1.00	2.00	4.00
I_2	20 s	40 s	10 s		I_2	1.00	2.00	0.50
I_3	40 s	10 s	20 s		I_3	1.00	0.25	0.50
mean:	23.33 s	23.33 s	23.33 s	me	ean:	1.00	1.42	1.67
med:	20.00 s	20.00 s	20.00 s					
geom:	20.00 s	20.00 s	20.00 s					

- Often, our data is somehow normalized.
- OK, so we get this table with normalized values, which allow us to make sense of the data at first glance.
- If we now compute the arithmetic mean, then A_1 is best and A_3 looks worst.

	A_1	A_2	A_3		A_1	A_2	A_{i}
I_1	10 s	20 s	40 s	I_1	1.00	2.00	4.00
I_2	20 s	40 s	10 s	I_2	1.00	2.00	0.50
I_3	40 s	10 s	20 s	I_3	1.00	0.25	0.50
mean:	23.33 s	23.33 s	23.33 s	 mean:	1.00	1.42	1.67
med:	20.00 s	20.00 s	20.00 s				
geom:	20.00 s	20.00 s	20.00 s				

- Often, our data is somehow normalized.
- OK, so we get this table with normalized values, which allow us to make sense of the data at first glance.
- If we now compute the arithmetic mean, then A_1 is best and A_3 looks worst.
- According to the median

	A_1	A_2	A_3			A_1	A_2	A_3
I_1	10 s	20 s	40 s		I_1	1.00	2.00	4.00
I_2	20 s	40 s	10 s		I_2	1.00	2.00	0.50
I_3	40 s	10 s	20 s		I_3	1.00	0.25	0.50
mean:	23.33 s	23.33 s	23.33 s	n	nean:	1.00	1.42	1.67
med:	20.00 s	20.00 s	20.00 s		med:	1.00	2.00	0.50
geom:	20.00 s	20.00 s	20.00 s					

- Often, our data is somehow normalized.
- If we now compute the arithmetic mean, then A_1 is best and A_3 looks worst.
- According to the median, A_3 is best

	A_1	A_2	A_3		A_1	A_2	A_3
I_1	10 s	20 s	40 s	I_1	1.00	2.00	4.00
I_2	20 s	40 s	10 s	I_2	1.00	2.00	0.50
I_3	40 s	10 s	20 s	I_3	1.00	0.25	0.50
mean:	23.33 s	23.33 s	23.33 s	mean:	1.00	1.42	1.67
med:	20.00 s	20.00 s	20.00 s	med:	1.00	2.00	0.50
geom:	20.00 s	20.00 s	20.00 s				

- Often, our data is somehow normalized.
- If we now compute the arithmetic mean, then A_1 is best and A_3 looks worst.
- According to the median, A_3 is best and A_2 is worst!

	A_1	A_2	A_3		A_1	A_2	A_3
I_1	10 s	20 s	40 s	I_1	1.00	2.00	4.00
I_2	20 s	40 s	10 s	I_2	1.00	2.00	0.50
I_3	40 s	10 s	20 s	I_3	1.00	0.25	0.50
mean:	23.33 s	23.33 s	23.33 s	mean:	1.00	1.42	1.67
med:	20.00 s	20.00 s	20.00 s	med:	1.00	2.00	0.50
geom:	20.00 s	20.00 s	20.00 s				

- Often, our data is somehow normalized.
- If we now compute the arithmetic mean, then A_1 is best and A_3 looks worst.
- According to the median, A_3 is best and A_2 is worst!
- Only the geometric mean still indicates that the algorithms perform the same. . .

	A_1	A_2	A_3		A_1	A_2	A_3
I_1	10 s	20 s	40 s	I_1	1.00	2.00	4.00
I_2	20 s	40 s	10 s	I_2	1.00	2.00	0.50
I_3	40 s	10 s	20 s	I_3	1.00	0.25	0.50
mean:	23.33 s	23.33 s	23.33 s	mean:	1.00	1.42	1.67
med:	20.00 s	20.00 s	20.00 s	med:	1.00	2.00	0.50
geom:	20.00 s	20.00 s	20.00 s	geom:	1.00	1.00	1.00

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- Hm.

		A_1	A_2	A_3		A_1	A_2	A_3
	I_1	10 s	20 s	40 s	I_1	1.00	2.00	4.00
	I_2	20 s	40 s	10 s	I_2	1.00	2.00	0.50
	I_3	40 s	10 s	20 s	I_3	1.00	0.25	0.50
	mean:	23.33 s	23.33 s	23.33 s	mean:	1.00	1.42	1.67
	med:	20.00 s	20.00 s	20.00 s	med :	1.00	2.00	0.50
į	geom:	20.00 s	20.00 s	20.00 s	geom:	1.00	1.00	1.00

- Often, our data is somehow normalized.
- ullet Hm. OK, then let's normalize using the results of A_2 instead.

	A_1	A_2	A_3
I_1	10 s	20 s	40 s
I_2	20 s	40 s	10 s
I_3	40 s	10 s	20 s
mean:	23.33 s	23.33 s	23.33 s
med:	20.00 s	20.00 s	20.00 s
geom:	20.00 s	20.00 s	20.00 s

med:

geom:

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20.00 s 20.00 s 20.00 s 20.00 s 20.00 s 20.00 s

• OK, so we get this table with normalized values.

	A_1	A_2	A_3		A_1	A_2	A_3
I_1	10 s	20 s	40 s	I_1	0.50	1.00	2.00
I_2	20 s	40 s	10 s	I_2	0.50	1.00	0.25
I_3	40 s	10 s	20 s	I_3	4.00	1.00	2.00
mean:	23.33 s	23.33 s	23.33 s				

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		A_1	A_2	A_3		A_1	A_2	A_3	
	I_1	10 s	20 s	40 s	I_1	0.50	1.00	2.00	
	I_2	20 s	40 s	10 s	I_2	0.50	1.00	0.25	
	I_3	40 s	10 s	20 s	I_3	4.00	1.00	2.00	
n	nean:	23.33 s	23.33 s	23.33 s	mean:	1.67	1.00	1.42	
	med:	20.00 s	20.00 s	20.00 s					
o	eom:	20 00 s	20 00 s	20.00 s					

- Often, our data is somehow normalized.
- OK, so we get this table with normalized values.
- If we now compute the arithmetic mean, then A_2 is best

		A_1	A_2	A_3			A_1	A_2	A_3	
	I_1	10 s	20 s	40 s		I_1	0.50	1.00	2.00	
	I_2	20 s	40 s	10 s		I_2	0.50	1.00	0.25	
	I_3	40 s	10 s	20 s		I_3	4.00	1.00	2.00	
_	mean:	23.33 s	23.33 s	23.33 s	_	mean:	1.67	1.00	1.42	
	med:	20.00 s	20.00 s	20.00 s						
	geom:	20 00 s	20 00 s	20.00 s						

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- If we now compute the arithmetic mean, then A_2 is best and A_1 looks worst.

	A_1	A_2	A_3			A_1	A_2	A_3	
I_1	10 s	20 s	40 s		I_1	0.50	1.00	2.00	
I_2	20 s	40 s	10 s		I_2	0.50	1.00	0.25	
I_3	40 s	10 s	20 s		I_3	4.00	1.00	2.00	
mean:	23.33 s	23.33 s	23.33 s	mea	an:	1.67	1.00	1.42	
med:	20.00 s	20.00 s	20.00 s						
geom:	20 00 s	20 00 s	20 00 s						

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- If we now compute the arithmetic mean, then A_2 is best and A_1 looks worst.
- According to the median

	A_1	A_2	A_3		A_1	A_2	A_3
I_1	10 s	20 s	40 s	I_1	0.50	1.00	2.00
I_2	20 s	40 s	10 s	I_2	0.50	1.00	0.25
I_3	40 s	10 s	20 s	I_3	4.00	1.00	2.00
mean:	23.33 s	23.33 s	23.33 s	mean:	1.67	1.00	1.42
med:	20.00 s	20.00 s	20.00 s	med:	0.50	1.00	2.00
geom:	20.00 s	20.00 s	20.00 s				

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- According to the median, A_1 is best

	A_1	A_2	A_3		A_1	A_2	A_3
I_1	10 s	20 s	40 s	I_1	0.50	1.00	2.00
I_2	20 s	40 s	10 s	I_2	0.50	1.00	0.25
I_3	40 s	10 s	20 s	I_3	4.00	1.00	2.00
mean:	23.33 s	23.33 s	23.33 s	mean:	1.67	1.00	1.42
med:	20.00 s	20.00 s	20.00 s	med:	0.50	1.00	2.00
geom:	20.00 s	20.00 s	20.00 s				

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	A_1	A_2	A_3		A_1	A_2	A_3
I_1	10 s	20 s	40 s	I_1	0.50	1.00	2.00
I_2	20 s	40 s	10 s	I_2	0.50	1.00	0.25
I_3	40 s	10 s	20 s	I_3	4.00	1.00	2.00
mean:	23.33 s	23.33 s	23.33 s	mean:	1.67	1.00	1.42
med:	20.00 s	20.00 s	20.00 s	med:	0.50	1.00	2.00
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I_3	40 s	10 s	20 s	I_3	4.00	1.00	2.00
mean:	23.33 s	23.33 s	23.33 s	mean:	1.67	1.00	1.42
med:	20.00 s	20.00 s	20.00 s	med:	0.50	1.00	2.00
geom:	20.00 s	20.00 s	20.00 s	geom:	1.00	1.00	1.00

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- The geometric mean is the only meaningful average if we have normalized data!²²
- And we very often have normalized data.
- For example, at least half of the papers on the Job Shop Scheduling Problem normalize
 the result qualities they obtain on benchmark instances with the Best Known Solutions
 (BKS).

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- The geometric mean is the only meaningful average if we have normalized data!²²
- And we very often have normalized data.
- For example, at least half of the papers on the Job Shop Scheduling Problem normalize the result qualities they obtain on benchmark instances with the *Best Known Solutions* (BKS) and then compute the arithmetic mean.

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 - If the median is much worse than the mean, then the mean is too optimistic, i.e., most of the time we should expect worse results.
- If there are outliers, the value of the arithmetic mean itself may be very different from any actually observed value, while the median is (almost always) similar to some actual measurements.

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- Then, the arithmetic mean and median can be very misleading and the geometric mean must be computed.
- I think: On raw data, compute all three measures of average, and pay special attention to the one looking the worst. On normalized data, compute the geometric mean, but also consider the arithmetic mean and median *if and only if they make* **your** *algorithm look worse*.

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- An average alone is not very meaningful if we known nothing about the range of the data.
- We can therefore compute a measure of dispersion, i.e., a value that tells us whether the
 observations are stretched and spread far or squeezed tight around the center.

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The variance is the expectation of the squared deviation of a random variable from its mean. The variance var(A) of a data sample $A = (a_0, a_1, \dots, a_{n-1})$ with n observations can be

estimated as:

$$var(A) = \frac{1}{n-1} \sum_{i=1}^{n-1} (a_i - mean(A))^2$$

Definition (Standard Deviation)

The statistical estimate $\operatorname{sd}(A)$ of the standard deviation of a data sample $A=(a_0,a_1,\ldots,a_{n-1})$ with n observations is the square root of the estimated variance $\operatorname{var}(A)$.

$$\operatorname{sd}(A) = \sqrt{\operatorname{var}(A)}$$

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- Large standard deviations indicate unreliable algorithms, but may also offer a potential that could be exploited: Given enough time, we can restart algorithms several times and expect to get different (and thus sometimes better) solutions.

Definition (Quantile)

The q-quantiles are the cut points that divide a sorted data sample $A=(a_0,a_1,\ldots,a_{n-1})$ where $a_{i-1}\leq a_i \ \forall i\in 1\ldots (n-1)$ into q-equally sized parts.

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$$\begin{array}{rcl} h&=&(n-1)\frac{k}{q}\\ &\text{quantile}_q^k(A)&=&\left\{\begin{array}{ll} a_h & \text{if h is integer}\\ a_{|h|}+(h-\lfloor h\rfloor)*\left(a_{|h|+1}-a_{|h|}\right) & \text{otherwise} \end{array}\right.$$

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- 4-quantiles are called *quartiles*.
- We often consider *percentiles* or write things like "98% quantile" or "0.98 percentile" or "98% percentile" meaning quantile 98/100.

$$\begin{array}{rcl} A & = & (1,3,4,4,4,5,6,6,6,6,7,7,9,9,9,10,11,12,14) \\ \operatorname{mean}(A) & = & 7 \\ B & = & (1,3,4,4,4,5,6,6,6,6,7,7,9,9,9,10,11,12,10'008) \\ \operatorname{mean}(B) & = & 533 \end{array}$$

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• Two data samples A and B with $n_a = n_b = 19$ values.

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 Being based on the arithmetic mean, the variance and standard deviation are heavily influenced by outliers – with all pros and cons coming with that...

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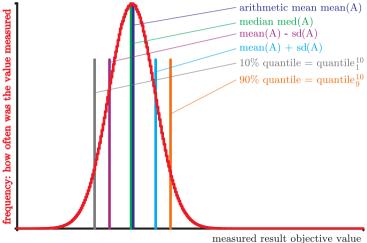
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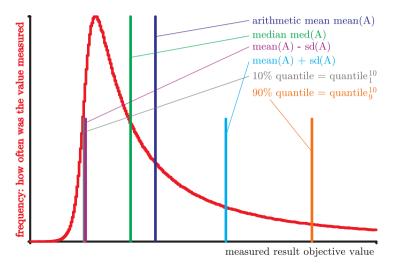
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 Being generalizations of the median, the quantiles are little influenced by outliers – with all pros and cons coming with that...

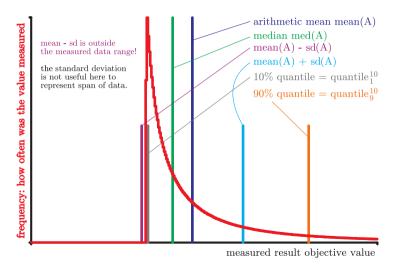
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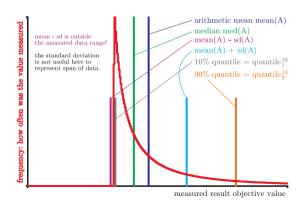
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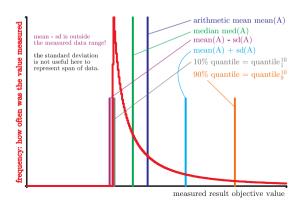
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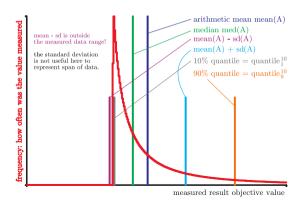
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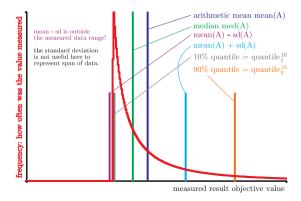
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 - ullet A statement such as "For this TSP instance, our algorithm can find tours for with a length of 100 ± 120 km." makes little sense. . .

Statistical Comparisons



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- The statement "A is better than B" makes only sense if we can give an upper bound α for the error probability p!

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- Disclaimer: I am not a mathematician. What follows are simplified explanations of concepts.

Example for Underlying Idea

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Example for Underlying Idea

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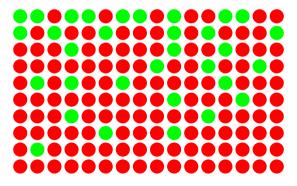




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- (What we will do right now is called *binomial test*.)

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$$= \frac{\frac{1'538'590'628'148'134'280'316'221'828'039'113}{365'375'409'332'725'729'550'921'208'179'070'754'913'983'135'744}$$

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- If the coin was an ideal coin, the chance that I win at least 128 out of 160 times is about $4\cdot 10^{-15}$.
- If you claim that I cheat, your chance to be wrong is about $4 \cdot 10^{-15}$.
- Thus, if we cannot accept a chance p to be wrong higher than a significance level $\alpha=1\%$, we can still say:

The observation is significant, I did likely cheat.

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- Use a program to test the combinations

```
/** an example class enumerating all combinations */
     public class EnumerateAtLeastAsExtremeScenarios {
       public static void main(String[] args) {
         int meanLowerOrEqualTo4 = 0; // how often did we find a mean <= 4
         int totalCombinations = 0; // total number of tested combinations

    A

         for (int i = 10: i > 0: i--) {
                                       // as 0 = numbers from 1 to 10
         for (int j = (i - 1); j > 0; j--) { // we can conveniently iterate
            for (int k = (j - 1); k > 0; k - - - - 1) { // over all 4-element combos
              for (int 1 = (k - 1); 1 > 0; 1--) { // with 4 such nested loops
                if (((i + j + k + 1) / 4.0) \le 4) { // check for the extreme cases

    If

                  meanLowerOrEqualTo4++; } // count the extreme case
                totalCombinations++; // add up combos, to verify

    Us

        } } } }
         System.out.println(meanLowerOrEqualTo4 + "" + totalCombinations);
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• Extreme cases into the other direction are the same, because if $mean(B) \le 4$ then $mean(A) \ge 6.5$ for any division $A \cup B = O$ and vice versa:

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 So – of course – we could have also done the test the other way around with the same result!

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- The method here is only feasible for small sample sets, real tests are more sophisticated

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- If I have two different algorithms A and B, logic dictates that their performance is also different.

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- To be practically significant, the measured difference of results should be statistically significant already with few runs, say, 11 or 21, not just with ≥ 100 runs.

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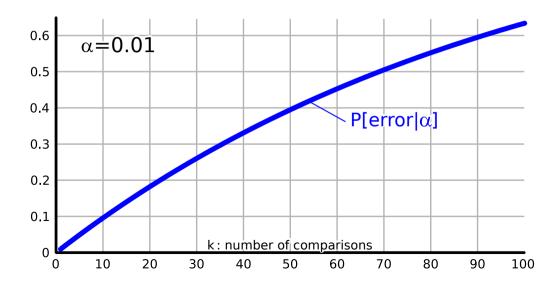
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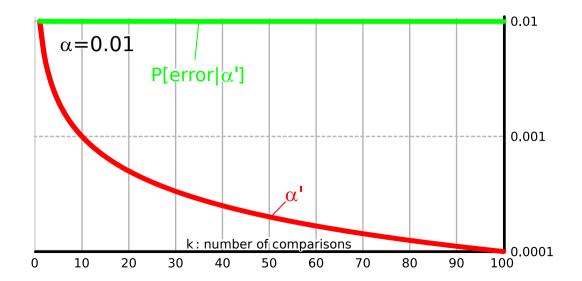
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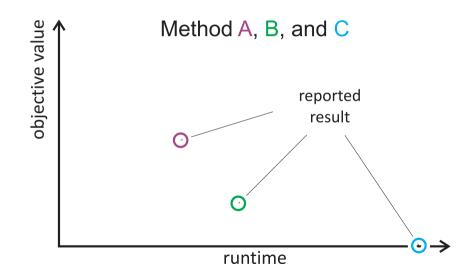


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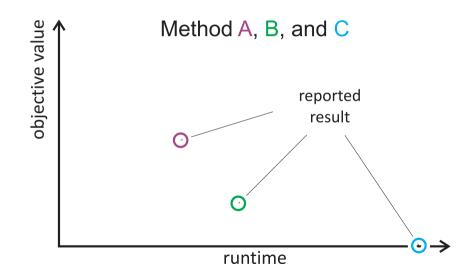
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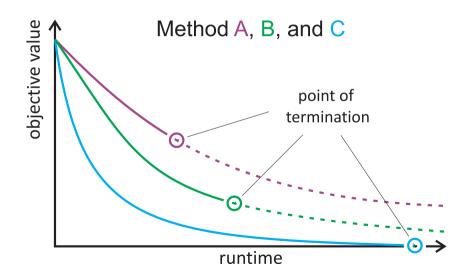


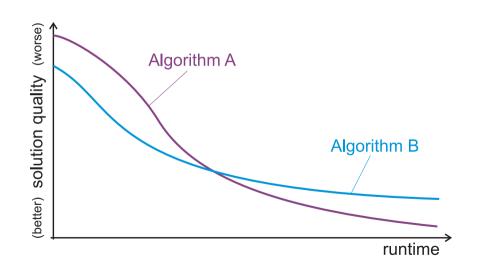
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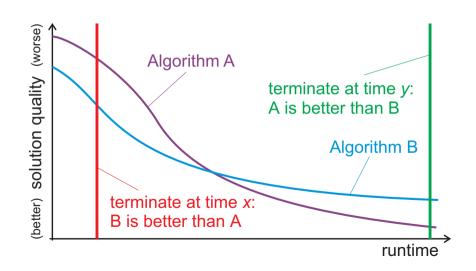
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Other Stuff



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- Know the standard benchmark instances for your field!

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Reproducibility prevents cheating and misunderstandings!

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 - 1. arithmetic and geometric mean and median of key performance indicators
 - 2. quartiles or top/bottom 1% quantile to get a feeling for the usual range of values
 - 3. don't trust just arithmetic mean or standard deviation alone
 - 4. geometric mean if the data is normalized
- Use non-parametric statistical tests with corrections for multiple comparisons.
- Do not only collect one data sample per run, try to plot progress curves.
- Use well-known benchmarks, provide your source code!

Thank you

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