合肥大學
HEFEI UNIVERSITY

Comparing Optimization Algorithms

Thomas Weise (汤卫思)
tweise@hfuu.edu.cn

Institute of Applied Optimization (IAO) | 应用优化研究所
School of Artificial Intelligence and Big Data | 人工智能与大数据学院
Hefei University | 合肥大学
Hefei, Anhui, China | 中国安徽省合肥市

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Outline

1. Introduction
2. Views on Performance and Time
3. Statistical Measures
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Introduction

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- What does this mean?
- And how do we find this algorithm?
- Hopefully this lesson will help answering these questions.
- As a complement to this lesson, I suggest the report *"Benchmarking in Optimization: Best Practice and Open Issues"*[6] on arXiv.

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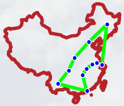

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- Let's look at the classical Traveling Salesperson Problem (TSP)[2,27,39,61].
  - Clearly, there is (at least) one shortest tour.
  - Theory proofs that the time needed to find this tour may grow exponentially with the number s of cities we want to visit in the worst case.[1,14,15,35,38]

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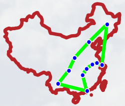

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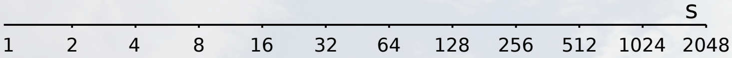
- What does exponential growth mean?
- Let's say we have a number of cities s.



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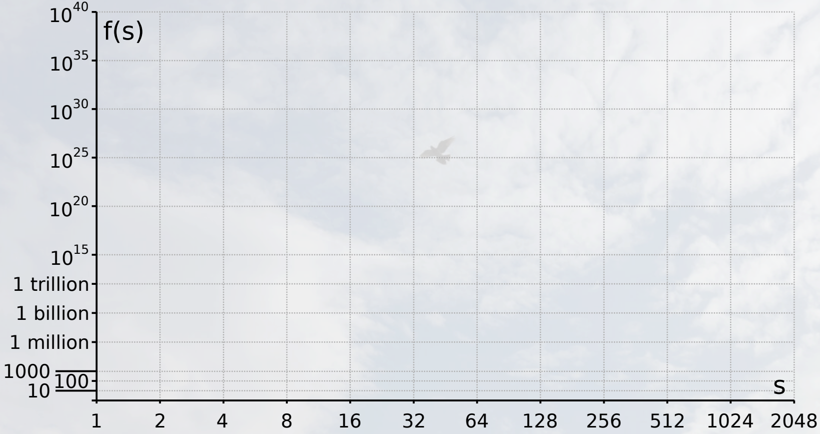

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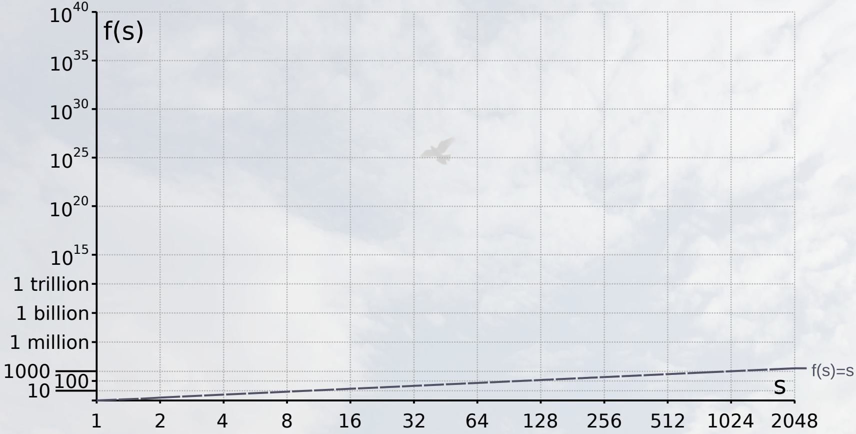
- A linear function means that the runtime $f(s)$ grows slowly with s.



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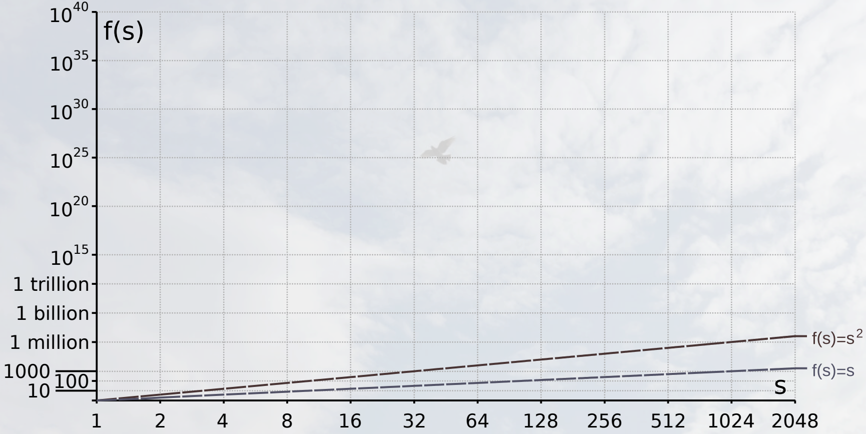
- A quadratic function (a straight line in log-log plots) is also OK.



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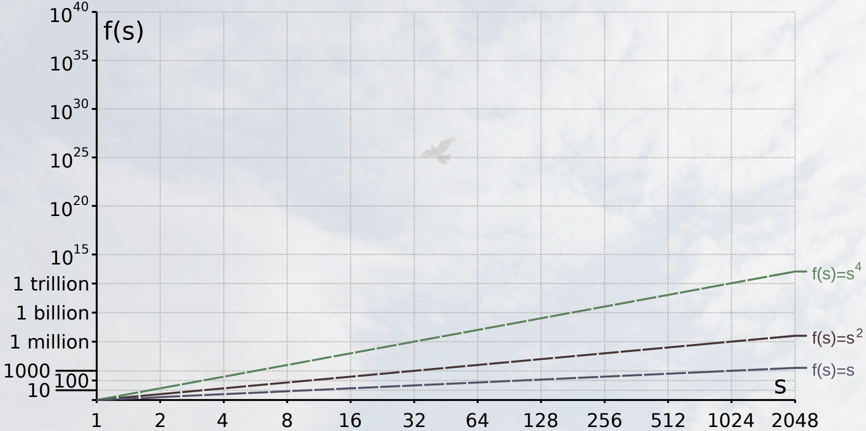
- A quartic function $f(s) = s^4$ gets quite large for growing s.



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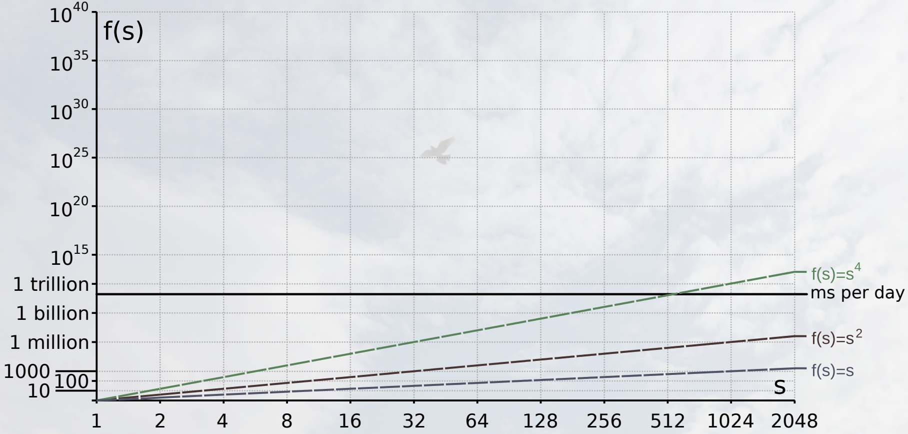

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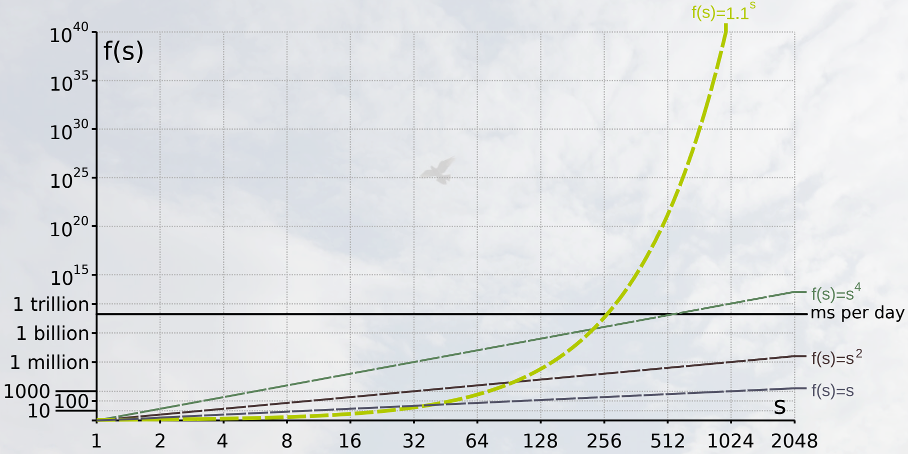
- But this is nothing compared to the exponential function $f(s) = 1.1^s \dots$



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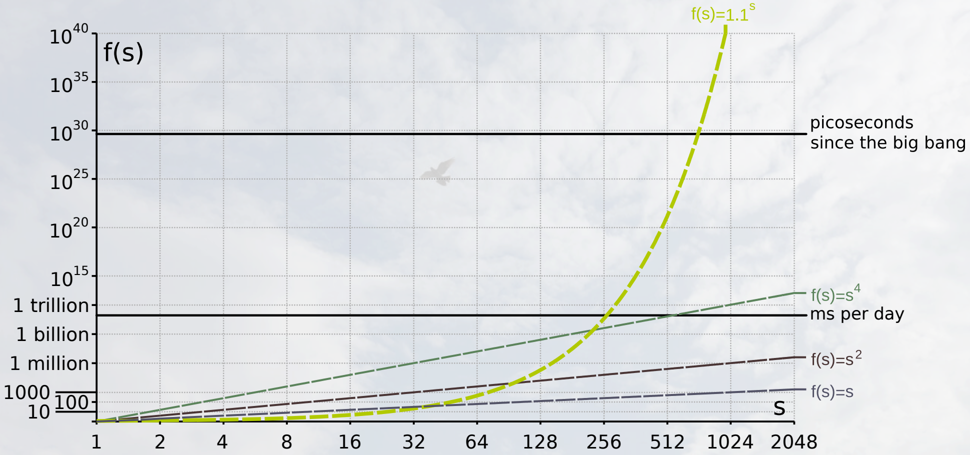

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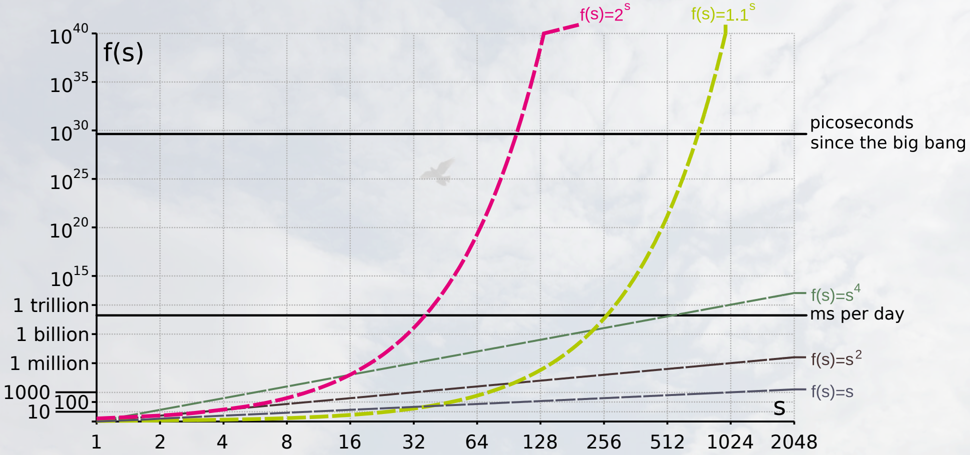

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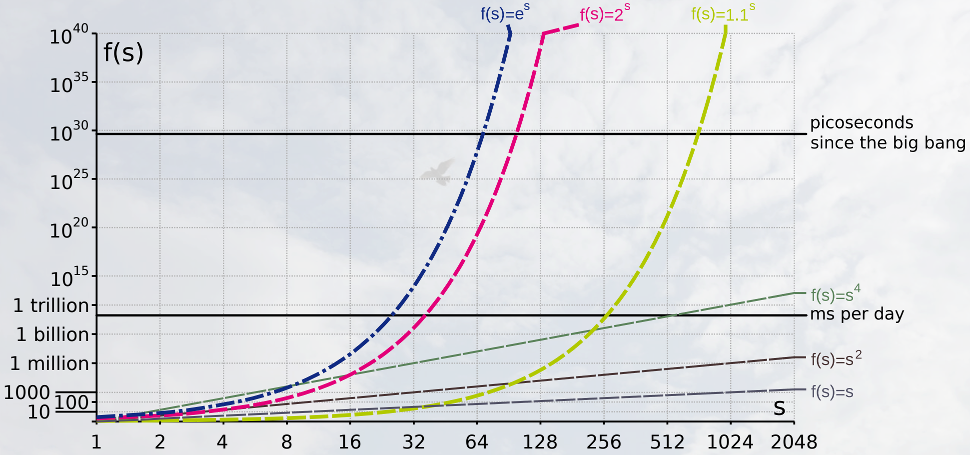

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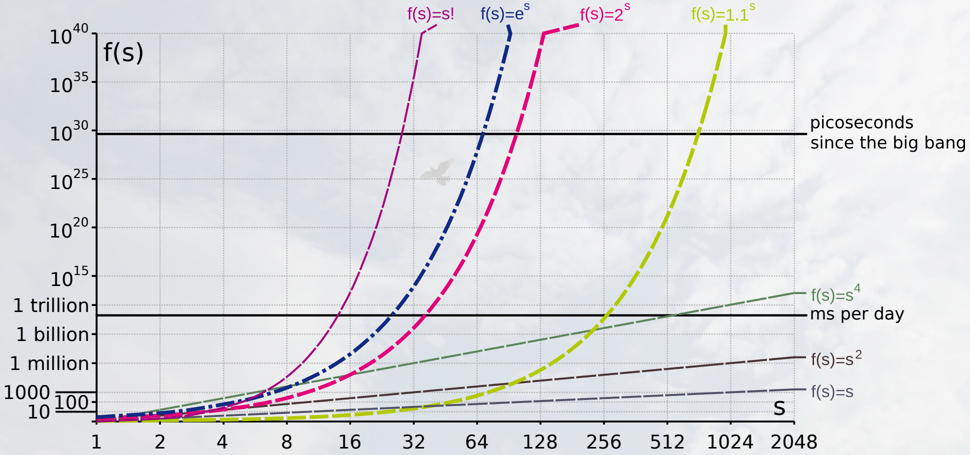
- If we would enumerate all possible tours of s cities in a TSP, that would be $s!$.



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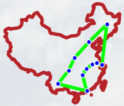

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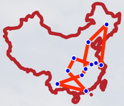

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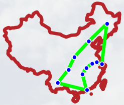

very little / fast — consumed runtime — very much / too (?) long

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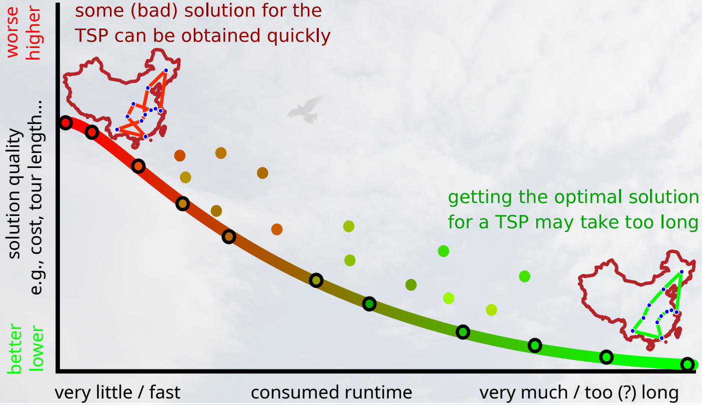

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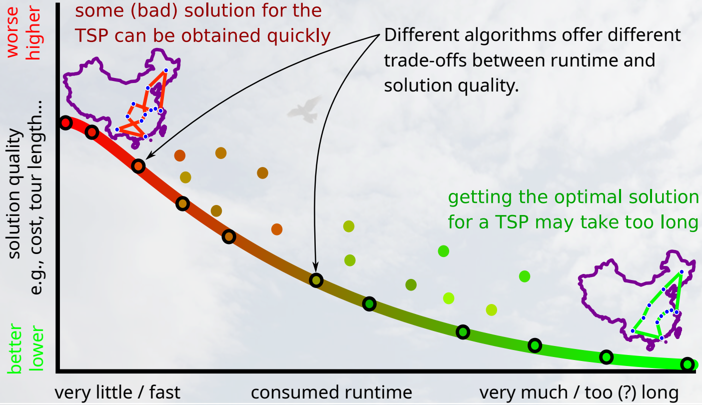

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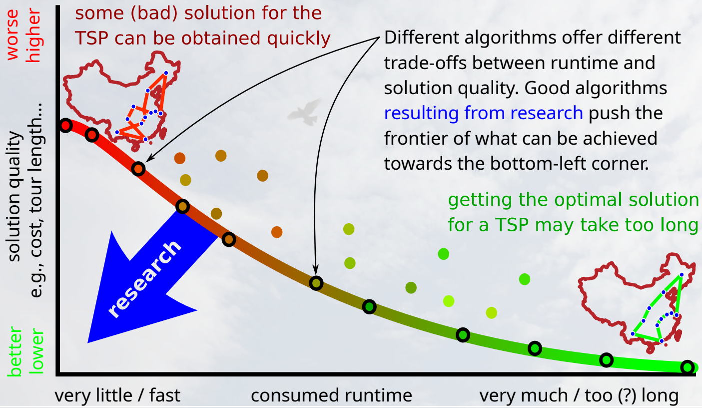

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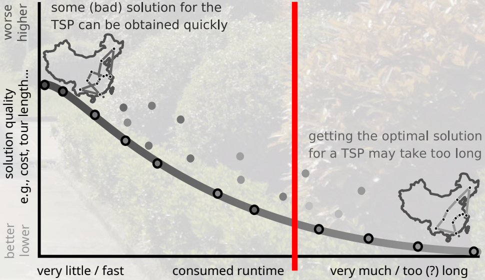

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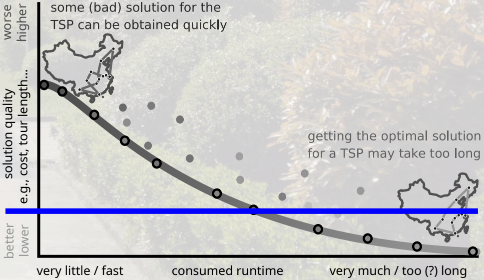

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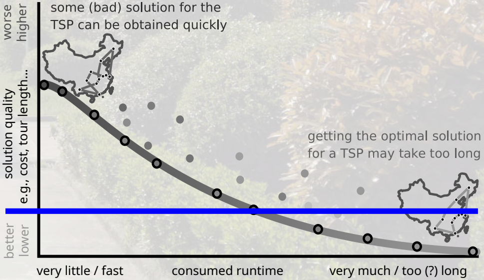

What is Runtime?

- What actually is runtime?

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

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    - When applying Ant Colony Optimization (ACO) instead, each FE takes $\mathcal{O}(s^2)$[61].
- Relevant for comparing algorithms, but not so much for the practical application or comparing implementations.

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    - Do you evaluate offspring solutions that are identical to their parents?

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

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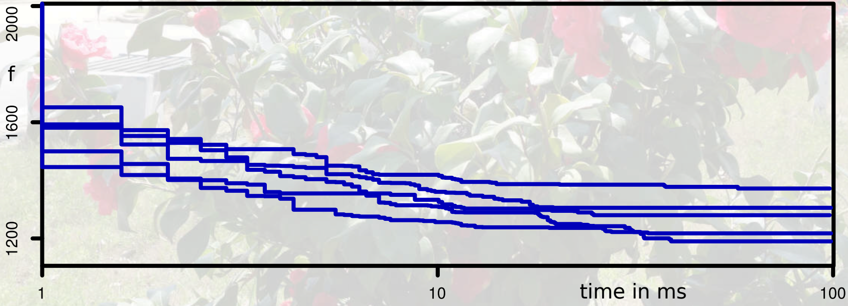
Views on Performance

- Which one is the “better” view on performance?



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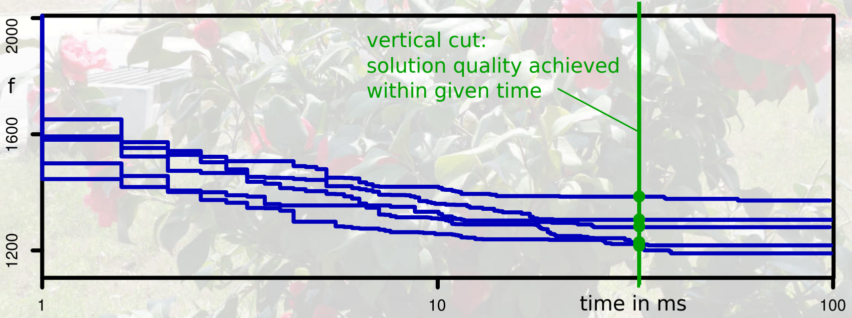

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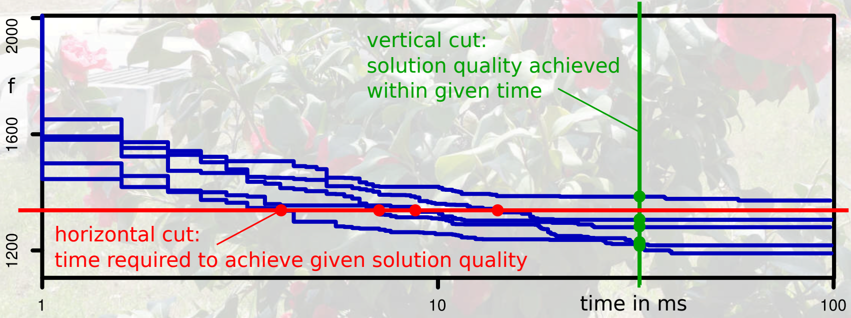

Views on Performance

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

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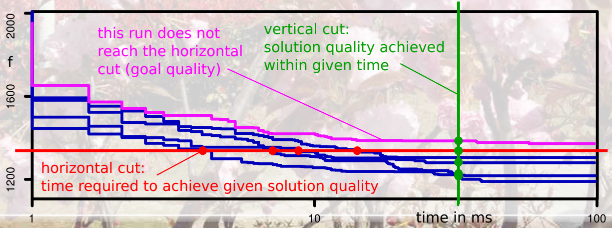

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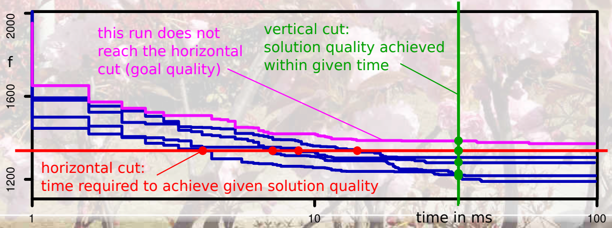
- Sometimes problematic: What if one run does not reach the goal quality?
- Then, alternative measures need to be computed, such as the ERT[3,47] or PAR2 and PAR10[8,36].



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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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- Otherwise, the best approach may be: Evaluate algorithm according to both methods.[61–63]
- Maybe cast a net of several horizontal and vertical cuts, to get a better picture. . .

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Statistical Measures

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  - Statistical evaluation over sets of runs necessary.

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- Example: Dice Throw
- How likely is it to roll a 1, 2, 3, 4, 5, or 6?

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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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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

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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
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

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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

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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

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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
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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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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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
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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

Important Distinction

- Crucial Difference: distribution and sample
- A sample is what we *measure*.
- A distribution is the asymptotic result of the ideal process.
- Statistical parameters of the distribution can be estimated from a sample.
- Example: Dice Throw
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- The parameters of a random process cannot be measured directly, but only be estimated from multiple measures.

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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 the arithmetic mean, the median, and the geometric mean.

Arithmetic Mean

Definition: Arithmetic Mean

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

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$$\mathrm{median}(A) = \begin{cases} a_{\frac{n-1}{2}} & \text{if } n \text{ is odd} \\ \frac{1}{2}\left(a_{\frac{n}{2}-1} + a_{\frac{n}{2}}\right) & \text{otherwise} \end{cases} \quad \text{if } a_{i-1} \leq a_i \; \forall i \in 1 \dots (n-1) \qquad (2)$$

Outliers

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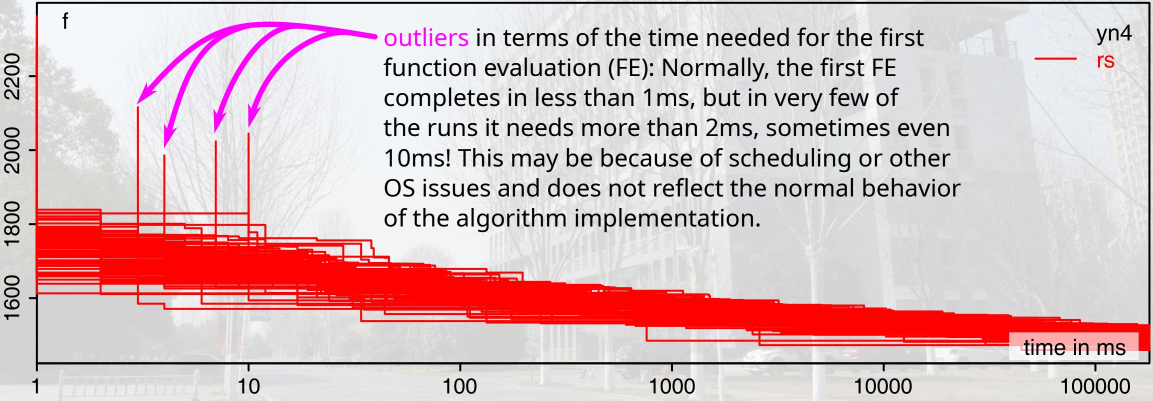

Outliers

- 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. . .

Example for Data Samples w/o Outlier

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

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

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

Outliers can be important!

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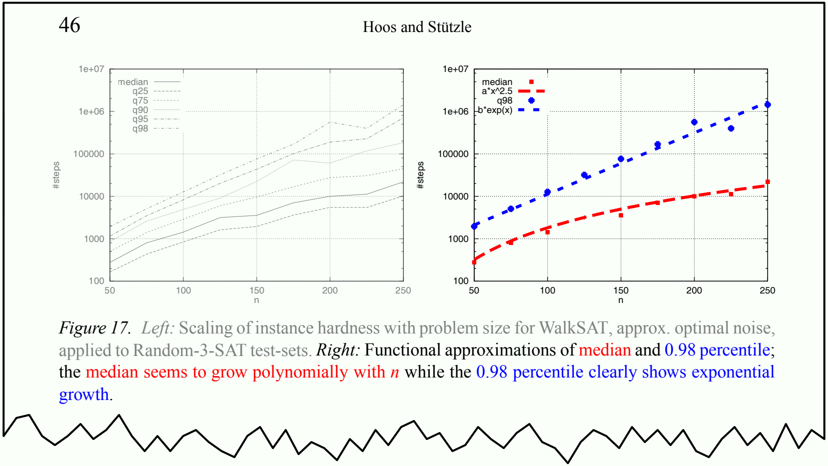
46 Hoos and Stützle

Figure 17. *Left:* Scaling of instance hardness with problem size for WalkSAT, approx. optimal noise, applied to Random-3-SAT test-sets. *Right:* Functional approximations of median and 0.98 percentile; the median seems to grow polynomially with *n* while the 0.98 percentile clearly shows exponential growth.

(Taken from the paper *“Local Search Algorithms for SAT: An Empirical Evaluation”* by Hoos and Stützle, coloring added manually[32].)

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- Thus, we may actually want that outliers influence our statistics...

Geometric Mean

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$$\tag{4}$$

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$$\mathrm{geom}(A) = \sqrt[n]{\prod_{i=0}^{n-1} a_i} \quad (3)$$

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

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	A_1	A_2	A_3
I_1			
I_2			
I_3			

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	A_1	A_2	A_3
I_1	10 s		
I_2			
I_3			

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I_2	20 s		
I_3	40 s		

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I_2	20 s		
I_3	40 s		

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- 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

Normalized Data

- 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
median:	20.00 s	20.00 s	20.00 s

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	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
median:	20.00 s	20.00 s	20.00 s
geom:	20.00 s	20.00 s	20.00 s

Normalized Data

- Often, our data is somehow normalized.
- The arithmetic mean, the median, and the geometric mean values are the same.
- We can conclude that the three algorithms offer the same performance in average over these benchmark instances.

	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
median:	20.00 s	20.00 s	20.00 s
geom:	20.00 s	20.00 s	20.00 s

Normalized Data

- Often, our data is somehow normalized.
- 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.

	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
median:	20.00 s	20.00 s	20.00 s
geom:	20.00 s	20.00 s	20.00 s

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- But often the measured numbers "look messier" and are harder to compare at first glance.
- So often we want to normalize them by picking one algorithm as "standard" and dividing them by its measurements.

	A_1	A_2	A_3
I_1	10 s	20 s	40 s
I_2	20 s	40 s	10 s
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- Let's say A_1 was a well-known heuristic, maybe we even took its results from a paper, and we want to use it as baseline for comparison and normalize our data by it.

	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
median:	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.

	A_1	A_2	A_3
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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
median:	20.00 s	20.00 s	20.00 s
geom:	20.00 s	20.00 s	20.00 s

	A_1	A_2	A_3
I_1	1.00	2.00	4.00
I_2	1.00	2.00	0.50
I_3	1.00	0.25	0.50

Normalized Data

- 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

	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
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	A_1	A_2	A_3
I_1	1.00	2.00	4.00
I_2	1.00	2.00	0.50
I_3	1.00	0.25	0.50
mean:	1.00	1.42	1.67

Normalized Data

- 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

	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
median:	20.00 s	20.00 s	20.00 s
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	A_1	A_2	A_3
I_1	1.00	2.00	4.00
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Normalized Data

- 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
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
median:	20.00 s	20.00 s	20.00 s
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	A_1	A_2	A_3
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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 and A_3 looks worst.
- According to the median

	A_1	A_2	A_3
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I_3	40 s	10 s	20 s
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Normalized Data

- 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
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
median:	20.00 s	20.00 s	20.00 s
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Normalized Data

- 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
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
median:	20.00 s	20.00 s	20.00 s
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	A_1	A_2	A_3
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Normalized Data

- 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
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
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	A_1	A_2	A_3
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mean:	1.00	1.42	1.67
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Normalized Data

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- Hm.

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Normalized Data

- Often, our data is somehow normalized.
- 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
median:	20.00 s	20.00 s	20.00 s
geom:	20.00 s	20.00 s	20.00 s

Normalized Data

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

	A_1	A_2	A_3
I_1	10 s	20 s	40 s
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mean:	23.33 s	23.33 s	23.33 s
median:	20.00 s	20.00 s	20.00 s
geom:	20.00 s	20.00 s	20.00 s

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I_1	0.50	1.00	2.00
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	A_1	A_2	A_3
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I_1	0.50	1.00	2.00
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mean:	1.67	1.00	1.42

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- If we now compute the arithmetic mean, then A_2 is best

	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
median:	20.00 s	20.00 s	20.00 s
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	A_1	A_2	A_3
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	A_1	A_2	A_3
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- And we very often have normalized data.
- For example, at least half of the papers on the Job Shop Scheduling Problem (JSSP) normalize the result qualities they obtain on benchmark instances with the Best Known Solutions (BKSes) and then compute the arithmetic mean.

Arithmetic Mean vs. Median vs. Geometric 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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  - if we normalize the runtime using another algorithm as standard.
- 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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- We do not know whether the data we have measured is very similar to the median or whether it may differ very much from the mean.
- An average alone is not very meaningful – if we known nothing about the range of the data.

Measures of the Spread

- The average gives us a good impression about the central value or location of a distribution.
- It does not tell us much about the range of the data.
- We do not know whether the data we have measured is very similar to the median or whether it may differ very much from the mean.
- 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.

Sample Variance

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The variance $\text{var}(A)$ of a data sample $A = (a_0, a_1, \ldots, a_{n-1})$ with n observations can be estimated as:

$$\text{var}(A) = \frac{1}{n-1}\sum_{i=0}^{n-1}(a_i - \text{mean}(A))^2 = \frac{1}{n-1}\left[\left(\sum_{i=0}^{n-1} a_i^2\right) - \frac{1}{n}\left(\sum_{i=0}^{n-1} a_i\right)^2\right]$$

Standard Deviation

Definition: Sample Standard Deviation

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

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

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Quantiles

Definition: Sample Quantile

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

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\begin{aligned}
h &= (n-1)\tfrac{k}{q} \\
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- The $\text{quantile}_1^2(A)$ is the median of A
- 4-quantiles are called *quartiles*.
- We often consider *percentiles* or write things like "98% quantile" or "0.98 percentile" or "98% percentile" meaning $\text{quantile}_{100}^{98}$.

Standard Deviation: Example

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

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

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\mathrm{mean}(B) &= 533 \\
\mathrm{var}(A) &= \frac{1}{19-1}\sum_{i=1}^{19}(a_i - \mathrm{mean}(A))^2 = \frac{198}{18} = 11 \\
\mathrm{var}(B) &= \frac{1}{19-1}\sum_{i=1}^{19}(b_i - \mathrm{mean}(B))^2 = \frac{94'763'306}{18} \approx 5'264'628
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\text{sd}(A) &= \sqrt{\text{var}\, A} = \sqrt{11} \approx 3.3 \\
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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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\text{quantile}^1_4(A) &= \text{quantile}^1_4(B) = 4.5 \\
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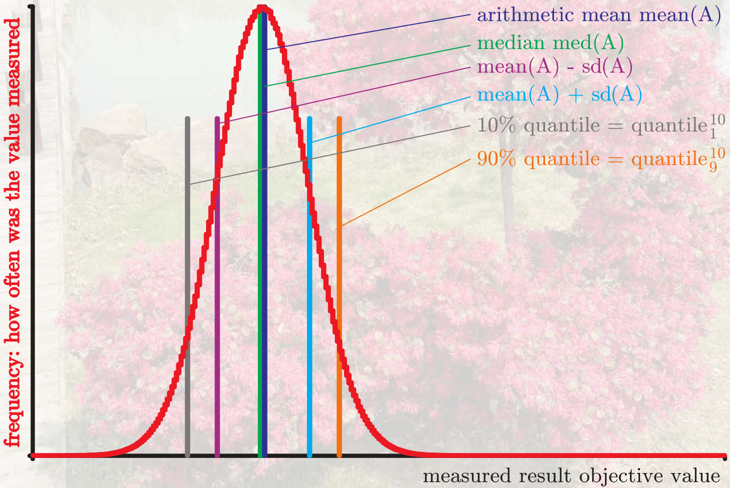
- Being generalizations of the median, the quantiles are little influenced by outliers – with all pros and cons coming with that. . .

Further Example

- The implicit assumption that $\text{mean} \pm \text{sd}$ is a meaningful range is not always true!



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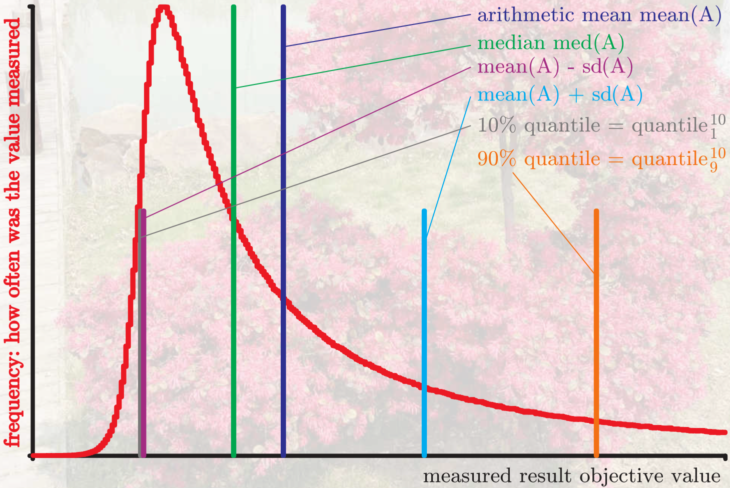

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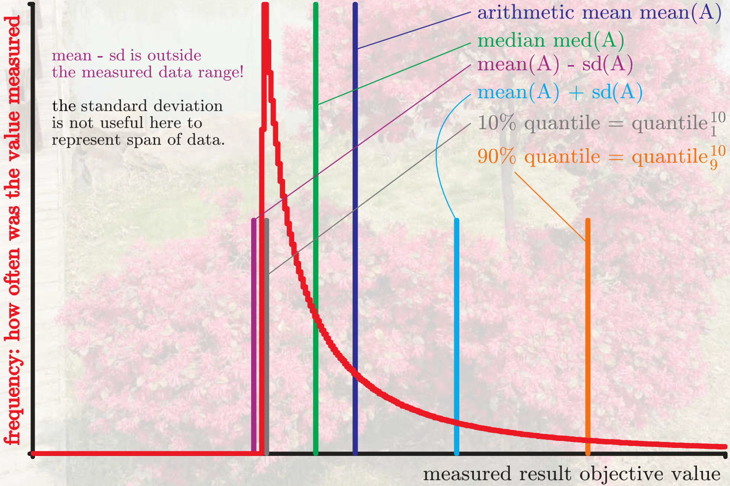

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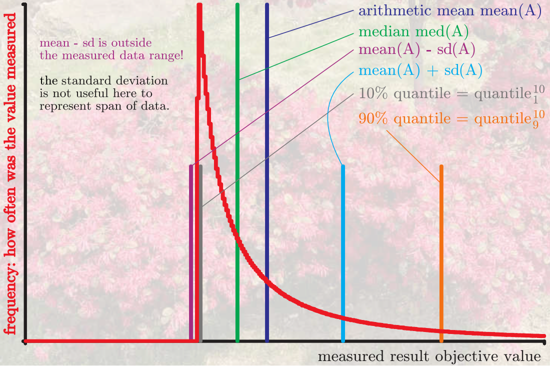

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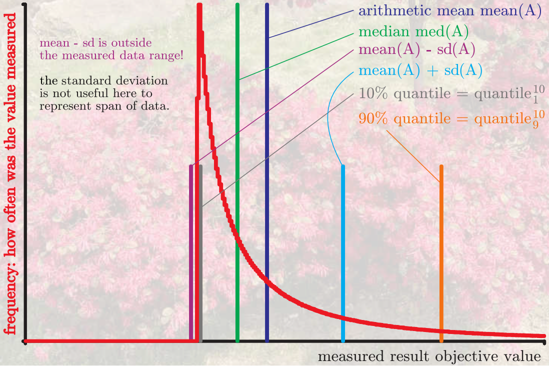

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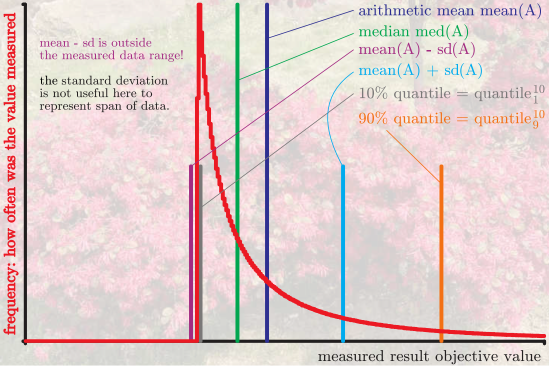

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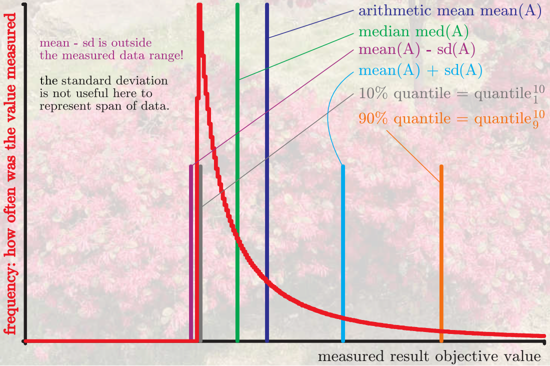

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  - A statement such as *"For this TSP instance, our algorithm can find tours with a length of* 100 ± 120 *km."* makes little sense...

Statistical Comparisons

Introduction

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- If we say *"A is better than B,"* we have a certain probability p to be wrong.
- The statement *"A is better than B"* makes only sense after we have decided about an upper bound α for the acceptable error probability p! (and if $p < \alpha$, obviously)

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

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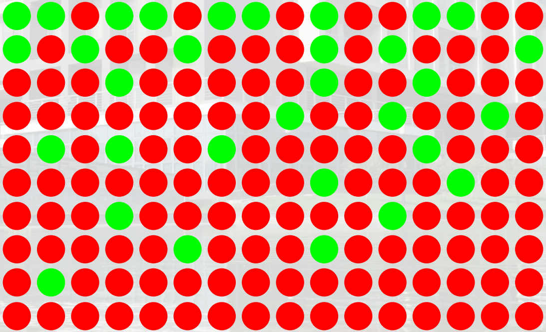

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- Flipping a coin n times is a Bernoulli Process

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- How likely is it that I win at least 128 times if I did not cheat?
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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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- Let's use a Python[60] program to test the combinations

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```python
"""Enumerate all combinations of numbers 1 to 10."""
mean_lower_or_equal_to_4 = 0  # how often did we find a mean <= 4
total_combinations       = 0  # total number of tested combinations

for i in range(1, 11):                  # i goes from 1 to 10
    for j in range(1, i):               # j goes from 1 to i - 1
        for k in range(1, j):           # k goes from 1 to j - 1
            for l in range(1, k):       # l goes from 1 to k - 1
                if ((i + j + k + l) / 4) <= 4:  # check for extreme case
                    mean_lower_or_equal_to_4 += 1  # count extreme case
                total_combinations += 1    # count all combinations

print(f" combinations with mean <= 4: {mean_lower_or_equal_to_4}")
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```

```
 combinations with mean <= 4: 27
total number of combinations: 210
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- Extreme cases into the other direction are the same, because if $\mathrm{mean}(B) \leq 4$ then $\mathrm{mean}(A) \geq 6.5$ 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

Statistical Tests: Types

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

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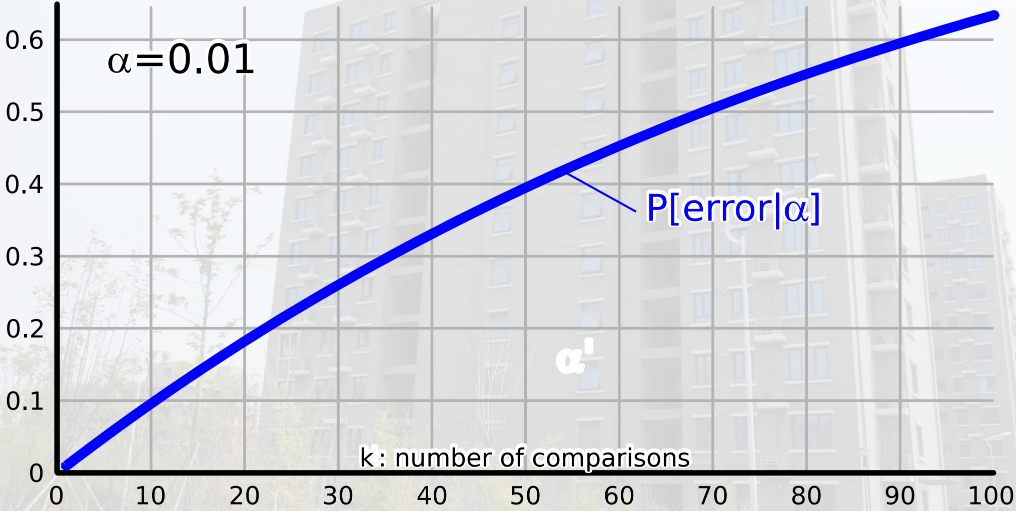

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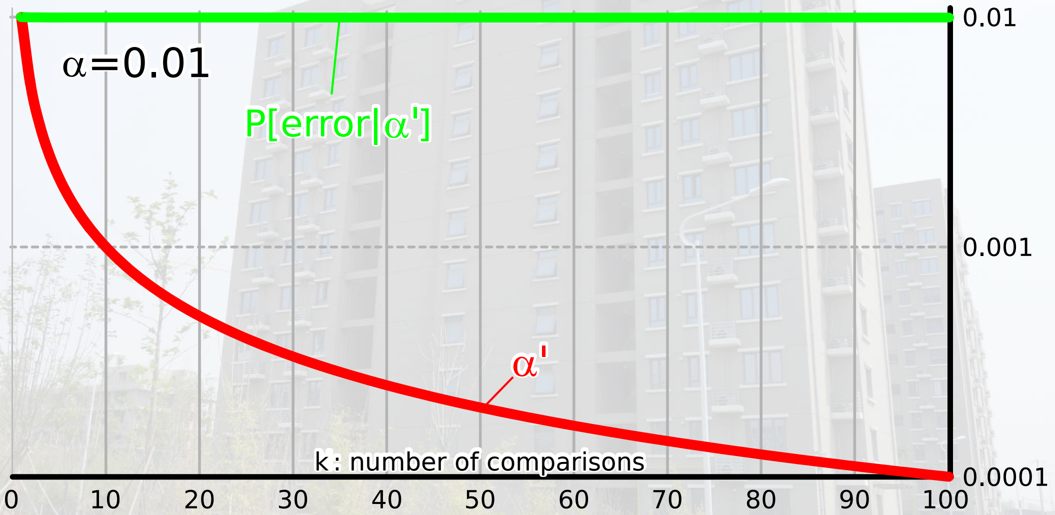

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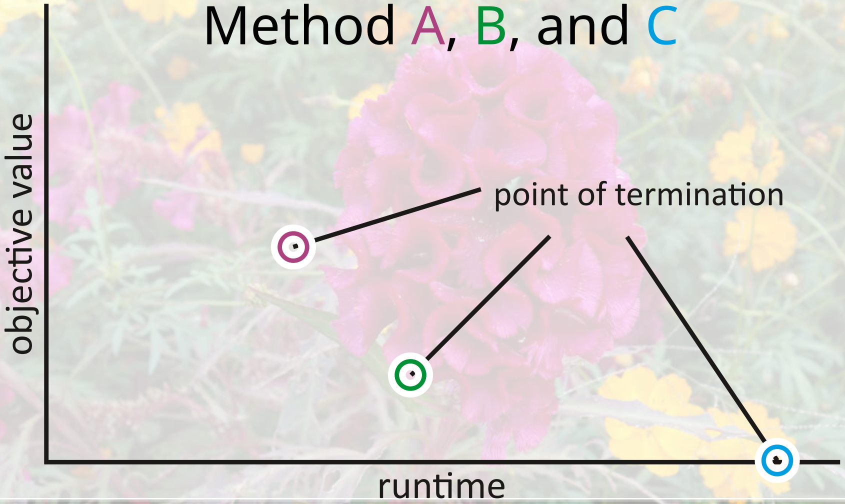

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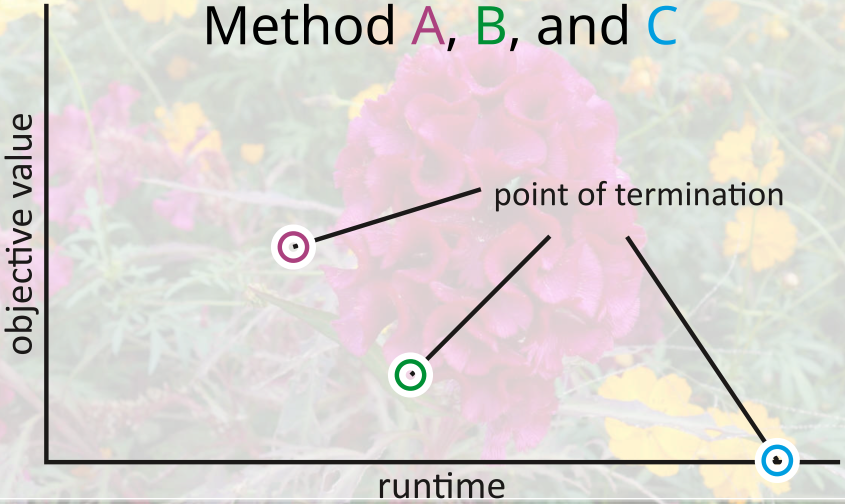

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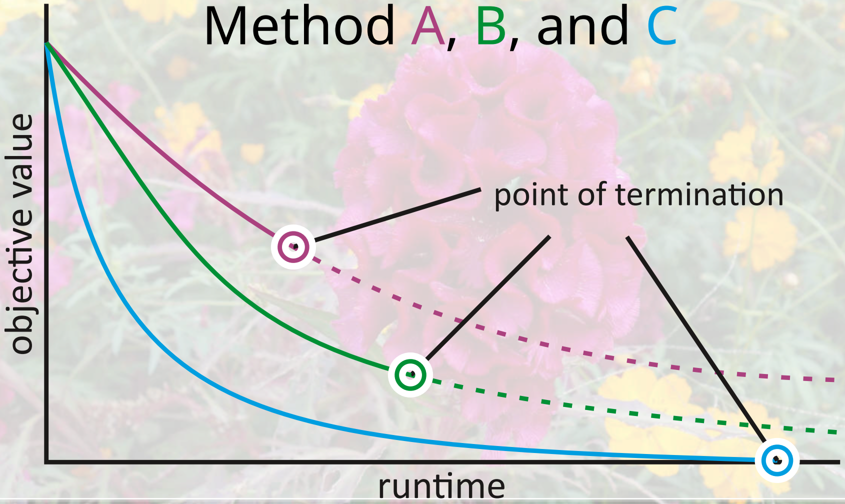

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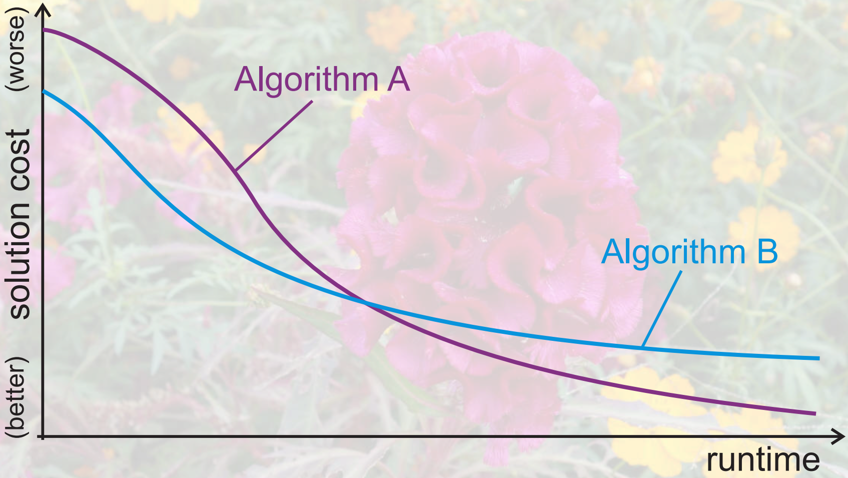

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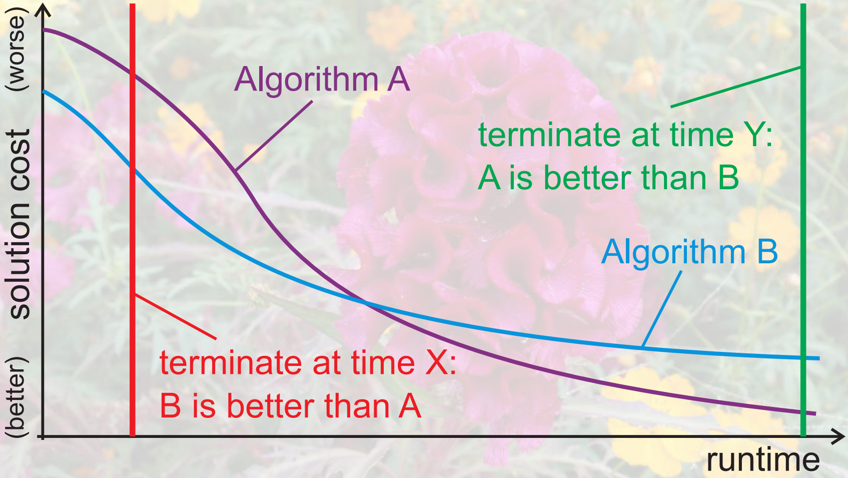

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Other Stuff

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- Use well-known benchmarks, provide your source code!

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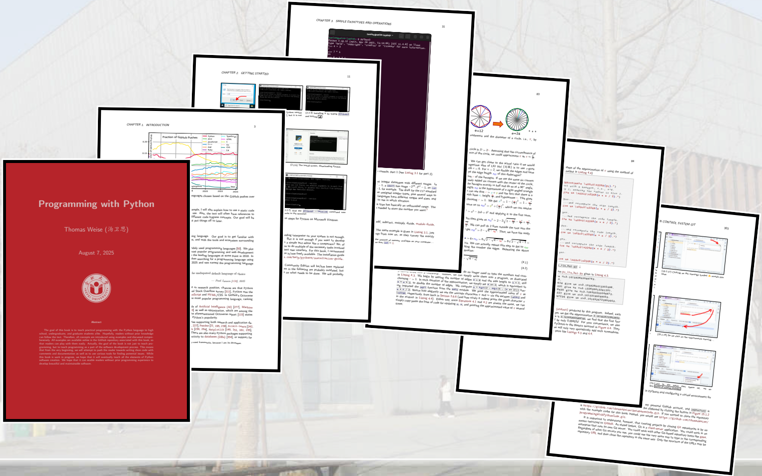
Programming with Python

We have a freely available course book on *Programming with Python* at https://thomasweise.github.io/programmingWithPython, with focus on practical software development using the Python ecosystem of tools[60].

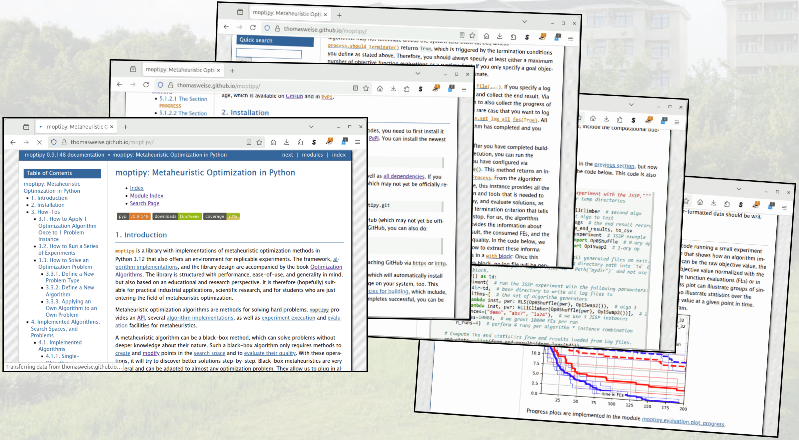


Databases

We have a freely available course book on *Databases* at https://thomasweise.github.io/databases, with actual practical examples using a real database management system (DBMS)[58].

Metaheuristic Optimization in Python: moptipy

We offer moptipy[64] a mature open source Python package for metaheuristic optimization, which implements several algorithms, can run self-documenting experiments in parallel and in a distributed fashion, and offers statistical evaluation tools.



谢谢您门！

Thank you!

Vielen Dank!

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Glossary I

EA An *evolutionary algorithm* is a metaheuristic optimization method that maintains a population of candidate solutions, which undergo selection (where better solutions are chosen with higher probability) and reproduction (where mutation and recombination create a new candidate solution from one or two existing ones, repectively)[5,59].

ACO *Ant Colony Optimization* is a nature-inspired optimization method for combinatorial problems where solutions are generated by "ants" that move from node to node in a graph choosing edges based on (1) the simulated pheromone on the edges and (2) a per-edge heuristic value[17–19]. If an ant produced a good solution, "pheromone" is distributed over the edges it visited, making it more likely to be re-visited by other ants.

BKS The *Best Known Solution* for an instance of an optimization problem is the best solution (measured based on the objective values) that has ever been reported in literature. BKSes are not necessarily globally optimal, as in many instances of $\mathcal{NP}$-hard problems, the true optima are unknown.

CSV *Comma-Separated Values* is a very common and simple text format for exchanging tabular or matrix data[52]. Each row in the text file represents one row in the table or matrix. The elements in the row are separated by a fixed delimiter, usually a comma (","), sometimes a semicolon (";"). Python offers some out-of-the-box CSV support in the `csv` module[16].

DB A *database* is an organized collection of structured information or data, typically stored electronically in a computer system. Databases are discussed in our book *Databases*[58].

DBMS A *database management system* is the software layer located between the user or application and the database (DB). The DBMS allows the user/application to create, read, write, update, delete, and otherwise manipulate the data in the DB[66].

FE *Objective function evaluations* are an implementation-independent measure of runtime for optimization algorithms[61]. 1 FE equals to one evaluated candidate solution during the optimization process.

Glossary II

Git is a distributed Version Control Systems (VCS) which allows multiple users to work on the same code while preserving the history of the code changes[54,57]. Learn more at https://git-scm.com.

GitHub is a website where software projects can be hosted and managed via the Git VCS[46,57]. Learn more at https://github.com.

JSSP The *Job Shop Scheduling Problem*[9,38] is one of the most prominent and well-studied scheduling tasks. In a JSSP instance, there are k machines and m jobs. Each job must be processed once by each machine in a job-specific sequence and has a job-specific processing time on each machine. The goal is to find an assignment of jobs to machines that results in an overall shortest makespan, i.e., the schedule which can complete all the jobs in the shortest time. The JSSP is $\mathcal{NP}$-complete[14,38].

MaxSAT The goal of satisfiablity problems is to find an assignment for n Boolean variables that make a given Boolean formula $F : \{0, 1\}^n \mapsto \{0, 1\}$ become true. In the *Maximum Satisfiability (MaxSAT)* problem[33], F is given in conjunctive normal form, i.e., the variables appear as literals either directly or negated in m "or" clauses, which are all combined into one "and." The objective function $f(x)$, subject to minimization, computes the number of clauses which are false under the variable setting x. If $f(x) = 0$, then all clauses of F are true, which solves the problem. The MaxSat problem is $\mathcal{NP}$-complete[15].

moptipy is the *Metaheuristic Optimization in Python* library[64]. Learn more at https://thomasweise.github.io/moptipy.

Python The Python programming language[34,40,42,60], i.e., what you will learn about in our book[60]. Learn more at https://python.org.

TSP In an instance of the *Traveling Salesperson Problem*, also known as *Traveling Salesman Problem*, a set of n cities or locations as well as the distances between them are defined[2,27,39,61]. The goal is to find the shortest round-trip tour that starts at one city, visits all the other cities one time each, and returns to the origin. The TSP is one of the most well-known $\mathcal{NP}$-hard combinatorial optimization problems.

Glossary III

TSPLib is a library of benchmark instances for the Traveling Salesperson Problem (TSP) available at http://comopt.ifi.uni-heidelberg.de/software/TSPLIB95[49,50].

unit test Software development is centered around creating the program code of an application, library, or otherwise useful system. A *unit test* is an *additional* code fragment that is not part of that productive code. It exists to execute (a part of) the productive code in a certain scenario (e.g., with specific parameters), to observe the behavior of that code, and to compare whether this behavior meets the specification[45,51,56]. If not, the unit test fails. The use of unit tests is at least threefold: First, they help us to detect errors in the code. Second, program code is usually not developed only once and, from then on, used without change indefinitely. Instead, programs are often updated, improved, extended, and maintained over a long time. Unit tests can help us to detect whether such changes in the program code, maybe after years, violate the specification or, maybe, cause another, depending, module of the program to violate its specification. Third, they are part of the documentation or even specification of a program.

VCS A *Version Control System* is a software which allows you to manage and preserve the historical development of your program code[57]. A distributed VCS allows multiple users to work on the same code and upload their changes to the server, which then preserves the change history. The most popular distributed VCS is Git.

$i!$ The factorial $a!$ of a natural number $a \in \mathbb{N}_1$ is the product of all positive natural numbers less than or equal to a, i.e., $a! = 1 * 2 * 3 * 4 * \cdots * (a-1) * a$[13,21,41].

$i..j$ with $i, j \in \mathbb{Z}$ and $i \leq j$ is the set that contains all integer numbers in the inclusive range from i to j. For example, 5..9 is equivalent to $\{5, 6, 7, 8, 9\}$

$\operatorname{geom}(A)$ The *geometric mean* $\operatorname{geom}(A)$ is the n^{th} root of the product of n *positive* values in a dataset $A = (a_0, a_1, \dots, a_{n-1})$ with $a_i > 0$ for all $i \in 0..n$, i.e., $\operatorname{geom}(A) = \sqrt[n]{\prod_{i=0}^{n-1} a_i} = \exp\left(\frac{1}{n}\sum_{i=0}^{n-1} \log a_i\right)$.

Glossary IV

$\text{mean}(A)$ The *arithmetic mean* $\text{mean}(A)$ is an estimate of the expected value of a distribution from which a data sample was, well, sampled. Its is computed on data sample $A = (a_0, a_1, \ldots, a_{n-1})$ as the sum of all n elements a_i in the sample data A divided by the total number n of values, i.e., $\text{mean}(A) = \frac{1}{n}\sum_{i=0}^{n-1} a_i$.

$\text{median}(A)$ The *median* $\text{median}(A)$ is the value separating the bigger-valued half from the smaller-valued half of a data sample or distribution. Its estimate is the value right in the middle of a *sorted* data sample $A = (a_0, a_1, \ldots, a_{n-1})$ where $a_{i-1} \leq a_i \; \forall i \in 1 \ldots (n-1)$ with an odd number of elements and the mean of the two values in the middle if n is even. In other words, $\text{median}(A) = a_{\frac{n-1}{2}}$ if n is odd and $\frac{1}{2}\left(a_{\frac{n}{2}-1} + a_{\frac{n}{2}}\right)$ otherwise, i.e., if n is even.

$\mathbb{N}_1$ the set of the natural numbers *excluding* 0, i.e., 1, 2, 3, 4, and so on. It holds that $\mathbb{N}_1 \subset \mathbb{Z}$.

$\mathcal{NP}$ $\mathcal{NP}$ is the class of computational problems that can be solved in polynomial time by a non-deterministic machine and can be verified in polynomial time by a deterministic machine (such as a normal computer)[25].

$\mathcal{NP}$-complete A decision problem is $\mathcal{NP}$-complete if it is in $\mathcal{NP}$ and all problems in $\mathcal{NP}$ are reducible to it in polynomial time[25,48]. A problem is $\mathcal{NP}$-complete if it is $\mathcal{NP}$-hard and if it is in $\mathcal{NP}$.

$\mathcal{NP}$-hard Algorithms that guarantee to find the correct solutions of $\mathcal{NP}$-hard problems[14,15,38] need a runtime that is exponential in the problem scale in the worst case. A problem is $\mathcal{NP}$-hard if all problems in $\mathcal{NP}$ are reducible to it in polynomial time[25].

$\mathcal{O}(g(x))$ If $f(x) = \mathcal{O}(g(x))$, then there exist positive numbers $x_0 \in \mathbb{R}^+$ and $c \in \mathbb{R}^+$ such that $f(x) \leq c * g(x) \forall x \geq x_0$[4,37]. In other words, $\mathcal{O}(g(x))$ describes an upper bound for function growth.

Glossary V

$\mathrm{quantile}_q^k(A)$ The q-*quantiles* are the cut points that divide a sorted data sample $A = (a_0, a_1, \dots, a_{n-1})$ where $a_{i-1} \leq a_i \; \forall i \in 1 \dots (n-1)$ into q equally-sized parts. $\mathrm{quantile}_q^k(A)$ be the k^{th} q-quantile, with $k \in 1 \dots (q-1)$, i.e., there are $q-1$ of the q-quantiles. In the context of this book, define $h = (n-1)\frac{k}{q}$. $\mathrm{quantile}_q^k(A)$ then can be computed as a_h if h is integer, i.e., $h \in \mathbb{Z}$, and as $a_{\lfloor h \rfloor} + (h - \lfloor h \rfloor) * \left(a_{\lfloor h \rfloor + 1} - a_{\lfloor h \rfloor}\right)$ otherwise. It holds that $\mathrm{quantile}_1^2(A) = \mathrm{median}(A)$

$\mathbb{R}$ the set of the real numbers.

$\mathbb{R}^+$ the set of the positive real numbers, i.e., $\mathbb{R}^+ = \{x \in \mathbb{R} : x > 0\}$.

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

$\mathrm{var}(A)$ The *variance* of a distribution is the expectation of the squared deviation of the underlying random variable from its mean. The variance $\mathrm{var}(A)$ of a data sample $A = (a_0, a_1, \dots, a_{n-1})$ with n observations can be estimated as $\mathrm{var}(A) = \frac{1}{n-1} \sum_{i=0}^{n-1} (a_i - \mathrm{mean}(A))^2$.

$\mathbb{Z}$ the set of the integers numbers including positive and negative numbers and 0, i.e., ..., -3, -2, -1, 0, 1, 2, 3, ..., and so on. It holds that $\mathbb{Z} \subset \mathbb{R}$.