# Optimization Algorithms

## A. Comparing Optimization Algorithms

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## Outline

1. Introduction
2. Performance Indicators and Time
3. Statistical Measures
4. Measures of Spread

# Introduction

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- For solving an optimization problem, we want to use the algorithm most suitable for it.
- What does this mean?

# Performance Indicators and Time

# Performance Indicators

- Key parameters[3–6]

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- Key parameters[3–6]:
  1. Solution quality reached after a certain runtime

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- Two key parameter[3–6]:
  1. Solution quality reached after a certain runtime
  2. Runtime to reach a certain solution quality
- Measure data samples $A$ containing the results from multiple runs and estimate key parameters.

# Runtime)

- What actually is runtime?

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

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- Disadvantages:
  - No clear relationship to real runtime
  - Does not contain "hidden complexities" of algorithm
  - 1 FE: very different costs in different situations!
- Relevant for comparing algorithms, but not so much for the practical application

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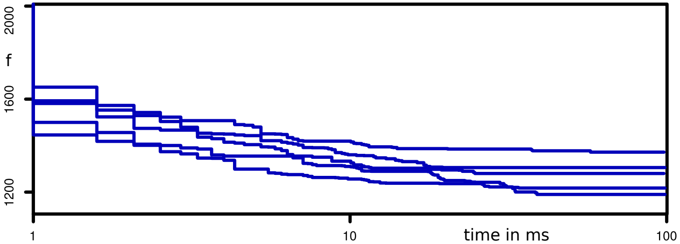
- Which one is the “better” performance indicator?



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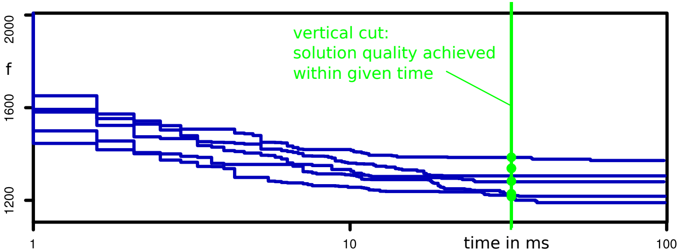

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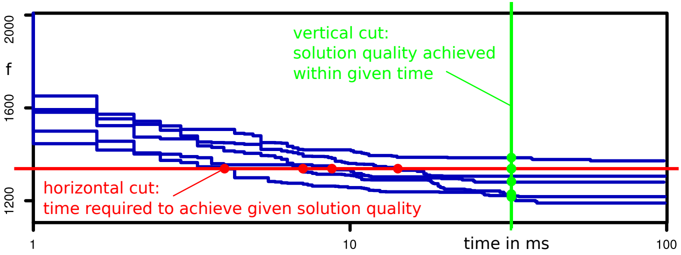

## Key Parameters

- Which one is the "better" performance indicator?
  1. Best objective function value reached after a certain number of FEs
  2. Number FEs needed to reach a certain objective function value
- This question actually does not really need an answer...

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- Number FEs needed to reach a certain objective function value
- Preferred by, e.g., the BBOB/COCO benchmark suite[3]:
  - Measures a time needed to reach a target function value $\Rightarrow$ "Algorithm $A$ is two/ten/hundred times faster than Algorithm $B$ in solving this problem."
  - Benchmark Perspective: No interpretable meaning to the fact that Algorithm $A$ reaches a function value that is two/ten/hundred times smaller than the one reached by Algorithm $B$.

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- Preferred by many benchmark suites such as[7].
- Practice Perspective: Best results achievable with given time budget wins.
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- This is the scenario in our JSSP example, too.

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- Best approach: Evaluate algorithm according to both methods.[5] [6] [8]

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  4. From prior, small-scale experiments.
  5. Based on known lower bounds

# Statistical Measures

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- Results can be different for each run!
- Executing a randomized algorithm one time does not give reliable information.
- Statistical evaluation over a set of runs necessary.

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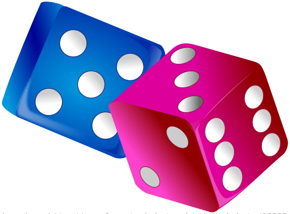
- Example: Dice Throw



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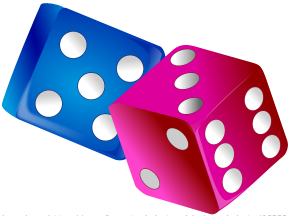
- Crucial Difference: distribution and sample
- A sample is what we *measure*.
- A distribution is the asymptotic result of the ideal process
- Statistical parameters of the distribution can be estimated from a sample
- Example: Dice Throw
- How likely is it to roll a 1, 2, 3, 4, 5, or 6?



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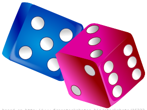
| # throws | number | f(1) | f(2) | f(3) | f(4) | f(5) | f(6) |
|---|---|---|---|---|---|---|---|
| 1 | 5 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 1.0000 | 0.0000 |



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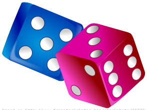

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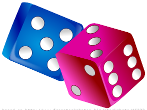
| 3 | 1 | 0.3333 | 0.0000 | 0.0000 | 0.3333 | 0.3333 | 0.0000 |



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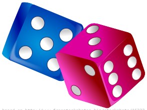
| 4 | 4 | 0.2500 | 0.0000 | 0.0000 | 0.5000 | 0.2500 | 0.0000 |



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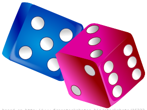
| 4 | 4 | 0.2500 | 0.0000 | 0.0000 | 0.5000 | 0.2500 | 0.0000 |
| 5 | 3 | 0.2000 | 0.0000 | 0.2000 | 0.4000 | 0.2000 | 0.0000 |



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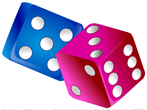
| 5 | 3 | 0.2000 | 0.0000 | 0.2000 | 0.4000 | 0.2000 | 0.0000 |
| 6 | 3 | 0.1667 | 0.0000 | 0.3333 | 0.3333 | 0.1667 | 0.0000 |



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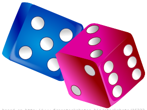
| 6 | 3 | 0.1667 | 0.0000 | 0.3333 | 0.3333 | 0.1667 | 0.0000 |
| 7 | 2 | 0.1429 | 0.1429 | 0.2857 | 0.2857 | 0.1429 | 0.0000 |
| 8 | 1 | 0.2500 | 0.1250 | 0.2500 | 0.2500 | 0.1250 | 0.0000 |
| 9 | 4 | 0.2222 | 0.1111 | 0.2222 | 0.3333 | 0.1111 | 0.0000 |
| 10 | 2 | 0.2000 | 0.2000 | 0.2000 | 0.3000 | 0.1000 | 0.0000 |



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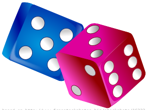
| 10 | 2 | 0.2000 | 0.2000 | 0.2000 | 0.3000 | 0.1000 | 0.0000 |
| 11 | 6 | 0.1818 | 0.1818 | 0.1818 | 0.2727 | 0.0909 | 0.0909 |
| 12 | 3 | 0.1667 | 0.1667 | 0.2500 | 0.2500 | 0.0833 | 0.0833 |



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| 11 | 6 | 0.1818 | 0.1818 | 0.1818 | 0.2727 | 0.0909 | 0.0909 |
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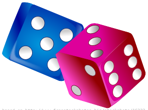
| 100 | ... | 0.1900 | 0.2100 | 0.1500 | 0.1600 | 0.1200 | 0.1700 |
| 1'000 | ... | 0.1700 | 0.1670 | 0.1620 | 0.1670 | 0.1570 | 0.1770 |
| 10'000 | ... | 0.1682 | 0.1699 | 0.1680 | 0.1661 | 0.1655 | 0.1623 |
| 100'000 | ... | 0.1671 | 0.1649 | 0.1664 | 0.1676 | 0.1668 | 0.1672 |
| 1'000'000 | ... | 0.1673 | 0.1663 | 0.1662 | 0.1673 | 0.1666 | 0.1664 |



based on http://www.freestockphotos.biz/stockphoto/16223

# Important Distinction

| # 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 |
| 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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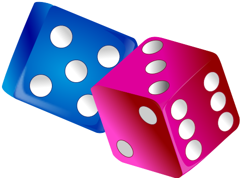
| 10'000'000 | ... | 0.1667 | 0.1667 | 0.1666 | 0.1668 | 0.1667 | 0.1665 |
| 100'000'000 | ... | 0.1667 | 0.1666 | 0.1666 | 0.1667 | 0.1667 | 0.1667 |
| 1'000'000'000 | ... | 0.1667 | 0.1667 | 0.1667 | 0.1667 | 0.1667 | 0.1667 |

# 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
- How likely is it to roll a 1, 2, 3, 4, 5, or 6?
- Never forget: All measured parameters are just estimates.



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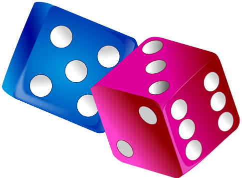

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- We usually want to reduce this set of numbers to a single value which can give us an impression of what the "average outcome" (or result quality is).
- Two of the most common options for doing so, for estimating the "center" of a distribution, are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

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

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

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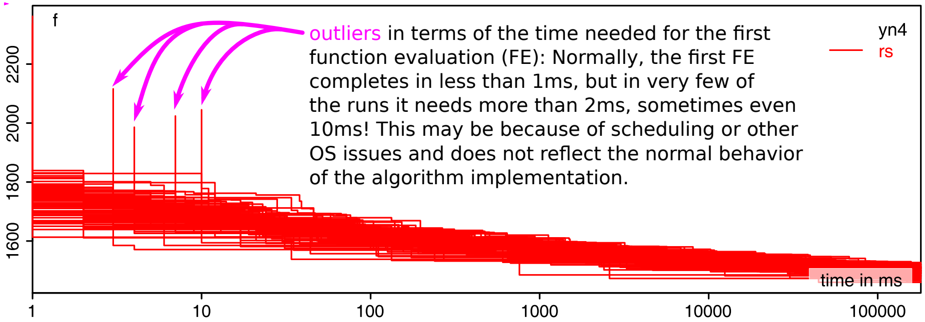
- For example, maybe the operating system was updating itself during a run of one of our JSSP algorithms and, thus, took away much of the 3 minute computation budget.
- We can see that such odd times are possible, as our experimental data shows that there are sometimes outliers in the time it takes to create and evaluate the first candidate solution.

# Outliers


f
outliers in terms of the time needed for the first function evaluation (FE): Normally, the first FE completes in less than 1ms, but in very few of the runs it needs more than 2ms, sometimes even 10ms! This may be because of scheduling or other OS issues and does not reflect the normal behavior of the algorithm implementation.
yn4
rs
2200
2000
1800
1600
time in ms
1
10
100
1000
10000
100000

# Outliers

# Example for Data Samples w/o Outlier

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

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\begin{aligned}
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- Thus, we often want that outliers influence our statistics.

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- So we can conclude: It is best to have both the mean and median statistic of a given performance indicator.

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- For this, we can 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.

## Variance

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

$$\mathrm{var}(A) = \frac{1}{n-1} \sum_{i=0}^{n-1} (a_i - \mathrm{mean}(A))^2$$

## Standard Deviation

### Definition (Standard Deviation)

The statistical estimate $\mathrm{sd}(A)$ 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 $\mathrm{var}(A)$.

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

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# Quantiles

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

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- The $\text{quantile}_1^2 A$ is the median of $A$
- 4-quantiles are called quartiles.
- We sometimes write things like "the 25% quantile," meaning $\text{quantile}_{100}^{25}$.

## Standard Deviation: Example

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

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

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\mathrm{mean}(A) &= 7 \\
B &= (1, 3, 4, 4, 4, 5, 6, 6, 6, 6, 7, 7, 9, 9, 9, 10, 11, 12, {\color{red}10'008}) \\
\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 5'264'628.1
\end{aligned}
$$

## Standard Deviation: Example

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

$$
\begin{aligned}
A &= (1,3,4,4,4,5,6,6,6,6,7,7,9,9,9,10,11,12,14) \\
\text{mean}(A) &= 7 \\
B &= (1,3,4,4,4,5,6,6,6,6,7,7,9,9,9,10,11,12,{\color{red}10'008}) \\
\text{mean}(B) &= 533 \\
\text{var}(A) &= \frac{1}{19-1}\sum_{i=1}^{19}(a_i - \text{mean}(a))^2 = \frac{198}{18} = 11 \\
\text{var}(B) &= \frac{1}{19-1}\sum_{i=1}^{19}(b_i - \text{mean}(b))^2 = \frac{94'763'306}{18} \approx 5'264'628.1 \\
\text{sd}(A) &= \sqrt{\text{var} A} = \sqrt{11} \approx 3.31662479 \\
\text{sd}(B) &= \sqrt{\text{var} B} = \sqrt{\frac{94'763'306}{18}} \approx 2294.477743
\end{aligned}
$$

## Quantiles: Example

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

$$A = (1, 3, 4, 4, 4, 5, 6, 6, 6, 6, 7, 7, 9, 9, 9, 10, 11, 12, 14)$$
$$B = (1, 3, 4, 4, 4, 5, 6, 6, 6, 6, 7, 7, 9, 9, 9, 10, 11, 12, 10'008)$$

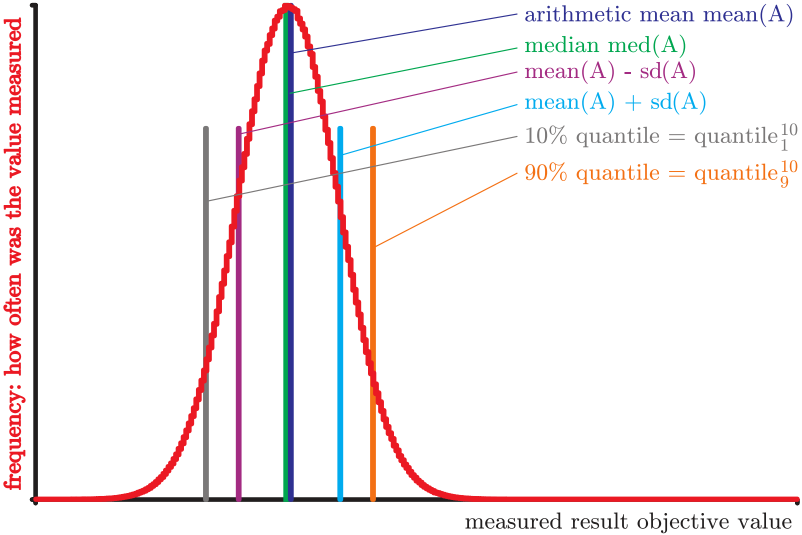
## Quantiles: Example

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

$$
\begin{aligned}
A &= (1, 3, 4, 4, 4, 5, 6, 6, 6, 6, 7, 7, 9, 9, 9, 10, 11, 12, 14) \\
B &= (1, 3, 4, 4, 4, 5, 6, 6, 6, 6, 7, 7, 9, 9, 9, 10, 11, 12, 10'008) \\
\text{quantile}_4^1(A) &= \text{quantile}_4^1(B) = 4.5 \\
\text{quantile}_4^3(A) &= \text{quantile}_4^3(B) = 9
\end{aligned}
$$

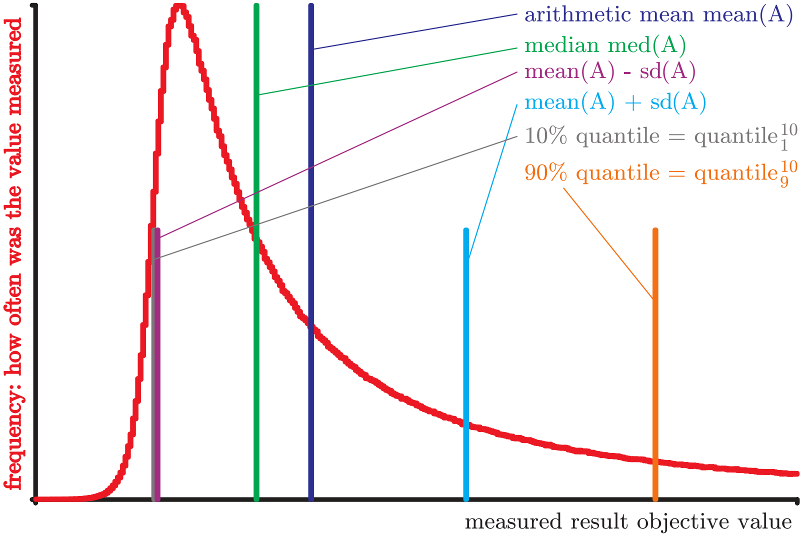
## Further Example

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



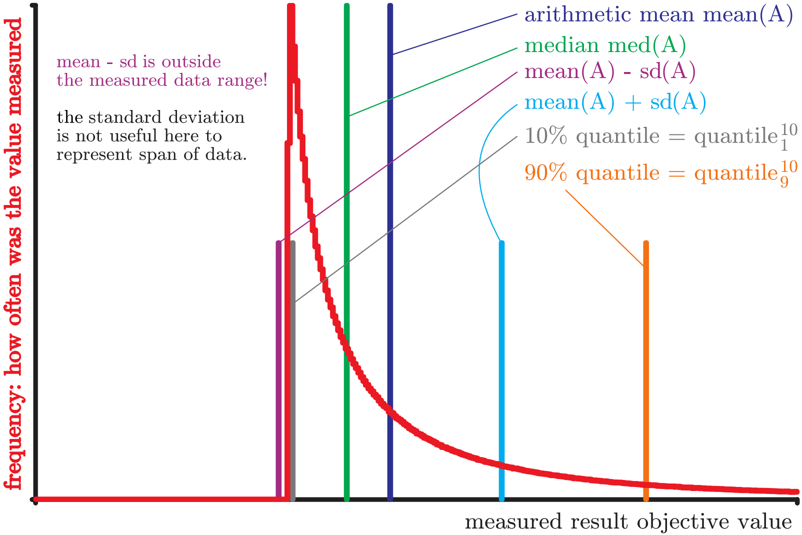
## Further Example

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



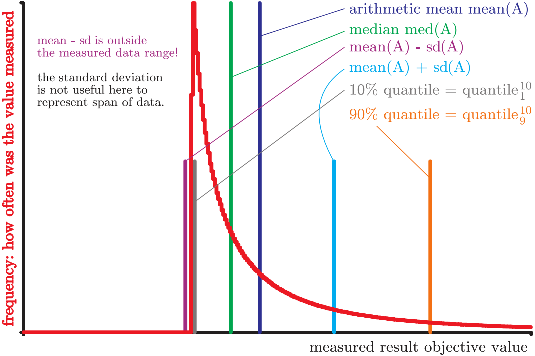
# Further Example

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



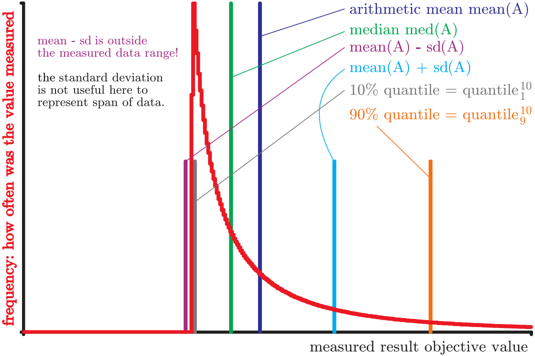
# Further Example

- The implicit assumption that $\mathrm{mean} \pm \mathrm{sd}$ is a meaningful range is not always true!
- Such a shape is possible in optimization!



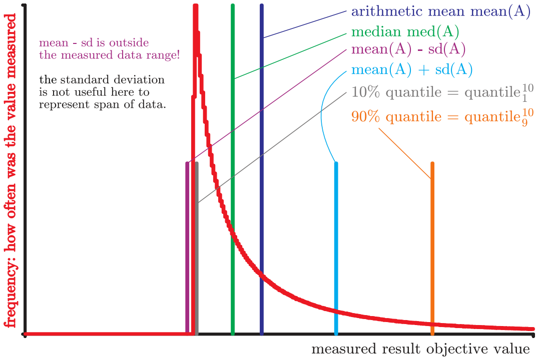
# Further Example

- The implicit assumption that $\mathrm{mean} \pm \mathrm{sd}$ is a meaningful range is not always true!
- Such a shape is possible in optimization:
  - The global optimum marks a lower bound for the possible objective values.



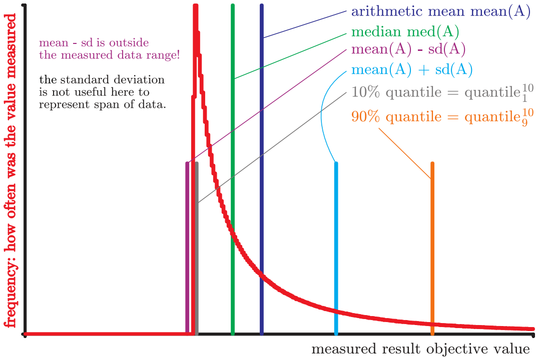
# Further Example

- The implicit assumption that $\mathrm{mean} \pm \mathrm{sd}$ is a meaningful range is not always true!
- Such a shape is possible in optimization:
  - The global optimum marks a lower bound for the possible objective values.
  - A good algorithm often returns results which are close-to-optimal.



# Further Example

- The implicit assumption that $\mathrm{mean} \pm \mathrm{sd}$ is a meaningful range is not always true!
- Such a shape is possible in optimization:
  - The global optimum marks a lower bound for the possible objective values.
  - A good algorithm often returns results which are close-to-optimal.
  - There may be a long tail of few but significantly worse runs.



谢谢

Thank you

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