# Theory of Estimation-of-Distribution Algorithms

PPSN 2024 Tutorial

## 1. Estimation-of-Distribution Algorithms (EDAs)

## 2. Theory

# 1. Estimation-of-Distribution Algorithms (EDAs)

» **What** are they?

# 2. Theory

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## 2. Theory

- **What** are they?
- **Focus** on the most commonly theoretically studied ones

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(Mathematical rigor)

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» **Selection** of important results

- **Understand** the basic idea

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- **What** are they?
- **Focus** on the most commonly theoretically studied ones

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(Mathematical rigor)

- **What** is studied?
- **Selection** of important results
  - **Understand** the basic idea

» **Depth over breadth**

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Carsten Witt



DOI: **10.1145/3377929.3389888**


(more **breadth**)

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(more **breadth**)

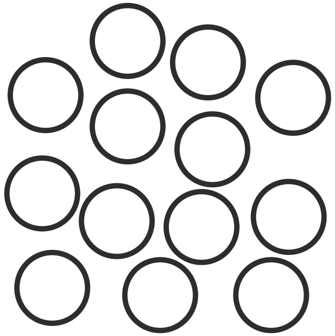
PPSN 2024

**Sunday, Sep. 15**

**9:30–12:30**

**30 Years of EDAs**

# Evolutionary Algorithms



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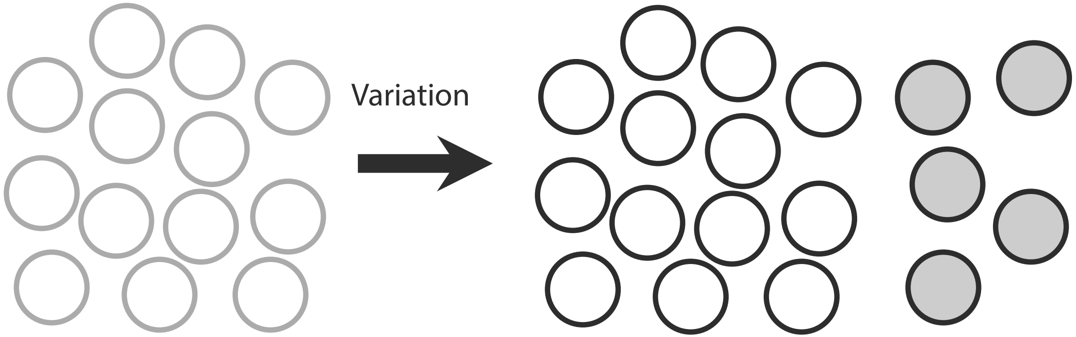

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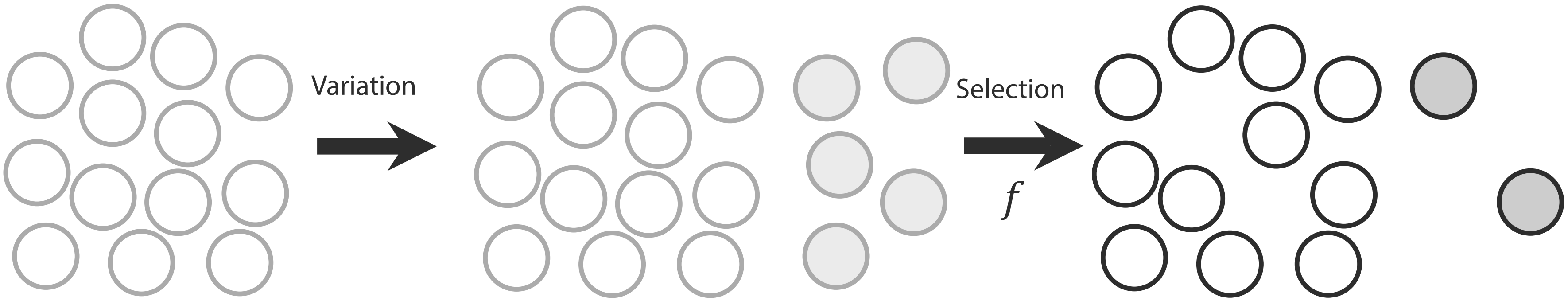

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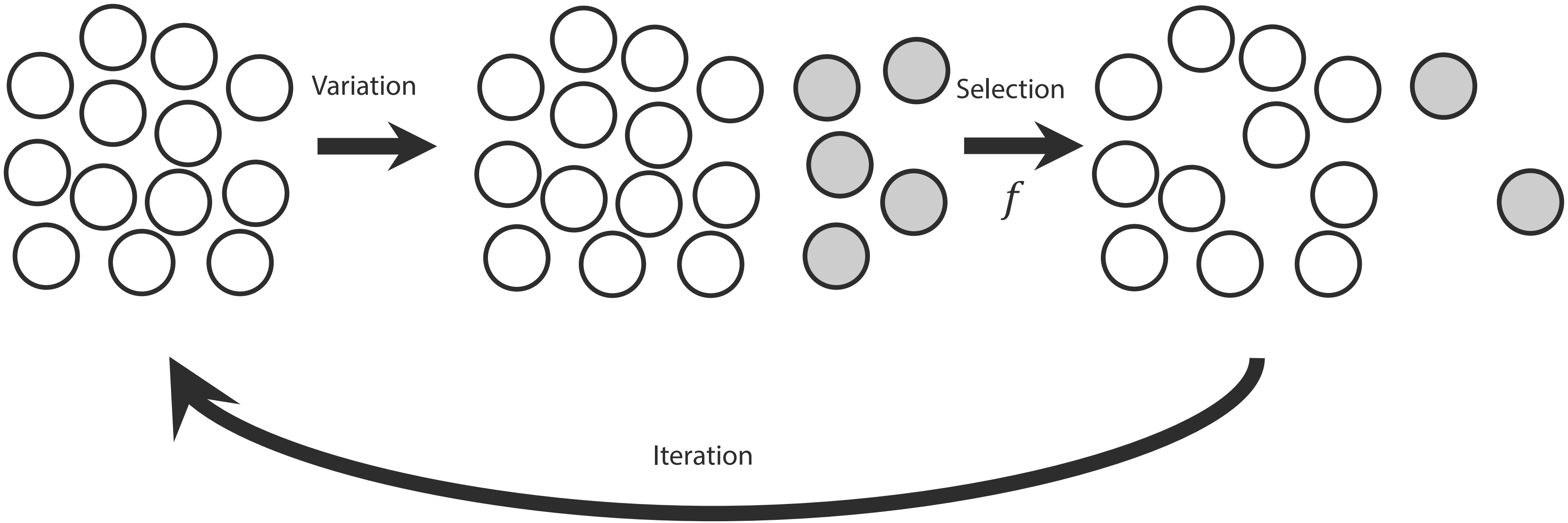
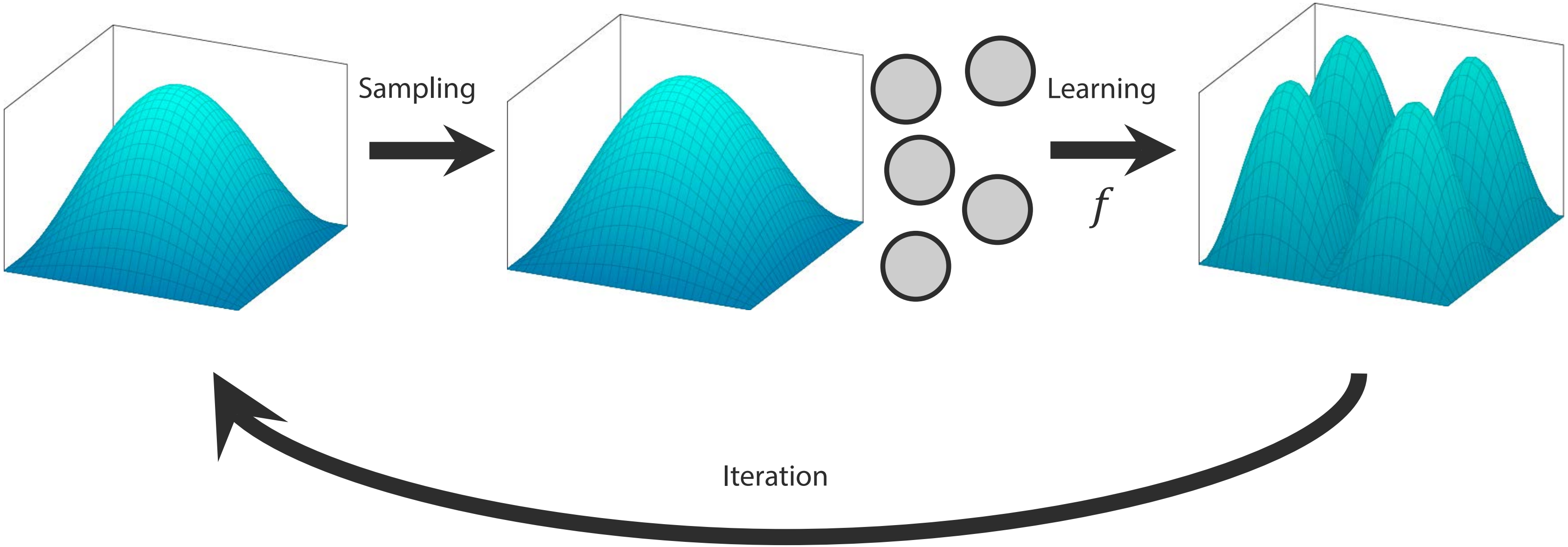
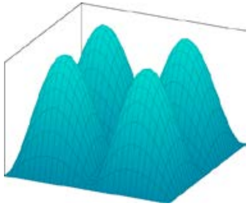


# Estimation-of-Distribution Algorithms



# Probabilistic Models



general

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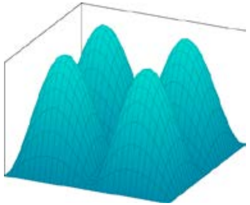
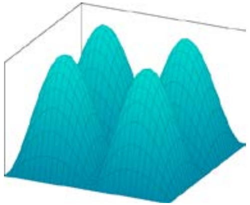


general

| $x_1$ | $x_2$ | $x_3$ | $x_4$ | $x_5$ |
|---|---|---|---|---|
| 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 1 |
| 0 | 0 | 0 | 0 | 2 |
| | | ⋮ | | |

# Probabilistic Models



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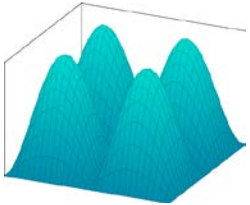
$$\prod_{i \in [\#\text{vars}]} \left(\#\text{vals}(x_i)\right) - 1$$

# Probabilistic Models



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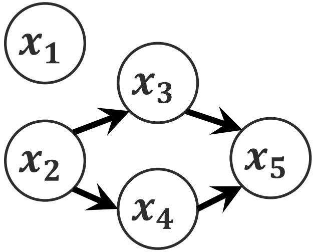
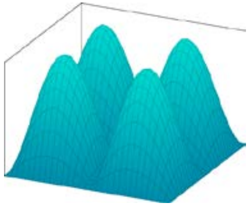



compressed, directed

# Probabilistic Models



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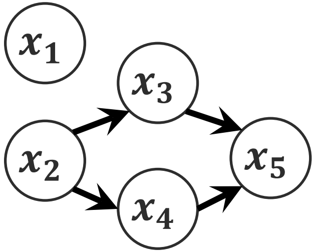


compressed, directed

| $x_1$ |
|---|
| 0 |
| 1 |
| 2 |
| ⋮ |

| $x_2$ |
|---|
| 0 |
| 1 |
| 2 |
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…

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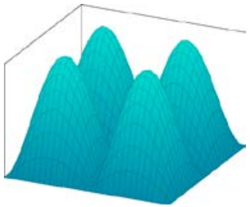

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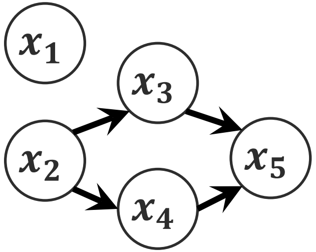
$$\prod_{i\in[\#\text{vars}]}\big(\#\text{vals}(x_i)\big) - 1$$

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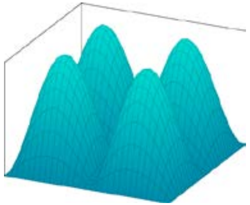
…

$$\sum_{i\in[\#\text{vars}]}(\#\text{vals}(x_i) - 1)\prod_{y\in\text{pred}(x_i)}\#\text{vals}(y)$$

# Probabilistic Models



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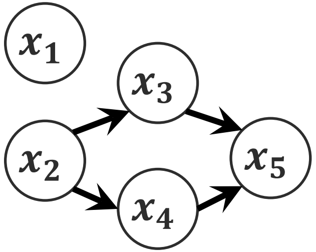
$$\prod_{i\in[\#\mathrm{vars}]}(\#\mathrm{vals}(x_i)) - 1$$

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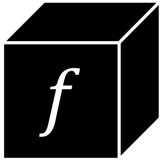
…

$$\sum_{i\in[\#\mathrm{vars}]}(\#\mathrm{vals}(x_i) - 1)\prod_{y\in\mathrm{pred}(x_i)}\#\mathrm{vals}(y)$$

**Theory**


**univariate**

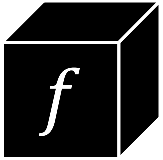
# Theory




$f: \{0,1\}^n \to \mathbf{R}$

» Pseudo-Boolean optimization

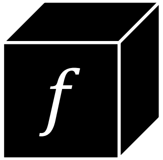
# Theory




$f : \{0,1\}^n \to \mathbf{R}$

- Pseudo-Boolean optimization
  - **Global optimum** often $1^n$

# Theory

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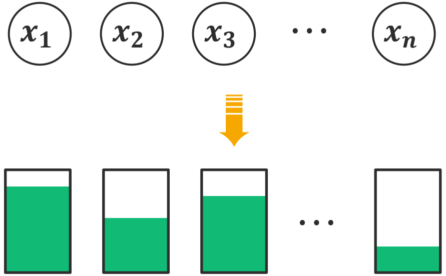

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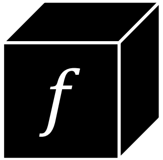


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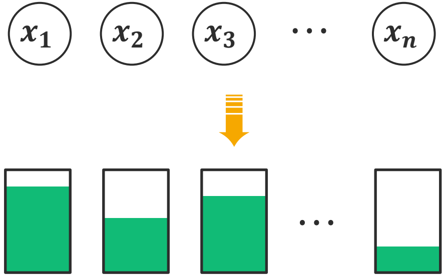
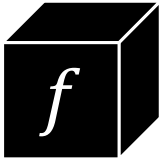



» *Frequency* vector $\boldsymbol{p}$

# Theory

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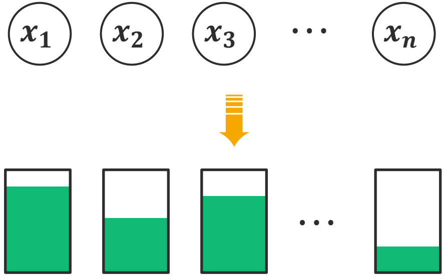
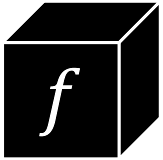



- *Frequency* vector $\boldsymbol{p}$
- $\boldsymbol{p}_i$ … probability to sample a 1 at $i$ (green mass)

# Theory

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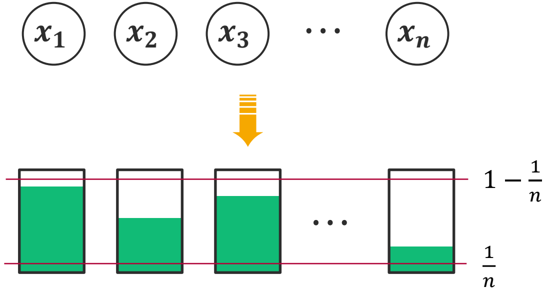


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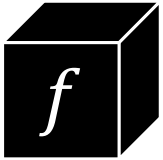


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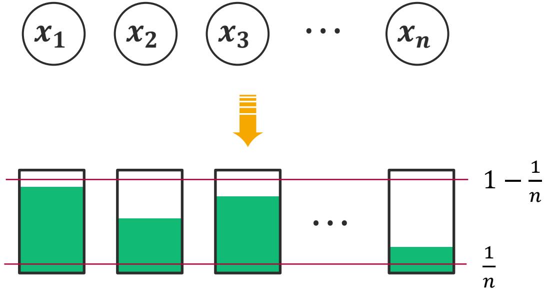


» *Frequency* vector $\boldsymbol{p}$

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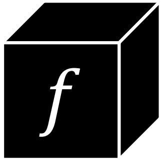
Multi-valued analyses

# Theory

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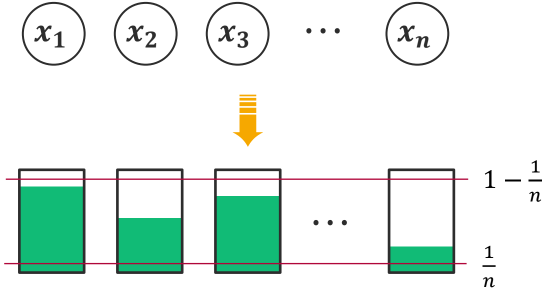


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Multi-valued analyses

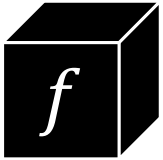
- DOI: **10.1016/j.tcs.2024.114622**

[Ben Jedidia, Doerr, K.'24]

- *Runtime Analysis of a Multi-Valued Compact Genetic Algorithm on Generalized OneMax*

[Adak, Witt'24]

# Theory

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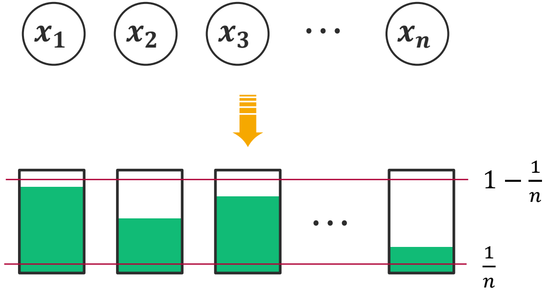
» Pseudo-Boolean optimization

❖ **Global optimum** often $1^n$

» **Run time** analysis

❖ Number of evaluations of $f$ until a global optimum is sampled

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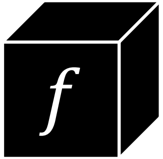


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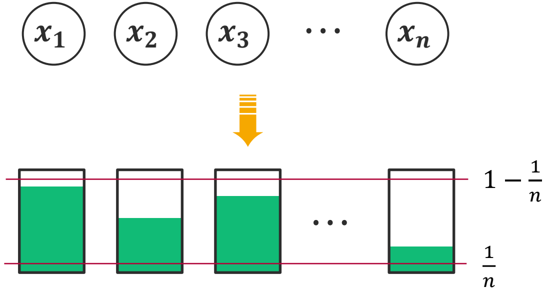


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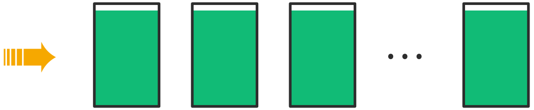
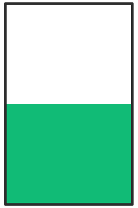


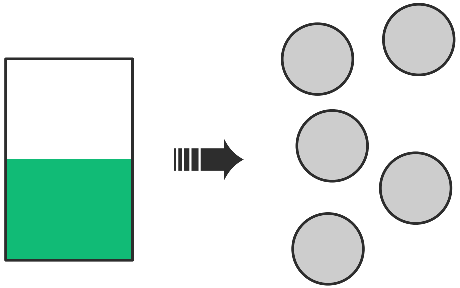
» Favorable albeit not necessary model

# Updating a Frequency (commonly)



$\boldsymbol{p}_i^{(t)}$

# Updating a Frequency (commonly)



$\boldsymbol{p}_i^{(t)}$

samples $\left\{\boldsymbol{x}^{(j)}\right\}_{j \in [\lambda]}$

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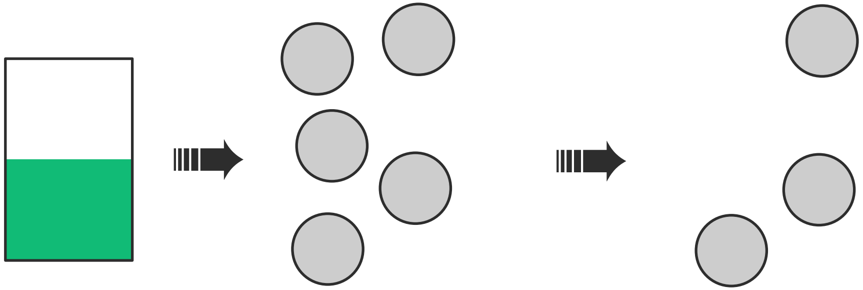


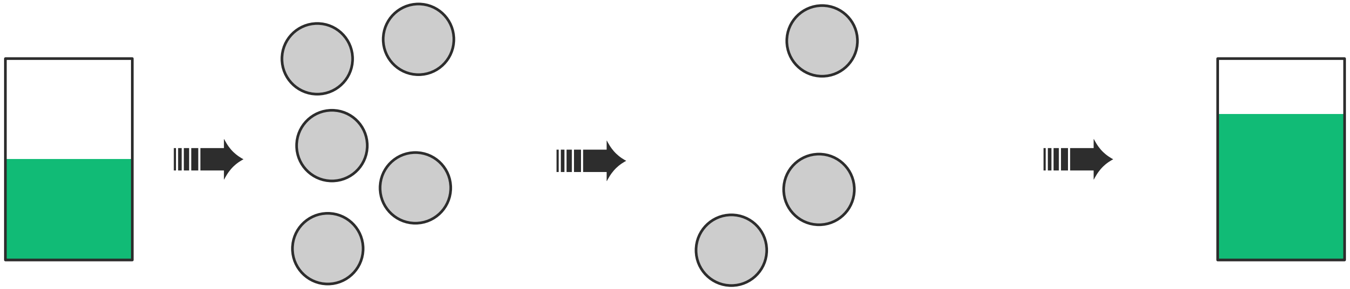
$\boldsymbol{p}_i^{(t)}$

samples $\left\{\boldsymbol{x}^{(j)}\right\}_{j\in[\lambda]}$

**selected** samples $\left\{\hat{\boldsymbol{x}}^{(k)}\right\}_{k\in[\mu]}$

(ordered by decreasing fitness)

# Updating a Frequency (commonly)



$\boldsymbol{p}_i^{(t)}$ samples $\left\{\boldsymbol{x}^{(j)}\right\}_{j\in[\lambda]}$ **selected** samples $\left\{\hat{\boldsymbol{x}}^{(k)}\right\}_{k\in[\mu]}$ (ordered by decreasing fitness) $\boldsymbol{p}_i^{(t+1)}$

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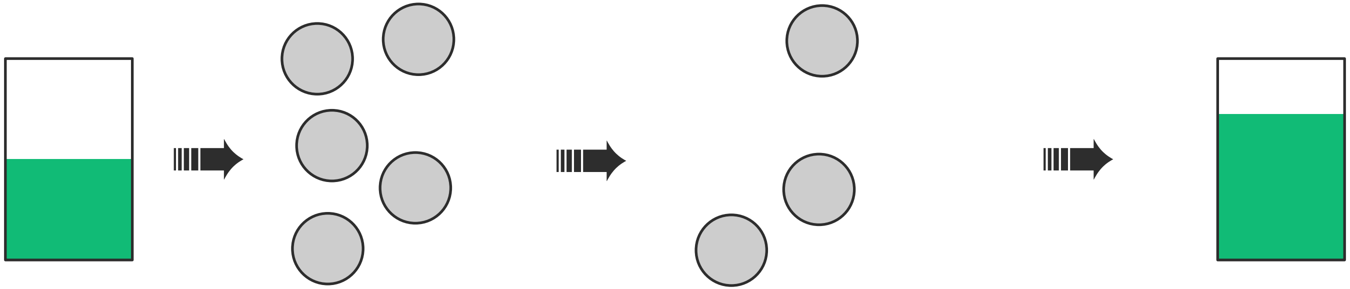

$\boldsymbol{p}_i^{(t)}$ samples $\left\{\boldsymbol{x}^{(j)}\right\}_{j\in[\lambda]}$ **selected** samples $\left\{\hat{\boldsymbol{x}}^{(k)}\right\}_{k\in[\mu]}$ (ordered by decreasing fitness) $\boldsymbol{p}_i^{(t+1)}$

$$\mathrm{E}\left[\boldsymbol{p}_i^{(t+1)} - \boldsymbol{p}_i^{(t)} \mid \boldsymbol{p}^{(t)}\right]$$

drift

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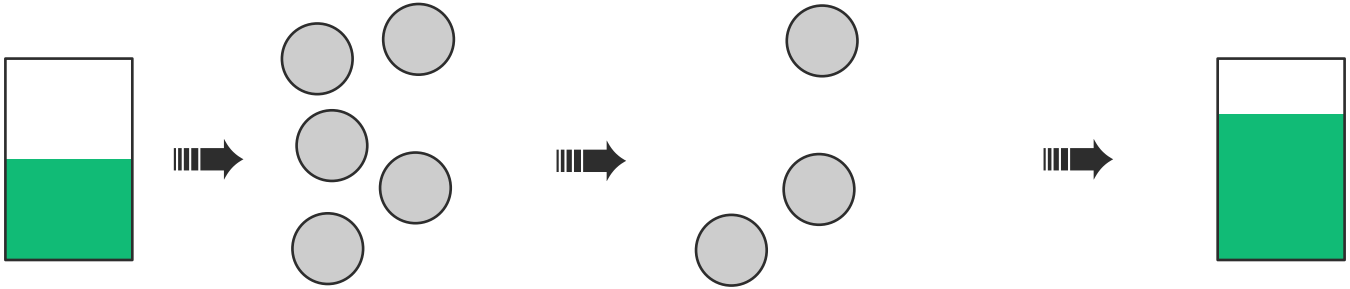

$\boldsymbol{p}_i^{(t)}$

samples $\left\{\boldsymbol{x}^{(j)}\right\}_{j\in[\lambda]}$

**selected** samples $\left\{\hat{\boldsymbol{x}}^{(k)}\right\}_{k\in[\mu]}$

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$\boldsymbol{p}_i^{(t+1)}$

$$\mathrm{E}\left[\boldsymbol{p}_i^{(t+1)} - \boldsymbol{p}_i^{(t)} \mid \boldsymbol{p}^{(t)}\right]$$

drift

» Estimating the drift, estimates the expected time that the frequency passes a specific value

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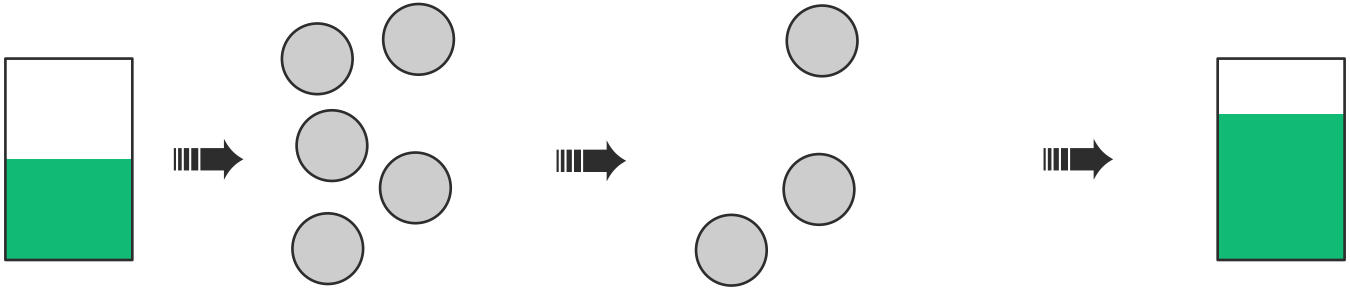

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drift

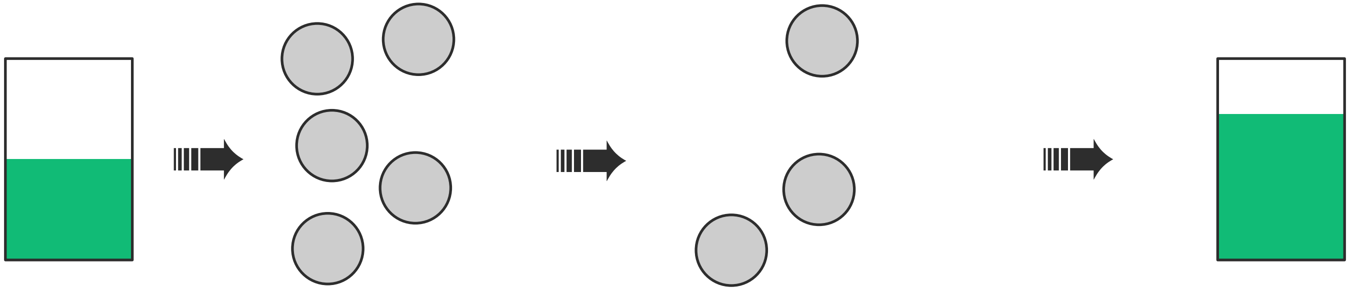
» Estimating the drift, estimates the expected time that the frequency passes a specific value

❖ **Drift analysis**

- 1712.00964 [Lengler'18]
- 2406.14589 [Kötzing'24]

# Updating a Frequency (commonly)

**Very tricky!**



$\boldsymbol{p}_i^{(t)}$ samples $\{\boldsymbol{x}^{(j)}\}_{j\in[\lambda]}$ **selected** samples $\{\hat{\boldsymbol{x}}^{(k)}\}_{k\in[\mu]}$ (ordered by decreasing fitness) $\boldsymbol{p}_i^{(t+1)}$

$$\mathrm{E}\left[\boldsymbol{p}_i^{(t+1)} - \boldsymbol{p}_i^{(t)} \mid \boldsymbol{p}^{(t)}\right]$$

drift

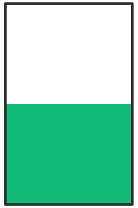
» Estimating the drift, estimates the expected time that the frequency passes a specific value

❖ **Drift analysis** 1712.00964 [Lengler'18]

2406.14589 [Kötzing'24]

# Updating a Frequency (Genetic drift)

» **What** happens if the samples are **not** informative?



$\boldsymbol{p}_i^{(t)}$

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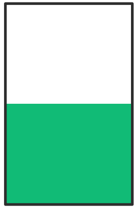

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» Can happen regularly during a run

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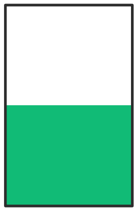

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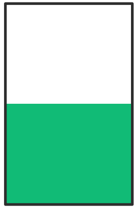

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- Typical property of univariate EDAs

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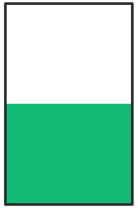

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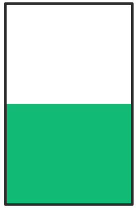

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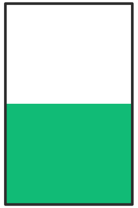

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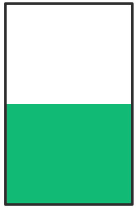

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drift via ➡ variance

$$\approx \frac{d}{\mathrm{Var}\left[\boldsymbol{p}_i^{(t+1)} \mid \boldsymbol{p}^{(t)}\right]}$$

[K.'19]

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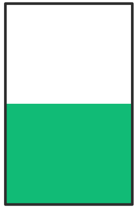

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[K.'19]

» This hitting time is **concentrated**

[Doerr, Zheng'20]

# Commonly Studied EDAs

Compact Genetic Algorithm (cGA)
[Harik, Lobo, Goldberg'99]

Univariate Marginal Distribution Algorithm (UMDA)
[Mühlenbein, Paaß'96]

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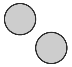

» $\lambda = 2$ samples each iteration

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[Mühlenbein, Paaß'96]

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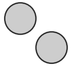

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$$p_i^{(t+1)} = p_i^{(t)} + \frac{1}{K}\left(\hat{x}_i^{(1)} - \hat{x}_i^{(2)}\right)$$

hypothetical population size

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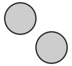

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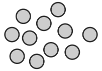

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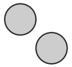

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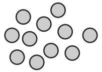

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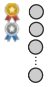

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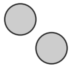

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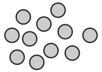

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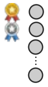

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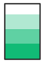

» **Set** to the relative number of 1s

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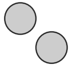

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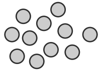

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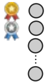

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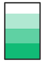

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$$\boldsymbol{p}_i^{(t+1)} = \frac{1}{\mu}\sum_{k\in[\mu]} \widehat{\boldsymbol{x}}_i^{(k)}$$

# Commonly Studied EDAs

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[Harik, Lobo, Goldberg'99]

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hypothetical population size

## Univariate Marginal Distribution Algorithm (UMDA)

[Mühlenbein, Paaß'96]

- » $\lambda$ samples each iteration
- » Select $\mu \leq \lambda$ best samples, ranking them
- » **Set** to the relative number of 1s

$$\boldsymbol{p}_i^{(t+1)} = \frac{1}{\mu}\sum_{k\in[\mu]} \widehat{\boldsymbol{x}}_i^{(k)}$$

- » Population-based incremental learning [Baluja'**94**]
- » 2-Max-Min ant system with iteration-best update [Neumann, Sudholt, Witt'10]

# Commonly Studied EDAs

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hypothetical population size ($K$)

## Univariate Marginal Distribution Algorithm (UMDA)

[Mühlenbein, Paaß'96]

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» Population-based incremental learning [Baluja'**94**]

» 2-Max-Min ant system with iteration-best update [Neumann, Sudholt, Witt'10]

All are **balanced!** (starting with the uniform distribution)

# Commonly Studied EDAs (variances)

## Compact Genetic Algorithm (cGA)

## Univariate Marginal Distribution Algorithm (UMDA)

$$\mathrm{Var}\left[\boldsymbol{p}_i^{(t+1)} \mid \boldsymbol{p}^{(t)}\right] = \mathrm{Var}\left[\boldsymbol{p}_i^{(t)} + \frac{1}{K}\left(\widehat{\boldsymbol{x}}_i^{(1)} - \widehat{\boldsymbol{x}}_i^{(2)}\right) \mid \boldsymbol{p}^{(t)}\right]$$

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$$= \frac{1}{K^2} \cdot \mathrm{Var}\left[\hat{\boldsymbol{x}}_i^{(1)} - \hat{\boldsymbol{x}}_i^{(2)} \mid \boldsymbol{p}^{(t)}\right]$$

## Univariate Marginal Distribution Algorithm (UMDA)

# Commonly Studied EDAs (variances)

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$$= \frac{1}{K^2} \cdot \left(\mathrm{Var}\left[\widehat{\boldsymbol{x}}_i^{(1)} \mid \boldsymbol{p}^{(t)}\right] + \mathrm{Var}\left[\widehat{\boldsymbol{x}}_i^{(2)} \mid \boldsymbol{p}^{(t)}\right]\right)$$

## Univariate Marginal Distribution Algorithm (UMDA)

# Commonly Studied EDAs (variances)

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$$= \frac{2}{K^2} \boldsymbol{p}_i{}^{(t)}\left(1 - \boldsymbol{p}_i{}^{(t)}\right)$$

## Univariate Marginal Distribution Algorithm (UMDA)

# Commonly Studied EDAs (variances)

## Compact Genetic Algorithm (cGA)

## Univariate Marginal Distribution Algorithm (UMDA)

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$$= \frac{2}{K^2}\, \boldsymbol{p}_i{}^{(t)}\left(1 - \boldsymbol{p}_i{}^{(t)}\right)$$

➡ $\boldsymbol{p}_i$ covers a distance of at most $\frac{1}{4}$ with constant probability within $\Theta(K^2)$ iterations

# Commonly Studied EDAs (variances)

## Compact Genetic Algorithm (cGA)

$$\mathrm{Var}\left[\boldsymbol{p}_i^{(t+1)} \mid \boldsymbol{p}^{(t)}\right] = \mathrm{Var}\left[\boldsymbol{p}_i^{(t)} + \frac{1}{K}\left(\widehat{\boldsymbol{x}}_i^{(1)} - \widehat{\boldsymbol{x}}_i^{(2)}\right) \mid \boldsymbol{p}^{(t)}\right]$$

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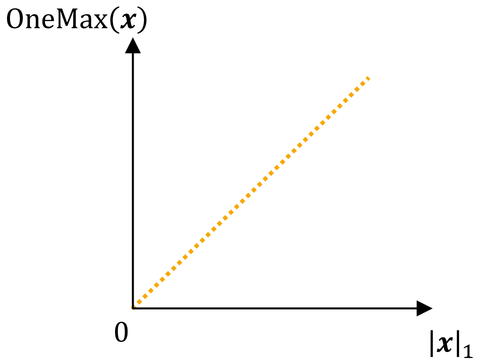
» The trick carries over to weak preferences of bit values [Doerr, Zheng'20]

# Commonly Studied Benchmarks

OneMax




$$\boldsymbol{x} \mapsto \sum_{i \in [n]} \boldsymbol{x}_i =: |\boldsymbol{x}|_1$$

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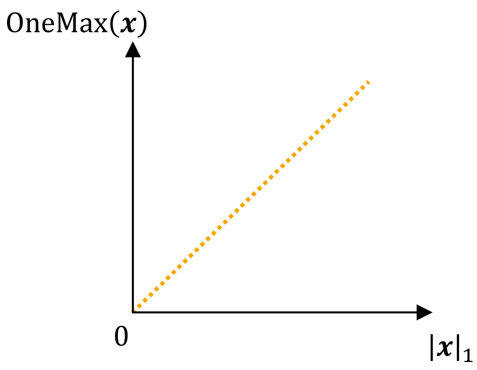


LeadingOnes

110000011010

111110000100

$\boldsymbol{x} \mapsto \sum_{i\in[n]} \boldsymbol{x}_i =: |\boldsymbol{x}|_1$ $\quad$ $\boldsymbol{x} \mapsto \max\{i \in [0..n] \mid \forall j \in [i]: \boldsymbol{x}_j = 1\}$

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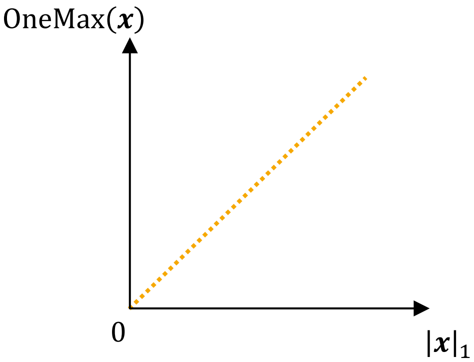


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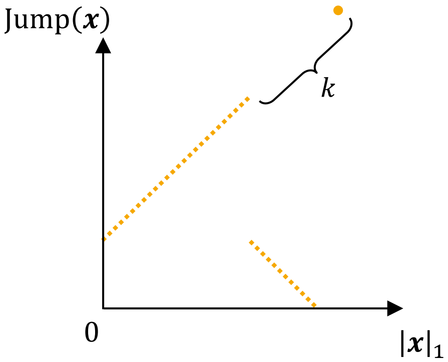
## Jump




$$\boldsymbol{x} \mapsto \begin{cases} k + |\boldsymbol{x}|_1 & \text{if } |\boldsymbol{x}|_1 \in [n-k] \cup \{n\} \\ n - |\boldsymbol{x}|_1 & \text{else} \end{cases}$$

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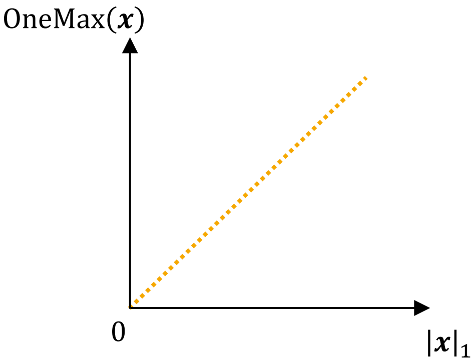


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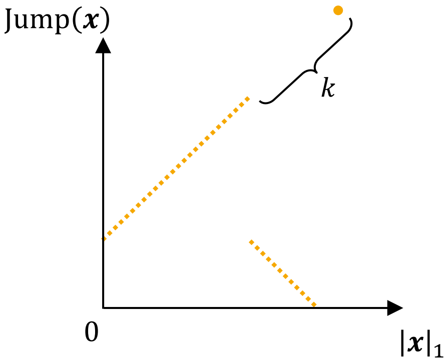


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$\boldsymbol{x} \mapsto \sum_{i \in [n]} 2^{n-i} \cdot \boldsymbol{x}_i$

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| | OneMax | LeadingOnes | Jump | BinVal |
|---|---|---|---|---|
| cGA | ✔ [Droste'06; Lengler, Sudholt, Witt'18; Sudholt, Witt'19] | ✖ | ✔ [Hasenöhrl, Sutton'18; Doerr'21; Witt'23] | ✔ [Droste'06; Witt'18] |
| UMDA | ✔ [Dang, Lehre, Nguyen'18; Witt'19; K., Witt'20] | ✔ [Dang, Lehre, Nguyen'18; Doerr, K.'21] | ✖ | ✔ [Dang, Lehre, Nguyen'18] |

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**Also:** (non-exhaustive)

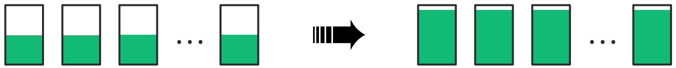
» Analyses on noise [Friedrich, Kötzing, K., Witt'17; Lehre, Nguyen'19; Lehre, Nguyen'21; Kötzing, Radhakrishnan'22]

» Analyses on deception [Lehre, Nguyen'19; Doerr, K.'21]

» New EDAs [Doerr, K.'20; Ajimakin, Devi'23]

» Multi-valued EDAs [Ben Jedidia, Doerr, K.'24; Adak, Witt'24]

# cGA on OneMax

Our aim: 

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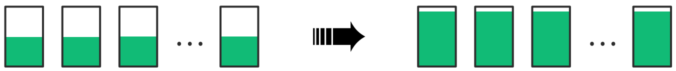
Our aim: 

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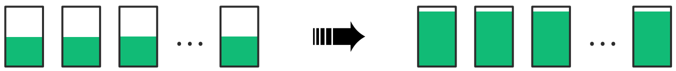
Our aim: 

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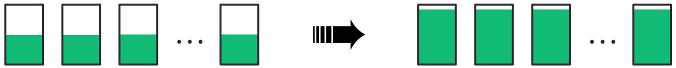
Our aim: 

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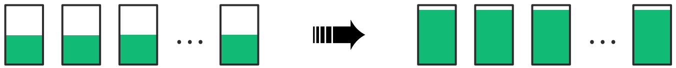
Our aim: 

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» Ignoring the case $D = 1$ does not change the result asymptotically here

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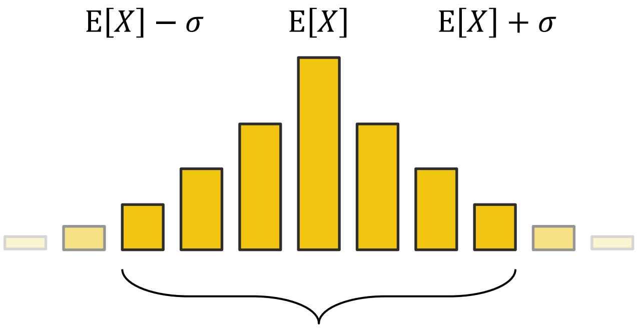


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# cGA on OneMax (the sampling variance)

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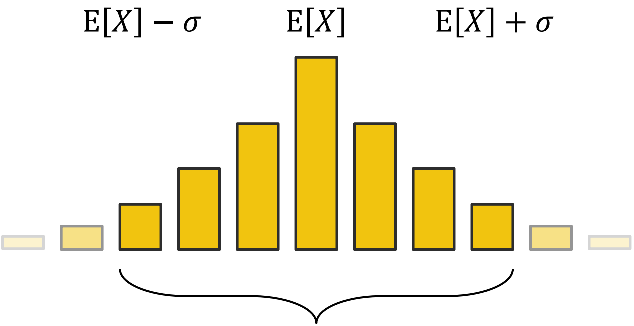


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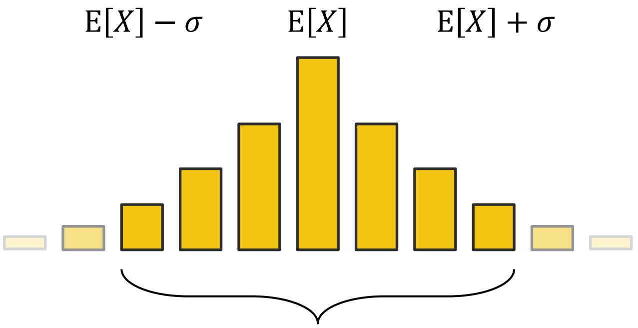


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sampling variance

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- For $K \in O\left(\frac{\sqrt{n}}{\log(n) \log \log n}\right)$ the run time is in $\Omega\left(K^{1/3}n + n \log n\right)$ [Lengler, Sudholt, Witt'18]
  - Covers **high** genetic drift

# UMDA on OneMax (with borders)

[Witt'18] 1. The UMDA with $\mu \in \Omega(\sqrt{n} \log n)$ and $\lambda = (1 + \Theta(1))\mu$ optimizes OneMax in $O(\lambda\sqrt{n})$ function evaluations in expectation. This is $O(n \log n)$ for minimal $\lambda$.

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» Analysis by Witt very similar to the cGA, but some steps are vastly different

- It analogously holds that $\mathrm{E}\left[\boldsymbol{p}_i^{(t+1)} - \boldsymbol{p}_i^{(t)} \mid \boldsymbol{p}^{(t)}\right] \gtrsim \boldsymbol{p}_i^{(t)}\left(1 - \boldsymbol{p}_i^{(t)}\right)$, but for different reasons, involving 1st- and 2nd-class individuals

# UMDA on OneMax (with borders)

[Witt'18] 1. The UMDA with $\mu \in \Omega(\sqrt{n}\log n)$ and $\lambda = (1+\Theta(1))\mu$ optimizes OneMax in $O(\lambda\sqrt{n})$ function evaluations in expectation. This is $O(n\log n)$ for minimal $\lambda$.

- **Low** genetic drift.
- Holds with high probability also without borders.

2. The UMDA with $\mu \in \Omega(\log n) \cap O(n^{1-\varepsilon})$ and $\lambda = (1+\Theta(1))\mu$ optimizes OneMax in $O(\lambda n)$ function evaluations in expectation. This is $O(n\log n)$ for minimal $\lambda$.

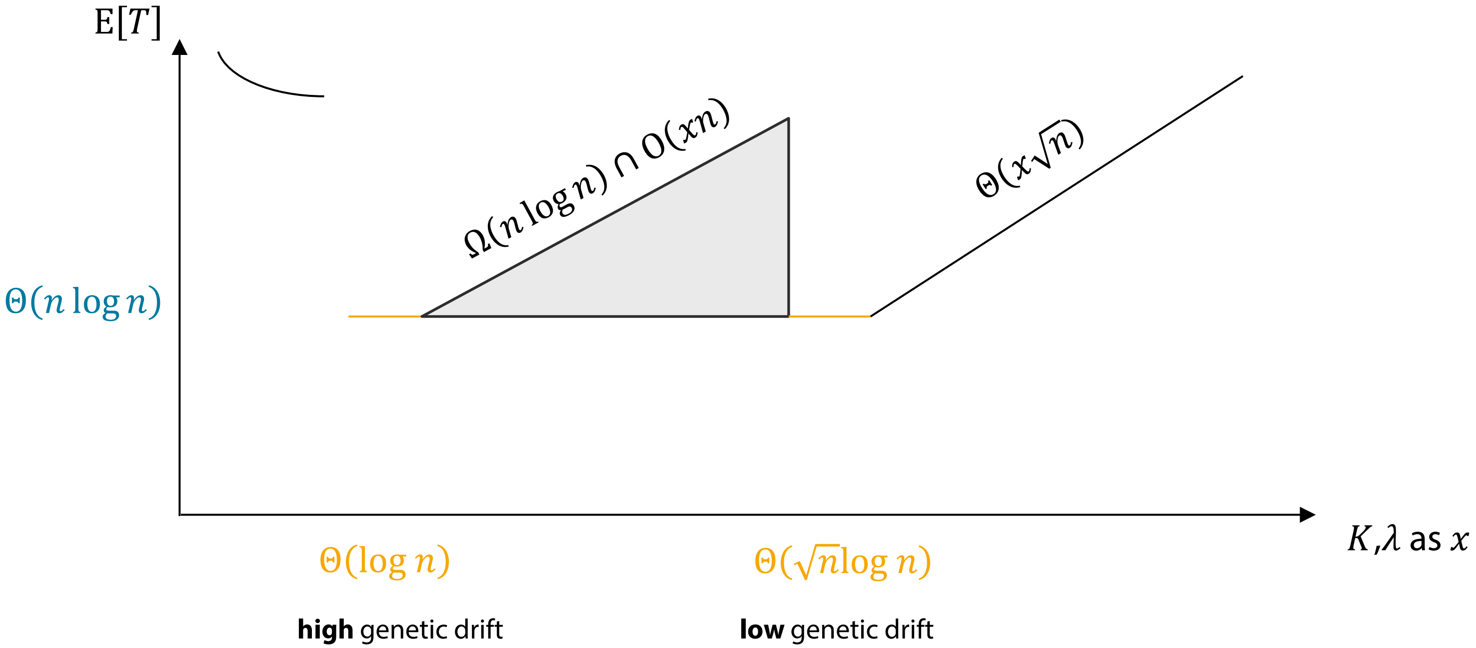
- **High** genetic drift.
- Only holds **with** borders, otherwise infinite even whp.

[Lehre, Nguyen'18] The UMDA with $\mu \in \Omega(\log n) \cap O(\sqrt{n})$ and $\lambda = (1+\Omega(1))\mu$ optimizes OneMax in $O(\lambda n)$ function evaluations in expectation. This is $O(n\log n)$ for minimal $\lambda$.

- **High** genetic drift.

- Analysis by Witt very similar to the cGA, but some steps are vastly different
  - It analogously holds that $\mathrm{E}\left[\boldsymbol{p}_i^{(t+1)} - \boldsymbol{p}_i^{(t)} \mid \boldsymbol{p}^{(t)}\right] \gtrsim \boldsymbol{p}_i^{(t)}\left(1-\boldsymbol{p}_i^{(t)}\right)$, but for different reasons, involving 1st- and 2nd-class individuals
- Analysis by Lehre and Nguyen simpler, utilizing a **level-based method**

# cGA and UMDA on OneMax



# cGA and UMDA on OneMax