Revisiting the Analysis of Population Variance in Differential Evolution Algorithms

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Context

- Current status:
  - most of knowledge on DE behavior relies on empirical analysis

    (intuition $\longrightarrow$ empirical validation $\longrightarrow$ practical guidelines)

  - most theoretical results rely on simplifying assumptions

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    (intuition $\longrightarrow$ empirical validation $\longrightarrow$ practical guidelines)
  - most theoretical results rely on simplifying assumptions
- Goal: develop robust guidelines and practical support for application development based on theoretical insights combined with empirical remarks
- Aim of this paper: revisit some theoretical results under more realistic assumptions
  - relationships between the expected variance of the trial population and the control parameters
    - influence of random reinitialization of trial components which violate the bound constraints
  - critical regions in the control parameter space which induces a decrease in the population variance even in the absence of selection pressure
    - comparison with empirically estimated regions of premature convergence

DE particularity

$$\underbrace{X(g)}_{\text{current population}} \xrightarrow[\text{mutation}]{} \underbrace{Y}_{\text{mutant population}} \xrightarrow[\text{crossover}]{} \underbrace{Z}_{\text{trial population}} \xrightarrow[\text{selection}]{} \underbrace{X(g+1)}_{\text{new population}}$$

- DE hallmark: difference based mutation

$$Y = \underbrace{\text{Base vector}}_{x_{r_1}(\text{random}), x_*(\text{best}), x_i(\text{current})\ldots} + \underbrace{\text{Scaled sampled difference}}_{F\cdot(x_{r_2} - x_{r_3}), \ldots}$$

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- Main control parameters: scale factor (F), crossover rate (CR)
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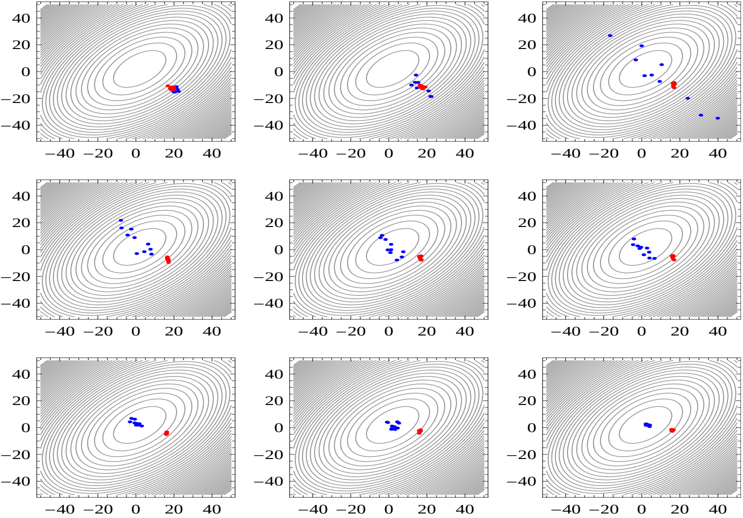
- Main control parameters: scale factor (F), crossover rate (CR)
- Mutation probability (p_m) controlled by crossover rate (CR)
- Main source of variation: population diversity

$\longrightarrow$ no progress in the absence of diversity $\longrightarrow$ premature convergence

DE particularity



CMA-ES

DE
DE/rand/1/bin,
$CR = 0.5$,
$F = 0.5$

Generations:
2,4,...,18
Premature
convergence

Neumaier function: $f(x) = \sum_{i=1}^{n}(x_i - 1)^2 - \sum_{i=2}^{n} x_i x_{i-1}$, $(n = 2)$

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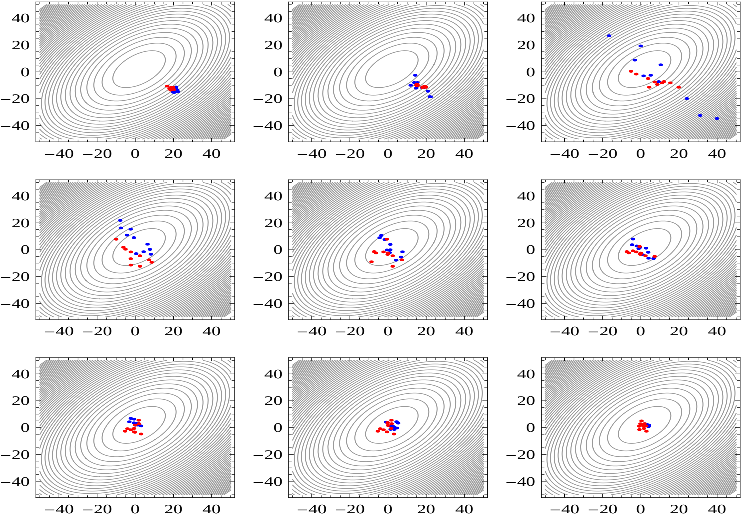

CMA-ES

DE

DE/rand/1/bin,

$CR = 0.5$,

$F = 0.8$

Generations:

2,4,...,18

Neumaier function: $f(x) = \sum_{i=1}^{n}(x_i - 1)^2 - \sum_{i=2}^{n} x_i x_{i-1}$, $(n = 2)$

Measuring the population diversity

- How is influenced the population diversity by changes in the control parameters?
- Measure of population diversity: averaged component-wise variance

$$
\begin{array}{ccccccc}
X_1 & = & [x_1^1, & x_1^2, & \ldots & x_1^j & \ldots & x_1^n] \\
\ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\
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X_m & = & [x_m^1, & x_m^2, & \ldots & x_m^j & \ldots & x_m^n] \\
\hline
 & & \mathrm{Var}(X^1) & \mathrm{Var}(X^2) & \ldots & \mathrm{Var}(X^j) & \ldots & \mathrm{Var}(X^n) & \underset{average}{\longrightarrow} & \underbrace{\langle \mathrm{Var}(X) \rangle}_{empirical \quad variance} \\
\hline
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Remark

The analysis of the variance is conducted at component level

Expected variance of trial population

$$\underbrace{Y_i}_{\text{mutant}} = \underbrace{x_{I_i}}_{\text{random base vector}} + \underbrace{\mathcal{P}_i}_{\text{random perturbation}}$$

$$Z_i^k = \begin{cases} x_i^k & \text{with probability } 1 - p_m \\ x_{I_i}^k + \mathcal{P}_i^k & \text{with probability } p_m \end{cases}, \qquad i = \overline{1, k}$$

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- $Z_i^k = x_i^k \mathbf{1}_{\overline{M}_i} + Y_i^k \mathbf{1}_{M_i}$
- M_i-mutation event, $prob(M_i) = p_m$
- component-wise analysis
  x_{I_i}, Y_i, Z_i - random variables
- $\mathbb{E}[\mathrm{Var}(Z)] = \frac{m-1}{2m}\mathbb{E}[(Z_i - Z_j)^2]$
  ($i \neq j$, selection without replacement)

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$$+2p_m(1 - p_m)\mathbb{E}[((X_i - X_{I_j}) - \mathcal{P}_j)^2]$$

$$+p_m^2\mathbb{E}[((X_{I_i} - X_{I_j}) + (\mathcal{P}_i - \mathcal{P}_j))^2]$$

Assumption: $\mathcal{P}$ independent of X (not true for DE)

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Trial population vs current population variance: linear dependence

$$\mathbb{E}[\mathrm{Var}(Z)] = \underbrace{\left(1 - \frac{p_m(2-p_m)}{m}\right)}_{c(p_m,m)}\mathrm{Var}(X) + \underbrace{p_m(2-p_m)\frac{m-1}{m}}_{d(p_m,m,\mathcal{P})}\mathrm{Var}(\mathcal{P})$$

Expected variance of trial population - DE/rand/*

DE case: Var($\mathcal{P}$) depends on Var(X) $\Longrightarrow d(p_m, m, ...) = 0$

DE/rand/1/*

$$Y_i = x_{I_i} + F \cdot (x_{J_i} - x_{K_i})$$

$$\mathbb{E}[\mathrm{Var}(Z)] = \left(1 + 2p_m F^2 - \frac{p_m(2 - p_m)}{m}\right) \mathrm{Var}(X)$$

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p_m vs CR

Binomial crossover:

$$p_m = CR\left(1 - \frac{1}{n}\right) + \frac{1}{n}$$

Exponential crossover:

$$p_m = \frac{1 - CR^n}{n(1 - CR)}$$

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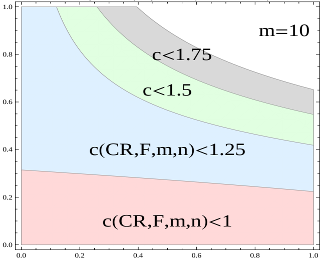
Remarks

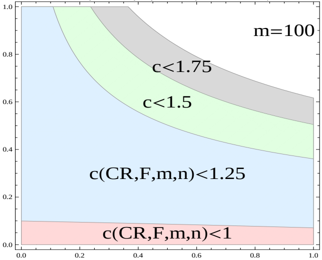
- influence of problem size - incorporated through the relationship between p_m and CR
- impact on variance of DE/rand/2/* $\Longleftrightarrow$ impact of DE/rand/1/* for $\sqrt{2}F$

$$c(CR, F, m, n) = \left(1 + 2p_m F^2 - \frac{p_m(2-p_m)}{m}\right), \qquad p_m = CR(1 - 1/n) + 1/n$$

DE/rand/1/bin (F vs CR)



DE/rand/1/bin (F vs CR)



Critical regions - DE/rand/1/bin

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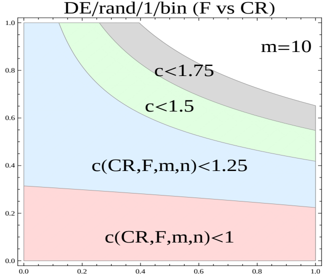
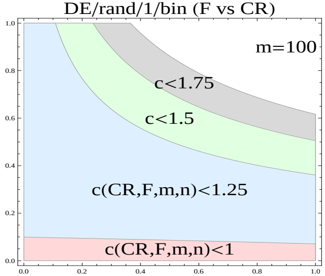
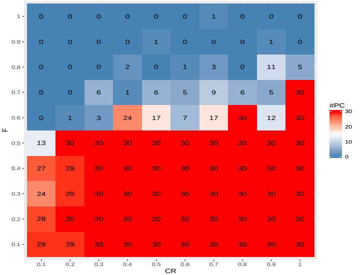




$c(CR, F, m, n) < 1 \Longrightarrow$ decrease of variance



Empirical estimation of premature convergence: $\text{Var}(X) < 10^{-8}$
Runs: 30
Function: Neumaier, $n = 6, m = 10$
Max. generations = 500
Bound constraint handling: resampling

Critical regions - DE/rand/1/bin

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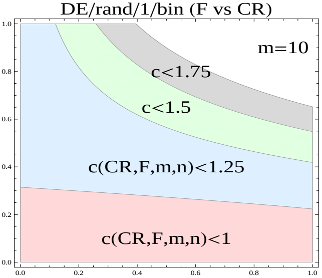
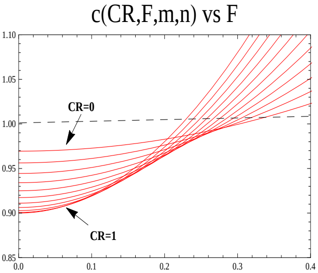
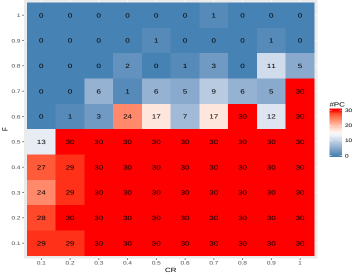
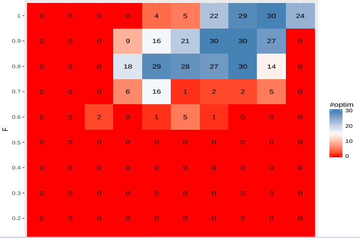




Premature convergence cases

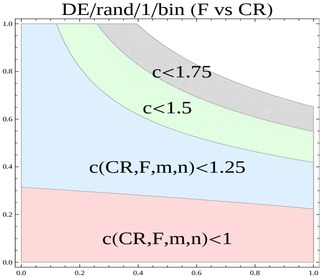


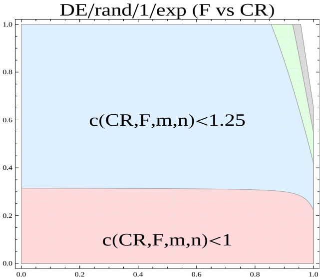
Successful cases



Critical regions - binomial vs exponential

$$c(CR, F, m, n) = \left(1 + 2p_m F^2 - \frac{p_m(2-p_m)}{m}\right)$$





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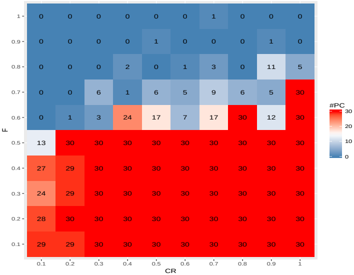

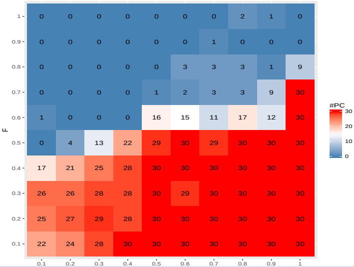

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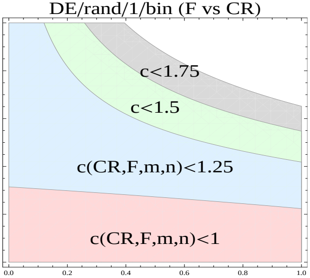

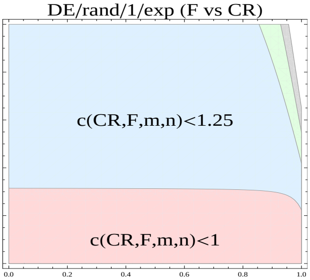

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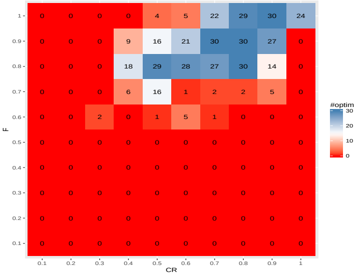
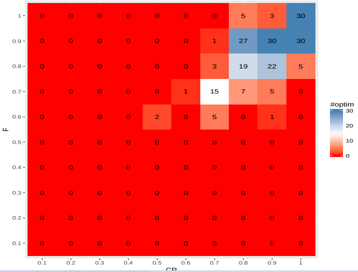




Expected variance of trial population

DE/either-or

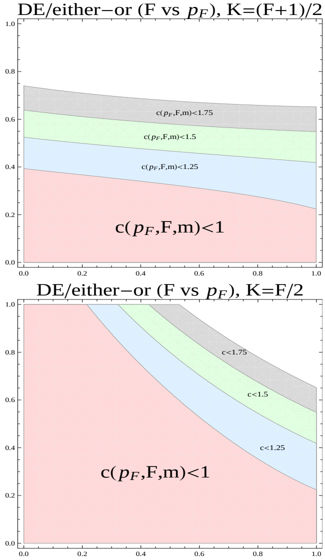
$$Z_i = \begin{cases} x_{I_i} + F \cdot (x_{J_i} - x_{K_i}) & \text{with probability } p_F \\ x_{I_i} + K \cdot (x_{J_i} + x_{K_i} - 2x_{I_i}) & \text{with probability } 1 - p_F \end{cases}$$

$$\mathbb{E}[\mathrm{Var}(Z)] = \Big(p_F^2(1 + 2F^2 - \tfrac{1}{m}) + 2p_F(1 - p_F)(\tfrac{m-1}{m} + F^2 + 3K^2 - 2K) + (1 - p_F)^2\left(\tfrac{m-1}{m} + 2\tfrac{m-2}{m}(3K^2 - 2K)\right)\Big)\,\mathrm{Var}(X)$$

Remarks

- no influence of current element on the trial element
- no influence of problem size on the variance

Critical regions - DE/either-or



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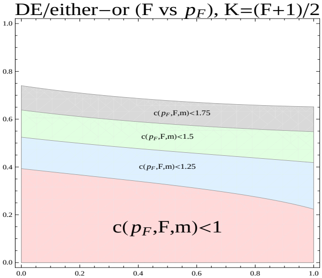

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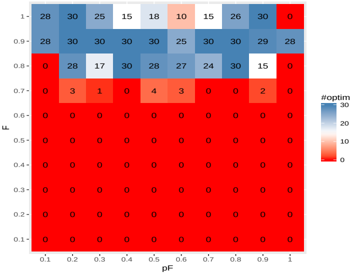
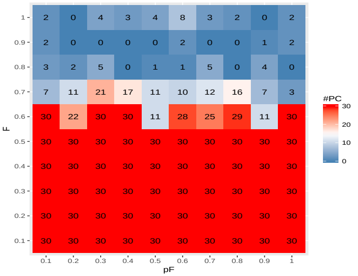
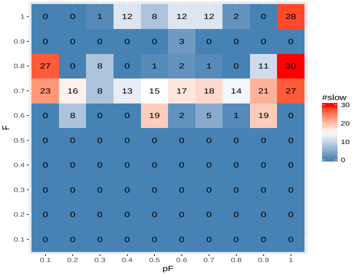


Premature convergence cases



Slow evolution cases



Expected variance of trial population

DE/best/1/*

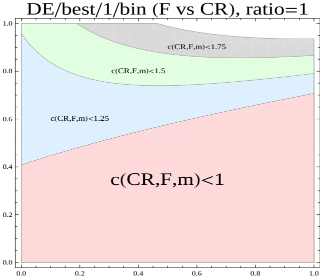
$$Y_i = x_* + F \cdot (x_{J_i} - x_{K_i})$$

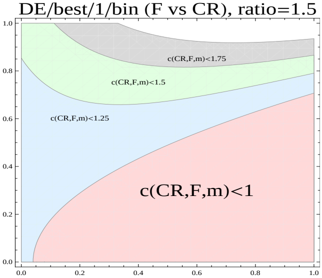
$$\mathbb{E}[\mathrm{Var}(Z)] = \left(1 + 2p_m F^2 - p_m - \frac{p_m(1-p_m)}{m}\right)\mathrm{Var}(X) + p_m(1-p_m)\frac{m-1}{m}(x_* - \overline{X})^2$$

Remarks

- the deviation of the best element with respect to the population average might act as a diversity promoter
- the ratio $\frac{(x_* - \overline{X})^2}{\mathrm{Var}(X)}$ takes values in $[0, 2+)$

Critical regions - DE/best/1/*





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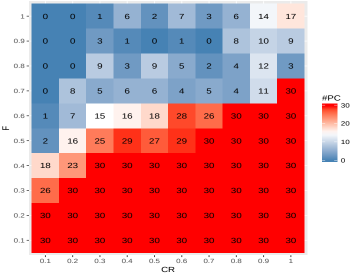

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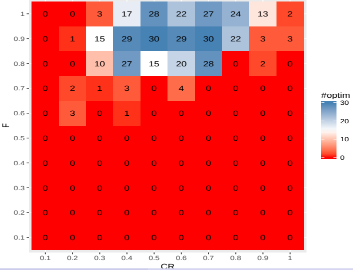
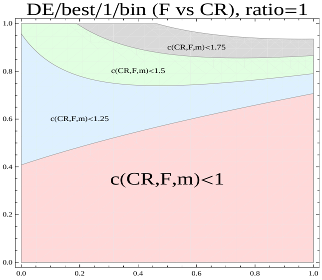
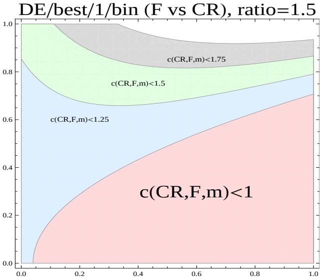
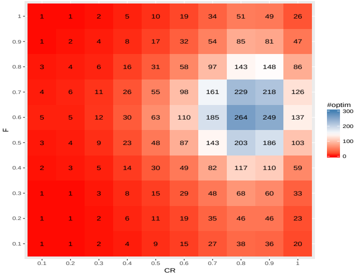


DE/best/1/* critical regions vs JADE parameters





Distribution of successful parameter values



How should be sampled the control parameter space?

- values outside the region characterized by $c(CR, F, m, n, ...) < 1$
- ... but close to the border

Handling bound constraints

- Bound constraint: $z \in [a, b]$ (for each component)
- Handling methods:
  - random reinitialization ($z \in \mathcal{U}_{[a,b]}$)
  - resampling (z is reconstructed based on newly selected parents)
  - projection on the closest bound ($z < a \longrightarrow z = a$, $z > b \longrightarrow z = b$)
  - reflection ($z < a \longrightarrow z = 2a - z$, $z > b \longrightarrow z = 2b - z$)

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- Questions:
  - How frequently are bound constraints violated by DE/rand/1 trial vectors?
  - Which is the impact of random reinitialization on the expected variance of the trial population?

Bound violation probability

- Assumptions: $a = 0$, $b = 1$, $F \in (0, 1]$,
- $Y = x_I + F \cdot (x_J - x_K) \longrightarrow Y \in [-F, 1 + F]$

[1] M. Ali, L. Fatti, A Differential Free Point Generation Scheme in the DE Algorithm, Journal of Global Optimization, 2006

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$$f_Y(y) = \begin{cases} (F + y)^2/(2F^2) & \text{if } -F \leq y \leq 0 \\ (F - y + 1)^2/(2F^2) & \text{if } 1 \leq y \leq 1 + F \end{cases}$$

- Probability of violating the bounds:
$P(Y \in [-F, 0) \cup (1, 1 + F] = \int_{-F}^{0} f_Y(y)dy + \int_{1}^{1+F} f_Y(y)dy$

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Violation probability

- if the population is almost uniformly distributed (i.e. during the first generations) then $p_v = F/3$

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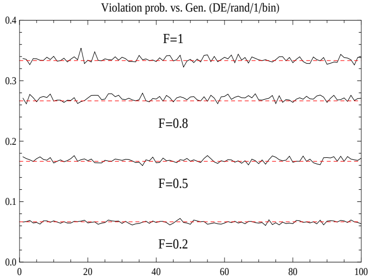
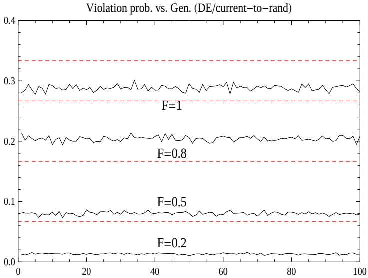
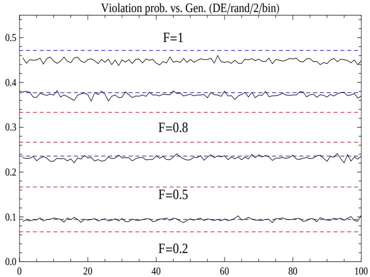
Violation probability (theoretical vs empirical)







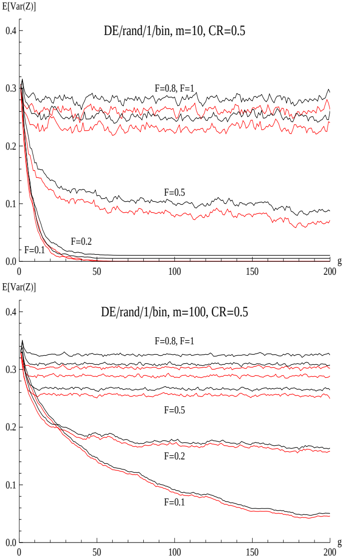
Remarks

- For DE/rand/2 the violation probability is close to $F\sqrt{2}$
- The violation probability is smaller if an interior point is used (as in DE/current-to-rand)

Expected variance of trial population - DE/rand/1 + random repairing

- $\mathbb{E}[\mathrm{Var}(Z)] = c(p_m, p_v, m, F)\cdot \mathrm{Var}(X) + d(p_m, p_v, m, a, b)$
- $$c(p_m, p_v, m, F) = (1-p_m)^2 + p_m p_v (1-p_m)\frac{m-1}{m} + p_m^2(1-p_v)^2 B\left[\frac{m-1}{m} + 2F^2\right]$$
  $$+2p_m(1-p_m)B\left[\frac{m-1}{m} + F^2\right] + 2p_m^2 p_v(1-p_v)B\left[\frac{(m-1)^2}{2m^2} + \frac{m-1}{m}F^2\right]$$
  $$B(u) = \begin{cases} u & \text{if } u \le 1 \\ 1 & \text{if } u > 1 \end{cases}$$
- $$d(p_m, p_v, m, a, b) = p_m p_v (1 - p_m p_v)\frac{m-1}{m}\left(\overline{X} - \frac{a+b}{2}\right)^2$$
  $$+p_m p_v\left(1 - \frac{1-p_m p_v}{m}\right)(b-a)^2/12$$

Expected variance vs empirical variance

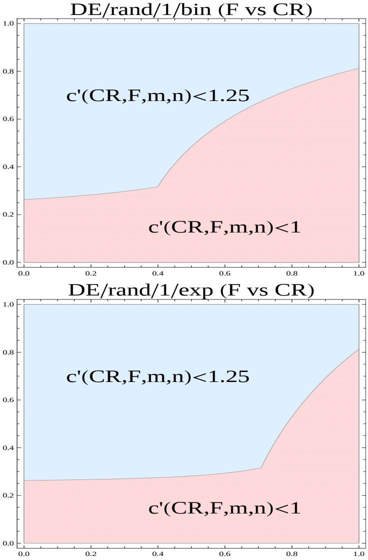


Assumptions

- flat landscape $\longrightarrow$ almost uniformly distributed population
- $\overline{X} - (a+b)/2 \simeq 0$
- $\mathrm{Var}(X) \simeq (b-a)^2/12$
- $\mathbb{E}[\mathrm{Var}(Z(g))] \simeq c'(p_m, p_v, m, F) \cdot \mathrm{Var}(X(g))$

Theoretical estimation - black line
Empirical estimation - red line

Critical regions - DE/rand/1 + random repairing



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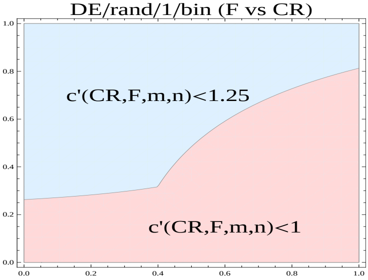

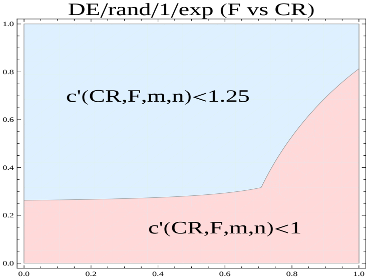

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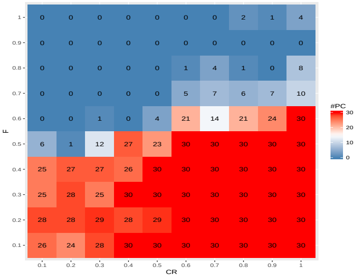
Premature convergence cases



Summary

- Different DE variants have different impact on the population diversity $\longrightarrow$ different critical regions
- The theoretical results on expected population variance might be used to guide the choice/adaptation of the control parameters in order to avoid systematic sampling from critical regions
- Bound constraints handling
  - probability of bound constraint violation is $F/3$ (DE/rand/1/* - first stage of evolution)
  - random reinitialization changes the shape of critical regions