On control charting normal variance

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Outline.

1. Introduction.
2. Modelling.
3. ARL calculation for Shiryaev-Roberts.
4. Competing statistics and 2-sided EWMA.
5. Summary.

Why should we apply SPC* to variance?

- Ensure appropriate control limits for mean chart.
- Detect deteriorated uniformity, repeatability, roughness, ...
  – increased variance level in general.

- Woodall & Montgomery (1999) demanded it ;-)

Woodall/Montgomery (1999), Research issues and ideas in statistical process control. *Journal of Quality Technology, 31, 376-386*

*Statistical Process Control

Two examples from a Mask Shop.

1. CD (critical dimension) uniformity:
   - Measure a certain number (20 ... 200) of, e. g., lines of nominal size 200 *nm* on a single plate,
   - calculate sample mean $\bar{CD}$ and standard deviation S_{CD},
   - chart both.

2. Gauge repeatibility – CD-SEM (scanning electron microscope):
   - Repeat a few times (e. g., 5) the measurement of one given line,
   - calculate standard deviation S_R,
   - chart it.

Modelling.

Modelling.

- Sequence $\{X_{ij}\}$, $i = 1, 2, \ldots$ and $j = 1, 2, \ldots, n \geq 1$ with $X_{ij} \sim \mathcal{N}(\mu, \sigma^2)$, independence.
- The change-point model: For a certain unknown m

$$\sigma^2 = \begin{cases} \sigma_0^2 = 1 & , \; i < m \\ \sigma_1^2 >(\neq)\; \sigma_0^2 & , \; i \geq m \end{cases} .$$

- Consider only changes between and not within samples.
- ... a lot of different statistics and control chart types.

Statistics.

$$R_i = \max_j X_{ij} - \min_j X_{ij} \, ,$$

$$S_i^2 = \frac{1}{n-1} \sum_{j=1}^{n} \left(X_{ij} - \bar{X}_i \right)^2 \qquad , \; \bar{X}_i = \frac{1}{n} \sum_{j=1}^{n} X_{ij} \, ,$$

$$S_i = \sqrt{S_i^2} \, ,$$

$$lS_i^2 = \log S_i^2 \qquad \text{– Crowder/Hamilton (1992) ,}$$

$$abcS_i^2 = a + b \, \log(S_i^2 + c) \qquad \text{– Castagliola (2005) .}$$

... control charts.

- Apply one of the statistics in
- control charts such as
  Shewhart, EWMA, CUSUM, Shiryaev-Roberts
- and consider performance measures such as
  zero-state and steady-state Average Run Length (ARL).

- Take $\sigma_1 = 1.5$
- and S^2 with batch size $n = 1$ (for given μ_0, here $\mu_0 = 0$) as illustrative example.

Shewhart Chart.

- Oldest scheme, natural extension of Shewhart's p and $\bar{X}$ chart.
- Flag if X_i^2 is large; more formal $L = \inf\{i \in I\!N : X_i^2 > c_u\}$.
- $X_i^2 \sim \chi_1^2$ for $i < m$, otherwise $X_i^2/\sigma_1^2 \sim \chi_1^2$
- Choose c_u so that $E_\infty(L) = A$.
- L is geometrically distributed with $p = P\left(X_i^2 > c_u\right)$.
  - $E_\infty(L) = p^{-1}$.
  - $c_u = F_{\chi_1^2}^{-1}\left(1 - A^{-1}\right)$.

CUSUM.

- Page (1954).
- Based on the log-likelihood ratio of pre- and post-change distribution.
- $$C_0 = 0\ , \quad C_i = \max\{0, C_i + X_i^2 - k\}\ , \quad k = \frac{2\log\sigma_1}{1-\sigma_1^{-2}}\ ,$$
  $$L = \inf\{i \in I\!N : C_i > c_u\}\ .$$
- Worst-case optimal –
  Lorden (1971), Moustakides (1986), Ritov (1990).

EWMA.

- Roberts (1959).
- No (log-)likelihood ratio involved.
- $$Z_0 = 1\,, \quad Z_i = (1-\lambda)Z_{i-1} + \lambda X_i^2\,, \quad \lambda \in (0,1]\,,$$
  $$L = \inf\{i \in I\!N : Z_i > c_u\}\,.$$
- EWMA (exponentially weighted moving average) is popular in finance, inventory forecasting, APC, ...

Shiryaev-Roberts (SR).

- Girshick/Rubin (1952), Shiryaev (1963), Roberts (1966)
- (log-)likelihood ratio of pre- and post-change distribution

$$Lik_i = \frac{(2\pi\sigma_1^2)^{-1/2}\, e^{-X_i^2/(2\sigma_1^2)}}{(2\pi)^{-1/2}\, e^{-X_i^2/2}} = \sigma_1^{-1}\, e^{\frac{1-\sigma_1^{-2}}{2} X_i^2} \,.$$

- $$R_0 = 0\,, \quad R_i = (1 + R_{i-1})\, Lik_i\,,$$
  $$L = \inf\{i \in I\!N : R_i > c_u\}\,.$$
- $\log(R_i) = r_i = \log\left(1 + e^{r_{i-1}}\right) - \log(\sigma_1) + \frac{1-\sigma_1^{-2}}{2} X_i^2\,.$
  – preferred appearance here.
- (asymptotically) steady-state optimal – Pollak (1985).
- rarely discussed for variance – Srivastava/Chow (1992), Bock (2007).

Performance measures.

Notation: $P_m(\cdot)$ and $E_m(\cdot)$ denote probability measure and expectation for given change point m.

- zero-state ARL: $E_\infty(L)$, $E_1(L)$ or $E_\sigma(L)$

  most popular measure in SPC.

- steady-state ARL: $\mathcal{D} = \lim_{m\to\infty} E_m\big(L - m + 1 | L \geq m\big)$.

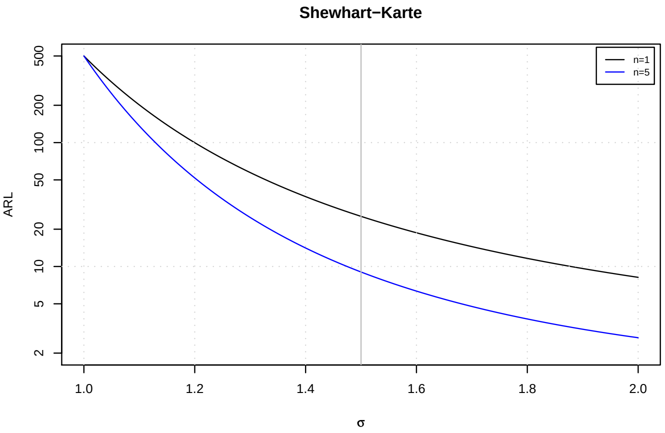
  link to Bayesian measures.

- worst case ARL: $\mathcal{W} := \sup_{m\geq 1} \operatorname{ess\,sup} E_m\big((L - m + 1)^+ \,|\, \mathcal{F}_{m-1}\big)$

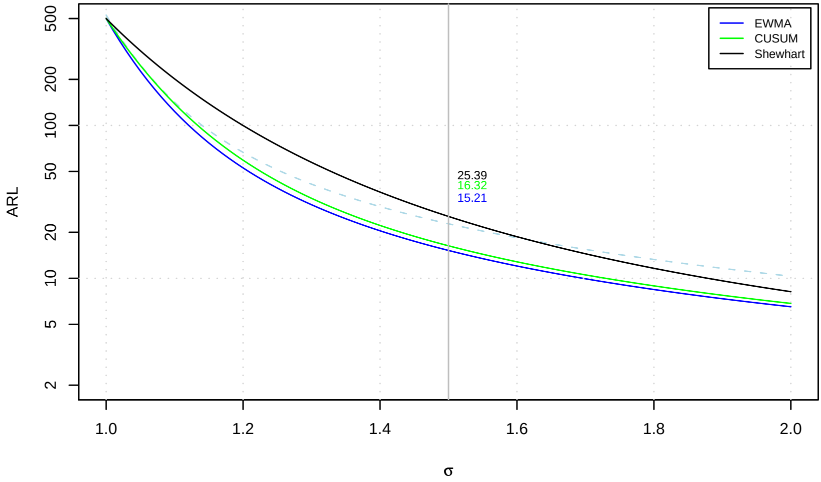
  most popular measure among (theoretical) statisticians.

Shewhart chart – ARL profile.

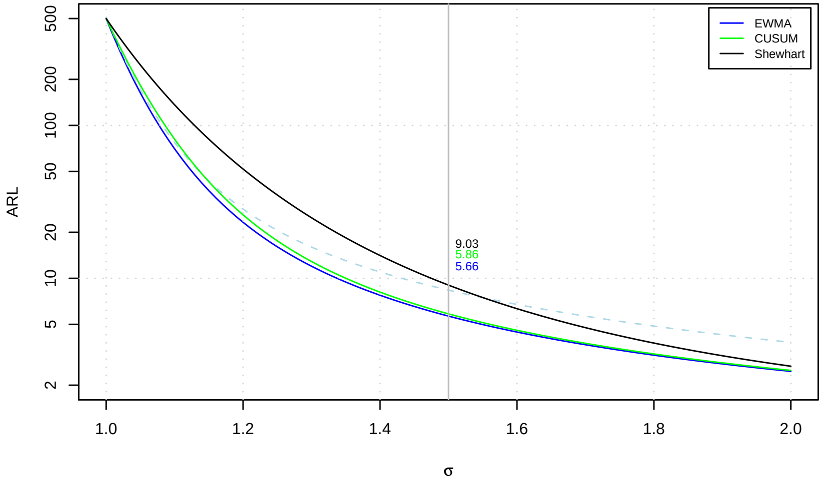
$$E_\sigma(L) = 1/\left(1 - F_{\chi^2_\nu}\left(c_u/\sigma^2\right)\right) \quad \left(c_u = \frac{1}{\nu} F^{-1}_{\chi^2_\nu}\left(1 - A^{-1}\right), A = 500\right).$$



... + EWMA & CUSUM ($n = 1$).



… + EWMA & CUSUM ($n = 5$).

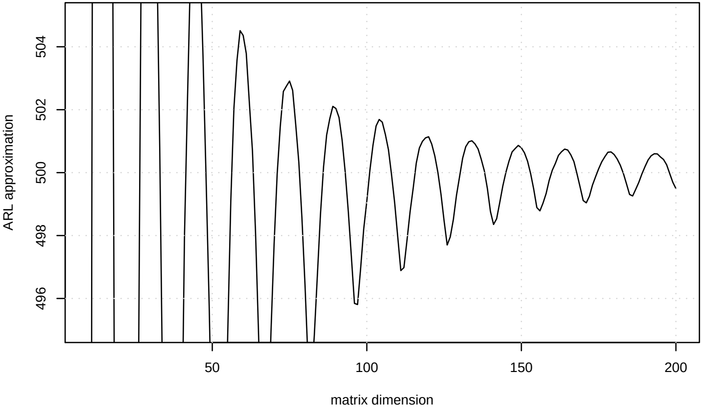


Shiryaev-Roberts?

Shiryaev-Roberts – Status Quo ARL calculation.

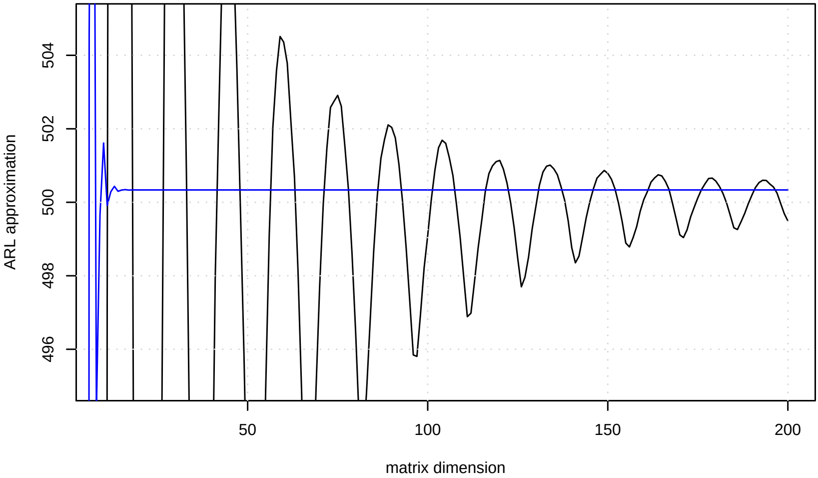
Methods applied so far:

Markov chain approximation and Monte Carlo simulation ...



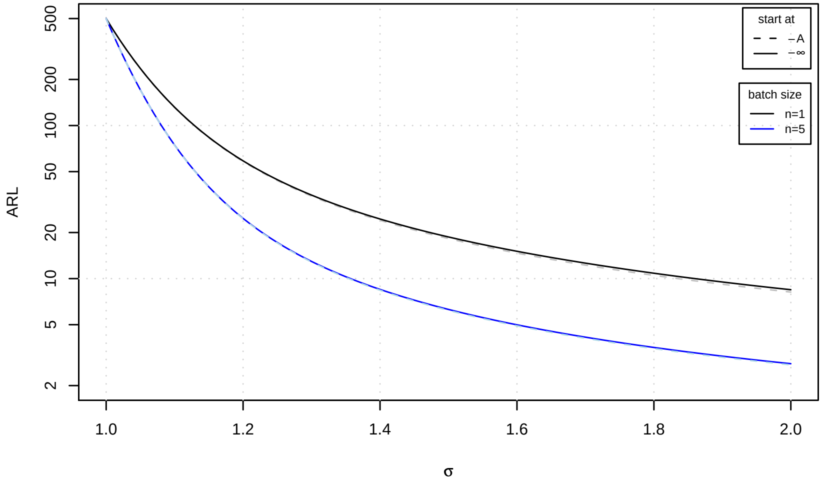
Solution: Appropriate piecewise collocation.

Result.



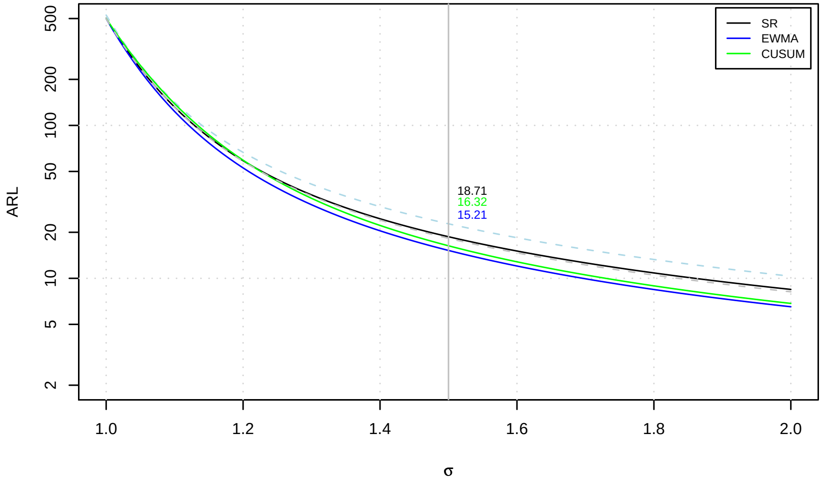
ARL approximation
504
502
500
498
496
50
100
150
200
matrix dimension

SR ARL profile.

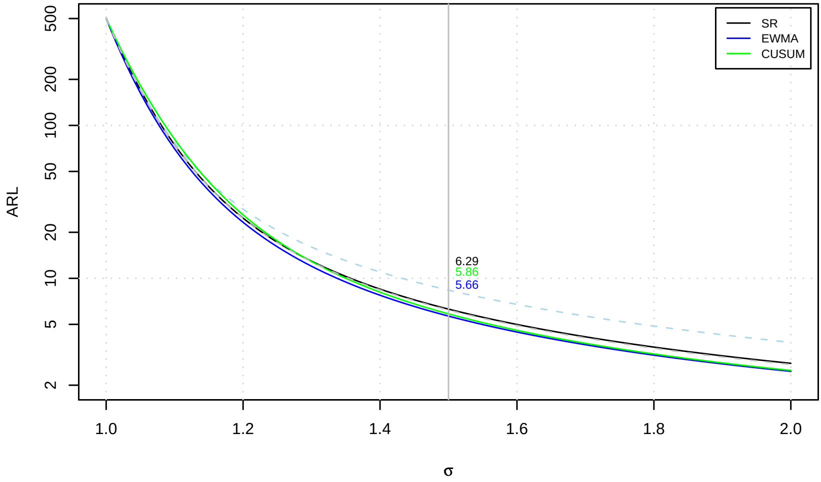


$-A = -\log(\sigma_1)$

All together: $n = 1$.



All together: $n = 5$.



Now the steady-state ARL.

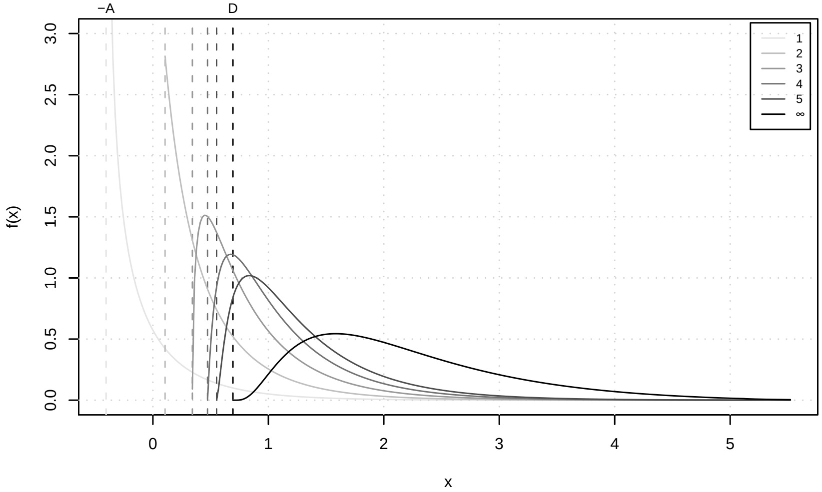
$$\mathcal{D} = \lim_{m\to\infty} E_m\big(L - m + 1 | L \geq m\big) \quad = \lim_{m\to\infty} \int_{-A}^{c_u} f_m(y)\, \mathcal{L}(y)\, dy$$

$$= \int_{-A}^{c_u} \psi(y)\, \mathcal{L}(y)\, dy$$

with $\psi()$ as left eigenfunction of the integral kernel (belonging to the largest in magnitude eigenvalue ρ):

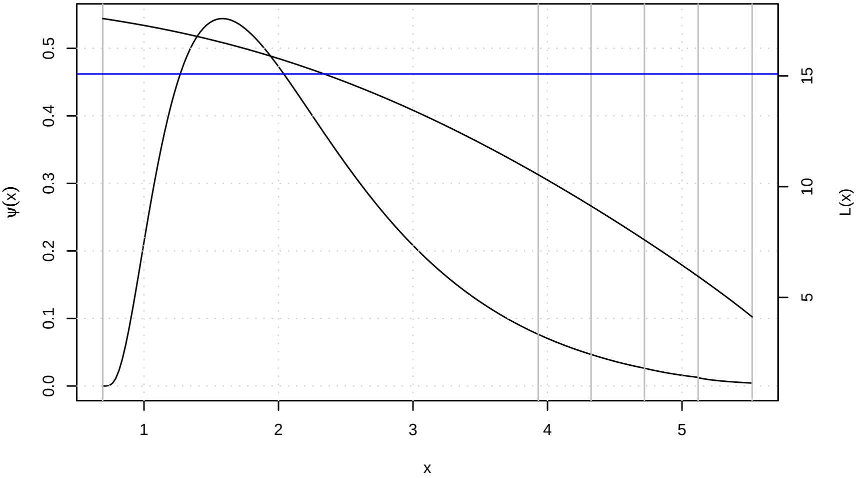
$$\psi(y) = \varrho \int_{-A}^{c_u} \psi(x)\, f_{\chi_1^2}\left(\frac{y + A - \log(1 + e^x)}{B\,\sigma^2}\right) \frac{1}{B\,\sigma^2}\, dx\,.$$

Density sequence $f_m(y)$ $(n = 1)$.

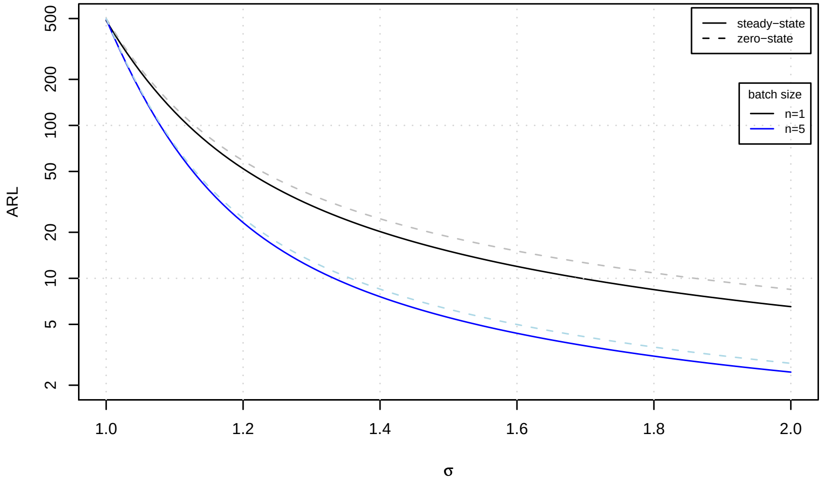


$-A = -\log(\sigma_1),\ D = -\log(e^{A} - 1) = -\log(\sigma_1 - 1)$

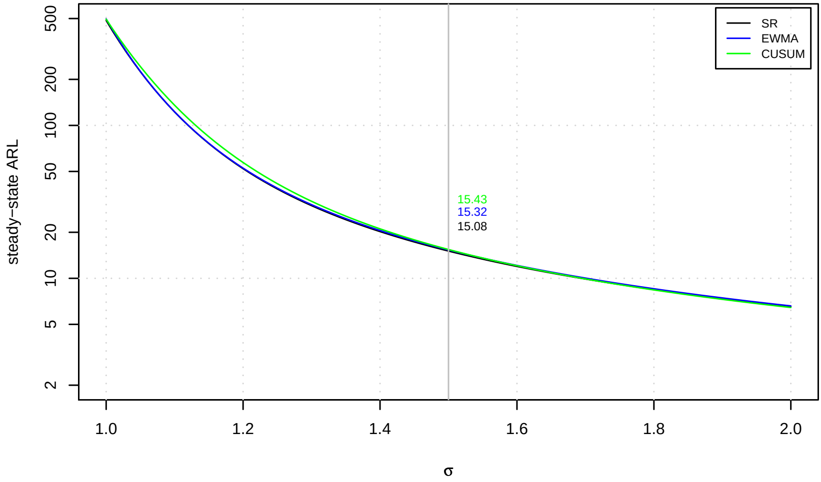
Bringing $\psi()$ and $\mathcal{L}()$ together.



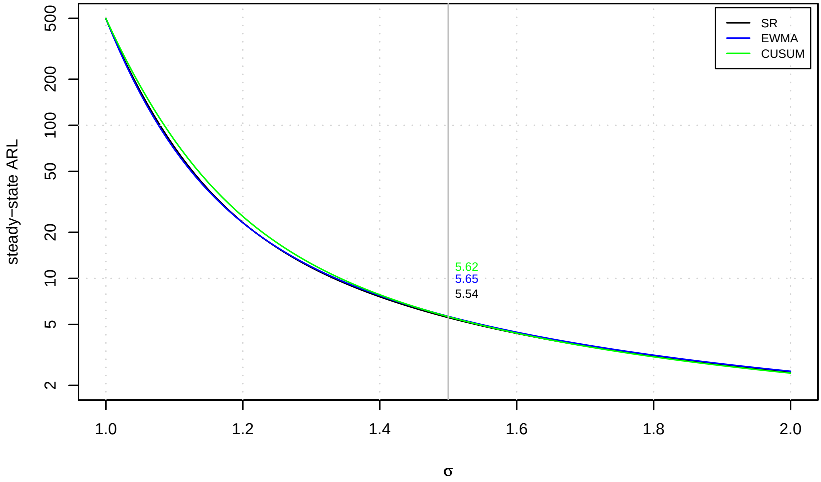
Zero-state vs. steady-state ARL.



Steady-state ARL profiles for all 3 charts: $n = 1$.



Steady-state ARL profiles for all 3 charts: $n = 5$.

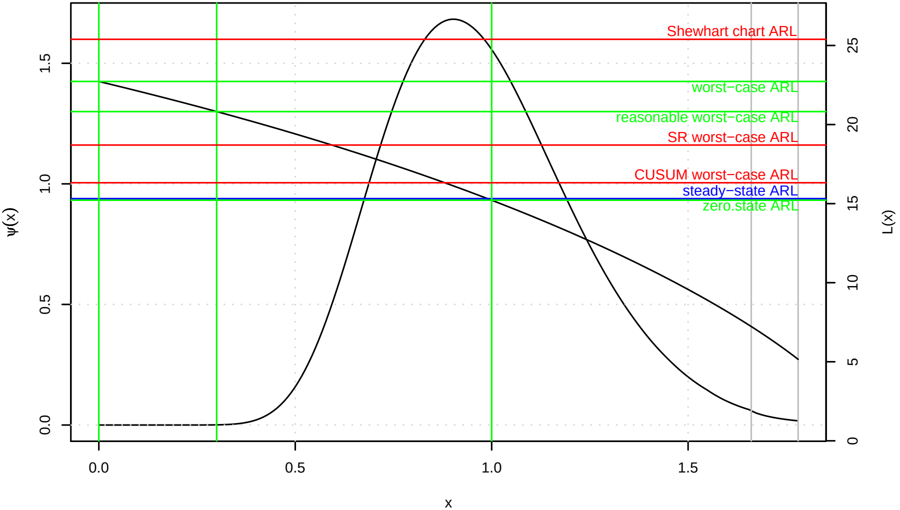


Что делать?

- All 3 exhibit the same steady-state performance (ARL).
- CUSUM is the best one in the worst case (, however, CUSUM is mostly in worst condition).
- Order by publicity/degree of esteem ...

1. Shewhart,
2. Shewhart with runs rules,
3. EWMA,
4. CUSUM,
5. Shiryaev-Roberts.

EWMA?


Shewhart chart ARL
worst−case ARL
reasonable worst−case ARL
SR worst−case ARL
CUSUM worst−case ARL
steady−state ARL
zero.state ARL
ψ(x)
L(x)
x
0.0
0.5
1.0
1.5
0
5
10
15
20
25

EWMA.

- On-line estimation of the monitored parameter,
- popular smoother in control schemes,
- more descriptive than CUSUM and SR,
- better than Shewhart (and Shewhart with runs rules),
- two-sided application is simple,
- also the setup as joint mean and variance monitoring scheme,
- single member of {CUSUM, EWMA, SR} that is contained in commercial SPC software packages.

(Jump)

Competing statistics and 2-sided EWMA.

$R, S^2, S, lS^2, abcS^2$ – batch size $n = 5$

Comparison study.

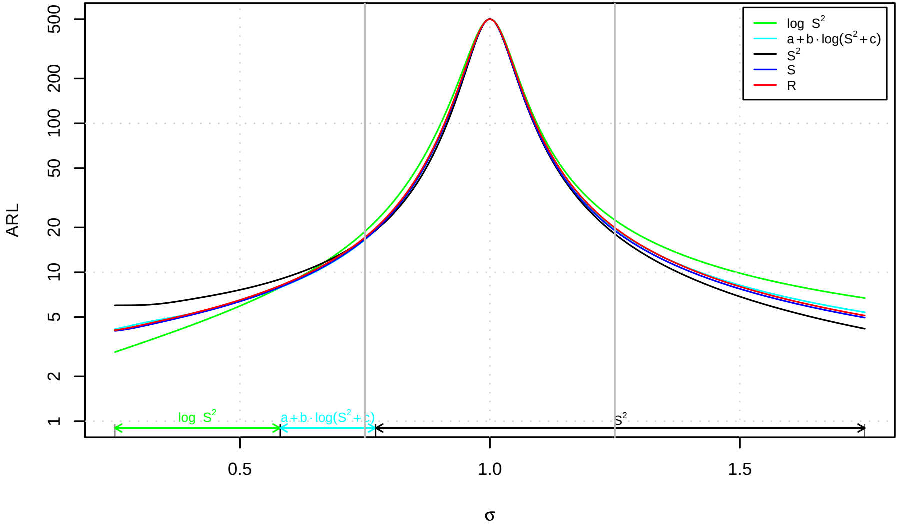
1. $E_\infty(L) = 500$ and $n = 5$.
2. "ARL unbiased" designs
   (see Acosta-Mejía, Pignatiello Jr. & Rao (1999)).
3. All schemes start from their in-control mean.
4. Look for "optimal" λ, that is, minimize

   $$\mathcal{L}_{0.75} + \mathcal{L}_{1.25} \quad \text{or} \quad \mathcal{L}_{0.5} + \mathcal{L}_{1.5}$$

   over $\lambda \in \{0.02, 0.03, \ldots, 0.99, 1.00\}$.
5. Resulting λ are:

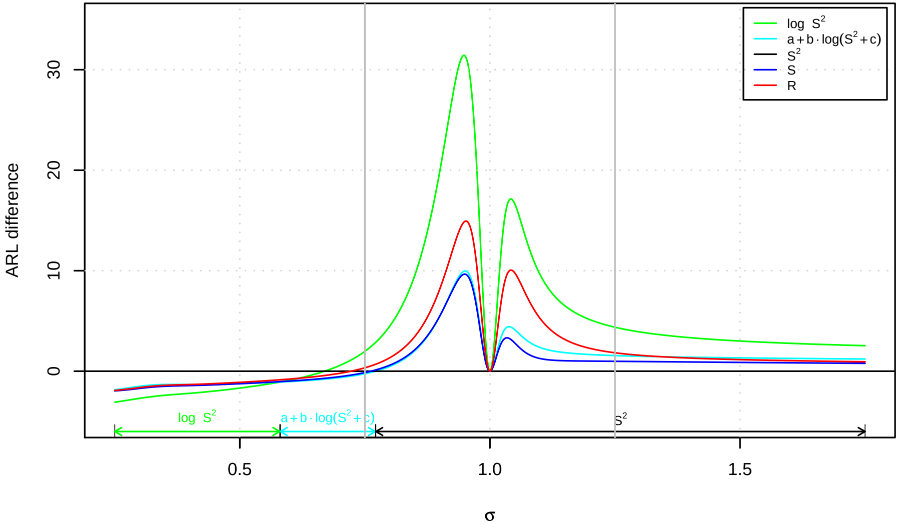
case	statistics				
	R	S^2	S	lS^2	$abcS^2$
$\mathcal{L}_{0.75} + \mathcal{L}_{1.25}$	0.08	0.08	0.08	0.07	0.08
$\mathcal{L}_{0.5} + \mathcal{L}_{1.5}$	0.23	0.25	0.24	0.20	0.27

Minimize $\mathcal{L}_{0.75} + \mathcal{L}_{1.25}$.



($n = 5$)

Minimize $\mathcal{L}_{0.75} + \mathcal{L}_{1.25}$ II.



$(n = 5)$

Minimize $\mathcal{L}_{0.75} + \mathcal{L}_{1.25}$ III.

σ	statistics				
	IS^2	$abcS^2$	S^2	S	R
0.4	**4.374**	5.251	6.575	*5.143*	5.249
0.5	**5.939**	6.389	7.619	*6.374*	6.514
0.6	8.547	**8.409**	9.438	*8.459*	8.660
0.7	13.74	**12.59**	13.17	*12.63*	12.96
0.75	18.78	**16.56**	16.81	*16.67*	17.14
0.8	27.94	*23.92*	**23.44**	24.04	24.78
0.9	96.70	*82.24*	**76.74**	82.26	84.96
1.0			500.000		
1.1	90.80	83.53	**81.16**	*82.43*	86.43
1.2	30.74	27.27	**25.61**	*26.61*	27.88
1.25	22.44	19.61	**18.06**	*19.04*	19.89
1.3	17.67	15.26	**13.77**	*14.73*	15.35
1.4	12.54	10.60	**9.206**	*10.12*	10.51
1.5	9.866	8.190	**6.864**	*7.740*	8.017
1.6	8.235	6.735	**5.460**	*6.295*	6.509

($n = 5$)

Summary.

Summary.

- Surveillance of the variance gained popularity.
- There are many competing control charts and statistics.
- Numerical difficulties during calculating of performance measures could be treated; methods could be applied to other designs too (distances, survival times, AR(1) CUSUM, ...)
- "Modern" schemes exhibit similar performance (ARL), all are better than established ones (Shewhart), EWMA resembles suitable compromise for practice.
- There is no need to replace the classics S^2/S or R by one of the popular log transformations.
- State of emergency in commercial SPC software packages: Shewhart charts (w/ and w/o runs rules) dominate, sometimes EWMA is implemented, rarely CUSUM and never SR.