Improved process capability assessment through semiparametric piecewise modeling

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Improved process capability assessment through semiparametric piecewise modeling

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Overview

Process capability indices

- Quality control ensures that products or services meet defined standards.

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- Process Capability Indices (PCIs) offer objective metrics to assess if produced items meet specifications by measuring the inherent variability of the process.

PCIs for normal data

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where USL and LSL represent the upper and lower specification limits, respectively. The variable d denotes the tolerance interval adjusted for process variation, T is the target value.

Classification

PCI	Classification	Interpretation
< 1.00	Incapable	over 2,700 items with nonconformities
$1.00 - 1.33$	Acceptable	between 64 and 2,700 nonconforming items
> 1.33	Capable	less than 64 nonconforming items

PCIs for non-normal data

The PCIs for non-normally distributed data are defined as follows:

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where U_p, M, and L_p represent the 99.865$^{\text{th}}$, 50$^{\text{th}}$, and 0.135$^{\text{th}}$ percentiles, respectively.

PE model

The Piecewise Exponential (PE) model with k change points can be represented by the following probability density function:

$$f(t;\boldsymbol{\lambda}) = \sum_{j=1}^{k+1} \lambda_j \exp\left\{-\lambda_j \left(t - \tau_{(j-1)}\right)\right\} C_{j-1} \mathbb{1}_{\mathcal{R}_j}(t),$$

where:

$$C_0 = 1 \quad \text{and} \quad C_i = \exp\left\{-\sum_{h=1}^{i} \lambda_h \left(\tau_{(h)} - \tau_{(h-1)}\right)\right\}, \quad i = 1, \ldots, k,$$

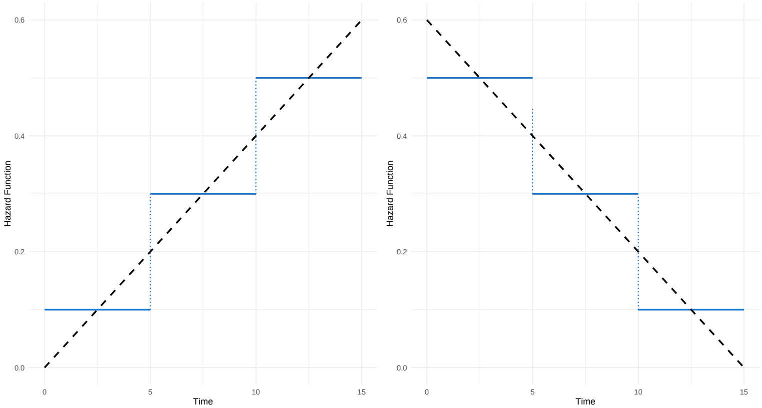
and $\mathbb{1}_{\mathcal{R}_j}(t) = 1$ if $t \in \mathcal{R}_j = \left(\tau_{(j-1)}, \tau_{(j)}\right]$, and 0 otherwise.

Why PE model?

The failure rate (or hazard) function of a PE model is given by:

$$h(t; \boldsymbol{\lambda}) = \sum_{j=1}^{k+1} \lambda_j \mathbb{1}_{\mathcal{R}_j}(t).$$

Why PE model?



0.6
0.4
0.2
0.0
Hazard Function
0
5
10
15
Time
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0.4
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Inference

The log-likelihood function is:

$$\ell(\boldsymbol{\lambda}, \boldsymbol{\tau}) = \sum_{j=1}^{k+1} \left[n_j \left(\log(\lambda_j) - \sum_{h=1}^{j-1} \lambda_h \left(\tau_{(h)} - \tau_{(h-1)} \right) \right) - \lambda_j \sum_{i:\, t_i \in \mathcal{R}_j} \left(t_i - \tau_{(j-1)} \right) \right],$$

where n_j is the number of observations in the j-th interval.

MLE

The maximum likelihood estimators (MLEs) of $\boldsymbol{\lambda}$ given $\boldsymbol{\tau}$ are given by:

$$\widehat{\lambda}_j(\boldsymbol{\tau}) = n_j \left(\sum_{i:\, t_i \in \mathcal{R}_j} \left(t_i - \tau_{(j-1)}\right) + \sum_{h=j}^{k} n_{h+1} \left(\tau_{(j)} - \tau_{(j-1)}\right) \right)^{-1}, \quad j = 1, \ldots, k,$$

$$\widehat{\lambda}_{k+1}(\boldsymbol{\tau}) = n_{k+1} \left(\sum_{i:\, t_i \in \mathcal{R}_{k+1}} \left(t_i - \tau_{(k)}\right) \right)^{-1}.$$

Asymptotic distribution

These estimators are asymptotically normally distributed:

$$\sqrt{n}(\widehat{\boldsymbol{\lambda}} - \boldsymbol{\lambda}) \xrightarrow{\mathcal{D}} \mathcal{N}_{(k+1)}\left(0, \mathcal{I}^{-1}\right), \quad \text{for } n \to +\infty,$$

where $\mathcal{I}$ is the Fisher information matrix, whose elements are given by

$$\mathcal{I}_{jj} = \frac{C_{j-1} - C_j}{\lambda_j^2}, \quad \text{for } j = 1, \ldots, k+1,$$

and $\mathcal{I}_{ij}(\boldsymbol{\lambda}) = 0$, for $i \neq j$.

CIs for the parameters

We can obtain approximate $100(1-\gamma)\%$ confidence intervals (CIs) for the parameters of each partition as follows:

$$\text{CI}\left[\lambda_j; 100(1-\gamma)\%\right] = \widehat{\lambda}_j \pm z_{\gamma/2}\frac{\widehat{\lambda}_j}{\sqrt{n\left(C_{j-1}-C_j\right)}},$$

where $z_{\gamma/2}$ is the $100(\gamma/2)$-th percentile of a standard normal distribution.

Goals

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2. Assess a change-point estimation method from the literature to identify changes in process behavior over time.
3. Calculate the standard error of the PCI estimators to measure their uncertainty.

Bias-corrected

Let us define the cumulante functions:

$$h_{ij}(\boldsymbol{\lambda}) = \mathbb{E}\left[\frac{\partial^2 \ell(\boldsymbol{\lambda})}{\partial \lambda_i \lambda_j}\right], \quad h_{ij}^{(l)}(\boldsymbol{\lambda}) = \frac{\partial h_{ij}(\boldsymbol{\lambda})}{\partial \lambda_l}, \quad h_{ijl}(\boldsymbol{\lambda}) = \mathbb{E}\left[\frac{\partial^3 \ell(\boldsymbol{\lambda})}{\partial \lambda_i \partial \lambda_j \partial \lambda_l}\right],$$

The bias of $\widehat{\boldsymbol{\lambda}}$ can be expressed as:

$$\text{Bias}(\widehat{\boldsymbol{\lambda}}) \approx \mathcal{I}^{-1} A \, \text{vec}\big(\mathcal{I}^{-1}\big),$$

where $A = \left[A^{(1)} \mid \ldots \mid A^{(p)}\right]$, with $A^{(l)} = \left\{h_{ij}^{(l)}(\boldsymbol{\lambda}) - 0.5 h_{ijl}(\boldsymbol{\lambda})\right\}$, for $i, j, l = 1, \ldots, k+1$.

Table: Calculating Bias and MSE from the estimates for the original parameters of the PE model, varying n with 10,000 simulated samples. The results of the traditional MLEs are shown between parentheses.

		Scenario 1		Scenario 2		Scenario 3	
	n	Bias	MSE	Bias	MSE	Bias	MSE
λ_1	10	-0.015 (0.008)	0.005 (0.006)	0.024 (0.032)	0.001 (0.002)	-0.097 (-0.085)	0.011 (0.009)
	20	-0.002 (0.010)	0.021 (0.023)	0.001 (0.004)	0.001 (0.002)	-0.041 (-0.033)	0.009 (0.009)
	30	-0.000 (0.008)	0.016 (0.017)	-0.002 (0.000)	0.001 (0.001)	-0.023 (-0.017)	0.006 (0.006)
	40	0.000 (0.006)	0.012 (0.013)	-0.001 (0.000)	0.001 (0.001)	-0.013 (-0.008)	0.005 (0.005)
	50	-0.000 (0.004)	0.010 (0.010)	0.000 (0.001)	0.001 (0.001)	-0.007 (-0.004)	0.004 (0.004)
λ_2	10	0.029 (0.094)	0.017 (0.029)	0.065 (0.077)	0.005 (0.006)	-0.314 (-0.294)	0.099 (0.087)
	20	0.010 (0.040)	0.054 (0.062)	0.015 (0.018)	0.001 (0.001)	-0.180 (-0.159)	0.037 (0.031)
	30	0.001 (0.020)	0.041 (0.045)	0.004 (0.006)	0.000 (0.000)	-0.107 (-0.089)	0.017 (0.014)
	40	-0.003 (0.011)	0.030 (0.032)	0.001 (0.002)	0.000 (0.000)	-0.067 (-0.051)	0.010 (0.009)
	50	0.000 (0.011)	0.024 (0.026)	0.000 (0.001)	0.000 (0.000)	-0.040 (-0.026)	0.008 (0.007)
λ_3	10	-0.002 (0.352)	0.482 (1.157)	0.016 (4.013)	59.740 (135.860)	-0.062 (0.952)	5.413 (14.637)
	20	0.007 (0.153)	0.183 (0.318)	0.002 (1.086)	12.354 (16.523)	-0.117 (0.833)	3.062 (7.845)
	30	0.004 (0.090)	0.081 (0.110)	-0.019 (0.621)	6.917 (8.250)	-0.090 (0.777)	2.378 (6.021)
	40	-0.002 (0.059)	0.054 (0.067)	0.037 (0.502)	5.022 (5.762)	-0.036 (0.721)	2.477 (5.662)
	50	0.002 (0.050)	0.040 (0.048)	0.016 (0.382)	3.889 (4.334)	-0.044 (0.609)	1.676 (3.773)

Change point estimation

The profile likelihood function is given by:

$$\ell_{\mathrm{P}}(\boldsymbol{\tau}) = \sum_{j=1}^{k+1} \left[n_j \left(\log\left(\widehat{\lambda}_j(\boldsymbol{\tau})\right) - \sum_{h=1}^{j-1} \widehat{\lambda}_h(\boldsymbol{\tau})(\tau_{(h)} - \tau_{(h-1)}) \right) - \widehat{\lambda}_j(\boldsymbol{\tau}) \sum_{i:\, t_i \in \mathcal{R}_j} \left(t_i - \tau_{(j-1)}\right) \right],$$

The estimated change-points can be determined through a simulated annealing algorithm, guided by the following linear constraints:

- **Trivial constraint**: $\tau_{(1)} < \ldots < \tau_{(k)}$.
- **Domain constraints**: $\tau_{(1)} > t_{\min} \wedge \tau_{(k)} < t_{\max}$.
- **Density constraints**: $\tau_{(j)} - \tau_{(j-1)} > m_j$.

Table: Bias and MSE estimates for the change-points, varying n with 10,000 samples.

		Scenario 1		Scenario 2		Scenario 3	
	n	Bias	MSE	Bias	MSE	Bias	MSE
$\tau_{(1)}$	10	0.034	0.152	-0.033	0.141	0.129	0.438
	20	0.103	0.202	0.047	0.089	-0.001	0.486
	30	0.111	0.182	0.044	0.081	-0.084	0.552
	40	0.116	0.164	0.061	0.077	-0.124	0.567
	50	0.106	0.150	0.070	0.075	-0.141	0.547
$\tau_{(2)}$	10	0.031	0.152	-0.012	0.053	0.183	0.409
	20	0.096	0.205	0.004	0.005	0.054	0.477
	30	0.104	0.185	0.003	0.002	-0.028	0.552
	40	0.109	0.165	0.003	0.000	-0.071	0.577
	50	0.101	0.151	0.002	0.000	-0.091	0.557

Delta method

The delta method suggests the following convergence:

$$\sqrt{n}\,(C(\boldsymbol{\lambda}) - C(\boldsymbol{\lambda})) \xrightarrow{\mathcal{D}} \mathcal{N}\left(0, [\nabla C(\boldsymbol{\lambda})]^\top \cdot \mathcal{I} \cdot \nabla C(\boldsymbol{\lambda})\right), \quad \text{for } n \to +\infty.$$

The CIs for the PCIs is given by:

$$\text{CI}\,[C(\boldsymbol{\lambda}); 100(1-\gamma)\%] = C(\boldsymbol{\lambda}) \pm z_{\gamma/2}\sqrt{[\nabla C(\boldsymbol{\lambda})]^\top \cdot \mathcal{I} \cdot \nabla C(\boldsymbol{\lambda})},$$

where $\nabla C(\boldsymbol{\lambda})$ is the gradient of C.

Table: Bias, MSE, and CP from the estimates of C_{pk} and C_{pm}, considering different values of n with 10,000 simulated samples.

		Scenario 1			Scenario 2			Scenario 3		
	n	Bias	MSE	CP	Bias	MSE	CP	Bias	MSE	CP
C_{pk}	150	-0.002	0.006	0.940	0.000	0.000	0.955	-0.030	0.029	0.926
	160	-0.002	0.006	0.937	0.000	0.000	0.959	-0.030	0.027	0.930
	170	-0.002	0.005	0.940	0.000	0.000	0.959	-0.027	0.026	0.926
	180	-0.001	0.005	0.946	0.000	0.000	0.956	-0.029	0.024	0.930
	190	-0.001	0.005	0.946	0.000	0.000	0.956	-0.028	0.022	0.937
	200	-0.001	0.005	0.940	0.000	0.000	0.956	-0.024	0.021	0.939
C_{pm}	150	-0.009	0.014	0.922	0.018	0.005	0.938	-0.110	0.061	0.933
	160	-0.007	0.011	0.935	0.015	0.004	0.943	-0.092	0.050	0.933
	170	-0.007	0.009	0.935	0.011	0.003	0.942	-0.078	0.042	0.935
	180	-0.006	0.008	0.937	0.009	0.002	0.948	-0.063	0.035	0.934
	190	-0.005	0.007	0.940	0.006	0.002	0.948	-0.060	0.032	0.932
	200	-0.004	0.006	0.940	0.005	0.001	0.948	-0.050	0.028	0.930

Table: Bias, MSE, and CP from the estimates of C^*_{pm} and C_{pmk}, considering different values of n with 10,000 simulated samples.

		Scenario 1			Scenario 2			Scenario 3		
	n	Bias	MSE	CP	Bias	MSE	CP	Bias	MSE	CP
C^*_{pm}	150	-0.000	0.000	0.943	0.001	0.000	0.950	-0.016	0.004	0.941
	160	-0.000	0.000	0.947	0.001	0.000	0.952	-0.015	0.004	0.943
	170	-0.000	0.000	0.946	0.001	0.000	0.952	-0.013	0.003	0.943
	180	-0.000	0.000	0.942	0.000	0.000	0.948	-0.013	0.003	0.941
	190	-0.000	0.000	0.943	0.000	0.000	0.951	-0.011	0.003	0.945
	200	-0.000	0.000	0.940	0.000	0.000	0.953	-0.012	0.003	0.939
C_{pmk}	150	-0.002	0.001	0.949	0.005	0.002	0.961	-0.030	0.015	0.947
	160	-0.002	0.001	0.946	0.004	0.001	0.967	-0.026	0.014	0.949
	170	-0.002	0.001	0.952	0.004	0.001	0.963	-0.025	0.013	0.949
	180	-0.001	0.001	0.952	0.004	0.001	0.964	-0.026	0.013	0.946
	190	-0.001	0.000	0.949	0.002	0.001	0.963	-0.023	0.012	0.947
	200	-0.001	0.000	0.948	0.002	0.001	0.959	-0.021	0.011	0.949

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- The Shapiro-Wilk test returned a p-value of 0.009553.

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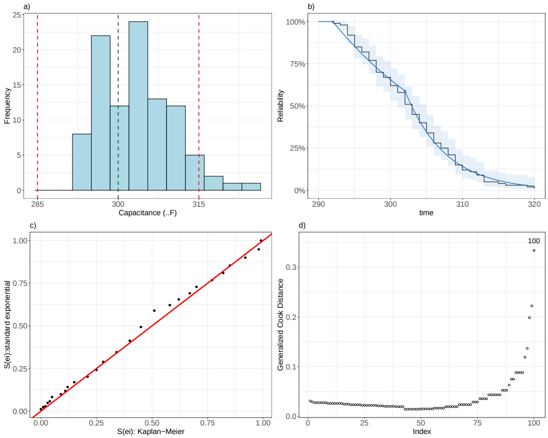

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Table: Estimates and 95% CIs for the parameters, change-points, and PCIs of the PE model.

Parameter/PCI	Estimate	CI (95%)
λ_1	0.05	(0.04, 0.07)
λ_2	0.18	(0.13, 0.22)
$\tau_{(1)}$	302	—
C_{pk}	0.36	(0.26, 0.47)
C_{pm}	0.67	(0.54, 0.80)
C^*_{pm}	0.33	(0.27, 0.40)
C_{pmk}	0.35	(0.25, 0.45)

Polymer Granules Data

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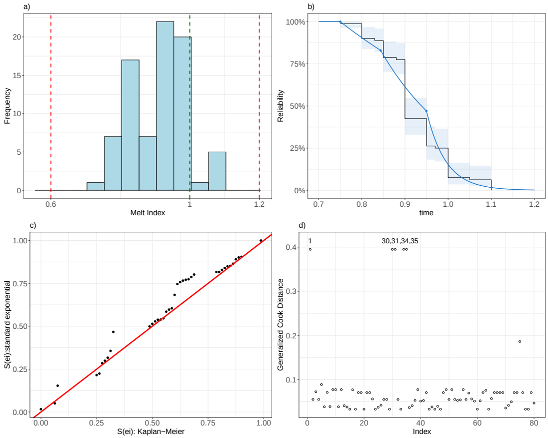

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Parameter/PCI	Estimate	CI (95%)
λ_1	2.00	(0.94, 3.06)
λ_2	5.34	(3.39, 7.29)
λ_2	22.28	(15.17, 29.4)
$\tau_{(1)}$	0.84	—
$\tau_{(2)}$	0.95	—
C_{pk}	0.95	(0.66, 1.25)
C_{pm}	1.21	(1.00, 1.41)
C^*_{pm}	0.40	(0.33, 0.47)
C_{pmk}	0.79	(0.60, 0.98)

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Improved process capability assessment through semiparametric piecewise modeling

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