Physikalisch-Technische Bundesanstalt
Braunschweig and Berlin
National Metrology Institute

A1.1.2: Straight-line regression in errors-in-variables models

Getting straight-line regression right

Examples of Measurement Uncertainty Evaluation

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WG 8.42 Data Analysis and Measurement Uncertainty

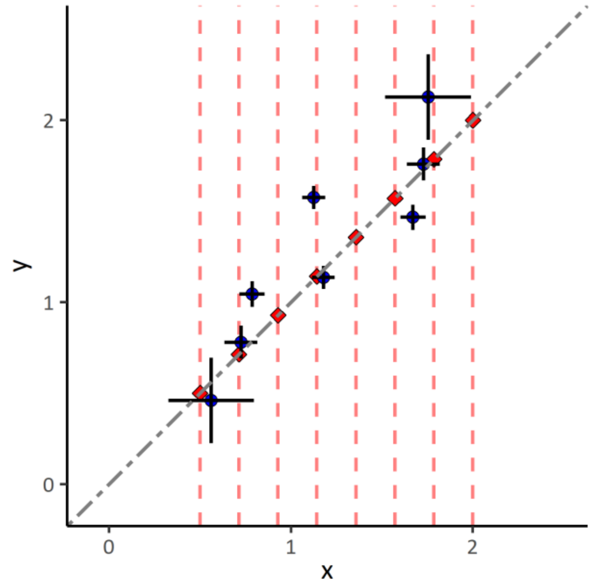
EMUE Workshop, 01/22/20, Paris

Straight line regression in Errors-in-Variables (EIV) models

[1]

ξ_i $\Rightarrow$ $\boxed{\eta_i = \beta_0 + \beta_1 \xi_i}$ $\Rightarrow$ $(y_i, \sigma_{y,i})$

$(x_i, \sigma_{x,i})$



- N pairs $(x_i, y_i)^{\mathrm{T}}$ of independent x_i and dependent variables y_i

$$(1a) \quad x_i = \xi_i + \epsilon_{x,i}$$

$$(1b) \quad y_i = \beta_0 + \beta_1 \xi_i + \epsilon_{y,i}$$

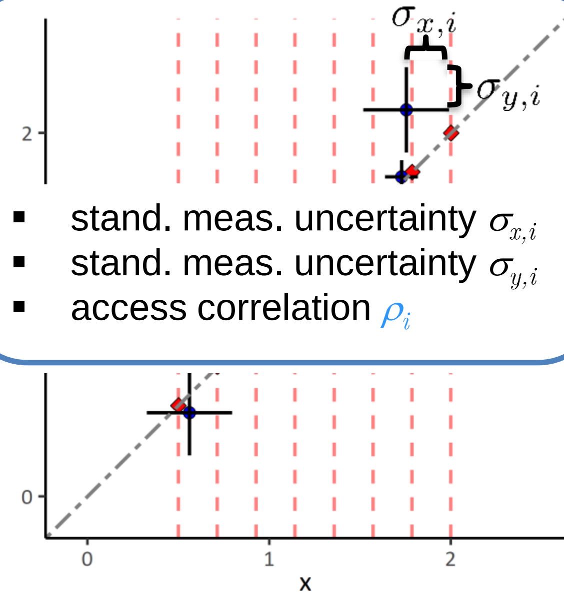
- is a common task in metrology including
  - calibration procedures
  - method comparision studies

[1] https://primosensor.de/produkt/ind4r13-digitalanzeige/
[2] https://nordiclifescience.org/wp-content/public_html/2018/05/lab-e1526288478439.jpg

Straight line regression in Errors-in-Variables (EIV) models

$\xi_i \Rightarrow \boxed{\eta_i = \beta_0 + \beta_1 \xi_i} \Rightarrow (y_i, \sigma_{y,i})$

$\xi_i \Rightarrow (x_i, \sigma_{x,i})$



- stand. meas. uncertainty $\sigma_{x,i}$
- stand. meas. uncertainty $\sigma_{y,i}$
- access correlation ρ_i

- N pairs $(x_i, y_i)^{\mathrm{T}}$ of independent x_i and dependent variables y_i

$$(1a)\quad x_i = \xi_i + \epsilon_{x,i}$$

$$(1b)\quad y_i = \beta_0 + \beta_1 \xi_i + \epsilon_{y,i}$$

- <u>assumptions:</u>
  a) errors of *i*-th measurement are drawn from a zero-mean, multivariate Gaussian distribution with *i*-th covariance

$$\boldsymbol{\Sigma}_i = \begin{pmatrix} \sigma_{x,i}^2 & \rho_i \sigma_{x,i} \sigma_{y,i} \\ \rho_i \sigma_{x,i} \sigma_{y,i} & \sigma_{y,i}^2 \end{pmatrix}$$

  b) $\boldsymbol{\Sigma}_i$ are known

Case 8 in ISO/TS 28037

ISO/TS 28037:2010(E), *Determination and use of straight-line calibration functions.*

Goal and open questions

- **Goal**: Find best estimates and their uncertainties

$$\hat{\beta}_0, \hat{\beta}_1, \hat{\xi}_i\,, u_{\hat{\beta}_0}, u_{\hat{\beta}_1}, u_{\hat{\xi}_i}, \mathbf{U}_{\hat{\beta}_0,\hat{\beta}_1,\hat{\boldsymbol{\xi}}}$$

- numerous approaches exist:
  - ➢ least-squares (LS)[1,2] methods
    - weighted TLS (WTLS)
      - o Deming regression[3]
      - o ordinary LS (OLS)
  - ➢ Bayesian regression[4,5]
  - ➢ maximum likelihood estimators [4]
  - ➢ instrumental variables[6]
  - ➢ methods-of-moments[7]
  - etc.

[1] Adcock *The Analyst* **4**, 183 (1877); **5**, 53 (1878), [2] Pearson *Philos Mag.* **2**, 559 (1901)
[3] W. E. Deming „Statistical adjustment of data“ (1943), [4] Zellner „An Introduction to Bayesian Inference Econometrics“ (1971)
[5] Carroll et al. „Measurement errors in Nonlinear models“ (2006), [6] 9 M. Y: Wong *Biometrika* **76**, 141 (1989),
[7] Pal *J. Econometrics* **14**, 349 (1980)

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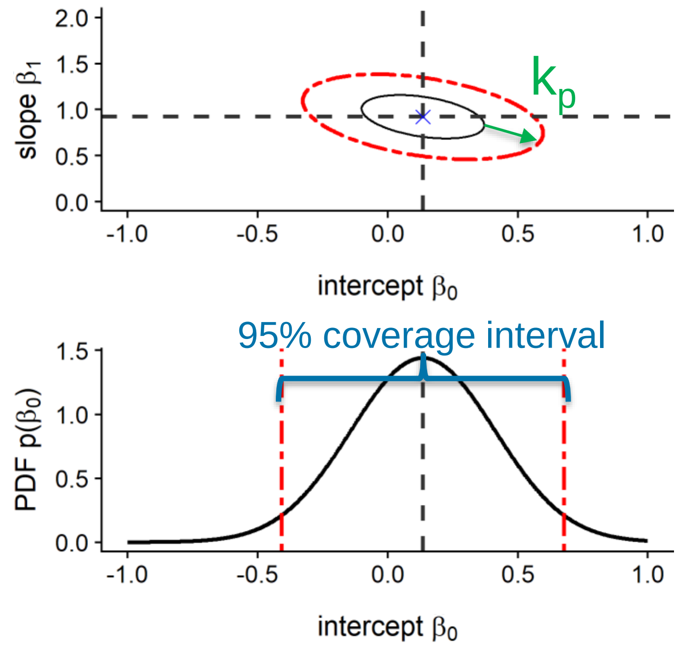

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- GUM documents advise uncertainties assessment based on
  1) propagation of uncertainties – **GUF** (GUM[1], GUM-S2[2])

[1] JCGM 100:2008, [2] JCGM 102:2011, [3] JCGM 101:2008

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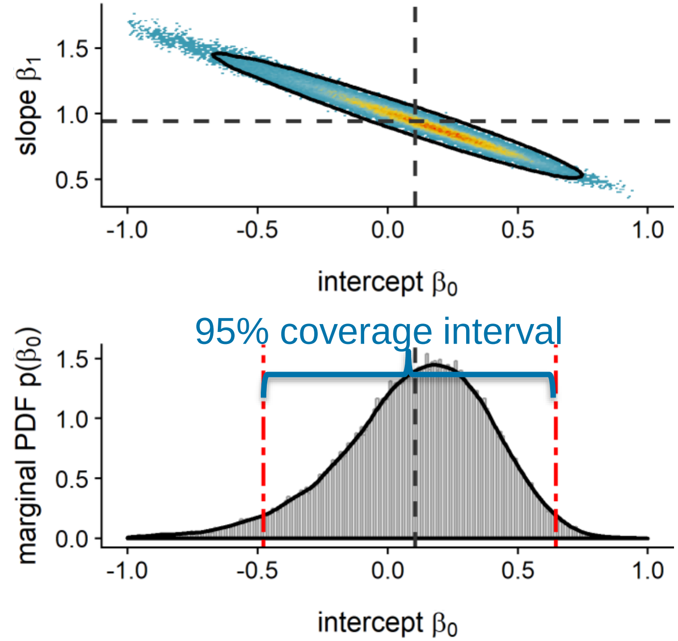

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  1) propagation of uncertainties – **GUF** (GUM[1], GUM-S2[2])
  2) propagation of distributions – **MC** methods (GUM-S1[3], GUM-S2[2])

- GUM documents do not give guidance for regressions problems

[1] JCGM 100:2008, [2] JCGM 102:2011, [3] JCGM 101:2008

Straight line regression in EIV models

- multiple standards recommend minimization of WTLS[1] functional

$$\begin{pmatrix} \hat{\boldsymbol{\beta}} \\ \hat{\boldsymbol{\xi}} \end{pmatrix} = \underset{\boldsymbol{\beta},\boldsymbol{\xi}}{\operatorname{argmin}} \sum_{i=1}^{N} \mathbf{v}_i^\top \boldsymbol{\Sigma}_i^{-1} \mathbf{v}_i \quad \text{with } \mathbf{v}_i = \begin{pmatrix} x_i - \xi_i \\ y_i - \beta_0 - \beta_1 \xi_i \end{pmatrix}, \boldsymbol{\beta} = \begin{pmatrix} \beta_0 \\ \beta_1 \end{pmatrix}$$

  - ❑ in general, only numerical approaches can be used
  - ❑ uncertainties might <u>depend</u> on chosen algorithm[2]
  - ❑ Does an uncertainty evaluation acc. to GUF and MC methods provide similar results for point estimates and their uncertainties?

- often, usage of OLS justified by „$\sigma_{x,i}$ is small compared to $\sigma_{y,i}$“ [3]
  - ❑ Under what conditions does OLS deliver valid results?

- Bayesian inference is generally applicable and more flexible
  - ❑ When and whether Bayesian inference with prior knowledge has advantages in comparison to MC methods?

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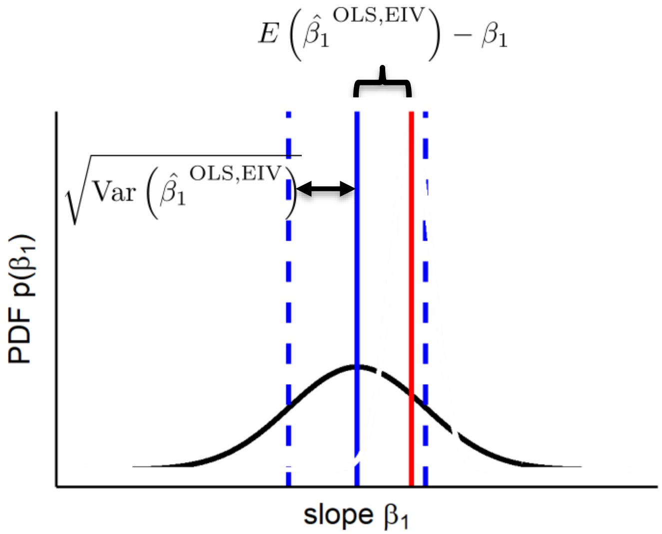
Validity of OLS in EIV models

- OLS point estimate is *biased* and *inconsistent*

<u>Reasonable conditions for usage of OLS:</u>

1. Deviation of estimator from true value must be compatible with the estimator's uncertainty.

$$\text{(2a)} \qquad \mathrm{Var}\left(\hat{\beta}_1^{\mathrm{OLS,EIV}}\right) \geq \left(E\left(\hat{\beta}_1^{\mathrm{OLS,EIV}}\right) - \beta_1\right)^2$$



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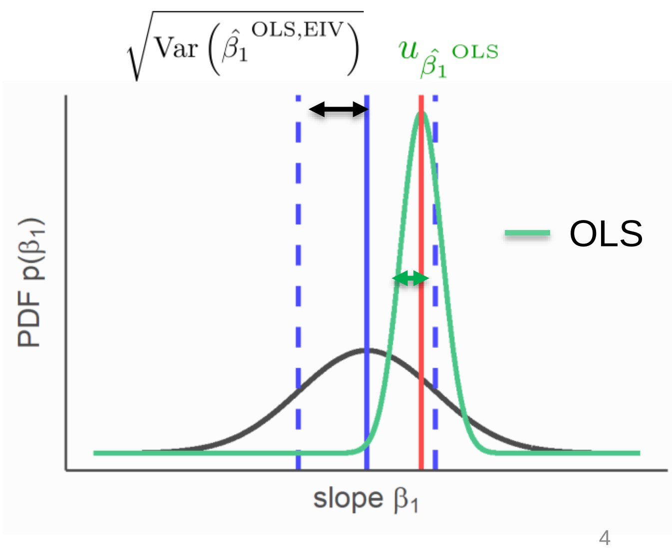
2. The uncertainty of the estimator should not be underestimated.

$$(2b) \quad \sqrt{\mathrm{Var}\left(\hat{\beta}_1^{\mathrm{OLS,EIV}}\right)} \leq u_{\hat{\beta}_1^{\mathrm{OLS}}}$$



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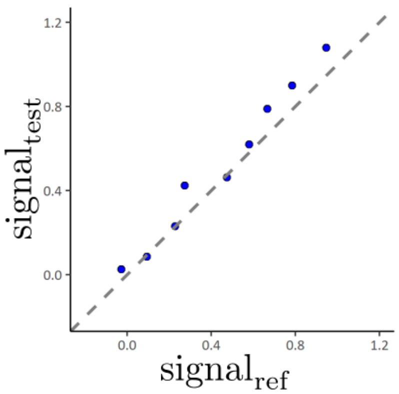
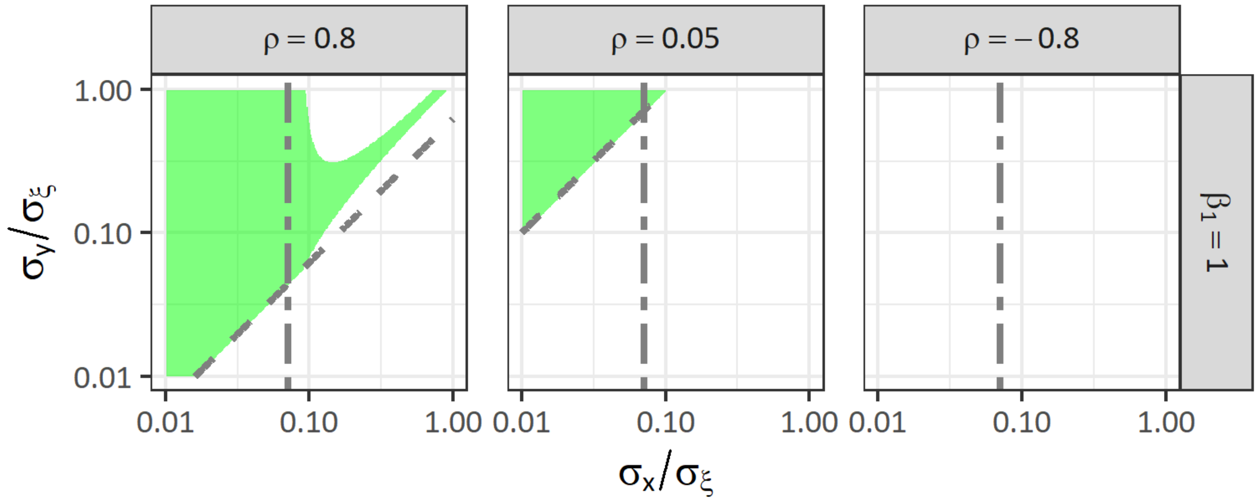
- in homosc. EIV ($\sigma_x = \sigma_{x,i}$, $\sigma_y = \sigma_{y,i}$, $\rho = \rho_i$), point estimates are *asymp. normally distributed* [1] and closed expressions for $E\left(\hat{\beta}_1^{\,\mathrm{OLS,EIV}}\right)$ and $\mathrm{Var}\left(\hat{\beta}_1^{\,\mathrm{OLS,EIV}}\right)$ exist

[1] Gleser et al., *Ann. Stat.* **15**, 220-233 (1987)

Validity of OLS in EIV models





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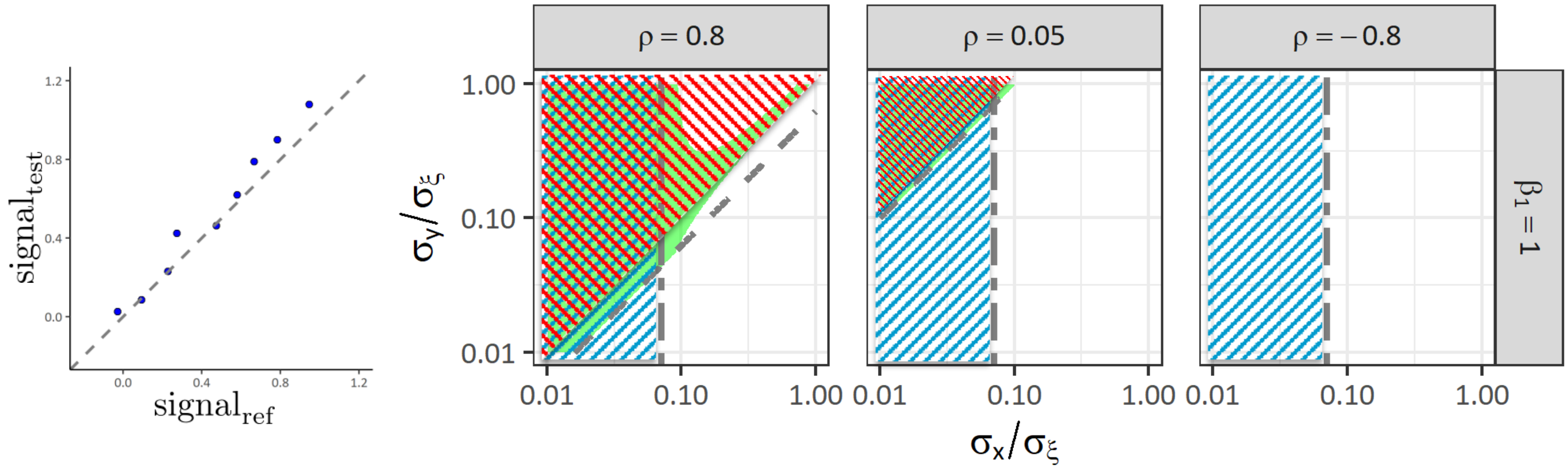


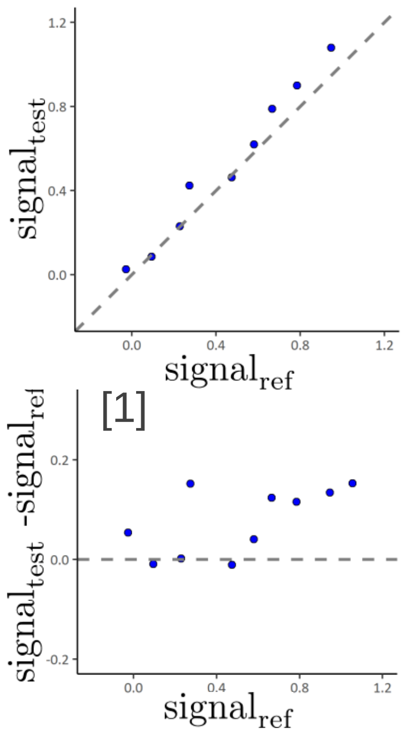
deviation condition $(2a)$ is fulfilled

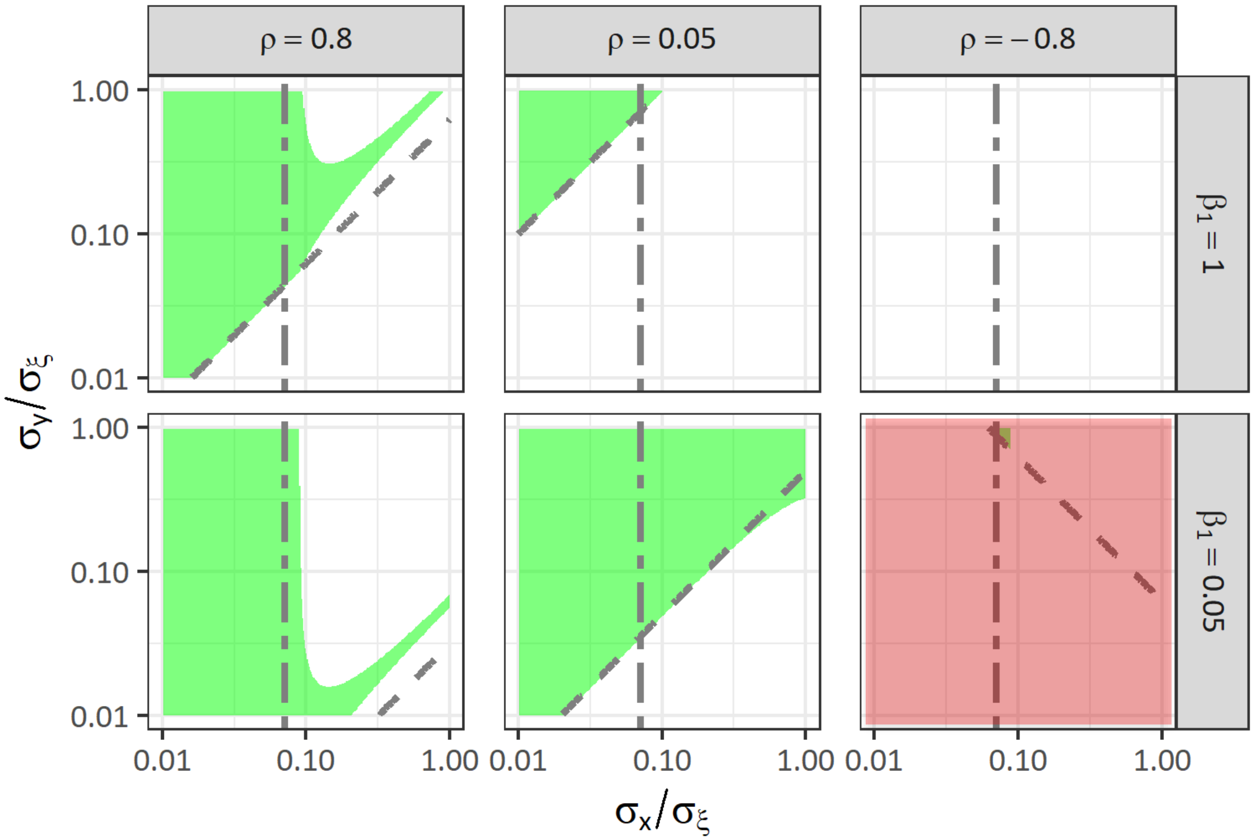
$$\sigma_x/\sigma_\xi < 1/\sqrt{N}$$

uncertainty condition $(2b)$ is obeyed

$$\frac{\sigma_y}{\sigma_\xi} > \frac{|\beta_1|}{|\rho|} \begin{cases} (\sigma_x/\sigma_\xi)^{-1}, & \operatorname{sgn}(\beta_1\rho) = -1 \\ 0.5(\sigma_x/\sigma_\xi), & \operatorname{sgn}(\beta_1\rho) = 1 \end{cases}$$

Validity of OLS in EIV models





- justification „$\sigma_{x,i}$ is small compared to $\sigma_{y,i}$“ is not sufficient
- in general, OLS cannot be recommended for EIV models especially if $\operatorname{sgn}(\rho\beta_1) = -1$

[1] example H.3 in JCGM 100:2008; OIML R 111-1 e04

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GUF vs. MC methods for WTLS

- multivariate measurand $\mathbf{Y} = (\beta_0, \beta_1, \boldsymbol{\xi})^T$

$$\hat{\mathbf{Y}} = \underset{\beta_0,\beta_1,\boldsymbol{\xi}}{\operatorname{argmin}} \sum_{i=1}^{N} \begin{pmatrix} x_i - \xi_i \\ y_i - \beta_0 - \beta_1 \xi_i \end{pmatrix}^\top \boldsymbol{\Sigma}_i^{-1} \begin{pmatrix} x_i - \xi_i \\ y_i - \beta_0 - \beta_1 \xi_i \end{pmatrix}$$

- evaluation of argmin leads to set of N+2 implicit normal equations

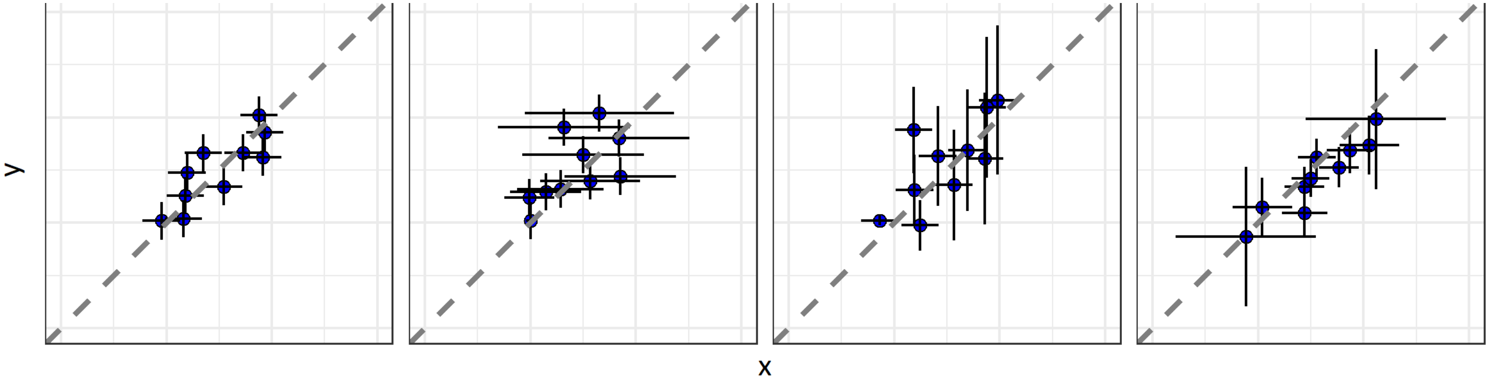
$$\mathbf{h}(\mathbf{X}, \mathbf{Y}) = 0, \quad \text{with input quantities} \quad \mathbf{X} = (x_1, y_1, \ldots, x_N, y_N)^\top$$

- supplement 2 to GUM (6.3) discusses this class of problems

GUF vs. MC methods for WTLS

- perform extensive numerical simulations
- generate „synthetic data“ according to stat. model (1a) - (1b)

N	ρ_i	σ_i^2/σ_ξ^2	MU Designs
{10, 100}	{-0.8,0,0.8}	{1%, 5%, 10%, 25%}	7



- for each combination
  $N_{rep} = 1000$ data sets + $N_{S1} = 5\ 10^4$ S1 sub-samples (Monte-Carlo)
- perform uncertainty evalutation accord. to GUF and MC methods

GUF vs. MC methods for WTLS

- ISO 28037[1] applies LPU to linearized problem (Gauss-Newton)

1) <u>coverage interval (CI) and frequentist coverage:</u>
   - 95% coverage intervals acc. to GUF yield 95% frequentist coverage
   - MC method provides slightly longer mean CI's length
     - effect strengthens with growing values for ($\sigma_{x,i},\ \sigma_{y,i}$)

2) <u>point estimates:</u>
   - GUF: point estimates are unbiased
   - MC method gives slightly larger estimates for β_1 and slightly smaller ones for β_0 $\rightarrow$ larger RMSEs
     - with growing N, difference between GUF and MC lessens

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> ➢ recommend ISO 28037:2010 WTLS implementation
>
> ➢ advise uncertainties evaluation acc. to the simpler propagation of uncertainties (**GUF**) approach

2)
   -
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Bayesian regression

- following Bayes' theorem, posterior for measurands $\boldsymbol{\theta} = (\beta_0, \beta_1, \boldsymbol{\xi}^\top)$

  $$p(\boldsymbol{\theta}|\text{data}) \propto \pi_0(\boldsymbol{\theta})\, \mathcal{L}(\boldsymbol{\theta}; \text{data})$$

  with prior $\pi_0(\boldsymbol{\theta})$, likelihood $\mathcal{L}(\boldsymbol{\theta}; \text{data})$, and <u>given</u> $\tilde{\boldsymbol{\Sigma}} = \text{diag}\left(\boldsymbol{\Sigma}_1, \ldots, \boldsymbol{\Sigma}_N\right)$

- assign flat prior to $\boldsymbol{\xi}$: $\pi_0(\boldsymbol{\theta}) = \pi_0(\boldsymbol{\beta})\pi_0(\boldsymbol{\xi}) \propto \pi_0(\boldsymbol{\beta})$

$$p(\boldsymbol{\beta}|\text{data}) \propto \pi_0(\boldsymbol{\beta}) \underbrace{\prod_{i=1}^{N} \sigma_{\text{eff,i}}^{-1}\left(\beta_1\right) \overbrace{\exp\left(-\frac{\left(y_i - \beta_0 - \beta_1 x_i\right)^2}{2\sigma_{\text{eff,i}}^2}\right)}^{\text{WTLS est. = ML est.}}}_{\text{MAP est. for } \beta_1 \neq \text{WTLS est.}},$$

$$\sigma_{\text{eff,i}}^2\left(\beta_1\right) = \sigma_{y,i}^2 - 2\rho_i\sigma_{x,i}\sigma_{y,i}\beta_1 + \beta_1^2\sigma_{x,i}^2$$

Bayesian regression

- select multivariate Normal prior for $\boldsymbol{\beta}$

$$\pi_0(\boldsymbol{\beta}) \propto \exp\left(-\frac{1}{2}\left(\boldsymbol{\beta}-\mu_\beta\right)^\top \boldsymbol{V}^{-1}\left(\boldsymbol{\beta}-\mu_\beta\right)\right), \text{with}\, \boldsymbol{\mu}_\beta = \begin{pmatrix}\mu_{\beta_0}\\ \mu_{\beta_1}\end{pmatrix}, \ \mathbf{V} = \mathrm{diag}(\sigma^2_{\beta_0}, \sigma^2_{\beta_1})$$

- closed expressions for marginal distributions can be derived

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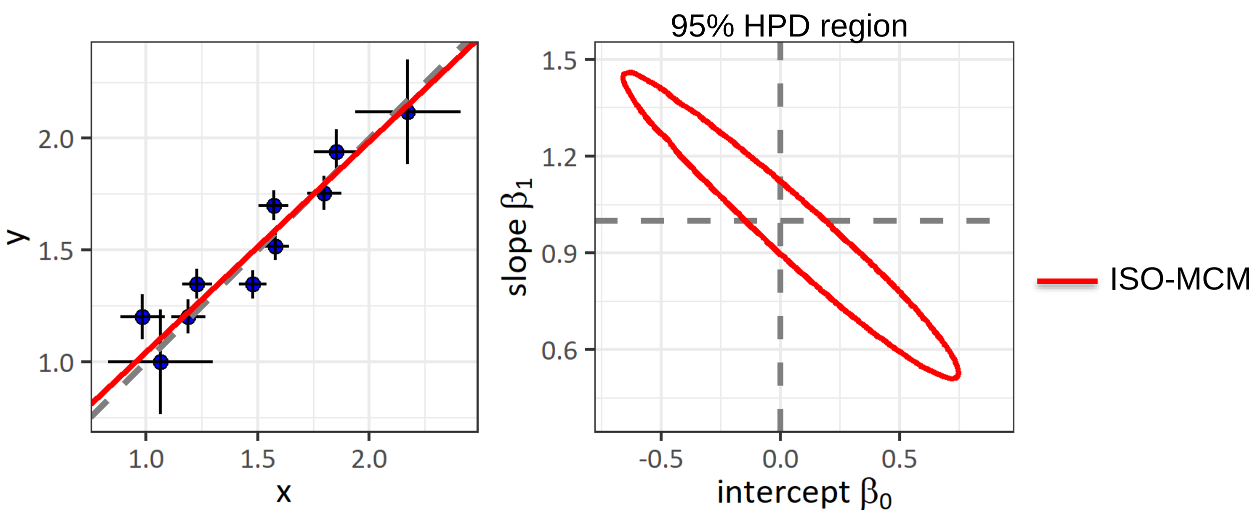

95% CI	LS estimate	Bayesian inference with normal prior		
	ISO – MCM			
β_0	(-0.48,0.65)			
β_1	(0.58,1.33)			

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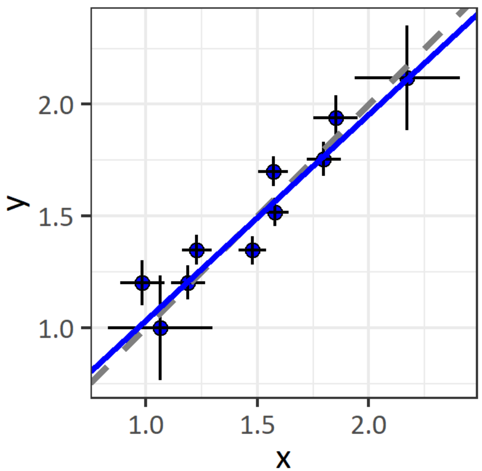
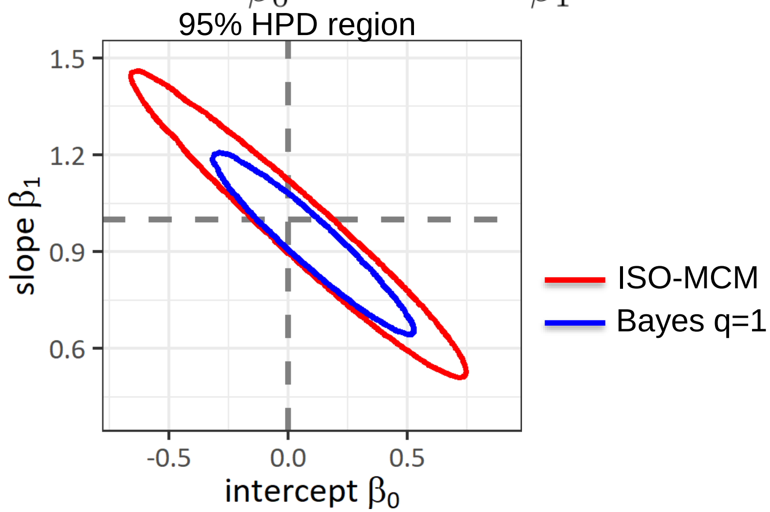
- closed expressions for marginal distributions can be derived
- set $(\mu_{\beta_0}, \mu_{\beta_1})^\top = (0,1)^\top$ and $(\sigma^2_{\beta_0}, \sigma^2_{\beta_1})^\top = q\left(u^2_{\hat{\beta}_0\,\mathrm{ISO-MCM}}, u^2_{\hat{\beta}_1\,\mathrm{ISO-MCM}}\right)^\top$





95% CI	LS estimate	Bayesian inference with normal prior		
	ISO – MCM		q=1	
β_0	(-0.48,0.65)		(-0.22,0.43)	
β_1	(0.58,1.33)		(0.71,1.15)	

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- closed expressions for marginal distributions can be derived
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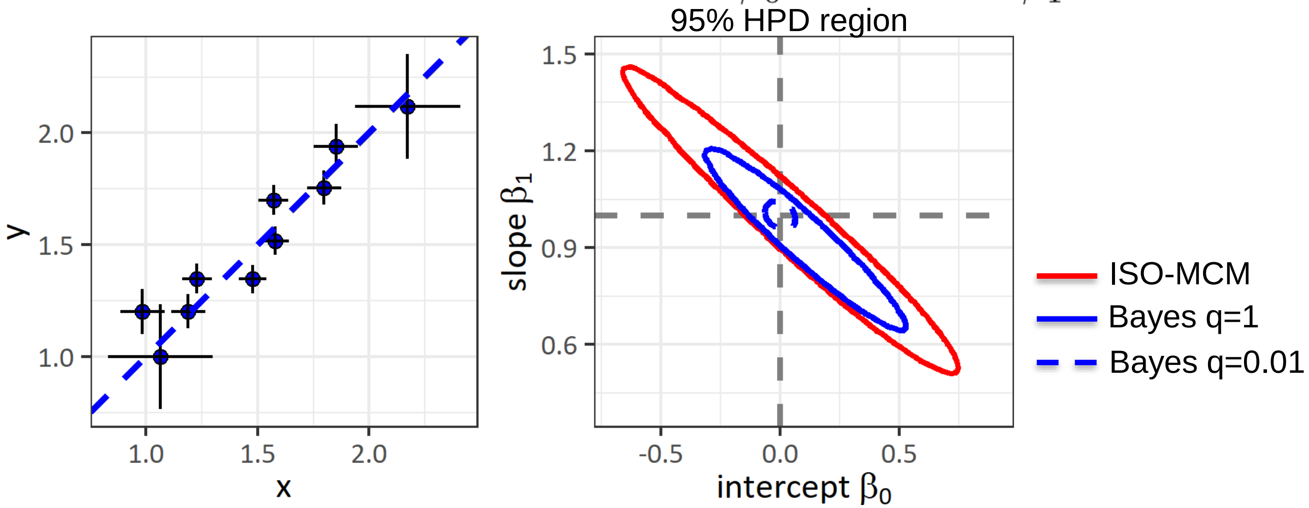


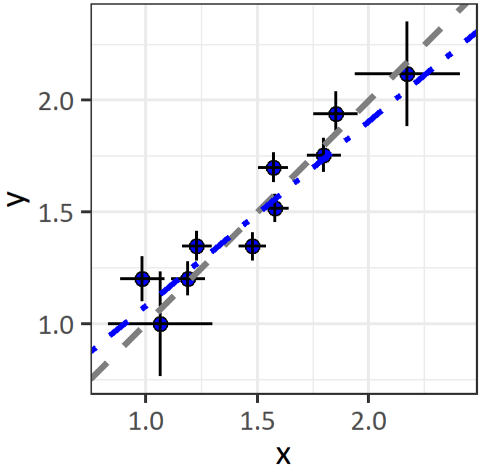
95% CI	LS estimate	Bayesian inference with normal prior		
	ISO – MCM	q=0.01	q=1	
β_0	(-0.48,0.65)	(-0.05,0.05)	(-0.22,0.43)	
β_1	(0.58,1.33)	(0.97,1.03)	(0.71,1.15)	

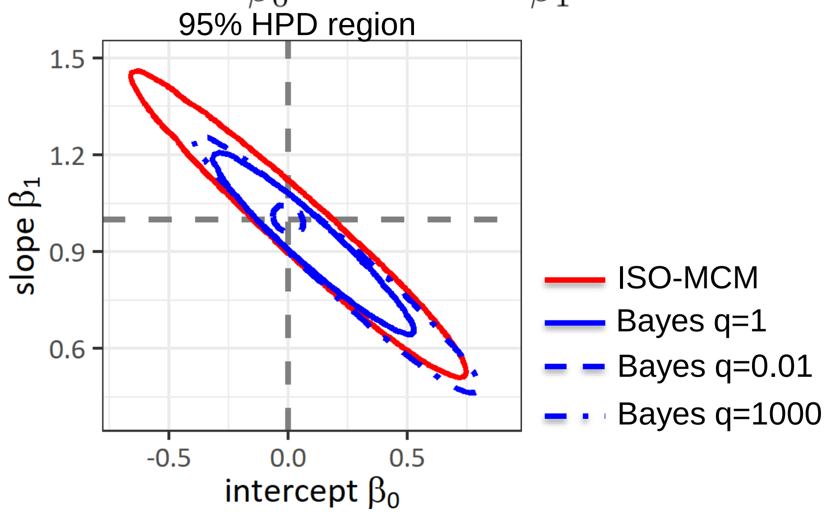
Bayesian regression

- select multivariate Normal prior for $\boldsymbol{\beta}$

$$\pi_0(\boldsymbol{\beta}) \propto \exp\left(-\frac{1}{2}(\boldsymbol{\beta}-\mu_\beta)^\top \boldsymbol{V}^{-1}(\boldsymbol{\beta}-\mu_\beta)\right), \text{with } \boldsymbol{\mu}_\beta = \begin{pmatrix}\mu_{\beta_0}\\ \mu_{\beta_1}\end{pmatrix}, \ \mathbf{V} = \mathrm{diag}(\sigma^2_{\beta_0}, \sigma^2_{\beta_1})$$

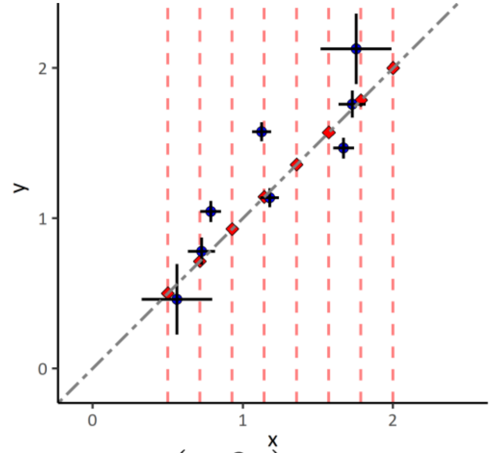
- closed expressions for marginal distributions can be derived
- set $(\mu_{\beta_0}, \mu_{\beta_1})^\top = (0,1)^\top$ and $(\sigma^2_{\beta_0}, \sigma^2_{\beta_1})^\top = q\,(u^2_{\hat{\beta}_0\,\mathrm{ISO-MCM}}, u^2_{\hat{\beta}_1\,\mathrm{ISO-MCM}})^\top$





95% CI	LS estimate	Bayesian inference with normal prior		
	ISO – MCM	q=0.01	q=1	q=1000
$\boldsymbol{\beta}_0$	(-0.48,0.65)	(-0.05,0.05)	(-0.22,0.43)	(-0.23,0.72)
$\boldsymbol{\beta}_1$	(0.58,1.33)	(0.97,1.03)	(0.71,1.15)	(0.52,1.15)

Conclusion



☑ present generic treatment of straight line regression in EIV models

☑ validity of OLS point estimates

- „$\sigma_{x,i}$ is small compared to $\sigma_{y,i}$“ is not sufficient
- especially, OLS cannot be recommended for EIV models if $\mathrm{sgn}(\rho\beta_1) = -1$

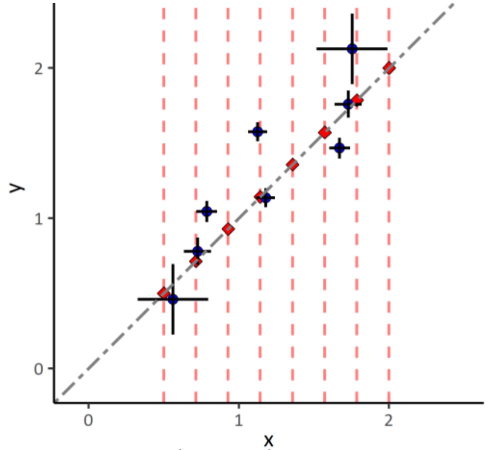
☑ uncertainty evaluation acc. to GUF or MC methods for WTLS point estimates

- advise uncertainty evaluation acc. to simpler GUF (LPU) approach
- recommend ISO 28037 implementation

☑ Bayesian inference with an informative prior

- is to be preferred if sufficient prior knowledge is available

Conclusion



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☑ ur **Straight line regression in errors-in-variables models – Comparison between the application of the GUM with its supplements and Bayesian analyses** ates

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☑ Ba

Steffen Martens[1], Katy Klauenberg[1], Maurice G. Cox[2], Alen Bošnjaković[3], John Greenwood[4], Adriaan M. H. van der Veen[5], and Clemens Elster[1]

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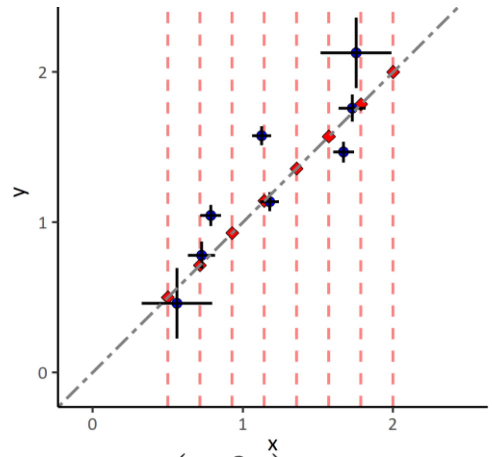
under revision

Conclusion



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