Physikalisch-Technische Bundesanstalt
Braunschweig and Berlin
National Metrology Institute

Uncertainty evaluation in curve fitting and regression problems

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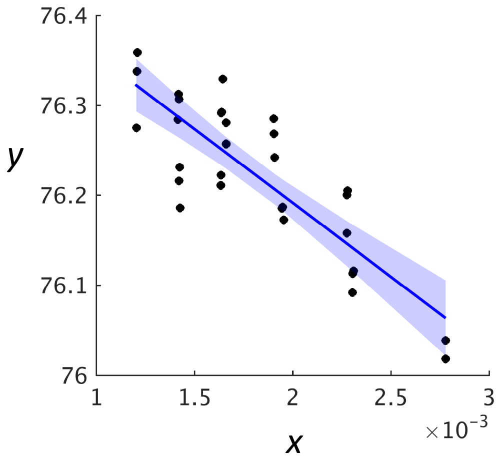
BIPM Workshop on Measurement Uncertainty

BIPM 15-16 June 2015

Motivation

- Curve fitting and regression problems relevant in metrology
- GUM and its supplements hardly give guidance
- Least-squares methods often applied
- Bayesian inference provides an alternative

Regression problem



$$y_i = f_{\boldsymbol{\theta}}(x_i) + \varepsilon_i \,,\; i = 1,\ldots,n$$

Data   Regression function   Errors

e.g. $\varepsilon_i \sim N(0,\sigma^2)$

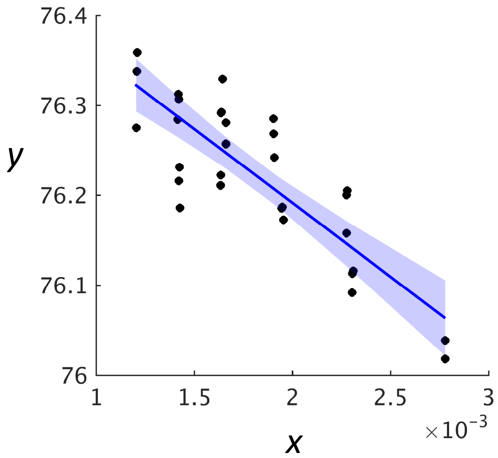
Measurand

– Regression parameters $\boldsymbol{\theta}$

– Regression function $f_{\boldsymbol{\theta}}(x)$

– Prediction of x from subsequent measurement of y

Bayesian inference



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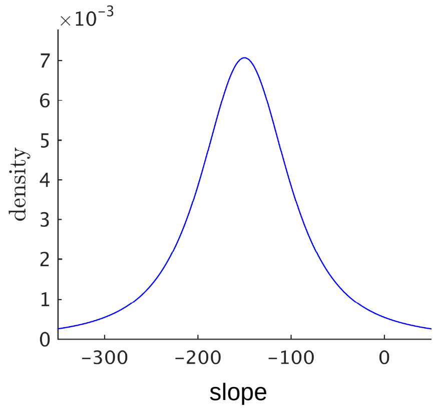
Prior knowledge

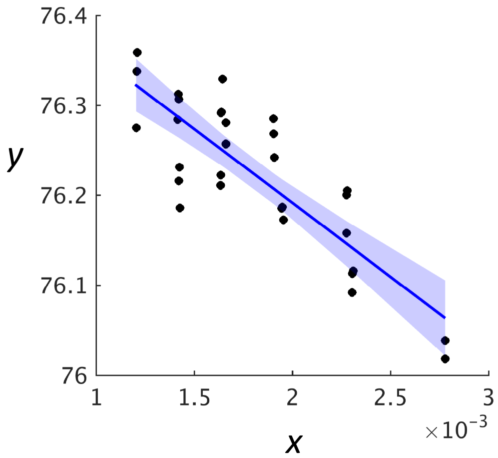


– Previous experiments

– Expert knowledge

– Known relations / constraints

Bayesian inference



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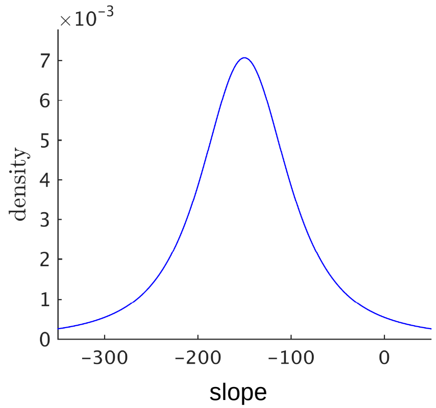
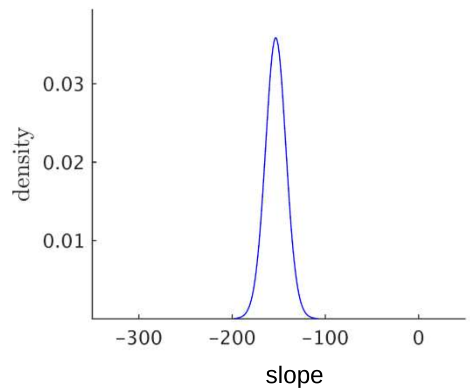


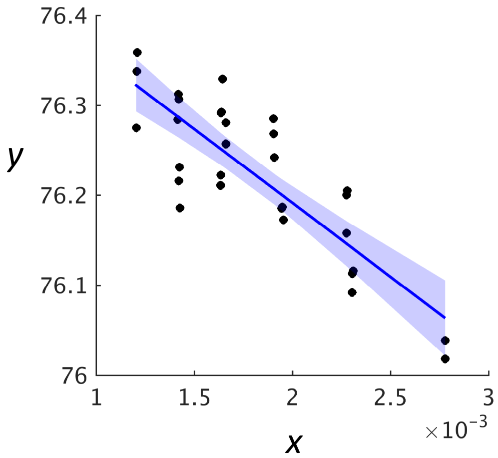
$\times$ Likelihood

Bayes theorem

Posterior distribution



Bayesian inference



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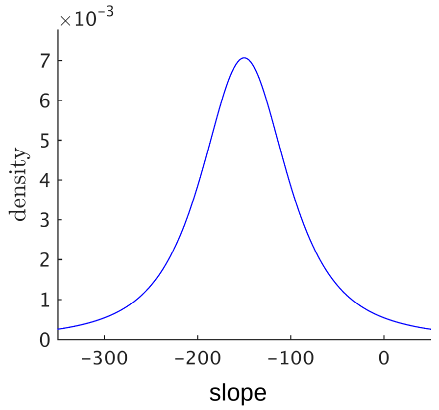

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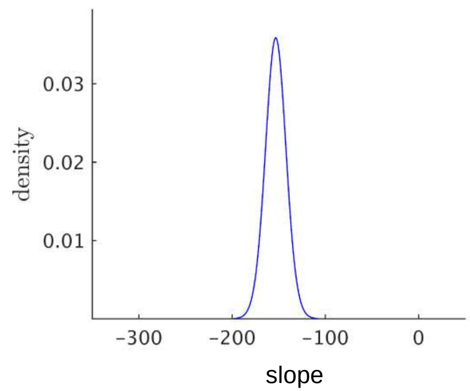
Likelihood

Bayes theorem

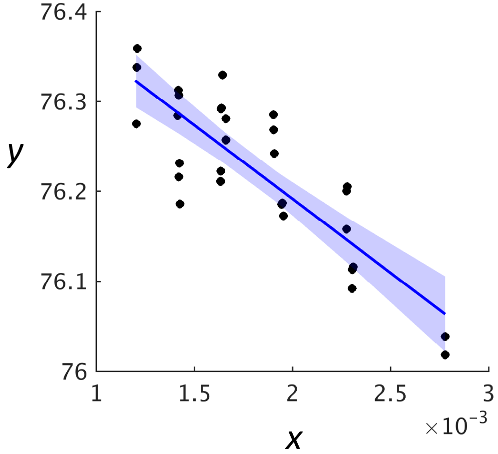
Posterior distribution



<u>Posterior distribution</u>

- Comprehensive characterization of uncertainty
- Basis for calculation of estimate and uncertainty
- Transferable (as prior in subsequent analyses)

Bayesian inference



Prior knowledge

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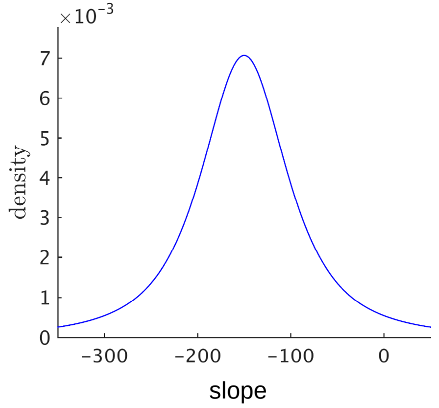
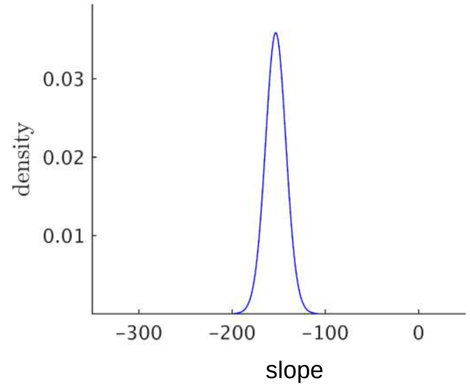
C P Robert (2007) The Bayesian choice: From Decision-Theoretic Foundations to Computational Implementations, Springer, New York

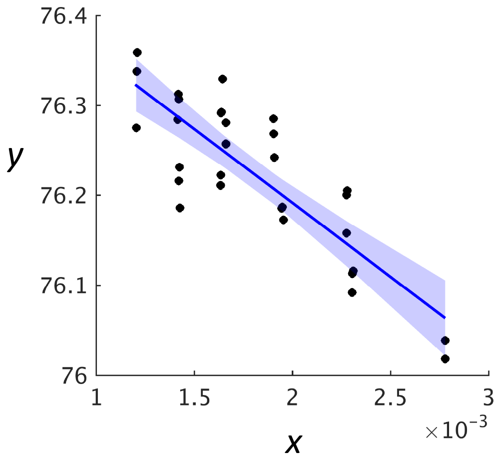


$\times$ Likelihood → Bayes theorem

Posterior distribution



Least-squares



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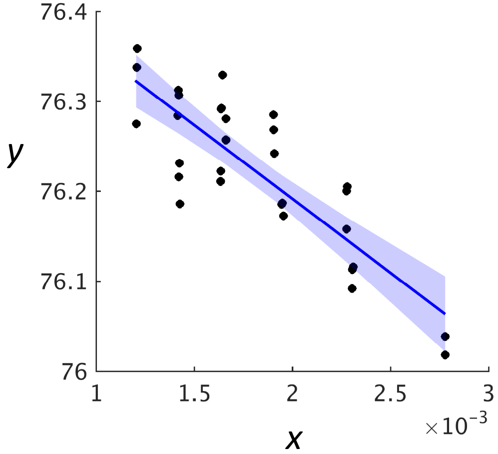
Data   Regression function   Errors

e.g. $\varepsilon_i \sim N(0,\sigma^2)$

$$\boxed{\hat{\boldsymbol{\theta}}: \quad \min_{\boldsymbol{\theta}} \sum_{i=1}^{n} \left(y_i - f_{\boldsymbol{\theta}}(x_i)\right)^2}$$

Least-squares



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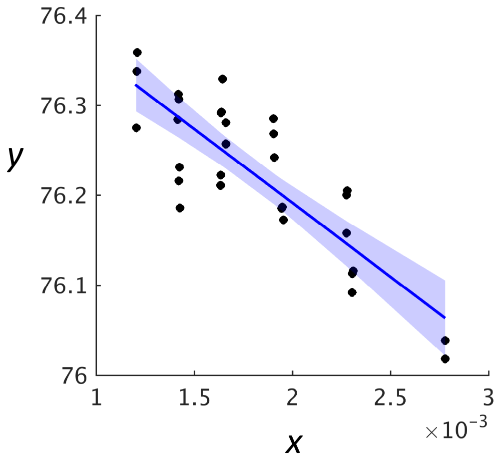
$$\mathbf{U}(\hat{\boldsymbol{\theta}}) = \hat{\sigma}^2 \left(\mathbf{J}^T\mathbf{J}\right)^{-1}, \quad u(\hat{\theta}_\alpha) = \sqrt{\hat{\sigma}^2 \left(\mathbf{J}^T\mathbf{J}\right)^{-1}_{\alpha\alpha}}\;, \quad \mathbf{J} = \partial f_{\boldsymbol{\theta}}(\mathbf{x}) / \partial \boldsymbol{\theta}$$

$$\frac{\boldsymbol{\psi}^T\hat{\boldsymbol{\theta}}}{\boldsymbol{\psi}^T\mathbf{U}(\hat{\boldsymbol{\theta}})\boldsymbol{\psi}} \sim t_{n-p}\,, \quad I_{\theta_\alpha} = \hat{\theta}_\alpha \pm t_{n-p}^{0.975} u(\hat{\theta}_\alpha)$$

G A F Seber and C J Wild (1989) **Nonlinear regression**, Wiley, New York

N R Draper and H Smith (1998) **Applied regression analysis**, Wiley, New York

Least-squares



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Data Regression function Errors

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$$\boxed{\hat{\boldsymbol{\theta}}: \quad \min_{\boldsymbol{\theta}} \sum_{i=1}^{n} \left(y_i - f_{\boldsymbol{\theta}}(x_i)\right)^2}$$

- Cannot include general prior knowledge (but possibly constraints)
- Different meaning of uncertainties than for Bayesian approach
- Typically (much) easier to compute than Bayesian approach
- Provides point estimates and uncertainties – no distribution

LS combined with GUM-S1/S2 versus Bayesian inference

- Combining LS methods with Supplement 1 (or 2) to the GUM also yields a distribution for the regression parameters

- Is such proceeding equivalent to a Bayesian inference?

LS combined with GUM-S1/S2 versus Bayesian inference

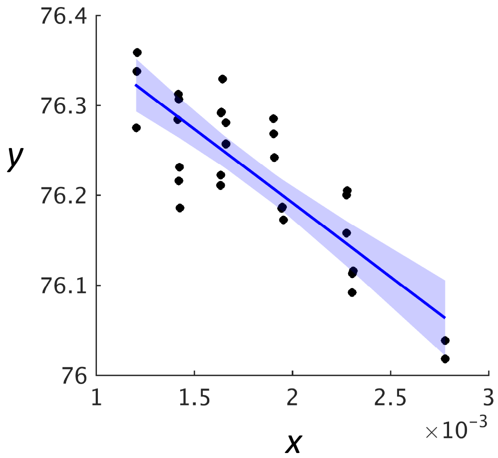
- Combining LS methods with Supplement 1 (or 2) to the GUM also yields a distribution for the regression parameters
- Is such proceeding equivalent to a Bayesian inference?
- In general it is not:
  - No account of prior knowledge (in terms of a distribution)
  - Generally even different to Bayesian inference with noninformative prior

C Elster and B Toman 2011 Bayesian uncertainty analysis for a regression model versus application of GUM Supplement 1 to the least-squares estimate *Metrologia* **48** 233-240

Normal linear straight line regression

$$y_i = \theta_1 + \theta_2 x_i + \varepsilon_i \qquad \varepsilon_i \sim N(0,\sigma^2)$$

[1)] Noninformative prior



	$\hat{\theta}_2$	$u(\theta_2)$	$I_{0.95}$
LS	-164.6	19.4	$[-204.3,-124.8]$
Bayes[1)]	-164.6	20.1	$[-204.3,-124.8]$

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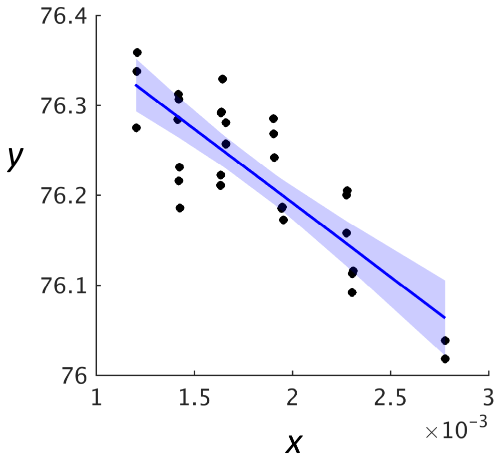

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– But different meaning of uncertainties

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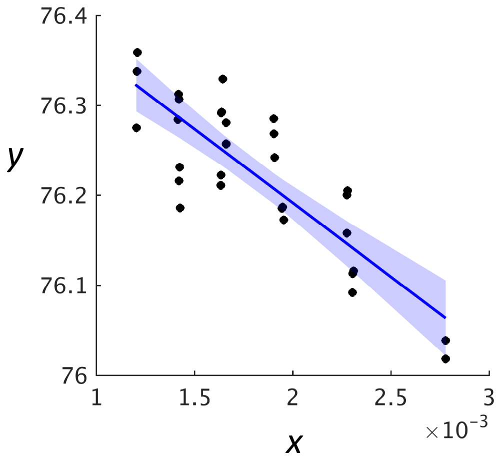

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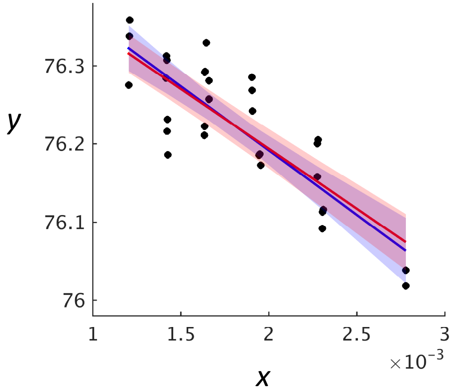

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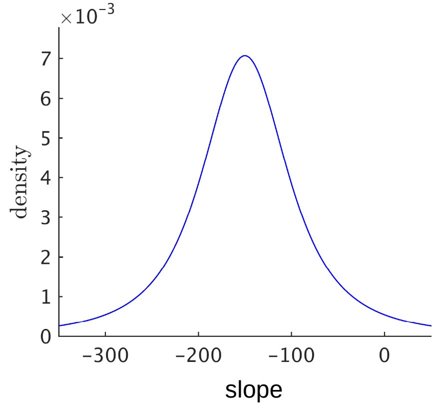
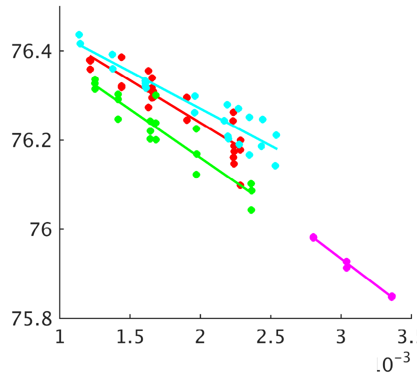


Prior knowledge from previous measurements[1]



[1]K Klauenberg, G Wübbeler, B Mickan, P M Harris and C Elster
A tutorial on Bayesian Normal linear regression, submitted to **Metrologia**

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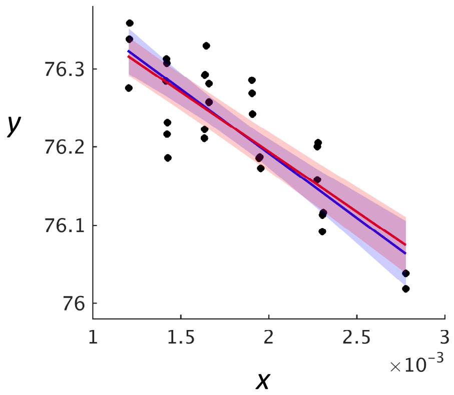

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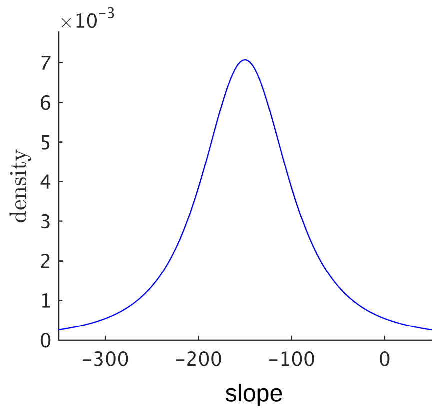

– Different estimates & intervals

– Bayesian inference can result in smaller uncertainties than LS

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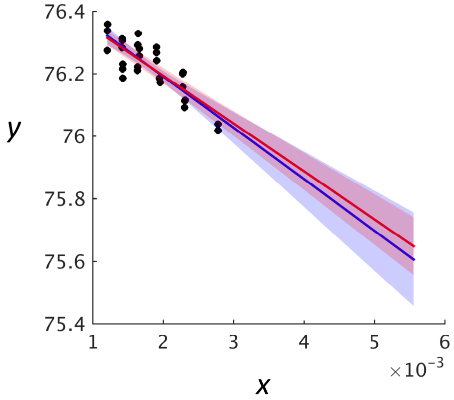

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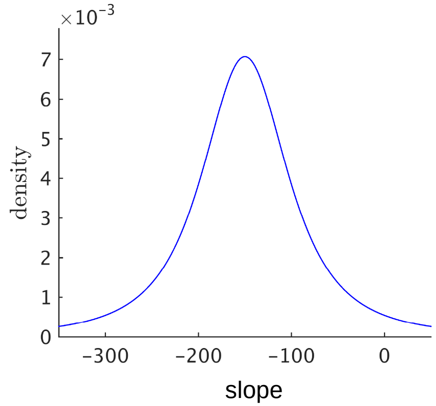

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– Relevant in particular for prediction beyond the range of data[1,2]

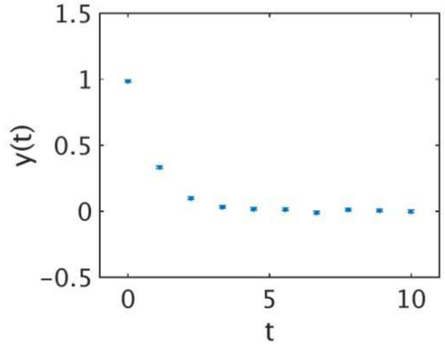
[1]G J P Kok, A M H van der Veen, P M Harris, I M Smith and C Elster (2015) *Bayesian analysis of a flow meter calibration problem*, **Metrologia**, 52, 400-405

[2]K Klauenberg, G Wübbeler, B Mickan, P M Harris and C Elster *A tutorial on Bayesian Normal linear regression*, submitted to **Metrologia**

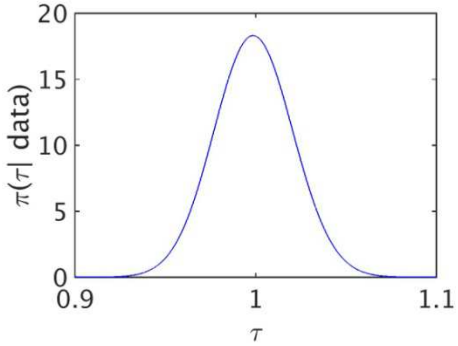
Nonlinear regression

Model $y(t_i) = ae^{-t_i/\tau} + \varepsilon_i,\ \ \varepsilon_i \sim N(0,\sigma^2),\ \ a,\sigma$ known, $\pi(\tau) \propto 1\ \ (0 < \tau < 10)$

Data



Posterior



	$\hat{\tau}$	$u(\tau)$	$I_{0.95}$
Bayes	1.0	0.02	[0.96,1.04]
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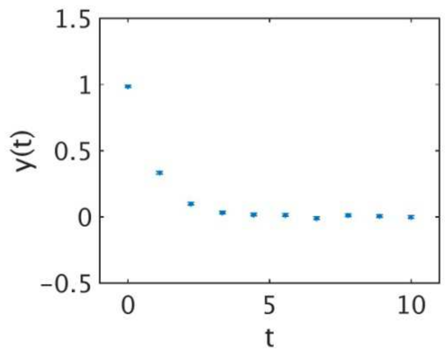

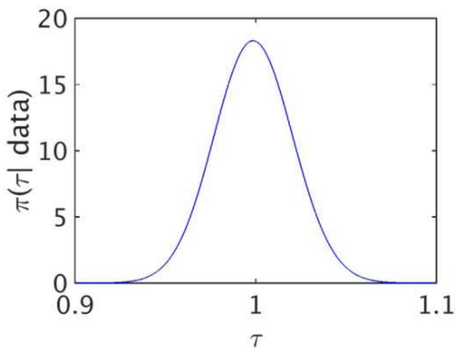

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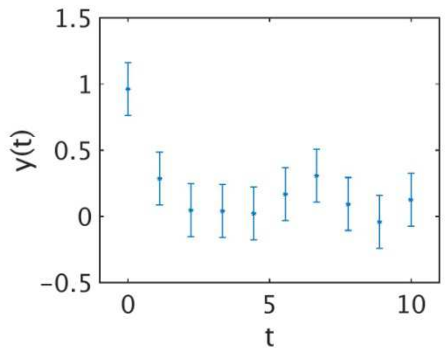

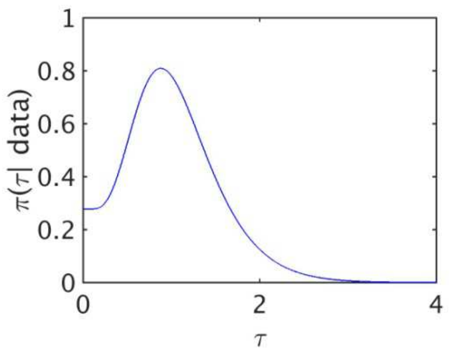

Bayes	1.00	0.54	[0.09,2.21]
LS	0.88	0.41	[0.06,1.70]

For large σ LS may underrate uncertainties due to nonlinearities

Conclusions

- LS and Bayesian inference different conceptually and typically also numerically

- Calculation of results usually easier for LS than for Bayesian inference

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- Calculation of results usually easier for LS than for Bayesian inference
- LS yields reasonable results when
  - Prior knowledge not available or not really informative, and
  - Simple statistical model appropriate, and
  - No severe nonlinearity in problem
- Bayesian inference advantageous when
  - Prior knowledge available and informative
  - Severe nonlinearity in problem
  - Non-trivial statistical model (e.g. heteroscedastic problem)

Acknowledgment & reference

- Gerd Wübbeler and Bodo Mickan for preparing figures and providing data

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- See also talks by Katy Klauenberg, Gertjan Kok, Nicolas Fischer

- C Elster, K Klauenberg, M Walzel, G Wübbeler, P Harris, M Cox, C Matthews, I Smith, L Wright, A Allard, N Fischer, S Cowen, S Ellison, P Wilson, F Pennecchi, G Kok, A van der Veen, L Pendrill (2015) *A Guide to Bayesian Inference for Regression Problems*, Deliverable of EMRP project NEW04 "Novel mathematical and statistical approaches to uncertainty evaluation" (available at http://www.ptb.de/emrp/new04-home.html)

References

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