Bayesian strategies for calibrating heteroskedastic static sensors with unknown model structures

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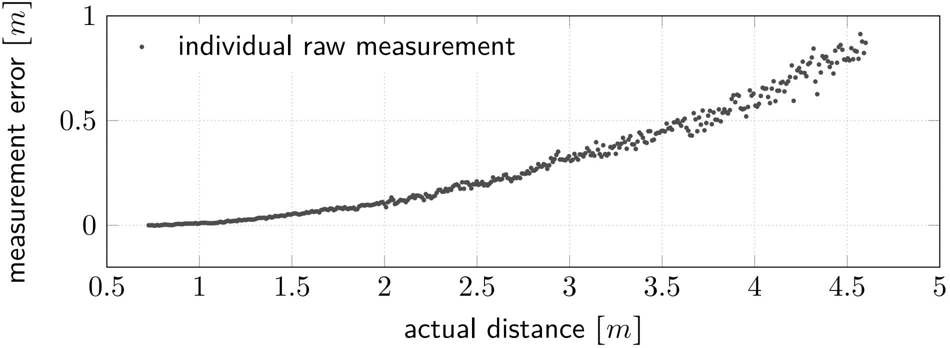
The problem in practice

How shall we calibrate a sensor that behaves in this way?



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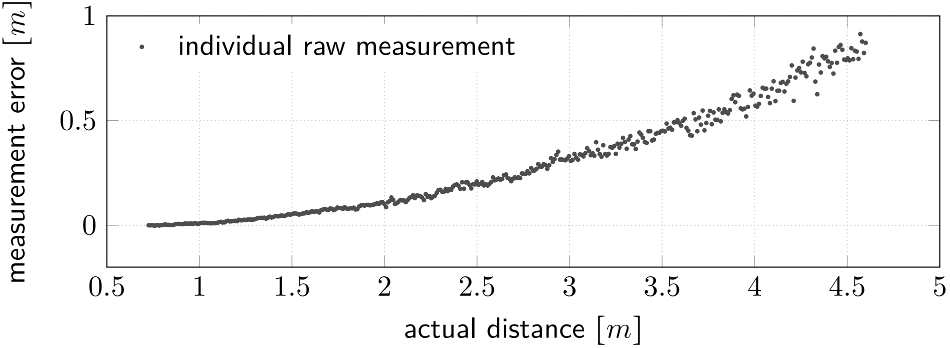

Rephrasing: how shall we account for:

- a systematic bias that smoothly depends on the measurand?
- a measurement noise whose variance also smoothly depends on the measurand?

The problem in practice – an illustrative example

The problem in formulas

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$$f_{\text{mean}}\left(x_i\right) = \begin{bmatrix} 1 & x_i & x_i^2 & \dots & x_i^N \end{bmatrix} \begin{bmatrix} \alpha_0 \\ \alpha_1 \\ \alpha_2 \\ \vdots \\ \alpha_N \end{bmatrix} \tag{2}$$

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$$\boldsymbol{\alpha} \sim \mathcal{N}\left(\boldsymbol{\mu}_{\boldsymbol{\alpha}}, \Sigma_{\boldsymbol{\alpha}}\right) \qquad \boldsymbol{\mu}_{\boldsymbol{\alpha}} := \begin{bmatrix} 0 & 1 & 0 & \cdots & 0 \end{bmatrix}^T \qquad \Sigma_{\boldsymbol{\alpha}} := \operatorname{diag}\left(\boldsymbol{\tau}_{\boldsymbol{\alpha}}^{-2}\right) \tag{3}$$

(assumption: $\boldsymbol{\mu}_{\boldsymbol{\alpha}}$ and $\boldsymbol{\tau}_{\boldsymbol{\alpha}}$ known)

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\text{Case II:} \quad & f_{\text{noise}}(x_i) &= \sigma_\nu x_i^\rho \\
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What do these models represent?

Case I: homoskedastic sensors

Case II: heteroskedasticity depending on the actual state

Case III: heteroskedasticity depending on the expected measurement

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Assumed priors

- $\sigma_\nu^{-2} = \tau_\nu \sim \text{Gamma}(a_\nu, b_\nu)$
- $\rho \in \mathcal{N}^+(a_\rho, b_\rho)$

The problem in formulas – summary

Given

$$y_i = \begin{bmatrix} 1 & \dots & x_i^N \end{bmatrix} \begin{bmatrix} \alpha_0 \\ \vdots \\ \alpha_N \end{bmatrix} + \begin{cases} \sigma_\nu \\ \sigma_\nu x_i^\rho \\ \sigma_\nu \left(\begin{bmatrix} 1 & \dots & x_1^N \end{bmatrix} \begin{bmatrix} \alpha_0 \\ \vdots \\ \alpha_N \end{bmatrix} \right)^\rho \end{cases}$$

a dataset $\mathcal{D} = \{(x_i, y_i)\}_{i=1}^M$ and opportune priors, estimate

- $\boldsymbol{\alpha}$
- σ_ν
- ρ

literature review

Literature review

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ordinary least squares $\implies$ unbiased estimate of the mean, biased estimate of the variance (that worsens with the degree of heteroskedasticity)

Box & Hill (1974)
Correcting inhomogeneity of variance with power transformation weighting
Technometrics

White (1980)
A heteroskedasticity-consistent cov. matrix estimator and a direct test for heteroskedasticity
Econometrica: Journal of the Econometric Society

Literature review

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other schemes focusing on simplified models $\implies$ Gibbs samplers, MCMC schemes

Geweke (1993)
Bayesian treatment of the independent Student-t linear model
Journal of applied econometrics

Boscardin & Gelman (1994)
Bayesian computation for parametric models of heteroscedasticity in the linear model
TODO

Tanizaki & Zhang (2001)
Posterior analysis of the multiplicative heteroscedasticity model
TODO

Our contributions

- slightly more generic model *(unknown ρ)*
- use exact likelihoods instead of approximated ones
- create a stepping stone for schemes where also the x_i's are unknown

the calibration algorithms

disclaimer: the models (and associated calibration procedures) are meaningful only for static sensors

Case I: $f_{\mathrm{noise}}(x_i) = \sigma_\nu$

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solution: Gibbs sampler, since we know the expressions of the conditional distributions & all the priors and likelihoods are conjugate

Algorithm for Case I: $f_{\text{noise}}(x_i) = \sigma_\nu$

1. initialization: $\boldsymbol{\alpha}^{(0)} = \boldsymbol{\mu}_{\boldsymbol{\alpha}}$ $\quad \tau_\nu^{(0)} \sim \text{Gamma}\,(a_\nu, b_\nu)$
2. for $k = 0, 1, \ldots$ up to convergence or k_{max}:
   1. update τ_ν and $\boldsymbol{\alpha}$ using Gibbs sampling:

$$
\begin{aligned}
\boldsymbol{\alpha}^{(k+1)} &\sim p\left(\boldsymbol{\alpha}^{(k)} \,\middle|\, \boldsymbol{x}, \tau_\nu^{(k)}\right) \\
\tau_\nu^{(k+1)} &\sim p\left(\tau_\nu^{(k)} \,\middle|\, \boldsymbol{x}, \boldsymbol{y}, \boldsymbol{\alpha}^{(k+1)}\right)
\end{aligned} \tag{5}
$$

where:

$$
\begin{aligned}
&p\left(\boldsymbol{\alpha}^{(k)} \,\middle|\, \boldsymbol{x}, \boldsymbol{y}, \tau_\nu^{(k)}\right) \propto \mathcal{N}\left(B^{(k)} A^{(k)}, B^{(k)}\right) \\
&A^{(k)} = \tau_\nu^{(k)} G_{\boldsymbol{x}}^T \boldsymbol{y} - \Sigma_{\boldsymbol{\alpha}}^{-1} \boldsymbol{\mu}_{\boldsymbol{\alpha}} \\
&B^{(k)} = \left(\tau_\nu^{(k)} G_{\boldsymbol{x}}^T G_{\boldsymbol{x}} + \Sigma_{\boldsymbol{\alpha}}^{-1}\right)^{-1} \\
&p\left(\tau_\nu^{(k)} \,\middle|\, \boldsymbol{x}, \boldsymbol{y}, \boldsymbol{\alpha}^{(k+1)}\right) \propto \text{Gamma}\left(a_\nu + \frac{M}{2}, \left(\frac{1}{b_\nu} + \frac{1}{2} {C^{(k+1)}}^T C^{(k+1)}\right)^{-1}\right) \\
&C^{(k+1)} = \left(\boldsymbol{y} - G_{\boldsymbol{x}} \boldsymbol{\alpha}^{(k+1)}\right)
\end{aligned} \tag{6}
$$

Case II: $f_{\text{noise}}(x_i) = \sigma_\nu x_i^\rho$

example: *MAP* $\Longrightarrow$ $$\arg \max_{\boldsymbol{\alpha}\in\mathbb{R}^N \; \sigma_\nu^2\in\mathbb{R}_+ \; \rho\in\mathbb{R}_+} p\left(\boldsymbol{\alpha}, \sigma_\nu^2, \rho \,|\, \boldsymbol{x}, \boldsymbol{y}\right) \tag{7}$$

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problem: now both σ_ν and ρ are unknown *(implying that also* $p(\rho \,|\, \boldsymbol{x}, \boldsymbol{y}, \boldsymbol{\alpha}, \tau_\nu)$ *is unknown)*

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problem: now both σ_ν and ρ are unknown *(implying that also $p\left(\rho \,|\, \boldsymbol{x}, \boldsymbol{y}, \boldsymbol{\alpha}, \tau_\nu\right)$ is unknown)*

solution: Single-Component Metropolis-Hastings scheme

Algorithm for Case II: $f_{\text{noise}}(x_i) = \sigma_\nu x_i^\rho$

1. initialization: $\boldsymbol{\alpha}^{(0)} = \boldsymbol{\mu}_{\boldsymbol{\alpha}}$ $\qquad \tau_\nu^{(0)} \sim \text{Gamma}(a_\nu, b_\nu)$ $\qquad \rho^{(0)} = 0$
2. for $k = 0, 1, \ldots$ up to convergence or k_{max}:
   1. update τ_ν and $\boldsymbol{\alpha}$ using the Gibbs sampler:
   $$\begin{aligned} \boldsymbol{\alpha}^{(k+1)} &\sim p\left(\boldsymbol{\alpha}^{(k)} \middle| \boldsymbol{x}, \tau_\nu^{(k)}, \rho^{(k)}\right) \\ \tau_\nu^{(k+1)} &\sim p\left(\tau_\nu^{(k)} \middle| \boldsymbol{x}, \boldsymbol{y}, \boldsymbol{\alpha}^{(k+1)}, \rho^{(k)}\right) \end{aligned} \tag{8}$$
   2. generate a new proposal:
   $$\rho^{(k+1)} \sim \mathcal{N}\left(\rho^{(k)}, \beta\right) \tag{9}$$
   3. calculate the acceptance probability:
   $$\gamma = \min\left[1, \frac{p\left(\boldsymbol{y} \middle| \boldsymbol{x}, \rho^{(k+1)}, \boldsymbol{\alpha}^{(k+1)}, \tau_\nu^{(k+1)}\right)}{p\left(\boldsymbol{y} \middle| \boldsymbol{x}, \rho^{(k)}, \boldsymbol{\alpha}^{(k+1)}, \tau_\nu^{(k+1)}\right)} \frac{p\left(\rho^{(k+1)}\right)}{p\left(\rho^{(k)}\right)}\right] \tag{10}$$
   4. accept the new proposal if $\gamma > \mathcal{U}[0,1]$ and $0 \le \rho \le 10$

Case III: $f_{\text{noise}}(x_i) = \sigma_\nu f_{\text{mean}}(x_i)^\rho$

$$f_{\text{mean}}(x_i) = \begin{bmatrix} 1 & \dots & x_i^N \end{bmatrix} \begin{bmatrix} \alpha_0 \\ \vdots \\ \alpha_N \end{bmatrix} \qquad \Sigma_\nu := \sigma_\nu^2 \operatorname{diag}\Big(f_{\text{mean}}(x_1)^{2\rho}, \dots, f_{\text{mean}}(x_M)^{2\rho} \Big)$$

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problem: now not only $p(\rho \,|\, \boldsymbol{x}, \boldsymbol{y}, \boldsymbol{\alpha}, \tau_\nu)$, but also $p(\boldsymbol{\alpha} \,|\, \boldsymbol{x}, \boldsymbol{y}, \tau_\nu, \rho)$ is unknown

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problem: now not only $p(\rho \,|\, \boldsymbol{x}, \boldsymbol{y}, \boldsymbol{\alpha}, \tau_\nu)$, but also $p(\boldsymbol{\alpha} \,|\, \boldsymbol{x}, \boldsymbol{y}, \tau_\nu, \rho)$ is unknown

solution: use acceptance/rejection mechanisms also for $\boldsymbol{\alpha}$

Algorithm for Case III: $f_{\text{noise}}(x_i) = \sigma_\nu f_{\text{mean}}(x_i)^\rho$

1. initialization: $\boldsymbol{\alpha}^{(0)} = \boldsymbol{\mu}_{\boldsymbol{\alpha}}$ $\quad \tau_\nu^{(0)} \sim \text{Gamma}(a_\nu, b_\nu)$ $\quad \rho^{(0)} = 0$
2. for $k = 0, 1, \ldots$ up to convergence or k_{max}:
   1. update τ_ν using the Gibbs sampler:
   $$\tau_\nu^{(k+1)} \sim p\left(\tau_\nu^{(k)} \middle| \boldsymbol{x}, \boldsymbol{y}, \boldsymbol{\alpha}^{(k)}\right) \tag{11}$$
   2. generate the new proposals:
   $$\boldsymbol{\alpha}^{(k+1)} \sim \mathcal{N}\left(\boldsymbol{\alpha}^{(k)}, \beta\right) \qquad \rho^{(k+1)} \sim \mathcal{N}\left(\rho^{(k)}, \beta'\right) \tag{12}$$
   3. calculate the acceptance probability:
   $$\gamma = \min\left[1, \frac{p\left(\boldsymbol{y} \middle| \boldsymbol{x}, \rho^{(k+1)}, \boldsymbol{\alpha}^{(k+1)}, \tau_\nu^{(k+1)}\right)}{p\left(\boldsymbol{y} \middle| \boldsymbol{x}, \rho^{(k)}, \boldsymbol{\alpha}^{(k)}, \tau_\nu^{(k+1)}\right)} \frac{p\left(\rho^{(k+1)}\right) p\left(\boldsymbol{\alpha}^{(k+1)}\right)}{p\left(\rho^{(k)}\right) p\left(\boldsymbol{\alpha}^{(k)}\right)}\right] \tag{13}$$
   4. accept the new proposal if $\gamma > \mathcal{U}[0, 1]$ and $0 \le \rho \le 10$

Recap

- $f_{\text{noise}}(x_i) = \sigma_\nu \implies$ we know all the conditional distributions $\implies$ we can use Gibbs samplers for $\boldsymbol{\alpha}$ and τ_ν

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- $f_{\text{noise}}(x_i) = \sigma_\nu x_i^\rho \implies$ we don't know the conditional distribution for $\rho \implies$ we shall use Gibbs samplers for $\boldsymbol{\alpha}$ and τ_ν, but a MH sampler for ρ

- $f_{\text{noise}}(x_i) = \sigma_\nu f_{\text{mean}}(x_i)^\rho \implies$ we don't know the conditional distributions for $\boldsymbol{\alpha}$ and $\rho \implies$ we shall use a Gibbs sampler for τ_ν, and MH samplers for $\boldsymbol{\alpha}$ and ρ

Test case: artificial setup

$$f_{\text{mean}}(x_i) = \sum_{n=0}^{3} \alpha_n x_i^n \qquad f_{\text{noise}}(x_i) = \sigma_\nu f_{\text{mean}}(x_i)^\rho$$

Test case: artificial setup

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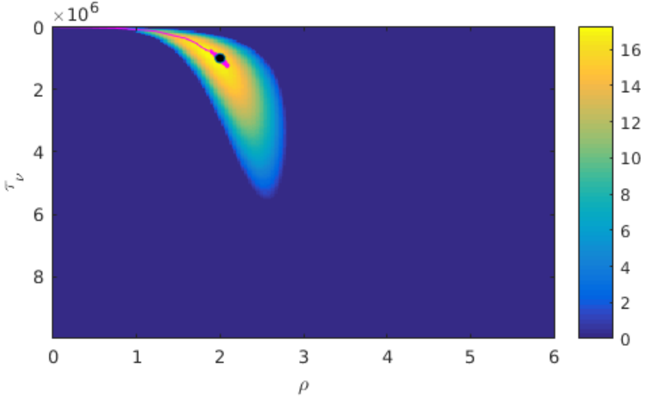
how does $p(\rho, \tau_\nu | \boldsymbol{x}, \boldsymbol{y})$ look like?

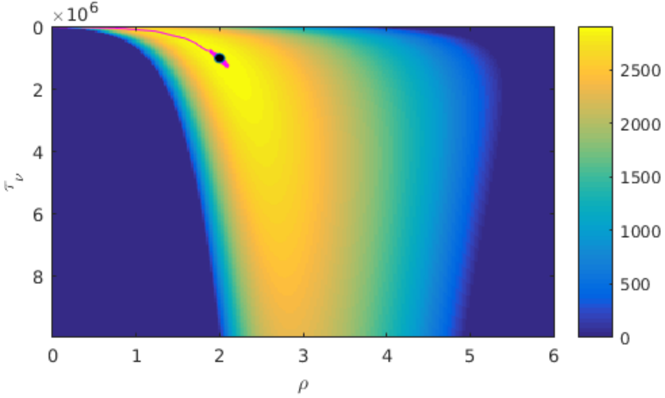
Test case: artificial setup - how does $p\left(\rho, \tau_\nu \middle| \boldsymbol{x}, \boldsymbol{y}\right)$ look like? ($M = 50$)

$$f_{\text{mean}}(x_i) = \sum_{n=0}^{3} \alpha_n x_i^n \qquad f_{\text{noise}}(x_i) = \sigma_\nu f_{\text{mean}}(x_i)^\rho$$

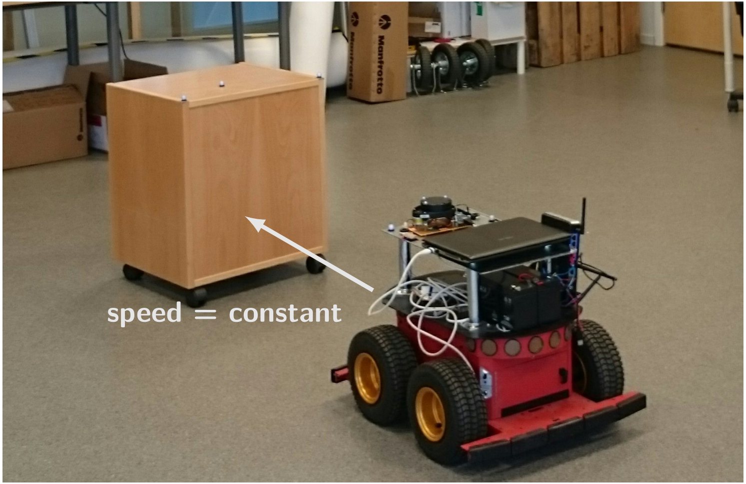


Test case: artificial setup - how does $p(\rho, \tau_\nu | \boldsymbol{x}, \boldsymbol{y})$ look like? ($M = 900$)

$$f_{\text{mean}}(x_i) = \sum_{n=0}^{3} \alpha_n x_i^n \qquad f_{\text{noise}}(x_i) = \sigma_\nu f_{\text{mean}}(x_i)^\rho$$

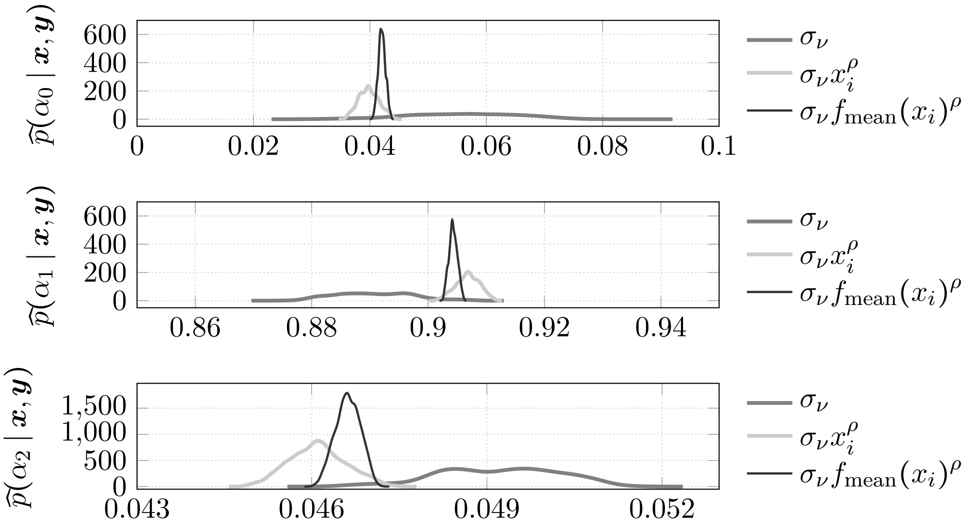


Test case: experimental setup



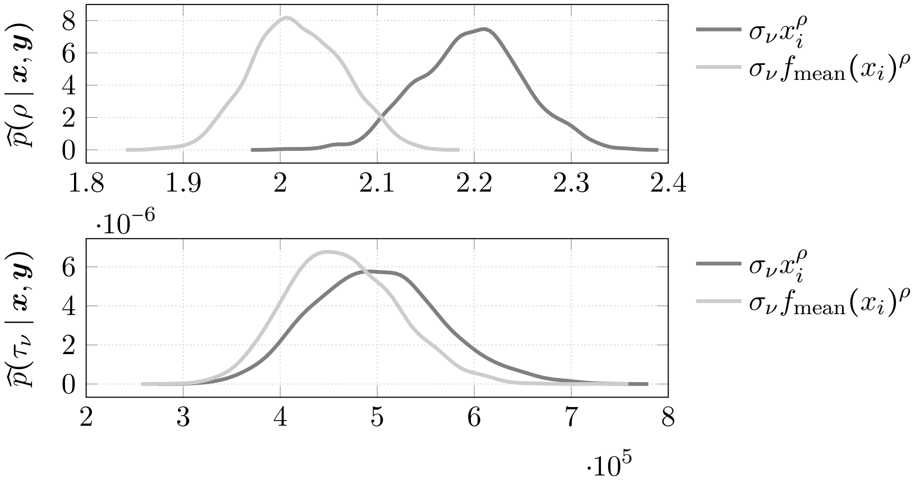
Test case: experimental results

Posteriors for α_0, α_1 and α_2



Test case: experimental results

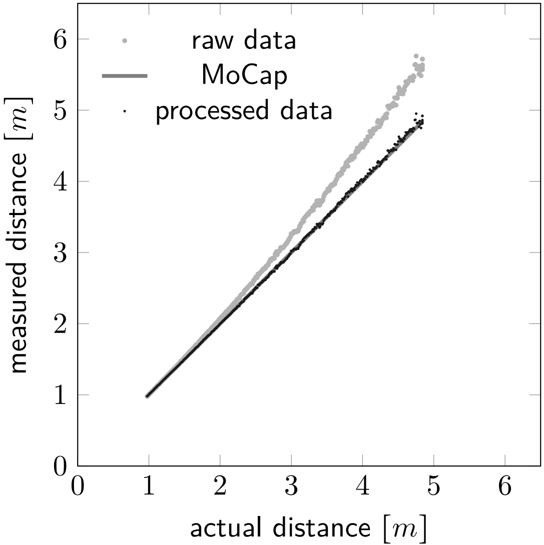
Posteriors for ρ and τ_ν



How shall we use the estimates?

$$\text{e.g.,} \quad \widehat{x}_i = \arg\max_{x_k \in \mathcal{X}} p\left(x_i \,|y_i, \boldsymbol{\alpha}, \sigma_\nu, \rho\right) \tag{14}$$

Test case: experimental results



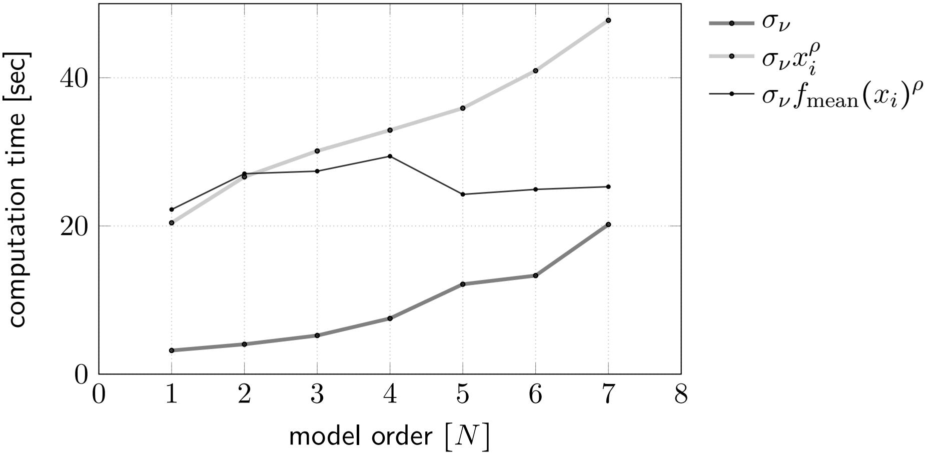
Test case: experimental results

MSE performance on the test set

N	σ_ν	$\sigma_\nu x_i^\rho$	$\sigma_\nu f_{\text{mean}}(x_i)^\rho$
1	1397.59261	50.14214	3220.53529
2	3.15795	0.27043	0.02243
3	0.49000	0.00507	**0.00185**
4	0.48642	0.00404	**0.00088**
5	0.48714	0.00220	**0.00092**
6	0.48675	0.00229	0.01049
7	0.48754	0.00285	0.45820

For completeness: computational times for estimating the models

Matlab on a standard laptop (Intel quad core i7-2640 CPUs 2.8GHz)



Conclusions

- heteroskedastic measurement noise + polynomial bias $\Longrightarrow$ great flexibility
- price: need for "advanced" estimation schemes
- Bayesian approach enables exploiting prior information
- meaningful results on both synthetic and field usecases

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- heteroskedastic measurement noise + polynomial bias $\implies$ great flexibility
- price: need for "advanced" estimation schemes
- Bayesian approach enables exploiting prior information
- meaningful results on both synthetic and field usecases

Next (ongoing) step: what if the x_i's are unknown?

$$y_i = \begin{bmatrix} 1 & \dots & x_i^N \end{bmatrix} \begin{bmatrix} \alpha_0 \\ \vdots \\ \alpha_N \end{bmatrix} + \begin{cases} \sigma_\nu \\ \sigma_\nu x_i^\rho \\ \sigma_\nu \left(\begin{bmatrix} 1 & \dots & x_1^N \end{bmatrix} \begin{bmatrix} \alpha_0 \\ \vdots \\ \alpha_N \end{bmatrix} \right)^\rho \end{cases}$$

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