calibration and uncertainty analysis: how well does a model accomplish its purpose

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Outline

Theoretical aspects of modeling

why do we model?

because we are uncertain about unmeasured quantities

- springflow under different conditions
- concentration at a compliance point
- potential subsidence in unstressed areas
- drawdown from different pumping

we need a **learning** framework to reduce uncertainty

What is calibration?
(and is calibration a **learning** framework?)

historical aspects of calibration

- computational resources were limited
- understanding of model usage was limited

$\therefore$ the best we could do **at that time**

what is calibration (thought to be)?

- “train” the model against reality
- improve the model’s representation of reality
- make the model more like reality

∴ the model simulates reality and yields the “truth”

dangers of calibration

GOAL: GET EXACTLY THE RIGHT ANSWER

"all models are **wrong** but some are **useful**"

Bayesian framework for uncertainty analysis
(a **learning** framework)

Bayes rule for uncertainty analysis

GOAL: BRACKET THE RIGHT ANSWER

Bayes rule for uncertainty analysis

$$\underbrace{P(\theta|\mathbf{D})}_{\substack{\text{what we}\\\text{know now}}} \propto \underbrace{\mathcal{L}(\theta|\mathbf{D})}_{\substack{\text{what we}\\\text{learned}}} \underbrace{P(\theta)}_{\substack{\text{what we}\\\text{knew}}}$$

$\mathbf{D}$	data
θ	model parameters
$P(\theta)$	prior parameter probability distribution
$\mathcal{L}(\theta\|\mathbf{D})$	likelihood of the model parameters given the data
$P(\theta\|\mathbf{D})$	posterior parameter probability distribution

the Prior

$$\underbrace{P(\theta|\mathbf{D})}_{\substack{\text{what we} \\ \text{know now}}} \propto \underbrace{\mathcal{L}(\theta|\mathbf{D})}_{\substack{\text{what we} \\ \text{learned}}} \; \underbrace{P(\theta)}_{\substack{\text{what we} \\ \text{knew}}}$$

- a useful modeler
- what we know **and don't know** about parameters
- initial ("best guess") ("mean value") parameters
- the spread around the "best guess"

likelihood

$$\underbrace{P(\theta|\mathbf{D})}_{\substack{\text{what we}\\ \text{know now}}} \propto \underbrace{\mathcal{L}(\theta|\mathbf{D})}_{\substack{\text{what we}\\ \text{learned}}} \underbrace{P(\theta)}_{\substack{\text{what we}\\ \text{knew}}}$$

- "model-based learning"
- information transfer observations → parameters
- smaller residuals→higher likelihood
- ugly
  - non-parametric
  - high dimensional
  - more on this later...

the Posterior

$$\underbrace{P(\theta|\mathbf{D})}_{\substack{\text{what we}\\\text{know now}}} \propto \underbrace{\mathcal{L}(\theta|\mathbf{D})}_{\substack{\text{what we}\\\text{learned}}} \underbrace{P(\theta)}_{\substack{\text{what we}\\\text{knew}}}$$

- combination of expert knowledge and information in data
- non-parametric
- high dimensional
- expense to fully characterize

calibration in context

$$\underbrace{P(\theta|\mathbf{D})}_{\substack{\text{what we}\\\text{know now}}} \propto \underbrace{\mathcal{L}(\theta|\mathbf{D})}_{\substack{\text{what we}\\\text{learned}}} \underbrace{P(\theta)}_{\substack{\text{what we}\\\text{knew}}}$$

- calibration→maximum likelihood estimation
- a single point in parameter space
- what about other points that fit the data? (non-uniqueness)
- ignores the Prior
- ignores us, the modelers

Synthetic example

why use synthetics?

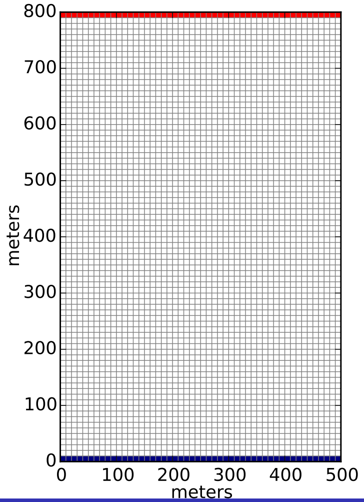
- demonstration
- runs quickly
- “cheating” (answers in the back of the book)

tools

- PEST++ V3 (Welter and others, 2015)
  - object-oriented version of PEST
  - integrated parallel run manager
  - global sensitivity analyses
  - builds on Windows,Linux, and Mac OS
  - **integrated linear-based uncertainty analyses**
- pyEMU (White and others, 2016)
  - python framework for linear-based uncertainty analyses
  - exploratory and data worth analyses
  - easy to use (says the guy who made it)

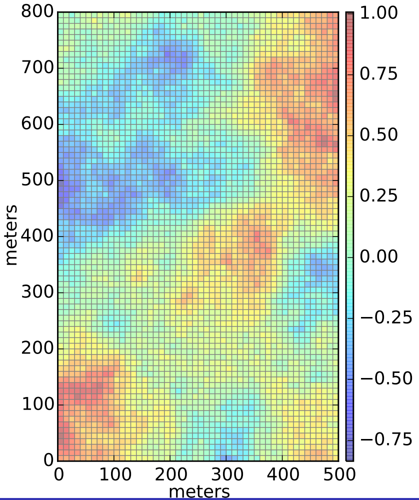
model details

- MODFLOW-2005
- MODPATH v6
- 1 stress period
- 1 layer
- 80 rows
- 50 columns



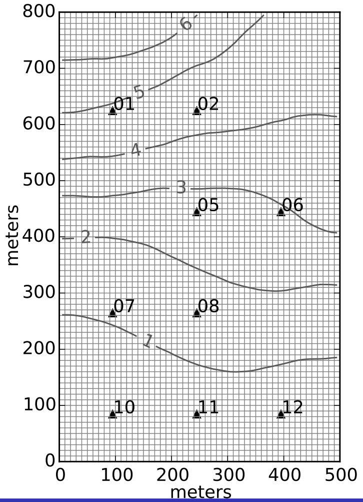
the “truth”

- exponential variogram
- range 600.0m
- sill 0.2 $log_{10}\frac{m}{d}$



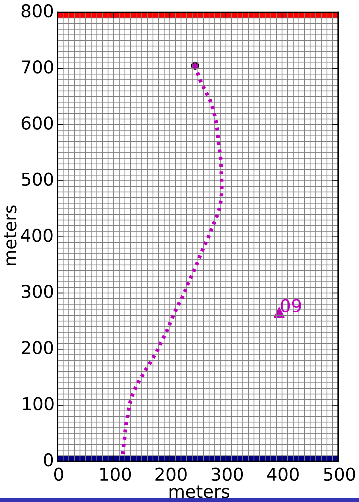
"observations"

- "observed" from the "true" model run
- heads at 9 locations
- Gaussian noise
- $\mathcal{N}(0, 0.1)$

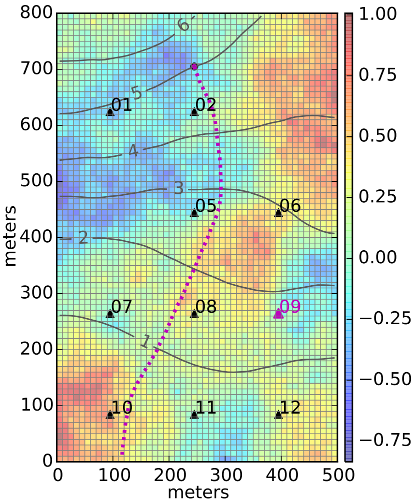


forecasts

- 1.)head at location #9
- 2.)particle exit point
- 3.)particle travel time



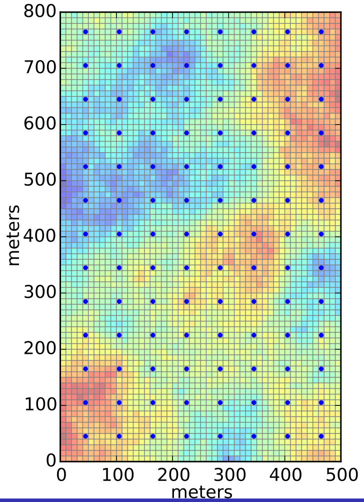
tying it all together



a tale of two models

two parameterizations

- only K is different
- 104 pilot points
- a single zone

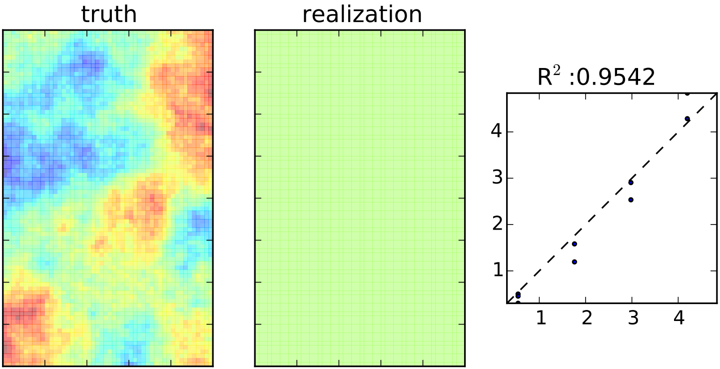


Calibration attempts

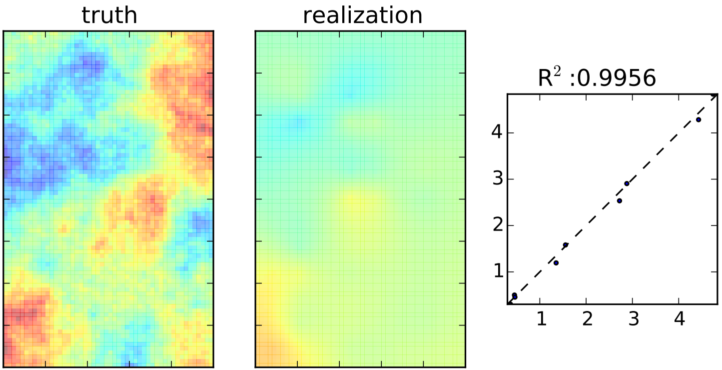
how

- PEST++ V3
- subspace and Tikhonov regularization

single parameter results

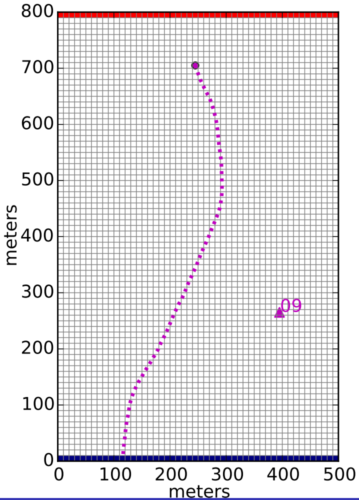


pilot point results

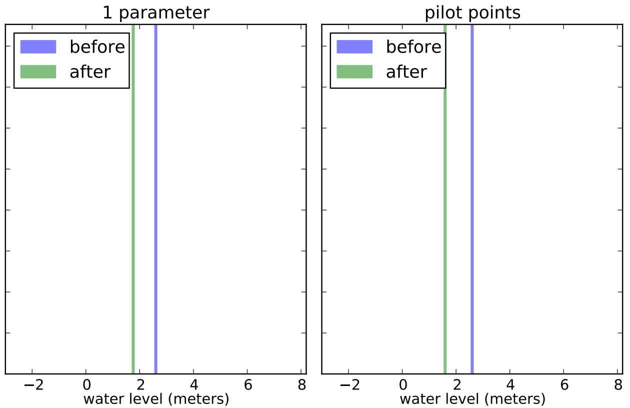


head forecast

- 1.)head at location #9
- 2.)particle exit point
- 3.)particle travel time

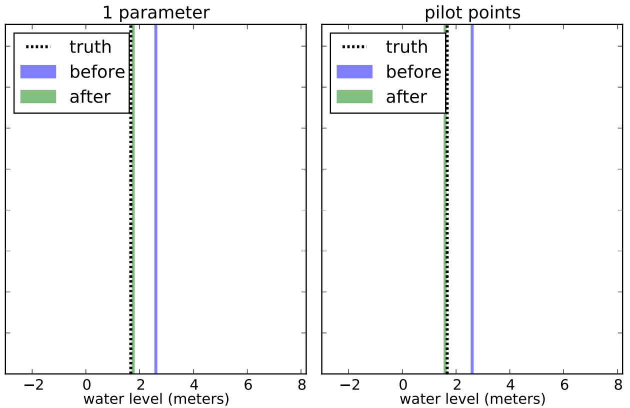


head forecast



- calibration has changed the value of the forecast from ≈2.2m to ≈ 2m

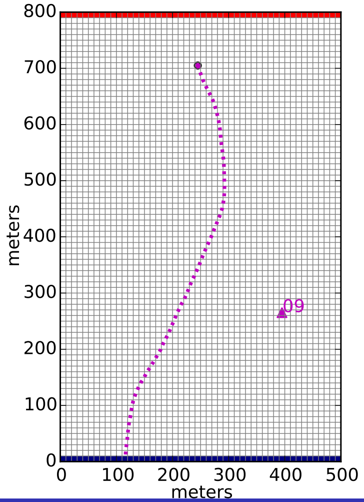
head forecast (with truth)



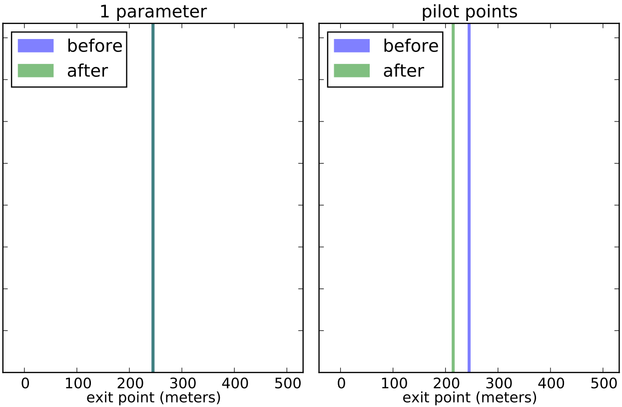
- both parameterizations calibrate to ≈ the true value

exit point forecast

- 1.)head at location #9
- 2.)particle exit point
- 3.)particle travel time

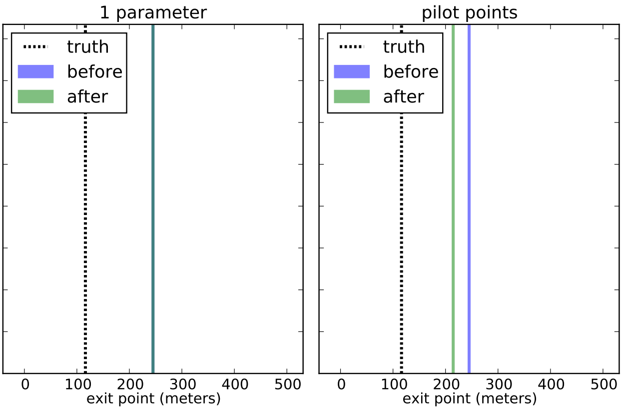


exit point forecast



- calibration of the single parameter model does not effect the forecast

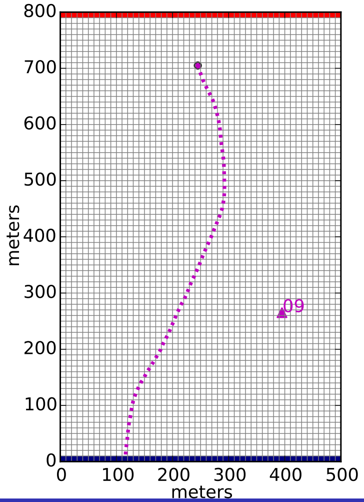
exit point forecast (with truth)



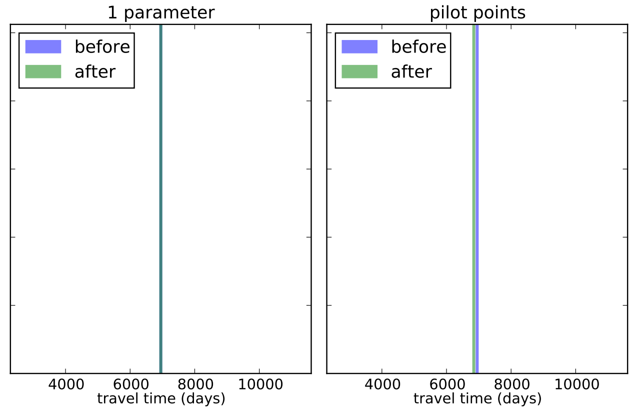
- both calibrated models are wrong

travel time forecast

- 1.)head at location #9
- 2.)particle exit point
- 3.)particle travel time

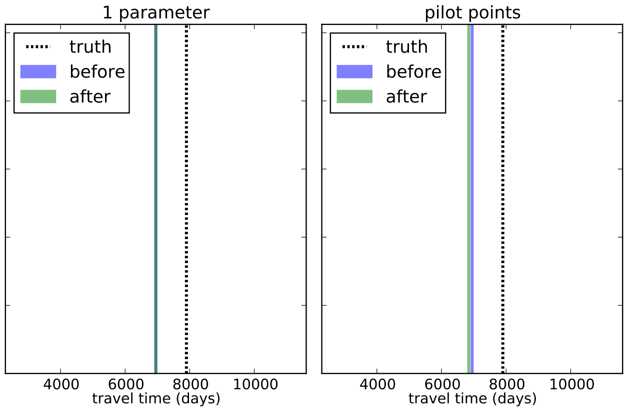


travel time forecast



- calibration does not effect the value of the forecast for either model

travel time forecast (with truth)



- both calibrated models are wrong

what did we learn about the model's purpose?

(Calibration as an learning framework)

- before calibration, each forecast had a value
- after calibration, each forecast has a (new) value
- increasing the number of parameters doesn't have any effect on our understanding of the model's purpose

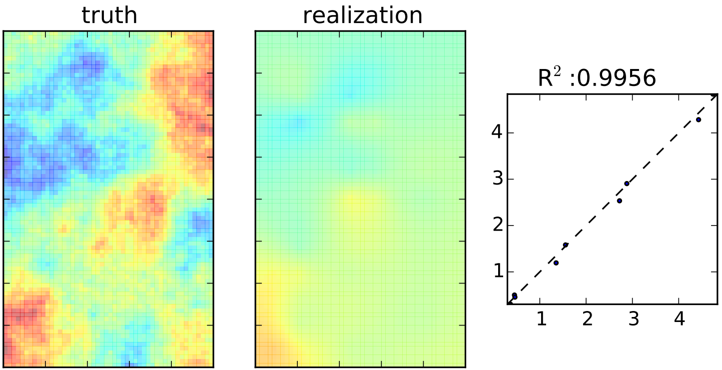
$\therefore$ we don't know what we learned about purpose

Check your work

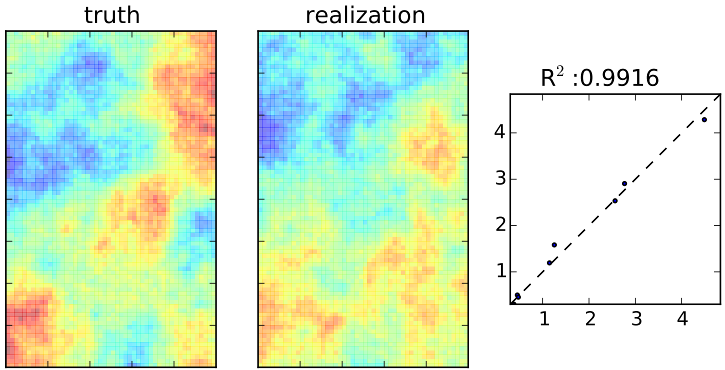
Since we know the “truth”... and this is a really simple model:

Why did we not get the correct forecast?

pilot point results



what did we learn?



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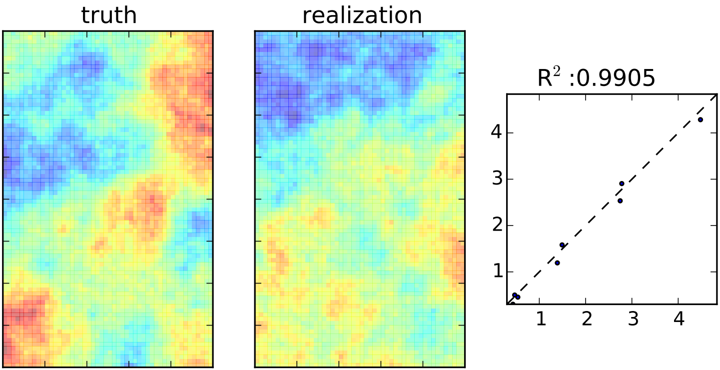

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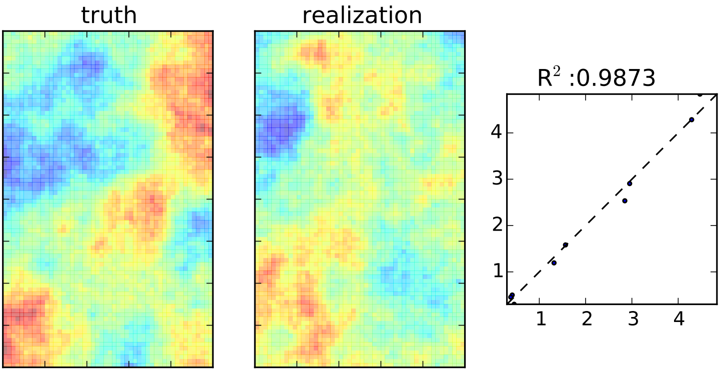
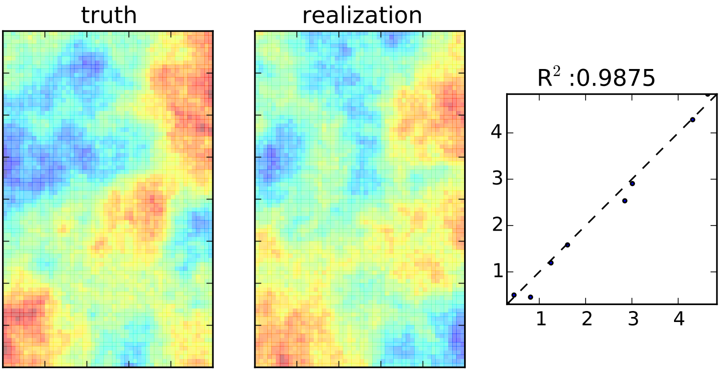


what did we learn?



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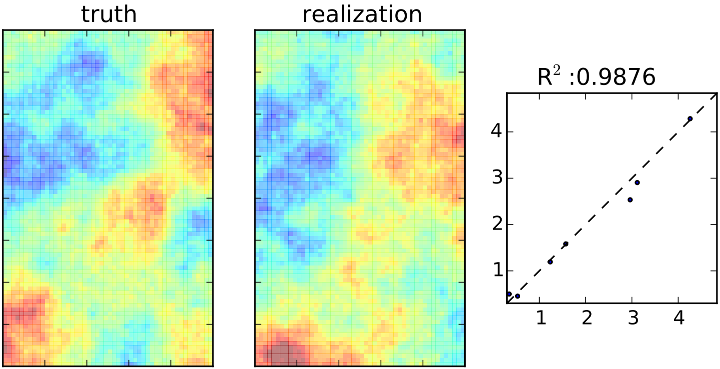
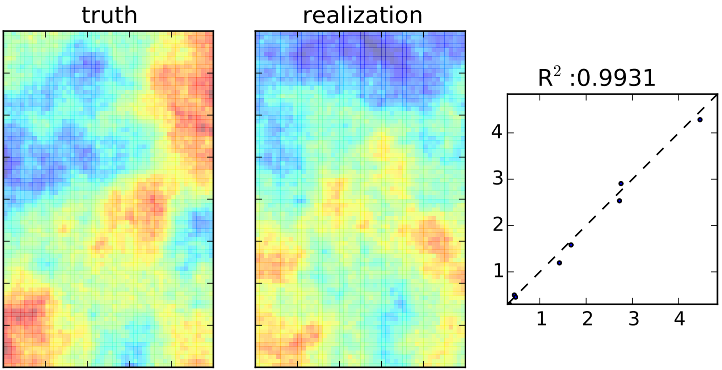
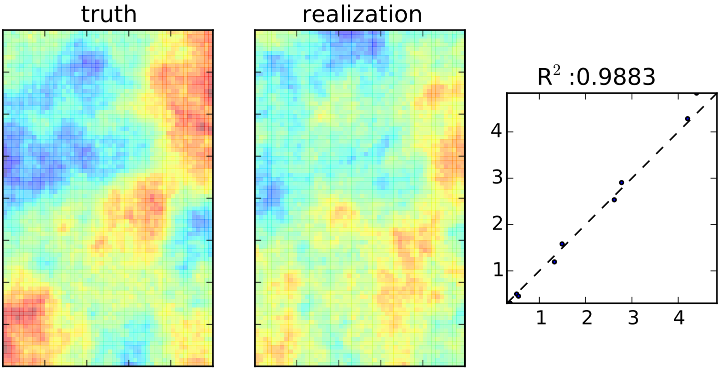


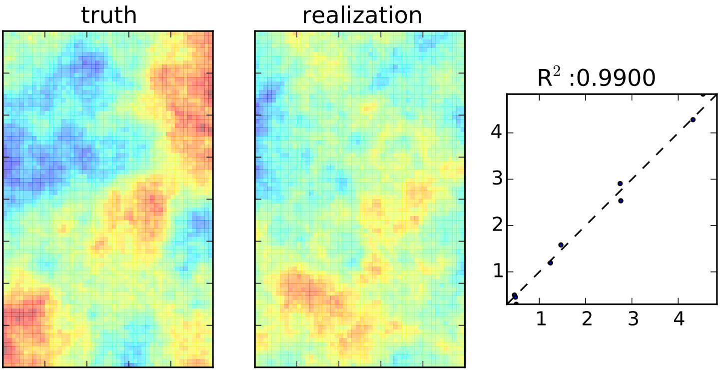
what did we learn?



what did we learn?



what did we learn?



Uncertainty analysis

Bayes for GW models

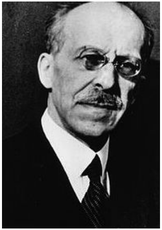
$$\underbrace{P(\theta|\mathbf{D})}_{\substack{\text{what we}\\\text{know now}}} \propto \underbrace{\mathcal{L}(\theta|\mathbf{D})}_{\substack{\text{what we}\\\text{learned}}} \underbrace{P(\theta)}_{\substack{\text{what we}\\\text{knew}}}$$

- in its purist form, Bayes is very difficult to apply to GW models
    - $\mathcal{L}$ is nonparameteric and high-dimensional
    - long model run times
- so...we make some simplifying assumptions:
    - linear-based uncertainty analysis

background on linear theory (FOSM)

- **F**irst **O**rder **S**econd **M**oment
- **FO**→linearity assumption
- **SM**→multivariate Gaussian posterior assumption
- $P(\theta|\mathbf{D}) \approx \mathcal{N}(\overline{\boldsymbol{\mu}}_{\boldsymbol{\theta}}, \overline{\boldsymbol{\Sigma}}_{\boldsymbol{\theta}})$
- requires only one run per parameter!





Schur's complement

$$\underbrace{\overline{\boldsymbol{\Sigma}}_{\boldsymbol{\theta}}}_{\substack{\text{what we}\\\text{still don't know}}} = \underbrace{\boldsymbol{\Sigma}_{\boldsymbol{\theta}}}_{\substack{\text{what we}\\\text{didn't know}}} - \underbrace{\boldsymbol{\Sigma}_{\boldsymbol{\theta}}\mathbf{J}^{\mathbf{T}}\left[\mathbf{J}\boldsymbol{\Sigma}_{\boldsymbol{\theta}}\mathbf{J}^{\mathbf{T}} + \boldsymbol{\Sigma}_{\boldsymbol{\epsilon}}\right]^{-1}\mathbf{J}\boldsymbol{\Sigma}_{\boldsymbol{\theta}}}_{\text{what we learned}}$$

$\boldsymbol{\Sigma}_{\boldsymbol{\theta}}$	prior parameter covariance matrix
$\mathbf{J}$	Jacobian matrix
$\boldsymbol{\Sigma}_{\boldsymbol{\epsilon}}$	measurement noise covariance matrix
$\overline{\boldsymbol{\Sigma}}_{\boldsymbol{\theta}}$	posterior parameter covariance matrix

parameters → forecasts

$$\sigma_s^2 = \mathbf{y}^\mathbf{T} \mathbf{\Sigma}_{\boldsymbol{\theta}} \mathbf{y}$$

$$\overline{\sigma}_s^2 = \mathbf{y}^\mathbf{T} \overline{\mathbf{\Sigma}}_{\boldsymbol{\theta}} \mathbf{y}$$

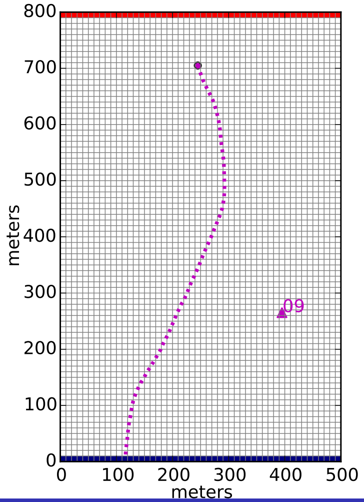
σ_s^2	prior variance of forecast s (what we didn't know)
$\overline{\sigma}_s^2$	posterior variance of forecast s (what we still don't know)
$\mathbf{y}$	forecast sensitivity vector

implementation - PEST++ V3

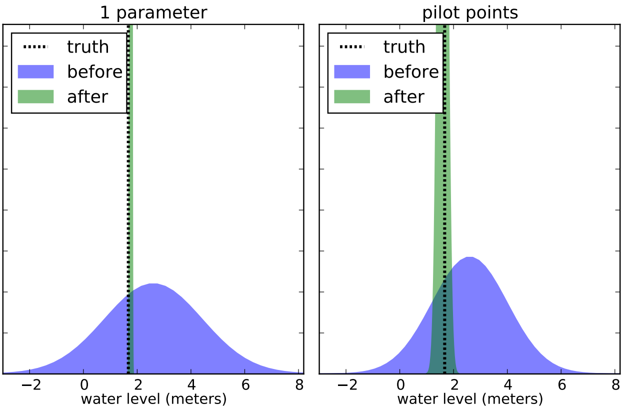
- no additional model runs required!
- no reason not to use this valuable information

head forecast

- 1.)head at location #9
- 2.)particle travel time
- 3.)particle exit point



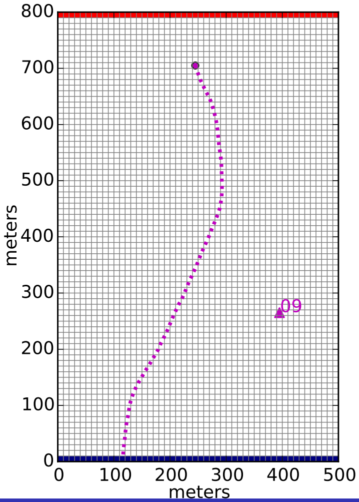
uncertainty: head forecast



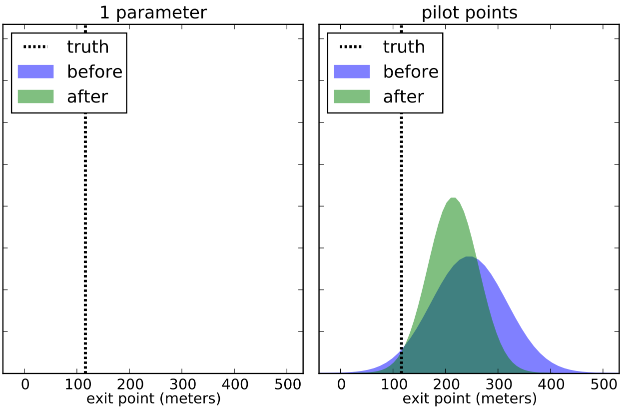
- calibration of both models reduces uncertainty
- pilot points model bracket the ”true” value

exit point forecast

- 1.)head at location #9
- 2.)particle exit point
- 3.)particle travel time



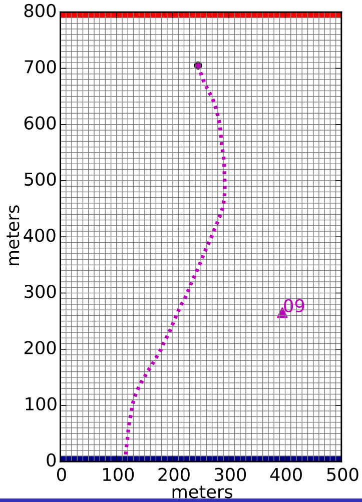
uncertainty: exit point forecast



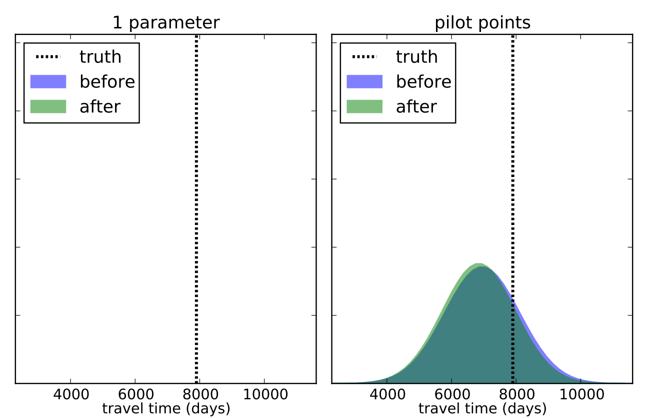
- 1 parameter model grossly underestimates uncertainty
- calibration only slightly reduces uncertainty

travel time forecast

- 1.)head at location #9
- 2.)particle exit point
- 3.)particle travel time



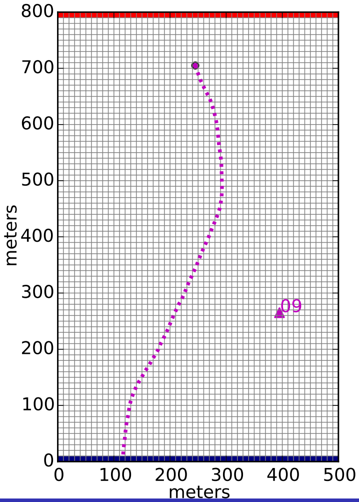
uncertainty: travel time forecast



- 1 parameter model grossly underestimates uncertainty
- calibration does not reduce uncertainty

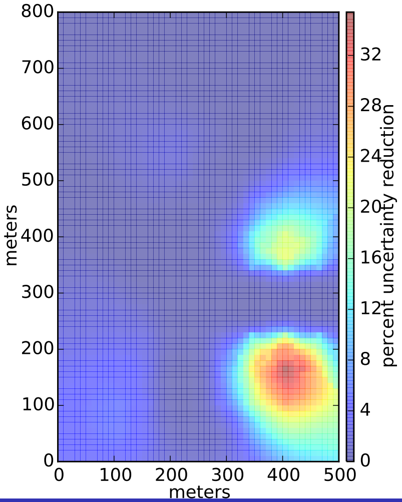
data worth analyses

- ”what if...” scenarios
- **data that we don’t have!!!**
- guide data acquisition
- where to ”learn” about K
  - most reduce uncertainty
  - **learn about model purpose**
- forecast specific
- no additional run required!
- pyEMU



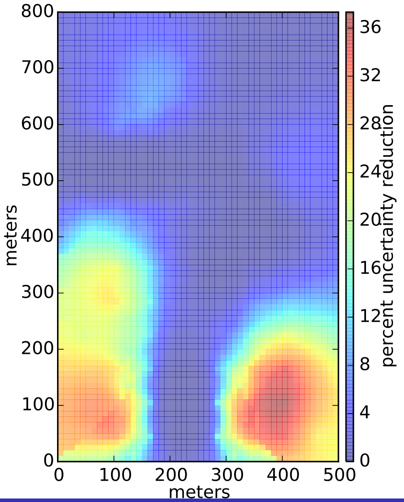
exploratory analysis: head forecast

- knowing K in the right place can reduce forecast uncertainty by 35%
- down gradient of forecast



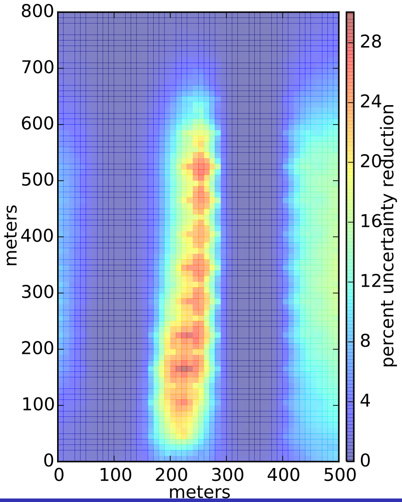
exploratory analysis: exit point forecast

- knowing K in the right place can reduce forecast uncertainty by 37%
- up gradient of forecast

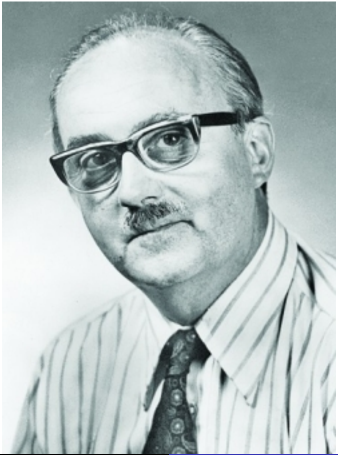


exploratory analysis: travel time forecast

- knowing K in the right place can reduce forecast uncertainty by 30%
- centerline of travel path



"all models are **wrong** but some are **useful**"



Why calibration is dangerous

- The **goal** of calibration: get the “right” answer
  - yikes!

Calibration doesn’t improve understanding (purpose)

why uncertainty analysis is better

- The **goal** of uncertainty analysis: bracket the "right" answer
    - a much better chance of being "right"
- **uncertainty analysis directly addresses learning**

data worth analyses

- great complement to uncertainty analysis
- super powerful tool for modeling analyses
- maximize value of expensive data collection
- very easy to apply
    - no additional model runs
    - pyEMU
- directly answers questions related to improved understanding of model purpose