

Probabilistic Inverse Theory

Lecture 5

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Optimization approach - direct search for best m

Optimization approach

$$S(\mathbf{m}) = \|\mathbf{d}^{obs} - \mathbf{d}^{th}(\mathbf{m})\| + \|\mathbf{m} - \mathbf{m}^{apr}\|$$

solution: search for \mathbf{m}^{ml} minimizing $S(\mathbf{m})$

$$S(\mathbf{m}^{ml}) = \min$$

Optimization approach - main steps

- ◆ selection *a priori* model \mathbf{m}^{apr}
- ◆ selection norms $\|\cdot\|_{\mathcal{D}}$ and $\|\cdot\|_{\mathcal{M}}$
- ◆ selection optimization algorithm
- ◆ run optimization
- ◆ post-optimization analysis (residua, resolution, etc.)

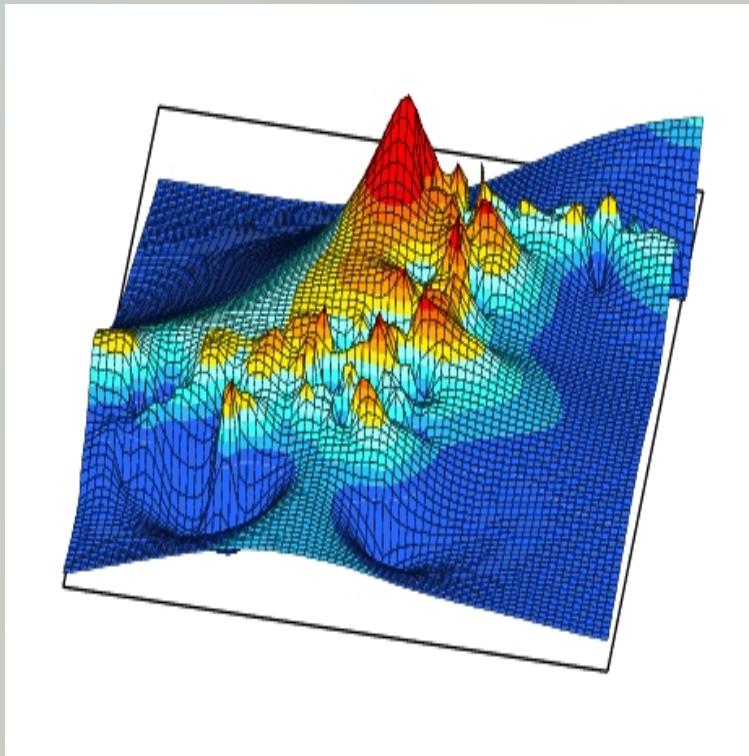
Optimization approach - features

- ◆ fully nonlinear method
- ◆ variety of existing optimization method
- ◆ choice of $S(\mathbf{m})$ - additional (*apriori*) constraints
- ◆ is solution unique ?
- ◆ problem with error estimation

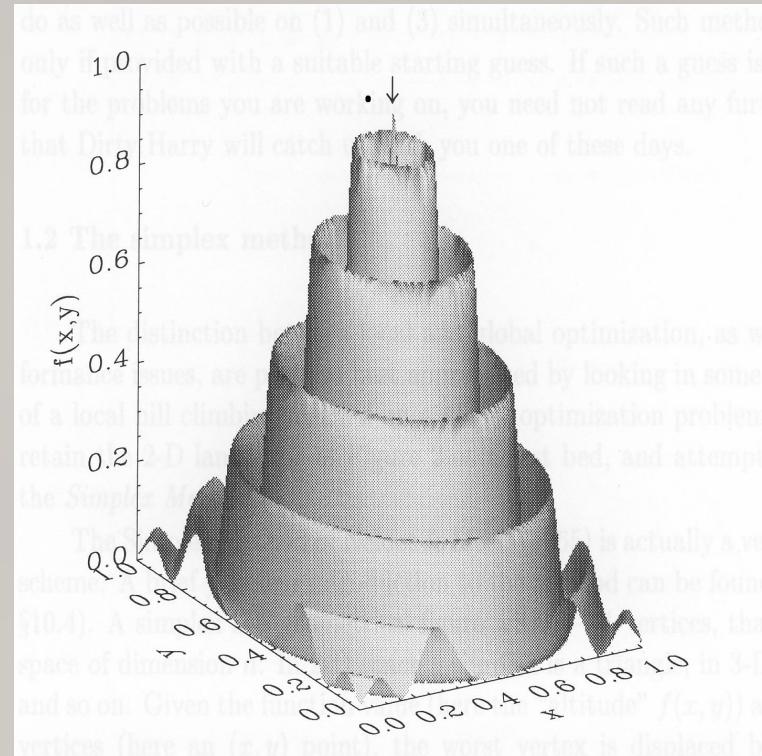
Optimization method - non-uniqueness

$$\sigma(\mathbf{m}) = \exp(-S(\mathbf{m}))$$

multi-modality



null space



Optimization approach - features

- ◆ fully nonlinear method
 - ◆ variety of existing optimization method
 - ◆ Choice of $S(\mathbf{m})$ - different norms + additional constraints
 - ◆ is solution unique ?
 - ◆ problem with error estimation
-

Inverse problem \equiv indirect measurement
Errors are important!

Solution errors

Optimization approach provides the “best fitting” **single** solution Estimation of accuracy of the find solution is, however, problematic and usually needs special additional afford and develop case-dependent approach. There is NO general method of uncertainty analysis for this approach!

Possible approaches

- ◆ skipping the problem
- ◆ linearization $G(\mathbf{m})$ around the optimum found and calculation of the covariance matrix
- ◆ Monte Carlo simulation

Inversion errors - linear problem and l_2 norms

Solution:

$$\mathbf{m}^{est} = \mathbf{m}^{apr} + \mathbf{C}_p^{-1} \mathbf{G}^T \mathbf{C}_d^{-1} \cdot (\mathbf{d}^{obs} - \mathbf{G} \cdot \mathbf{m}^{apr})$$

where

$$C_p = (\mathbf{G}^T \mathbf{C}_d^{-1} \mathbf{G} + \mathbf{C}_m^{-1})$$

Moreover

$$S(\mathbf{m}) = (\mathbf{m} - \mathbf{m}^{est})^T \mathbf{C}_p^{-1} (\mathbf{m} - \mathbf{m}^{est})$$

Inversion errors - Monte Carlo approach

$$\|\mathbf{d}^{obs} - \mathbf{d}^{th}(\mathbf{m}^{est})\|_D + \|\mathbf{m}^{est} - \mathbf{m}^{apr}\|_M = \min$$

$$\begin{aligned} & \|\mathbf{d}^{obs} - \mathbf{d}^{th}(\mathbf{m}^{est}) + \epsilon^{obs} + \epsilon^{th}(\mathbf{m})\|_D + \\ & \|\mathbf{m}^{est} - \mathbf{m}^{apr} + \epsilon^{apr}\|_M = \min \end{aligned}$$



$$\mathbf{m}_{ijk}^{est} = \mathbf{m}^{est} (\epsilon_i^{obs}, \epsilon_j^{th}(\mathbf{m}^{est}), \epsilon_k^{apr})$$

Estimating measurement errors - what does it mean

When measuring parameter p we provide (or should do) result in the form

$$\mathbf{p} = \mathbf{p}^o \pm \delta\mathbf{p}$$

where $\delta\mathbf{p}$ is an error measurement. What this notion does it mean?

Uncertainties - repeated measurements

$$\mathbf{p}_1, \mathbf{p}_2, \dots, \mathbf{p}_N$$

calculate the average value:

$$\bar{\mathbf{p}} = \frac{1}{N} \sum_{i=1}^N \mathbf{p}_i$$

and its variance

$$\delta^2 \mathbf{p} = \frac{1}{N} \sum_1^N (\mathbf{p} - \bar{\mathbf{p}})^2$$

then

$$\mathbf{p} = \bar{\mathbf{p}} \pm \delta \mathbf{p}$$

Uncertainties - stochastic point of view (1)

$N(p)$ - number of measurement results with values in range
 $[p - h/2, p + h/2]$

then histogram (probability distribution)

$$H(p) = \frac{N(p)}{N}$$

average value

$$\bar{p} = \sum_p p H(p)$$

dispersion

$$\delta^2 p = \sum_p (p - \bar{p})^2 H(p)$$

Uncertainties - stochastic point of view (2)

stochastic errors

$$p^{obs} = p^{true} + \epsilon$$

with given probability distribution $\rho(\epsilon)$ (usually unknown)

if sufficient number of measurements and measurements are unbiased ($\bar{\epsilon} = 0$)

$$\rho(\epsilon) \approx H(p - \bar{p})$$

is approximate statistics of errors

then (sometimes) a good estimator of p^{true} is

$$\mathbf{p}^{est} = \bar{\mathbf{p}} \pm \delta \mathbf{p}$$

Uncertainties - stochastic point of view (2)

However, the error statistics can be quite complex, multi-modal, etc. Then, the formula

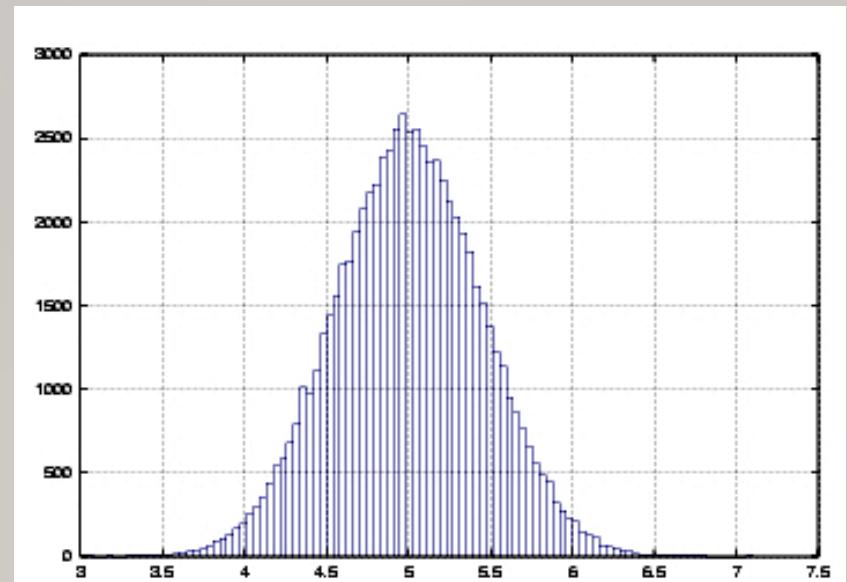
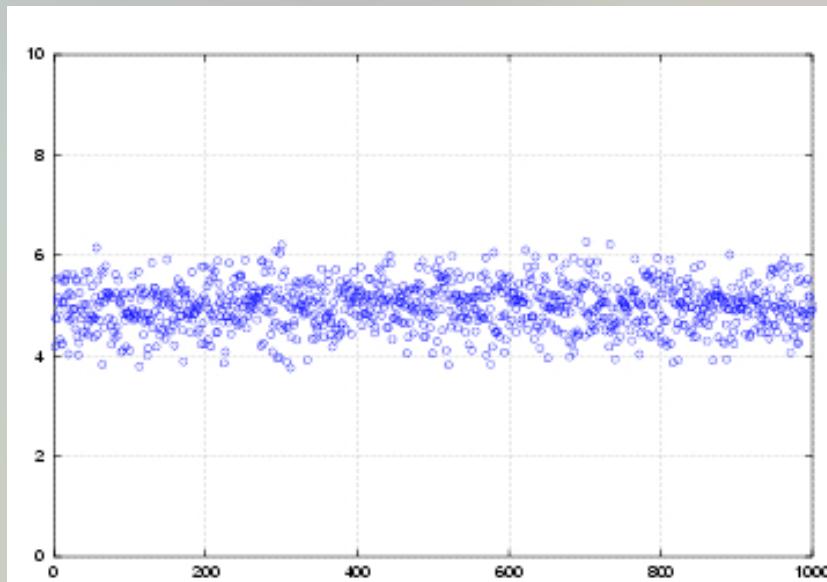
$$\mathbf{p}^{est} = \bar{\mathbf{p}} \pm \delta \mathbf{p}$$

cannot be used

Than, the correct error estimation requires providing the **complete** error statistics $\rho(\epsilon)$

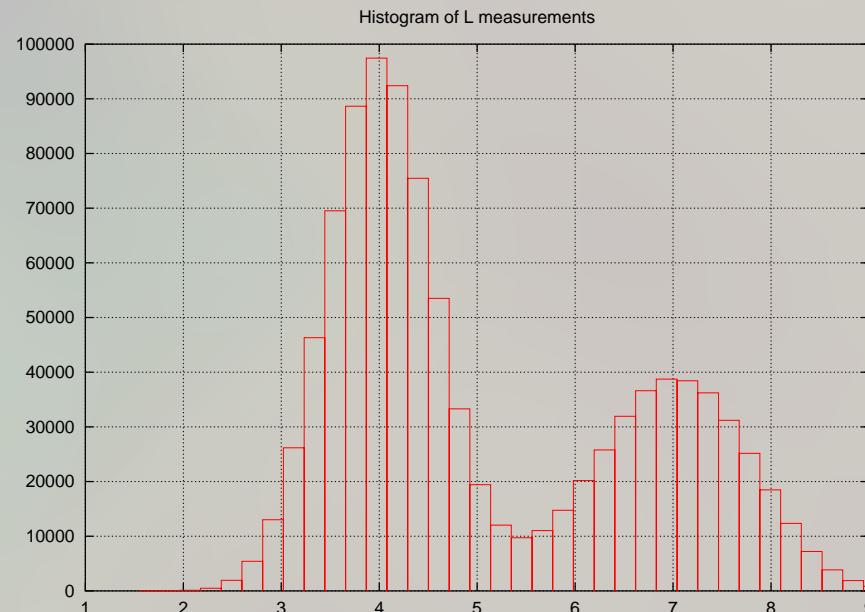
This is what we need in case of inverse problems

Uncertainties - Gaussian errors



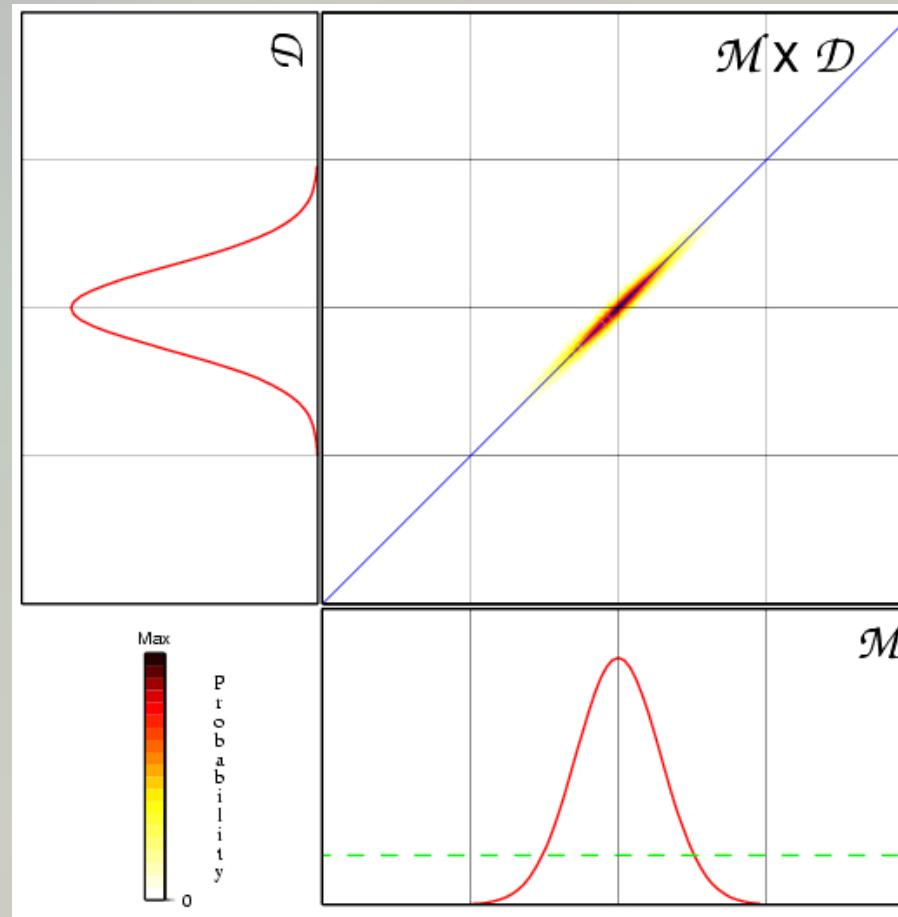
$$P(\bar{p} - \delta < p < \bar{p} + \delta) = 0.68$$

Uncertainties - non-Gaussian errors

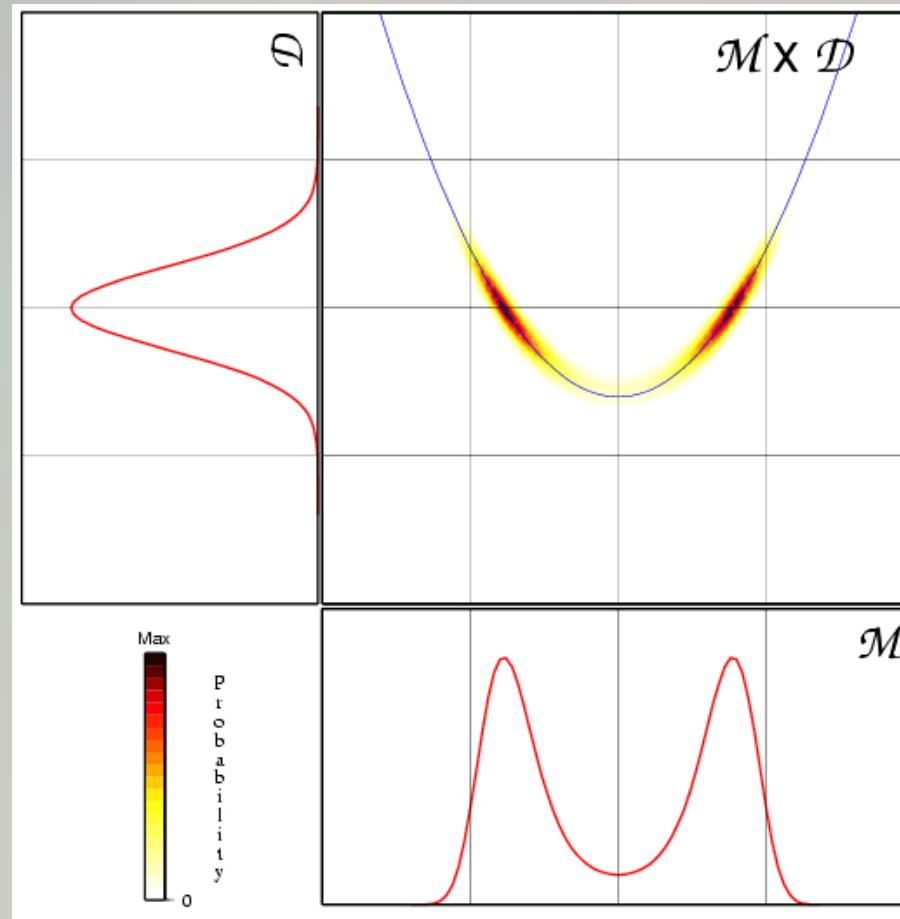


$$\mathbf{p}^{est} \neq \bar{\mathbf{p}} \pm \delta \mathbf{p}$$

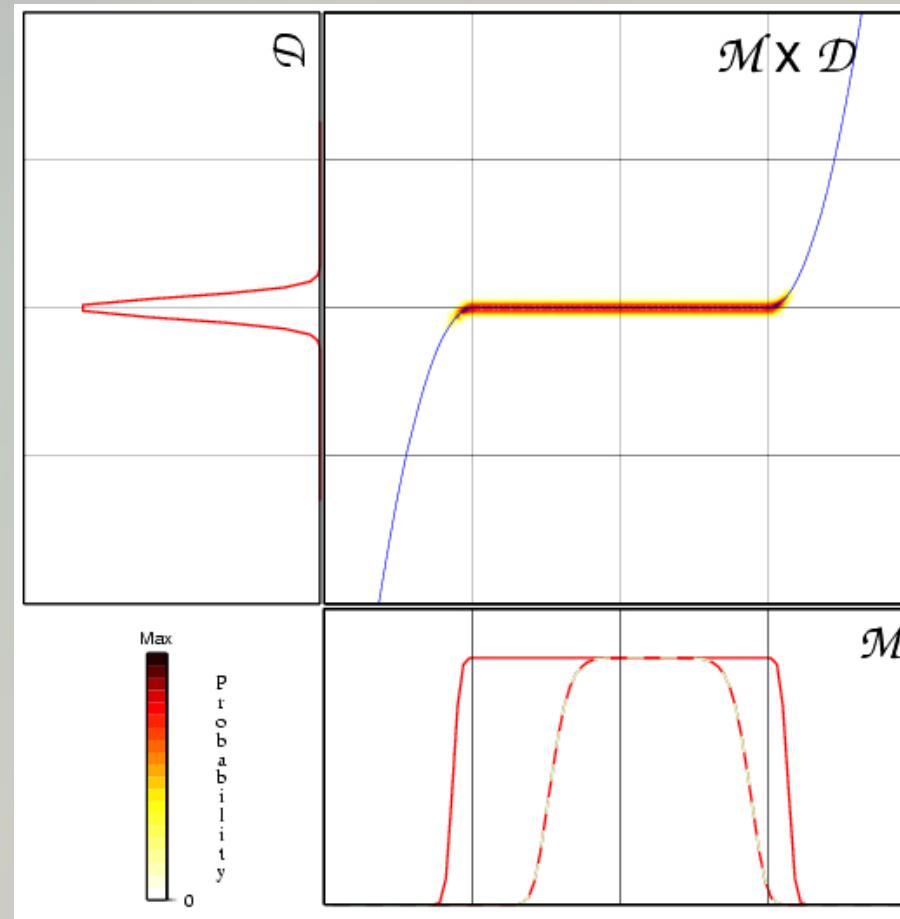
Uncertainties - inverse problems (1)



Uncertainties - inverse problems (2)



Uncertainties - inverse problems (3)



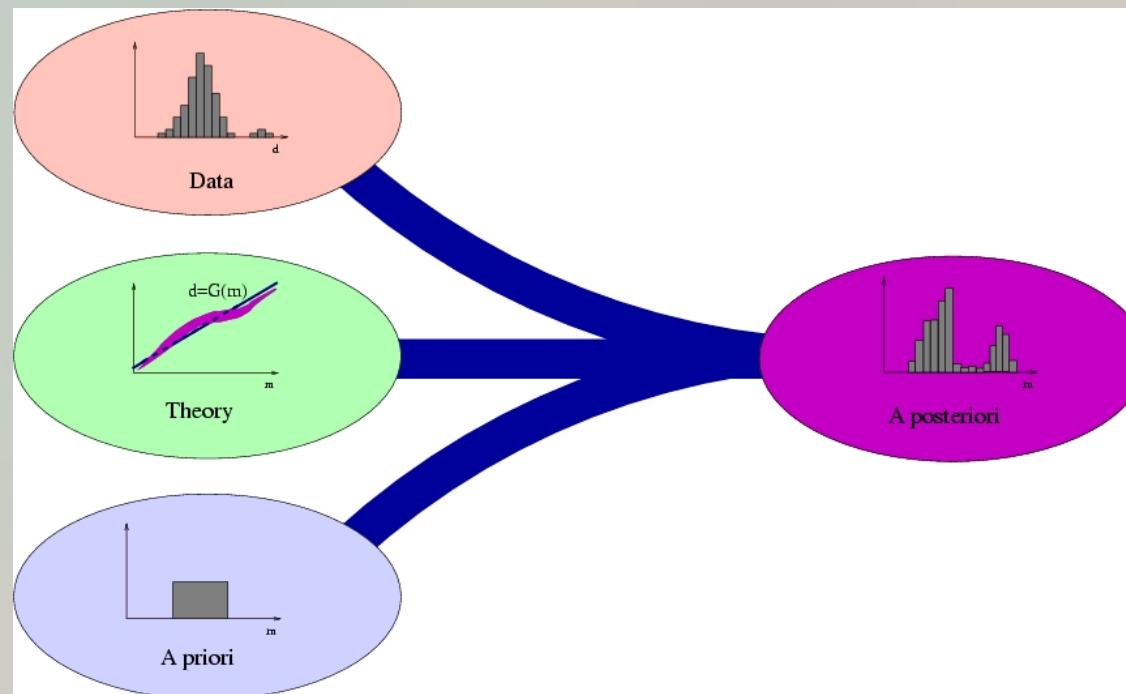
Uncertainties - inverse problems (3)

Nonlinearity of forward problem can significantly modify “observational” errors. If, in addition we consider that forward modelling can also be imprecise (e.g. due to theoretical simplification) we conclude that final inversion errors can have complex distribution. Without full knowledge of it, the inversion error analysis is practically

IMPOSSIBLE

Generalization - probabilistic approach

Solution \equiv searching for
probability distribution
describing *a posteriori* uncertainties



Generalization - probabilistic approach

Method

Algebraic

Optimization

Solution

model given by math formula

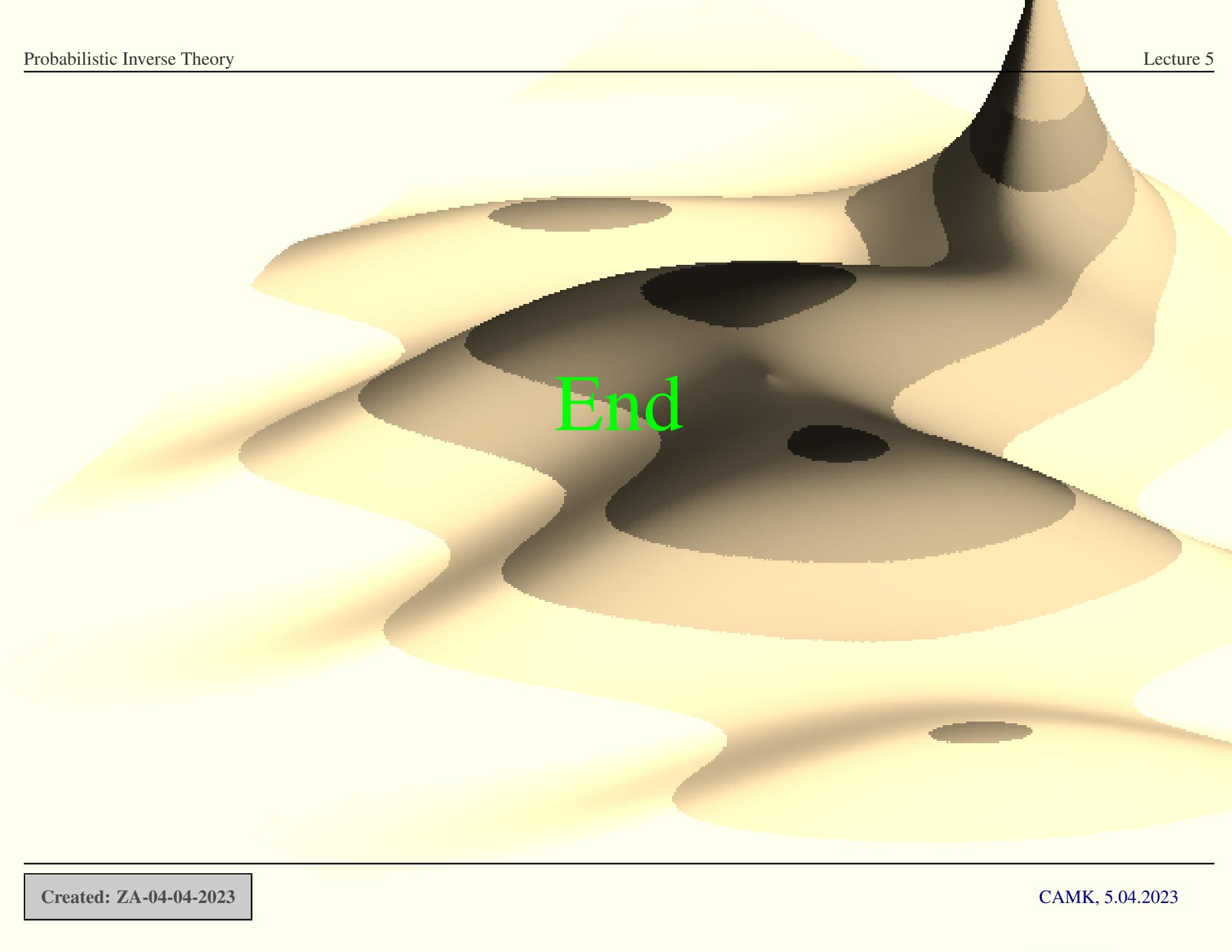
single “optimum” model



Probabilistic

probability distribution

This *a posteriori* distribution is supposed to describe (at least) inversion errors



The background of the slide features a 3D surface plot of a function with multiple local minima and one prominent global minimum. The surface is rendered in a color gradient from light yellow to dark grey, with the global minimum at the top right being the darkest point. The word "End" is overlaid in bright green text in the center of the plot.

End