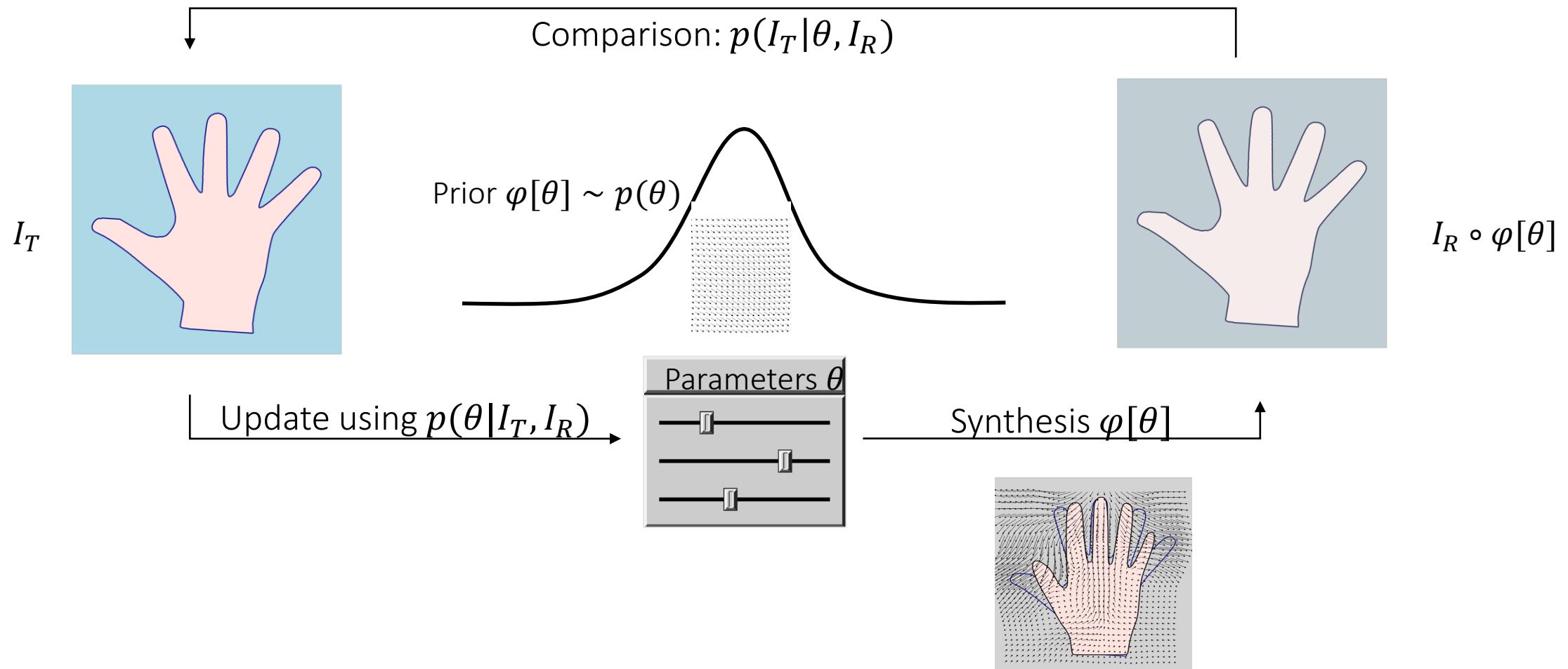


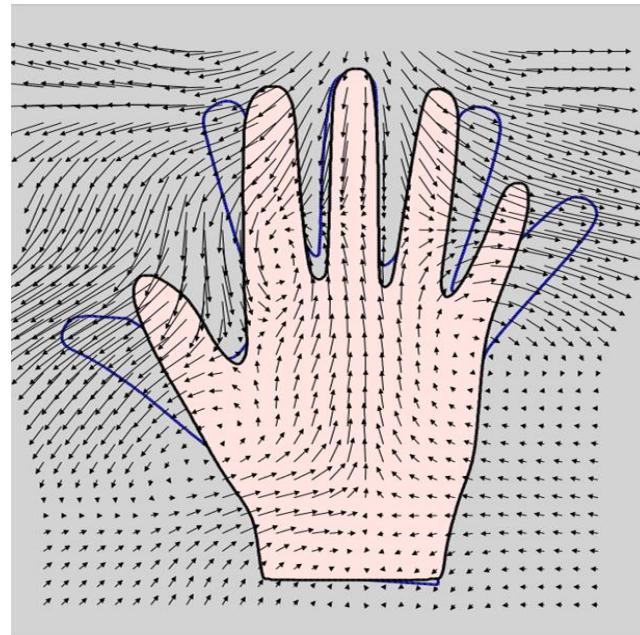
## Probabilistic Fitting

Marcel Lüthi,  
University of Basel

# Reminder: Registration as analysis by synthesis



# Reminder: Priors



Gaussian process

$$u \sim GP(\mu, k)$$

Represented using first  $r$  components

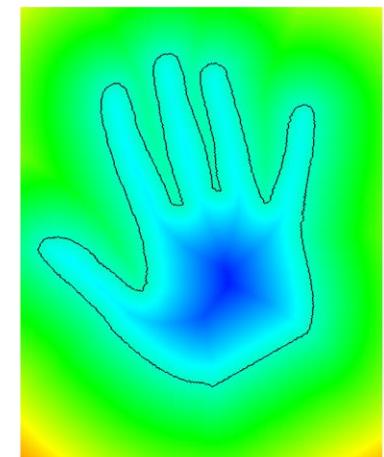
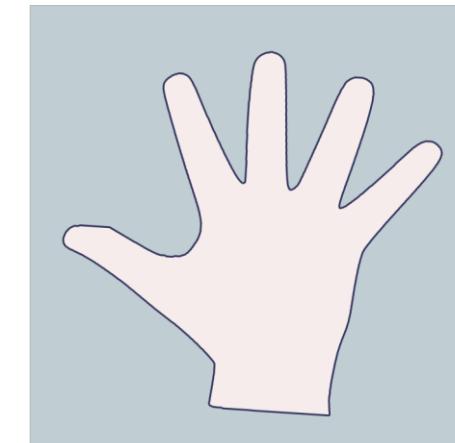
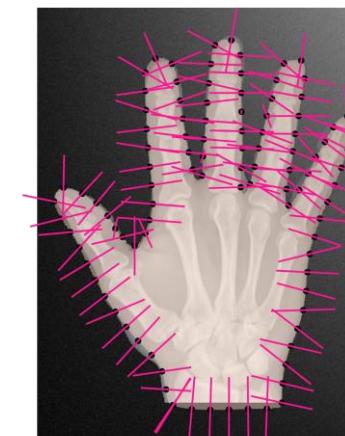
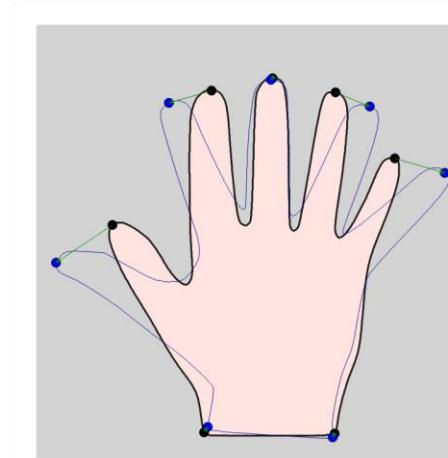
$$u = \mu + \sum_{i=1}^r \alpha_i \sqrt{\lambda_i} \phi_i, \quad \alpha_i \sim N(0, 1)$$

*Different GP-s lead to very different deformation models*

- All of them are parametric  $u \sim p(\theta)$ .

# Reminder: Likelihood functions

Likelihood function:  $p(I_T | \theta, I_R)$



Information in likelihood

Position of landmark points

Intensity profiles at surface boundary

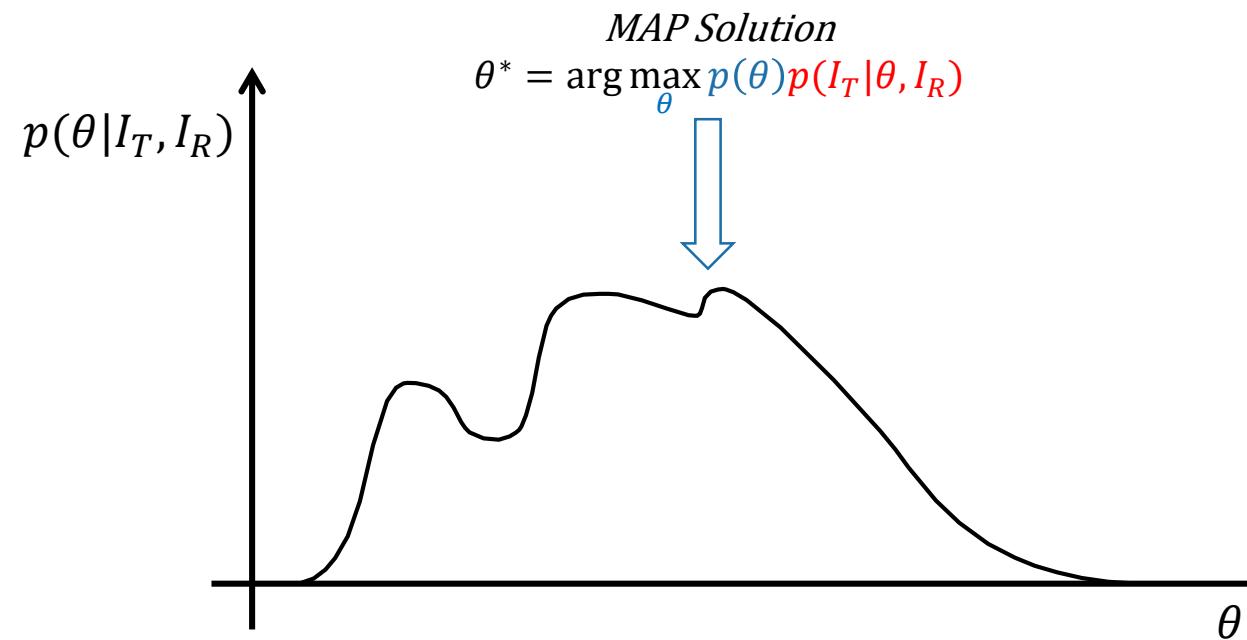
Image intensity on full image

Distance to surface

# Reminder: Obtaining the posterior parameters

MAP-Estimate

$$\theta^* = \arg \max_{\theta} p(\theta | I_T, I_R) = \arg \max_{\theta} p(\theta) p(I_T | \theta, I_R)$$

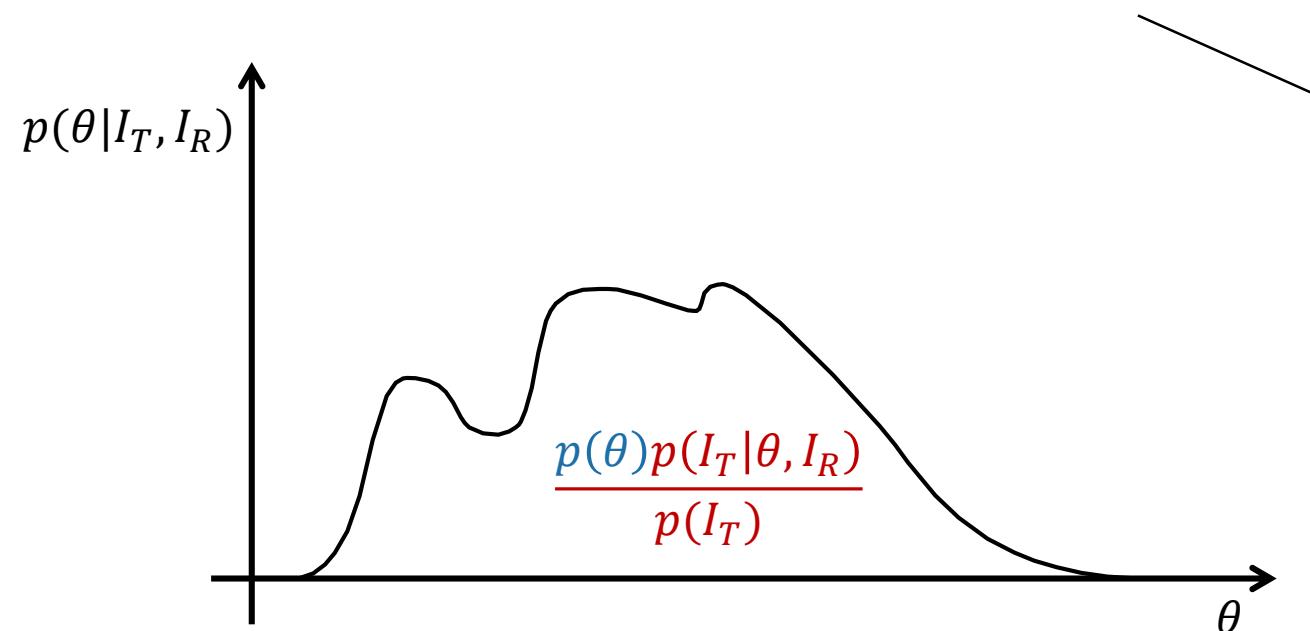


- Solving an optimization problem

# Obtaining the posterior distribution

Full posterior distribution

$$p(\theta|I_T, I_R) = \frac{p(\theta)p(I_T|\theta, I_R)}{p(I_T)}$$



Infeasible to compute:  
 $p(I_T) = \int p(\theta)p(I_T|\theta) d\theta$

- Doing (approximate) Bayesian inference

# Outline

- Basic idea: Sampling methods and MCMC
- The Metropolis-Hastings algorithm
  - The Metropolis algorithm
  - Implementing the Metropolis algorithm
  - The Metropolis-Hastings algorithm
- Example: 3D Landmark fitting
- *Next time: Guest lecture T. Vetter. Probabilistic fitting of 2D Face photographs*

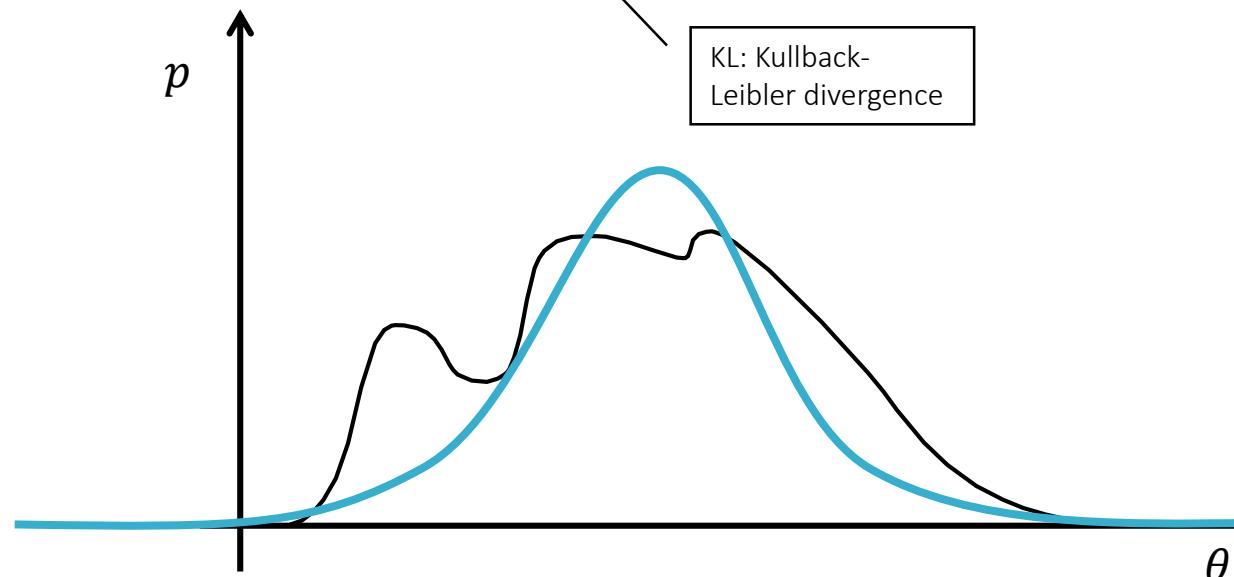
# Approximate Bayesian Inference

## Variational methods

- Function approximation  $q(\theta)$

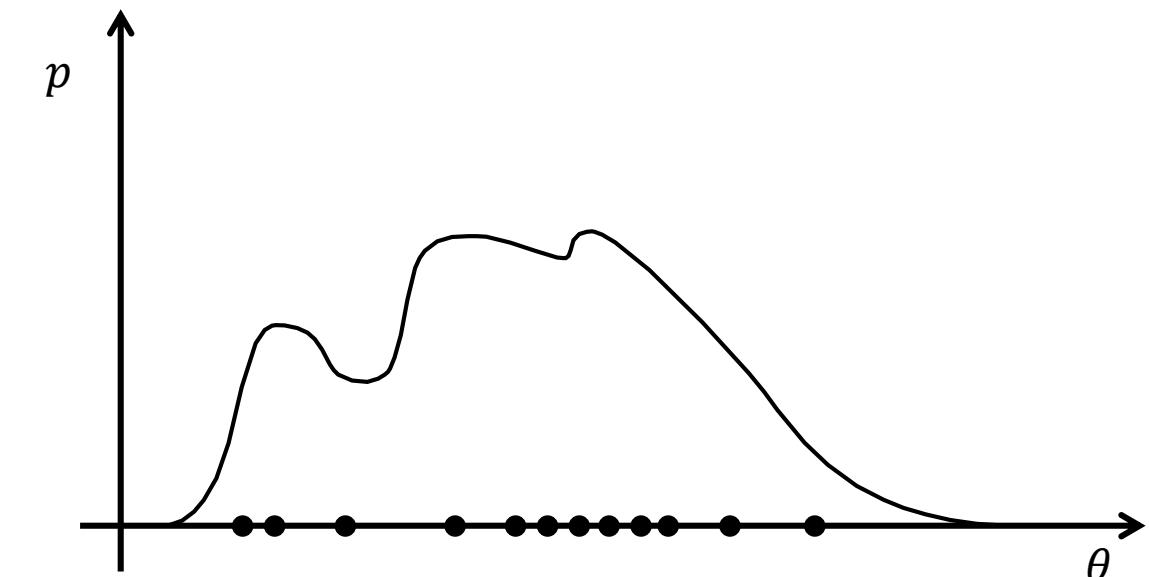
$$\arg \max_q \text{KL}(q(\theta) \| p(\theta | D))$$

KL: Kullback-  
Leibler divergence



## Sampling methods

- Numeric approximations through simulation



# Sampling Methods

- Simulate a distribution  $p$  through random samples  $x_i$
- Evaluate expectation (of some function  $f$  of random variable  $X$ )

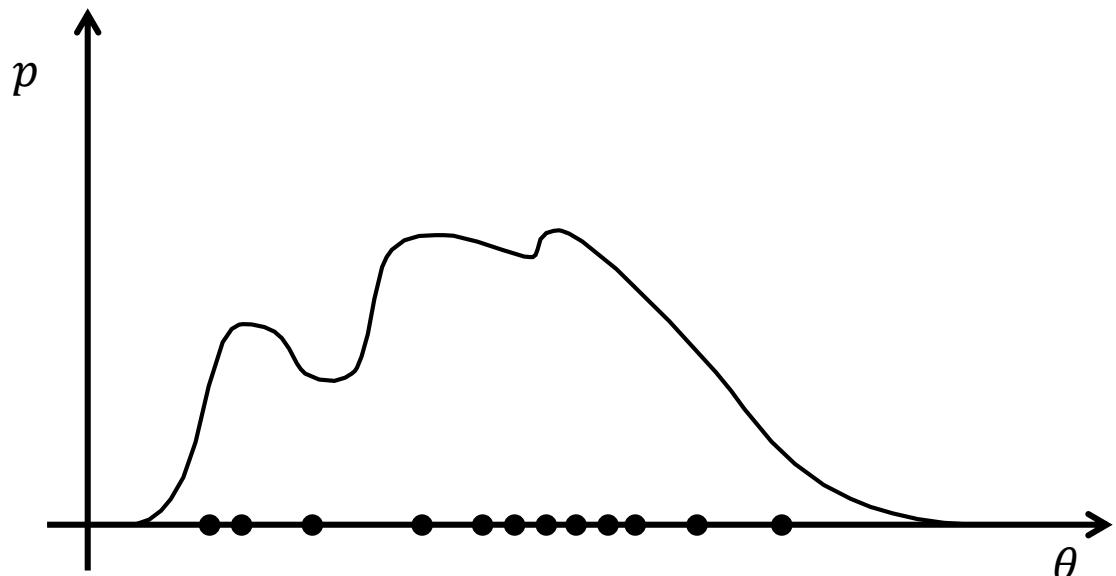
$$E[f(X)] = \int f(x)p(x)dx$$

$$E[f(X)] \approx \hat{f} = \frac{1}{N} \sum_i^N f(x_i), \quad x_i \sim p(x)$$

This is difficult!

$$V[\hat{f}(X)] \sim O\left(\frac{1}{N}\right)$$

- “Independent” of dimensionality of  $X$
- More samples increase accuracy



# Sampling from a Distribution

- Easy for standard distributions ... is it?
  - Uniform
  - Gaussian
- How to sample from more complex distributions?
  - Beta, Exponential, Chi square, Gamma, ...
  - Posteriors are very often not in a “nice” standard text book form
- *We need to sample from an unknown posterior with only unnormalized, expensive point-wise evaluation* 😞

```
Random.nextDouble()  
Random.nextGaussian()
```

# Markov Chain Monte Carlo

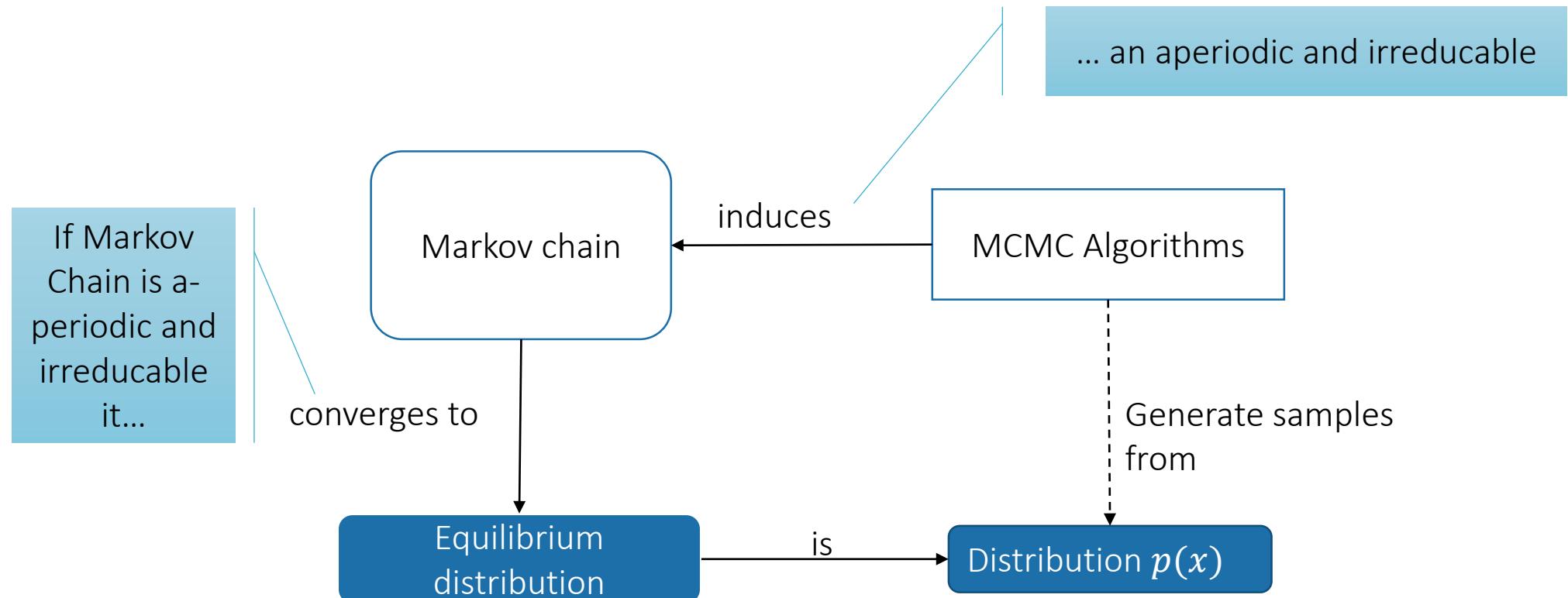
## Markov Chain Monte Carlo Methods (MCMC)

Idea: Design a *Markov Chain* such that samples  $x$  obey the target distribution  $p$

Concept: “*Use an already existing sample to produce the next one*”

- Many successful practical applications
  - Proven: developed in the 1950/1970ies (Metropolis/Hastings)
- Direct mapping of computing power to approximation accuracy

# MCMC: An ingenious mathematical construction



*No need to understand this now: more details follow!*

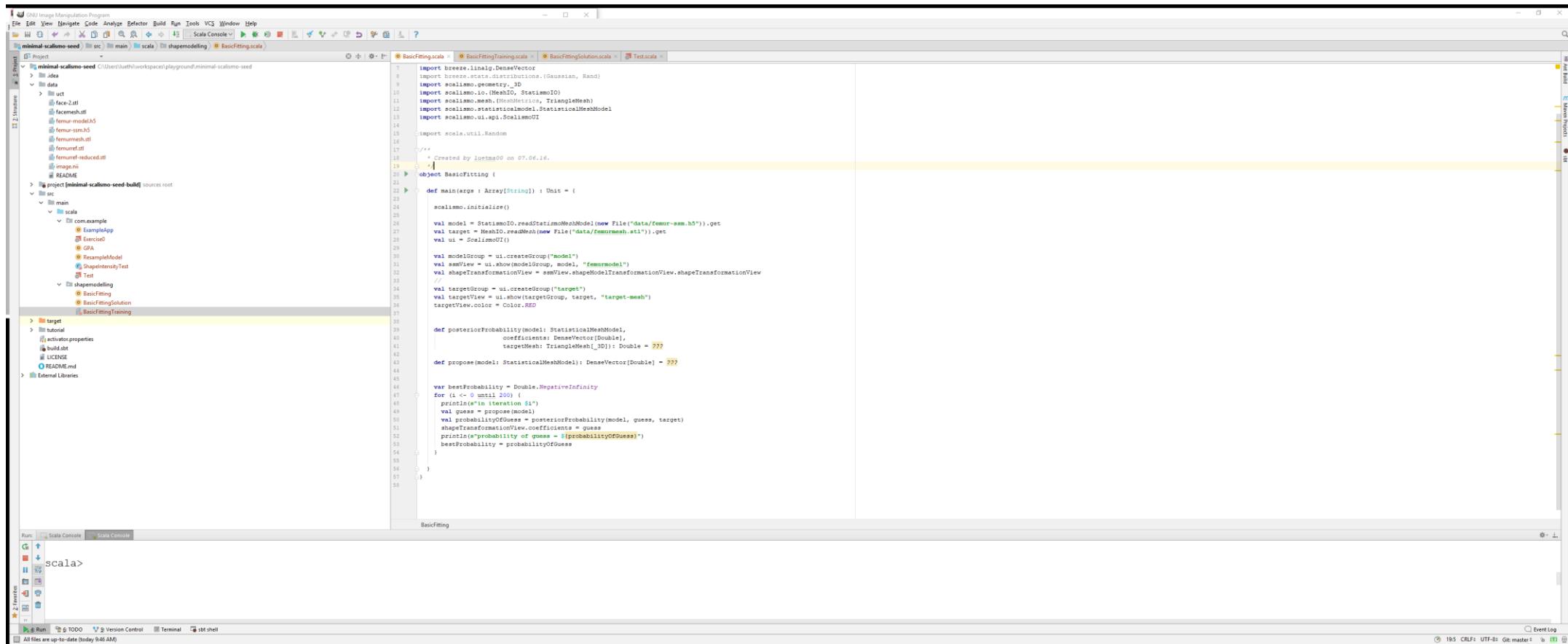
# The Metropolis Algorithm

Requirements:

- Proposal distribution  $Q(\mathbf{x}'|\mathbf{x})$  – *must generate samples, symmetric*
- Target distribution  $P(\mathbf{x})$  – *with point-wise evaluation*

Result:

- Stream of samples approximately from  $P(\mathbf{x})$
- Initialize with sample  $\mathbf{x}$
- Generate next sample, with current sample  $\mathbf{x}$ 
  1. Draw a sample  $\mathbf{x}'$  from  $Q(\mathbf{x}'|\mathbf{x})$  (“proposal”)
  2. With *probability*  $\alpha = \min\left\{\frac{P(\mathbf{x}')}{P(\mathbf{x})}, 1\right\}$  accept  $\mathbf{x}'$  as new state  $\mathbf{x}$
  3. Emit current state  $\mathbf{x}$  as sample



```
1  // Scalismo Image Manipulation Program
2  // File Edit View Navigate Code Analyze Refactor Build Run Tools VCS Window Help
3  // minimal-scalismo-seed C:\Users\luethi\workspace\playground\minimal-scalismo-seed
4  // Project S: src main scala shapemodelling BasicFitting.scala
5  // 2. Favorites
6  // minimal-scalismo-seed C:\Users\luethi\workspace\playground\minimal-scalismo-seed
7  // > minimal-scalismo-seed
8  //   > idea
9  //   > data
10 //     > uct
11 //       face2.stl
12 //       femurmesh.stl
13 //       femur-mesh.h5
14 //       femur-mesh5.stl
15 //       femur-mesh5.h5
16 //       femur-mesh.stl
17 //       femur-mesh5.stl
18 //       femur-reduced.stl
19 //       image.nii
20 //       README
21 //   > project [minimal-scalismo-seed-build] sources root
22 //   > bin
23 //     > main
24 //       > scala
25 //         > com.example
26 //           ExampleApp
27 //           Exercise0
28 //           GPA
29 //           ResampleModel
30 //           ShapeInferenceTest
31 //           target
32 //           shapemodelling
33 //             > BasicFitting
34 //             > BasicFittingSolution
35 //             > BasicFittingTraining
36 //           target
37 //           tutorial
38 //           actoroperator.properties
39 //           LICENSE
40 //           README.md
41 //   > External Libraries
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# Example: 2D Gaussian

- Target:  $P(\mathbf{x}) = \frac{1}{2\pi\sqrt{|\Sigma|}} e^{-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^T \Sigma^{-1} (\mathbf{x}-\boldsymbol{\mu})}$
- Proposal:  $Q(\mathbf{x}'|\mathbf{x}) = \mathcal{N}(\mathbf{x}'|\mathbf{x}, \sigma^2 I_2)$

← Random walk

Target

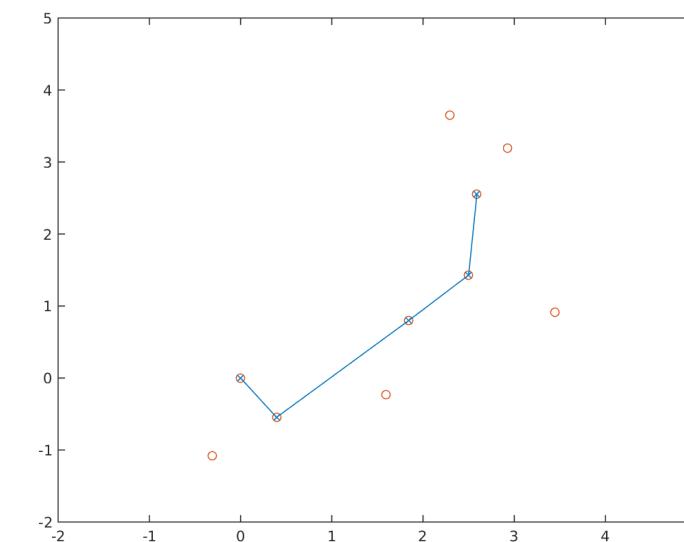
$$\boldsymbol{\mu} = \begin{bmatrix} 1.5 \\ 1.5 \end{bmatrix}$$

$$\Sigma = \begin{bmatrix} 1.25 & 0.75 \\ 0.75 & 1.25 \end{bmatrix}$$

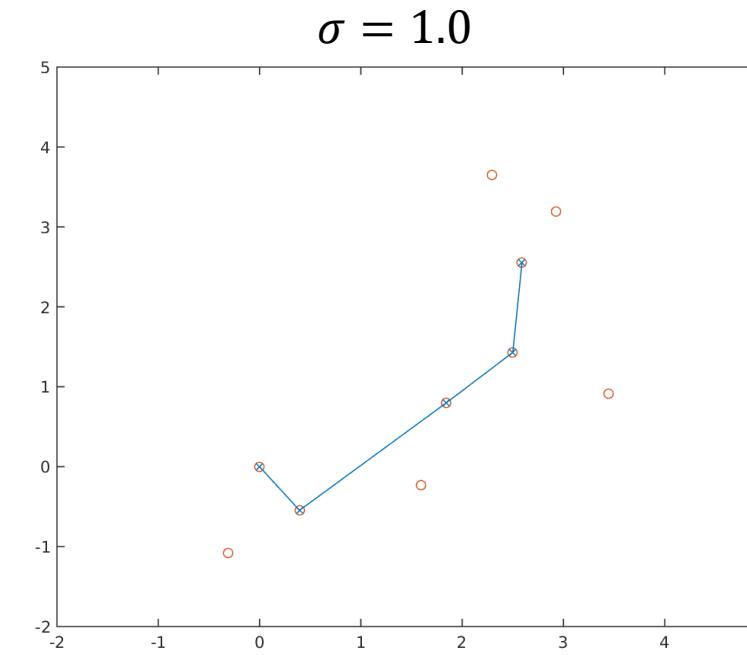
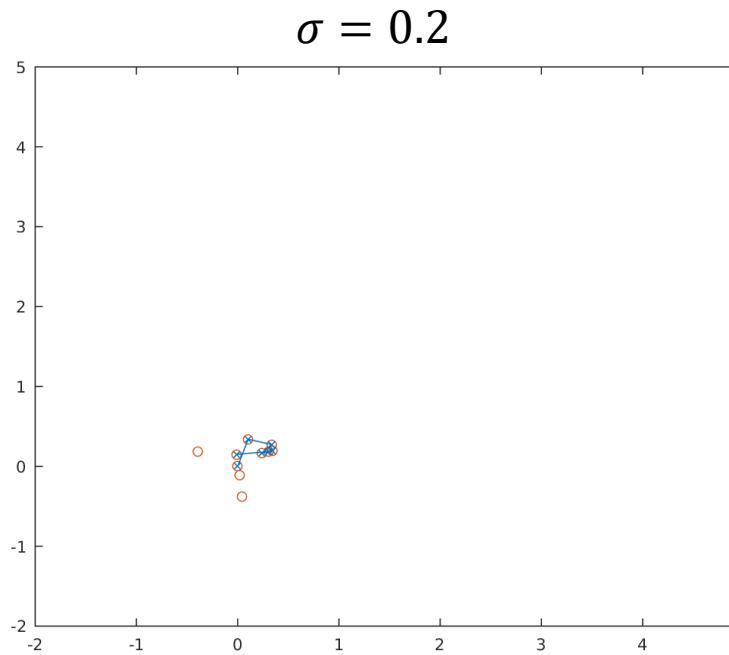
Sampled Estimate

$$\hat{\boldsymbol{\mu}} = \begin{bmatrix} 1.56 \\ 1.68 \end{bmatrix}$$

$$\hat{\Sigma} = \begin{bmatrix} 1.09 & 0.63 \\ 0.63 & 1.07 \end{bmatrix}$$



# 2D Gaussian: Different Proposals



# The Metropolis-Hastings Algorithm

- Initialize with sample  $\mathbf{x}$
- Generate next sample, with current sample  $\mathbf{x}$ 
  1. Draw a sample  $\mathbf{x}'$  from  $Q(\mathbf{x}'|\mathbf{x})$  ("proposal")
  2. With probability  $\alpha = \min\left\{\frac{P(\mathbf{x}')}{P(\mathbf{x})} \frac{Q(\mathbf{x}|\mathbf{x}')}{Q(\mathbf{x}'|\mathbf{x})}, 1\right\}$  accept  $\mathbf{x}'$  as new state  $\mathbf{x}$
  3. Emit current state  $\mathbf{x}$  as sample
- Generalization of Metropolis algorithm to asymmetric Proposal distribution

$$Q(\mathbf{x}'|\mathbf{x}) \neq Q(\mathbf{x}|\mathbf{x}')$$

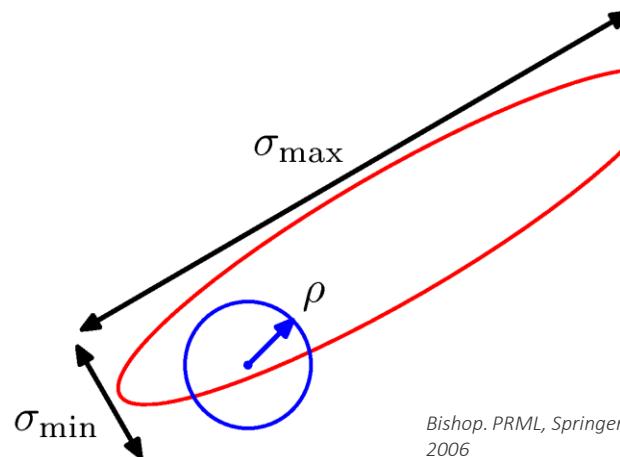
$$Q(\mathbf{x}'|\mathbf{x}) > 0 \Leftrightarrow Q(\mathbf{x}|\mathbf{x}') > 0$$

# Properties

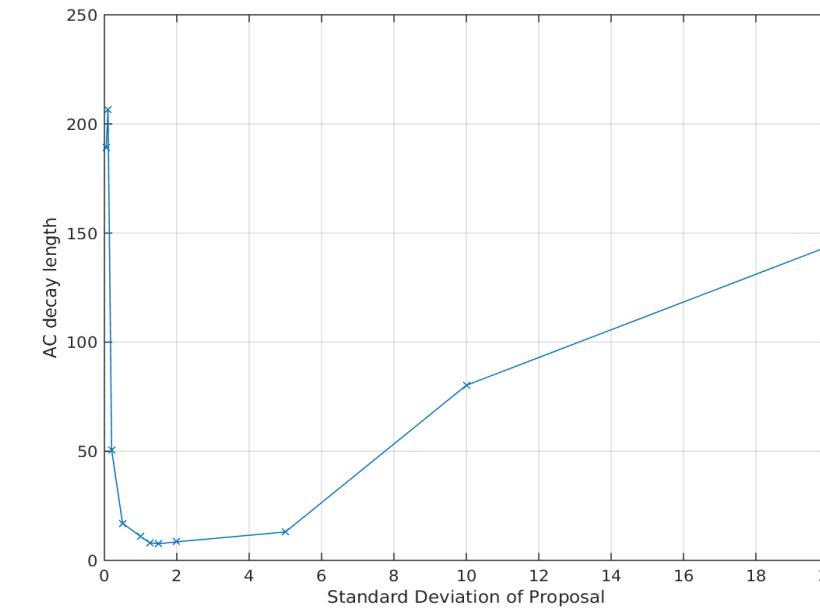
- **Approximation:** Samples  $x_1, x_2, \dots$  approximate  $P(x)$   
Unbiased but correlated (not *i.i.d.*)
- **Normalization:**  $P(x)$  does not need to be normalized  
Algorithm only considers ratios  $P(x')/P(x)$
- **Dependent Proposals:**  $Q(x'|x)$  depends on current sample  $x$   
Algorithm adapts to target with simple 1-step memory

# Metropolis - Hastings: Limitations

- Highly correlated targets  
Proposal should match target to avoid too many rejections



- Serial correlation
  - Results from rejection and too small stepping
  - Subsampling



# Propose-and-Verify Algorithm

- Metropolis algorithm formalizes: *propose-and-verify*
- *Steps are completely independent.*

## Propose

Draw a sample  $x'$  from  $Q(x'|x)$

## Verify

With probability  $\alpha = \min \left\{ \frac{P(x')}{P(x)} \frac{Q(x|x')}{Q(x'|x)}, 1 \right\}$  accept  $x'$  as new sample

# MH as Propose and Verify

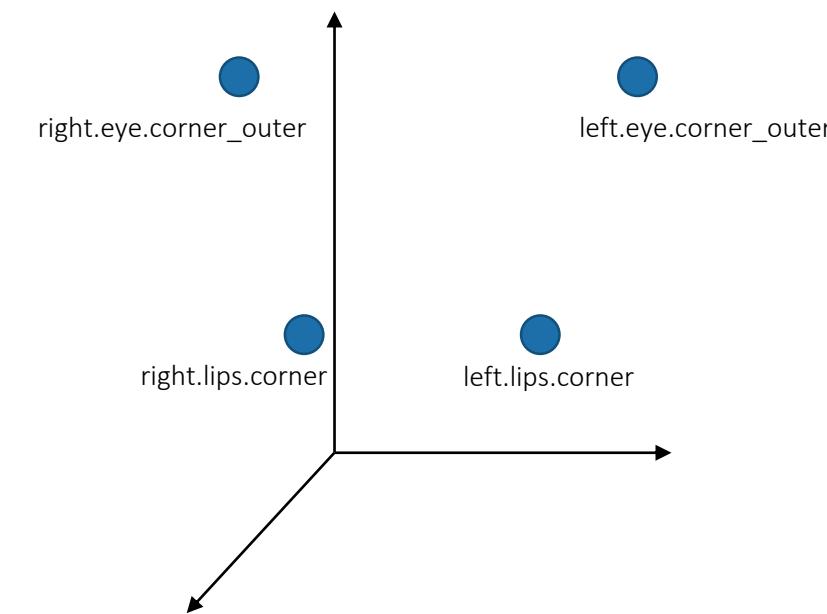
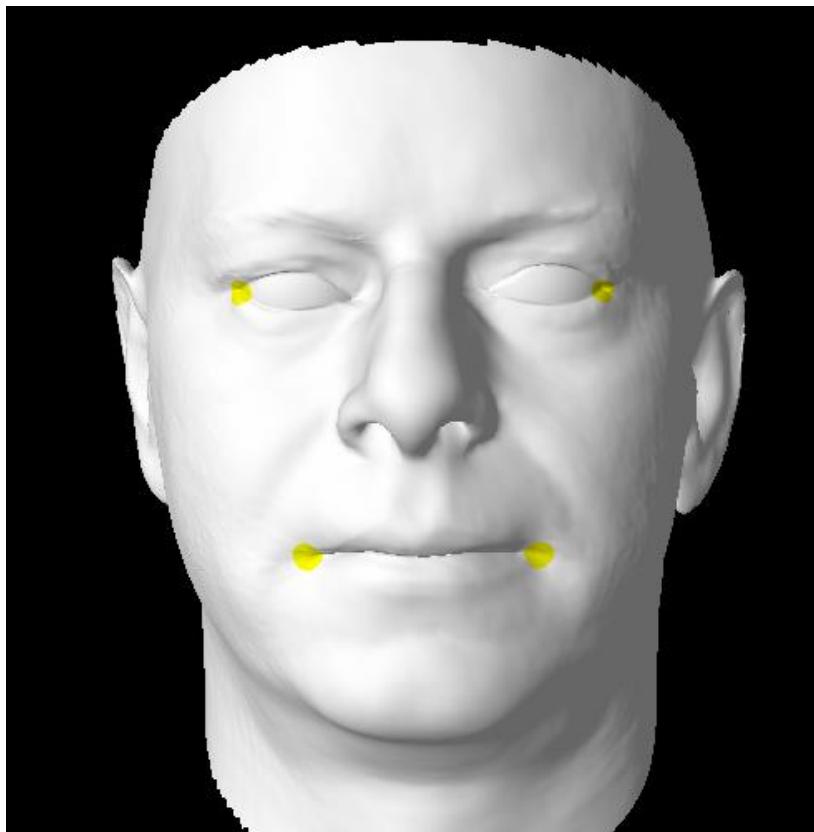
- Decouples the steps of finding the solution from validating a solution
- Natural to integrate uncertain proposals  $Q$   
(e.g. automatically detected landmarks, ...)
- Possibility to include “local optimization” (e.g. a ICP or ASM updates, gradient step, ...) as proposal

*Anything more “informed” than random walk should improve convergence.*

# Fitting 3D Landmarks

3D Alignment with Shape and Pose

# 3D Fitting Example



# 3D Fitting Setup

*Goal: Find posterior distribution for arbitrary pose and shape*

Shape transformation

$$\varphi_s[\alpha] = \mu(x) + \sum_{i=1}^r \alpha_i \sqrt{\lambda_i} \Phi_i(x)$$

Rigid transformation

- 3 angles (pitch, yaw, roll)  $\varphi, \psi, \vartheta$
- Translation  $t = (t_x, t_y, t_z)$

$$\varphi_R[\varphi, \psi, \vartheta, t] = R_\vartheta R_\psi R_\varphi(x) + t$$

Full transformation

$$\varphi[\theta](x) = (\varphi_R \circ \varphi_s)[\theta](x)$$

Observations

- Observed positions  $l_T^1, \dots, l_T^n$
- Correspondence:  $l_R^1, \dots, l_R^n$

Parameters

$$\theta = (\alpha, \varphi, \psi, \vartheta, t)$$

Posterior distribution:

$$P(\theta | l_T^1, \dots, l_T^n) \propto p(l_T^1, \dots, l_T^n | \theta) P(\theta)$$

# Proposals

- Gaussian random walk proposals

$$"Q(\theta'|\theta) = N(\theta'|\theta, \Sigma_\theta)"$$

- Update different parameter types block-wise

• Shape	$N(\alpha' \alpha, \sigma_s^2 I_{m \times m})$
• Rotation	$N(\varphi' \varphi, \sigma_\varphi^2), N(\psi' \psi, \sigma_\psi^2), N(\vartheta' \vartheta, \sigma_\vartheta^2)$
• Translation	$N(t' t, \sigma_t^2 I_{3 \times 3})$

- Large mixture distributions as proposals

- Choose proposal  $Q_i$  with probability  $c_i$

$$Q(\theta'|\theta) = \sum c_i Q_i(\theta'|\theta)$$

# 3DMM Landmarks Likelihood

Simple models: **Independent Gaussians**

Observation of  $L$  landmark locations  $l_T^i$  in image

- Single *landmark position* model:

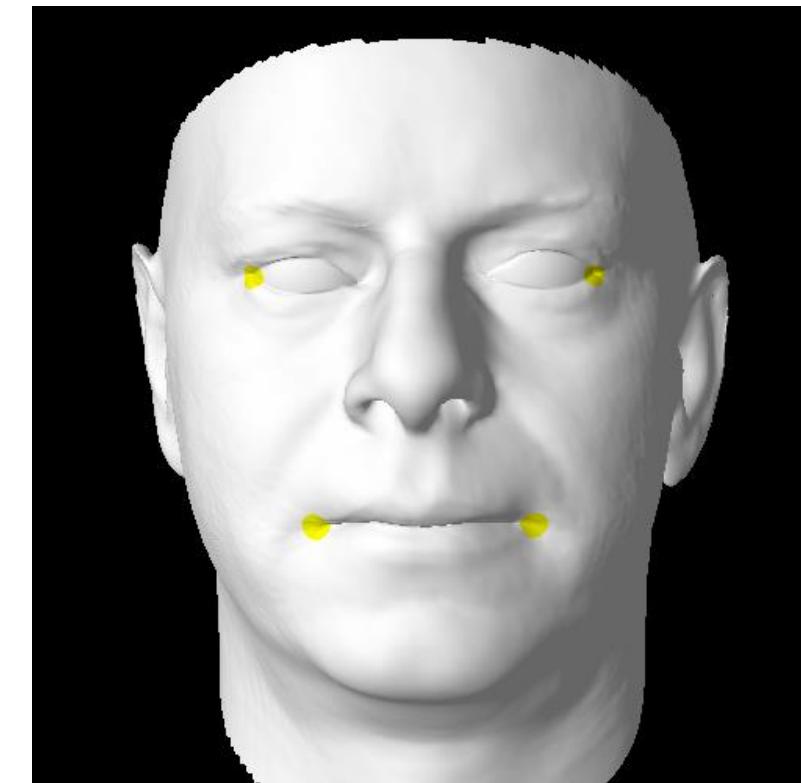
$$p(l_T | \theta, l_R) = N(\varphi[\theta](l_R), I_{3 \times 3} \sigma^2)$$

- *Independent* model (conditional independence):

$$p(l_T^1, \dots, l_T^n | \theta) = \prod_{i=1}^L p_i(l_T^i | \theta)$$

# 3D Fit to landmarks

- Influence of landmarks uncertainty on final posterior?
  - $\sigma_{LM} = 1\text{mm}$
  - $\sigma_{LM} = 4\text{mm}$
  - $\sigma_{LM} = 10\text{mm}$
- Only 4 landmark observations:
  - Expect only weak shape impact
  - Should still constrain pose
- Uncertain landmarks should be looser



# Posterior: Pose & Shape, 4mm



$$\begin{aligned}\hat{\mu}_{yaw} &= 0.511 \\ \hat{\sigma}_{yaw} &= 0.073 (4^\circ)\end{aligned}$$

$$\begin{aligned}\hat{\mu}_{t_x} &= -1 \text{ mm} \\ \hat{\sigma}_{t_x} &= 4 \text{ mm}\end{aligned}$$

$$\begin{aligned}\hat{\mu}_{\alpha_1} &= 0.4 \\ \hat{\sigma}_{\alpha_1} &= 0.6\end{aligned}$$

(Estimation from samples)

# Posterior: Pose & Shape, 1mm

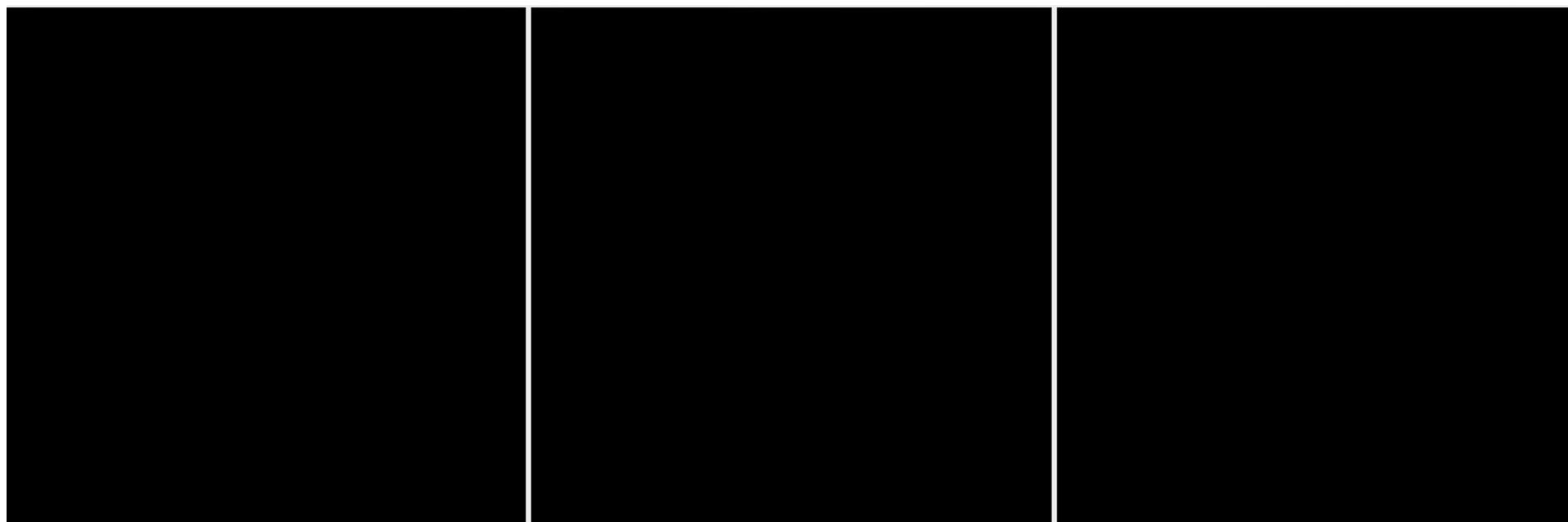


$$\begin{aligned}\hat{\mu}_{\text{yaw}} &= 0.50 \\ \hat{\sigma}_{\text{yaw}} &= 0.041 \text{ (} 2.4^\circ \text{)}\end{aligned}$$

$$\begin{aligned}\hat{\mu}_{t_x} &= -2 \text{ mm} \\ \hat{\sigma}_{t_x} &= 0.8 \text{ mm}\end{aligned}$$

$$\begin{aligned}\hat{\mu}_{\alpha_1} &= 1.5 \\ \hat{\sigma}_{\alpha_1} &= 0.35\end{aligned}$$

# Posterior: Pose & Shape, 10mm



$$\begin{aligned}\hat{\mu}_{\text{yaw}} &= 0.49 \\ \hat{\sigma}_{\text{yaw}} &= 0.11 (7^\circ)\end{aligned}$$

$$\begin{aligned}\hat{\mu}_{t_x} &= -5 \text{ mm} \\ \hat{\sigma}_{t_x} &= 10 \text{ mm}\end{aligned}$$

$$\begin{aligned}\hat{\mu}_{\alpha_1} &= 0 \\ \hat{\sigma}_{\alpha_1} &= 0.6\end{aligned}$$

# Summary: MCMC for 3D Fitting

- Probabilistic inference for fitting probabilistic models
  - Bayesian inference: posterior distribution
- Probabilistic inference is often intractable
  - Use *approximate* inference methods
- MCMC methods provide a powerful sampling framework
  - Metropolis-Hastings algorithm
    - Propose update step
    - Verify and accept with probability
- Samples converge to true distribution: More about this later!