University of Basel

The Metropolis-Hastings algorithm

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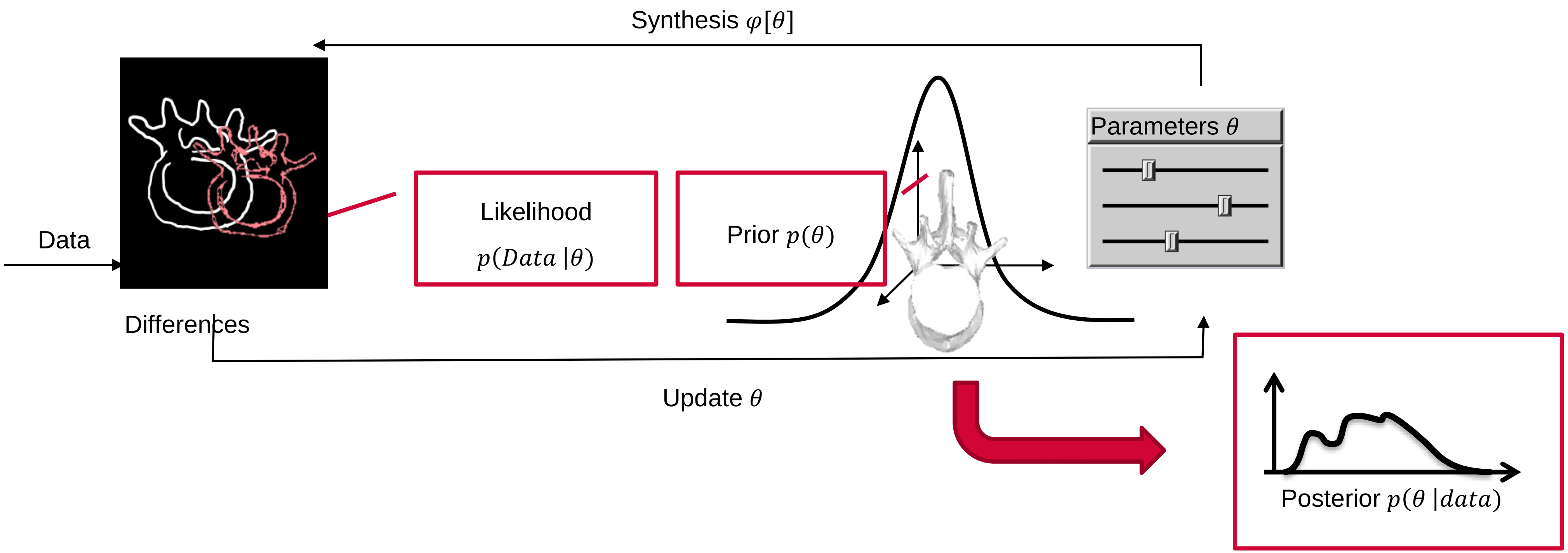
Analysis by Synthesis and Bayesian Inference



Bayes rule

$$p(\theta|D) = \frac{p(D|\theta)p(\theta)}{p(D)} = \frac{p(D|\theta)p(\theta)}{\int p(D|\theta)p(\theta)d\theta}$$

Analysis by synthesis – Computational problem

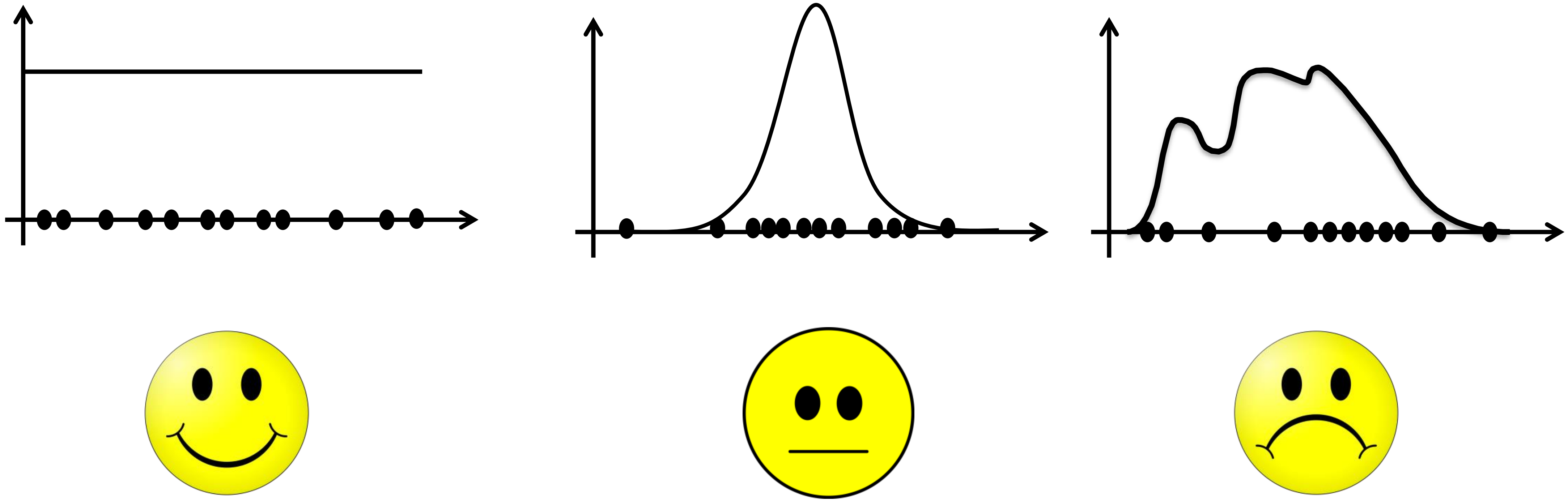
- Non-linear
- Impossible to evaluate directly
- Can only be approximated

- Usually non-linear
- Expensive to evaluate
- Can only be evaluated pointwise

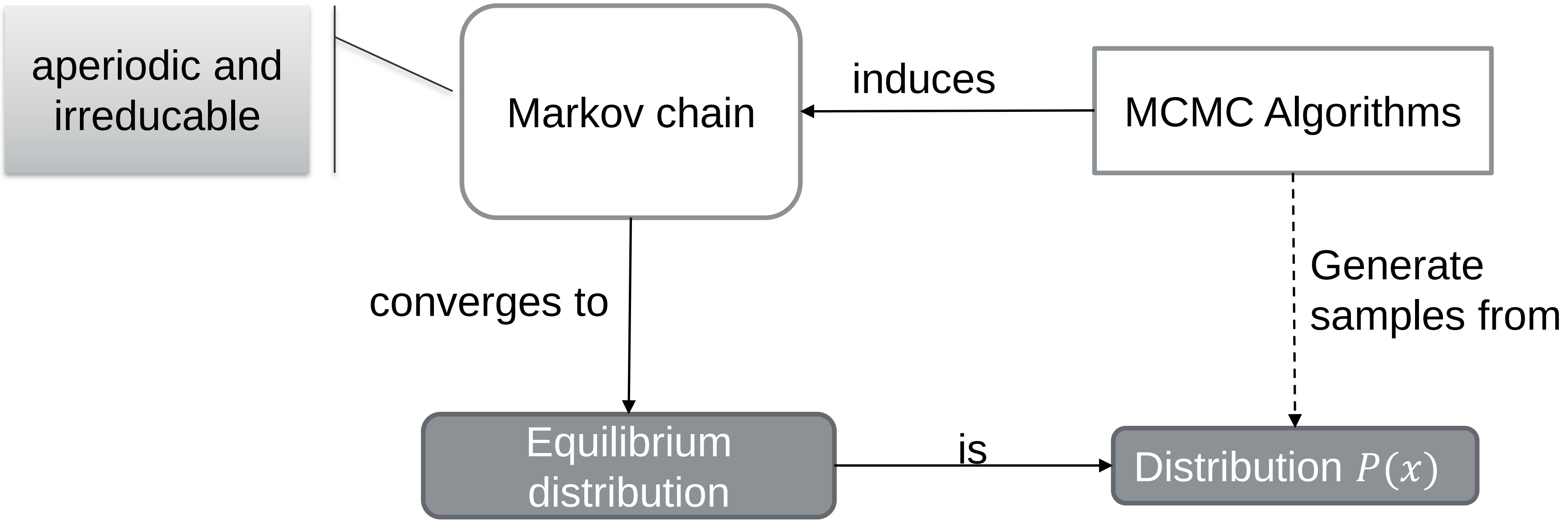
$$p(\theta|\mathrm{D}) = \frac{p(\theta)p(\mathrm{D}|\theta)}{\int p(\theta)p(D|\theta)d\theta}$$

High dimensional

Drawing samples from a distribution



Markov Chain Monte Carlo Methods



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

The Metropolis Algorithm

Requirements:

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

Result:

- Stream of samples approximately from $P(\boldsymbol{x})$

Initialize with sample $\boldsymbol{x}$
Generate next sample, with current sample $\boldsymbol{x}$

1. Draw a sample $\boldsymbol{x}'$ from $Q(\boldsymbol{x}'|\boldsymbol{x})$ (“proposal”)
2. With *probability* $\alpha = \min\left\{\frac{P(\boldsymbol{x}')}{P(\boldsymbol{x})}, 1\right\}$ accept $\boldsymbol{x}'$ as new state $\boldsymbol{x}$
3. Emit current state $\boldsymbol{x}$ as sample

Example: 2D Gaussian

Target: $$P(\boldsymbol{x}) = \frac{1}{2\pi\sqrt{|\Sigma|}} e^{-\frac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu})^T \Sigma^{-1} (\boldsymbol{x}-\boldsymbol{\mu})}$$

Target

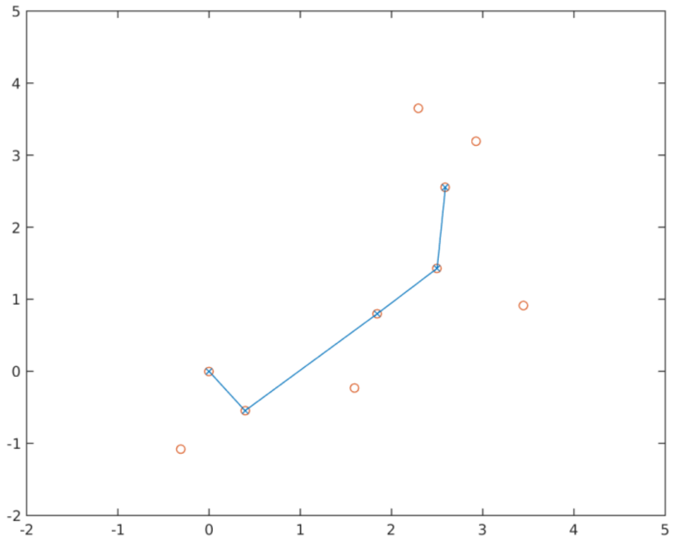
$$\mu = \begin{bmatrix} 1.5 \\ 1.5 \end{bmatrix}$$
$$\Sigma = \begin{bmatrix} 1.25 & 0.75 \\ 0.75 & 1.25 \end{bmatrix}$$

Sampled Estimate

$$\hat{\mu} = \begin{bmatrix} 1.56 \\ 1.68 \end{bmatrix}$$
$$\hat{\Sigma} = \begin{bmatrix} 1.09 & 0.63 \\ 0.63 & 1.07 \end{bmatrix}$$

Proposal: $$Q(\boldsymbol{x}'|\boldsymbol{x}) = \mathcal{N}(\boldsymbol{x}'|\boldsymbol{x}, \sigma^2 I_2)$$

Random walk



Animation: S. Schönborn, University of Basel

The Metropolis-Hastings Algorithm

Generalization of Metropolis algorithm to asymmetric proposal distribution

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

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

Initialize with sample $\boldsymbol{x}$
Generate next sample, with current sample $\boldsymbol{x}$

1. Draw a sample $\boldsymbol{x}'$ from $Q(\boldsymbol{x}'|\boldsymbol{x})$ (“proposal”)
2. With *probability* $\alpha = \min\left\{\frac{P(x')}{P(x)} \frac{\mathbf{Q}(\mathbf{x}|\boldsymbol{x}')}{\mathbf{Q}(\boldsymbol{x}'|\boldsymbol{x})}, 1\right\}$ accept $\boldsymbol{x}'$ as new state $\boldsymbol{x}$
3. Emit current state $\boldsymbol{x}$ as sample

Metropolis-Hastings for analysis by synthesis

Computational problem

$$p(\theta|D) = \frac{p(D|\theta)p(\theta)}{p(D)} = \frac{p(D|\theta)p(\theta)}{\int p(D|\theta)p(\theta)d\theta}$$