# Markov chain Monte Carlo (MCMC)

TMA4300: Computer Intensive Statistical Methods (Spring 2016)

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## Bayesian point estimates

Statistical inference about  $\theta$  is based solely on the posterior distribution  $f(\theta|x)$ . Suitable point estimates are location parameters, such as:

• Posterior mean  $E(\theta|x)$ :

$$\mathsf{E}(\theta|x) = \int \theta f(\theta|x) d\theta.$$

• Posterior mode  $Mod(\theta|x)$ :

$$\mathsf{Mod}(\theta|x) = \arg\max_{\theta} f(\theta|x)$$

• Posterior median  $Med(\theta|x)$  is defined as the value a which satisfies

$$\int_{-\infty}^{a} f(\theta|x)d\theta = 0.5 \quad \text{and} \quad \int_{a}^{\infty} f(\theta|x)d\theta = 0.5$$

## Lecture 7: Brief reminder - Bayesian model

• data: x

• likelihood model:  $x|\theta \sim f(x|\theta)$ 

• prior distribution:  $\theta \sim f(\theta)$ 

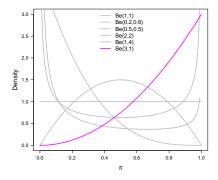
• posterior distribution:

$$\underbrace{f(\theta|x)}_{\text{Posterior}} \propto \underbrace{f(x|\theta)}_{\text{Likelihood}} \times \underbrace{f(\theta)}_{\text{Prior}}$$

## Binomial experiment

Let  $X \sim \text{Bin}(n, p)$  with n known and  $p \in \Pi = (0, 1)$  unknown.

Since p is constrained to be within 0 and 1, a usual prior distribution is a beta distribution, so that  $p \sim \text{Be}(\alpha, \beta)$  with  $\alpha, \beta > 0$  and  $\mathcal{T} = (0, 1)$ .



## Binomial experiment (2)

$$X \sim \text{Bin}(n, p), \ x = 0, 1, \dots, n, \qquad p \sim \text{Be}(\alpha, \beta), \ 0 
$$\downarrow \qquad \qquad \downarrow$$

$$L(p) = f(x|p) = \binom{n}{x} p^x (1-p)^{n-x} \quad f(p) = \frac{1}{B(\alpha, \beta)} p^{\alpha-1} (1-p)^{\beta-1}$$

$$\propto p^x (1-p)^{n-x} \qquad \propto p^{\alpha-1} (1-p)^{\beta-1}$$$$

Thus, the posterior distribution results as:

$$f(p|x) \propto f(x|p) \times f(p)$$

$$= p^{x} (1-p)^{n-x} \times p^{\alpha-1} (1-p)^{\beta-1}$$

$$= p^{\alpha+x-1} (1-p)^{\beta+n-x-1}$$

This corresponds to the core of a beta distribution, so that

$$p|x \sim \text{Be}(\alpha + \underbrace{x}_{\text{successes}}, \beta + \underbrace{n-x}_{\text{failures}})$$

#### Credible interval

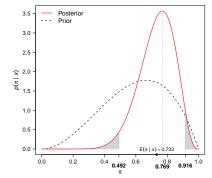
For fixed  $\alpha \in (0,1)$ , a  $(1-\alpha)$  credible interval is defined through two real numbers  $t_l$  and  $t_u$ , so that

$$\int_{t_l}^{t_u} f(\theta|x)d\theta = 1 - \alpha.$$

The number  $1 - \alpha$  is called the credible level of the credible interval  $[t_l, t_u]$ .

There are infinitely many (1 -  $\alpha$ )-credible intervals for fixed  $\alpha$ . (At least if  $\theta$  is continuous.)

### Binomial experiment: Simple example



Posterior density of p|x for a Be(3,2) prior and observation x=8 in a binomial experiment with n=10 trials. An equi-tailed 95% credible interval is also shown.

Using a Be(1,1) the posterior mode equals the Maximum Likelihood (ML) estimate.

## Credible interval (II)

### Equi-tailed credible interval

The same amount  $(\alpha/2)$  of probability mass is cut from the left and right tail of the posterior distribution, i.e. choose  $t_l$  as the  $\alpha/2$ -quantile and  $t_u$  as the  $1-\alpha/2$ -quantile.

### Highest posterior density (HPD) intervals

Feature: The posterior density at any value of  $\theta$  inside the credible interval must be larger than anywhere outside the credible interval. HPD-interval have the smallest width among all  $(1-\alpha)$  credible intervals. For symmetric posterior distributions HPD intervals are also equi-tailed.

### Properties of the beta-distribution

Be $(\alpha, \beta)$  can be interpreted as that which would have arisen if we had started with an "improper" Be(0,0) prior and then observed  $\alpha$  successes in  $\alpha + \beta$  trials.  $\Rightarrow n_0 = \alpha + \beta$  can be viewed as a prior sample size and  $\alpha/(\alpha + \beta)$  as prior mean.

The posterior mean is given by:

$$\mathsf{E}(p|x) = \frac{\alpha + x}{\alpha + \beta + n} = \underbrace{\frac{\alpha + \beta}{\alpha + \beta + n} \cdot \frac{\alpha}{\alpha + \beta}}_{\text{Weighted prior mean}} + \underbrace{\frac{n}{\alpha + \beta + n} \cdot \frac{x}{n}}_{\text{Weighted ML-estimate}}$$

The weights are proportional to the prior sample size and the data sample size.

 $\Rightarrow$  Observing more data leads to a decreasing influence of the prior.

## Choice of prior distributions

• Under a uniform prior the posterior mode equals the MLE, as

$$f(\theta|x) \propto L_x(\theta)$$

- The prior distribution has to be chosen appropriately, which often causes concerns to practitioners.
- It should reflect the knowledge about the parameter of interest (e.g. a relative risk parameter in an epidemiological study).
- Ideally it should be elicited from experts.
- In the absence of expert opinions, simple informative prior distributions may still be a reasonable choice.

### Bayesian learning

An important feature of Bayesian inference is the consistent processing of sequentially arising data.

- Suppose new independent data  $x_2$  from a Bin(n, p) arrive.
- The posterior distribution from the original observation (with x now called x<sub>1</sub>) becomes the prior for x<sub>2</sub>:

$$f(p|x_1, x_2) \propto f(x_2|p, x_1) \times f(p|x_1)$$
  
  $\propto f(x_2|p) \times f(p|x_1)$ 

Using  $f(p|x_1) \propto f(x_1|p) \times f(p)$  an alternative formula is

$$f(p|x_1, x_2) \propto f(x_2|p) \times f(x_1|p) \times f(p)$$
  
=  $f(x_1, x_2|p) \times f(p)$ 

Thus,  $f(p|x_1, x_2)$  is the same whether or not the data are processed sequentially.

## Choice of the prior distribution

Prior distributions incorporate prior beliefs in the Bayesian analysis. A pragmatic approach is to choose a prior distribution.

#### Conjugate prior distribution

Let  $L_x(\theta) = p(x|\theta)$  denote a likelihood function based on the observation X = x. A class  $\mathcal G$  of distributions is called conjugate with respect to  $L_x(\theta)$  if the posterior distribution  $p(\theta|x)$  is in  $\mathcal G$  for all x whenever the prior distribution  $p(\theta)$  is in  $\mathcal G$ .

### Example

Binomial experiment Let  $X|p \sim \text{Bin}(n,p)$ . The family of beta distributions,  $p \sim \text{Be}(\alpha,\beta)$ , is conjugate with respect to  $L_x(p)$ , since the posterior distribution is again a beta distribution:

$$p|x \sim \text{Be}(\alpha + x, \beta + n - x)$$

## List of conjugate prior distributions

#### Sequential processing:

- Sufficient to study conjugacy for one member of a random sample  $X_1, \ldots, X_n$ .
- The posterior after observing the first observation is of the same type as the prior and serves as new prior distribution for the next observation.
- Sequentially processing the data, only the parameters will change and not the type of prior.

### Improper prior distributions

Maybe you feel uncomfortable putting a prior on an unknown parameter. If you use a normal prior you can use a very large variance. In the limit this leads to an improper prior distribution.

### Improper prior distribution

For example, let  $\mu \sim \mathcal{N}(\mu, \infty)$ , i.e.  $f(\mu) \propto \text{const.} > 0$ .

$$\int f(\mu)d\mu \approx \infty$$

Priors such as  $f(\mu) = \text{const.}, f(\sigma) = 1/\sigma$  are improper, because they do not integrate to 1.

### List of conjugate prior distributions

Likelihood	Conjugate prior	Posterior distribution
$X p \sim Bin(n,p)$	$ extcolor{black}{ ho} \sim Be(lpha,eta)$	$p x \sim Be(\alpha + x, \beta + n - x)$
$X p \sim Geom(p)$	$ extcolor{black}{p} \sim Be(lpha,eta)$	$p x \sim Be(lpha+1,eta+x-1)$
$X \lambda \sim Po(e \cdot \lambda)$	$\lambda \sim G(lpha,eta)$	$\lambda   x \sim G(\alpha + x, \beta + e)$
$X \lambda \sim Exp(\lambda)$	$\lambda \sim G(lpha,eta)$	$\lambda   x \sim G(\alpha + 1, \beta + x)$
$X \mu \sim \mathcal{N}(\mu, \sigma_{\star}^2)$	$\mu \sim \mathcal{N}( u,  au^2)$	$\mu   \mathbf{x} \sim \mathcal{N} \left[ (\mathbf{A})^{-1} \left( \frac{\mathbf{x}}{\sigma^2} + \frac{\nu}{\tau^2} \right), (\mathbf{A})^{-1} \right]$
$X \sigma^2 \sim \mathcal{N}(\mu_\star, \sigma^2)$	$\sigma^2 \sim IG(lpha,eta)$	$\sigma^2 x\sim IG(\alpha+\frac{1}{2},\beta+\frac{1}{2}(x-\mu)^2)$

\*: known.

$$A = \frac{1}{\sigma^2} + \frac{1}{\tau^2}$$

## Improper prior distributions (II)

In most cases, improper priors can be used in Bayesian analyses without major problems. However, things to watch out for are:

- In a few models, the use of improper priors can result in improper posteriors.
- Use of improper priors makes model selection difficult.

## Uninformative priors

Though conjugate priors are computationally nice, priors might be preferred which do not strongly influence the posterior distribution. Such a prior is called an uninformative prior.

- The historical approach, followed by Laplace and Bayes, was to assign flat priors.
- This prior seems reasonably uninformative. We do not know where the actual value lies in the parameter space, so we might as well consider all values equi-probable.
- However, this prior is not invariant to one-to-one transformations.

## Jeffreys' prior for the geometric distribution

The geometric distribution models the number X of Bernoulli trials needed to get the first success. Let  $X|\pi \sim \text{Geom}(\pi)$ , i.e.

$$P(x|\pi) = \pi \cdot (1-\pi)^{x-1}$$
.

Thus:

$$I_x(\pi) = \log(\pi) + (x-1)\log(1-\pi)$$

$$I_x'(\pi)=\frac{1}{\pi}-\frac{x-1}{1-\pi}$$

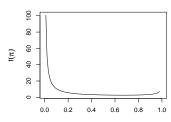
$$I_{x}^{"}(\pi) = -\frac{1}{\pi^{2}} - \frac{x-1}{(1-\pi)^{2}}$$

$$J(\pi) = -E\left(-\frac{1}{\pi^2} - \frac{x-1}{(1-\pi)^2}\right)$$
$$= \frac{1}{\pi^2} + \frac{\frac{1}{\pi} - 1}{(1-\pi)^2}$$
$$= \frac{1}{\pi^2} + \frac{1-\pi}{\pi(1-\pi)^2}$$
$$= \pi^{-2}(1-\pi)^{-1}$$

Jeffreys' prior results as:

$$f(\pi) \propto \sqrt{J(\pi)} = \pi^{-1} (1-\pi)^{-1/2}$$

(can be seen as "Be(0, 0.5)")



 $\Rightarrow$  Small values are favoured.

## Harold Jeffreys' prior

#### Definition

Let X denote a random variable with likelihood function  $p(x|\theta)$  where  $\theta$  is an unknown scalar parameter. Jeffreys' prior or Jeffreys' rule is defined as

$$f(\theta) \propto \sqrt{J(\theta)}$$
,

where  $J(\theta)$  is the expected Fisher information of  $\theta$ .

Jeffreys' prior has certain desired properties, e.g. invariance property.

## New concept: Penalised complexity (PC) priors

There was recently a new concept developed here at NTNU to choose interpretable and meaningful prior distributions.

For more information see here

http://arxiv.org/abs/1403.4630

We may come back to this later, when we talk about Bayesian hierarchical models.