# Bayesian data analysis: Theory & practice

## Part 2: Parameter estimation, MCMC & simple linear regression in BRMS

Michael Franke

# Practical goal for today

## master this!

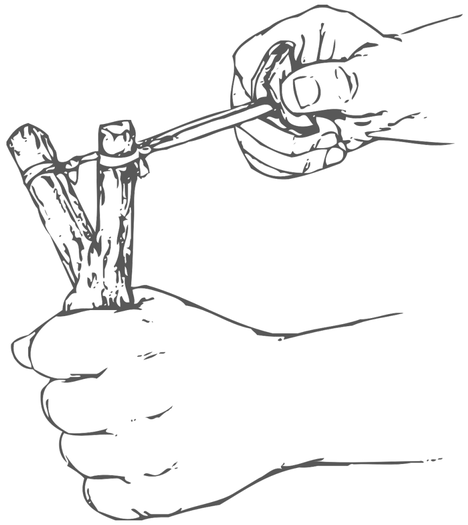
```
 Family: gaussian
  Links: mu = identity; sigma = identity
Formula: murder_rate ~ unemployment
   Data: murder_data (Number of observations: 20)
Samples: 4 chains, each with iter = 2000; warmup = 1000; thin = 1;
         total post-warmup samples = 4000

Population-Level Effects:
             Estimate Est.Error l-95% CI u-95% CI Rhat Bulk_ESS Tail_ESS
Intercept      -28.48      7.32   -42.05   -13.79 1.00     3014     2362
unemployment     7.07      1.04     4.97     9.04 1.00     2978     2451

Family Specific Parameters:
      Estimate Est.Error l-95% CI u-95% CI Rhat Bulk_ESS Tail_ESS
sigma     5.42      0.96     3.88     7.63 1.00     2664     2196

Samples were drawn using sampling(NUTS). For each parameter, Eff.Sample
is a crude measure of effective sample size, and Rhat is the potential
scale reduction factor on split chains (at convergence, Rhat = 1).
```

# Main learning goals
for this part



1. Bayesian parameter estimation
    a. sampling-based approaches
    b. Bayesian summary statistics
2. Markov Chain Monte Carlo sampling
    a. Metropolis Hastings
    b. Hamiltonian Monte Carlo
    c. diagnostics and tuning-parameters
3. Bayesian regression with the `BRMS` package
    a. extracting samples
    b. priors & predictive functions
    c. plotting

# parameter estimation

# Computing posterior distributions

problem of computational complexity

$$P(\theta \mid D) = \frac{P(D \mid \theta)\, P(\theta)}{\int P(D \mid \theta)\, P(\theta)\, \mathrm{d}\theta}$$

✓fast & easy

✓fast & easy

✗☠ possibly intractable ☠✗



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# Excursion: Posteriors from conjugacy

closed-form posteriors from clever choice of priors

- prior $P(\theta)$ is a **conjugate prior** for likelihood $P(D \mid \theta)$ iff prior $P(\theta)$ and posterior $P(\theta \mid D)$ are the same kind of probability distribution, e.g.:
  - prior: $\theta \sim \text{Beta}(1,1)$
  - posterior: $\theta \mid D \sim \text{Beta}(8,18)$
- **claim:** the beta distribution is a conjugate prior for the binomial likelihood function
  - proof:

$$P(\theta \mid k, N) \propto \text{Binomial}(k; N, \theta)\ \text{Beta}(\theta \mid a, b)$$

$$P(\theta \mid k, N) \propto \theta^{k} (1-\theta)^{N-k} \theta^{a-1} (1-\theta)^{b-1}$$

$$P(\theta \mid k, N) \propto \theta^{k+a-1} (1-\theta)^{N-k+b-1}$$

$$P(\theta \mid k, N) = \text{Beta}(\theta \mid k+a, N-k+b)$$


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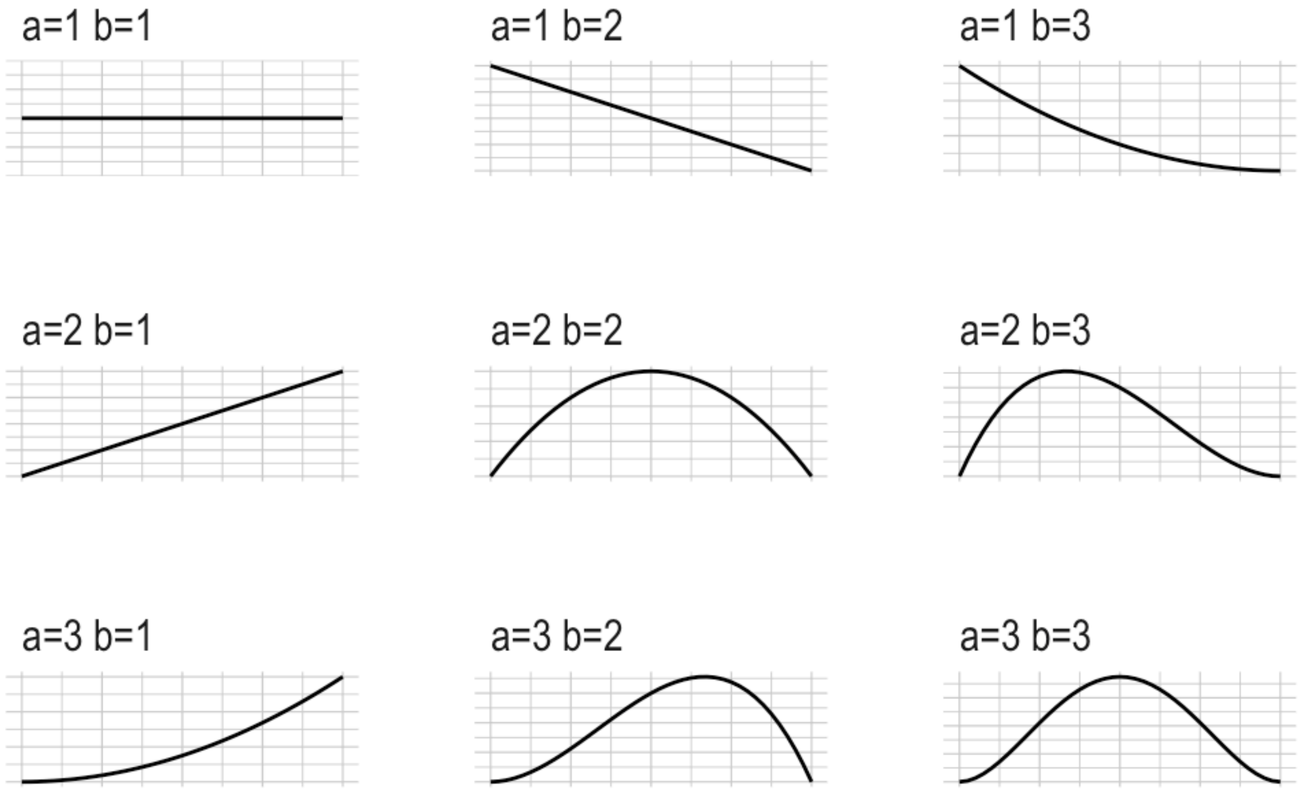
# Excursion: Sequential updating

## for the beta-binomial model

- sequence of updating does not matter
  - any order of single-observation updates
  - any ‘chunking’: whole data set, different subsets in whatever sequence (as long as disjoined)
- “today’s posterior is tomorrow’s prior”

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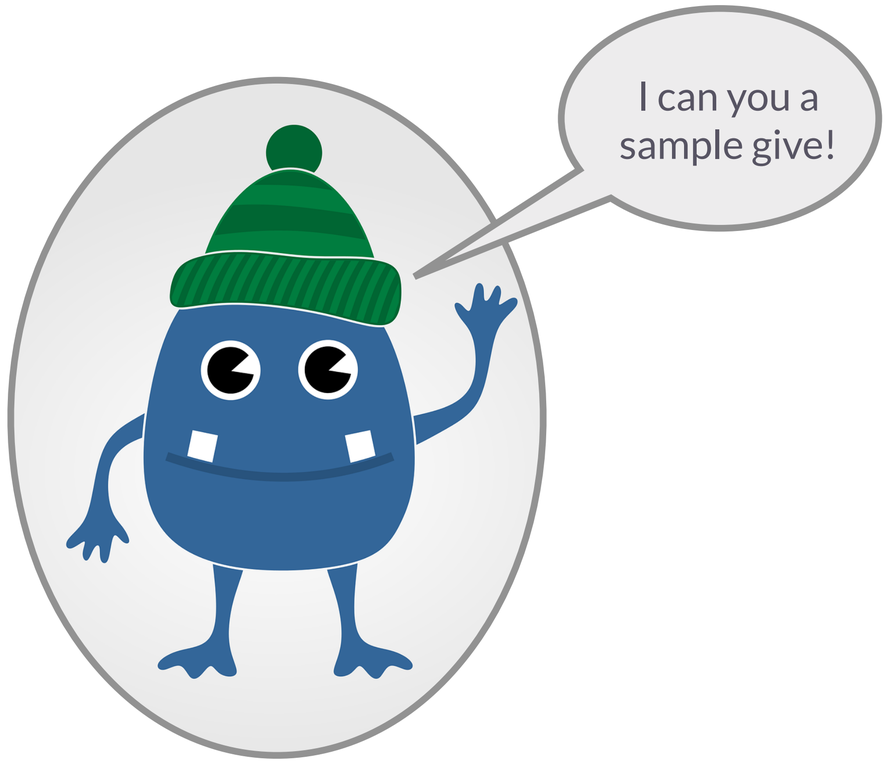
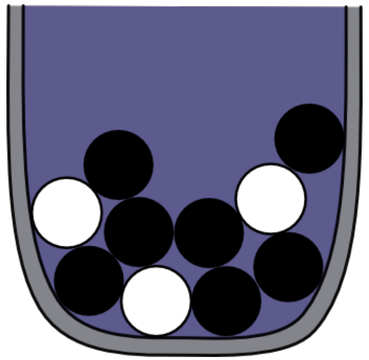
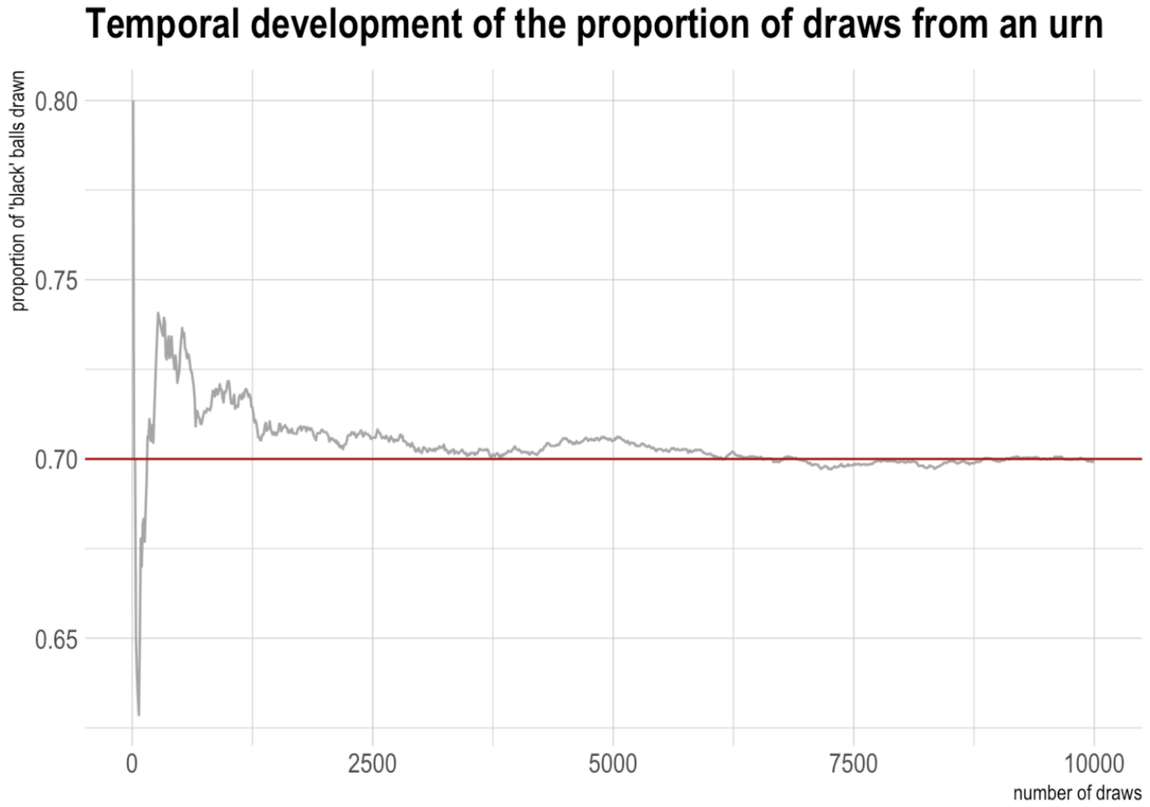
# Approximating distributions via sampling

## our go-to solution for approximating posterior distributions beyond conjugacy

- we can approximate many summary statistics of a probability distribution by either:
  - a large set of representative samples; or
  - an oracle that returns a sample if needed.





# summary statistics

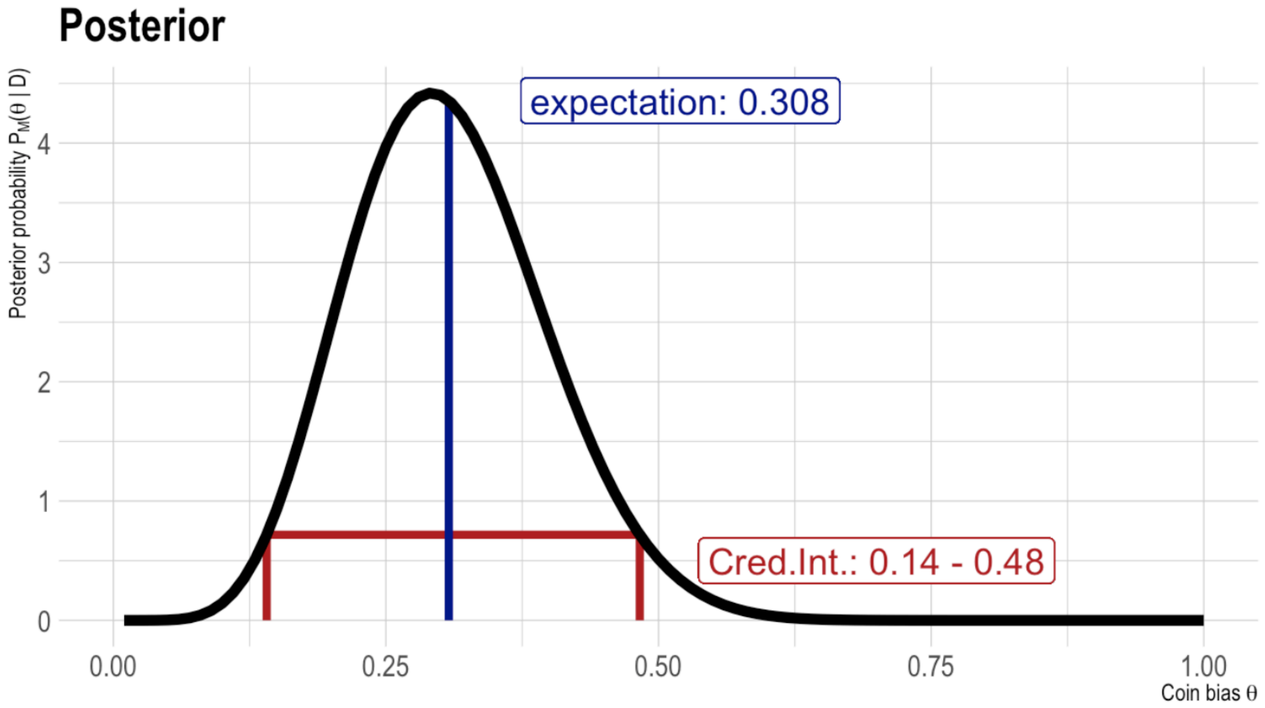
# Parameter estimation

## point- and interval-valued estimates

- Bayes' rule for parameter estimation:

$$P(\theta \mid D) = \frac{P(D \mid \theta)\ P(\theta)}{\int P(D \mid \theta)\ P(\theta)\ \mathrm{d}\theta}$$

- common point estimates ("best" values):
  - maximum likelihood estimate (MLE)
  - maximum a posteriori (MAP)
  - **posterior mean / expected value**
- common interval estimates (range of "good" values):
  - confidence intervals
  - inner quantile ranges
  - **credible intervals**

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# Point-valued estimates

## MLE, MAP and (posterior) expected value

- **MLE:**

$$\arg\max_{\theta} P(D \mid \theta)$$

  - doesn't take prior into account (not Bayesian)
  - not necessarily unique

- **MAP:**

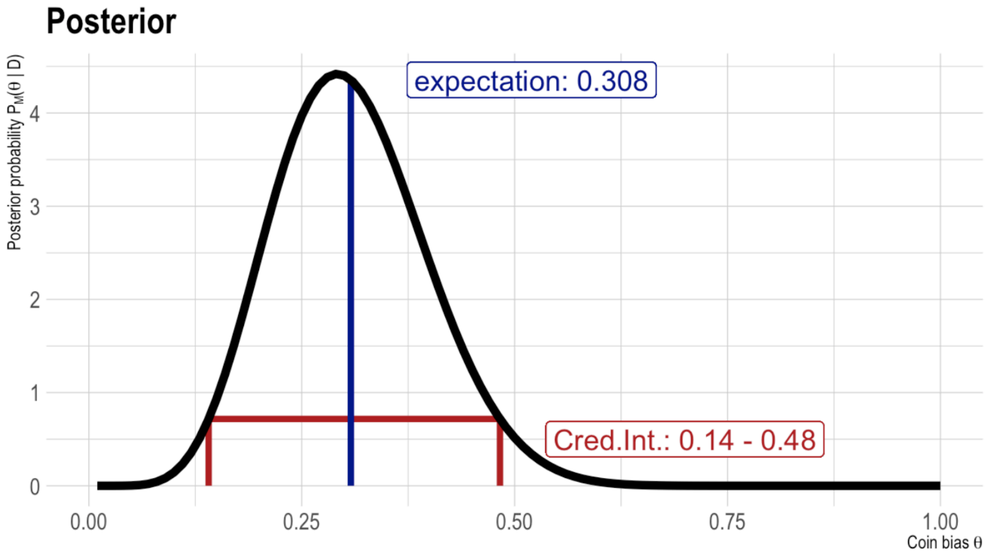
$$\arg\max_{\theta} P(\theta \mid D)$$

  - local / does not consider full distribution (not fully Bayesian)
  - increasingly uninformative in larger parameter spaces
  - not necessarily unique

- **posterior mean / expected valued**

$$\mathbb{E}_{P(\theta|D)} = \int \theta \; P(\theta \mid D) \; \mathrm{d}\theta$$

  - holistic / depends on full distribution ("genuinely Bayesian")
  - always unique (for proper priors/posteriors)

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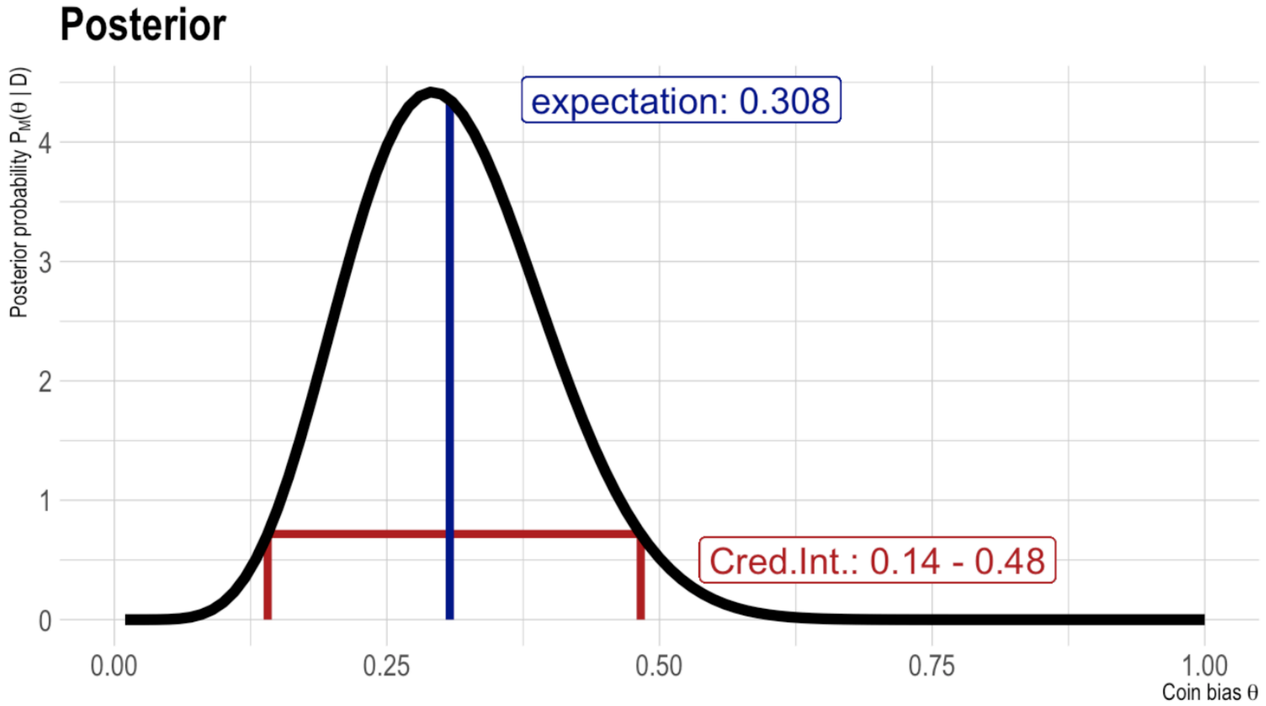
# Bayesian credible intervals

a.k.a.: highest density interval …

An interval $I$ is a $\gamma\%$ credible interval, if:

1. the probability that $\theta \in I$ is $\frac{\gamma}{100}$, and
2. no value outside of $I$ is more likely than any point inside of $I$.

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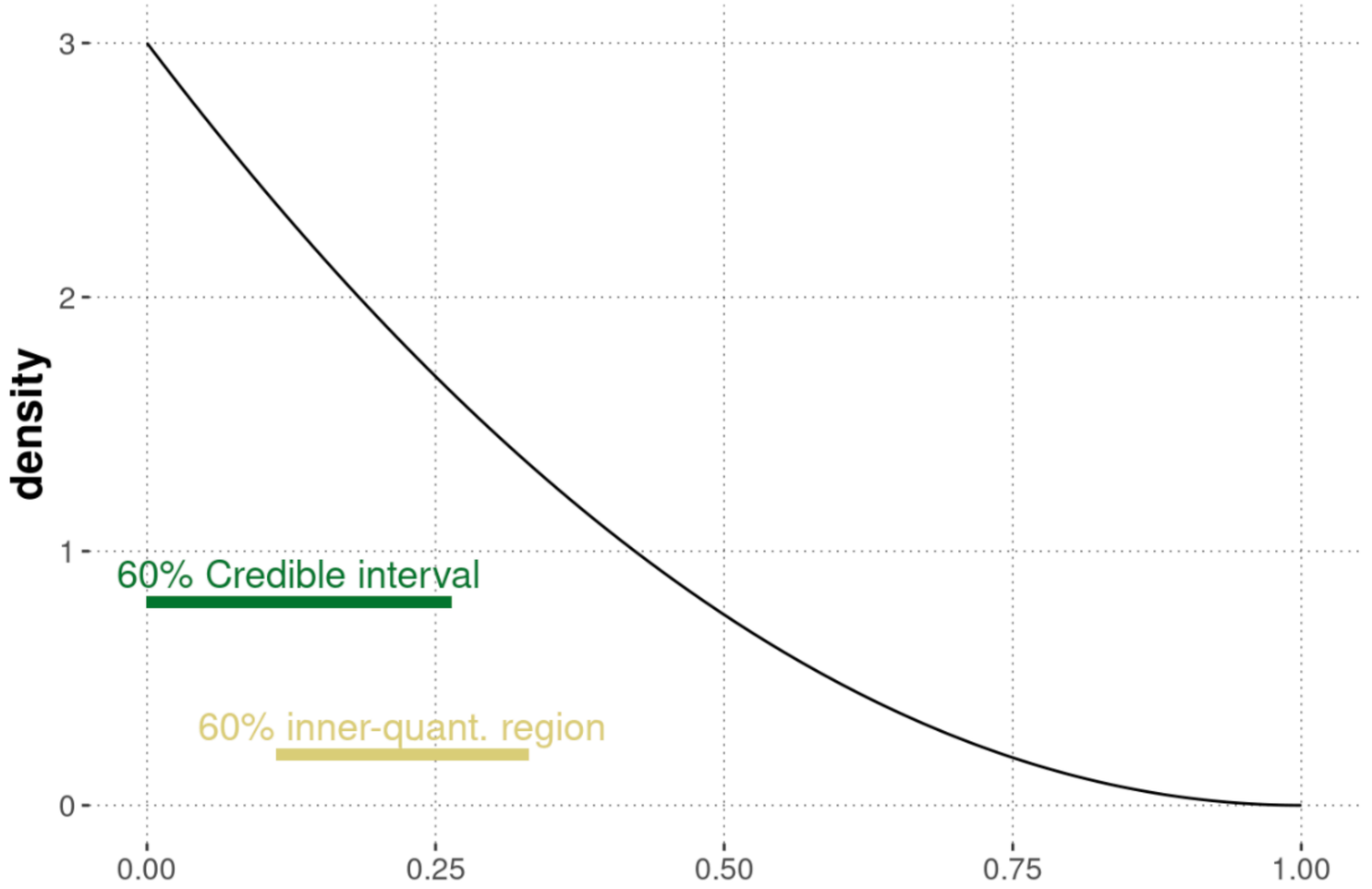
# Inner quantile regions

!!!are not credible intervals!!!

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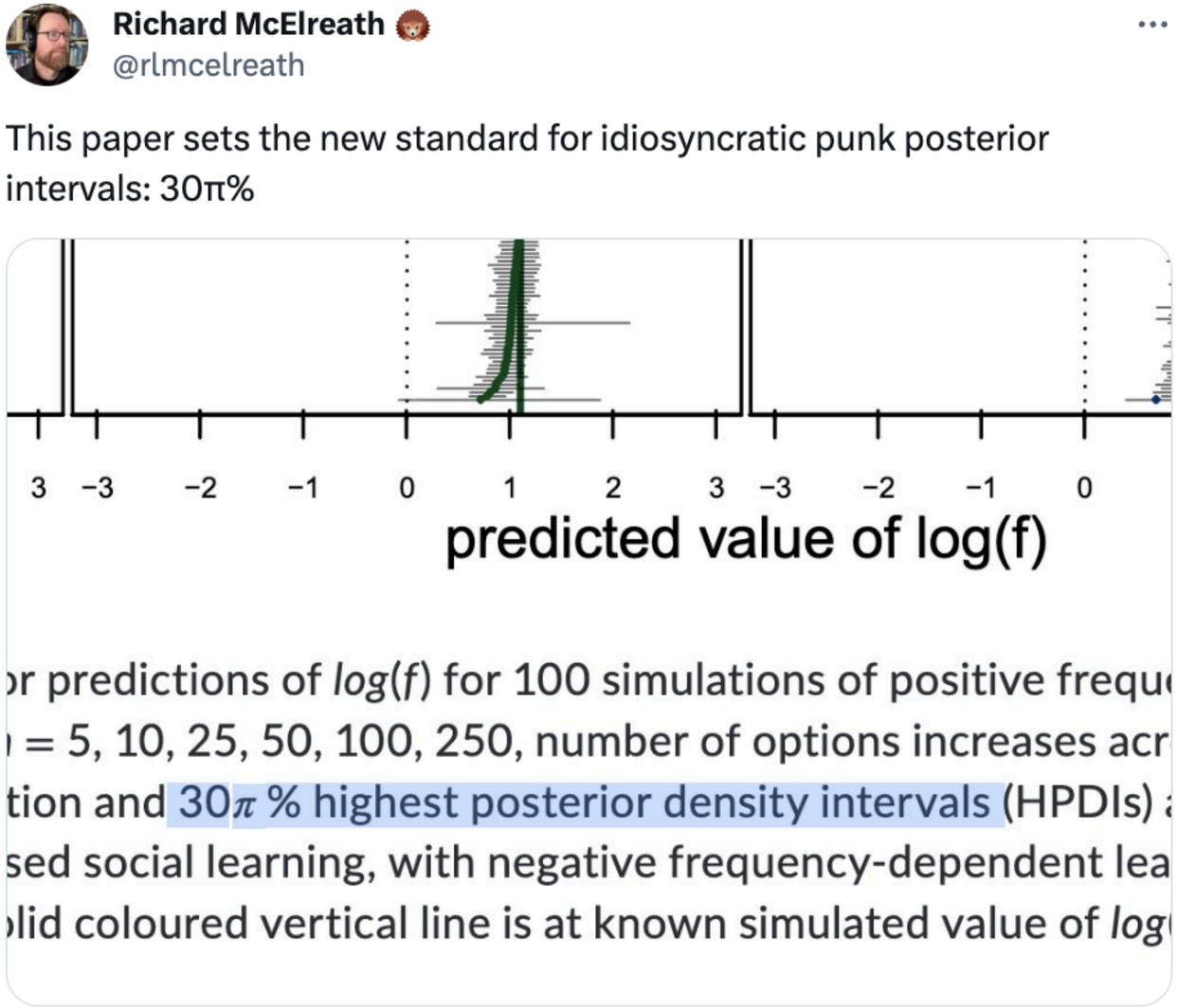
# Post-everything choice of bounds

## if you want to signal that it's all arbitrary

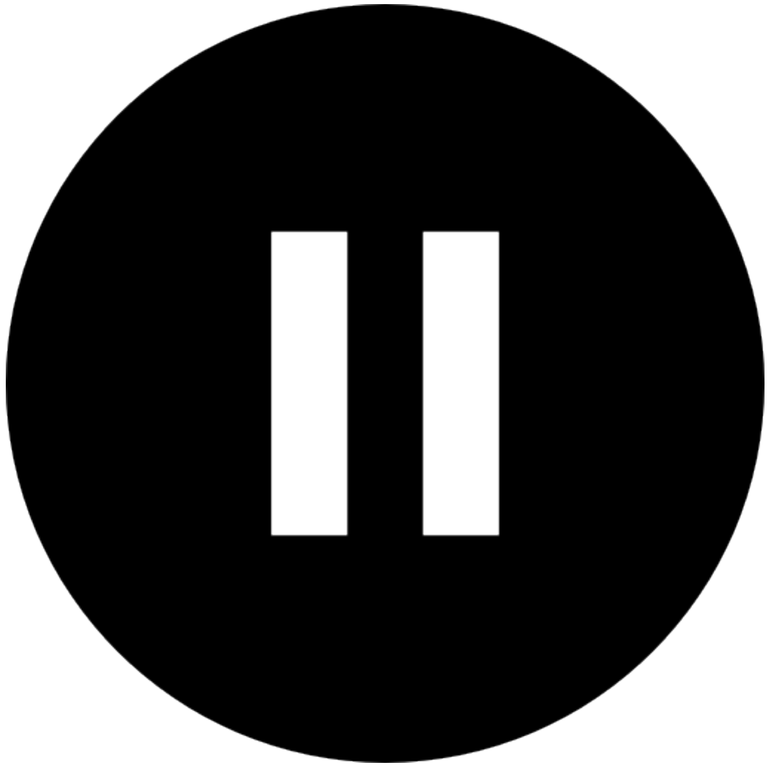


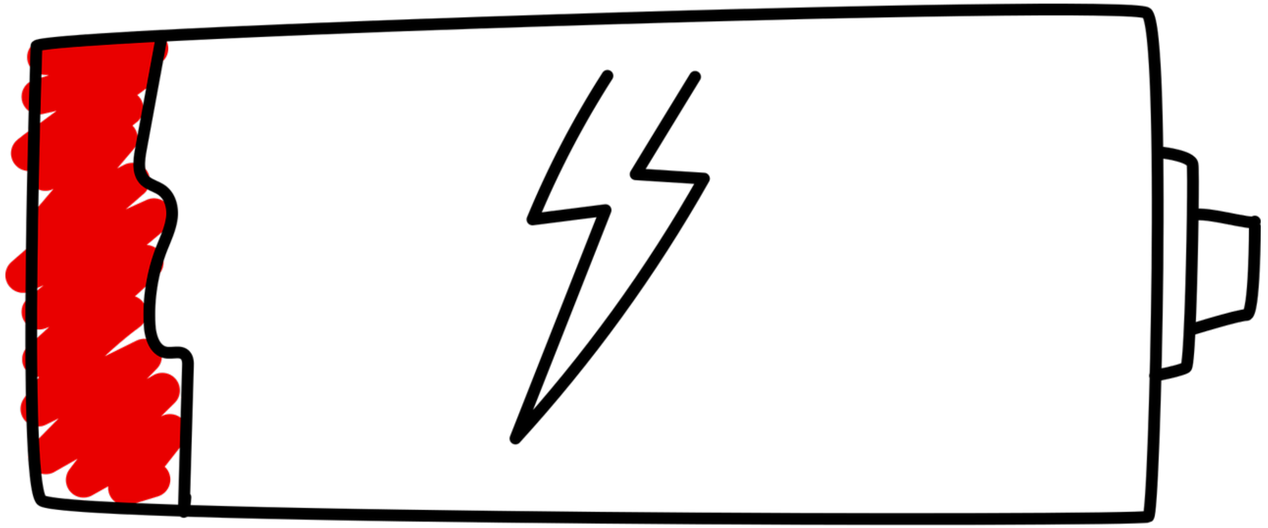
**Richard McElreath** 🦔
@rlmcelreath

This paper sets the new standard for idiosyncratic punk posterior intervals: 30π%



or predictions of *log*(*f*) for 100 simulations of positive frequ
= 5, 10, 25, 50, 100, 250, number of options increases acr
tion and 30$\pi$ % highest posterior density intervals (HPDIs) a
sed social learning, with negative frequency-dependent lea
olid coloured vertical line is at known simulated value of *log*





# Bayesian regression in BRMS

# Bayesian linear regression in R

## using BRMS and Stan

- R package BRMS provides high-level interface for Bayesian linear regression
- models are specified with R's formula syntax
- returns samples from the posterior distribution
  - alternatives: MAPs, variational inference
- builds on probabilistic programming language Stan
  - powerful, cutting-edge tool for Bayesian computation
  - strong, non-commercial development team
  - many interfaces: stand-alone, R, Python, Julia, …

```r
fit_brms_murder <- brm(
  # specify what to explain in terms of what
  #  using the formula syntax
  formula = murder_rate ~ unemployment,
  # which data to use
  data = murder_data
)
```

# Navigating BRMS output

```
summary(fit_brms_murder)
```

model & data we used

information about sampling

main model parameters

additional model parameters

information about sampling

```
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Formula: murder_rate ~ unemployment
   Data: murder_data (Number of observations: 20)
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Samples were drawn using sampling(NUTS). For each parameter, Eff.Sample
is a crude measure of effective sample size, and Rhat is the potential
scale reduction factor on split chains (at convergence, Rhat = 1).
```

# demo

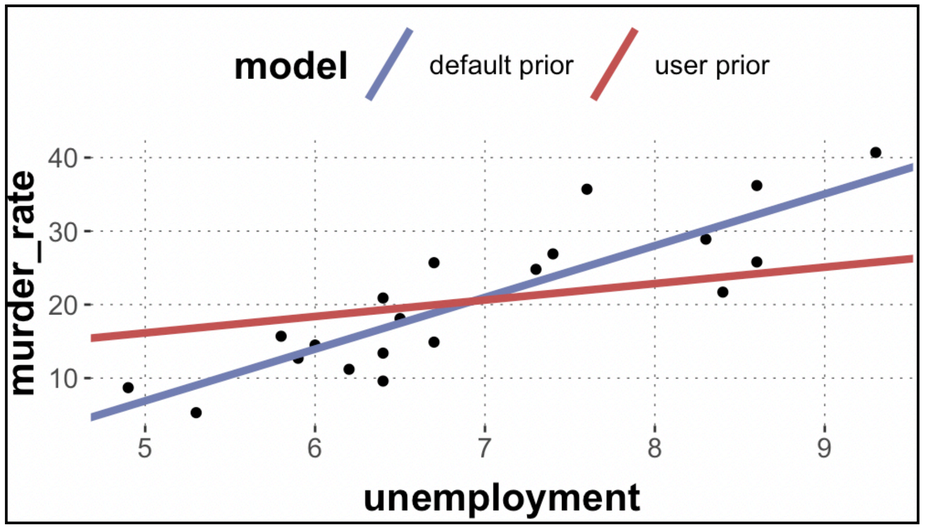
hands-on exploration of a simple linear model in BRMS

# Setting priors in `brms`

# Setting priors in BRMS

```r
fit_brms_murder <- brm(
  formula = murder_rate ~ unemployment,
  data = aida::data_murder
)

fit_brms_murder_wPrior <- brm(
  formula = murder_rate ~ unemployment,
  data = aida::data_murder,
  prior = prior(normal(0,1), class = "b")
)
```




```
> brms::prior_summary(fit_brms_murder)
                   prior     class         coef group resp dpar nlpar lb ub       source
                  (flat)         b                                                default
                  (flat)         b unemployment                               (vectorized)
 student_t(3, 19.5, 9.7) Intercept                                             default
    student_t(3, 0, 9.7)     sigma                                  0         default
> brms::prior_summary(fit_brms_murder_wPrior)
                   prior     class         coef group resp dpar nlpar lb ub       source
            normal(0, 1)         b                                                user
            normal(0, 1)         b unemployment                               (vectorized)
 student_t(3, 19.5, 9.7) Intercept                                             default
    student_t(3, 0, 9.7)     sigma                                  0         default
```

```
> tidybayes::summarise_draws(fit_brms_murder)
# A tibble: 5 × 10
  variable          mean median     sd    mad     q5     q95  rhat ess_bulk ess_tail
  <chr>            <dbl>  <dbl>  <dbl>  <dbl>  <dbl>   <dbl> <dbl>    <dbl>    <dbl>
1 b_Intercept    -28.3   -28.3   7.45   6.99   -40.3  -16.0    1.00    2945.    2304.
2 b_unemployment   7.04    7.04  1.06   1.01     5.31   8.76   1.00    2929.    2337.
3 sigma            5.44    5.28  0.994  0.897    4.12   7.26   1.00    2667.    2319.
4 lprior          -6.07   -6.06  0.0816 0.0655  -6.23  -5.98   1.00    2369.    2121.
5 lp__           -66.0   -65.6   1.36   1.10   -68.7  -64.5    1.00    1516.    2070.
> tidybayes::summarise_draws(fit_brms_murder_wPrior)
# A tibble: 5 × 10
  variable          mean median     sd    mad      q5     q95  rhat ess_bulk ess_tail
  <chr>            <dbl>  <dbl>  <dbl>  <dbl>   <dbl>   <dbl> <dbl>    <dbl>    <dbl>
1 b_Intercept      4.96    4.84   7.19   7.28  -6.77    17.1    1.00    2299.    2440.
2 b_unemployment   2.24    2.24   1.01   1.02   0.584    3.89   1.00    2313.    2499.
3 sigma            8.02    7.81   1.65   1.50   5.67    11.1    1.00    2268.    2218.
4 lprior         -10.2    -9.72   2.27   2.06 -14.7     -7.56   1.00    2398.    2541.
5 lp__           -77.8   -77.5    1.28   1.05 -80.2    -76.4    1.00    1881.    2436.
```

read more here

# Stan code generated by BRMS

- brms generates Stan code implicitly
- show it using: `brms::stancode(fitted_model)`
- prior information increases the log-score
- priors specified in `brms` must use Stan-like syntax

```
transformed parameters {
  real lprior = 0;  // prior contributions to the log posterior
  lprior += normal_lpdf(b | 0, 1);
  lprior += student_t_lpdf(Intercept | 3, 19.5, 9.7);
  lprior += student_t_lpdf(sigma | 3, 0, 9.7)
    - 1 * student_t_lccdf(0 | 3, 0, 9.7);
}
```

```
// generated with brms 2.18.0
functions {
}
data {
  int<lower=1> N;  // total number of observations
  vector[N] Y;  // response variable
  int<lower=1> K;  // number of population-level effects
  matrix[N, K] X;  // population-level design matrix
  int prior_only;  // should the likelihood be ignored?
}
transformed data {
  int Kc = K - 1;
  matrix[N, Kc] Xc;  // centered version of X without an intercept
  vector[Kc] means_X;  // column means of X before centering
  for (i in 2:K) {
    means_X[i - 1] = mean(X[, i]);
    Xc[, i - 1] = X[, i] - means_X[i - 1];
  }
}
parameters {
  vector[Kc] b;  // population-level effects
  real Intercept;  // temporary intercept for centered predictors
  real<lower=0> sigma;  // dispersion parameter
}
transformed parameters {
  real lprior = 0;  // prior contributions to the log posterior
  lprior += normal_lpdf(b | 0, 1);
  lprior += student_t_lpdf(Intercept | 3, 19.5, 9.7);
  lprior += student_t_lpdf(sigma | 3, 0, 9.7)
    - 1 * student_t_lccdf(0 | 3, 0, 9.7);
}
model {
  // likelihood including constants
  if (!prior_only) {
    target += normal_id_glm_lpdf(Y | Xc, Intercept, b, sigma);
  }
  // priors including constants
  target += lprior;
}
generated quantities {
  // actual population-level intercept
  real b_Intercept = Intercept - dot_product(means_X, b);
}
```

read more here

# Prior & posterior predictions

# Three pillars of BDA

1. parameter estimation / inference [which parameter values are credible given data and model?]

$$\underbrace{P(\theta \mid D)}_{\text{posterior}} \propto \underbrace{P(\theta)}_{\text{prior}} \times \underbrace{P(D \mid \theta)}_{\text{likelihood}}$$

---

2. predictions [which future data observations are likely given my model?]

a. prior

$$P(D_{\text{pred}}) = \int P(\theta)\ P(D_{\text{pred}} \mid \theta)\ \mathrm{d}\theta$$

b. posterior

$$P(D_{\text{pred}} \mid D_{\text{obs}}) = \int P(\theta \mid D_{\text{obs}})\ P(D_{\text{pred}} \mid \theta)\ \mathrm{d}\theta$$

---

3. model comparison [which model of two models is more likely to have generated the data?]

$$\underbrace{\frac{P(M_1 \mid D)}{P(M_2 \mid D)}}_{\text{posterior odds}} = \underbrace{\frac{P(D \mid M_1)}{P(D \mid M_2)}}_{\text{Bayes factor}} \underbrace{\frac{P(M_1)}{P(M_2)}}_{\text{prior odds}}$$

# Prior and posterior (data) predictions

## Monte Carlo sampling

- fix a model with $P(D \mid X, \theta)$ and $P(\theta)$
  - latter can be prior or post. conditioned on $D'$
- sample from the predictive distribution by:

  (i) sampling a vector of parameters $\theta^* \sim P(\theta)$

  (ii) sampling "fake" data $D^*$ from the likelihood function, conditioned on the sampled $\theta^*$ (given the relevant predictor values $X$) :
  $D^* \sim P(D \mid X, \theta^*)$
- Monte Carlo sampling:
  - by taking many samples and "aggregating", we approximate the integrals
    - "aggregating" means that (i) we usually don't care for just one sample, but the distributional information in a lot of samples, and (ii) we might want to focus on particular aspects of each sampled "fake" data (e.g., a particular **summary statistic**)

**prior predictive**

$$P(D_{\text{pred}}) = \int P(\theta)\ P(D_{\text{pred}} \mid \theta)\ \mathrm{d}\theta$$

**posterior predictive**

$$P(D_{\text{pred}} \mid D_{\text{obs}}) = \int P(\theta \mid D_{\text{obs}})\ P(D_{\text{pred}} \mid \theta)\ \mathrm{d}\theta$$

**predicted linear predictor**

- fix a linear model with $P(\theta)$
  - $P(\theta)$ can be prior or posterior
- sample a linear predictor $\mu^* \sim P(\mu^* \mid X, \theta)$
  - $X$ is a matrix of independent variables

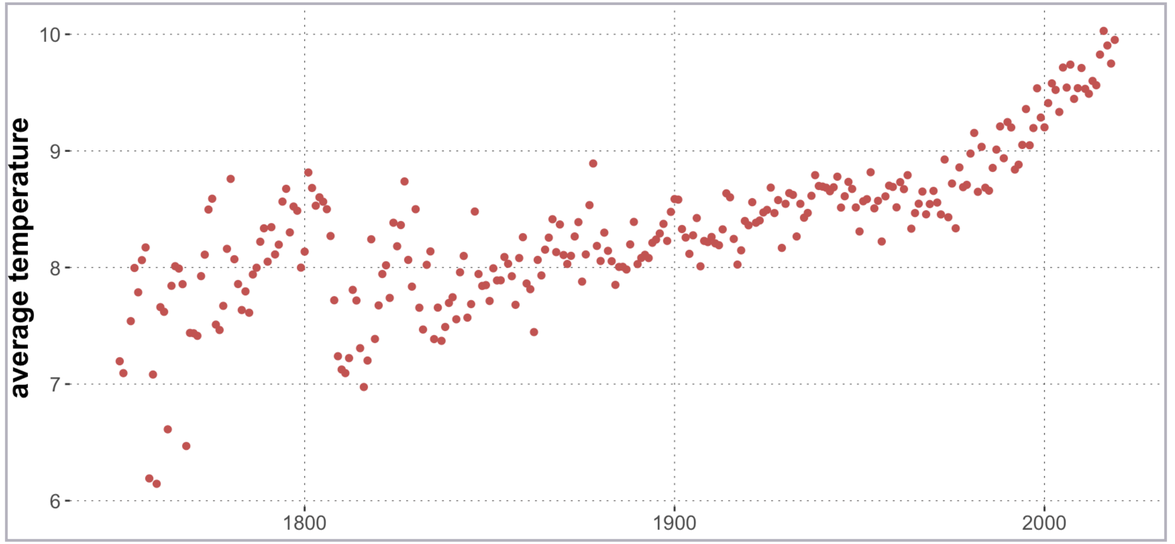
# Example: World-temperature data

data, model and posterior predictions

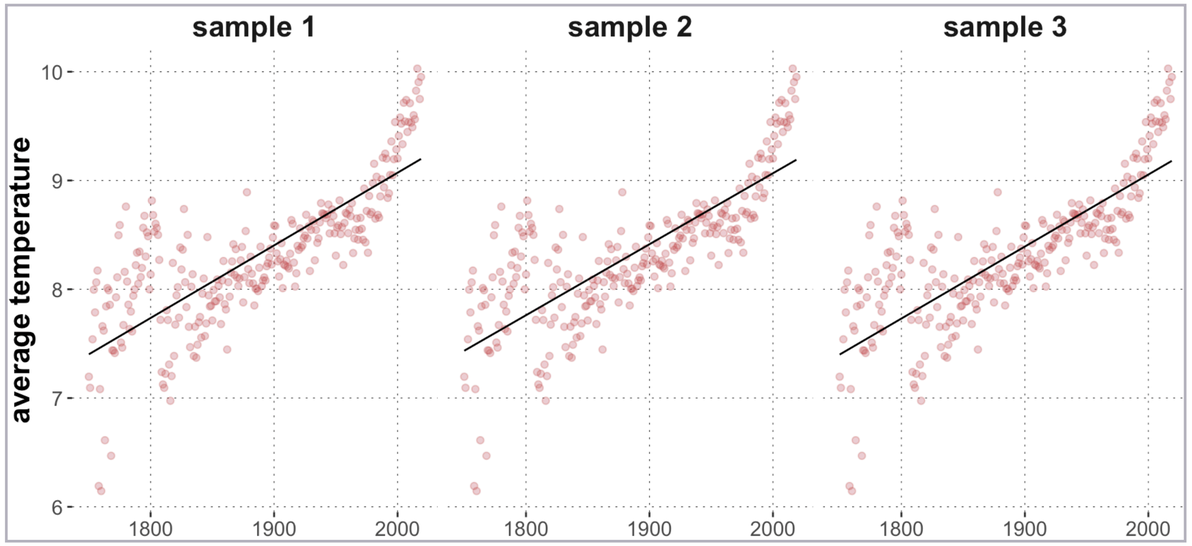
- data:
  - average world temperature 1750-2019
- model:

```
fit_worldTemp <- brm(
  avg_temp ~ year,
  data = aida::data_WorldTemp,
  prior = prior(student_t(1,0,5), class = "b")
  )
```

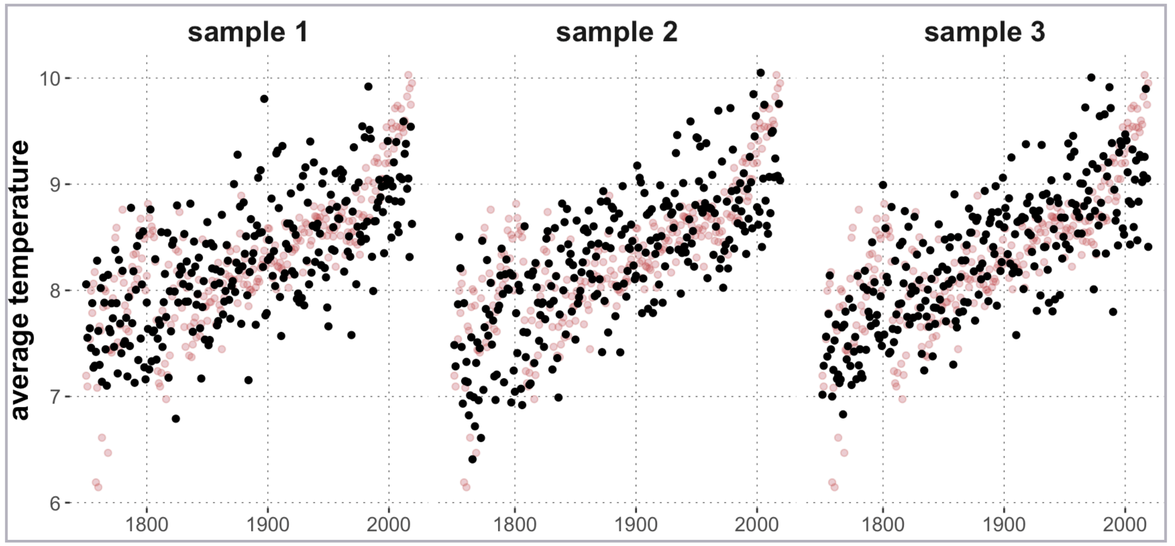
## Data




## Posterior samples for the central tendency



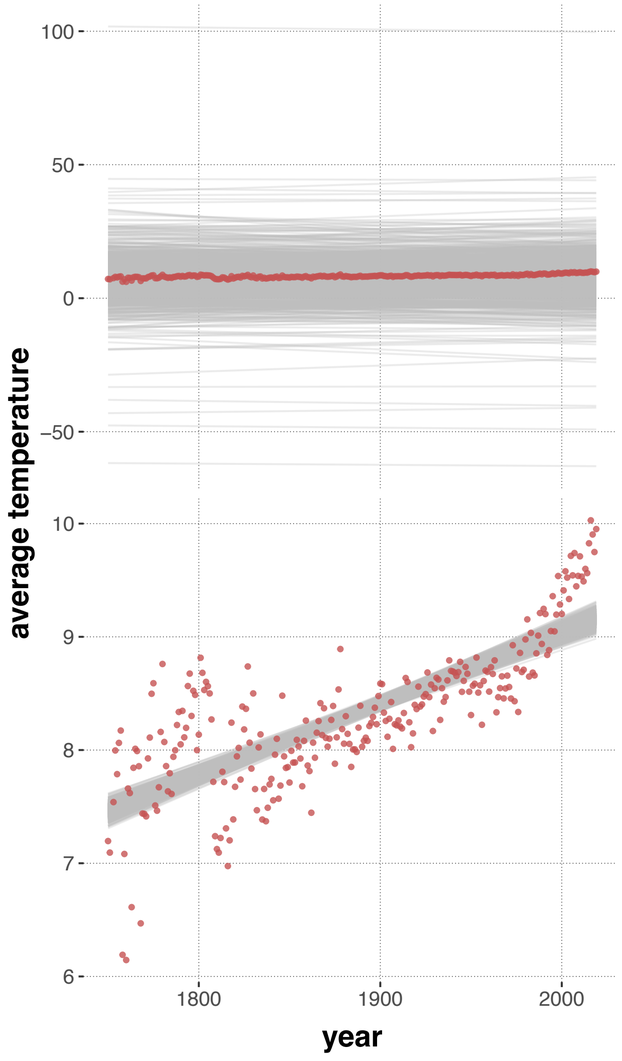

## Samples from the posterior predictive (data)



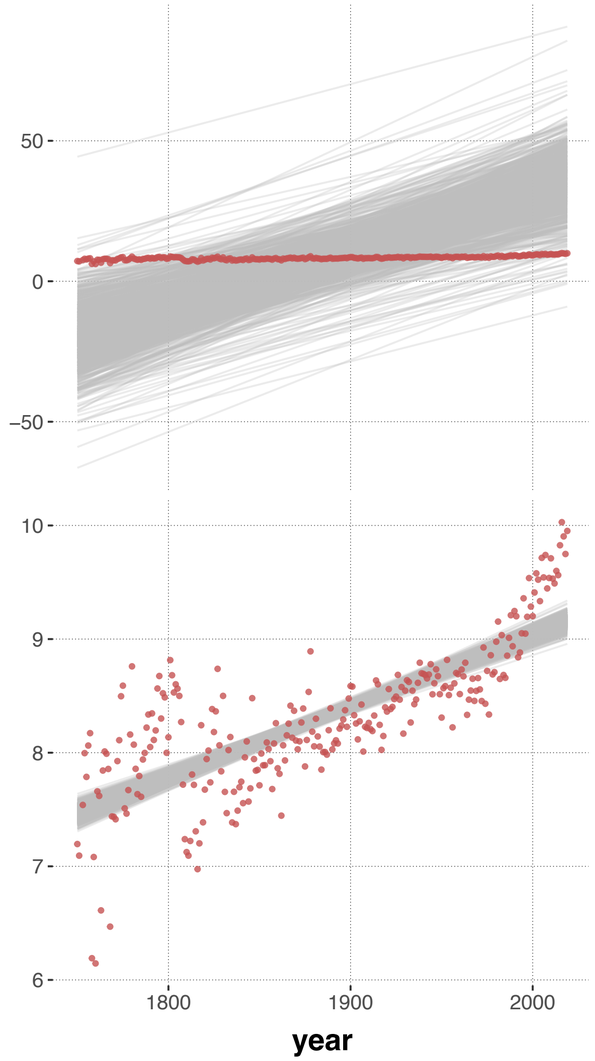
# Exploring prior and posterior prediction

## Prior & posterior samples of linear predictor value ($\mu$)

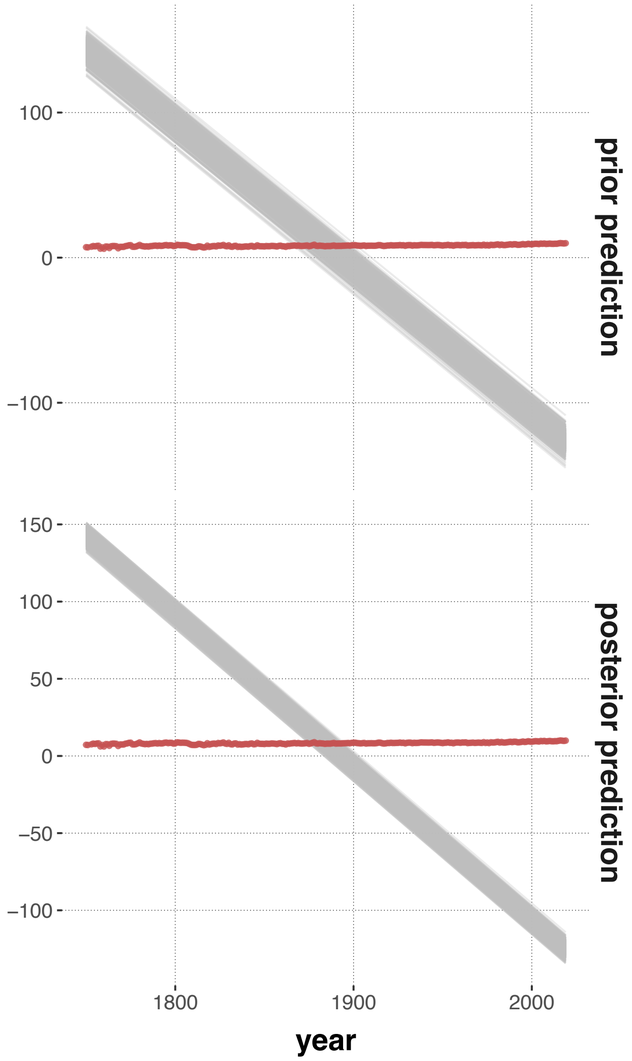
$\beta_{\text{year}} \sim \text{Normal}(0, 0.02)$




$\beta_{\text{year}} \sim \text{Normal}(0.2, 0.05)$




$\beta_{\text{year}} \sim \text{Normal}(-1, 0.005)$



# demo

assessing predictive samples in BRMS