Chapter 7

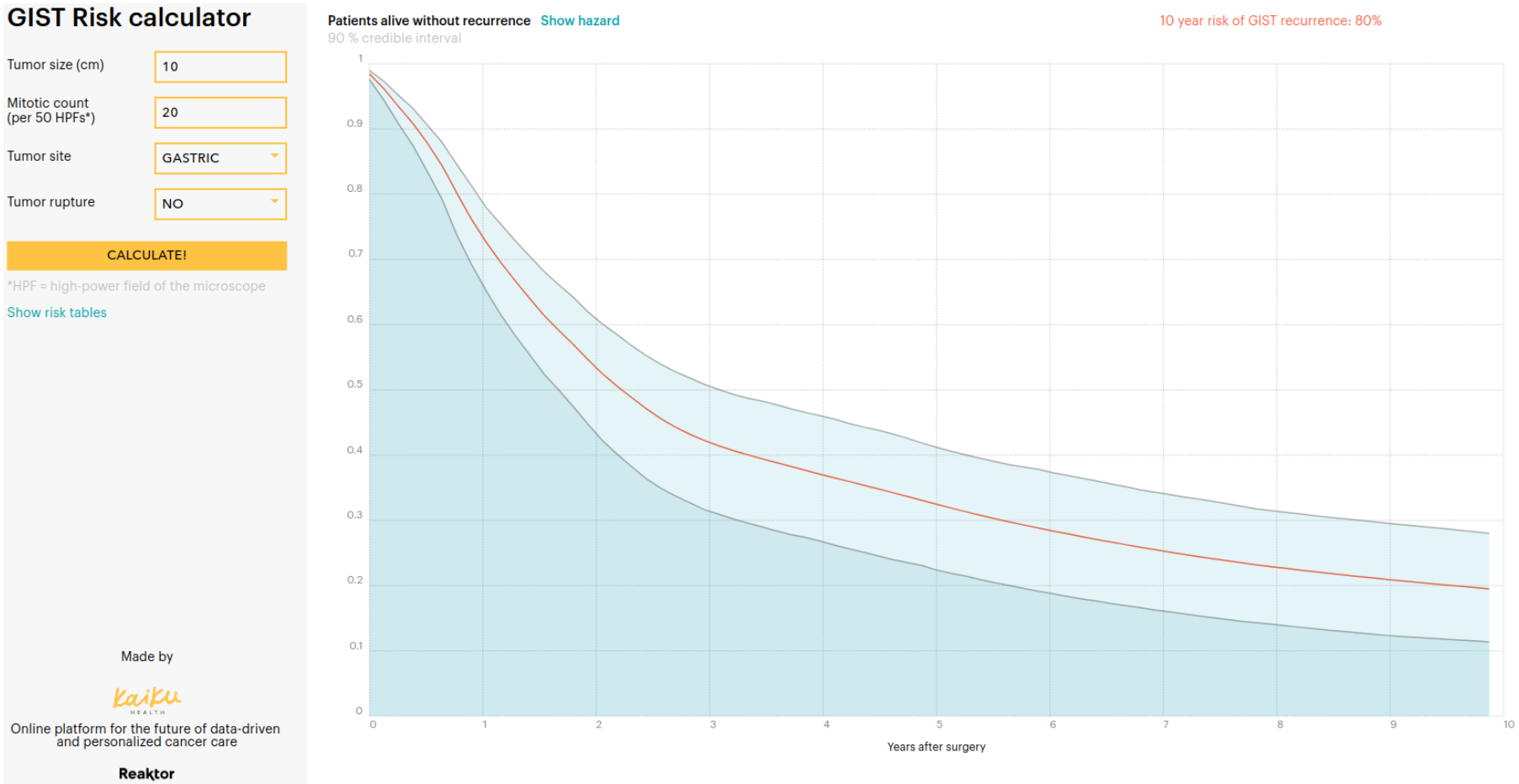
- 7.1 Measures of predictive accuracy
- 7.2 Information criteria and cross-validation
  - Instead of 7.2, read:
    Vehtari, A., Gelman, A., Gabry, J. (2017). Practical Bayesian model evaluation using leave-one-out cross-validation and WAIC. Statistics and Computing. 27(5):1413–1432. arXiv preprint.
- 7.3 Model comparison based on predictive performance
- 7.4 Model comparison using Bayes factors
- 7.5 Continuous model expansion / sensitivity analysis
- 7.5 Example (may be skipped)

Model assessment, selection and inference after selection

- Extra material at https://avehtari.github.io/modelselection/
  - Videos, Slides, Notebooks, References
  - The most relevant for the course is the first part of the talk “Model assessment, comparison and selection at Master class in Bayesian statistics, CIRM, Marseille”

Predicting concrete quality

Predicting cancer recurrence



Predictive performance

- True predictive performance is found out by using it to make predictions and comparing predictions to true observations
  - external validation

Predictive performance

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  - external validation
- Expected predictive performance
  - approximates the external validation

Predictive performance

- We need to choose the utility/cost function
- Application specific utility/cost functions are important
  - eg. money, life years, quality adjusted life years, etc.

Predictive performance

- We need to choose the utility/cost function
- Application specific utility/cost functions are important
  - eg. money, life years, quality adjusted life years, etc.
- If are interested overall in the goodness of the predictive distribution, or we don't know (yet) the application specific utility, then good information theoretically justified choice is log-score

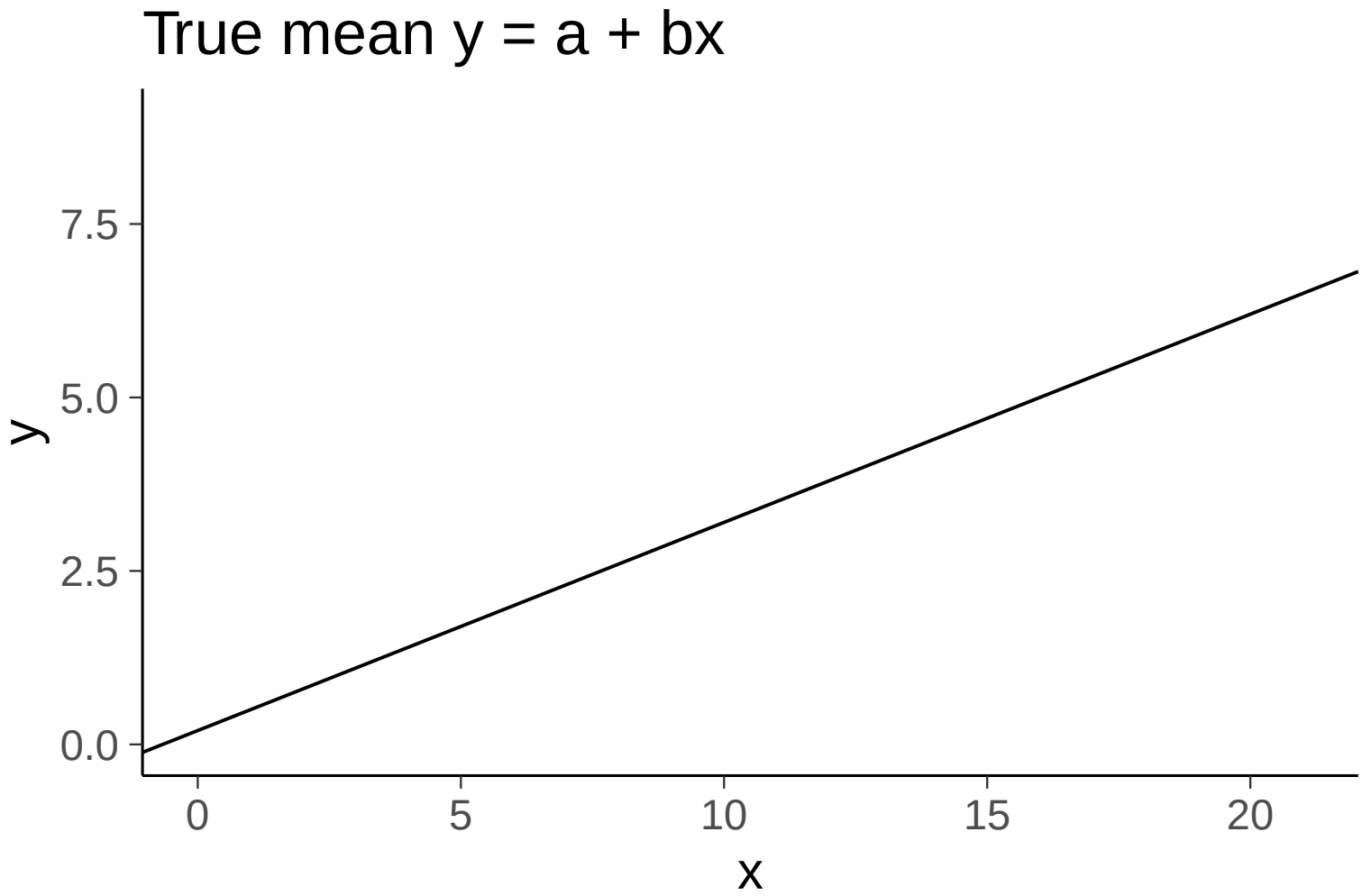
$$\log p(y^{\text{rep}}|y, M),$$

Outline

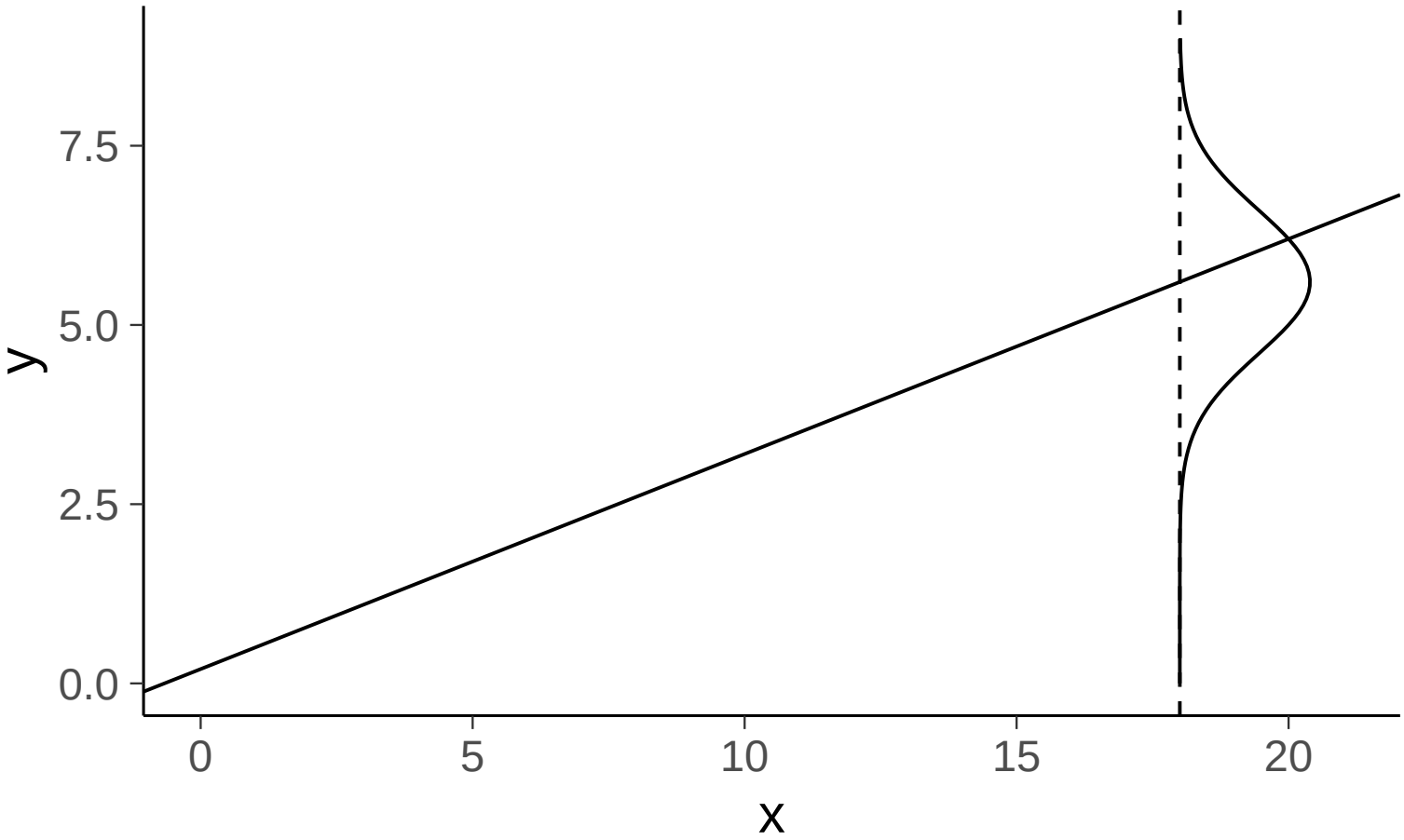
- What is cross-validation
  - Leave-one-out cross-validation (elpd_loo, p_loo)
  - Uncertainty in LOO (SE)
- When is cross-validation applicable?
  - data generating mechanisms and prediction tasks
  - leave-many-out cross-validation
- Fast cross-validation
  - PSIS and diagnostics in loo package (Pareto k, n_eff, Monte Carlo SE)
  - K-fold cross-validation
- Related methods (WAIC, *IC, BF)
- Model comparison and selection (elpd_diff, se)
- Model averaging with Bayesian stacking

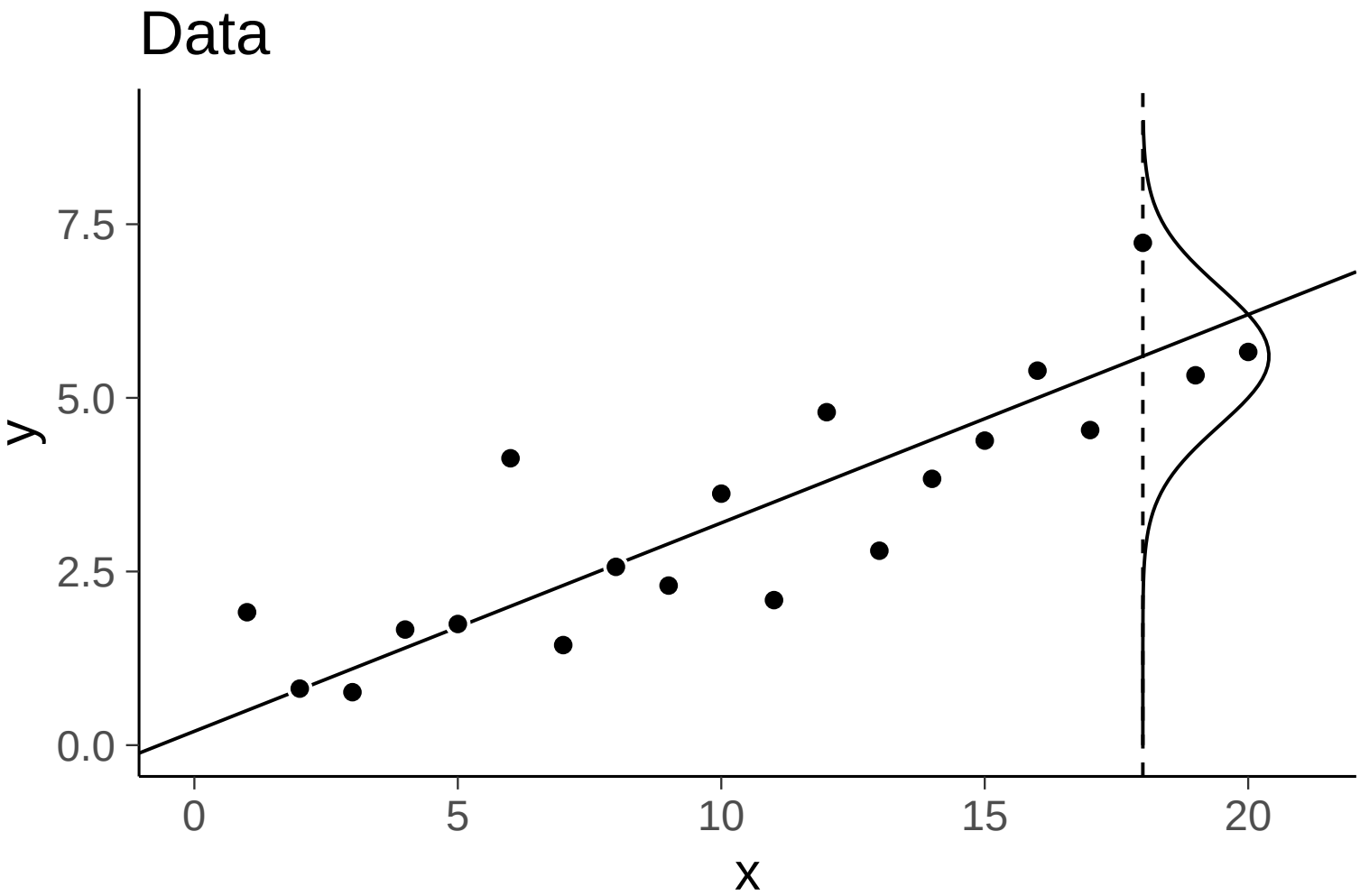
Stan and `loo` package

```
 Computed from 4000 by 20 log-likelihood matrix

          Estimate  SE
elpd_loo    -29.5 3.3
p_loo         2.7 1.0
------

Monte Carlo SE of elpd_loo is 0.1.

Pareto k diagnostic values:
                         Count Pct.    Min. n_eff
(-Inf, 0.5]   (good)     18    90.0%   899
 (0.5, 0.7]   (ok)        2    10.0%   459
   (0.7, 1]   (bad)       0     0.0%   <NA>
   (1, Inf)   (very bad)  0     0.0%   <NA>

All Pareto k estimates are ok (k < 0.7).
See help('pareto-k-diagnostic') for details.

Model comparison:
(negative 'elpd_diff' favors 1st model, positive favors 2nd)

elpd_diff        se
     -0.2        0.1
```

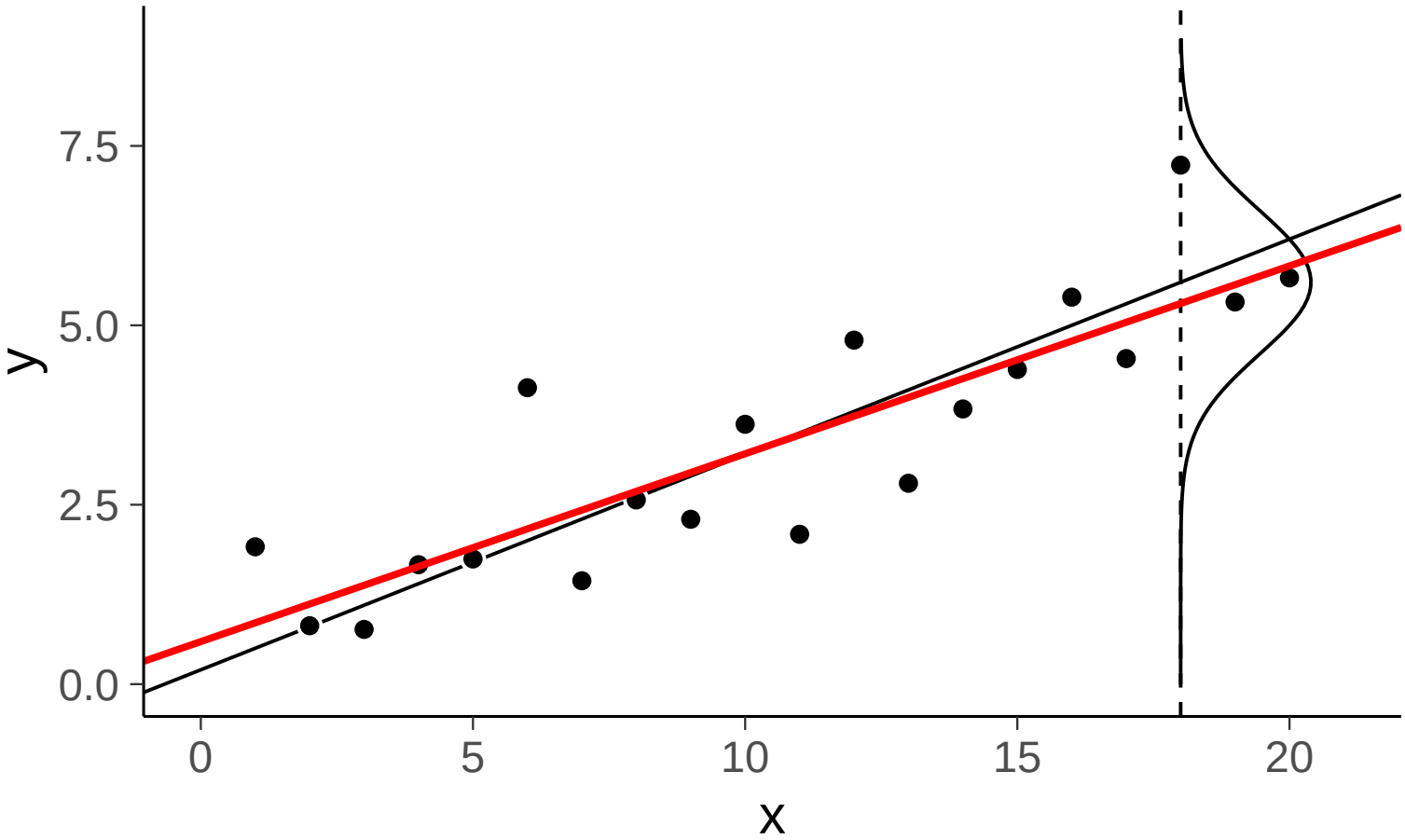

True mean y = a + bx
7.5
5.0
2.5
0.0
y
0
5
10
15
20
x

True mean and sigma

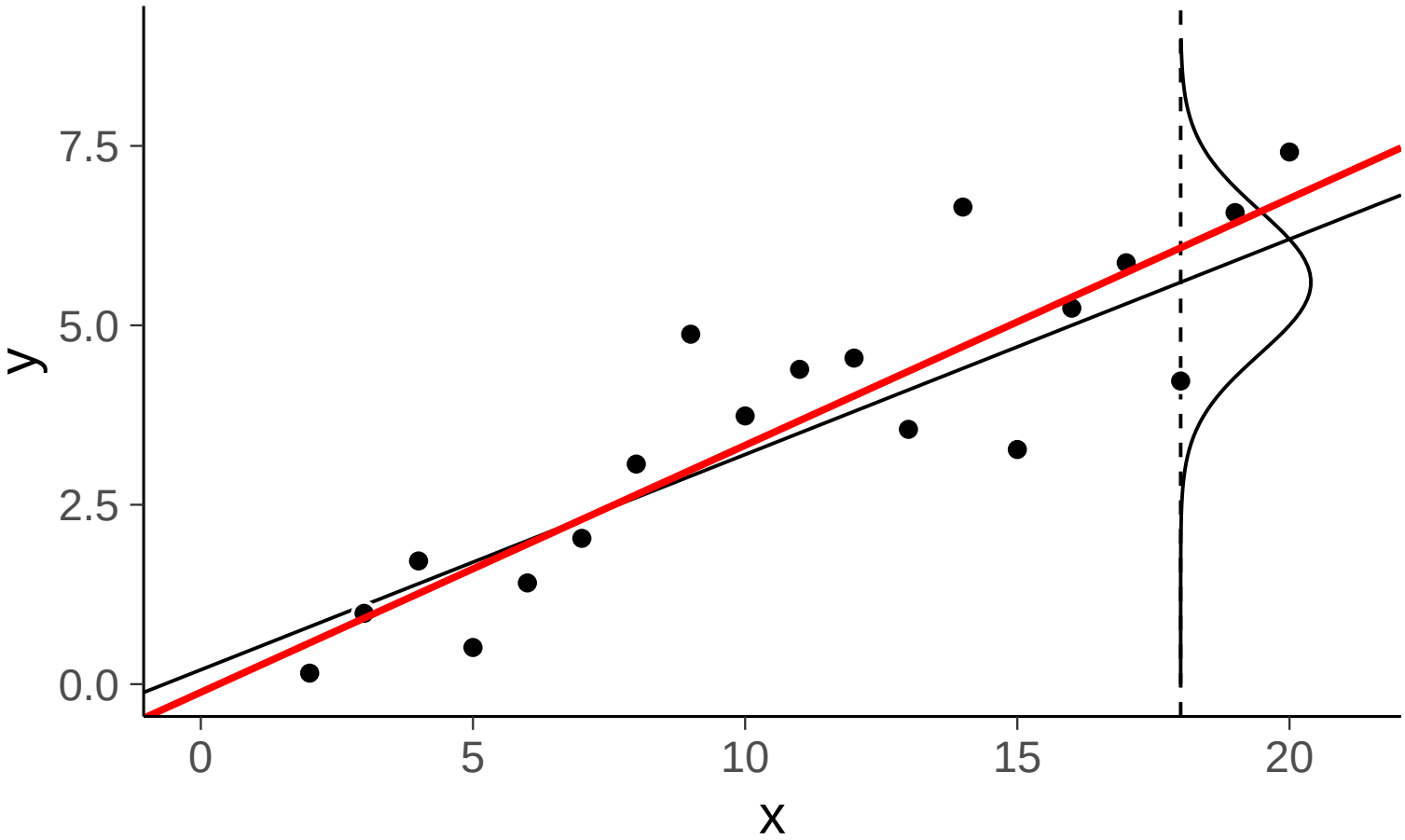



Data
7.5
5.0
2.5
0.0
y
0
5
10
15
20
x

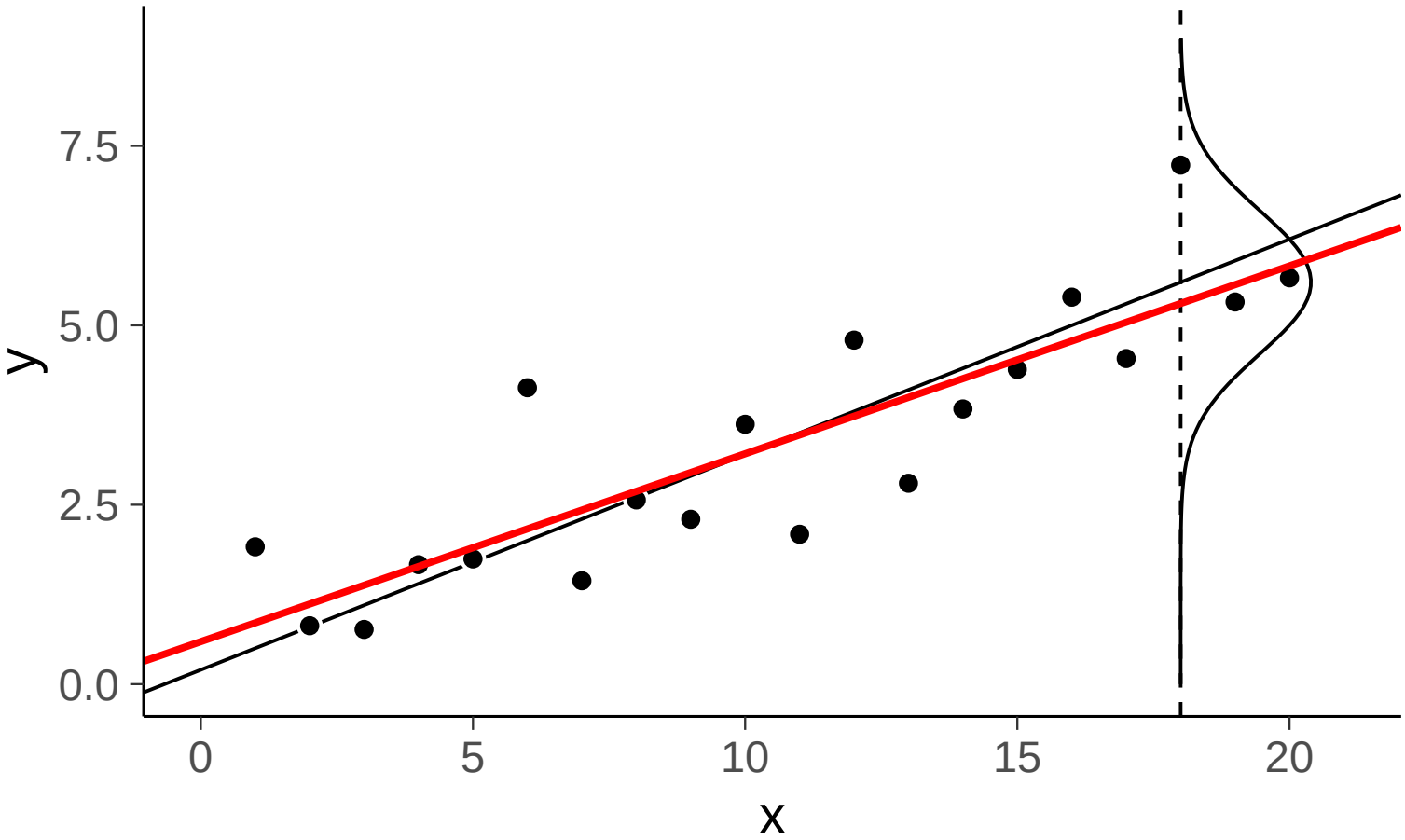
Posterior mean

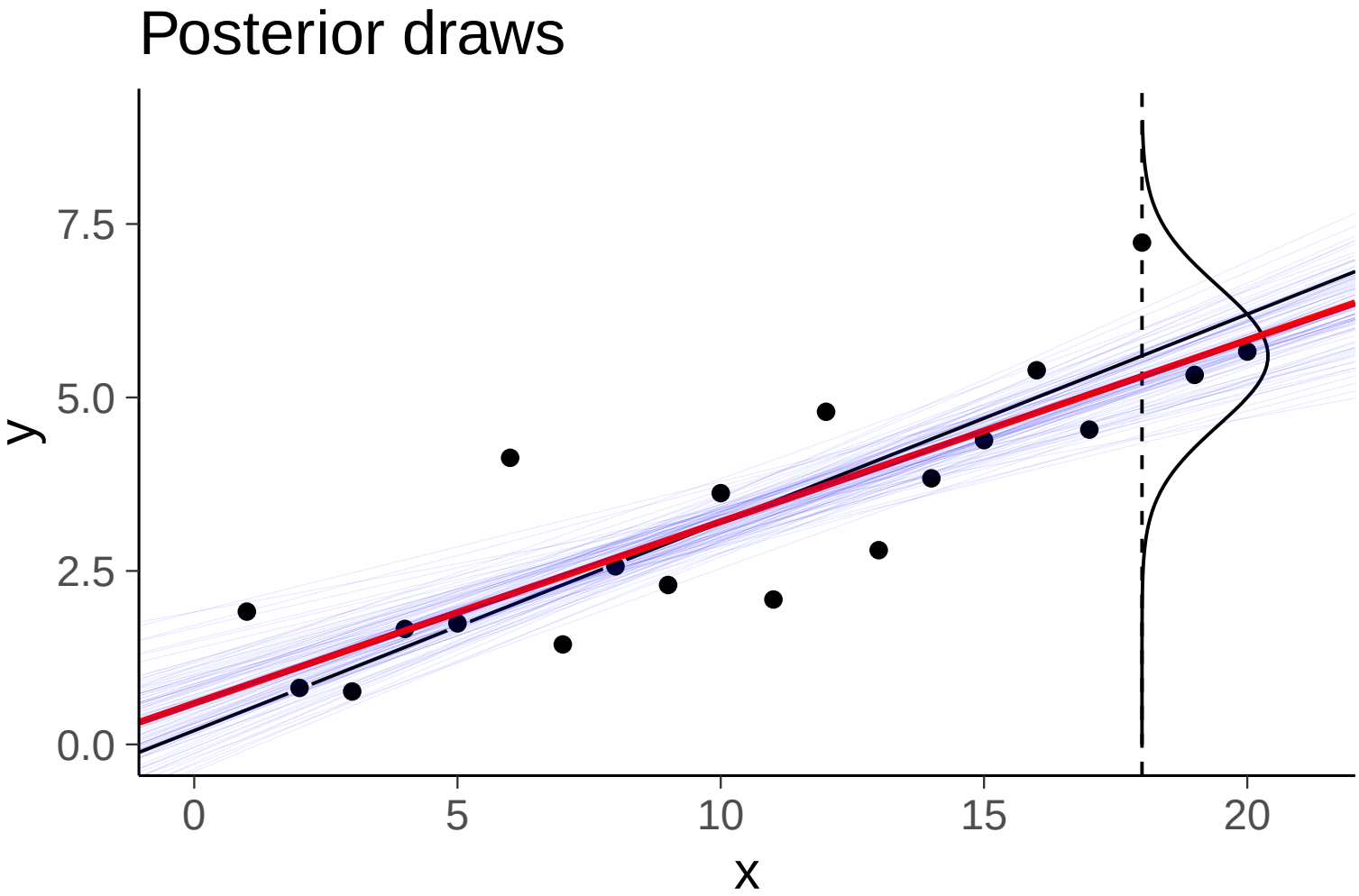


Posterior mean, alternative data realisation

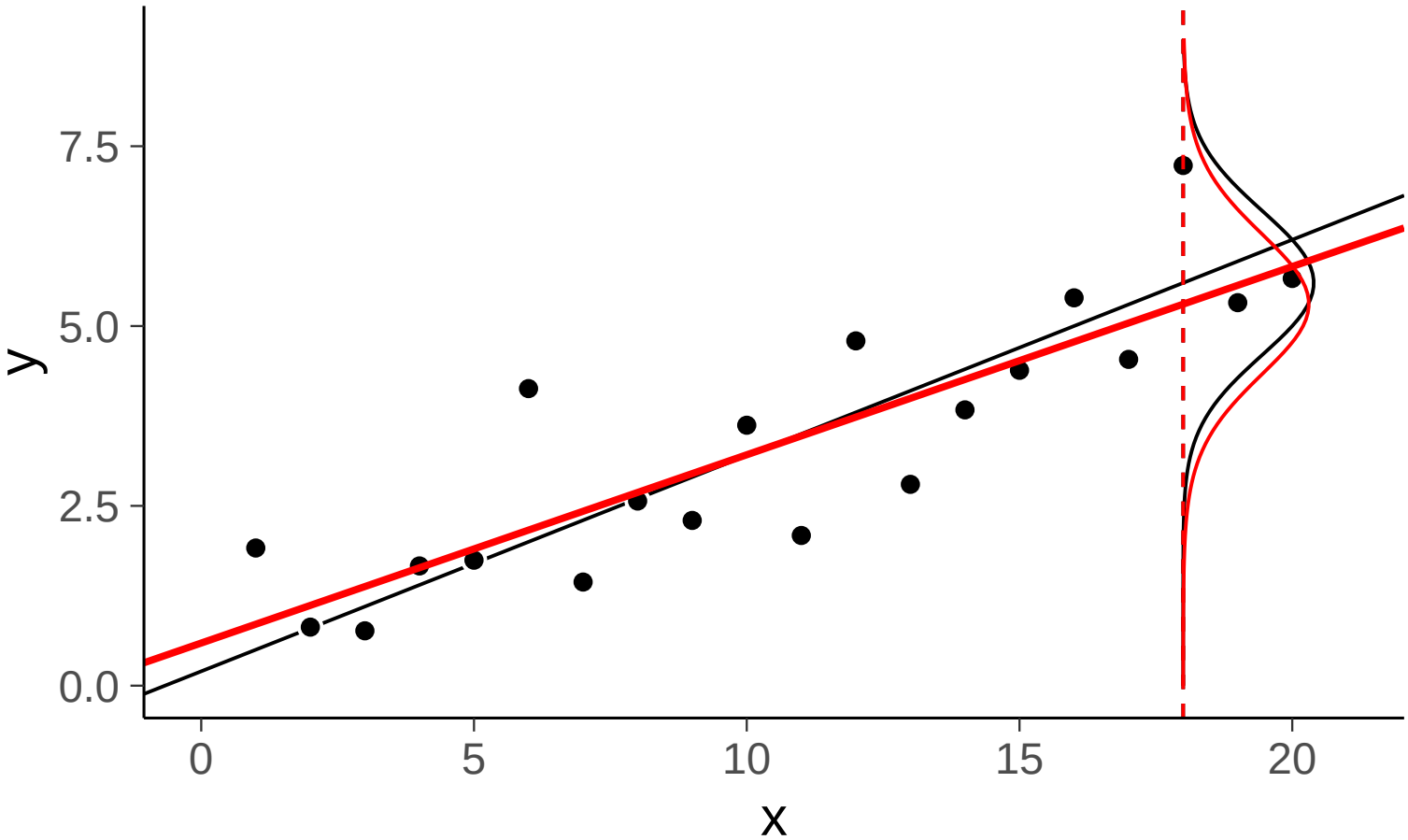


Posterior mean

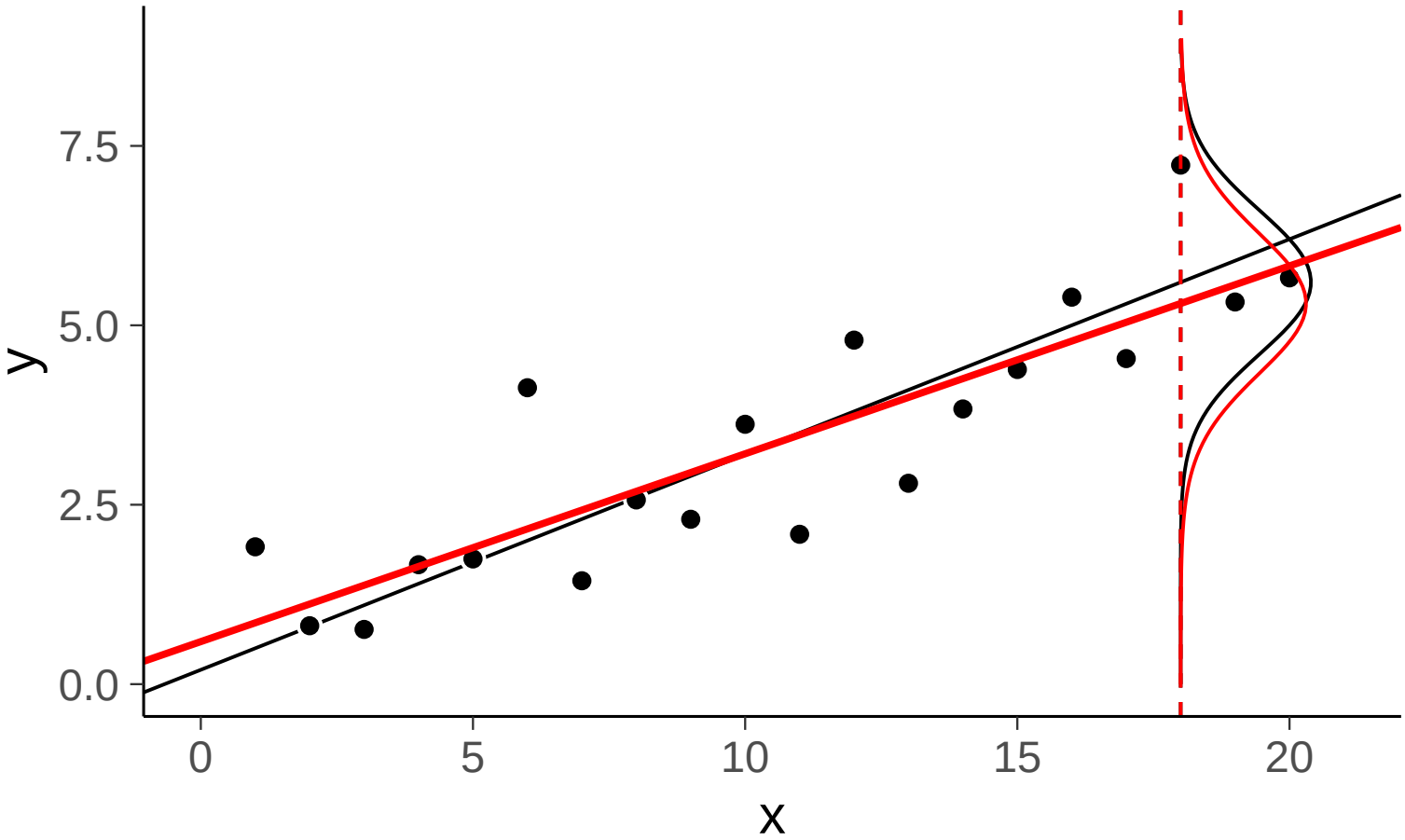



Posterior draws
7.5
5.0
2.5
0.0
y
0
5
10
15
20
x

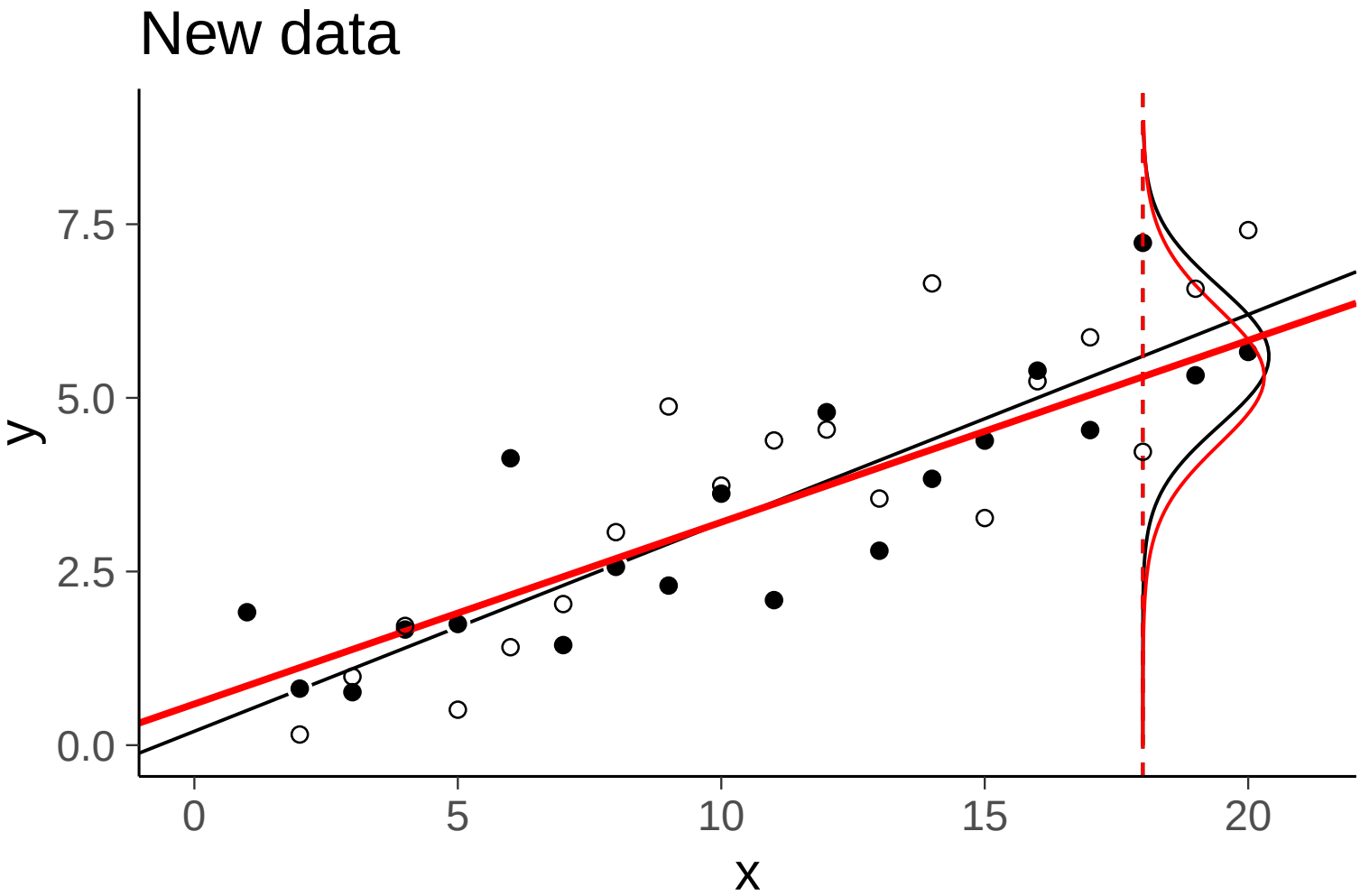
Posterior predictive distribution



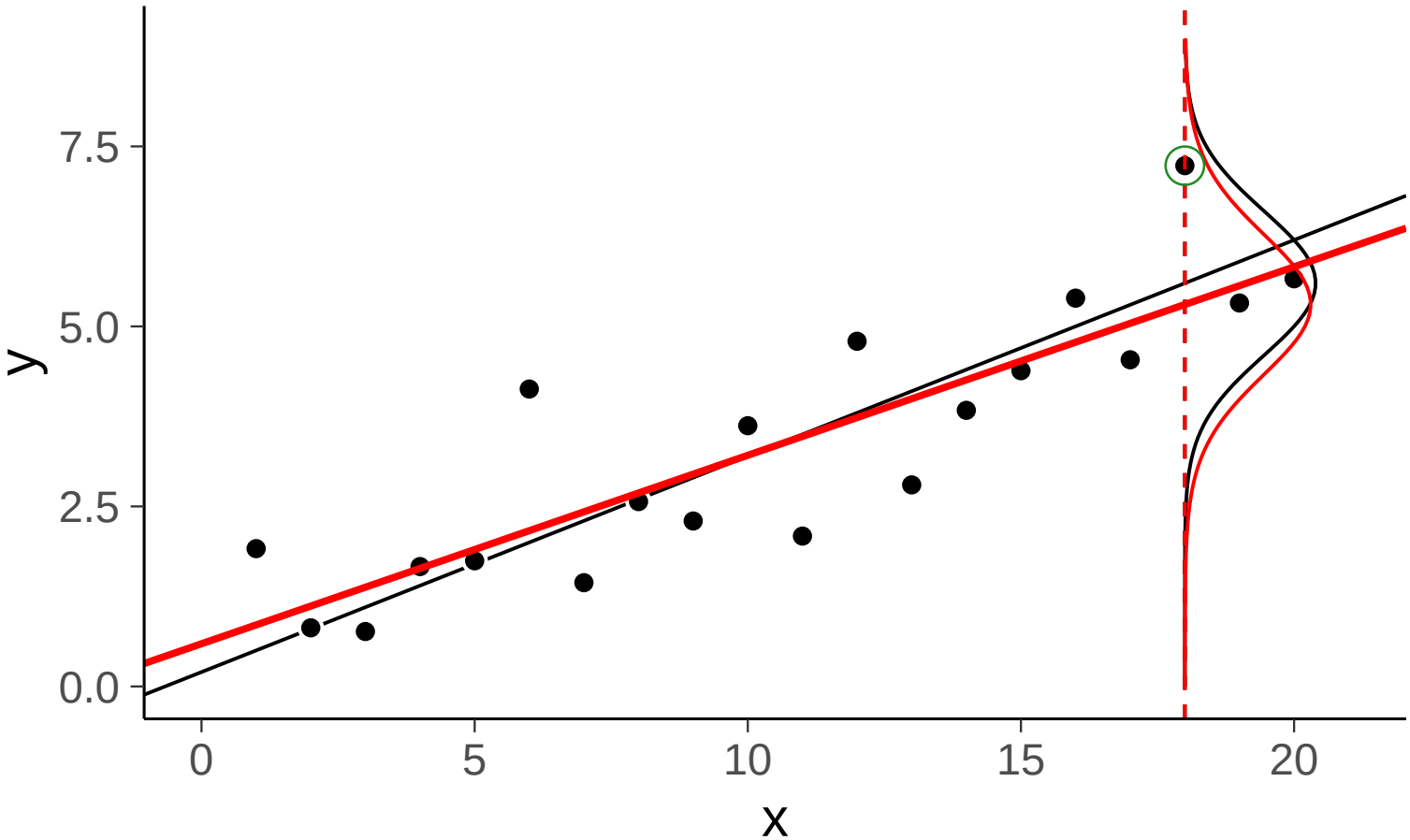
Posterior predictive distribution



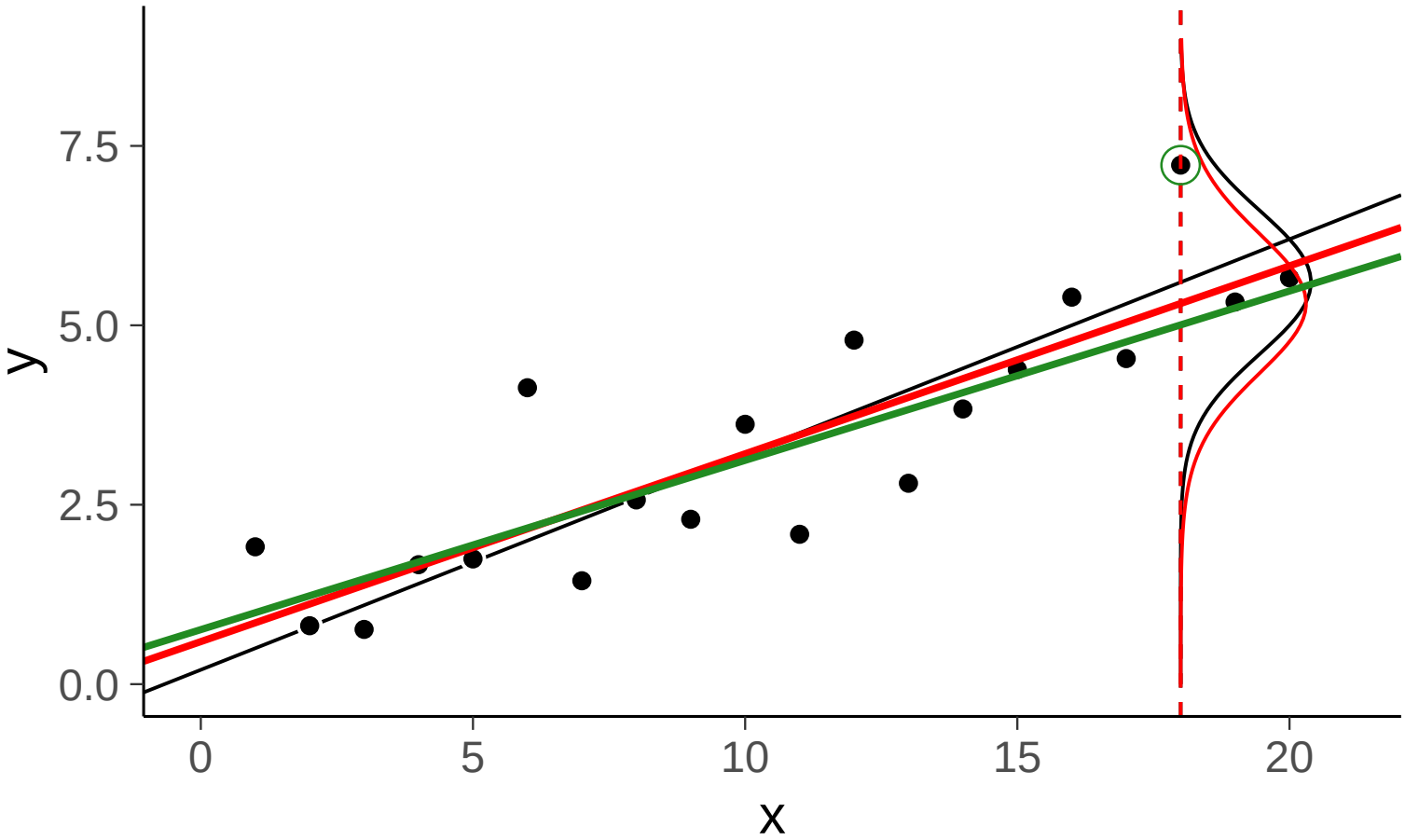
$$p(\tilde{y}|\tilde{x} = 18, x, y) = \int p(\tilde{y}|\tilde{x} = 18, \theta)p(\theta|x, y)d\theta$$


New data
7.5
5.0
2.5
0.0
y
0
5
10
15
20
x

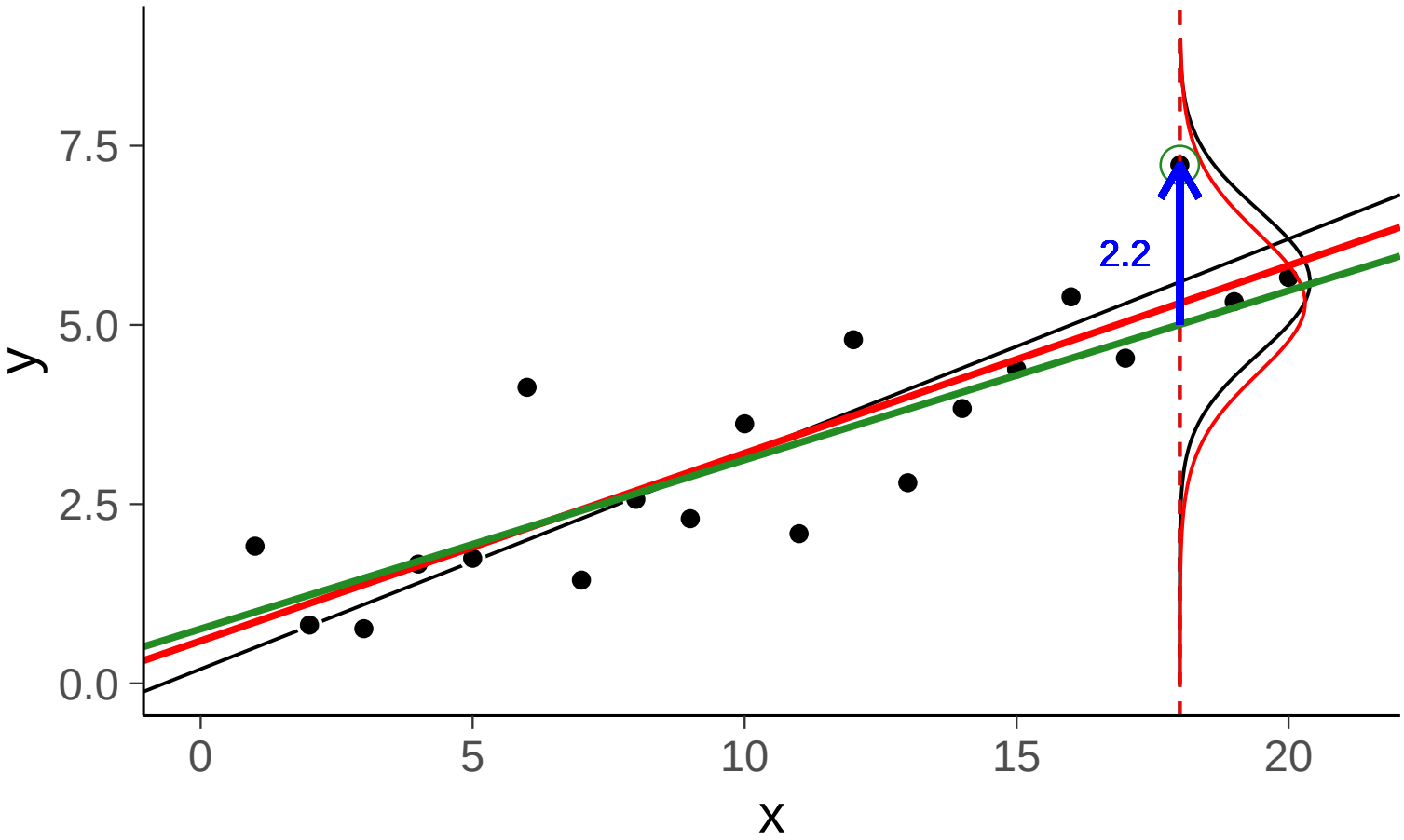
Posterior predictive distribution



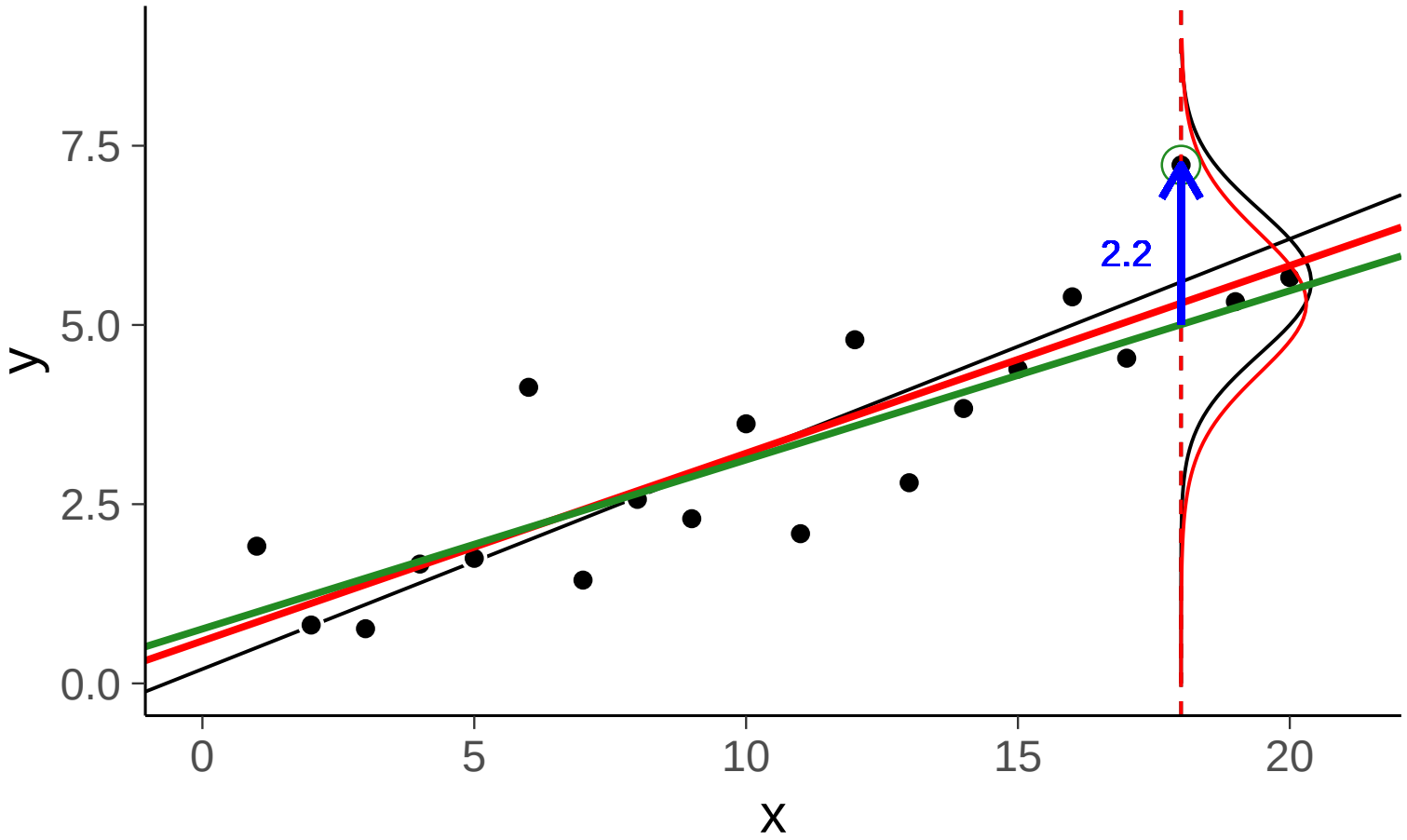
Leave−one−out mean



Leave−one−out residual

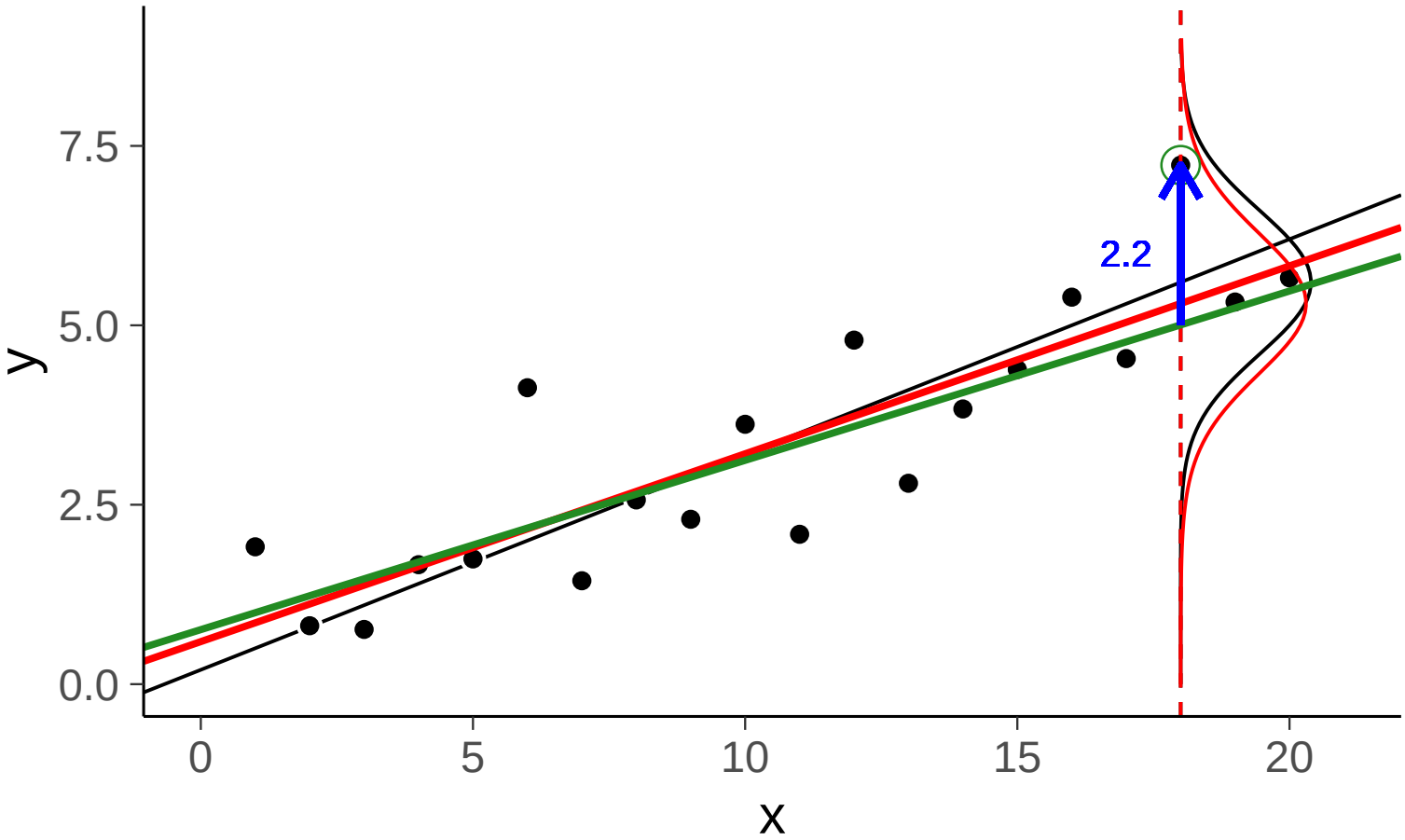


Leave−one−out residual



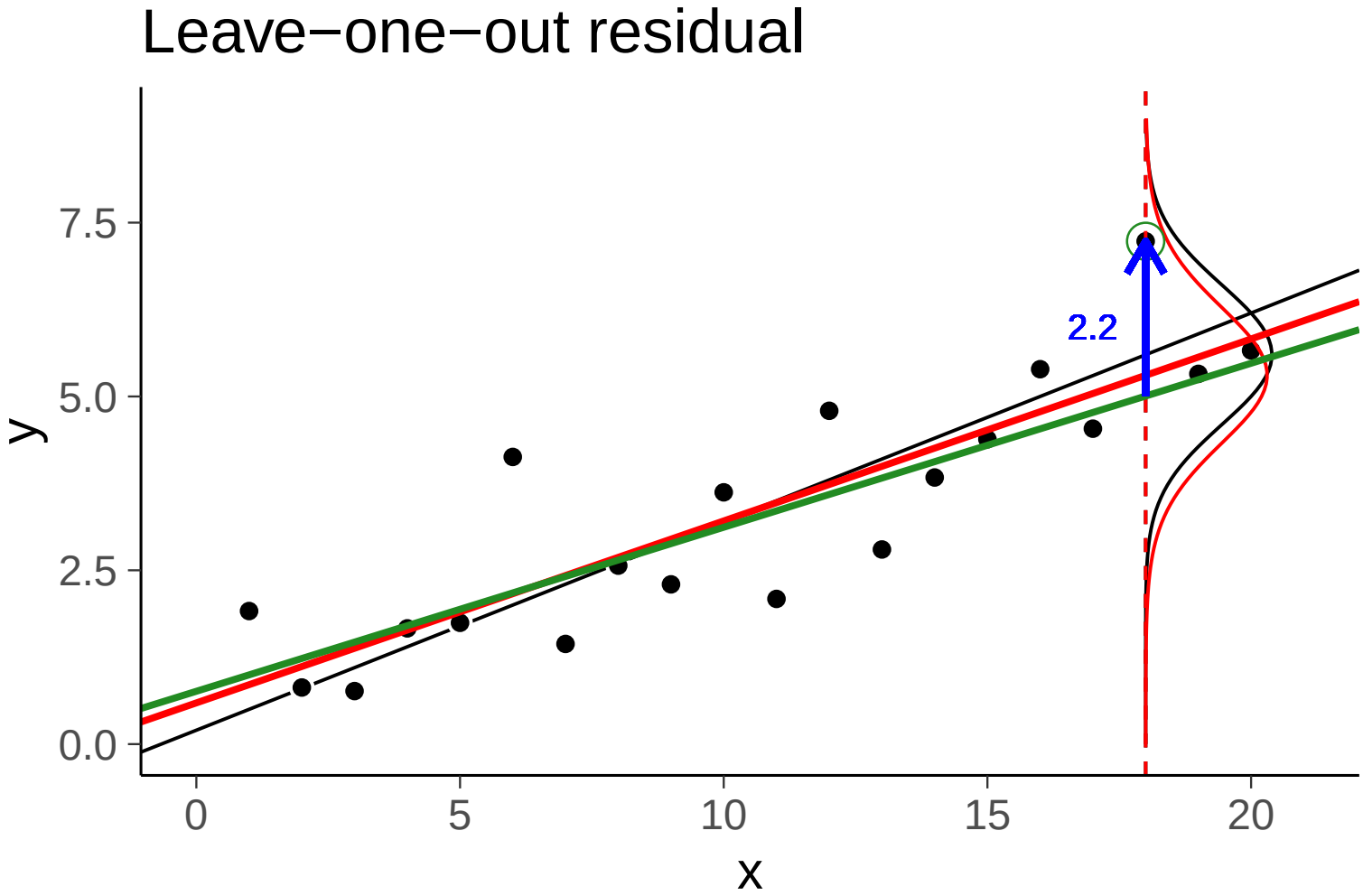
$y_{18} - E[p(\tilde{y}|\tilde{x} = 18, x_{-18}, y_{-18})]$

Leave−one−out residual



$y_{18} - E[p(\tilde{y}|\tilde{x} = 18, x_{-18}, y_{-18})]$

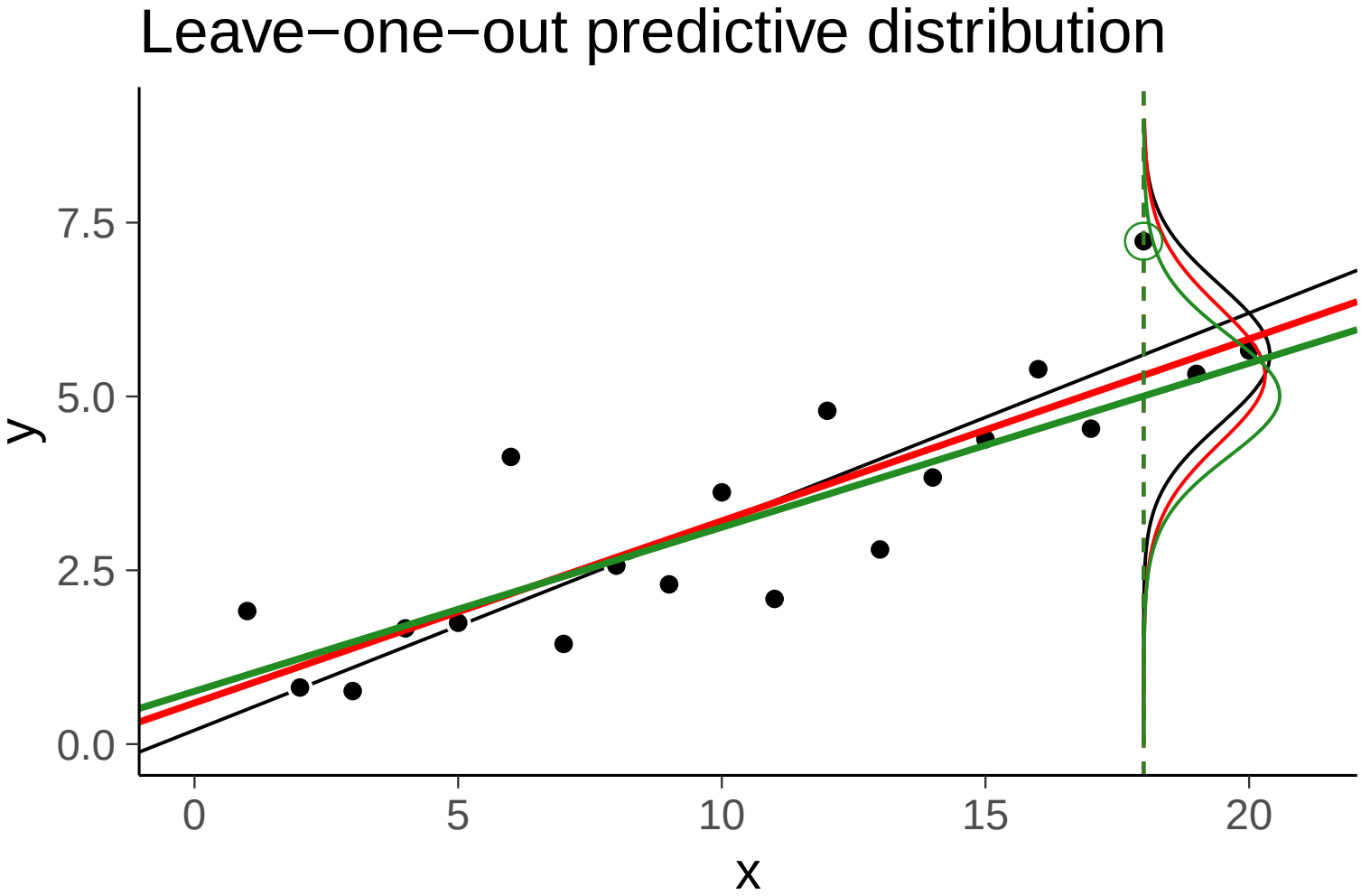
Can be use to compute, e.g., RMSE, R^2, 90% error



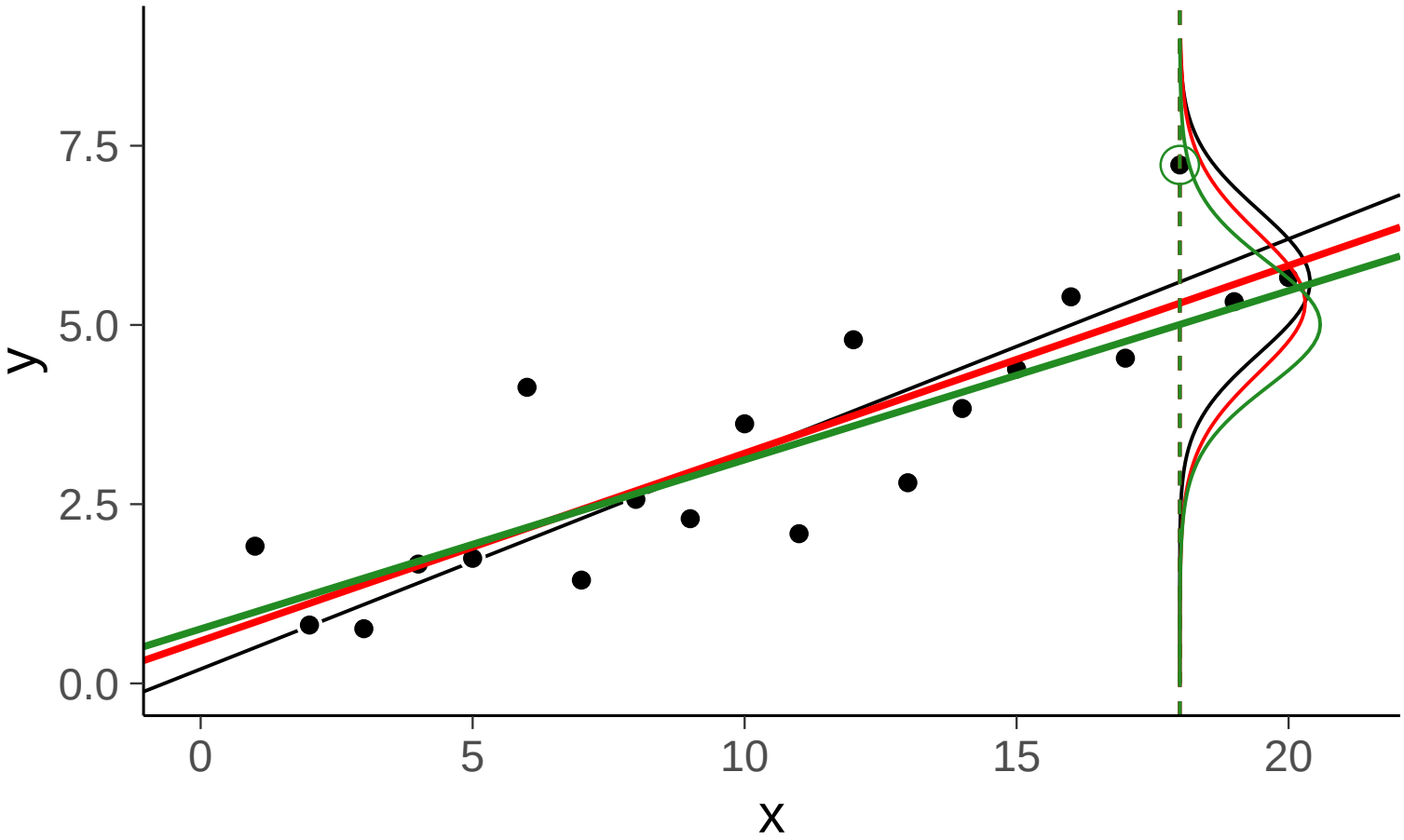
$y_{18} - E[p(\tilde{y}|\tilde{x} = 18, x_{-18}, y_{-18})]$

Can be use to compute, e.g., RMSE, R^2, 90% error

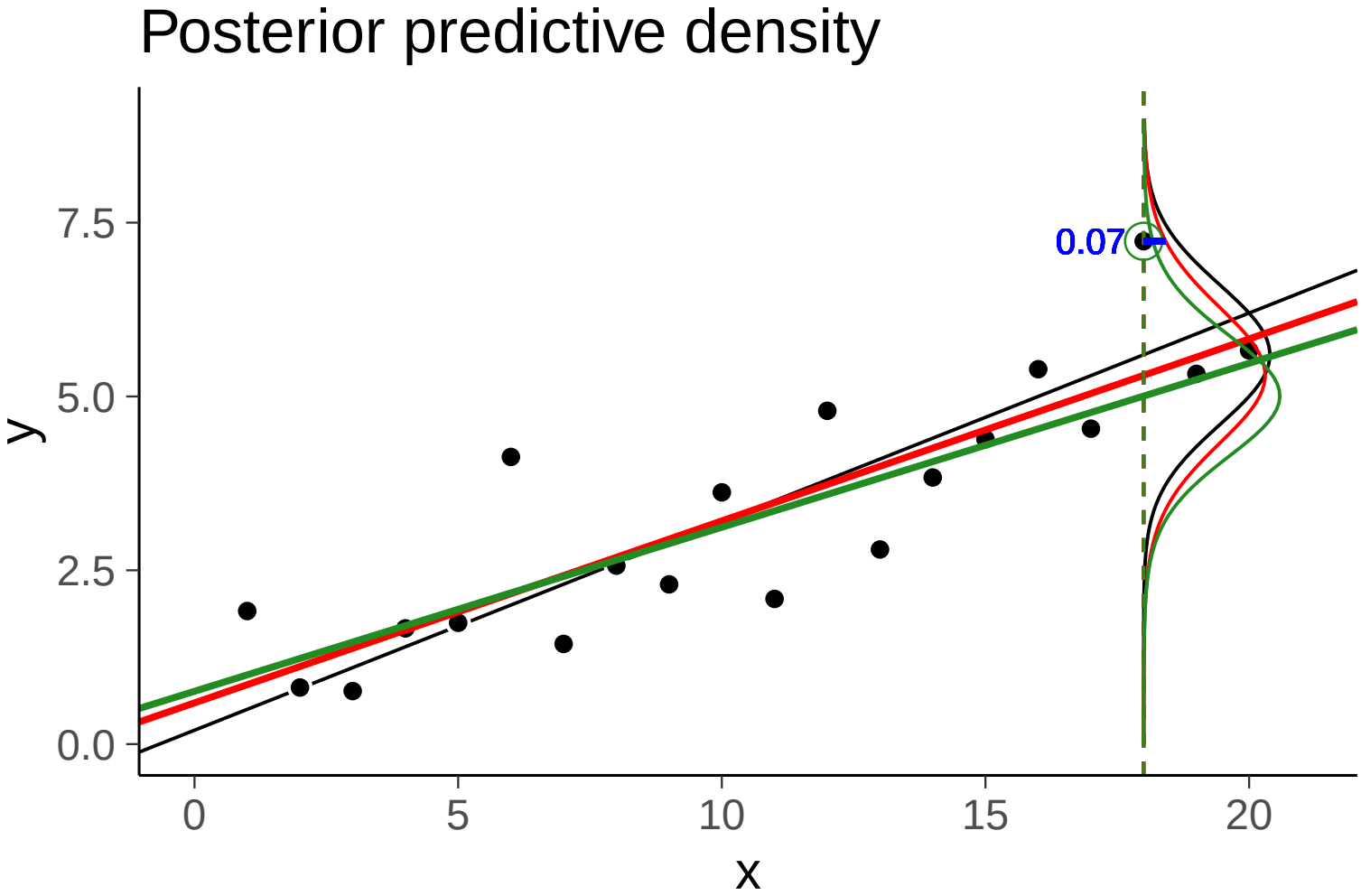
See LOO-R^2 at avehtari.github.io/bayes_R2/bayes_R2.html


Leave−one−out predictive distribution
7.5
5.0
2.5
0.0
y
0
5
10
15
20
x

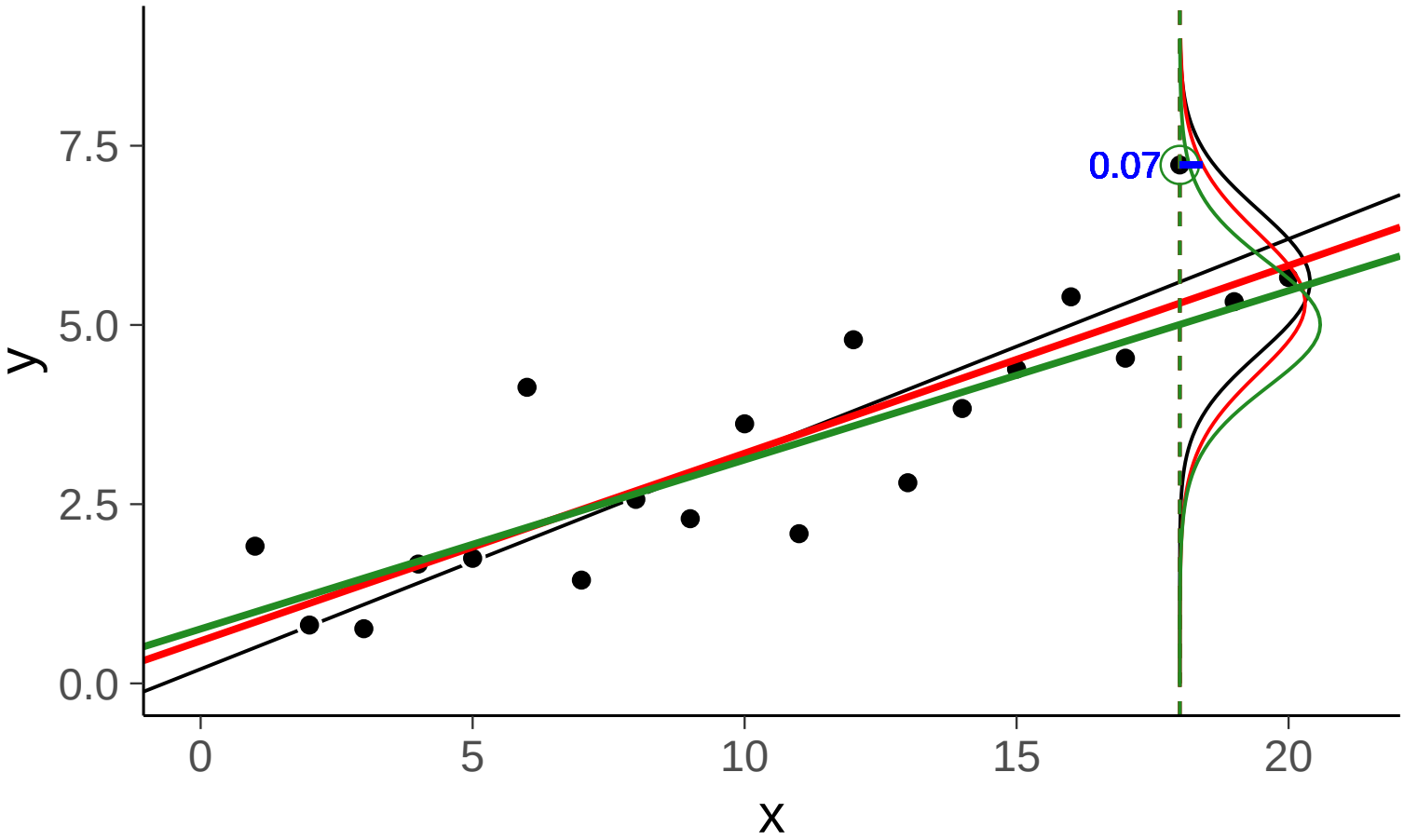
Leave−one−out predictive distribution



$$p(\tilde{y}|\tilde{x} = 18, x_{-18}, y_{-18}) = \int p(\tilde{y}|\tilde{x} = 18, \theta) p(\theta|x_{-18}, y_{-18}) d\theta$$

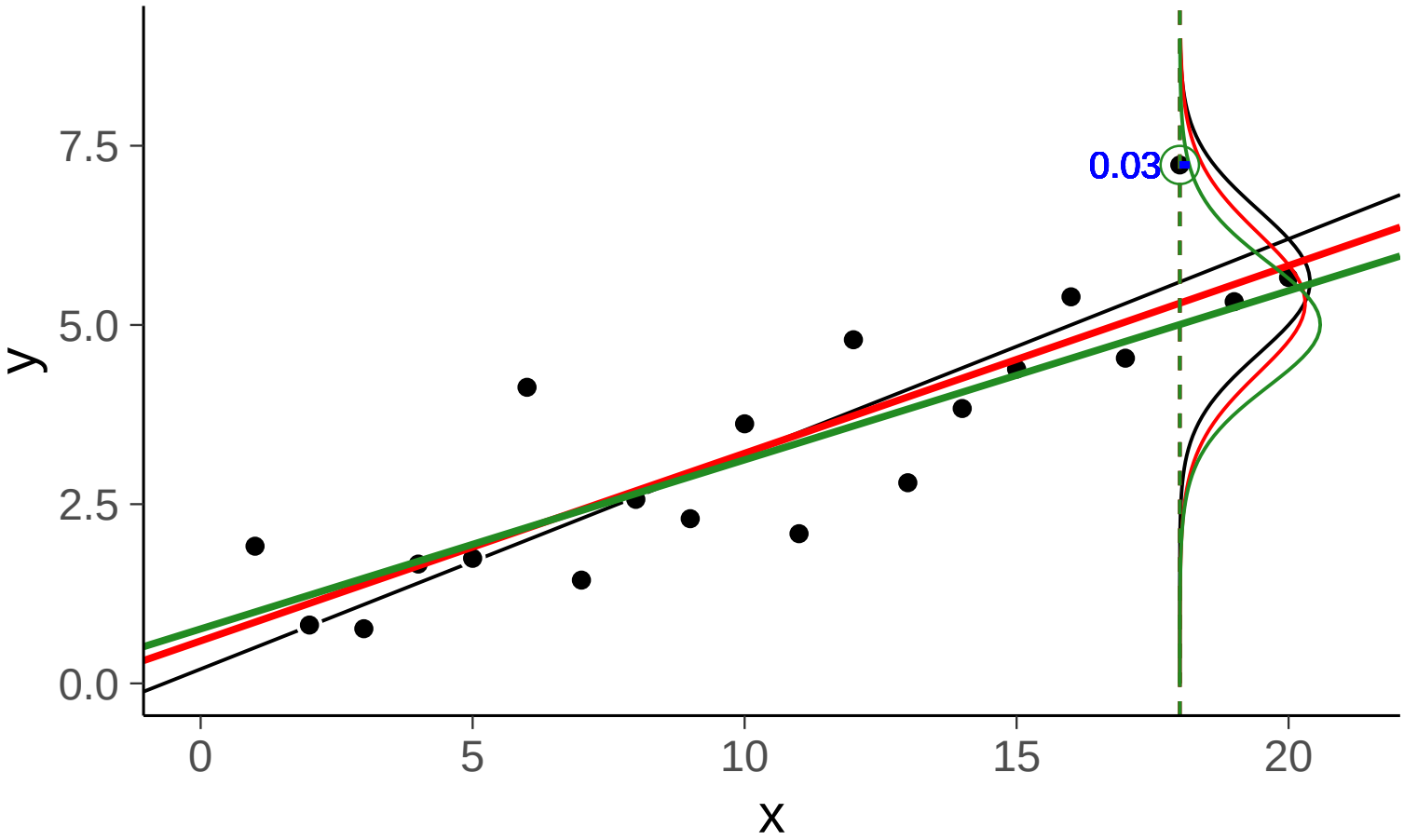

Posterior predictive density
7.5
5.0
2.5
0.0
y
0
5
10
15
20
x
0.07

Posterior predictive density



$p(\tilde{y} = y_{18} | \tilde{x} = 18, x, y) \approx 0.07$

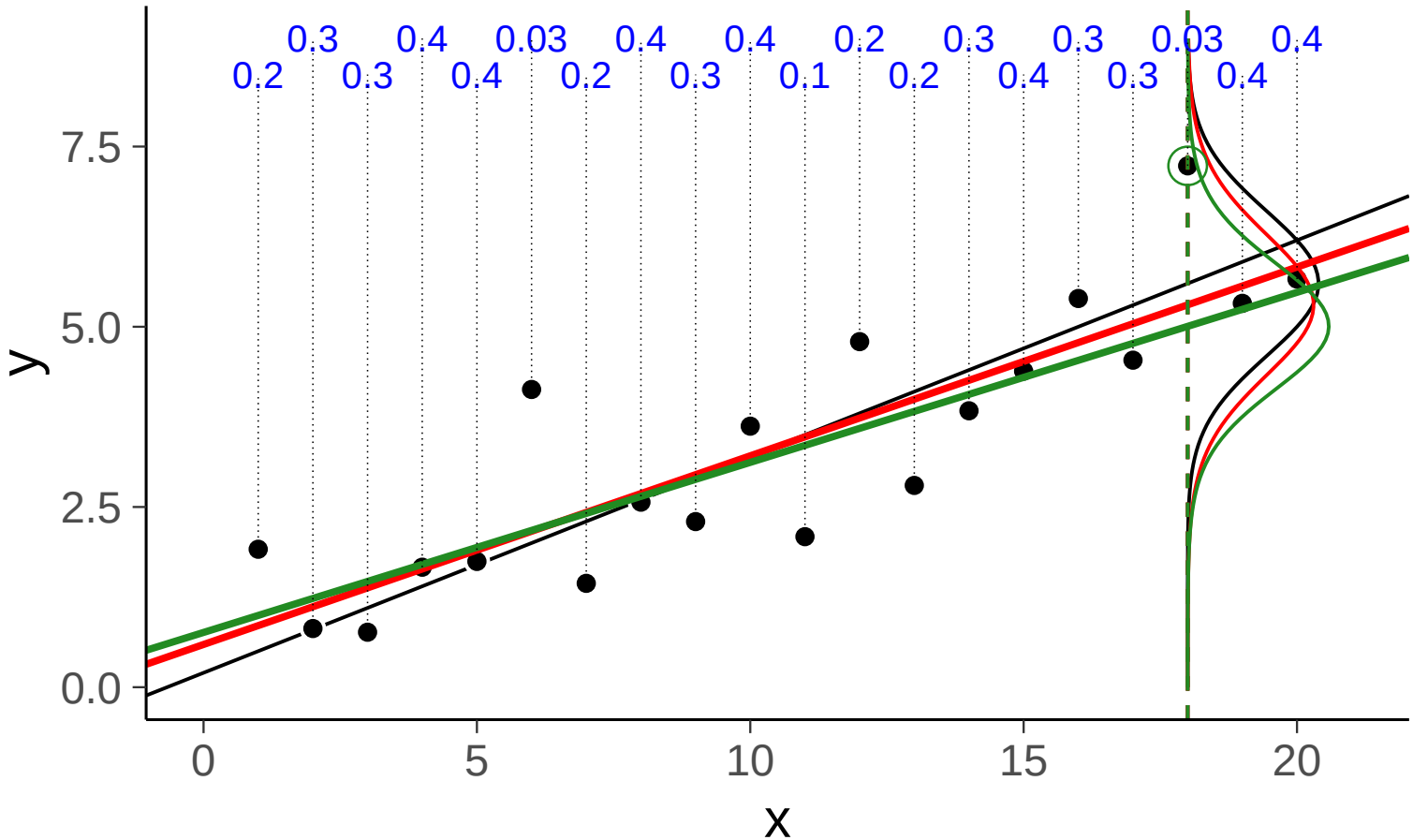
Leave−one−out predictive density



$p(\tilde{y} = y_{18} | \tilde{x} = 18, x, y) \approx 0.07$

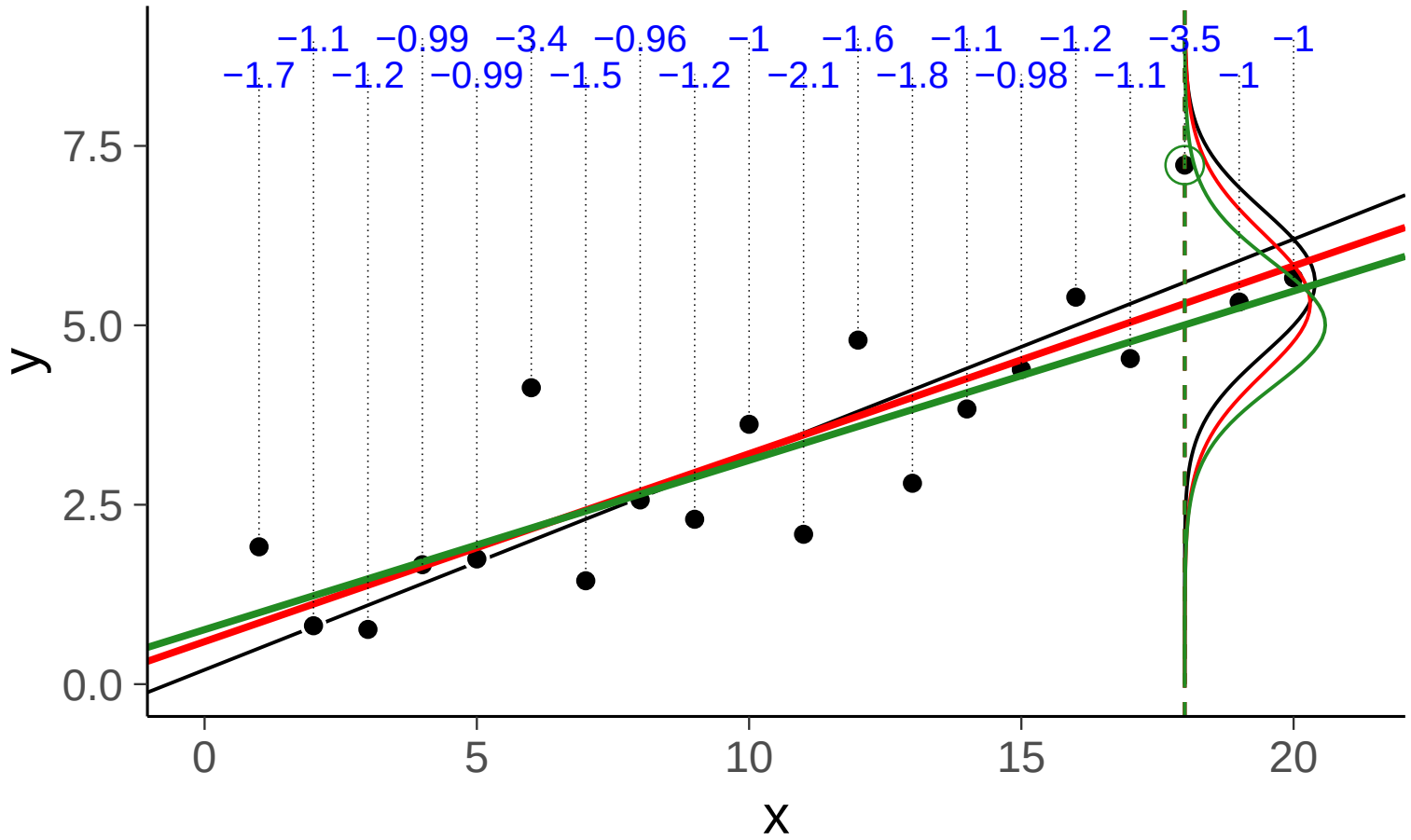
$p(\tilde{y} = y_{18} | \tilde{x} = 18, x_{-18}, y_{-18}) \approx 0.03$

Leave−one−out predictive densities



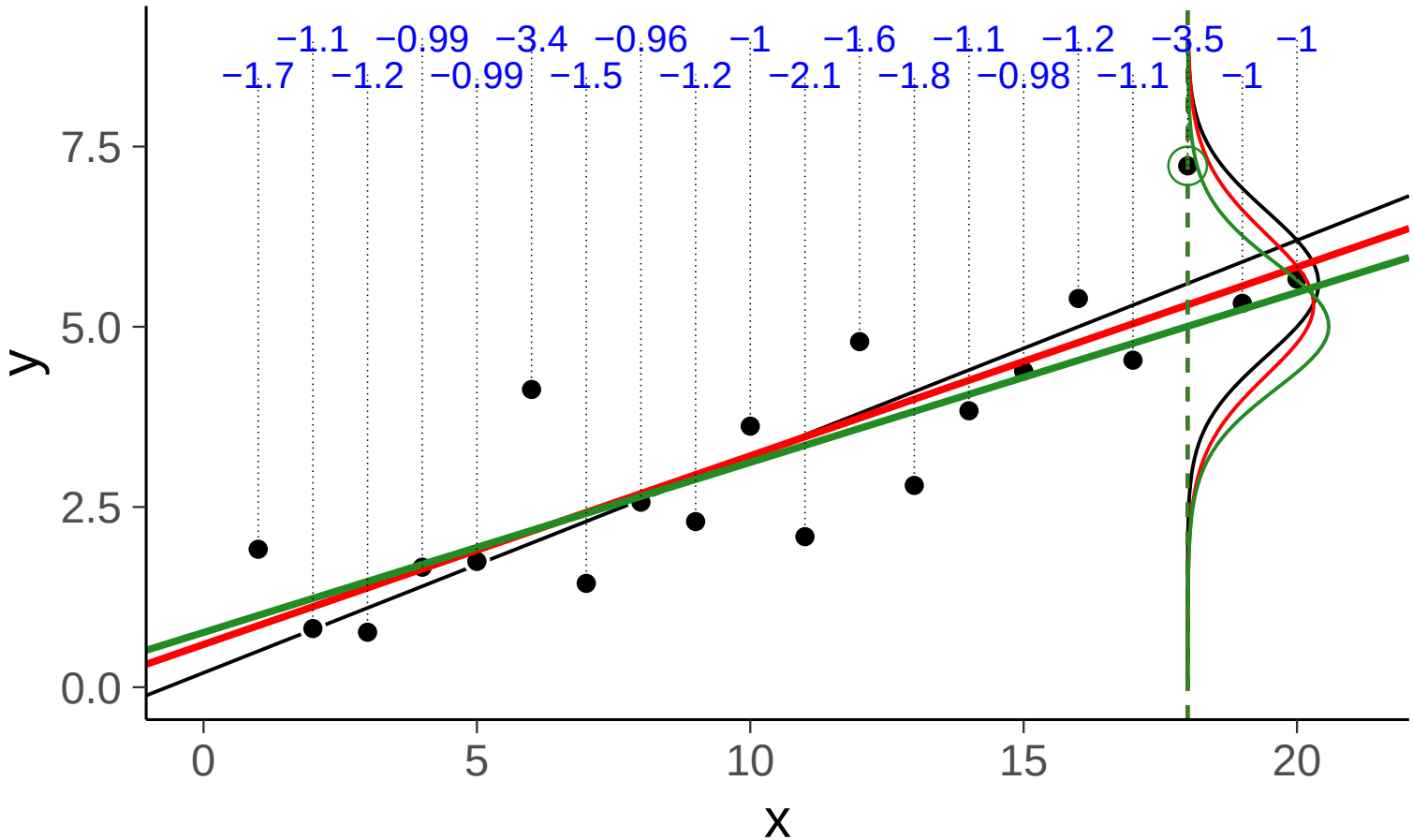
$p(y_i|x_i, x_{-i}, y_{-i}), \quad i = 1, \ldots, 20$

Leave−one−out log predictive densities



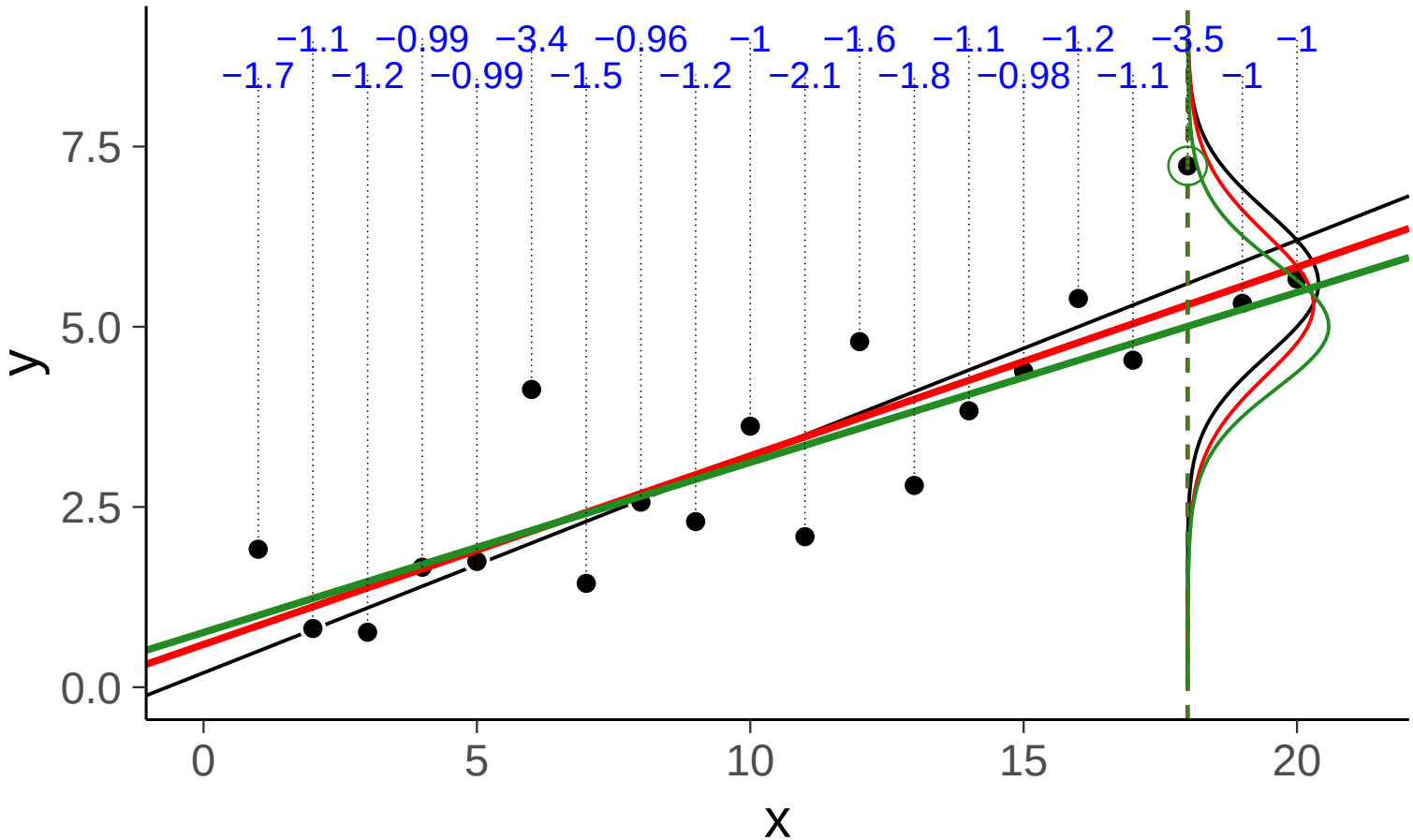
$\log p(y_i|x_i, x_{-i}, y_{-i}), \quad i = 1, \ldots, 20$

Leave−one−out log predictive densities



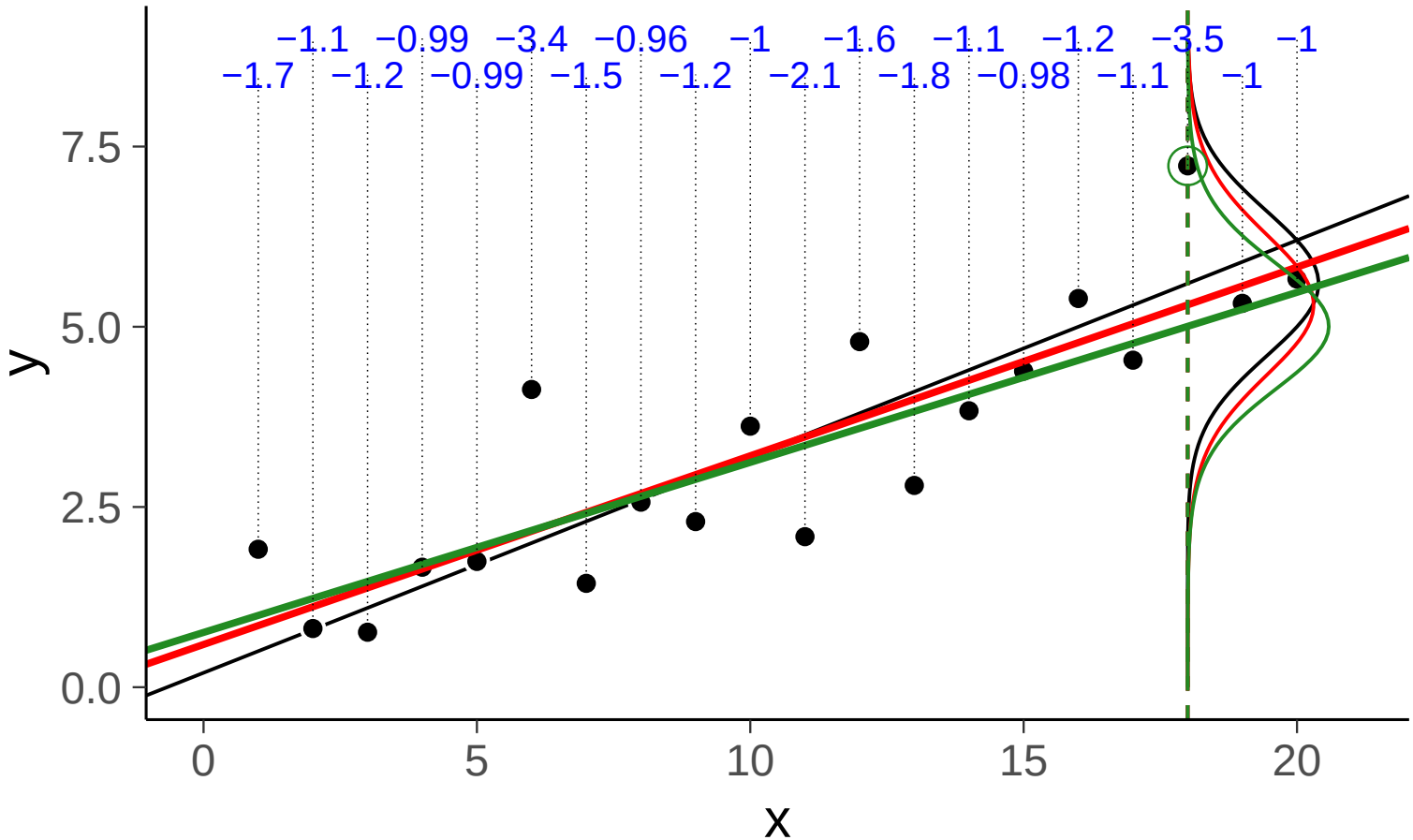
$\sum_{i=1}^{20} \log p(y_i|x_i, x_{-i}, y_{-i}) \approx -29.5$

Leave−one−out log predictive densities



$$\text{elpd\_loo} = \sum_{i=1}^{20} \log p(y_i | x_i, x_{-i}, y_{-i}) \approx -29.5$$

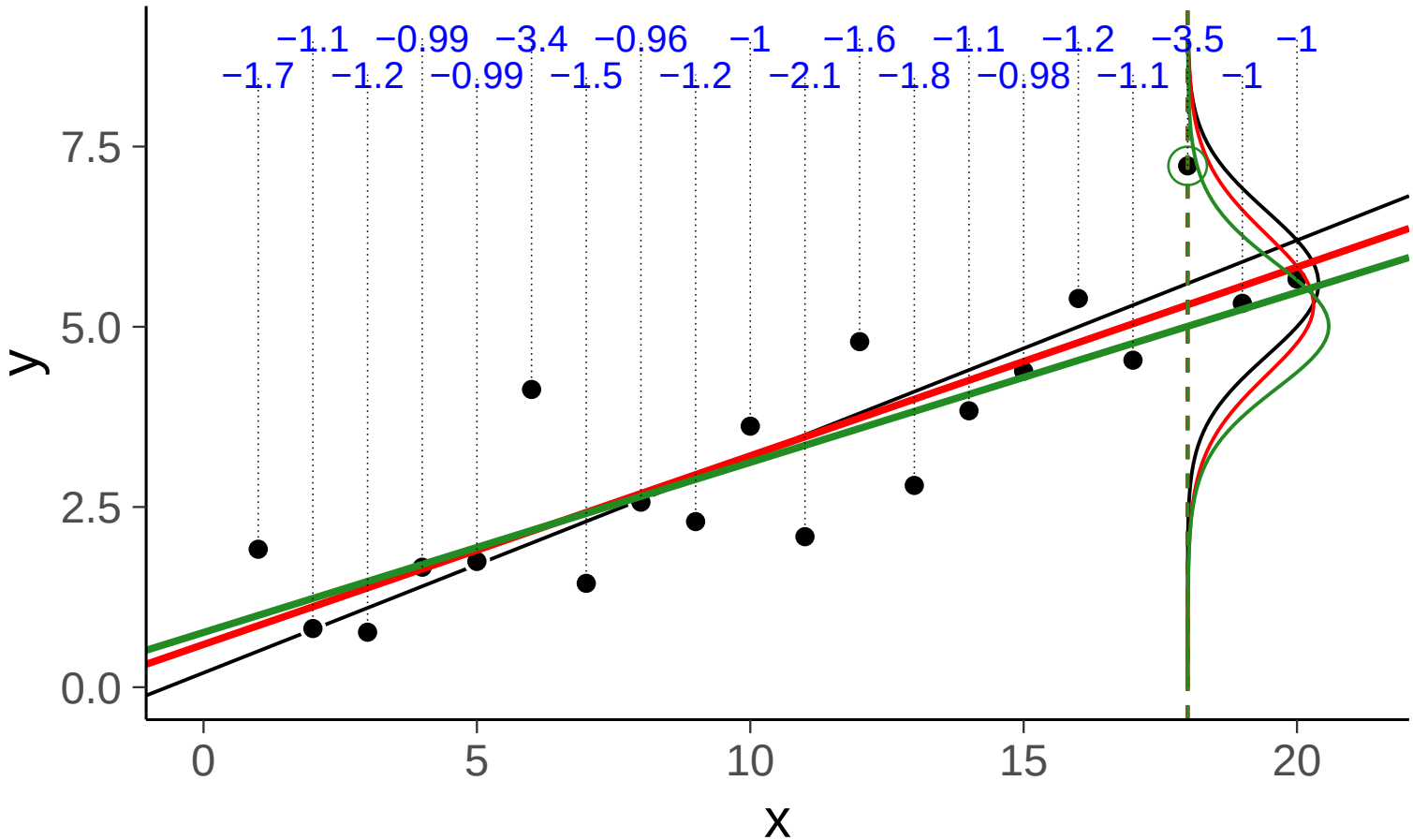
Leave−one−out log predictive densities



$\text{elpd\_loo} = \sum_{i=1}^{20} \log p(y_i | x_i, x_{-i}, y_{-i}) \approx -29.5$

unbiased estimate of log posterior pred. density for new data

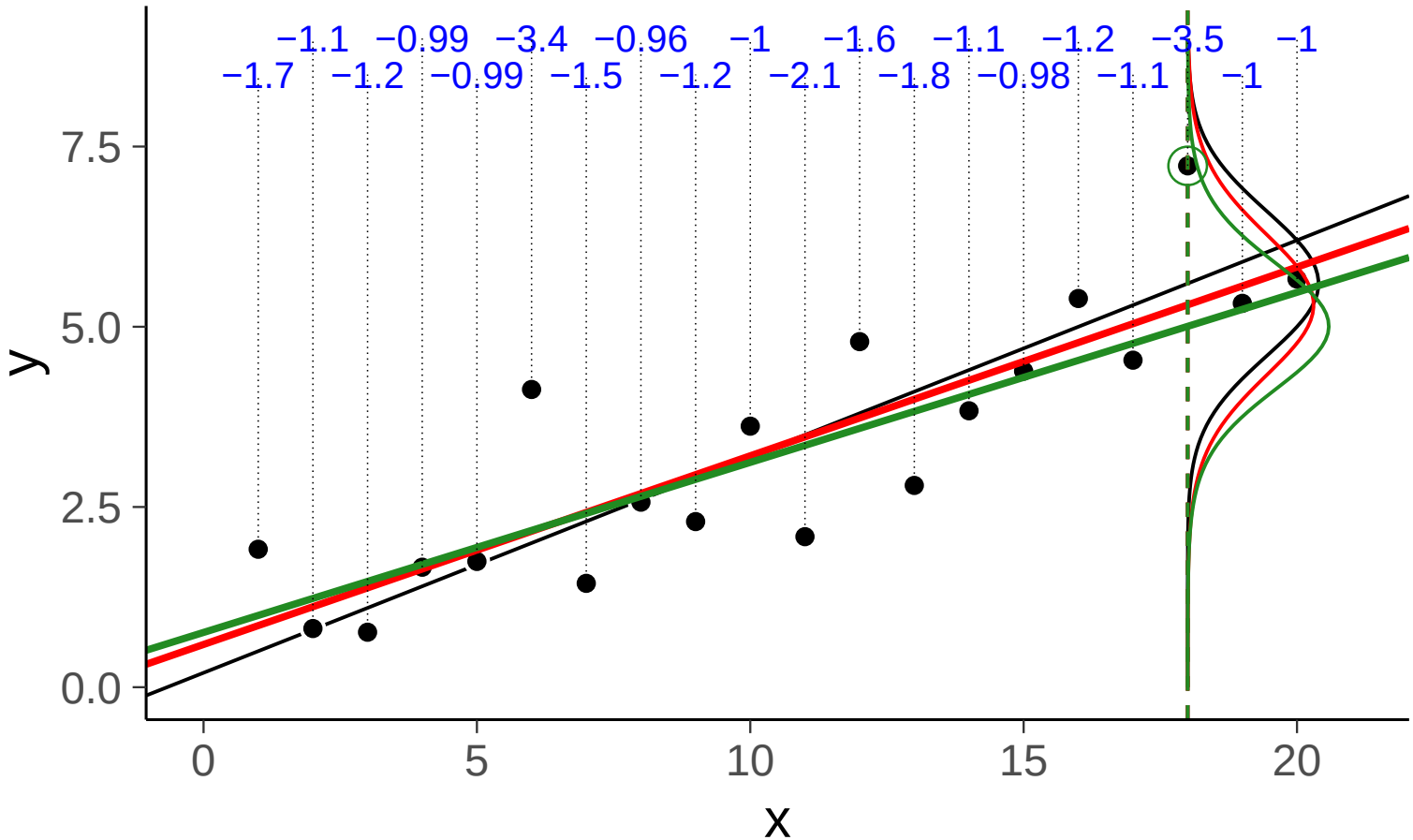
Leave−one−out log predictive densities



$\text{elpd\_loo} = \sum_{i=1}^{20} \log p(y_i|x_i, x_{-i}, y_{-i}) \approx -29.5$

$\text{lpd} = \sum_{i=1}^{20} \log p(y_i|x_i, x, y) \approx -26.8$

Leave−one−out log predictive densities

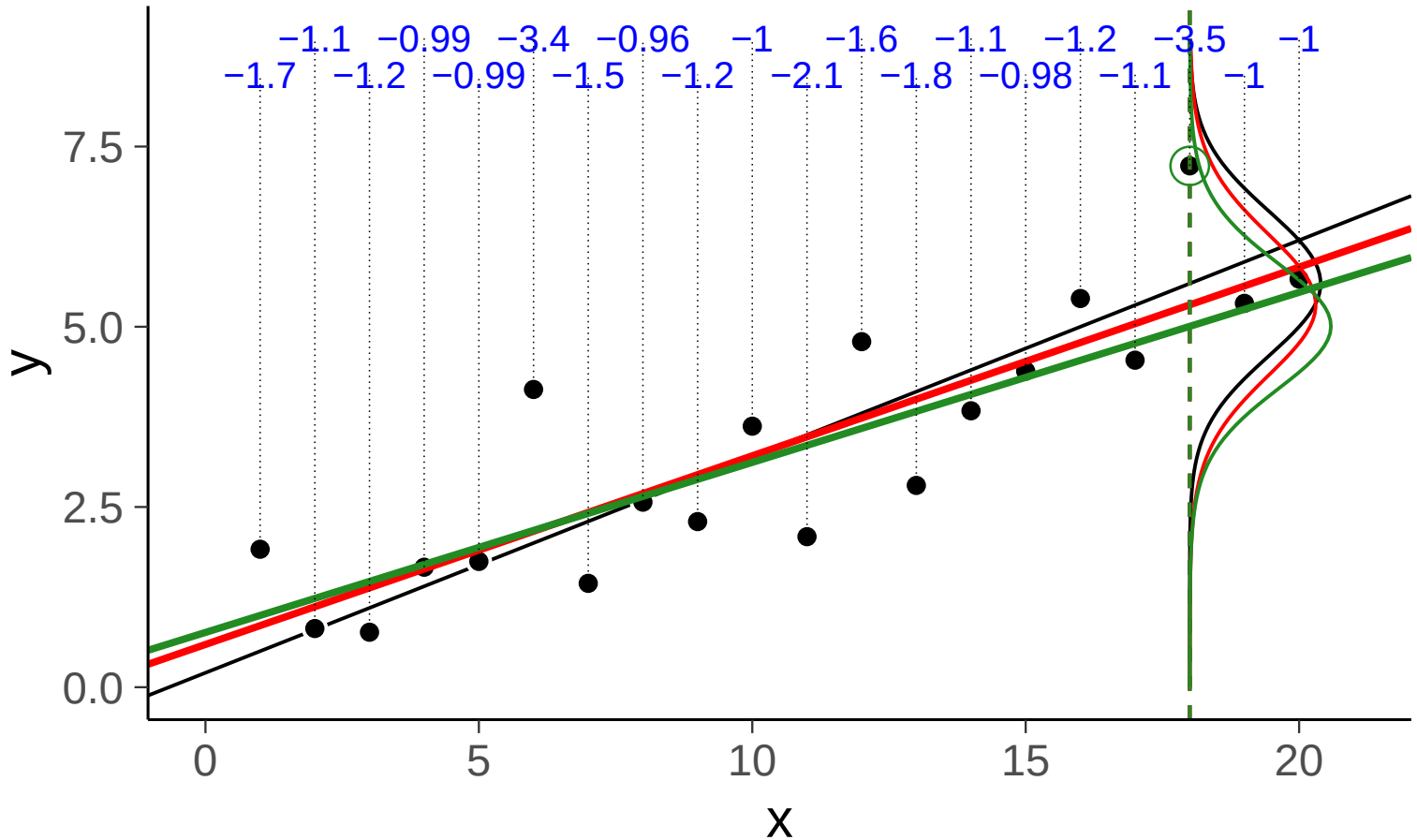


$\text{elpd\_loo} = \sum_{i=1}^{20} \log p(y_i|x_i, x_{-i}, y_{-i}) \approx -29.5$

$\text{lpd} = \sum_{i=1}^{20} \log p(y_i|x_i, x, y) \approx -26.8$

$\text{p\_loo} = \text{lpd} - \text{elpd\_loo} \approx 2.7$

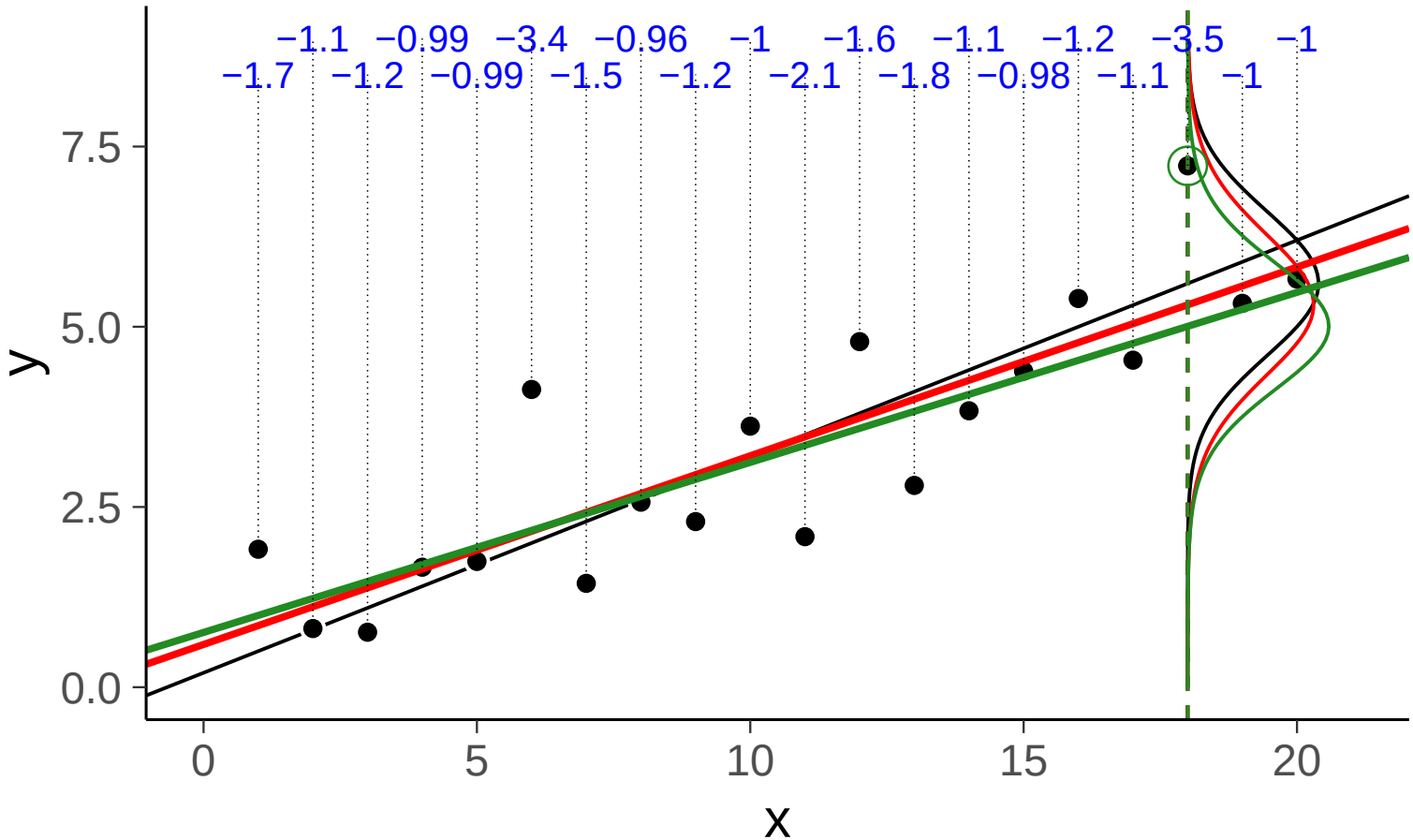
Leave−one−out log predictive densities



$$\text{elpd\_loo} = \sum_{i=1}^{20} \log p(y_i|x_i, x_{-i}, y_{-i}) \approx -29.5$$

$$\text{SE} = \text{sd}(\log p(y_i|x_i, x_{-i}, y_{-i})) \cdot \sqrt{20} \approx 3.3$$

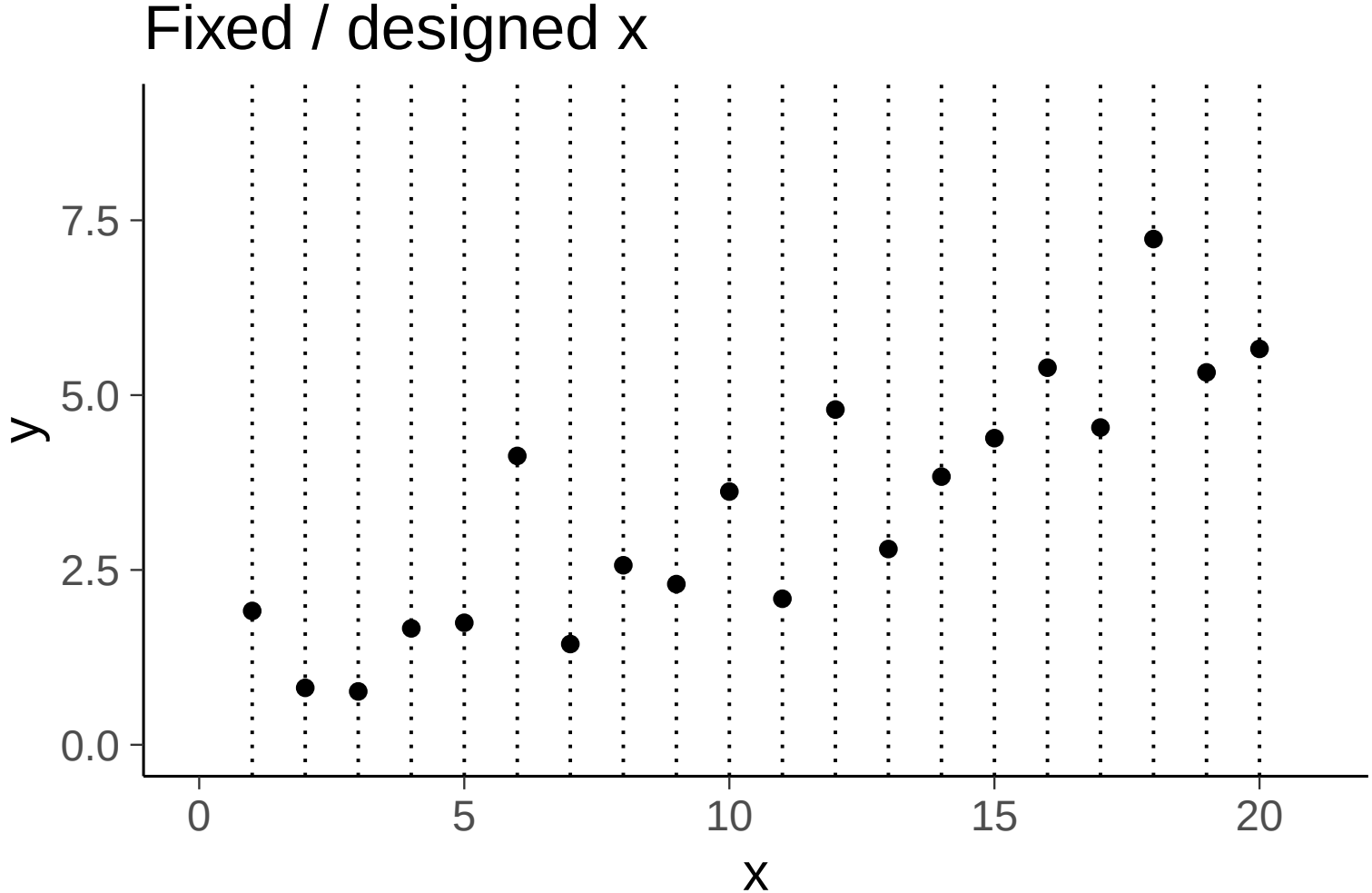
Leave−one−out log predictive densities



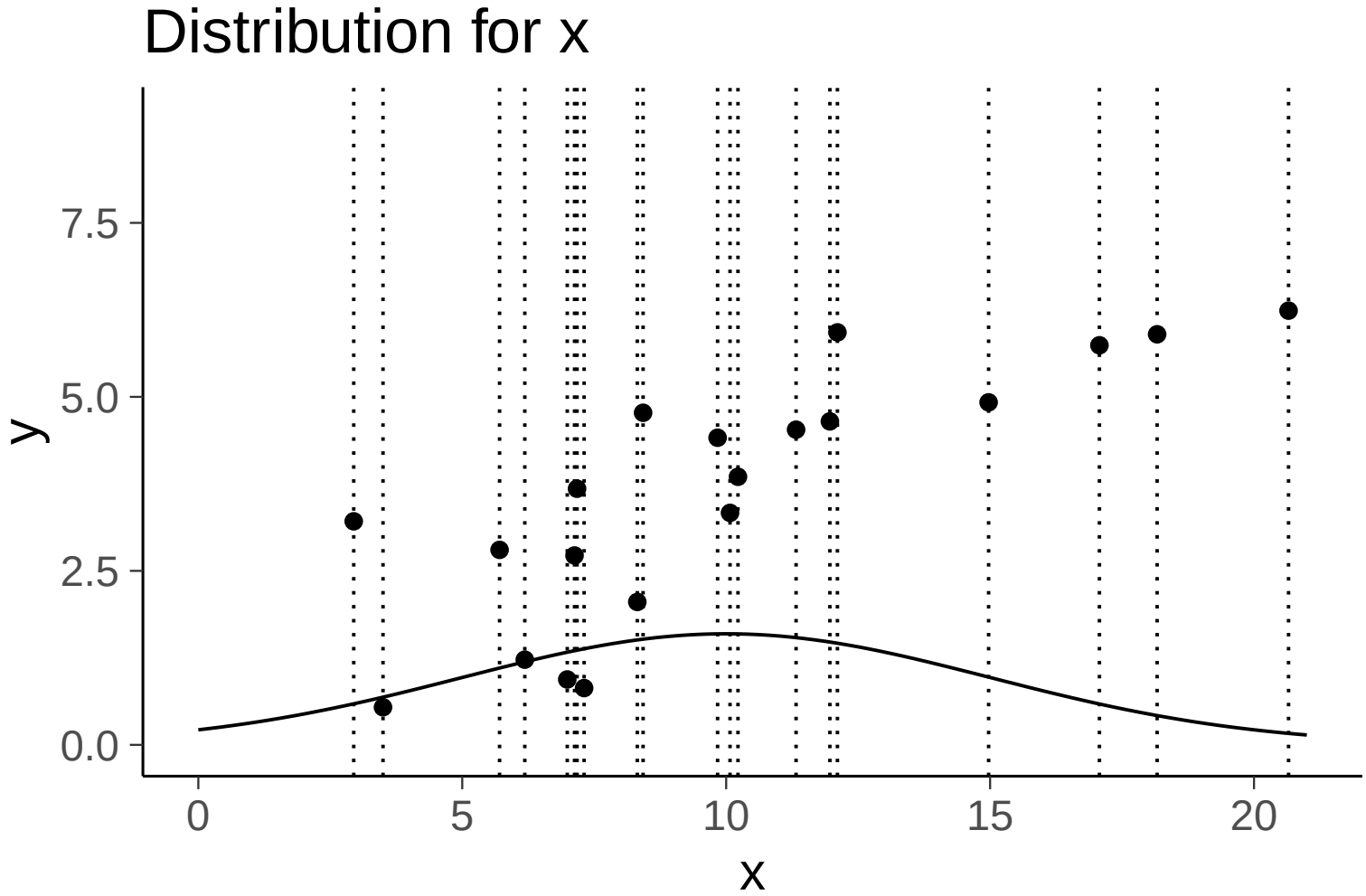
$$\text{elpd\_loo} = \sum_{i=1}^{20} \log p(y_i|x_i, x_{-i}, y_{-i}) \approx -29.5$$

$$\text{SE} = \text{sd}(\log p(y_i|x_i, x_{-i}, y_{-i})) \cdot \sqrt{20} \approx 3.3$$

see Vehtari, Gelman & Gabry (2017a) and Vehtari & Ojanen (2012) for more



LOO is ok for fixed / designed x. SE is uncertainty about $y|x$.
see Vehtari & Ojanen (2012)



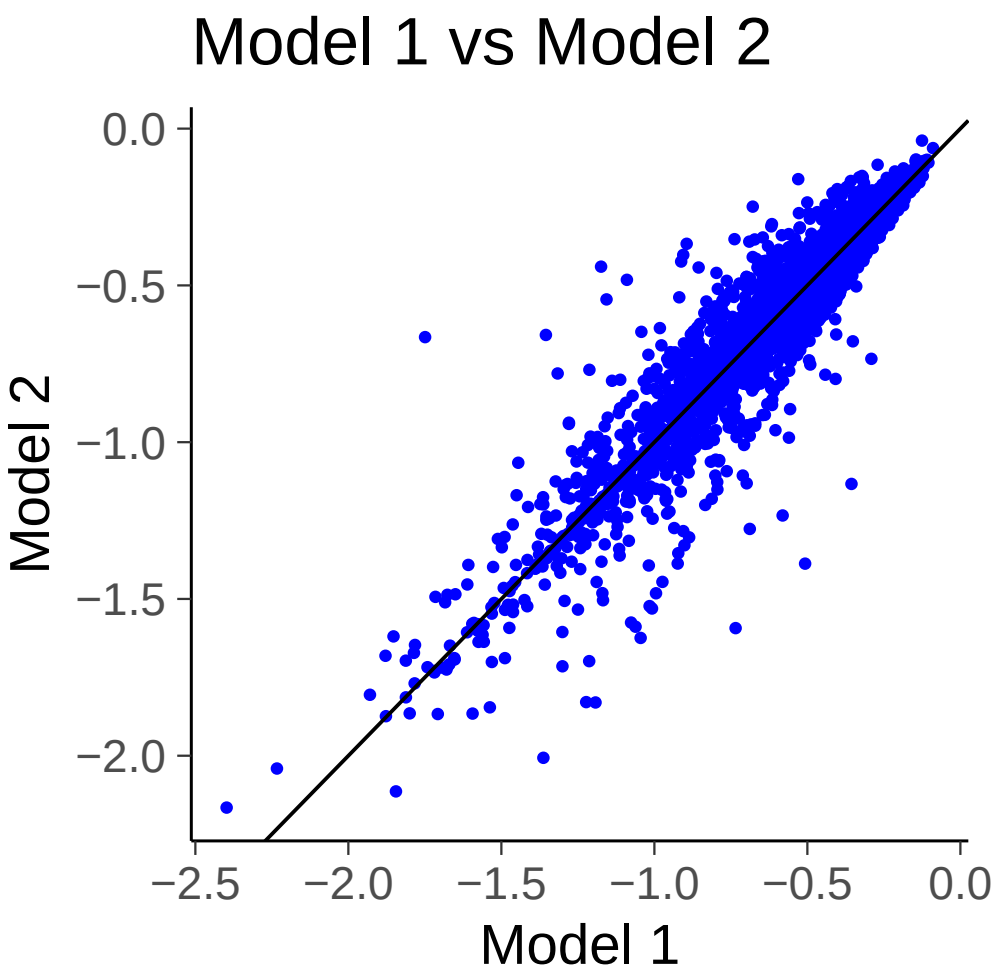
LOO is ok for random x. SE is uncertainty about $y|x$ and x.
see Vehtari & Ojanen (2012)

Arsenic well example – Model comparison

- Probability of switching well with high arsenic level in rural Bangladesh
  - Model 1 covariates: log(arsenic) and distance
  - Model 2 covariates: log(arsenic), distance and education level

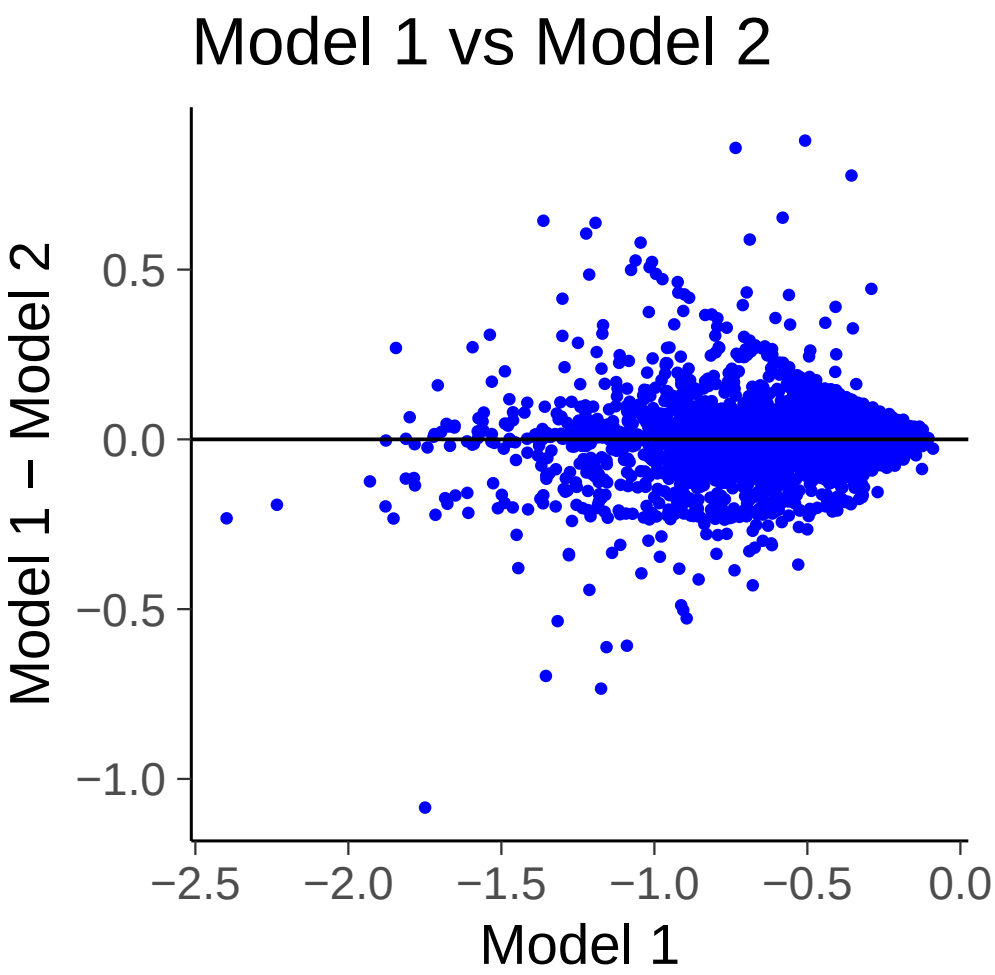
Gelman, Hill & Vehtari (2020): Regression and Other Stories, Chapter 13.

Arsenic well example – Model comparison



Model 1 elpd_loo $\approx$ -1952, SE=16
Model 2 elpd_loo $\approx$ -1938, SE=17

Arsenic well example – Model comparison




```
> loo_compare(model1, model2)
       elpd_diff se_diff
model2    0.0       0.0
model1  −14.4       6.1
```

see Vehtari, Gelman & Gabry (2017a)

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`se_diff` and normal approximation for the uncertainty in the difference is good only if models are well specified and the number of observations is relatively big (more details in a forthcoming article).

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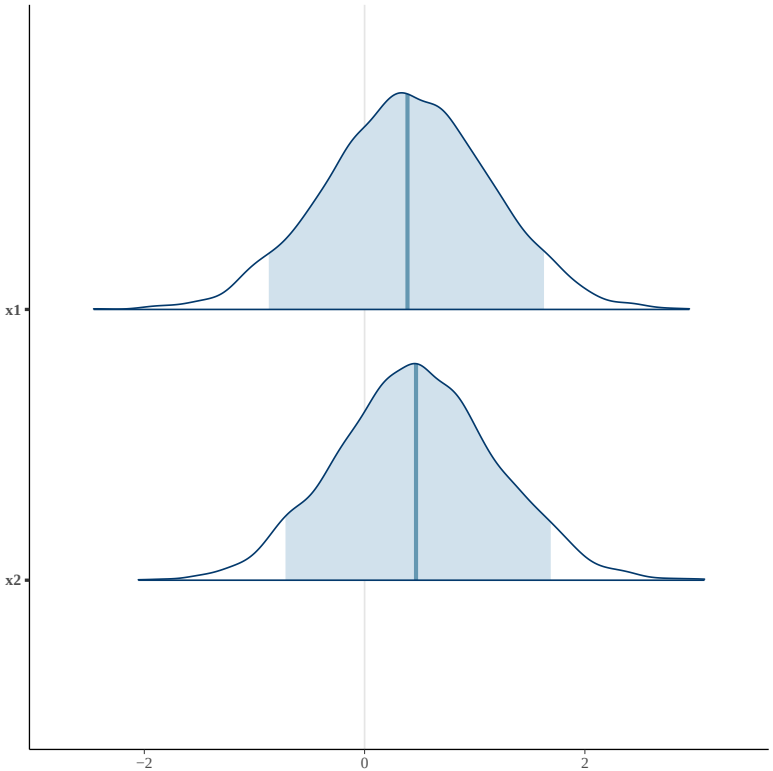
- In nested case, often easier and more accurate to analyse posterior distribution of more complex model directly
  avehtari.github.io/modelselection/betablockers.html

Sometimes predictive model comparison can be useful



Marginal posterior intervals

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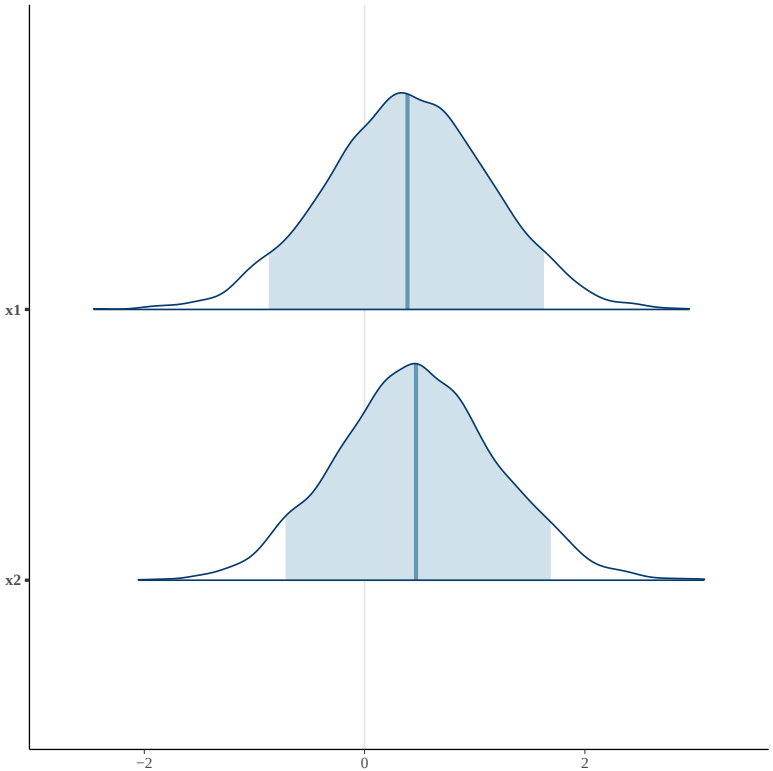

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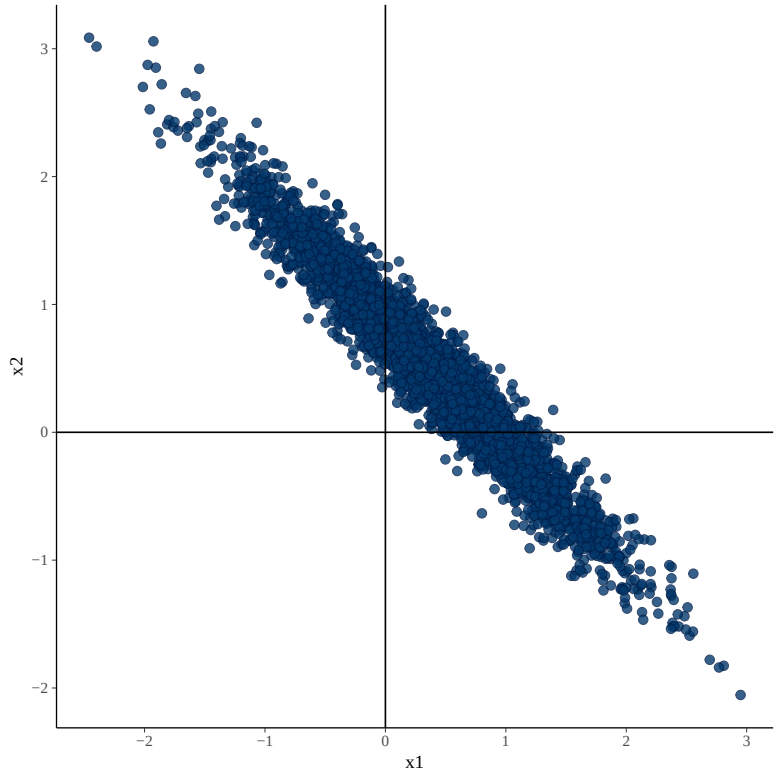

Joint posterior density

rstanarm + bayesplot

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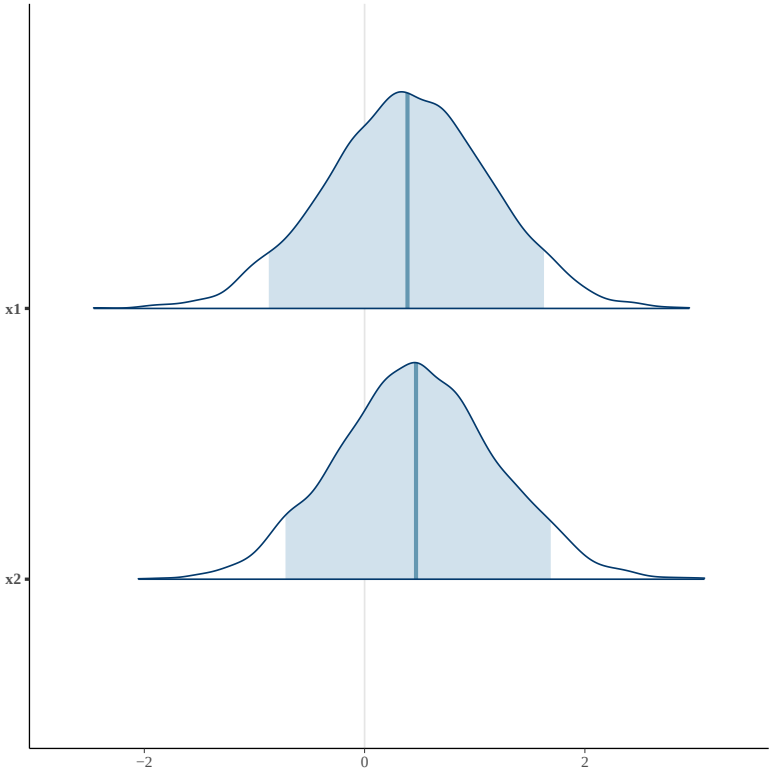

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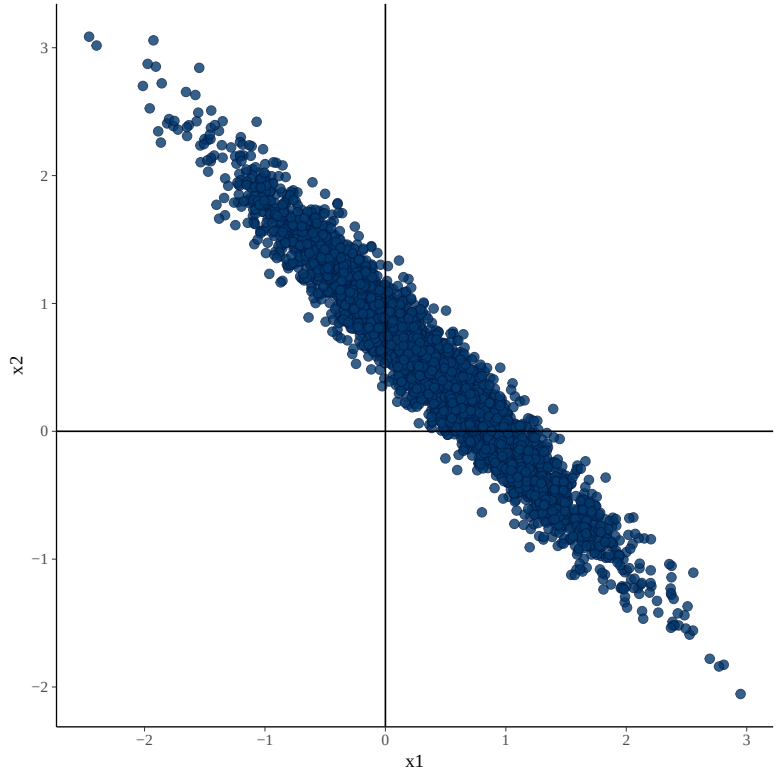

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see also Collinear demo

What if one is not clearly better than others?

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- Continuous expansion including all models?
  - and then analyse the posterior distribution directly
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  - sparse priors like regularized horseshoe prior instead of variable selection
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- Bayesian stacking may work better than BMA
    - Yao, Vehtari, Simpson, & Gelman (2018)

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- Overfitting in selection process is not unique for cross-validation

Selection induced bias and overfitting

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  - same data is used to assess the performance and make the selection
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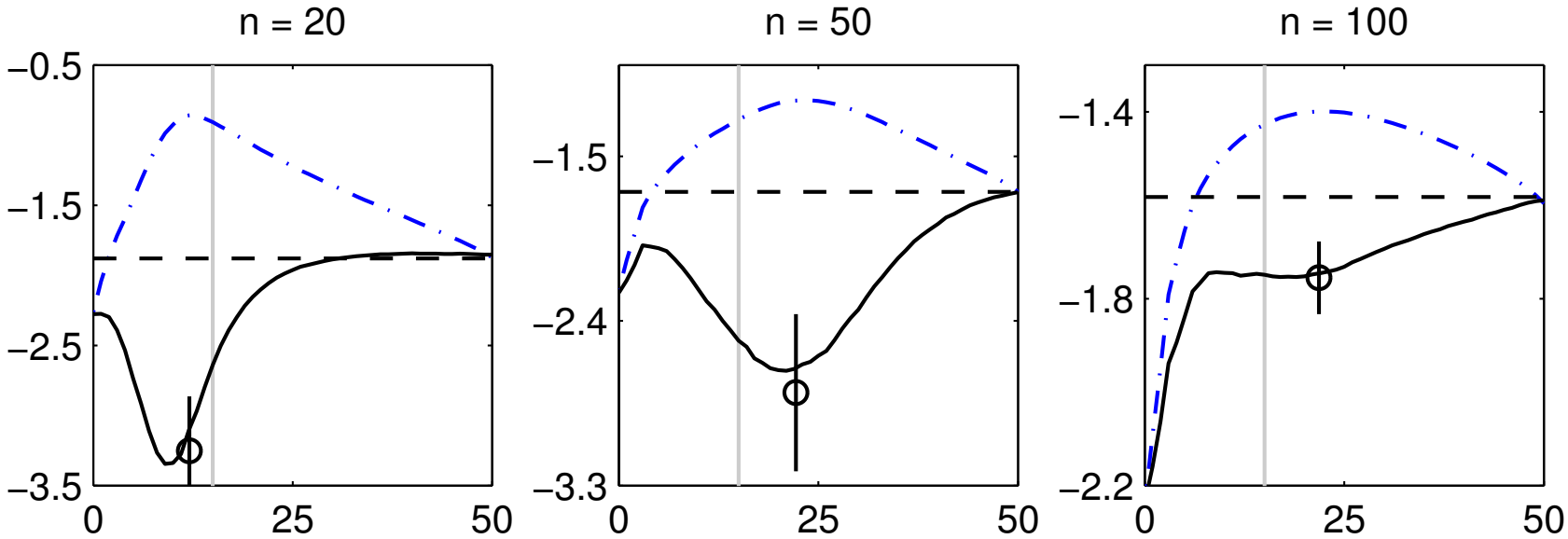
- Bigger problem if there is a large number of models as in covariate selection

Selection induced bias in variable selection



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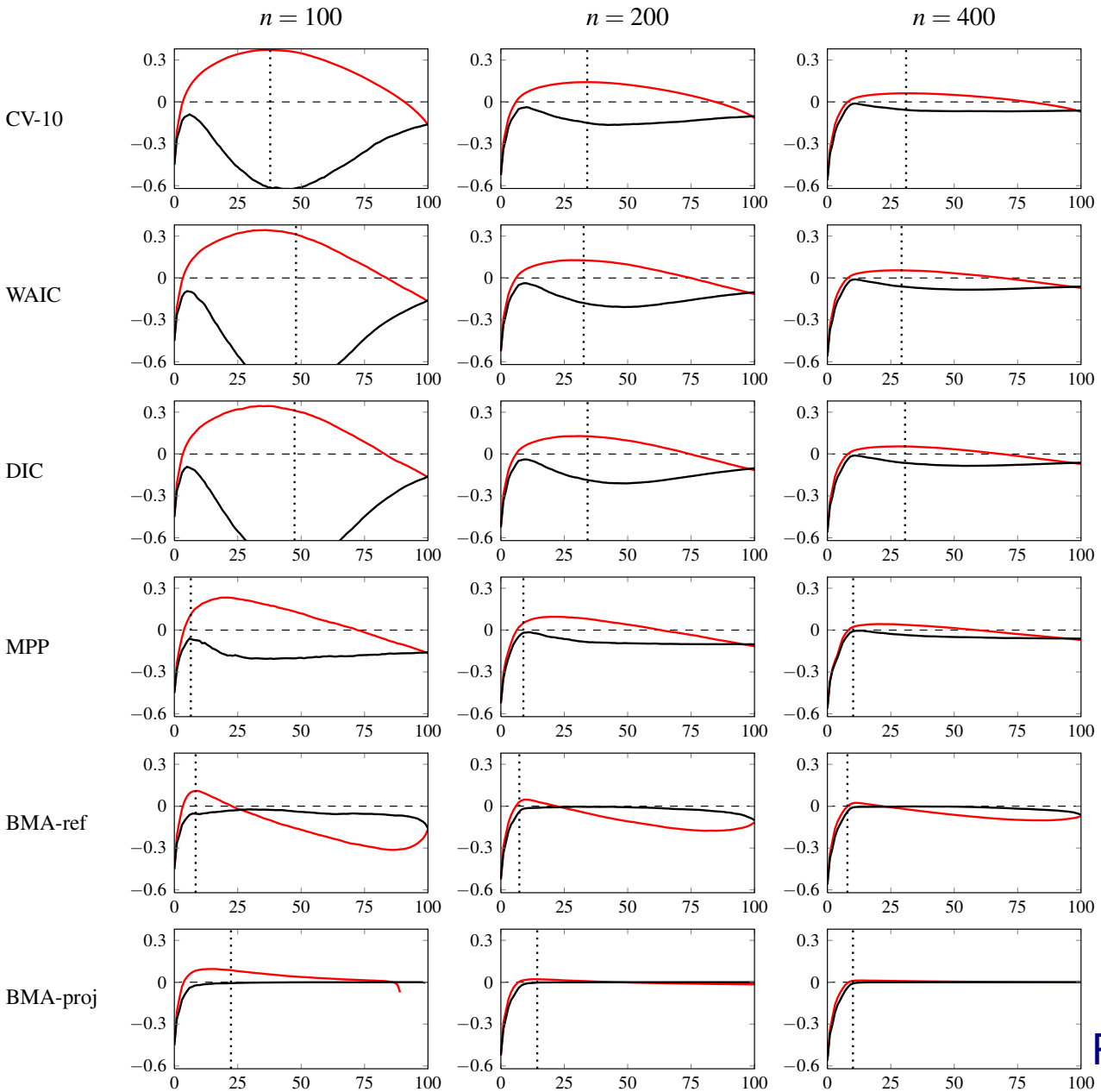

Piironen & Vehtari (2017)

Take-home messages

- It's good to think predictions of observables, because observables are the only ones we can observe
- Cross-validation can simulate predicting and observing new data
- Cross-validation is good if you don't trust your model
- Different variants of cross-validation are useful in different scenarios
- Cross-validation has high variance, and **if** you trust your model you can beat cross-validation in accuracy

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