Lecture #11: Hierarchical Models

AM 207: Advanced Scientific Computing

Stochastic Methods for Data Analysis, Inference and Optimization

Fall, 2020

IACS

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Outline

1. Review of Statistical Modeling
2. Motivation for Hierarchical Models
3. Hierarchical Models and Empirical Bayes

Review of Statistical Modeling

What We Can Do So Far: Models

1. **(Likelihood Models with Observed Variables)** When we have observed data Y_{Obs}, we can model Y_{Obs} as a random variable $Y_{\text{Obs}} \sim p(Y|\theta)$ with a known distribution p.

    - if Y_{Obs} is a label, we can model it as a *Categorical* or *Bernoulli* variable
    - if Y_{Obs} is a count, we can model it as a *Binomial*, *Multinomial* or *Poisson*
    - if Y_{Obs} is continuous, we can model it as a *Gaussian*, *Exponential*, *Dirichlet* etc

2. **(Likelihood Models with Latent Variables)** When we also have unobserved data Z_{Latent}, we can model Z_{Latent} and Y_{Obs} jointly $p(Y_{\text{Obs}}, Z_{\text{Latent}}|\theta)$.

3. **(Bayesian Models)** When we are being Bayesian, we *assume* a prior for θ, encoding our knowledge and uncertainty about θ. We model parameters and data jointly $p(Y_{\text{Obs}}, \theta)$ or $p(Y_{\text{Obs}}, Z_{\text{Latent}}, \theta)$.

What We Can Do So Far: Inference

We can make statements about θ by performing:

I. *Maximum Likelihood Estimation:* for likelihood models, we compute a fixed value θ_{MLE} that maximizes the likelihood of the observed data Y.

II. *Bayesian Inference:* for Bayesian models, we compute the posterior distribution $p(\theta|Y)$.

We choose an ***inference algorithm or method*** to perform inference:

I. *Maximum Likelihood Estimation:*
A. For *models with observed variables*, we *analytically* solve an unconstrained or contrained optimization problem to obtain θ_{MLE}.
B. For *latent variable models*, we use ***expectation maximization*** to approximately find θ_{MLE}.

II. *Bayesian Inference:*
A. If the prior and likelihood are ***conjugate***, *analytically* derive the posterior distribution
B. If the posterior distribution does not have a known form, sample from it using a ***sampler***.
C. If the posterior distribution does not have a known form, approximate it using ***variational inference***.

What Can We Not Do?

1. (***Regression Models***) We don't have any models where some observed variables Y_{Obs} depend on other observed variables X_{Obs}, i.e. none of our models have covariates that we condition on.

2. (***Gradient Descent Methods***) Analytically optimizing the log-likelihood is not always possible, and when possible it is extremely annoying to do by hand. *Can we find a way to black-box optimize any objective function?*

3. (***Hamiltonian Monte Carlo***) MCMC samplers can be extremely inefficient in high-dimensions where the samplers struggle to find area of high mass in the target distribution. *Can we build a proposal distribution with an indicator of where the target distribution mass is located?*

4. (***Black-box Variational Inference etc***) Variational inference sounds like a great idea but maximizing the ELBO using coordinate ascent is an artisenal process that requires a massive amount of derivations per model. *Can we find an algorithm to compute/estimate the gradient of the ELBO that is model independent? Can we perform black-box variational inference?*

What Happens After Inference?

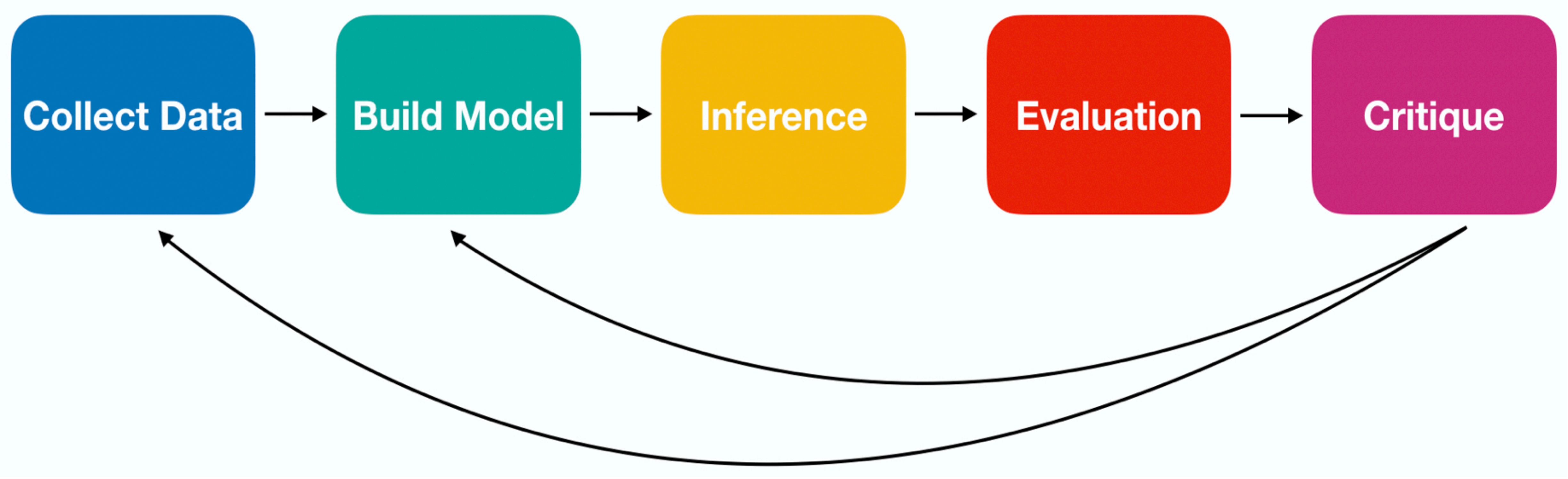
1. **(Predictive Evaluation)** In practice, we do not know the true model θ_{True}! Thus, θ_{MLE} and $p(\theta|Y)$ cannot be evaluated by comparison to θ_{True}.

   - ***Maximimum Likelihood Estimation:*** we compute θ_{MLE} on multiple bootstrap samples of the data; for each θ_{MLE} we sample $Y \sim p(Y|\theta_{\text{MLE}})$. We compare these samples with observed data Y_{Obs}.
   - ***Bayesian Inference:*** we sample θ's from the posterior, for each $\theta \sim p(\theta | Y^{\text{OBS}})$ sample $Y \sim p(Y|\theta)$. We compare these ***posterior predictive samples*** with the observed data Y_{Obs}.

2. **(Uncertainty Evaluation)** Before making decisions with real-life consequence based on your model, you should check the precision of your estimate or uncertainty of you model.

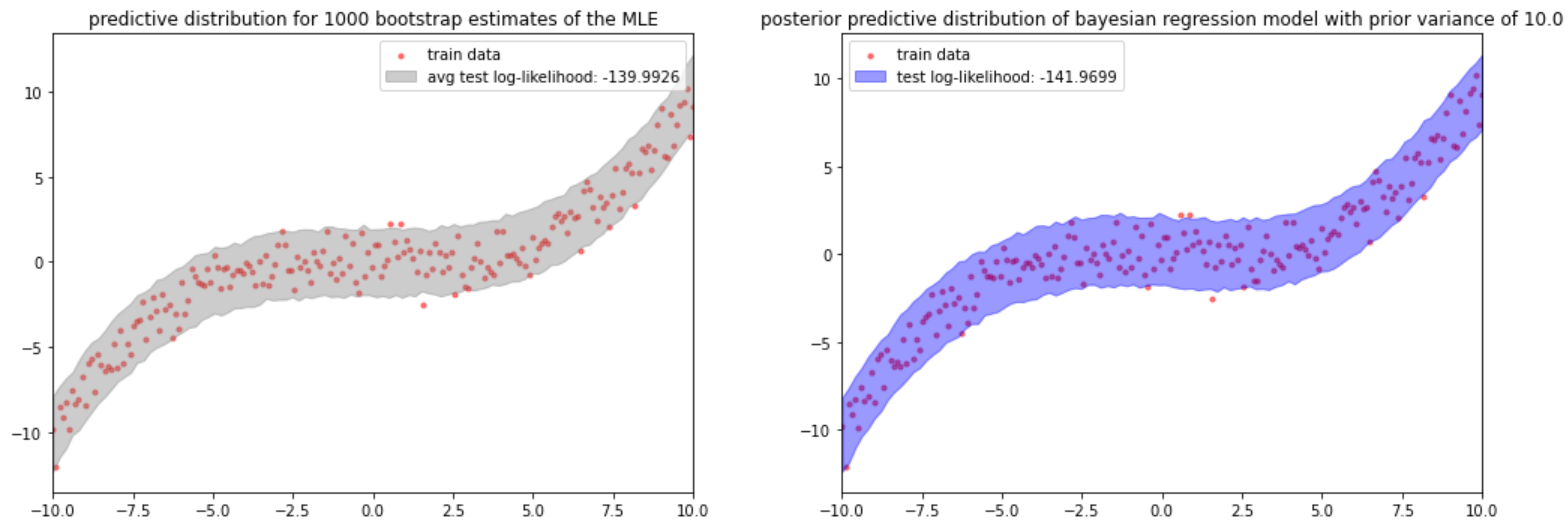
   - ***Maximimum Likelihood Estimation:*** repeat the MLE computation on many bootstrap samples of Y_{Obs}. Compute the confidence interval of θ and the predictive interval for Y. These intervals indicate *precision*.
   - ***Bayesian Inference:*** Compute credible intervals for the posterior $p(\theta|Y)$ and the predictive intervals of the posterior predictive. These intervals indicate *model uncertainty*.

The Modeling Process



Interpreting the Data Log-Likelihood

In [5]:
```
fig, ax = plt.subplots(1, 2, figsize=(15, 5))
prior_var = 10.
ax, log_likelihood_bayes = mle_vs_bayesian(x_2, y_2, ax, prior_var=prior_var)
plt.tight_layout()
plt.show()
```



Evaluating and Quantifying Uncertainty

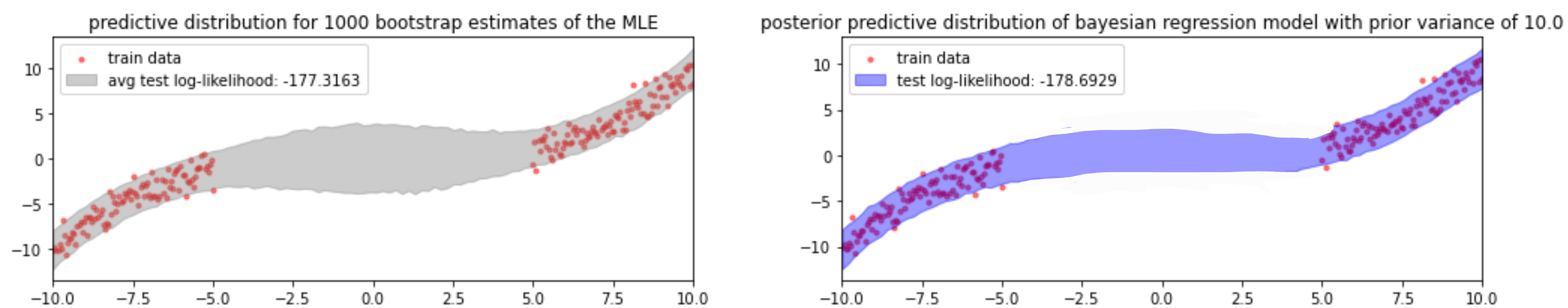
How do we know our model uncertainties (confidence intervals, credible intervals, predcitive intervals, posterior predictive intervals) are any good? What information about the data/model do we want our uncertainties to capture?

Epistemic Uncertainty: uncertainty due to small number of samples across all scenarios. This can be reduced by more samples!

Aleatoric Uncertainty: uncertainty due to the underlying randomness of the data generation process. This cannot be reduced no matter what.

Can we use log-likelihood of as a metric for the quality of predictive uncertainty?

In [6]:
```
fig, ax = plt.subplots(1, 2, figsize=(15, 3))
ax = mle_vs_bayesian(x_1, y_1, ax, prior_var=prior_var)
plt.tight_layout()
plt.show()
```



Motivation for Hierarchical Models

A Binomial Model for Movie Rankings

We model the number of likes Y_n received by the n-th movie as a binomial variable $Y_n|\theta_n \sim Bin(R_n, \theta_n)$, where R_n is the number of times the n-th movies was rated and θ_n is the "likeability" of the movie.

In [11]:

```
#Print results of ranking
print('Top 10 Movies')
print('***************************')
for movie, likes, total_ratings, likable in top_movies:
    print (movie, ':', likable, '({}/{})'.format(likes, total_ratings))
```

```
Top 10 Movies
****************************
French Twist (Gazon maudit) (1995) : 1.0 (2.0/2.0)
Exotica (1994) : 1.0 (2.0/2.0)
Three Colors: Red (1994) : 1.0 (12.0/12.0)
Three Colors: White (1994) : 1.0 (8.0/8.0)
Shawshank Redemption, The (1994) : 1.0 (39.0/39.0)
Brother Minister: The Assassination of Malcolm X (1994) : 1.0 (1.0/1.0)
Carlito's Way (1993) : 1.0 (4.0/4.0)
Robert A. Heinlein's The Puppet Masters (1994) : 1.0 (2.0/2.0)
Horseman on the Roof, The (Hussard sur le toit, Le) (1995) : 1.0 (2.0/2.0)
Wallace & Gromit: The Best of Aardman Animation (1996) : 1.0 (6.0/6.0)
```

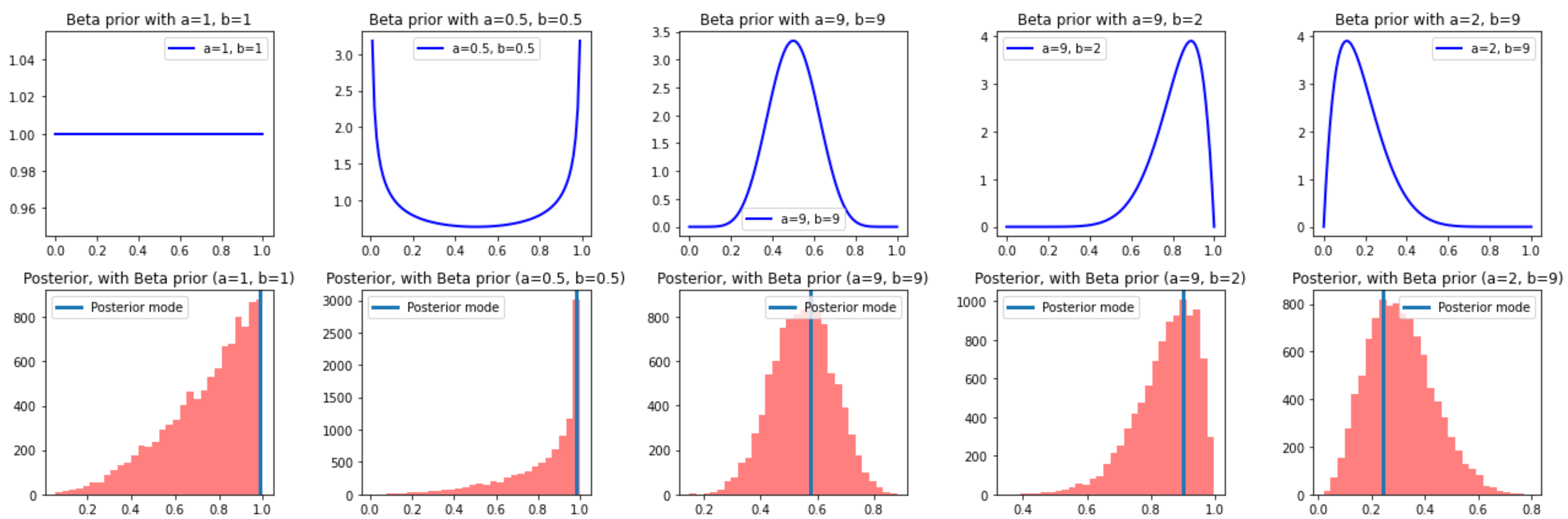
A Beta-Binomial Model for Movie Rankings

We model the number of likes Y_n received by the n-th movie as a binomial variable $Y_n|\theta_n \sim Bin(R_n, \theta_n)$, we model our prior beliefs and uncertainty about θ using a beta distribution $\theta_n \sim Beta(\alpha, \beta)$.

In [13]:

```
print('{}: {} ({}/{})'.format(movie_name, likability, likes, total_ratings))
fig, ax = plt.subplots(2, n, figsize=(18, 6))
ax = plot_priors_with_posteriors(ax, beta_shapes, likes, total_ratings, samples)
plt.tight_layout()
plt.show()
```

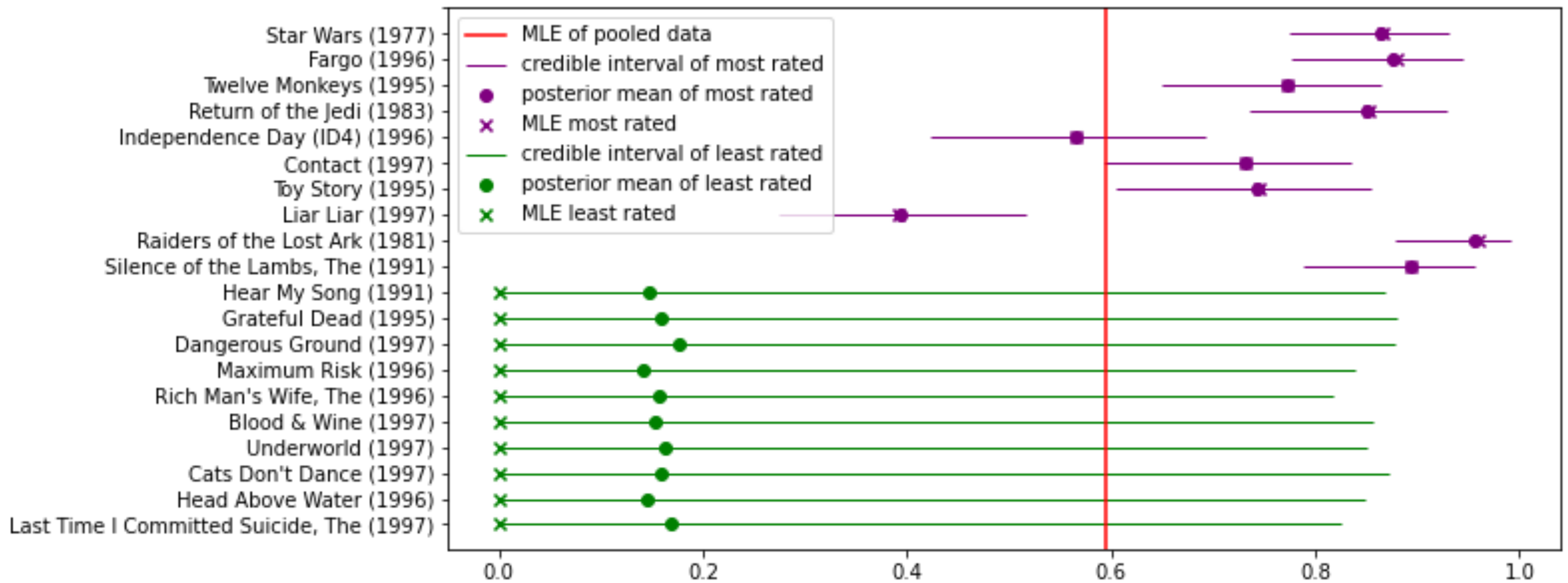
```
French Twist (Gazon maudit) (1995): 1.0 (2.0/2.0)
```



Credible Intervals for Movies with the Most and the Least Number of Ratings

In [15]:

```
fig, ax = plt.subplots(1, 1, figsize=(10, 5))
ax = plot_credible_intervals(a, b, ax)
plt.show()
```



Emprirical Bayes (ML-II) For the Beta-Binomial Model

Since the prior has a significant impact on the posterior when the number of ratings is small, we want to choose a prior that is appropriate for the data.

Idea: choose the hyperparameters α, β for the beta prior such that the expected likelihood of the data, over $\theta_n \sim Beta(\alpha, \beta)$, is maximized:

$$p(Y_1, \ldots, Y_N | \alpha, \beta) = \prod_{n=1}^{N} \int_0^1 Bin(Y_n | R_n, \theta_n) Beta(\theta_n | \alpha, \beta) d\theta_n = \prod_{n=1}^{N} \binom{R_n}{Y_n} \frac{B(\alpha + Y_n, \beta + R_n - Y_n)}{B(\alpha, \beta)}$$

where B is the beta function. The marginal likelihood of the data $p(Y_1, \ldots, Y_N | a, b)$ is called ***evidence***.

This method of choosing the hyperparameters of the prior based on the data is called ***empirical Bayes*** or ***type-II maximum likelihood***.

Question: doens't this violate the principle of choosing the prior independent of the data?

Method of Moments for Empirical Bayes (ML-II)

Since each marginal $p(Y_n|\alpha, \beta)$ is a Beta-Binomial distribution, we know its first two moments:

$$
\begin{aligned}
\mathbb{E}\left[Y_n\right] &= R_n \frac{\alpha}{\alpha+\beta} \\
\mathrm{Var}\left[Y_n\right] &= \frac{R_n \alpha\beta}{(\alpha+\beta)^2} \frac{\alpha+\beta+R_n}{\alpha+\beta+1}
\end{aligned}
$$

Now we can make the simplyfying approximations that the Y_n's are iid data from the *same* binomial, i.e. all have the same moments as above. Then we can use empirical moments to approximate the theoretical moments and solve for α, β:

$$
\begin{aligned}
\widehat{\mathbb{E}}\left[\frac{Y_n}{R_n}\right] &= \frac{\alpha}{\alpha+\beta} \\
\widehat{\mathrm{Var}}\left[\frac{Y_n}{R_n}\right] &= \frac{\alpha\beta}{\overline{R}_n(\alpha+\beta)^2} \frac{\alpha+\beta+\overline{R}_n}{\alpha+\beta+1}
\end{aligned}
$$

where $\widehat{\mathbb{E}}$ is sample mean and $\widehat{\mathrm{Var}}$ is sample variance and $\overline{R}_n$ is the average total number of ratings.

Processing math: 100%

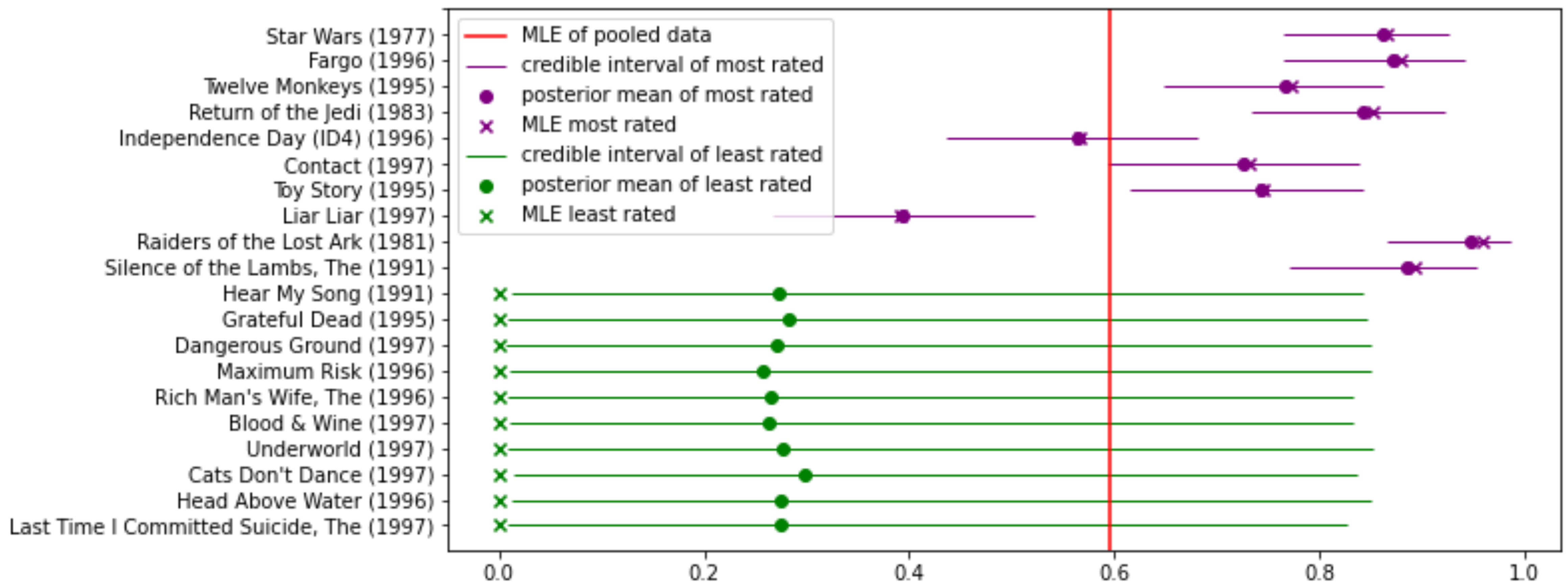
Empirical Bayes and Shrinkage

Computing the hyperparameters α, β of the beta prior on θ from the data, allows the ratings rich movies to influence the prior of ratings poor movies, since all movies contribute to the empirical Bayes estimate.

As a result, the estimates from ratings poor movies tend to ***shrink*** towards the population mean more so than ratings rich movies.

In [17]:

```
fig, ax = plt.subplots(1, 1, figsize=(10, 5))
ax = plot_credible_intervals(alpha_eb, beta_eb, ax)
plt.show()
```



Hierarchical Models and Empirical Bayes

A Hierarchical Model for Movie Rankings

We model the number of likes Y_n received by the n-th movie as a binomial variable $Y_n|\theta_n \sim Bin(R_n, \theta_n)$, we model our prior beliefs and uncertainty about θ using a beta distribution $\theta_n \sim Beta(\alpha, \beta)$; finally, we model our uncertainty about α, β using uniform distributions $\alpha, \beta \sim U(0.5, 100)$:

$$\begin{aligned} \alpha, \beta &\sim U(0.5, 100) \\ \theta_n|\alpha, \beta &\sim Beta(\alpha, \beta) \\ Y_n|\theta_n &\sim Bin(R_n, \theta_n) \end{aligned}$$

This is an example of a ***hierarchical model*** -- a model with multiple layers of unknown variables.

There are overlaps between hierarchical models and latent variable models. Generally, we want the hiearchy in a ***hierarchical model*** to express scientifically meaningful conditional relationships. In ***latent variable models*** we want the latent variable to represent unknown aspects of the data rather than unknown parameters of our model.

Point Estimate Approximations of Inference in Hierachical Models (MAP-II)

The posterior of the hierarchical model for movie ratings is $p(\alpha, \beta, \theta_1, \ldots, \theta_N | Y_1, \ldots, Y_N)$, but since we know how θ_n is conditioned on α, β, it is often easier to marginalize out θ_n and work with $p(\alpha, \beta | Y_1, \ldots, Y_N)$.

The central idea is that by infering the posterior $p(\alpha, \beta | Y_1, \ldots, Y_N)$, α and β are influenced by the entire data set and thus ratings poor movies can ***borrow statistical strength*** from ratings rich movies through the way θ_n depends on α, β.

However, performing full Bayesian inference on hierarchical models can be difficult. Thus, we can make a point estimate approximation of $p(\alpha, \beta | Y_1, \ldots, Y_N)$:

$$\alpha^*, \beta^* = \mathrm{argmax}_{\alpha,\beta} p(\alpha, \beta | Y_1, \ldots, Y_N).$$

When we perform the usual Bayesian inference on $p(Y_n | \theta_n) p(\theta_n | \alpha^*, \beta^*)$, this is called the ***type-II MAP method***.

But when α, β are uniform random varibles, the above becomes:

$$\alpha^*, \beta^* = \mathrm{argmax}_{\alpha,\beta} p(Y_1, \ldots, Y_N | \alpha, \beta),$$

When we perform the usual Bayesian inference on $p(Y_n | \theta_n) p(\theta_n | \alpha^*, \beta^*)$, this is just our empirical Bayes or type-II MLE method!