02477 – Bayesian Machine Learning: Lecture 2

Michael Riis Andersen

Technical University of Denmark,
DTU Compute, Department of Applied Math and Computer Science

Outline

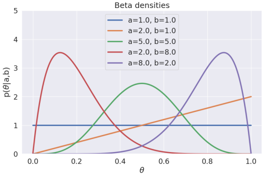
1. Quick re-cap of last week
2. Probabilistic machine learning
3. The plug-in approximation
4. Grid approximations for non-conjugate models
5. Introduction to exercise: towards logistic regression

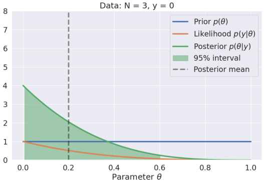
Quick re-cap of last week

Quick re-cap of Beta-binomial model and what's next

- *Bayes' rule* provides a systematic way to combine data with prior knowledge

$$p(\theta|y) = \frac{p(y|\theta)p(\theta)}{p(y)}$$





Quick re-cap of Beta-binomial model and what's next

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$$p(\theta|y) = \frac{p(y|\theta)p(\theta)}{p(y)}$$

- *The beta-binomial model* is a *conjugate* model

$$p(\theta) = \text{Beta}(\theta|a_0, b_0) \qquad (\textit{Prior})$$

$$p(y|\theta) = \binom{N}{y}\theta^y(1-\theta)^{N-y} \qquad (\textit{Likelihood})$$

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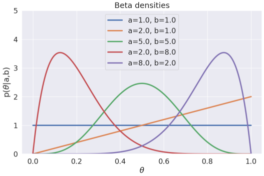

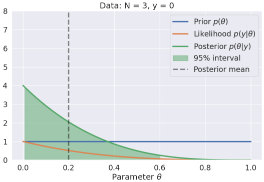

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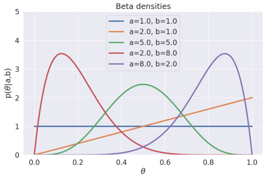

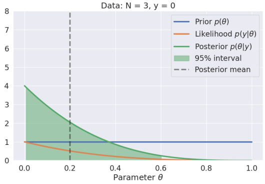

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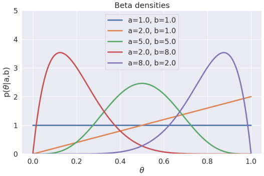
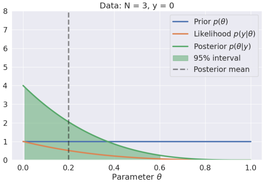
- .. and use *credibility intervals* of the posterior to *quantify the uncertainty*

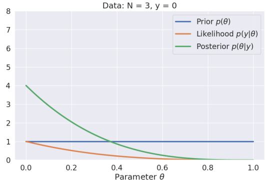
$$P(\theta \in [0.01, 0.60]\,|y) = 0.95$$





What about making predictions?

Example continued: suppose we have this website ad with $N = 3$ views and $y = 0$ clicks.



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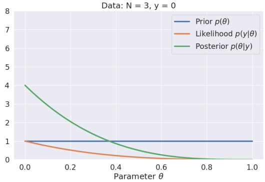

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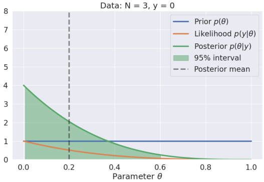

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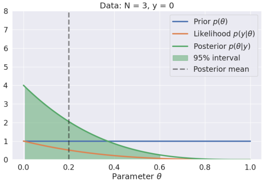

- **Goal**: *predict* number of clicks y^* in the next $N^* = 50$ views?

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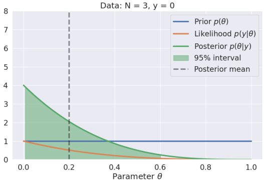

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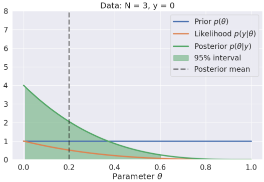

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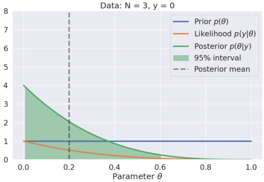

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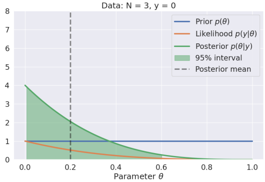

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Which value of θ to use? How do we use the *posterior knowledge* to make predictions? How do we take the *uncertainty* into account?

Probabilistic machine learning

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Product rule
$p(\boldsymbol{a}, \boldsymbol{b}) = p(\boldsymbol{b}|\boldsymbol{a})p(\boldsymbol{a})$

Sum rule
$p(\boldsymbol{b}) = \int p(\boldsymbol{a}, \boldsymbol{b})\mathrm{d}\boldsymbol{a}$

Conditional
$p(\boldsymbol{a}|\boldsymbol{b}) = \frac{p(\boldsymbol{a},\boldsymbol{b})}{p(\boldsymbol{b})}$

Conditional independence
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Product rule	Sum rule	Conditional	Conditional independence
$p(\boldsymbol{a}, \boldsymbol{b}) = p(\boldsymbol{b}\vert\boldsymbol{a})p(\boldsymbol{a})$	$p(\boldsymbol{b}) = \int p(\boldsymbol{a}, \boldsymbol{b})\mathrm{d}\boldsymbol{a}$	$p(\boldsymbol{a}\vert\boldsymbol{b}) = \frac{p(\boldsymbol{a},\boldsymbol{b})}{p(\boldsymbol{b})}$	$p(\boldsymbol{a}, \boldsymbol{b}\vert\boldsymbol{c}) = p(\boldsymbol{a}\vert\boldsymbol{c})p(\boldsymbol{b}\vert\boldsymbol{c})$

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$$p(y) = \int p(y, \theta)\mathrm{d}\theta = \int p(y|\theta)p(\theta)\mathrm{d}\theta$$

- Hence, in theory, we can derive *all quantities of interest* from the *joint distribution*

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- ... or more generally for $\boldsymbol{y} = \begin{bmatrix} y_1 & y_2 & \dots & y_N \end{bmatrix}$

$$p(\boldsymbol{y}|\theta) = p(y_1|\theta)p(y_2|\theta)\dots p(y_N|\theta) = \prod_{n=1}^{N} p(y_n|\theta)$$

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- The *joint distribution* becomes

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Website ad example continued: Making predictions

- **Example continued:** Your website ad has been shown $N = 123$ times and generated $y = 12$ clicks. Suppose you pay for another $N^* = 50$ views, how many clicks y^* should you expect *given the observed data*?

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- The assumption of *conditional independence* implies

$$p(y, y^*|\theta) = p(y|\theta)p(y^*|\theta) =$$

Website ad example continued: Making predictions

- **Example continued:** Your website ad has been shown $N = 123$ times and generated $y = 12$ clicks. Suppose you pay for another $N^* = 50$ views, how many clicks y^* should you expect *given the observed data*?

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$$p(\theta) = \text{Beta}(\theta|a_0, b_0)$$

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- **Goal**: compute *predictive distribution* of y^* given we have observed $y = 12$, i.e. $p(y^*|y = 12)$.

A probabilistic perspective on making predictions

Product rule
$p(\boldsymbol{a}, \boldsymbol{b}) = p(\boldsymbol{b}|\boldsymbol{a})p(\boldsymbol{a})$

Sum rule
$p(\boldsymbol{b}) = \int p(\boldsymbol{a}, \boldsymbol{b})\mathrm{d}\boldsymbol{a}$

Conditional
$p(\boldsymbol{a}|\boldsymbol{b}) = \frac{p(\boldsymbol{a},\boldsymbol{b})}{p(\boldsymbol{b})}$

Conditional independence
$p(\boldsymbol{a}, \boldsymbol{b}|\boldsymbol{c}) = p(\boldsymbol{a}|\boldsymbol{c})p(\boldsymbol{b}|\boldsymbol{c})$

Goal: Given some data y, what can we say about a new observation y^*?

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$$p(y^*, y, \theta) = p(y^*, y|\theta)p(\theta) =$$

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- **Key take-away**: To reason about *y^* given y*, we need to *average the likelihood* for y^* wrt. to the *posterior distribution* $p(\theta|y)$.

Quiz time

Take the quiz called
Lecture 2: Prior, likelihood, posterior, posterior predictive
to test your understanding.

Website example

- **Example continued:** Your website ad has been shown $N = 123$ times and generated $y = 12$ clicks. Suppose you pay for another $N^* = 50$ views, how many clicks y^* should you expect *given the observed data*?

Website example

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- We already defined the model

$$
\begin{aligned}
p(y|\theta) &= \text{Bin}(y|N, \theta) && (\textit{Likelihood}) \\
p(y^*|\theta) &= \text{Bin}(y^*|N^*, \theta) && (\textit{Predictive likelihood}) \\
p(\theta) &= \text{Beta}(\theta|a_0, b_0) && (\textit{Prior})
\end{aligned}
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- We know how to compute the *posterior distribution*

$$p(\theta|y) = \text{Beta}(\theta|y + a_0, N - y + b_0)$$

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$$p(\theta|y) = \text{Beta}(\theta|y + a_0, N - y + b_0)$$

- Next, we want to compute the *posterior predictive distribution*

$$p(y^*|y) = \int p(y^*|\theta)p(\theta|y)\mathrm{d}\theta =$$

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$$p(y^*|y) = \int p(y^*|\theta)p(\theta|y)\mathrm{d}\theta = \int \text{Bin}(y|N^*, \theta)\text{Beta}(\theta|y + a_0, N - y + b_0)\mathrm{d}\theta$$

- *Intuition*: Instead of plugging in a single value for the parameter estimate, we plug in all possible values for θ and weight the result according to $p(\theta|y)$

Website example

- Compute *posterior predictive distribution*

$$p(y^* = k|y) = \int \mathrm{Bin}(y = k|N^*, \theta)\mathrm{Beta}(\theta|y + a_0, N - y + b_0)\mathrm{d}\theta$$

Website example

- Compute *posterior predictive distribution*

$$
\begin{aligned}
p(y^* = k|y) &= \int \text{Bin}(y = k|N^*, \theta)\text{Beta}(\theta|y + a_0, N - y + b_0)\text{d}\theta \\
&= \int \binom{N^*}{k}\theta^k(1-\theta)^{N^*-k}\frac{1}{B(\alpha,\beta)}\theta^{\alpha-1}(1-\theta)^{\beta-1}\text{d}\theta
\end{aligned}
$$

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\end{aligned}
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\end{aligned}
$$

- We recognize the terms in green as the *functional form* of a Beta density, and hence, we know how to compute the integral

$$
p(y^* = k|y) = \binom{N^*}{k}\frac{B(\alpha+k, \beta+N^*-k)}{B(\alpha,\beta)}
$$

for $\alpha = y + a_0$ and $\beta = N - y + b_0$.

Website example: putting everything together

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p(\theta|y) &= \text{Beta}(\theta|13,112) && \text{(\textit{Posterior})}
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- Distribution of clicks y^* based on views $N^* = 50$ views

$$p(y^* = k|y) = \binom{N^*}{k} \frac{B(\alpha + k, \beta + N^* - k)}{B(\alpha, \beta)} =$$

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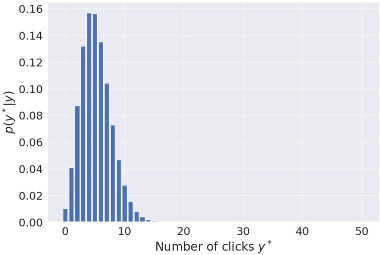

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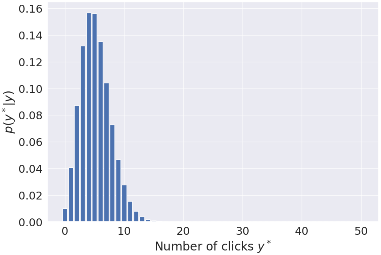

- Distribution of clicks y^* based on views $N^* = 50$ views

$$p(y^* = k|y) = \binom{N^*}{k} \frac{B(\alpha + k, \beta + N^* - k)}{B(\alpha, \beta)} = \binom{50}{k} \frac{B(13 + k, 162 - k)}{B(13, 112)}$$

- The expected number of clicks given the data is

$$\mathbb{E}_{p(y^*|y)}[y^*] = \sum_{k=0}^{50} k p(y^* = k|y) \approx 5.2$$

The plug-in approximation

A few prerequisites first

Univariate Gaussians

- The *normal distribution* (also known as the Gaussian) is distribution over $x \in \mathbb{R}$ with density

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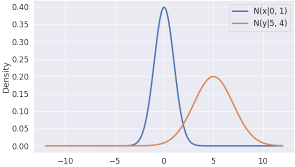

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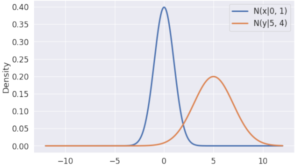

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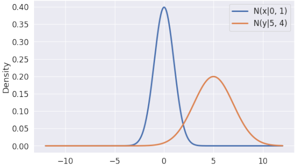

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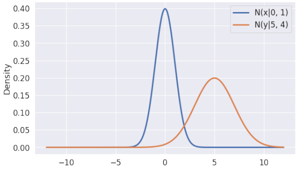

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- We will talk more about Gaussians later in this course

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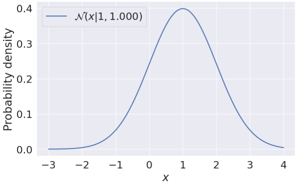

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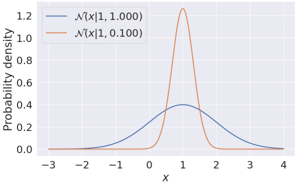

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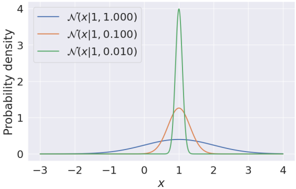

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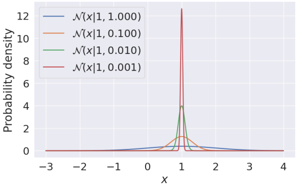

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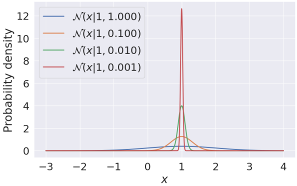

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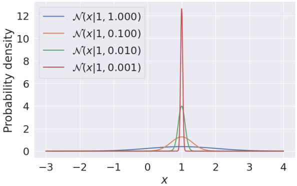

(3)

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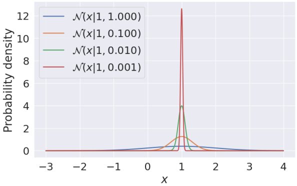

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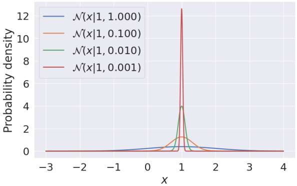

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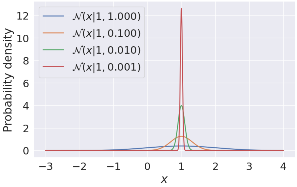
- Eq. (3) is called the *sifting property* and implies

$$\mathbb{E}_{\delta(x-\mu)}\left[f(x)\right] = f(\mu)$$



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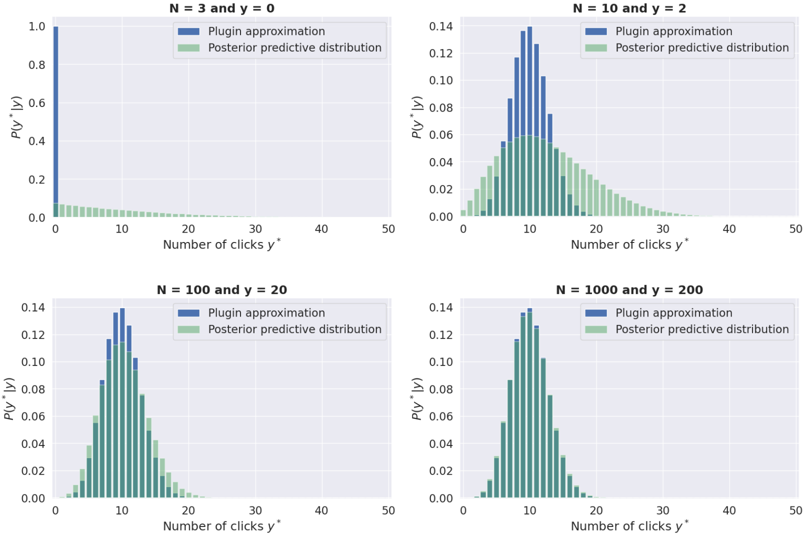
- This is how we make predictions in deep learning...

The posterior predictive distribution and plugin approximations



Grid approximations for non-conjugate models

Introduction to non-conjugate models

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- We studied the binomial model for estimating proportions and imposed a Beta prior for θ for Bayesian inference
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- Unfortunately, we *cannot* evaluate the evidence, i.e. $p(y)$ analytically *intractable* for most models of practical interest...

Approximate inference methods

- **In this course**: We will study several computational tools and approximation inference methods for dealing with such *intractable distributions*

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  2. Laplace approximations
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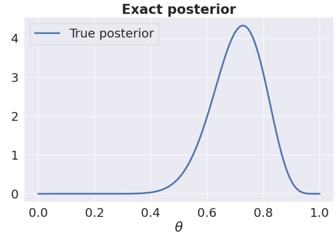
- **This week**: We will focus on *grid approximations*, which are easy to understand and apply, and they will help build our intuition about marginalization.

The grid approximation

- **Constructing the grid approximation for $p(\theta|y)$**



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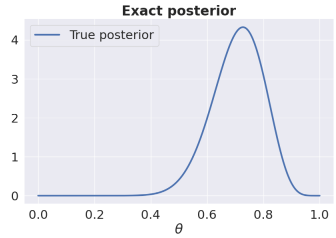

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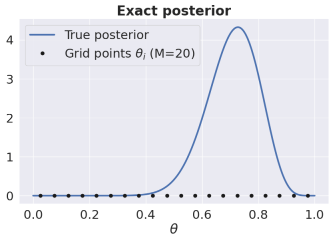

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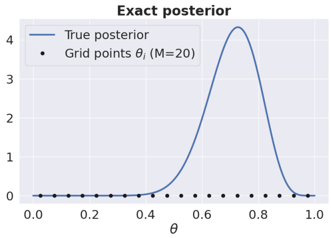

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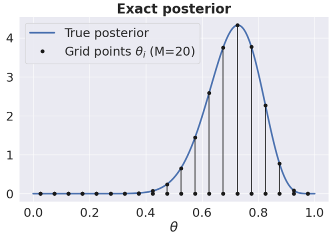

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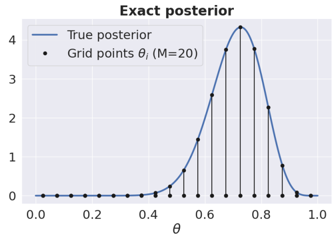

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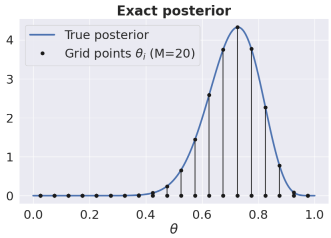

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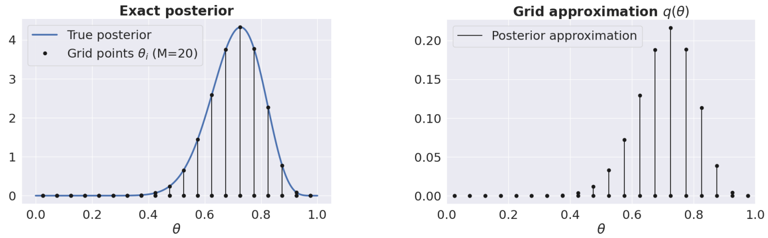

The grid approximation

Posterior summaries

- The grid approximation is a discrete distribution, so computing summaries is easy, e.g the posterior mean

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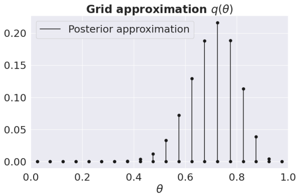

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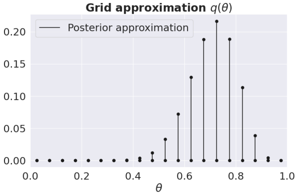

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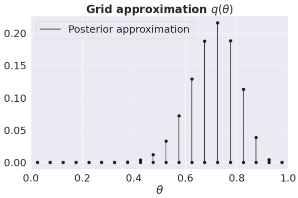

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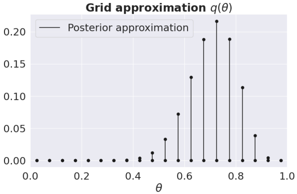

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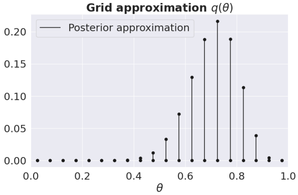

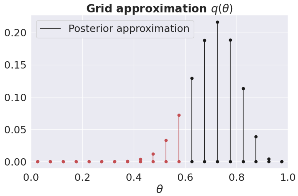

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The posterior predictive distribution

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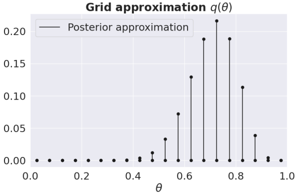

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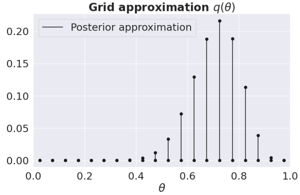

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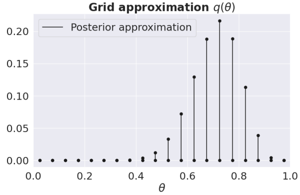

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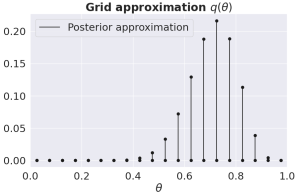

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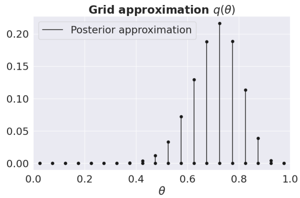

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- To make predictions we literally compute a weighted sum of all possible parameter values

The grid approximation

A few practical considerations

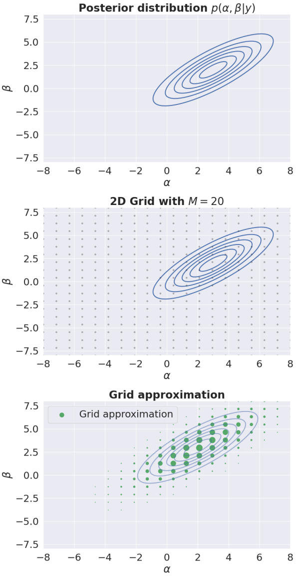
- Choosing the grid range
  - Range for $\theta \in [0, 1]$ is easy
  - For a different parameter $\alpha \in \mathbb{R}$, we need to choose an interval $[a, b]$ for the grid. Often identified visually.
- Scaling with model dimensionality
  - Suppose we use $M = 20$ points for each dimension

    1D: 20 evaluations

    2D: $20^2 = 400$ evaluations

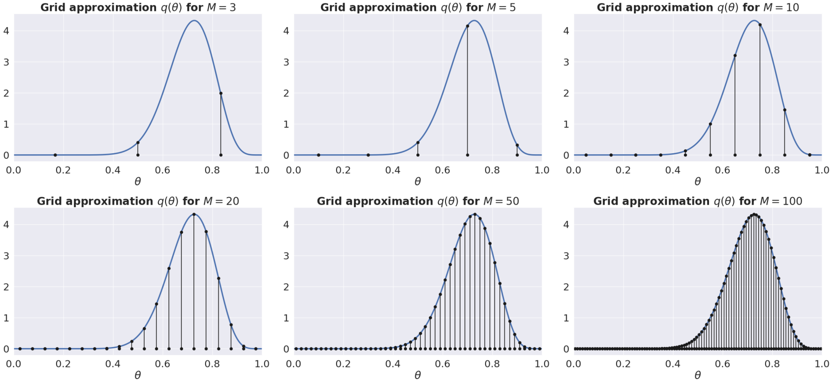
    3D: $20^3 = 8000$ evaluations

    4D: $16000^4 = 160000$ evaluations
  - Grid approximations do not scale well beyond 3-4 dimensions
- Number of grid points M
  - M is balance between computational cost and accuracy
  - Grid approximation is zero when evaluated outside the grid points
  - Often diminishing returns as M increases (next slide)



The grid approximation

Summary



- **Pros:** Simple, easy and intuitive.
- **Cons:** Suffers from curse of dimensionality and does not scale beyond 3-4 dimensions

Introduction to exercise: towards logistic regression

Towards logistic regression

- So far we focussed on modelling *proportions*, i.e. $\theta \in [0, 1]$ given data about y successes in N *conditionally independent trials*

- The binomial likelihood is also often used in *dose-response* models, which is key for determining "safe" dosages for drugs, pollution, foods etc.

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- **Example**: A company wants to study side effects of their new drug

x **(Dose in mg)**	y **(# side effects)**	N **(# patients)**
80	0	69
160	4	832
320	13	835
480	20	459
640	12	324
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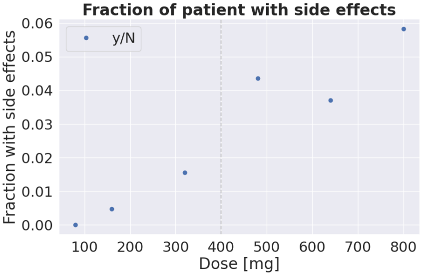
- We could analyze the data for each dose independently using a beta-binomial model, but we would like to ...

  1. understand how dose affect the probability of side effects
  2. make predictions for new dosages x^*
  3. borrow "statistical strength" across dosages

Towards logistic regression

Example & motivation II

x (Dose in mg)	y (# side effects)	N (# patients)	y/N
80	0	69	0
160	4	832	0.005
320	13	835	0.016
480	20	459	0.044
640	12	324	0.037
800	6	103	0.058



- How accurate can we predict the probability of side effects for $x^* = 400mg$?

Towards logistic regression
Setting up the likelihood

- For each dose x_i, we assume

$$y_i|x_i \sim \text{Bin}(y_i|N_i, \theta_i), \quad \theta_i \in [0, 1]$$

Towards logistic regression

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$$\theta_i \equiv \theta(x_i) = \sigma(\alpha + \beta x),$$

where $\sigma(x) : \mathbb{R} \to [0, 1]$ is a sigmoid function and $\alpha, \beta \in \mathbb{R}$ are model parameters.

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$$p(\mathbf{y}|\mathbf{x}, \alpha, \beta) = \prod_{i=1}^{M} p(y_i|x_i, \alpha, \beta) = \prod_{i=1}^{M} \text{Bin}(y_i|N_i, \theta_i),$$
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- The predictive likelihood for y^* is

$$p(y^*|x^*, \alpha, \beta) = \text{Bin}(y^*|N_i, \theta^*)$$

  where $\theta^* \equiv \theta(x^*)$

Towards logistic regression

Setting up the prior

- The model parameters are α (intercept) and β (slope) of the generalized linear model

Towards logistic regression

Setting up the prior

- The model parameters are α (intercept) and β (slope) of the generalized linear model
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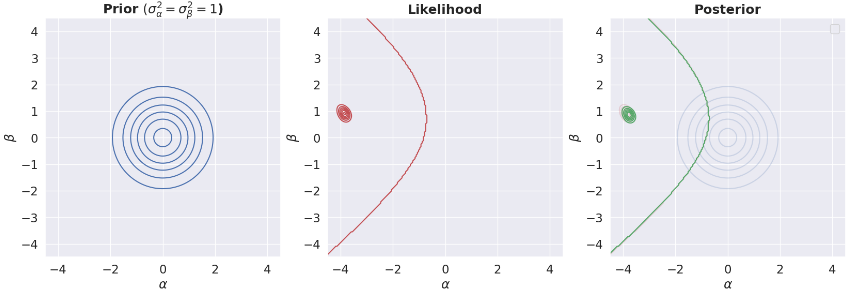
- The *posterior predictive distribution* is by *conditioning on* $\mathbf{y}$ and *marginalizing out the parameters* via the sum rule

$$p(y^*|\mathbf{y}, \mathbf{x}, x^*) = \iint p(y^*, \alpha, \beta|\mathbf{y}, \mathbf{x}, x^*)\mathrm{d}\alpha\mathrm{d}\beta = \iint \underbrace{p(y^*|x^*, \alpha, \beta)}_{\text{likelihood for } y^*} \underbrace{p(\alpha, \beta|\mathbf{y}, \mathbf{x})}_{\text{posterior distribution}} \mathrm{d}\alpha\mathrm{d}\beta$$

- After obtaining the posterior of α, β, we can *propagate* the posterior uncertainty of the parameters to any quantity that depends on α, β, i.e. $\theta(x) = \sigma(\alpha + \beta x)$, the fraction of people with side effects y^*/N etc.

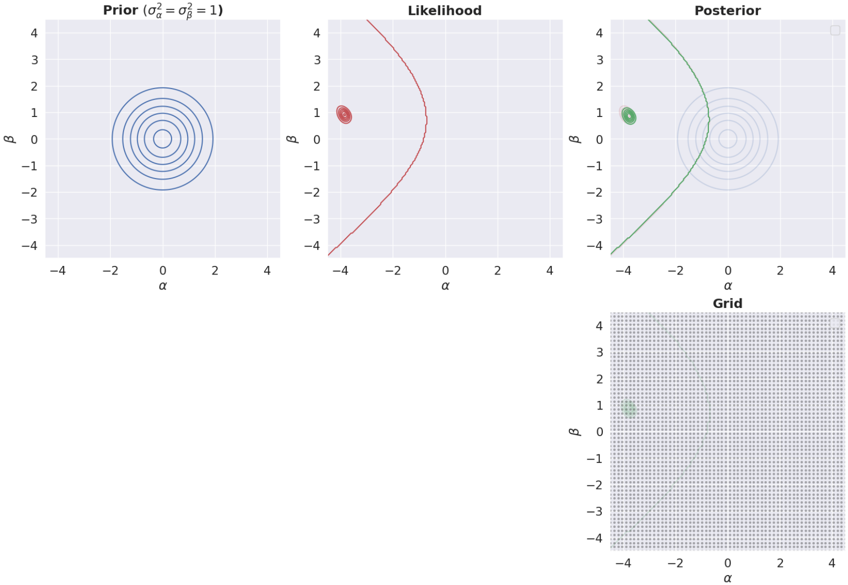
Towards logistic regression

Visualizing the distributions



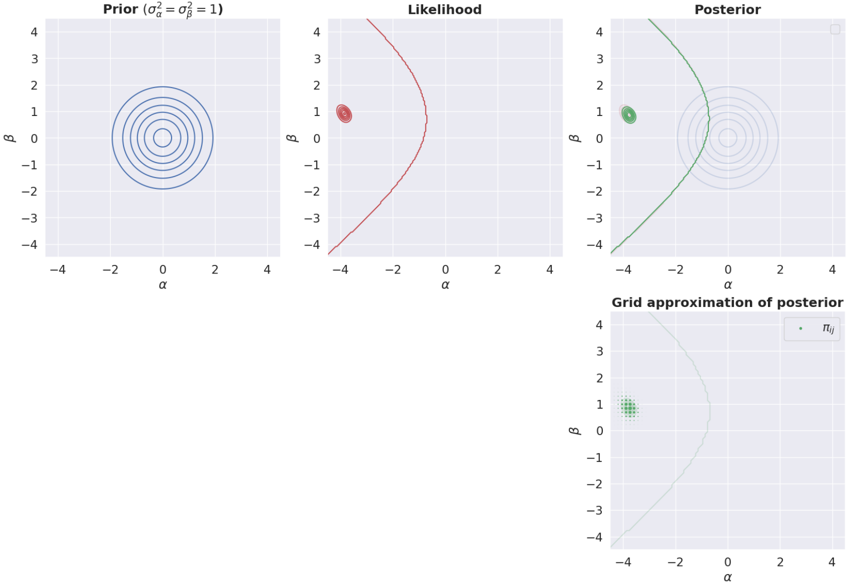
Towards logistic regression

Visualizing the distributions



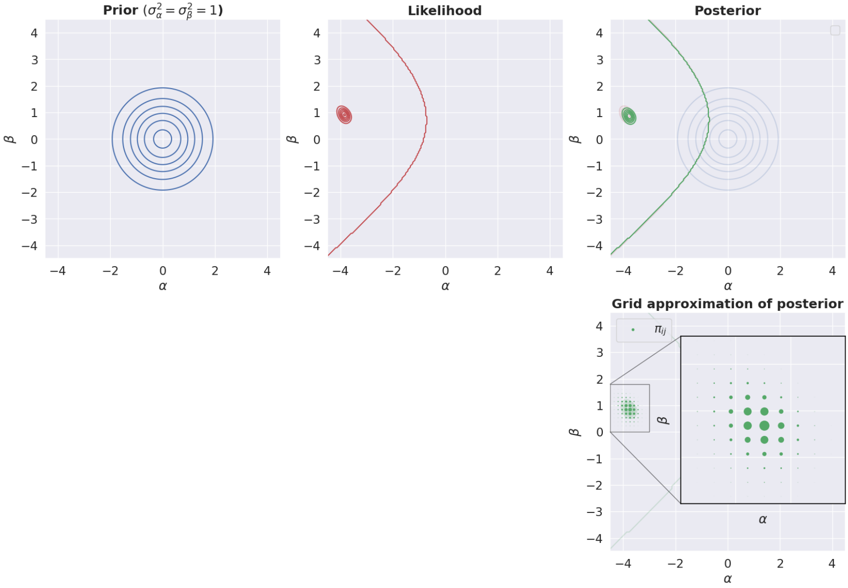
Towards logistic regression

Visualizing the distributions



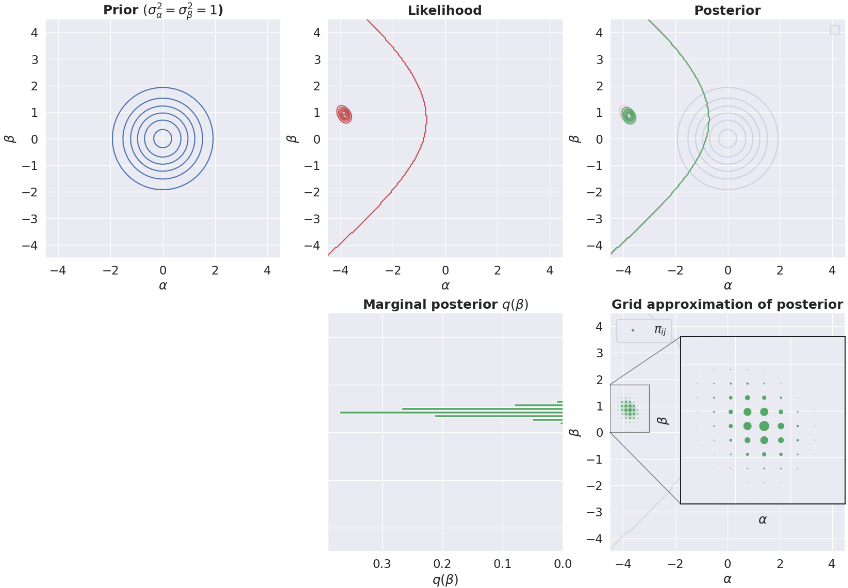
Towards logistic regression

Visualizing the distributions



Towards logistic regression

Visualizing the distributions



Towards logistic regression

Making predictions

Computing the posterior predictive distribution $p(y^* = k|\mathbf{y}, \mathbf{x}, x^*)$ for $x^* = 400$mg and $N^* = 500$

$$p(y^* = k|\mathbf{y}, \mathbf{x}, x^*) = \iint \underbrace{p(y^* = k|x^*, \alpha, \beta)}_{\text{likelihood for } y^*} \underbrace{p(\alpha, \beta|\boldsymbol{y}, \boldsymbol{x})}_{\text{posterior distribution}} \, \mathrm{d}\alpha \mathrm{d}\beta \qquad \text{(Sum rule)}$$

Towards logistic regression

Making predictions

Computing the posterior predictive distribution $p(y^* = k|\mathbf{y}, \mathbf{x}, x^*)$ for $x^* = 400$mg and $N^* = 500$

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$$= \mathbb{E}_{p(\alpha,\beta|\mathbf{y},\mathbf{x},x^*)}\left[p(y^* = k|x^*, \alpha, \beta)\right] \qquad \text{(Integrals as expectation)}$$

Computing the posterior predictive distribution $p(y^* = k|\mathbf{y}, \mathbf{x}, x^*)$ for $x^* = 400$mg and $N^* = 500$

$$\begin{aligned}
p(y^* = k|\mathbf{y}, \mathbf{x}, x^*) &= \iint \underbrace{p(y^* = k|x^*, \alpha, \beta)}_{\text{likelihood for } y^*} \underbrace{p(\alpha, \beta|\mathbf{y}, \boldsymbol{x})}_{\text{posterior distribution}} \, \mathrm{d}\alpha \mathrm{d}\beta && \text{(Sum rule)} \\
&= \mathbb{E}_{p(\alpha,\beta|\mathbf{y},\mathbf{x},x^*)} \left[p(y^* = k|x^*, \alpha, \beta) \right] && \text{(Integrals as expectation)} \\
&= \mathbb{E}_{p(\alpha,\beta|\mathbf{y},\mathbf{x},x^*)} \left[\mathrm{Bin}(y^*|N^*, \theta^*) \right] && \text{(Inserting dist.)}
\end{aligned}$$

Computing the posterior predictive distribution $p(y^* = k|\mathbf{y}, \mathbf{x}, x^*)$ for $x^* = 400$mg and $N^* = 500$

$$p(y^* = k|\mathbf{y}, \mathbf{x}, x^*) = \iint \underbrace{p(y^* = k|x^*, \alpha, \beta)}_{\text{likelihood for } y^*} \underbrace{p(\alpha, \beta|\mathbf{y}, \boldsymbol{x})}_{\text{posterior distribution}} \, \mathrm{d}\alpha \mathrm{d}\beta \qquad \text{(Sum rule)}$$

$$= \mathbb{E}_{p(\alpha,\beta|\mathbf{y},\mathbf{x},x^*)}\left[p(y^* = k|x^*, \alpha, \beta)\right] \qquad \text{(Integrals as expectation)}$$

$$= \mathbb{E}_{p(\alpha,\beta|\mathbf{y},\mathbf{x},x^*)}\left[\mathrm{Bin}(y^*|N^*, \theta^*)\right] \qquad \text{(Inserting dist.)}$$

$$\approx \mathbb{E}_{q(\alpha,\beta)}\left[\mathrm{Bin}(y^*|N^*, \theta^*)\right] \qquad \text{(Grid approx.)}$$

Towards logistic regression

Making predictions

Computing the posterior predictive distribution $p(y^* = k|\mathbf{y}, \mathbf{x}, x^*)$ for $x^* = 400$mg and $N^* = 500$

$$p(y^* = k|\mathbf{y}, \mathbf{x}, x^*) = \iint \underbrace{p(y^* = k|x^*, \alpha, \beta)}_{\text{likelihood for } y^*} \underbrace{p(\alpha, \beta|\mathbf{y}, \boldsymbol{x})}_{\text{posterior distribution}} \, \mathrm{d}\alpha \mathrm{d}\beta \qquad \text{(Sum rule)}$$

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$$= \mathbb{E}_{p(\alpha,\beta|\mathbf{y},\mathbf{x},x^*)}\left[\text{Bin}(y^*|N^*, \theta^*)\right] \qquad \text{(Inserting dist.)}$$

$$\approx \mathbb{E}_{q(\alpha,\beta)}\left[\text{Bin}(y^*|N^*, \theta^*)\right] \qquad \text{(Grid approx.)}$$

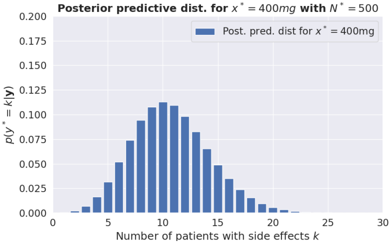
$$= \sum_{i,j} \text{Bin}(y^*|N^*, \sigma(\alpha_i + \beta_j x^*))\pi_{ij}$$

Towards logistic regression

Making predictions

Computing the posterior predictive distribution $p(y^* = k|\mathbf{y}, \mathbf{x}, x^*)$ for $x^* = 400$mg and $N^* = 500$

$$
\begin{aligned}
p(y^* = k|\mathbf{y}, \mathbf{x}, x^*) &= \iint \underbrace{p(y^* = k|x^*, \alpha, \beta)}_{\text{likelihood for } y^*} \underbrace{p(\alpha, \beta|\mathbf{y}, \mathbf{x})}_{\text{posterior distribution}} \, \mathrm{d}\alpha \mathrm{d}\beta && \text{(Sum rule)} \\
&= \mathbb{E}_{p(\alpha,\beta|\mathbf{y},\mathbf{x},x^*)} \left[p(y^* = k|x^*, \alpha, \beta) \right] && \text{(Integrals as expectation)} \\
&= \mathbb{E}_{p(\alpha,\beta|\mathbf{y},\mathbf{x},x^*)} \left[\mathrm{Bin}(y^*|N^*, \theta^*) \right] && \text{(Inserting dist.)} \\
&\approx \mathbb{E}_{q(\alpha,\beta)} \left[\mathrm{Bin}(y^*|N^*, \theta^*) \right] && \text{(Grid approx.)} \\
&= \sum_{i,j} \mathrm{Bin}(y^*|N^*, \sigma(\alpha_i + \beta_j x^*)) \pi_{ij}
\end{aligned}
$$



Towards logistic regression

Making predictions

Computing the posterior predictive distribution $p(y^* = k|\mathbf{y}, \mathbf{x}, x^*)$ for $x^* = 400\text{mg}$ and $N^* = 500$

$$p(y^* = k|\mathbf{y}, \mathbf{x}, x^*) = \iint \underbrace{p(y^* = k|x^*, \alpha, \beta)}_{\text{likelihood for } y^*} \underbrace{p(\alpha, \beta|\mathbf{y}, \mathbf{x})}_{\text{posterior distribution}} \, \mathrm{d}\alpha \mathrm{d}\beta \qquad \text{(Sum rule)}$$

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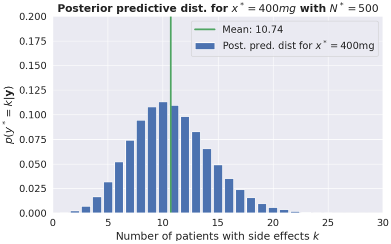

Towards logistic regression

Making predictions

Computing the posterior predictive distribution $p(y^* = k|\mathbf{y}, \mathbf{x}, x^*)$ **for** $x^* = 400$**mg and** $N^* = 500$

$$p(y^* = k|\mathbf{y}, \mathbf{x}, x^*) = \iint \underbrace{p(y^* = k|x^*, \alpha, \beta)}_{\text{likelihood for } y^*} \underbrace{p(\alpha, \beta|\mathbf{y}, \mathbf{x})}_{\text{posterior distribution}} \, \mathrm{d}\alpha \mathrm{d}\beta \qquad \text{(Sum rule)}$$

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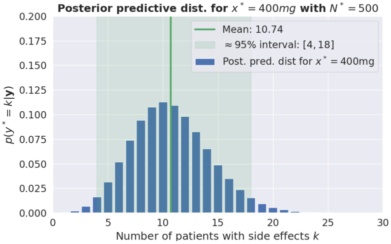

Intro to exercise

- On DTU Learn you will find an exercise for each week in notebook format
- We will spend all 4 hours from 13-17 working with the exercises
- In this exercise you will
  - Dive deeper into the Bayesian framework
  - Study and implement the probabilistic model for logistic regression for the Challenger Distaster dataset
  - Study and implement the grid approximations
  - Practice probabilistic reasoning
- Mix of pen&paper, programming and discussion questions
- Feel free to collaborate with your peers
- Ask for help!
  - Ask for help when stuck
  - Use teachers/TAs to check your understanding
  - Engage in discussion to practice
- Feedbacks persons: Meet at 16:45