

3.4 Prediction: Posterior Predictive Distributions

From parameter inference to forecasting the next data points

4BIC

Inference vs prediction: what changes?

Inference (what we've done so far)

You observe data $Y_1, \dots, Y_N$ and build a model with parameter θ .

$$\text{Prior } \pi(\theta) \longrightarrow \text{Posterior } \pi(\theta \mid y).$$

Inference vs prediction: what changes?

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Now ask:

“What are the next data points likely to be?”

Formally, introduce a future observation Z and want the distribution

$$\pi(z \mid y).$$

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Key message

Inference learns *parameters*. Prediction learns *future outcomes*, and must propagate parameter uncertainty into the forecast.

Definition 3.3: Posterior predictive distribution

Set-up

- Observe data y under a model parameterised by θ .
- Choose a prior $\pi(\theta)$ and compute posterior $\pi(\theta \mid y)$.
- Interested in a future observation Z generated by the same model.

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$$\pi(z | y) = \int \pi(z | \theta) \pi(\theta | y) d\theta.$$

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$$\pi(z \mid y) = \int \pi(z \mid \theta) \pi(\theta \mid y) d\theta.$$

One-sentence interpretation

It is the model's prediction $\pi(z \mid \theta)$ *averaged* over the posterior uncertainty in θ .

The historical intuition: Bayes and the beanbag

(Story / intuition)

Think of Bayes repeatedly throwing a beanbag over his shoulder and recording where it lands.

- Past observations: y (where it landed previously).
- Unknown “parameter”: θ (the underlying tendency / bias).
- Next throw: Z (where will the next beanbag land?).

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What does Bayes really want?

Not only “what is θ ?”, but also:

“Given what I’ve seen, where will the *next* one land?”

That is exactly $\pi(z \mid y)$.

Thomas Bayes: the “beanbag” (billiard table) experiment

The story (why this appears in Bayes' original essay)

Imagine a flat table.

- A ball/beanbag is tossed (or rolled) onto the table and lands at some position.
- Bayes repeats this many times and records where the toss lands.
- He wants to use past tosses to predict the next one.

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Modern translation

- Past data: $Y_1, \dots, Y_n$ (previous landing outcomes)
- Unknown “bias” parameter: θ (how likely the toss is to land in a region)
- Future outcome: Z (next landing outcome)

What the beanbag story teaches

Two uncertainties

- **Parameter uncertainty:** we do not know θ exactly.
- **Outcome randomness:** even if θ were known, the next toss is still random.

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Posterior predictive combines them

$$\pi(z \mid \text{data}) = \int \pi(z \mid \theta) \pi(\theta \mid \text{data}) d\theta.$$

It averages the next-outcome model over all plausible θ values.

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Why it feels reasonable

If the data strongly pin down θ , the predictive becomes sharp. If the data are weak, the predictive stays diffuse (more cautious).

What do the two factors mean?

$$\pi(z \mid \theta)$$

Sampling model for new data.

Fix a candidate parameter value θ .

Ask: “If θ were true, how likely is each z ?”

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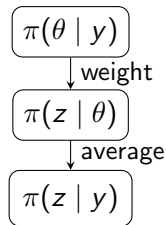
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Posterior over parameters.

After seeing y , which θ values are plausible, and how plausible?



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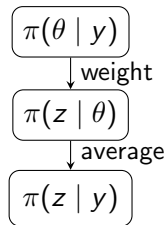
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Mixture picture

For each θ you get a different predictive curve $\pi(z \mid \theta)$. The posterior predictive is the weighted average of all those curves.

A “mental algorithm” for prediction

Two-stage sampling view (very important intuition)

To draw a predictive sample $Z^* \sim \pi(z \mid y)$:

- 1 Sample $\theta^* \sim \pi(\theta \mid y)$ (pick a plausible world)
- 2 Sample $Z^* \sim \pi(z \mid \theta^*)$ (simulate the next outcome)

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Why this is helpful

Even if the integral is messy, simulation often remains simple.

Why “constants don’t matter” breaks here

Earlier: posterior up to proportionality

For parameter inference we often write

$$\pi(\theta \mid y) \propto \pi(y \mid \theta)\pi(\theta)$$

and say “ignore the normalising constant”.

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The posterior predictive $\pi(z \mid y)$ is a **proper** density/pmf in z . If you want to compute numbers like $\Pr(Z \leq 8 \mid y)$, you need the **correct normalisation**.

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Practical consequence

You must keep track of constants (or use a known conjugacy result / a computer). That is why the algebra can feel “painful” in predictive calculations.

Example 3.6: late coursework submissions (set-up)

Problem

Last year: $y = 3$ late submissions out of $n_0 = 30$ students.

This year: $n = 30$ students. Predict how many will be late.

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Model

Let θ be the probability a student submits late.

$$Y \mid \theta \sim \text{Bin}(n_0, \theta), \quad Z \mid \theta \sim \text{Bin}(n, \theta).$$

We assume the same θ carries over from last year to this year.

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Prior (Uniform / “non-informative” on $[0, 1]$)

$$\theta \sim \text{Unif}[0, 1] = \text{Beta}(1, 1).$$

Step 1: posterior for θ (conjugacy)

Beta–Binomial conjugacy

If

$$Y \mid \theta \sim \text{Bin}(n_0, \theta), \quad \theta \sim \text{Beta}(\alpha, \beta),$$

then

$$\theta \mid y \sim \text{Beta}(\alpha + y, \beta + n_0 - y).$$

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Here ($n_0 = 30$, $y = 3$, $\alpha = \beta = 1$)

$$\theta \mid y \sim \text{Beta}(1 + 3, 1 + 30 - 3) = \text{Beta}(4, 28).$$

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Posterior mean (for intuition)

$$\mathbb{E}[\theta \mid y] = \frac{4}{4 + 28} = \frac{1}{8} = 0.125.$$

Step 2: set up the posterior predictive integral

We want

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Write each factor

$$\pi(z | \theta) = \binom{30}{z} \theta^z (1 - \theta)^{30-z},$$

$$\pi(\theta | y) = \frac{1}{B(4, 28)} \theta^{4-1} (1 - \theta)^{28-1} = \frac{1}{B(4, 28)} \theta^3 (1 - \theta)^{27}.$$

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Combine like terms

$$\pi(z | y) = \binom{30}{z} \frac{1}{B(4, 28)} \int_0^1 \theta^{z+3} (1 - \theta)^{57-z} d\theta.$$

The “cheat step”: recognise a Beta integral

Recall the Beta function

$$B(a, b) = \int_0^1 t^{a-1} (1-t)^{b-1} dt.$$

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Match exponents

$$\theta^{z+3} = \theta^{(z+4)-1}, \quad (1-\theta)^{57-z} = (1-\theta)^{(58-z)-1}.$$

So

$$\int_0^1 \theta^{z+3} (1-\theta)^{57-z} d\theta = B(z+4, 58-z).$$

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Posterior predictive pmf (Beta–Binomial)

$$\Pr(Z = z \mid y) = \binom{30}{z} \frac{B(z+4, 58-z)}{B(4, 28)}, \quad z = 0, 1, \dots, 30.$$

Predictive mean (fast route, no summing)

Law of iterated expectation

$$\mathbb{E}[Z \mid y] = \mathbb{E}_{\theta|y}[\mathbb{E}[Z \mid \theta]].$$

For $Z \mid \theta \sim \text{Bin}(30, \theta)$, $\mathbb{E}[Z \mid \theta] = 30\theta$, hence

$$\mathbb{E}[Z \mid y] = 30 \mathbb{E}[\theta \mid y] = 30 \cdot \frac{4}{4 + 28} = 30 \cdot \frac{1}{8} = 3.75.$$

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Interpretation

Given last year's data, we expect about **3.75** students to hand in late this year.

Computing the pmf in R (Beta via Gamma)

Beta function identity

$$B(a, b) = \frac{\Gamma(a)\Gamma(b)}{\Gamma(a+b)}.$$

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```
pmf: choose(n,z) * B(z+alpha, n-z+beta) / B(alpha,beta) num <- gamma(z + alpha) *  
gamma(n - z + beta) * gamma(alpha + beta) den <- gamma(alpha) * gamma(beta) *  
gamma(n + alpha + beta)  
out <- choose(n, z) * (num / den) return(out)
```

Check it is a valid pmf + plot

```
sum(ppd)  should be 1 (up to numerical error)
plot(z, ppd, xlab = "z", ylab = "Posterior predictive mass", main = "Posterior
predictive (Beta-Binomial)")
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Sanity checks you should always do

- Non-negativity: $\Pr(Z = z \mid y) \geq 0$ for all z .
- Sums to 1: $\sum_{z=0}^n \Pr(Z = z \mid y) = 1$.
- Shape makes sense: mode near the expected value.

Predictive CDF, intervals, and a probability statement

```
CDF cdf <- cumsum(ppd) cbind(z, cdf)  
Probability up to 8 late submissions sum(ppd[z <= 8])
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Interpreting outputs

- $\mathbb{E}[Z \mid y] = 3.75$ means: **expected number** of late submissions is 3.75.
- $\Pr(Z \leq 8 \mid y) \approx 0.954$ means: **about a 95.4% chance** of up to 8 late submissions.

What changed compared to a plug-in estimate?

A common non-Bayesian “plug-in” approach

Estimate θ first (e.g. MLE $\hat{\theta} = y/n_0 = 3/30 = 0.1$), then predict:

$$Z \approx \text{Bin}(30, 0.1).$$

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Instead of fixing θ at one value, we average over $\theta \mid y$:

$$\pi(z \mid y) = \int \text{Bin}(z; 30, \theta) \pi(\theta \mid y) d\theta.$$

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Practical implication

Bayesian prediction is typically **more uncertain** than plug-in prediction (because it includes parameter uncertainty, not just Binomial noise).

Example 3.7: Bayesian linear model (setup)

For $i = 1, \dots, n$:

$$Y_i = x_i^\top \beta + \varepsilon_i, \quad \varepsilon_i \stackrel{i.i.d}{\sim} \mathcal{N}(0, \sigma^2),$$

where $x_i \in \mathbb{R}^p$ are fixed covariates and $\beta \in \mathbb{R}^p$ are unknown coefficients.

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$$Y = X\beta + \varepsilon, \quad \varepsilon \sim \mathcal{N}(0, \sigma^2 I_{n \times n}).$$

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Two tasks

- 1 Posterior distribution: $\pi(\beta \mid y)$
- 2 Posterior predictive for a new covariate x' :

$$Y' = x'^\top \beta + \varepsilon', \quad \varepsilon' \sim \mathcal{N}(0, \sigma^2)$$

Find $\pi(y' \mid y, x')$.

Likelihood

Because $Y \mid \beta \sim \mathcal{N}(X\beta, \sigma^2 I)$,

$$\pi(y \mid \beta) \propto \exp\left(-\frac{1}{2\sigma^2} \|y - X\beta\|_2^2\right).$$

Prior and likelihood

Likelihood

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Prior (Gaussian)

Assume

$$\beta \sim \mathcal{N}(0, c^2 I_{p \times p}).$$

So

$$\pi(\beta) \propto \exp\left(-\frac{1}{2c^2} \|\beta\|_2^2\right).$$

Why this is convenient

Normal prior + Normal likelihood $\Rightarrow$ Normal posterior (conjugacy).

Posterior distribution (Gaussian update / Bayes rule for Gaussians)

Posterior is multivariate Normal

$$\beta \mid y \sim \mathcal{N}(\mu, \Sigma)$$

with

$$\mu = (X^\top X + \frac{\sigma^2}{c^2} I)^{-1} X^\top y,$$

$$\Sigma = \left(\frac{1}{\sigma^2} X^\top X + \frac{1}{c^2} I \right)^{-1}.$$

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Interpretation

- $X^\top X$ measures how informative the design is.
- σ^2 controls observation noise (less noise $\Rightarrow$ sharper posterior).
- c^2 controls prior strength (smaller $c^2 \Rightarrow$ more shrinkage toward 0).

Connection to ridge regression

OLS estimator (frequentist)

If $X^\top X$ is invertible (typically $n > p$),

$$\hat{\beta}_{\text{OLS}} = (X^\top X)^{-1} X^\top y = \arg \min_{\beta \in \mathbb{R}^p} \|y - X\beta\|_2^2.$$

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Ridge estimator

$$\hat{\beta}_\lambda^{\text{ridge}} = \arg \min_{\beta \in \mathbb{R}^p} \{ \|y - X\beta\|_2^2 + \lambda \|\beta\|_2^2 \} = (X^\top X + \lambda I)^{-1} X^\top y.$$

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Bayesian link

Posterior mean equals ridge estimator with

$$\lambda = \frac{\sigma^2}{c^2}, \quad \mu = (X^\top X + \lambda I)^{-1} X^\top y.$$

MAP viewpoint: why ridge appears

Posterior mode (MAP)

$$\beta_{\text{MAP}} = \arg \max_{\beta} \pi(\beta \mid y) = \arg \max_{\beta} \pi(y \mid \beta)\pi(\beta).$$

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Take logs and flip sign

$$\begin{aligned} \beta_{\text{MAP}} &= \arg \max_{\beta} \{ \log \pi(y \mid \beta) + \log \pi(\beta) \} \\ &= \arg \min_{\beta} \left\{ \frac{1}{\sigma^2} \|y - X\beta\|_2^2 + \frac{1}{c^2} \|\beta\|_2^2 \right\}. \end{aligned}$$

Multiply by σ^2 :

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Posterior predictive for a new input x'

New observation model

$$Y' = x'^{\top} \beta + \varepsilon', \quad \varepsilon' \sim \mathcal{N}(0, \sigma^2), \quad \varepsilon' \perp \beta.$$

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Posterior predictive definition

$$\pi(y' | y, x') = \int \pi(y' | \beta, x') \pi(\beta | y) d\beta.$$

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Key simplification

$\pi(y' | \beta, x')$ is Normal and $\pi(\beta | y)$ is Normal, so the integral is analytic and the posterior predictive is also Normal.

Posterior predictive via “linear combination of Gaussians”

Write

$$Y' = x'^{\top} \beta + \varepsilon'.$$

Given y , we have $\beta \mid y \sim \mathcal{N}(\mu, \Sigma)$ and $\varepsilon' \sim \mathcal{N}(0, \sigma^2)$ independent.

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Mean

$$\mathbb{E}[Y' \mid y, x'] = \mathbb{E}[x'^{\top} \beta \mid y] + \mathbb{E}[\varepsilon'] = x'^{\top} \mu.$$

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Mean

$$\mathbb{E}[Y' \mid y, \mathbf{x}'] = \mathbb{E}[\mathbf{x}'^\top \beta \mid y] + \mathbb{E}[\varepsilon'] = \mathbf{x}'^\top \mu.$$

Variance

$$\text{Var}(Y' \mid y, \mathbf{x}') = \text{Var}(\mathbf{x}'^\top \beta \mid y) + \text{Var}(\varepsilon') = \mathbf{x}'^\top \Sigma \mathbf{x}' + \sigma^2.$$

Posterior predictive via “linear combination of Gaussians”

Write

$$Y' = x'^{\top} \beta + \varepsilon'.$$

Given y , we have $\beta \mid y \sim \mathcal{N}(\mu, \Sigma)$ and $\varepsilon' \sim \mathcal{N}(0, \sigma^2)$ independent.

Mean

$$\mathbb{E}[Y' \mid y, x'] = \mathbb{E}[x'^{\top} \beta \mid y] + \mathbb{E}[\varepsilon'] = x'^{\top} \mu.$$

Variance

$$\text{Var}(Y' \mid y, x') = \text{Var}(x'^{\top} \beta \mid y) + \text{Var}(\varepsilon') = x'^{\top} \Sigma x' + \sigma^2.$$

Posterior predictive distribution

$$Y' \mid y, x' \sim \mathcal{N}\left(x'^{\top} \mu, x'^{\top} \Sigma x' + \sigma^2\right).$$

Interpretation: what contributes to predictive uncertainty?

Two sources

$$\text{Var}(Y' \mid y, x') = \underbrace{x'^{\top} \Sigma x'}_{\text{parameter uncertainty}} + \underbrace{\sigma^2}_{\text{irreducible noise}} .$$

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Intuition

- If you have tons of data, Σ shrinks and $x'^{\top} \Sigma x'$ gets small.
- Even with infinite data, you cannot beat the observation noise σ^2 .

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Prediction interval

A 95% predictive interval is approximately

$$x'^{\top} \mu \pm 1.96 \sqrt{x'^{\top} \Sigma x' + \sigma^2}.$$

Three common computation routes

1) Closed form (conjugacy)

- Beta–Binomial $\Rightarrow$ Beta–Binomial predictive
- Normal–Normal $\Rightarrow$ Normal predictive
- Gaussian linear model (with known σ^2) $\Rightarrow$ Normal predictive

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Approximate the integral in (3.1) by:

$$\pi(z | y) \approx \frac{1}{M} \sum_{m=1}^M \pi(z | \theta^{(m)}), \quad \theta^{(m)} \sim \pi(\theta | y).$$

Or simulate $Z^{(m)}$ by two-stage sampling.

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3) Approximate posteriors

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Laplace approximation, variational Bayes, etc. give an approximate $\pi(\theta \mid y)$, then plug into (3.1).

Posterior predictive sampling algorithm

- 1 Draw $\theta^{(1)}, \dots, \theta^{(M)} \sim \pi(\theta | y)$.
- 2 For each draw, simulate $Z^{(m)} \sim \pi(z | \theta^{(m)})$.
- 3 Approximate:

$$\mathbb{E}[Z | y] \approx \frac{1}{M} \sum_{m=1}^M Z^{(m)}, \quad \Pr(Z \leq k | y) \approx \frac{1}{M} \sum_{m=1}^M \mathbb{1}\{Z^{(m)} \leq k\}.$$

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Why this is conceptually perfect

It literally follows the Bayesian generative story:

$$\theta | y \rightarrow Z | \theta.$$

Summary: what you must remember

Posterior predictive (core formula)

$$\pi(z | y) = \int \pi(z | \theta) \pi(\theta | y) d\theta.$$

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Interpretation

“The posterior predictive averages the sampling model for new data over the posterior uncertainty in the parameters.”

Quick practice questions (good revision)

- 1 (Concept) Explain why $\pi(z | y)$ is typically more dispersed than $\pi(z | \hat{\theta})$ for a plug-in estimate $\hat{\theta}$.
- 2 (Beta-Binomial) If y successes out of n_0 and prior $\theta \sim \text{Beta}(\alpha, \beta)$, write down $\Pr(Z = z | y)$ for $Z | \theta \sim \text{Bin}(n, \theta)$.
- 3 (Linear model) Identify which term in $x'^T \Sigma x' + \sigma^2$ comes from parameter uncertainty and which term is irreducible noise.
- 4 (Computation) Describe the two-stage Monte Carlo method to draw from $\pi(z | y)$.

Optional: one-slide cheat sheet

Object	Formula / meaning
Posterior	$\pi(\theta y) \propto \pi(y \theta)\pi(\theta)$
Posterior predictive	$\pi(z y) = \int \pi(z \theta)\pi(\theta y) d\theta$
Predictive mean	$\mathbb{E}[Z y] = \mathbb{E}_{\theta y}[\mathbb{E}[Z \theta]]$
Beta-Binomial PPD	$\Pr(Z = z y) = \binom{n}{z} \frac{B(z + \alpha, n - z + \beta)}{B(\alpha, \beta)}$
Bayes linear posterior	$\beta y \sim \mathcal{N}(\mu, \Sigma), \mu = (X^\top X + \sigma^2/c^2 I)^{-1} X^\top y, \Sigma = (\frac{1}{\sigma^2} X^\top X + \frac{1}{c^2} I)^{-1}$
Bayes linear predictive	$Y' y, x' \sim \mathcal{N}(x'^\top \mu, x'^\top \Sigma x' + \sigma^2)$

Non-informative priors: the idea and the snag

Definition 3.4 (informal)

A prior is “non-informative” if it places equal weight across plausible values of θ . On a bounded interval, this suggests:

$$\theta \sim \text{Unif}[a, b].$$

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Practical takeaway

Uniform(0,1) is genuinely simple for probabilities. For unbounded parameters, “non-informative” needs more care.

Unintended consequence: non-informative is not invariant

Example: reparameterisation

Let $\theta \sim \text{Unif}(0, 1)$ with density $\pi(\theta) = 1$. Define $\phi = \theta^2$.

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Example: reparameterisation

Let $\theta \sim \text{Unif}(0, 1)$ with density $\pi(\theta) = 1$. Define $\phi = \theta^2$.

Change of variables

$\theta = \sqrt{\phi}$ and

$$\left| \frac{d\theta}{d\phi} \right| = \frac{1}{2\sqrt{\phi}}.$$

So

$$\pi_{\phi}(\phi) = \pi_{\theta}(\sqrt{\phi}) \left| \frac{d\theta}{d\phi} \right| = 1 \cdot \frac{1}{2\sqrt{\phi}}, \quad 0 < \phi < 1.$$

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Meaning

Flat in θ is **not** flat in ϕ . A “non-informative” prior depends on the parameterisation.

Picture intuition for the reparameterisation issue

Why does $\phi = \theta^2$ bias toward small values?

For $\theta \in (0, 1)$, squaring makes numbers smaller:

$$0.3^2 = 0.09, \quad 0.8^2 = 0.64.$$

So lots of θ values get “squeezed” near $\phi = 0$.

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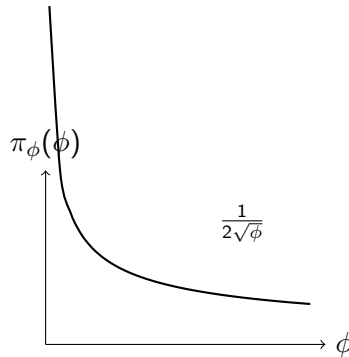
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Density behaviour

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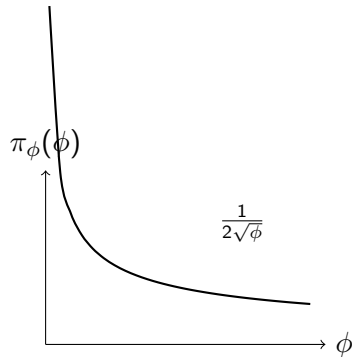
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Preview

Summary: what to remember for prediction

Posterior predictive = mixture over posterior

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Interpretation you can always write in words

- $\pi(z | \theta)$: how the model generates new data if θ were known.
- $\pi(\theta | y)$: uncertainty about θ after seeing data.
- integral: average predictions over all plausible θ values.

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- $\pi(z | \theta)$: how the model generates new data if θ were known.
- $\pi(\theta | y)$: uncertainty about θ after seeing data.
- integral: average predictions over all plausible θ values.

Example 3.6

Beta prior + Binomial likelihood $\Rightarrow$ Beta posterior, and Binomial + Beta $\Rightarrow$ Beta-Binomial predictive.

Revision questions (quick checks)

- 1 Explain (in one sentence) why $\pi(z | y)$ is a mixture distribution.
- 2 In Example 3.6, identify $\pi(z | \theta)$ and $\pi(\theta | y)$ explicitly.
- 3 Compute $\mathbb{E}[Z | y]$ using $\mathbb{E}[Z | y] = 30 \mathbb{E}[\theta | y]$.
- 4 Why do “constants” matter more for posterior predictive than for MAP estimation?
- 5 Give an example showing that “uniform prior” is not invariant under reparameterisation.