

Bayesian Methods

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1 Foundations

1.1 Definitions, identities

Notation

- Upper-case letters (A, B, C, X, Y): random variables
- Lower-case letters (a, b, c, x, y): real numbers
- $P(X = x) =: P(x)$
- $P(X = x \text{ and } Y = y) =: P(x, y)$
- $P(A = a, \text{ given } B = b) =: P(a | b)$
- $\int_{-\infty}^{+\infty} [\dots] da =: \sum_{a \in \mathbb{R}} [\dots] =: \sum_a [\dots]$

Conditional probability

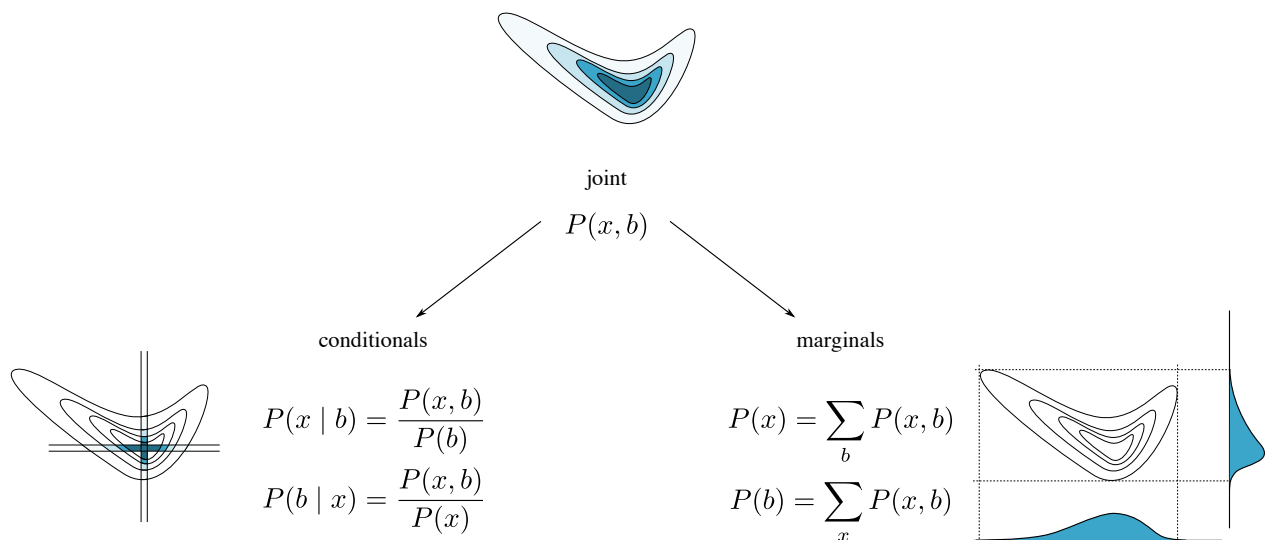
- $P(a | b) = \frac{P(a, b)}{P(b)}$
- $P(a, b) = P(a | b) P(b)$
- $P(a, b | c) = P(a | b, c) P(b | c)$
- $\sum_a P(a | b) = 1$, but $\sum_b P(a | b) \neq 1$, in general
- $\sum_b P(a | b) P(b) = \sum_b P(a, b) = P(a)$

Marginal

- $P(a) = \sum_b P(a | b) P(b)$

Bayes theorem

- $P(b | x) = \frac{1}{P(x)} P(x | b) P(b)$



1.2 Bayesian inference

Prior, likelihood, posterior

- Data: $D = \{x_1, x_2, \dots, x_n\}$, independent measurements.
- Model: M with θ : parameter(s) to estimate
- Prior: $P(\theta)$
- Likelihood: $P(D | \theta) = P(x_1 | \theta) P(x_2 | \theta) \dots P(x_n | \theta) = \prod_{i=1}^n P(x_i | \theta)$
- Unnormalized posterior: $P^*(\theta | D) = P(D | \theta) P(\theta)$
- Normalization: $Z = \sum_{\theta} P^*(\theta | D)$
- Posterior: $P(\theta | D) = \frac{1}{Z} P^*(\theta | D)$

Example

“Three light bulbs of the same make lasted 1, 2 and 5 months of continuous use. Let us estimate the lifetime of this kind of light bulb.”

- $D = \{t_1, t_2, t_3\} = \{1, 2, 5\}$
- M : Light bulbs have average lifetime of T months.
- $P(T) = \frac{1}{1000}$, uniform on $[0, 1000]$.
- $P(t | T) = \frac{1}{T} \exp\left(-\frac{t}{T}\right)$
- $P(D | T) = \prod_i P(t_i | T) = \prod_{i=1}^3 \frac{1}{T} \exp\left(-\frac{t_i}{T}\right) = \frac{1}{T^3} \exp\left(-\frac{1+2+5}{T}\right)$
- $P^*(T | D) = \frac{1}{T^3} \exp\left(-\frac{8}{T}\right)$
- Z and $P(T | D)$ can be determined numerically:

```
1 import numpy as np
2
3 T_arr = np.linspace(0.1, 1000, 10_000)
4 Pstar_arr = 1.0/T_arr**3 * np.exp(-8/T_arr)
5 Z = np.sum(Pstar_arr)
6 P_arr = Pstar_arr / Z
```

yielding $Z = 0.1562$

- $\mathbb{E}(T | D) = \sum_T T P(T | D)$
- $\text{std}(T | D) = \sqrt{\sum_T (T - \mathbb{E}(T))^2 P(T | D)}$

```
1 T_ev = np.sum(T_arr * P_arr)
2 T_std = np.sqrt(np.sum((T_arr - T_ev)**2 * P_arr))
```

yielding $\mathbb{E}(T | D) = 7.937$, $\text{std}(T | D) = 14.48$.

1.3 Model comparison

New definition: Evidence

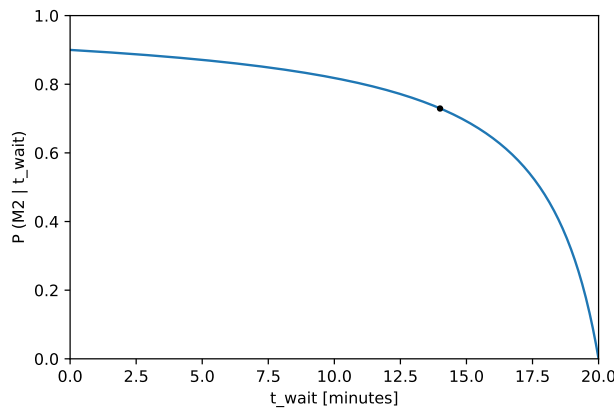
- Data: D
- Model 1: M_1 with parameter θ_1 and prior $P(\theta_1 | M_1)$, and likelihood $P(D | \theta_1, M_1)$
- Model 2: M_2 with parameter θ_2 and prior $P(\theta_2 | M_2)$, and likelihood $P(D | \theta_2, M_2)$
- Prior on models: $P(M_1) = 0.5$, $P(M_2) = 0.5$.
- Evidence for each model: $P(D | M_i) = \sum_{\theta} P(D | \theta_i, M_i) P(\theta_i | M_i)$
- Unnormalized posterior: $P^*(M_1 | D) = P(D | M_1) P(M_1)$, and $P^*(M_2 | D) = P(D | M_2) P(M_2)$
- Normalization: $Z = P^*(M_1 | D) + P^*(M_2 | D)$.

Example

“Waiting for my baggage at the airport carousel, there are two possibilities: 1) It could miss the plane, and will never come, or 2) It was on the plane and it had a $1/20$ chance of arriving within any of the 1-minute intervals between 0 and 20 minutes. Now, given what is the posterior probability of model 2 given that 14 minutes has passed and the bag has not arrived?”

- $D = \{\text{Bag has not arrived after } t_{\text{wait}} = 14 \text{ minutes}\}$
- M_1 : It never arrives, $P(D | M_1) = 1$
- M_2 : It shows up some time between 0 and 20 minutes, $P(t_{\text{bag}} | M_2) = 1/20$ for $t_{\text{bag}} \in [0, 20]$, and the likelihood is $P(D | t_{\text{bag}}, M_2) = 1$, if $t_{\text{bag}} > t_{\text{wait}}$, and 0 otherwise.
- $P(M_1) = 0.1$, $P(M_2) = 0.9$
- $P(D | M_1) = 1$
- $P(D | M_2) = \sum_{t_{\text{bag}}} P(D | t_{\text{bag}}, M_2) P(t_{\text{bag}} | M_2) = \sum_{t_{\text{bag}}} [t_{\text{bag}} > 14] \times \frac{1}{20} = \frac{20-14}{20}$
- $P^*(M_1 | D) = 1 \times 0.1$, $P^*(M_2 | D) = \frac{20-14}{20} \times 0.9$
- $Z = 0.1 + \frac{3}{10} \times 0.9 = 0.37$
- $P(M_2 | D) = P^*(M_2 | D)/Z = 0.7297$.

We can also plot $P(M_2 | t_{\text{wait}})$ for all waiting times between 0 and 20 minutes.



1.4 Prediction

New definition: Predictive distribution

- Data: $D = \{x_1, x_2, \dots, x_n\}$
- Model: M with parameter θ , prior $P(\theta)$ and likelihood $P(x | \theta)$
- Posterior: $P(\theta | D) = P^*(\theta | D)/Z = \dots$ (see previous sections)
- Predictive distribution: $P(X_{n+1} = x | D) = \sum_{\theta} P(x | \theta) P(\theta | D)$
- Customized prediction: $P(f(\theta) | D) = \sum_{\theta} f(\theta) P(\theta | D)$

Example

“Two player, A and B are playing a game of luck, where at the beginning of the game a ball is rolled on a pool table to divide the table in two un-equal halves: A’s side and B’s side. In each subsequent round, a ball is rolled. A point is given to the player on whose side the ball stops. A and B are playing this game until one of them reaches 6 points. The current score is 5 to 3 in favor of A. What is the chance that A will win this game?”

- $D = \{n_A = 5, n_B = 3\}$
- M , first ball: $P(b) = 1$ in $[0, 1]$
- $P(\text{A scores} | b) = b$
- $P(D | b) = \text{Binomial}(5 | 5 + 3, b)$
- $P^*(b_0 | D) = \text{Binomial}(5 | 8, b) \times 1$
- $Z = \sum_b \text{Binomial}(5 | 8, b)$ can be calculated numerically

```
1 import numpy as np
2 from scipy.stats import binom
3
4 b_arr = np.linspace(0, 1, 1000)
5 Pstar_arr = binom.pmf(5, 8, b_arr)
6 Z = np.sum(Pstar_arr)
```

- $P(\text{A wins} | b, D) = 1 - P(\text{B wins} | b, D) = 1 - (1 - b)^3 = f(b)$
- $P(\text{A wins} | D) = \sum_b f(b) P^*(b | D) / Z$

```
1 P_arr = Pstar_arr / Z
2 P_Awins = np.sum((1 - (1 - b_arr)**3) * P_arr)
```

yielding $P(\text{A wins} | D) = 0.909$

2 Exact inference and Maximum Likelihood Estimate

2.1 Maximum likelihood estimate

MLE-method

- Data: $D = \{x_1, x_2, \dots, x_N\}$
- Parameter: θ
- Likelihood: $P(x_i | \theta)$
- Total log likelihood: $L(\theta) = \log P(D | \theta) = \sum_{i=1}^N \log P(x_i | \theta)$
- Maximum likelihood estimate $\theta_{\text{MLE}} = \operatorname{argmax}_{\theta} \log P(D | \theta)$,
Numerically: with gradient descent or EM methods,
Analytically: equating first derivatives to 0, and solving the system of equations.

Example 1: Normal model

- Data: $D = \{x_i\}_{i=1}^N$
- Parameters: $\mu \in \mathbb{R}, \sigma^2 > 0$
- Likelihood: $P(x_i | \mu, \sigma^2) = \text{Normal}(x_i | \mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{(x_i - \mu)^2}{2\sigma^2}\right]$
- Total log likelihood:

$$L(\mu, \sigma^2) = \sum_{i=1}^N \log \text{Normal}(x_i | \mu, \sigma^2) = -\frac{N}{2} \log(\sigma^2) - \sum_{i=1}^N \frac{(x_i - \mu)^2}{2\sigma^2} + \text{const.}$$

- Analytical solution:

$$\begin{aligned} 0 &= \left[\frac{\partial L}{\partial \mu} \right]_{\text{MLE}} = \left[\sum_{i=1}^N \frac{\mu - x_i}{\sigma^2} \right]_{\text{MLE}} \Rightarrow \mu_{\text{MLE}} = \frac{1}{N} \sum_{i=1}^N x_i. \\ 0 &= \left[\frac{\partial L}{\partial (\sigma^2)} \right]_{\text{MLE}} = \left[-\frac{N}{2\sigma^2} + \sum_{i=1}^N \frac{(x_i - \mu)^2}{2(\sigma^2)^2} \right]_{\text{MLE}} \Rightarrow (\sigma^2)_{\text{MLE}} = \frac{1}{N} \sum_{i=1}^N (x_i - \mu_{\text{MLE}})^2 \end{aligned}$$

Example 2: Cauchy distribution

- Data: $D = \{-10, 1, 2, 5, 20\}$
- Parameters: $m \in \mathbb{R}, \quad s > 0.$
- Likelihood: $P(x_i | m, s) = \text{Cauchy}(x_i | m, s) = \frac{1}{s\pi} \frac{1}{1 + [(x_i - m)/s]^2}$
- Total log likelihood:

$$L(m, s) = \sum_{i=1}^N \log \text{Cauchy}(x_i | m, s) = -N \log(s) - \sum_{i=1}^N \log \left(1 + \left[\frac{x_i - m}{s} \right]^2 \right)$$

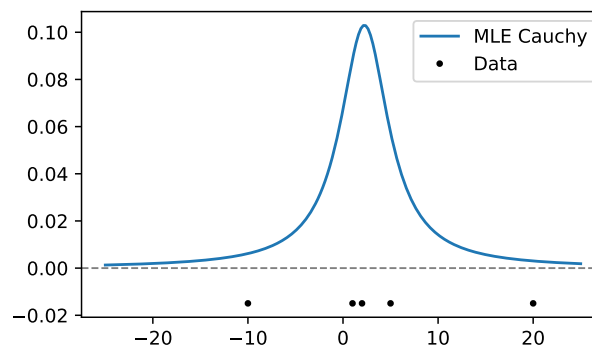
- Numerical maximization (starting from $m_0 = 0, s_0 = 10$):

```

1 import numpy as np
2 from scipy.optimize import minimize
3
4 def cauchy_total_log_likelihood(X, m, s):
5     X = np.array(X)
6
7     L = 0
8     L += -len(X)/2 * np.log(s**2)
9     L += -np.sum( np.log(1 + (X - m)**2 / s**2 ) )
10
11     return L
12
13 X = [-10, 1, 2, 5, 20]
14 def func_to_minimize(theta):
15     m = theta[0]
16     s = theta[1]
17     return - cauchy_total_log_likelihood(X, m, s)
18
19 m0 = 0
20 s0 = 10
21 result = minimize(func_to_minimize, [m0, s0])
22 m_MLE, s_MLE = result.x

```

yielding $m_{\text{MLE}} = 2.251$, $s_{\text{MLE}} = 3.090$, the resulting MLE fit is shown below.



2.2 Exact inference examples

Binomial model

- Data: $D = \{(k_1, n_1), (k_2, n_2), \dots, (k_N, n_N)\}$, where k_i (successes), n_i (attempts) $\in \mathbb{N}$ and $k_i \leq n_i$
- Parameter: p (probability of success) $\in [0, 1]$, flat prior: $P(p) = 1$, on $[0, 1]$
- Likelihood: $P(k_i | n_i, p) = \text{Binomial}(k_i | n_i, p) = \binom{n_i}{k_i} p^{k_i} (1-p)^{n_i-k_i}$
- Posterior:

$$\begin{aligned} P(p | D) &= \frac{1}{Z} \prod_{i=1}^N [p^{k_i} (1-p)^{n_i-k_i}] = \frac{1}{Z} p^{k_{\text{tot}}} (1-p)^{n_{\text{tot}}-k_{\text{tot}}} \\ &= \frac{\Gamma(\alpha + \beta)}{\Gamma(\alpha)\Gamma(\beta)} p^{\alpha-1} (1-p)^{\beta-1} = \text{Beta}(p | \alpha = k_{\text{tot}} + 1, \beta = n_{\text{tot}} - k_{\text{tot}} + 1), \end{aligned}$$

where $k_{\text{tot}} = \sum_i k_i$ and $n_{\text{tot}} = \sum_i n_i$. Mean, mode and standard deviation are

$$\begin{aligned} \mathbb{E}(p) &= \frac{\alpha}{\alpha + \beta} = \frac{k_{\text{tot}} + 1}{n_{\text{tot}} + 2}, \quad \text{mode}(p) = \frac{\alpha - 1}{\alpha + \beta - 2} = \frac{k_{\text{tot}}}{n_{\text{tot}}}, \\ \text{std}(p) &= \frac{\sqrt{\alpha\beta}}{(\alpha + \beta)\sqrt{\alpha + \beta + 1}} = \frac{\sqrt{(k_{\text{tot}} + 1)(n_{\text{tot}} - k_{\text{tot}} + 1)}}{(n_{\text{tot}} + 2)\sqrt{n_{\text{tot}} + 3}} \end{aligned}$$

Poisson model

- Data: $D = \{k_1, k_2, \dots, k_N\}$, where k_i (number of events) $\in \mathbb{N}$
- Parameters: λ (expected number of events) > 0 , flat prior: $P(\lambda) = \text{const.}$
- Likelihood: $P(k_i | \lambda) = \text{Poisson}(k_i | \lambda) = e^{-\lambda} \frac{\lambda^{k_i}}{k_i!}$
- Posterior:

$$P(\lambda | D) = \frac{1}{Z} \prod_{i=1}^N [e^{-\lambda} \lambda^{k_i}] = \frac{1}{Z} e^{-N\lambda} \lambda^{k_{\text{tot}}} = \frac{\beta^\alpha}{\Gamma(\alpha)} \lambda^{\alpha-1} e^{-\beta\lambda} = \text{Gamma}(\lambda | \alpha = k_{\text{tot}} + 1, \beta = N),$$

where $k_{\text{tot}} = \sum_i k_i$. Mean, mode and standard deviation are

$$\mathbb{E}(\lambda) = \frac{\alpha}{\beta} = \frac{k_{\text{tot}} + 1}{N}, \quad \text{mode}(\lambda) = \frac{\alpha - 1}{\beta} = \frac{k_{\text{tot}}}{N}, \quad \text{std}(\lambda) = \frac{\sqrt{\alpha}}{\beta} = \frac{\sqrt{k_{\text{tot}} + 1}}{N}$$

Multinomial model

- Data: $D = \{(k_{1,1}, k_{1,2}, \dots, k_{1,M}), (k_{2,1}, k_{2,2}, \dots, k_{2,M}), \dots, (k_{N,1}, k_{N,2}, \dots, k_{N,M})\}$, where $k_{i,j}$ (counts of outcome j) $\in \mathbb{N}$, and $\sum_j k_{i,j} = 1, \forall i$.
- Parameters: $p = (p_1, p_2, \dots, p_M)$, where p_j (probability of outcome j) > 0 and $\sum_j p_j = 1$; flat prior: $P(p) = \text{const.}$
- Likelihood: $P(\{k_{i,j}\}_{j=1}^M | p) = \text{Multinomial}(\{k_{i,j}\}_{j=1}^M | p) = k_{i,\text{tot}}! \prod_j \frac{p_j^{k_{i,j}}}{k_{i,j}!}$
- Posterior:

$$P(p | D) = \frac{1}{Z} \prod_{i=1}^N \prod_{j=1}^M (p_j)^{k_{i,j}} = \frac{1}{Z} \prod_{j=1}^M (p_j)^{k_{\text{tot},j}} = \Gamma(\alpha_{\text{tot}}) \prod_{j=1}^M \frac{(p_j)^{\alpha_j - 1}}{\Gamma(\alpha_j)} = \text{Dirichlet}(p | \alpha_j = k_{\text{tot},j} + 1),$$

where $k_{i,\text{tot}} = \sum_j k_{i,j}$, $k_{\text{tot},j} = \sum_i k_{i,j}$, and $\alpha_{\text{tot}} = \sum_j \alpha_j = k_{\text{tot},\text{tot}} + M$. Mean, mode and marginal standard deviation are

$$\begin{aligned} \mathbb{E}(p_j) &= \frac{\alpha_j}{\alpha_{\text{tot}}} = \frac{k_{\text{tot},j} + 1}{k_{\text{tot},\text{tot}} + M}, \quad \text{mode}(p) : p_j = \frac{\alpha_j - 1}{\alpha_{\text{tot}} - M} = \frac{k_{\text{tot},j}}{k_{\text{tot},\text{tot}}} \\ \text{std}(p_j) &= \frac{\sqrt{\alpha_j(\alpha_{\text{tot}} - \alpha_j)}}{\alpha_{\text{tot}} \sqrt{\alpha_{\text{tot}} + 1}} = \frac{\sqrt{(k_{\text{tot},j} + 1)(k_{\text{tot},\text{tot}} - k_{\text{tot},j} + M - 1)}}{(k_{\text{tot},\text{tot}} + M) \sqrt{k_{\text{tot},\text{tot}} + M + 1}} \end{aligned}$$

Exponential model

- Data: $D = \{t_1, t_2, \dots, t_N\}$, where t_i (waiting times) > 0
- Parameter: γ (rate) > 0 , flat prior: $P(\gamma) = \text{const.}$
- Likelihood: $P(t_i | \gamma) = \text{Exponential}(t_i | \gamma) = \gamma e^{-\gamma t_i}$
- Posterior:

$$P(\gamma | D) = \frac{1}{Z} \prod_{i=1}^N [\gamma e^{-\gamma t_i}] = \frac{1}{Z} \gamma^N e^{-\gamma t_{\text{tot}}} = \frac{\beta^\alpha}{\Gamma(\alpha)} \gamma^{\alpha-1} e^{-\beta \gamma} = \text{Gamma}(\gamma | \alpha = N + 1, \beta = t_{\text{tot}}),$$

where $t_{\text{tot}} = \sum_i t_i$. Mean, mode, standard deviation are

$$\mathbb{E}(\gamma) = \frac{\alpha}{\beta} = \frac{N + 1}{t_{\text{tot}}}, \quad \text{mode}(\gamma) = \frac{\alpha - 1}{\beta} = \frac{N}{t_{\text{tot}}}, \quad \text{std}(\gamma) = \frac{\sqrt{\alpha}}{\beta} = \frac{\sqrt{N + 1}}{t_{\text{tot}}}$$

Normal

- Data: $D = \{x_1, x_2, \dots, x_N\}$, where x (value) $\in \mathbb{R}$
- Parameters: μ (expected value) $\in \mathbb{R}$, σ^2 (variance) > 0 , uninformative prior: $P(\mu, \sigma^2) = \text{const.}$
- Likelihood: $P(x_i | \mu, \sigma^2) = \text{Normal}(x_i | \mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{(x_i - \mu)^2}{2\sigma^2}\right]$
- Posterior:

$$\begin{aligned}
P(\mu, \sigma^2 | D) &= \frac{1}{Z} \prod_{i=1}^N \left\{ \frac{1}{\sqrt{\sigma^2}} \exp\left[-\frac{(x_i - \mu)^2}{2\sigma^2}\right] \right\} = \frac{1}{Z} \left(\frac{1}{\sigma^2}\right)^{N/2} \exp\left[-\frac{Ns^2 + N(\mu - m)^2}{2\sigma^2}\right] \\
&= \frac{\sqrt{\lambda}}{\sqrt{2\pi\sigma^2}} \frac{\beta^\alpha}{\Gamma(\alpha)} \left(\frac{1}{\sigma^2}\right)^{\alpha+1} \exp\left[-\frac{2\beta + \lambda(\mu - \mu_c)^2}{2\sigma^2}\right] \\
&= \text{Normal-Inverse-Gamma}\left(\mu, \sigma^2 \mid \alpha = \frac{N-3}{2}, \beta = \frac{Ns^2}{2}, \mu_c = m, \lambda = N\right),
\end{aligned}$$

where $m = \frac{1}{N} \sum_i x_i$ is the empirical mean, $s^2 = \frac{1}{N} \sum_i (x_i - m)^2$ is the empirical variance. The mode is identical to the MLE result

$$\text{mode}(\mu, \sigma^2) = (m, s^2).$$

The marginal, and mean, mode and standard deviation of μ is

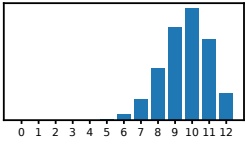
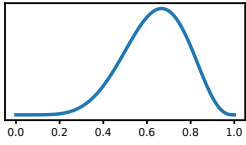
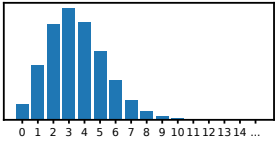
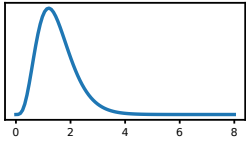
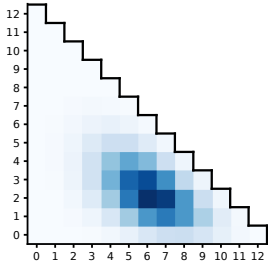
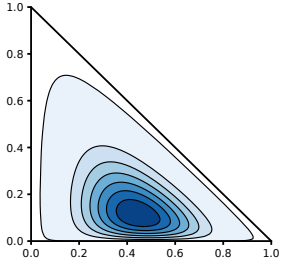
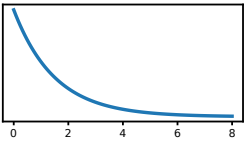
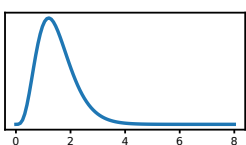
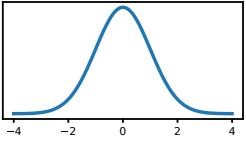
$$\begin{aligned}
P(\mu | D) &= \sum_{\sigma^2} P(\mu, \sigma^2 | D) = \frac{\Gamma\left(\frac{N-2}{2}\right)}{\Gamma\left(\frac{N-3}{2}\right)} \frac{1}{\sqrt{\pi s^2}} \left[1 + \frac{(\mu - m)^2}{s^2}\right]^{-(N-2)/2} \\
&= \frac{\Gamma\left(\frac{\nu+1}{2}\right)}{\Gamma\left(\frac{\nu}{2}\right)} \frac{1}{\sqrt{\pi\nu}} \left[1 + \frac{1}{\nu} \left(\frac{\mu - \text{loc}}{\text{scale}}\right)^2\right]^{-(\nu+1)/2} \frac{1}{\text{scale}} \\
&= \text{t-distr}\left(\mu \mid \text{loc} = m, \text{scale} = \frac{s}{\sqrt{N-3}}, \nu = N-3\right),
\end{aligned}$$

$$\mathbb{E}(\mu) = m, \quad \text{mode}(\mu) = m, \quad \text{std}(\mu) = \frac{s}{\sqrt{N-3}} \sqrt{\frac{\nu}{\nu-2}} = \frac{s}{\sqrt{N-5}},$$

where ν is the “degrees of freedom” of the Student’s t-distribution. The marginal, and mean, mode and standard deviation of σ^2 is

$$\begin{aligned}
P(\sigma^2 | D) &= \sum_{\mu} P(\mu, \sigma^2 | D) = \frac{\beta^\alpha}{\Gamma(\alpha)} \left(\frac{1}{\sigma^2}\right)^{\alpha+1} \exp\left(-\frac{\beta}{\sigma^2}\right) \\
&= \text{Inverse-Gamma}\left(\sigma^2 \mid \alpha = \frac{N-3}{2}, \beta = \frac{Ns^2}{2}\right)
\end{aligned}$$

$$\mathbb{E}(\sigma^2) = \frac{\beta}{\alpha-1} = s^2 \frac{N}{N-5}, \quad \text{mode}(\sigma^2) = \frac{\beta}{\alpha+1} = s^2 \frac{N}{N-1}, \quad \text{std}(\sigma^2) = \frac{\beta}{(\alpha-1)\sqrt{\alpha-2}} = s^2 \frac{\sqrt{2}N}{(N-5)\sqrt{N-7}}$$

Model	Posterior
Binomial 	Beta 
Poisson 	Gamma 
Multinomial 	Dirichlet 
Exponential 	Gamma 
Normal 	Normal-Inverse-Gamma 