Bayesian Methods

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Contents

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
- $P(X = x) \ =: \ P(x)$
- $P(X = x \text{ and } Y = y) \ =: \ P(x, y)$
- $P(A = a, \text{ given } B = b) \ =: \ P(a \mid b)$
- $\int_{\infty}^{+\infty} [\ldots] da \ =: \ \sum_{a \in \mathbb{R}} [\ldots] \ =: \ \sum_a [\ldots]$

Conditional probability

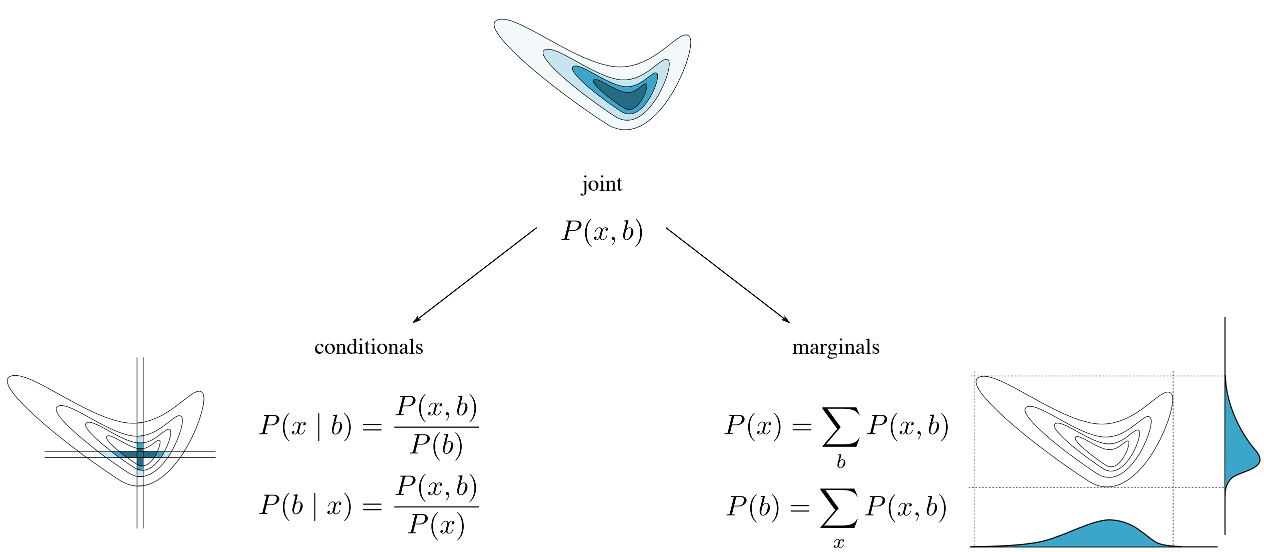
- $P(a \mid b) \ = \ \frac{P(a,b)}{P(b)}$
- $P(a, b) \ = \ P(a \mid b) \, P(b)$
- $P(a, b \mid c) \ = \ P(a \mid b, c) \, P(b \mid c)$
- $\sum_a P(a \mid b) \ = \ 1, \quad \text{but} \ \ \sum_b P(a \mid b) \neq 1$, in general
- $\sum_b P(a \mid b) \, P(b) \ = \ \sum_b P(a, b) \ = \ P(a)$

Marginal

- $P(a) \ = \ \sum_b P(a \mid b) \, P(b)$

Bayes theorem

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



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: $P(D \mid \theta) = P(x_1 \mid \theta)\, P(x_2 \mid \theta)\, \dots\, P(x_n \mid \theta) = \prod_{i=1}^{n} P(x_i \mid \theta)$
- Unnormalized posterior: $P^*(\theta \mid D) \;=\; P(D \mid \theta)\, P(\theta)$
- Normalization: $Z = \sum_\theta P^*(\theta \mid D)$
- Posterior: $P(\theta \mid D) = \frac{1}{Z} P^*(\theta \mid D)$

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].
- $P(t \mid T) = \frac{1}{T} \exp\left(-\frac{t}{T}\right)$
- $P(D \mid T) = \prod_i P(t_i \mid T) = \prod_{i=1}^{3} \frac{1}{T} \exp\left(-\frac{t_i}{T}\right) = \frac{1}{T^3} \exp\left(-\frac{1+2+5}{T}\right)$
- $P^*(T \mid D) = \frac{1}{T^3} \exp\left(-\frac{8}{T}\right)$
- Z and $P(T \mid D)$ can be determined numerically:

```
import numpy as np

T_arr = np.linspace(0.1, 1000, 10_000)
Pstar_arr = 1.0/T_arr**3 * np.exp(-8/T_arr)
Z = np.sum(Pstar_arr)
P_arr = Pstar_arr / Z
```

  yielding $Z = 0.1562$

- $\mathbb{E}(T \mid D) = \sum_T T\; P(T \mid D)$
- $\mathrm{std}(T \mid D) = \sqrt{\sum_T (T - \mathbb{E}(T))^2\; P(T \mid D)}$

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

  yielding $\mathbb{E}(T \mid D) = 7.937, \quad \mathrm{std}(T \mid D) = 14.48.$

1.3 Model comparison

New definition: Evidence

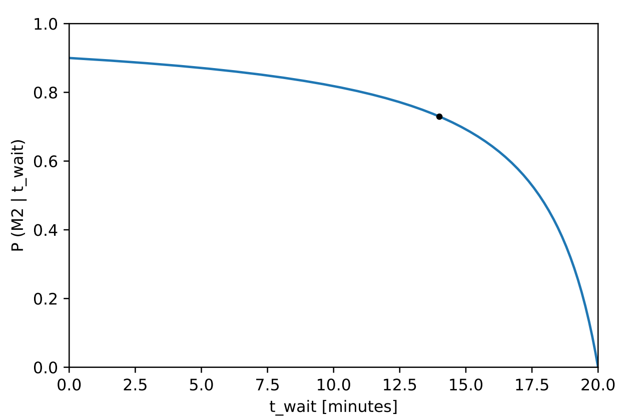
- Data: D
- Model 1: M_1 with parameter θ_1 and prior $P(\theta_1 \mid M_1)$, and likelihood $P(D \mid \theta_1, M_1)$
- Model 2: M_2 with parameter θ_2 and prior $P(\theta_2 \mid M_2)$, and likelihood $P(D \mid \theta_2, M_2)$
- Prior on models: $P(M_1) = 0.5, \quad P(M_2) = 0.5$.
- Evidence for each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

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, $P(D \mid M_1) = 1$
- M_2: It shows up some time between 0 and 20 minutes, $P(t_{\text{bag}} \mid M_2) = 1/20$ for $t_{\text{bag}} \in [0, 20]$, and the likelihood is $P(D \mid t_{\text{bag}}, M_2) = 1$, if $t_{\text{bag}} > t_{\text{wait}}$, and 0 otherwise.
- $P(M_1) = 0.1, \quad P(M_2) = 0.9$
- $P(D \mid M_1) = 1$
- $P(D \mid M_2) = \sum_{t_{\text{bag}}} P(D \mid t_{\text{bag}}, M_2)\ P(t_{\text{bag}} \mid M_2) = \sum_{t_{\text{bag}}} [t_{\text{bag}} > 14] \times \frac{1}{20} = \frac{20-14}{20}$
- $P^*(M_1 \mid D) = 1 \times 0.1, \quad P^*(M_2 \mid D) = \frac{20-14}{20} \times 0.9$
- $Z = 0.1 + \frac{3}{10} \times 0.9 = 0.37$
- $P(M_2 \mid D) = P^*(M_2 \mid D)/Z = 0.7297$.

We can also plot $P(M_2 \mid t_{\text{wait}})$ 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 $P(x \mid \theta)$
- Posterior: $P(\theta \mid D) = P^*(\theta \mid D)/Z = \dots$ (see previous sections)
- Predictive distribution: $P(X_{n+1} = x \mid D) = \sum_\theta P(x \mid \theta)\; P(\theta \mid D)$
- Customized prediction: $P(f(\theta) \mid D) = \sum_\theta f(\theta)\; P(\theta \mid D)$

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 $[0, 1]$
- $P(\text{A scores} \mid b) = b$
- $P(D \mid b) = \text{Binomial}(5 \mid 5 + 3,\ b)$
- $P^*(b_0 \mid D) = \text{Binomial}(5 \mid 8, b) \times 1$
- $Z = \sum_b \text{Binomial}(5 \mid 8, b)$ can be calculated numerically

```
import numpy as np
from scipy.stats import binom

b_arr = np.linspace(0, 1, 1000)
Pstar_arr = binom.pmf(5, 8, b_arr)
Z = np.sum(Pstar_arr)
```

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

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

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

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: $P(x_i \mid \theta)$
- Total log likelihood: $L(\theta) = \log P(D \mid \theta) = \sum_{i=1}^{N} \log P(x_i \mid \theta)$
- Maximum likelihood estimate $\theta_{\mathrm{MLE}} = \mathrm{argmax}_\theta \log P(D \mid \theta)$,
  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: $\mu \in \mathbb{R}, \quad \sigma^2 > 0$
- Likelihood: $P(x_i \mid \mu, \sigma^2) = \mathrm{Normal}(x_i \mid \mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{(x_i-\mu)^2}{2\sigma^2}\right]$
- Total log likelihood:

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

- Analytical solution:

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

- Note: These MLE results coincide with the modes of the exact posterior obtained from the non-informative prior $P(\mu, \sigma^2) = \frac{\mathrm{const.}}{\sigma}$. (See “Exact inference examples” section.)

Example 2: Cauchy distribution

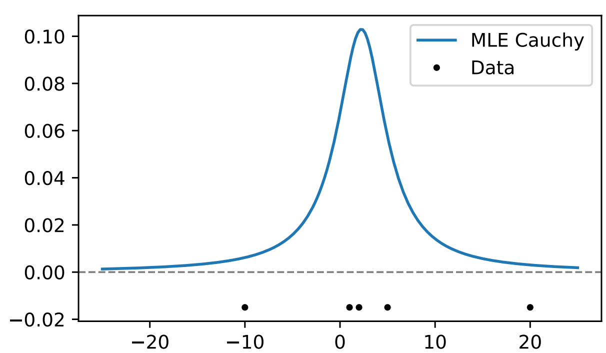
- Data: $D = \{-10, 1, 2, 5, 20\}$
- Parameters: $m \in \mathbb{R}, \quad s > 0.$
- Likelihood: $P(x_i \mid m, s) = \text{Cauchy}(x_i \mid m, s) = \frac{1}{s\pi}\frac{1}{1+[(x_i-m)/s]^2}$
- Total log likelihood:

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

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

```
import numpy as np
from scipy.optimize import minimize

def cauchy_total_log_likelihood(X, m, s):
    X = np.array(X)

    L = 0
    L += -len(X)/2 * np.log(s**2)
    L += -np.sum( np.log(1 + (X - m)**2 / s**2 ) )

    return L

X = [-10, 1, 2, 5, 20]
def func_to_minimize(theta):
    m = theta[0]
    s = theta[1]
    return - cauchy_total_log_likelihood(X, m, s)

m0 = 0
s0 = 10
result = minimize(func_to_minimize, [m0, s0])
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 $k_i \le n_i$
- Parameter: p (probability of success) $\in [0,1]$, flat prior: $P(p) = 1$, on $[0,1]$
- Likelihood: $P(k_i \mid n_i, p) = \text{Binomial}(k_i \mid n_i, p) = \binom{n_i}{k_i}\, p^{k_i}(1-p)^{n_i - k_i}$
- Posterior:

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

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

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

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: $P(k_i \mid \lambda) = \text{Poisson}(k \mid \lambda) = e^{-\lambda}\frac{\lambda^{k_i}}{k_i!}$
- Posterior:

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

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: $P(\{k_{i,j}\}_{j=1}^M \mid p) = \text{Multinomial}(\{k_{i,j}\}_{j=1}^M \mid p) = k_{i,\text{tot}}! \prod_j \frac{p_j^{k_{i,j}}}{k_{i,j}!}$
- Posterior:

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

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

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

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: $P(t_i \mid \gamma) = \text{Exponential}(t_i \mid \gamma) = \gamma e^{-\gamma t_i}$
- Posterior:

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

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

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

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: $P(\mu, \sigma^2) = \frac{\text{const.}}{\sigma}$
- Likelihood: $P(x_i \mid \mu, \sigma^2) = \text{Normal}(x_i \mid \mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{(x_i-\mu)^2}{2\sigma^2}\right]$
- Posterior:

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

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

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

$$
\mathbb{E}(\mu) = m, \quad \text{mode}(\mu) = m, \quad \text{std}(\mu) = \frac{s}{\sqrt{N-2}}\sqrt{\frac{\nu}{\nu-2}} = \frac{s}{\sqrt{N-4}},
$$

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

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

$$
\mathbb{E}(\sigma^2) = \frac{\beta}{\alpha-1} = s^2\frac{N}{N-4}, \quad \text{mode}(\sigma^2) = \frac{\beta}{\alpha+1} = s^2, \quad \text{std}(\sigma^2) = \frac{\beta}{(\alpha-1)\sqrt{\alpha-2}} = s^2\frac{\sqrt{2}N}{(N-4)\sqrt{N-6}}
$$