Probabilistic Machine Learning

EBERHARD KARLS
UNIVERSITÄT
TÜBINGEN

Exercise 3

Summer Term 2023

Full Name	Matriculation No
Batuhan Özcömlekci	6300476
Aakarsh Nair	6546577

Eberhards Karls University of Tübingen, May 13, 2023 a)

$$p(x|a,b) = g(x;a,b) = \frac{b^a}{\Gamma(a)} x^{a-1} e^{-bx} \quad \text{with } \Gamma(z)=\int_0^\infty t^{z-1}e^{-t}\,dt$$

$$\tilde p(x|a,b) = x^{a-1}e^{-bx}$$

$$\log \tilde p(x|a,b) = (a-1)\log x - bx$$

$$\frac{\partial \log\tilde p}{\partial x} = \frac{a-1}{x} - b = 0 \Rightarrow a-1 = bx \Rightarrow x^* = \frac{a-1}{b} = \hat x \text{ (mode)}$$

$$\left.\frac{\partial^2 \log \tilde p}{\partial x^2}\right|_{x=x^*} = \left.\frac{1-a}{x^2}\right|_{x=x^*} = \frac{(1-a)b^2}{(a-1)^2} = -\frac{b^2}{a-1} \quad \text{and thus } \sigma^2 = \frac{a-1}{b^2}$$

Finally $$\underbrace{q(x|a,b)}_{\text{approximation}} = N\left(x; \frac{a-1}{b}, \frac{a-1}{b^2}\right) = \frac{b\, e^{-\frac{b^2\left(x-\frac{a-1}{b}\right)^2}{2(a-1)}}}{\sqrt{2\pi(a-1)}}$$

For $b=1$, $$q(x|a,b) = N(x; a-1, a-1) = \frac{\exp\left[\frac{(x-a+1)^2}{2(a-1)}\right]}{\sqrt{2\pi(a-1)}}$$

To find Stirling approximation:

We know that $$\Gamma(a) = \int_0^\infty x^{a-1}e^{-x}\,dx = (a-1)!$$

we also know $$\int p(x|a,b) \approx p(\hat x)\int \exp\left[\frac{(x-\hat x)^2}{2\sigma^2}\right]dx = 1$$

L03, slide 35

$$1 \approx \frac{\hat x^{a-1}\, e^{-\hat x}}{\Gamma(a)} \int \exp\left[\frac{-(x-\hat x)^2}{2(a-1)}\right]dx$$

$$1 \approx \frac{(a-1)^{a-1}\, e^{-(a-1)}}{\Gamma(a)}\sqrt{2\pi(a-1)}$$

$a-1=n$

$$\Gamma(a) \approx (a-1)^{a-1}\, e^{-(a-1)}\sqrt{2\pi(a-1)} = \boxed{\sqrt{2\pi(a-1)}\left(\frac{a-1}{e}\right)^{a-1}}$$

$$\Gamma(n+1) \approx \sqrt{2\pi n}\left(\frac{n}{e}\right)^n$$

Q.E.D.

b)

$$\mathcal{N}(x_i;\mu,\Sigma) = \frac{|\Sigma^{-1}|^{\frac{1}{2}}}{(2\pi)^{\frac{d}{2}}} \exp\left[\frac{-(x_i-\mu)^T \Sigma^{-1} (x_i-\mu)}{2}\right] = p(x_i \mid \mu, \Sigma)$$

(or use $p(x_i \mid \mu, \Sigma^{-1})$)

Show conjugate prior under this likelihood:

$$p(\Sigma^{-1} \mid W, v) = \mathcal{W}(\Sigma^{-1} \mid W, v) = \frac{|\Sigma^{-1}|^{(v-d-1)/2} \exp\left(-\frac{tr(W^{-1}\Sigma^{-1})}{2}\right)}{2^{dv/2} |W|^{v/2} \Gamma_d(v/2)}$$

Where tr is the trace and $\Gamma_d = \pi^{d(d-1)/4} \prod_{i=1}^{d} \Gamma\left(z + \frac{1-i}{2}\right)$

We need to prove that the posterior distribution of Σ^{-1} after observing data $\{x_i\}$ is also in the same distributional family as the prior. In other words

$$\underbrace{p(\Sigma^{-1} \mid W, v, X)}_{\text{Wishart}} \propto p(X \mid \mu, \Sigma^{-1}) \overbrace{p(\Sigma^{-1} \mid W, v)}^{\text{Wishart}}$$

$$\propto \underbrace{\prod_i p(x_i \mid \mu, \Sigma^{-1})}_{\substack{\text{By i.i.d assumption} \\ \text{It is also a Gaussian}}} p(\Sigma^{-1} \mid W, v)$$

Using the property for positive definite square matrix Σ^{-1}:

$$(x_i-\mu)^T \Sigma^{-1} (x_i-\mu) = tr\left((x_i-\mu)(x_i-\mu)^T \Sigma^{-1}\right)$$

For the multiplication of i.i.d. Gaussians this takes the form:

$$\prod_{i=1}^{n} A_i \exp\left[-tr\left((x_i-\mu)(x_i-\mu)^T \Sigma^{-1}\right)/2\right] = B \exp\left[-tr\left(\sum_{i=1}^{n} (x_i-\mu)(x_i-\mu)^T \Sigma^{-1}\right)/2\right]$$

Finally multiplying the exponentials of the combined Gaussians and the Wishart prior, we have

$$p(\Sigma^{-1} | W^t, v^t, X) \propto \prod_{i=1}^{n \to \text{number of observed points}} p(x_i | \mu, \Sigma^{-1})\, p(\Sigma^{-1} | W, v)$$

$$\propto \frac{|\Sigma^{-1}|^{n}}{(2\pi)^{\frac{nd}{2}}} \exp\left[-\mathrm{tr}\left[\left(\sum_{i=1}^{n}(x_i-\mu)(x_i-\mu)^T\right)\Sigma^{-1}/2\right]\right]$$

$$\times \frac{|\Sigma^{-1}|^{(v-d-1)/2}}{2^{vd/2}|W|^{v/2}\Gamma(v/2)} \exp\left[\mathrm{tr}(W^{-1}\Sigma^{-1})\right]$$

$$\propto \frac{|\Sigma^{-1}|^{(v+n-d-1)/2}}{2^{(v+n)/2}\, C} \exp\left[-\mathrm{tr}\left(\left(W^{-1}+\sum_{i=1}^{n}(x_i-\mu)(x_i-\mu)^T\right)\Sigma^{-1}\right)/2\right]$$

where C denotes normalization constant. From this we clearly see that the posterior takes the form:

$$p(\Sigma^{-1} | W', v', X) = p\left(\Sigma^{-1} \,\middle|\, \left(W^{-1}+\sum_{i=1}^{n}(x_i-\mu)(x_i-\mu)^T\right)^{-1}, v+n\right)$$

$$= \mathrm{Wishart}\left(\Sigma^{-1} \,\middle|\, \left(W^{-1}+\sum_{i=1}^{n}(x_i-\mu)(x_i-\mu)^T\right)^{-1}, v+n\right)$$

Q.E.D

See also: Normal Wishart Distribution

Probabilistic Machine Learning

University of Tübingen, Summer Term 2023 © 2023 P. Hennig

Exercise Sheet No. 3 — Exponential Families

Submission by:

- Batuhan, Oezcoemlekci, Matrikelnummer: 6300476
- Aakarsh, Nair, Matrikelnummer: 6546577

Exercise 3.2 (Coding Exercise)

Consider the abstract base class `ExponentialFamily` introduced in the lecture (reproduced below for easy reference).

In [110…

```
import jax
import numpy as np
import logging

from jax import numpy as jnp
from matplotlib import pyplot as plt
from numpy.typing import ArrayLike

from tueplots import bundles
from tueplots.constants.color import rgb

plt.rcParams.update(bundles.beamer_moml())
plt.rcParams.update({"figure.dpi": 200})


logging.getLogger("matplotlib.font_manager").setLevel(logging.ERROR)
```

In [111…

```
import abc
import functools

class ExponentialFamily(abc.ABC):
    @abc.abstractmethod
    def sufficient_statistics(self, x: ArrayLike | jnp.ndarray, /) -> jnp.nd
        """Signature `(D)->(P)`"""

    @abc.abstractmethod
    def log_base_measure(self, x: ArrayLike | jnp.ndarray, /) -> jnp.ndarray
        """Signature `(D)->()`"""

    @abc.abstractmethod
```

```python
    def log_partition(self, parameters: ArrayLike | jnp.ndarray, /) -> jnp.r
        """Signature `(P)->()`"""

    def parameters_to_natural_parameters(
        self, parameters: ArrayLike | jnp.ndarray, /
    ) -> jnp.ndarray:
        """Signature `(P)->(P)`
        In some EF's, the canonical parameters are
        actually a transformation of the natural parameters.
        In such cases, this method should be overwritten to
        provide the inverse transformation.
        """
        return jnp.asarray(parameters)

    def logpdf(
        self, x: ArrayLike | jnp.ndarray, parameters: ArrayLike | jnp.ndarra
    ) -> jnp.ndarray:
        """Signature `(D),(P)->()`
        log p(x|parameters)
            = log h(x) + sufficient_statistics(x) @ natural_parameters - log
            = log base measure + linear term - log partition
        """
        x = jnp.asarray(x).astype(jnp.float32)
        log_base_measure = self.log_base_measure(x)
        natural_parameters = self.parameters_to_natural_parameters(parameter
        st = self.sufficient_statistics(x)[..., None, :]
        linear_term = (st  @ natural_parameters[..., None])[..., 0, 0]
        log_partition = self.log_partition(parameters)
        return log_base_measure + linear_term - log_partition

    def conjugate_log_partition(
        self, alpha: ArrayLike | jnp.ndarray, nu: ArrayLike | jnp.ndarray, /
    ) -> jnp.ndarray:
        """The log partition function of the conjugate exponential family.
        Signature `(P),()->()`
        If(!) this is available, it allows analytic construction of the conj
        """
        raise NotImplementedError()

    def conjugate_prior(self) -> "ConjugateFamily":
        return ConjugateFamily(self)

    def predictive_log_marginal_pdf(
        self,
        x: ArrayLike | jnp.ndarray,
        conjugate_natural_parameters: ArrayLike | jnp.ndarray,
    ) -> jnp.ndarray:
        """ Signature `(D),(P)->()`
            log p(x|conjugate_natural_parameters)
            Your answer to Part B below should be implemented here.
        """
        # Implement $p(x) = h(x)\frac{F(\phi(x)+\alpha, \nu+1)}{F(\alpha, \r
        lbm = self.log_base_measure(x)
        st = self.sufficient_statistics(x)
        alpha = conjugate_natural_parameters[:-1]
        nu =   conjugate_natural_parameters[-1]
```

```python
        plm =  (lbm \
            + self.conjugate_log_partition(st + alpha, nu + 1))[...,0] \
            - self.conjugate_log_partition(alpha, nu)
        return plm


    def Laplace_predictive_log_marginal_pdf(
        self,
        x: ArrayLike | jnp.ndarray,
        conjugate_natural_parameters: ArrayLike | jnp.ndarray,
        mode: ArrayLike | jnp.ndarray,
    ) -> jnp.ndarray:
        """ Signature `(D),(P)->()`
            log p(x|conjugate_natural_parameters)
            Your answer to Part B below should be implemented here.
        """
        def log_pdf_fun(y):
            return -self.logpdf(y, conjugate_natural_parameters)
        hessian = jax.hessian(log_pdf_fun)(mode)
        hessian_inv = np.linalg.inv(hessian)
        return jax.scipy.stats.multivariate_normal.logpdf(jnp.asarray(x), mo

    def posterior_parameters(
        self,
        prior_natural_parameters: ArrayLike | jnp.ndarray,
        data: ArrayLike | jnp.ndarray,
    ) -> jnp.ndarray:
        """Computes the natural parameters of the posterior distribution unc
        conjugate prior.
        Signature `(P),(D)->(P)`
        This can be implemented already in the abc and inherited by all subc
        even if the conjugate log partition function is not available.
        (In the latter case, only the unnormalized posterior is immediately
        """

        prior_natural_parameters = jnp.asarray(prior_natural_parameters)

        sufficient_statistics = self.sufficient_statistics(data)
        n = sufficient_statistics[..., 0].size

        expected_sufficient_statistics = jnp.sum(
            sufficient_statistics,
            axis=tuple(range(sufficient_statistics.ndim)),
        )

        alpha_prior, nu_prior = (
            prior_natural_parameters[:-1],
            prior_natural_parameters[-1],
        )
        return jnp.append(alpha_prior + expected_sufficient_statistics, nu_p


class ConjugateFamily(ExponentialFamily):
    def __init__(self, likelihood: ExponentialFamily) -> None:
        self._likelihood = likelihood
```

```
    @functools.partial(jnp.vectorize, excluded={0}, signature="(d)->(p)")
    def sufficient_statistics(self, w: ArrayLike | jnp.ndarray, /) -> jnp.nd
        """Signature `(D)->(P)`
        the sufficient statistics of the conjugate family are
        the natural parameters and the (negative) log partition function of
        """
        return jnp.append(
            self._likelihood.parameters_to_natural_parameters(w),
            -self._likelihood.log_partition(w),
        )

    def log_base_measure(self, w: ArrayLike | jnp.ndarray, /) -> jnp.ndarray
        """Signature `(D)->()`
        the base measure of the conjugate family is, implicitly, the Lebesgu
        """
        w = jnp.asarray(w)
        return jnp.zeros_like(w[..., 0])

    def log_partition(
        self, natural_parameters: ArrayLike | jnp.ndarray, /
    ) -> jnp.ndarray:
        """Signature `(P)->()`
        If the conjugate log partition function is available,
        we can use it to compute the log partition function of the conjugate
        """
        natural_parameters = jnp.asarray(natural_parameters)

        alpha, nu = natural_parameters[:-1], natural_parameters[-1]

        return self._likelihood.conjugate_log_partition(alpha, nu)

    def unnormalized_logpdf(
        self, w: ArrayLike | jnp.ndarray, natural_parameters: ArrayLike | jn
    ) -> jnp.ndarray:
        """Signature `(D),(P)->()`
        Even if the conjugate log partition function is not available,
        we can still compute the unnormalized log pdf of the conjugate famil
        """
        return self.sufficient_statistics(w) @ jnp.asarray(natural_parameter

    def laplace_precision(
        self,
        natural_parameters: ArrayLike | jnp.ndarray,
        mode: ArrayLike | jnp.ndarray,
        /,
    ) -> jnp.ndarray:
        """Signature `(P),(D)->()`
        If the conjugate log partition function is _not_ available,
        we can still compute the Laplace approximation to the posterior,
        using only structure provided by the likelihood.
        This requires the mode of the likelihood, which is not available in
        but may be found by numerical optimization if necessary.
        """
        return -jax.hessian(self.unnormalized_logpdf, argnums=0)(
            jnp.asarray(mode), natural_parameters
        )
```

TaskrA.

Implement a concrete realization of the binomial exponential family parametrized by log odds ratio $w = \log \frac{p}{1-p}$, i.e.

$$p(k \mid w) = \exp\big(\log h(k) + \phi(k)^T w - \log Z(w)\big),$$

where

- $\log h(k) := \log \binom{n}{k}$,
- $\phi(k) := k$, and
- $\log Z(w) := n \log(1 + \exp(w))$.

(Note that n is a constant in this definition, not a parameter). The normalization constant of the conjugate family

$$\begin{aligned} F(\alpha, \nu) &:= \int_{-\infty}^{\infty} \exp(\alpha w - \nu \log Z(w)) \mathrm{d}w \\ &= \int_{-\infty}^{\infty} \exp(w)^{\alpha} (1 + \exp(w))^{-n\nu} \mathrm{d}w \\ &= \int_0^1 \left(\frac{p}{1-p}\right)^{\alpha} \left(1 + \frac{p}{1-p}\right)^{-n\nu} \left|\frac{1}{p(1-p)}\right| \mathrm{d}p \\ &= \int_0^1 p^{\alpha-1}(1-p)^{(n\nu-\alpha)-1} \mathrm{d}p \\ &= B(\alpha, n\nu - \alpha), \end{aligned}$$

since $p = \frac{1}{1+\exp(-w)}$ and $\frac{\mathrm{d}p}{\mathrm{d}w} = \frac{\exp(-w)}{(1+\exp(-w))^2} = p(1-p)$. This is also the normalization constant of the type VI logistic or logistic-beta distribution.

In [112…

```
# thus, the following transformation is a useful utility:
def sigmoid_logpdf_transform(logpdf_logodds):
    """Transform the log-pdf of a random variable X into the
    log-pdf of the random variable sigmoid(X)"""

    def logpdf_p(ps):
        logps = jnp.log(ps)
        log1mps = jnp.log1p(-ps)
        logodds = logps - log1mps

        return logpdf_logodds(logodds) - logps - log1mps

    return logpdf_p
```

In [113…

```
import jax.numpy as jnp
from jax.lax import lgamma

class BinomialLogOdds(ExponentialFamily):
        def __init__(self, n) -> None:
```

```python
        """The BinomialLogOdds has one fixed parameter."""
        super().__init__()
        self.n = jnp.array(n).astype(jnp.float32)

    def sufficient_statistics(self, k: ArrayLike | jnp.ndarray) -> jnp.r
        """Both the Poisson distribution and the Bionomial
        Log odds distribution us the identity function as
        sufficient statistics."""
        return jnp.asarray(k)

    def log_base_measure(self, k: ArrayLike | jnp.ndarray) -> jnp.ndarra
        """log(h(k) = log(n choose k):= log(n choose k = n! / (k! (n-k)!
        k = jnp.asarray(k).astype(jnp.float32)
        k_value = k[..., 0]
        choose_value = lgamma(self.n + 1) - lgamma(k_value + 1) - lgamma
        return choose_value

    def log_partition(self, parameters: ArrayLike | jnp.ndarray) -> jnp.
        # \log Z(w) := n \log (1 + \exp(w))
        n_value = self.n #parameters[..., 0].size
        return n_value * jnp.log(1 + jnp.exp(parameters[..., 0]))

    def parameters_to_natural_parameters(
        self, logodds: ArrayLike | jnp.ndarray
    ) -> jnp.ndarray:
        """We are getting input directly interms of log odds."""
        logodds = jnp.asarray(logodds)
        return logodds

    def conjugate_log_partition(self, alpha: ArrayLike | jnp.ndarray, nu
        """
        + Beta(\alpha, n*\nu - \alpha)
        """
        alpha = jnp.asarray(alpha).astype(jnp.float32)
        nu = jnp.asarray(nu).astype(jnp.float32)

        def log_beta(a, b):
            return lgamma(a) + lgamma(b) - lgamma(a + b)
        return log_beta(alpha, ((self.n * nu) - alpha))
```

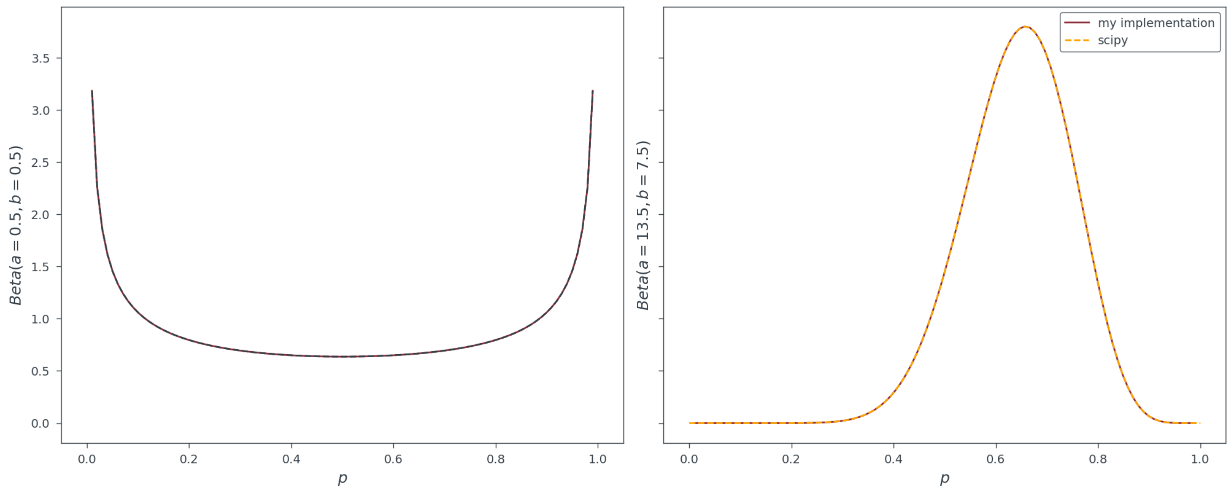
In [114…

```python
# Some unit tests to make sure your implementation is correct:
# instantiate your EF, and its conjugate prior:
likelihood = BinomialLogOdds(n=1)

prior = likelihood.conjugate_prior()

# Prior Natural Parameters: are alpha, nu.
a, b = 0.5, 0.5
prior_natural_parameters = [
    a,  # alpha
    a + b, # nu
]  # => Logistic-Beta(a, b)

# create some data:
key = jax.random.PRNGKey(0)
data = jax.random.bernoulli(key, 0.75, shape=(20, 1))
```

```python
posterior = prior
posterior_natural_parameters = likelihood.posterior_parameters(
    prior_natural_parameters,
    data,
)

# A: Check your implementation of the conjugate prior is correctly normalize
import scipy.integrate

np.testing.assert_allclose(
    scipy.integrate.quad(
        lambda logodds: np.exp(prior.logpdf(
            [logodds], prior_natural_parameters)),
        -30,
        30,
    )[0],
    1.0,
    rtol=1e-5,
    err_msg="The conjugate prior is not correctly normalized.",
)


# B: check your log pdf against the scipy implementation:
fig, axs = plt.subplots(1,2, sharex=True, sharey=True)
fig.set_size_inches(10, 4)
plt_ps = np.linspace(0.0, 1.0, 100)

# first for the prior:
axs[0].plot(
    plt_ps,
    jnp.exp(
        sigmoid_logpdf_transform(
            lambda logodds: prior.logpdf(
                logodds[..., None], prior_natural_parameters)
        )(plt_ps[..., None])
    ),
    label='my implementation'
)

axs[0].plot(plt_ps, jax.scipy.stats.beta.pdf(plt_ps, a, b),'--', label='scip
axs[0].set_xlabel(r"$p$")
axs[0].set_ylabel(f"$Beta(a={a}, b={b})$")

# then for the posterior:
axs[1].plot(
    plt_ps,
    jnp.exp(
        sigmoid_logpdf_transform(
            lambda logodds: posterior.logpdf(
                logodds[..., None], posterior_natural_parameters)
        )(plt_ps[..., None])
    ),
    label='my implementation'
)
```

```
axs[1].plot(plt_ps, jax.scipy.stats.beta.pdf(plt_ps, a + data.sum(), b + dat
axs[1].set_xlabel(r"$p$")
axs[1].set_ylabel(f"$Beta(a={a + data.sum()}, b={b + data.size - data.sum()}
axs[1].legend()
```

Out[114]: `<matplotlib.legend.Legend at 0x7f9ae3767fd0>`



Task B.

Add a `predictive_log_marginal_pdf(x, natural_parameters)` function to the `ExponentialFamily` above (a placeholder has already been included). It should compute

$$\log p(x \mid \alpha, \nu) = \log \int_{\mathbb{W}} p(x \mid w) p(w \mid \alpha, \nu) \mathrm{d}w.$$

This can be explicitly implemented in the abstract base class if the `conjugate_log_partition` is available. Revisit slide 10 of Lecture 5 for reference.

In fact, it is still possible to provide this functionality **approximately** even if `conjugate_log_partition` is *not* available, using the Laplace approximation. Add a `Laplace_predictive_log_marginal_pdf(self,x,natural_parameters, mode)` function to `ExponentialFamily`, which approximates the functionality of `predictive_log_marginal_pdf` when given a `mode` $w* = \arg\max_w p(w \mid \alpha, \nu)$ (compare with the `laplace_precision` function already in `ConjugateFamily`). Revisit slide 7 of Lecture 6 for reference.

Test your implementation for the concrete example of the Binomial above (for the binomial, this marginal is known as the Beta-Binomial distribution).

In [115…

```
def conjugate_mode(conjugate_natural_parameters):
    """Closed-form expression for the mode of the conjugate exponential fami
    log-odds parametrized Binomial distribution."""
    return jnp.atleast_1d(
        jnp.log(
```

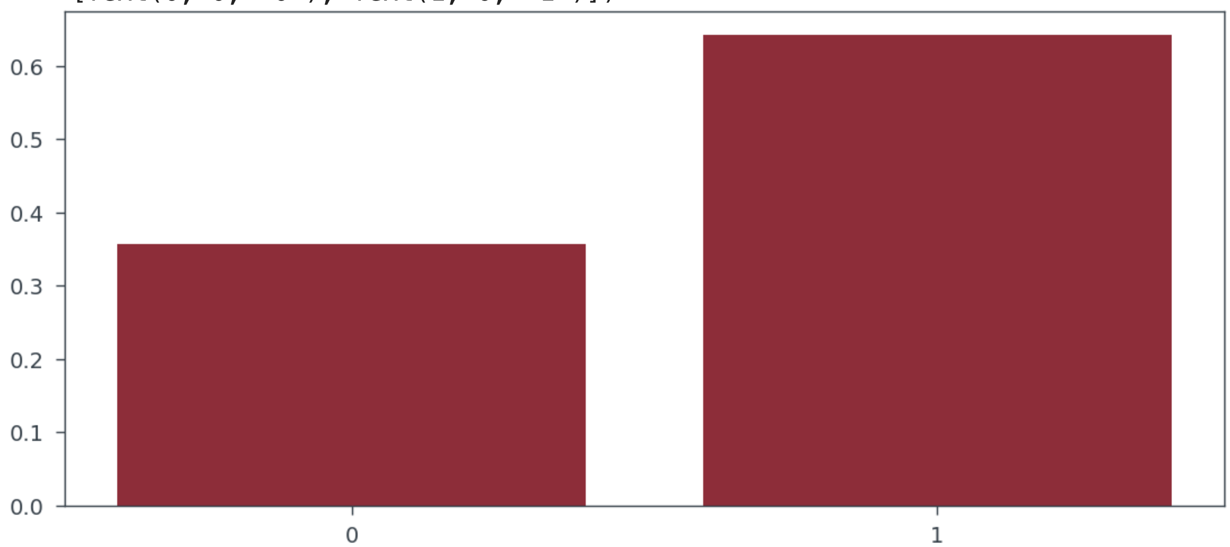
```
            conjugate_natural_parameters[0]
            / (conjugate_natural_parameters[1] - conjugate_natural_parameter
        )
    )
```

In [116…

```
plt.bar(
    [0, 1],
    np.exp(
        likelihood.predictive_log_marginal_pdf(
            [[0], [1]],
            posterior_natural_parameters,
        )
    ),
)
plt.xticks([0, 1])
```

Out[116]:

```
([<matplotlib.axis.XTick at 0x7f9a90e087f0>,
  <matplotlib.axis.XTick at 0x7f9a90e085e0>],
 [Text(0, 0, '0'), Text(1, 0, '1')])
```

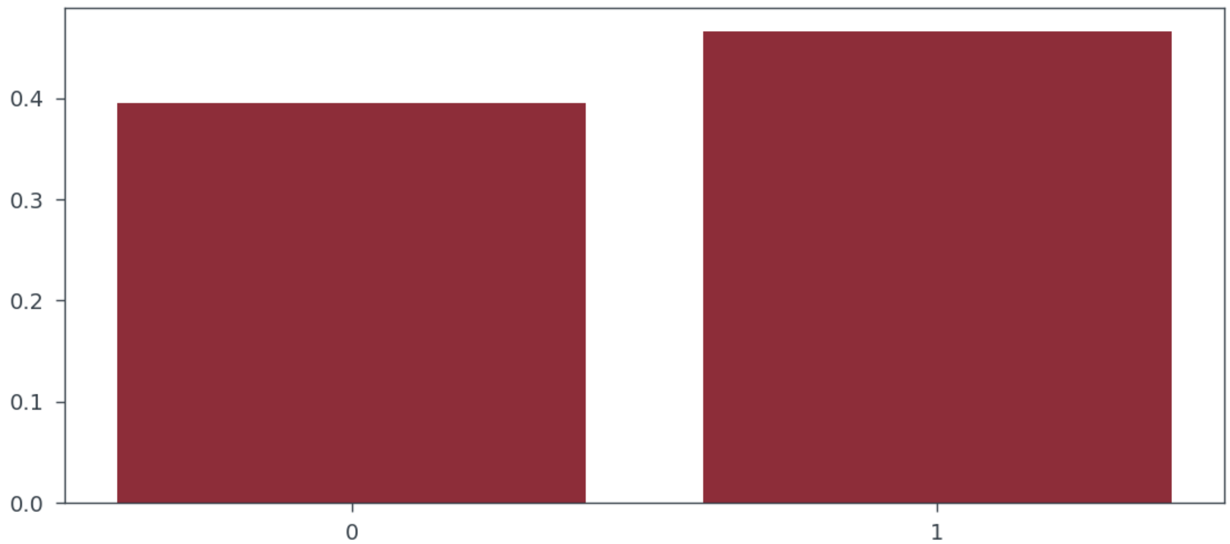


In [117…

```
plt.bar(
    [0, 1],
    np.exp(
        likelihood.Laplace_predictive_log_marginal_pdf(
            [[0], [1]],
            jnp.reshape(posterior_natural_parameters, (2,1)), #posterior_nat
            conjugate_mode(posterior_natural_parameters),
        )
    )
)
plt.xticks([0, 1])
```

Out[117]:

```
([<matplotlib.axis.XTick at 0x7f9a90e82da0>,
  <matplotlib.axis.XTick at 0x7f9a90e83190>],
 [Text(0, 0, '0'), Text(1, 0, '1')])
```

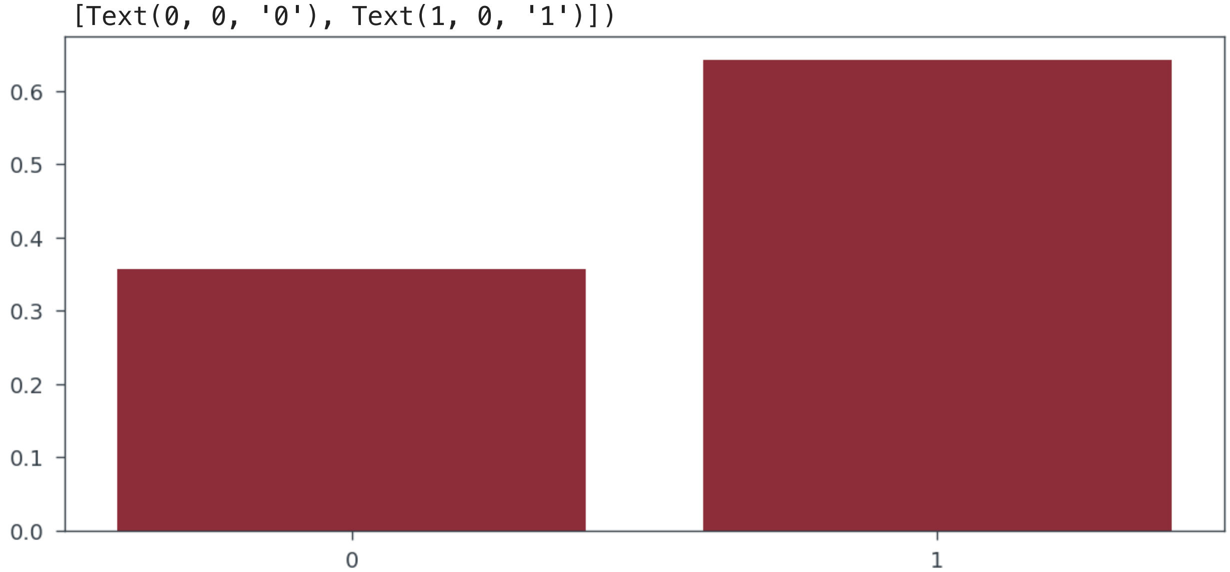


In [118…

```
plt.bar(
    [0, 1],
    np.exp(
        likelihood.logpdf(
            [[0], [1]],
            conjugate_mode(posterior_natural_parameters),
        )
    )
)
plt.xticks([0, 1])
```

Out[118]:

```
([<matplotlib.axis.XTick at 0x7f9aa8678670>,
  <matplotlib.axis.XTick at 0x7f9aa8678640>],
 [Text(0, 0, '0'), Text(1, 0, '1')])
```



How to submit your work:

Export your answer into a pdf (for example using jupyter's `Save and Export Notebook as` feature in the `File` menu). Make sure to include all outputs, in particular plots. Also include your answer to the theory question, either by adding it as LaTeX code directly in the notebook, or by adding it as an extra page (e.g. a scan) to the pdf. Submit the exercise on Ilias, in the associated folder. **Do not forget to add your name(s) and matrikel number(s) above!)**