E1

January 16, 2024

1 Statistical Parameter Estimation 2024

1.1 Exercise 1

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Let us consider a simple exponential decay

$$y(t) = a\ exp(-bt) + \epsilon(t).$$

Let the data be

$$y(t) = (0.3573, 0.3618, 0.1920, 0.1585, 0.1041, 0.1100, 0.0560, 0.0291, 0.0252, 0.0249, 0.04160)^T,$$

$$t = (0.0, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1.0)^T,$$

$$\varepsilon(t)\ N(0, \sigma^2), \text{with } \sigma = 0.02.$$

Original simulation values are a = 0.4 and b = 3. We denote

$$\theta := (a, b)^T$$

1. Likelihood density

- Write the likelihood density of θ given y(t).
- Derive the negative log-likelihood

The likelihood density, given a fixed variance, can be formulated as follows:

$$p(y(t)|\theta) = L(\theta) = \frac{1}{\sqrt{(2\pi)|\sigma^2 \mathbf{I}|}} \exp(-\frac{1}{2}\frac{\sum_{i=1}^{11}(y(t_i) - a\ \exp(-bt_i))^2}{\sigma^2})$$

Furthermore the negative log-likelihood goes as follows:

$$
\begin{aligned}
-\log(L(\theta)) &= -\log(\frac{1}{\sqrt{(2\pi)|\sigma^2\mathbf{I}|}}\exp(-\frac{1}{2}\frac{\sum_{i=1}^{11}(y(t_i)-a\ \exp(-bt_i))^2}{\sigma^2})) \\
&= -\log(\frac{1}{\sqrt{(2\pi)|\sigma^2\mathbf{I}|}}) - \log(\exp(-\frac{1}{2}\frac{\sum_{i=1}^{11}(y(t_i)-a\ \exp(-bt_i))^2}{\sigma^2})) \\
&= \log(\sqrt{(2\pi)|\sigma^2\mathbf{I}|}) + \frac{1}{2}\frac{\sum_{i=1}^{11}(y(t_i)-a\ \exp(-bt_i))^2}{\sigma^2} \\
&= \frac{1}{2}\log(2\pi) + \log(\sigma) + \frac{1}{2\sigma^2}\sum_{i=1}^{11}(y(t_i)-a\ \exp(-bt_i))^2
\end{aligned}
$$

2. Optimisation: use the methods in the optimisation toolbox e.g. fminsearch in Matlab, to obtain a numerical optimizer for the maximum likelihood estimator of θ.

[50]:
```python
import scipy
import numpy as np
import matplotlib.pyplot as plt
import warnings

warnings.filterwarnings("ignore")


t = np.array([0.0, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1.0])
y_t = np.array([0.3573, 0.3618, 0.1920, 0.1585, 0.1041, 0.1100, 0.0560, 0.0291,␣
↪0.0252, 0.0249, 0.04160])
sigma = 0.02

gt = 0.3 * np.exp(-3 * t)

neg_log_likelihood = (
    lambda theta: 1 / 2 * np.log(2 * np.pi)
    + np.log(sigma)
    + 1 / (2 * sigma**2) * np.sum((y_t - theta[0] * np.exp(-theta[1] * t)) ** 2)
)

x0 = np.zeros(shape=(2,))

optim = scipy.optimize.fmin(neg_log_likelihood, x0=x0)

print(f"Found maximum likelihood estimators: a = {optim[0]}, b = {optim[1]}")
```

```
Optimization terminated successfully.
         Current function value: 7.699880
         Iterations: 73
         Function evaluations: 143
Found maximum likelihood estimators: a = 0.3910576244325278, b =
2.95856657099285
```

3. Integration

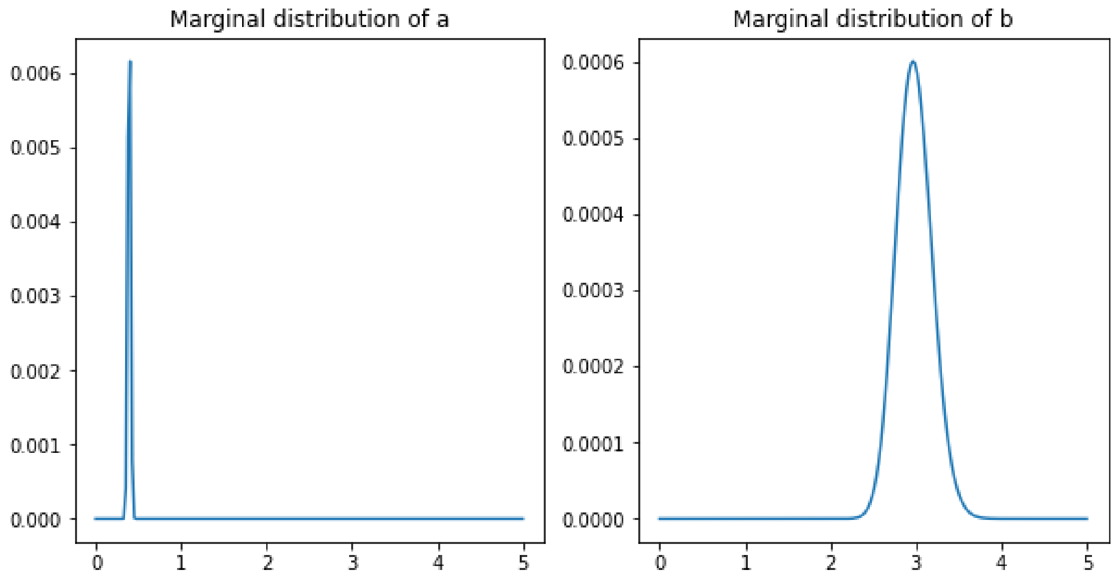
- Use numerical integration to calculate the conditional mean estimator of θ. Any standard quadrature will do.
- Similarly, calculate numerically marginal densities for a and b.

[51]:
```
likelihood = (
    lambda a, b: 1 / (np.sqrt(2 * np.pi * sigma**2))
    * np.exp(-1 / 2 * np.sum((y_t - a * np.exp(-b * t)) ** 2) / sigma**2)
)

evidence = scipy.integrate.dblquad(likelihood, -np.inf, np.inf, -np.inf, np.inf)
CM_fun_a = lambda a, b: a * likelihood(a, b)
CM_fun_b = lambda a, b: b * likelihood(a, b)


integral_a = scipy.integrate.dblquad(CM_fun_a, -np.inf, np.inf, -np.inf, np.inf)
integral_b = scipy.integrate.dblquad(CM_fun_b, -np.inf, np.inf, -np.inf, np.inf)
print(
    f"Conditional mean estimator values with prior 1 for a and b: {integral_a[0]/
 ↪evidence[0], integral_b[0]/evidence[0]}"
)
```

```
Conditional mean estimator values with prior 1 for a and b: (0.3916385023902581,
2.9818569339442993)
```

Marginal distributions of a and b

[52]:
```
a = np.linspace(0, 5, 200)
b = np.linspace(0, 5, 200)

dist = np.zeros((len(a), len(b)))

for i, a_i in enumerate(a):
    for j, b_j in enumerate(b):
        dist[i, j] = likelihood(a_i, b_j)

marg_a = np.sum(dist, axis=1)
marg_b = np.sum(dist, axis=0)


plt.figure(figsize=(10, 5))
plt.subplot(121)
plt.plot(a, marg_a)
plt.title("Marginal distribution of a")
plt.subplot(122)
plt.plot(b, marg_b)
plt.title("Marginal distribution of b")
plt.show()
```



4. Priors

- Choose a Gaussian prior for θ and define a posterior distribution. Calculate the negative log posterior. Calculate the MAP and CM estimators.
- Do the same as above, but choose a prior distribution that is uniformly distributed.

Posterior:

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

$$p(\theta) = \frac{1}{\sqrt{2\pi|\Sigma|}} exp(-\frac{1}{2}(\theta - \mu)^T \Sigma^{-11}(\theta - \mu))$$

$$p(y|\theta) = \frac{1}{\sqrt{(2\pi)|\sigma^2 \mathbf{I}|}} \exp(-\frac{1}{2}\frac{\sum_{i=1}^{11}(y(t_i) - a \exp(-bt_i))^2}{\sigma^2})$$

So the unnormalized posterior is of the form:

$$p(\theta|y) \propto p(\theta)p(y|\theta)$$

Thus the negative log posterior is of the form:

$$\begin{aligned}
-L_{post}(\theta) &= -log(p(\theta|y)) \\
&= -log(p(\theta)) - log(p(y|\theta)) \\
&= -log(p(\theta)) + \frac{1}{2}\log(2\pi) + \log(\sigma) + \frac{1}{2\sigma^2}\sum_{i=1}^{11}(y(t_i) - a\exp(-bt_i))^2
\end{aligned}$$

Priors and MAP

[53]:
```python
# Gaussian priors for theta
G_prior_a = lambda a: scipy.stats.norm.pdf(a, loc=2, scale=0.5)
G_prior_b = lambda b: scipy.stats.norm.pdf(b, loc=2, scale=1)

G_prior_theta = lambda theta: [G_prior_a(theta[0]), G_prior_b(theta[1])]
# Uniform priors

U_prior_a = lambda a: scipy.stats.uniform.pdf(a, loc=0.05, scale=4.9)
U_prior_b = lambda b: scipy.stats.uniform.pdf(b, loc=1, scale=3)

U_prior_theta = lambda theta: [U_prior_a(theta[0]), U_prior_b(theta[1])]

neg_log_posterior = lambda theta, prior: -np.log(prior(theta)) +␣
↪neg_log_likelihood(
    theta
)


def minimize(f, prior, a, b):
    optim = [None, None]
    min_a = np.inf
    min_b = np.inf
    for a_i in a:
        for b_j in b:
            theta = [a_i, b_j]
            val = f(theta, prior)
            val_a = val[0]
            val_b = val[1]
            if val_a < min_a:
                min_a = val_a
                optim[0] = a_i
            if val_b < min_b:
                min_b = val_b
                optim[1] = b_j
    return optim


optim_G = minimize(neg_log_posterior, G_prior_theta, a, b)
optim_U = minimize(neg_log_posterior, U_prior_theta, a, b)


print(
    f"Found maximum a posteriori for Gaussian priors: a = {optim_G[0]:.3f}, b =␣
↪{optim_G[1]:.3f}"
)
```

```
print(
    f"Found maximum a posteriori for Uniform priors: a = {optim_U[0]:.3f}, b =␣
 ↪{optim_U[1]:.3f}"
)
```

```
Found maximum a posteriori for Gaussian priors: a = 0.402, b = 2.839
Found maximum a posteriori for Uniform priors: a = 0.402, b = 3.040
```

CM estimation

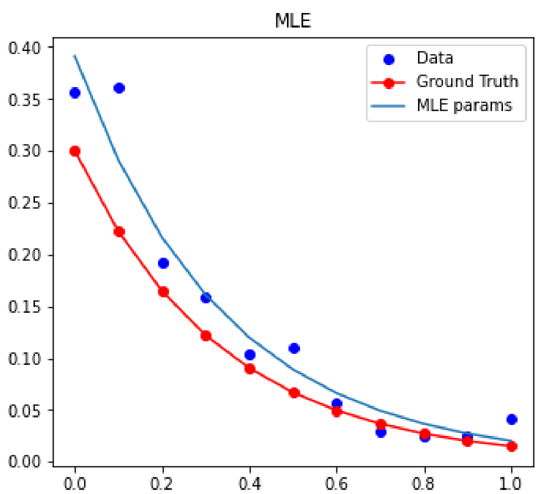
[54]:
```
GCM_fun_a = lambda a, b: a * G_prior_a(a) * likelihood(a, b)
GCM_fun_b = lambda a, b: b * G_prior_b(b) * likelihood(a, b)


Gintegral_a = scipy.integrate.dblquad(GCM_fun_a, -np.inf, np.inf, -np.inf, np.
 ↪inf)
Gintegral_b = scipy.integrate.dblquad(GCM_fun_b, -np.inf, np.inf, -np.inf, np.
 ↪inf)

GCM_a = Gintegral_a[0] / evidence[0]
GCM_b = Gintegral_b[0] / evidence[0]

UCM_fun_a = lambda a, b: a * U_prior_a(a) * likelihood(a, b)
UCM_fun_b = lambda a, b: b * U_prior_b(b) * likelihood(a, b)

Uintegral_a = scipy.integrate.dblquad(UCM_fun_a, -np.inf, np.inf, -np.inf, np.
 ↪inf)
Uintegral_b = scipy.integrate.dblquad(UCM_fun_b, -np.inf, np.inf, -np.inf, np.
 ↪inf)

UCM_a = Uintegral_a[0] / evidence[0]
UCM_b = Uintegral_b[0] / evidence[0]

print(f"CM estimator values with Gaussian priors for a and b: {GCM_a, GCM_b}")

print(f"CM estimator values with Uniform priors for a and b: {UCM_a, UCM_b}")
```

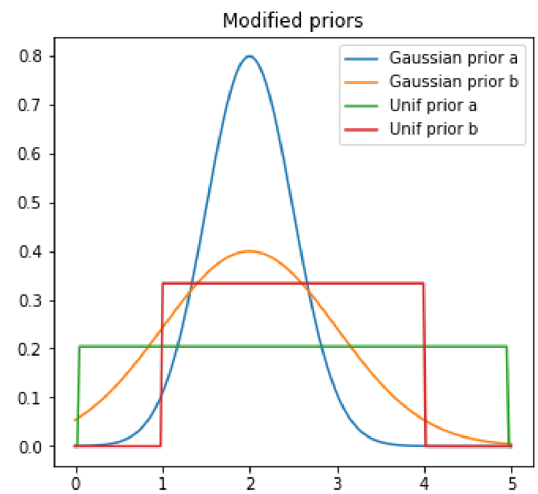
```
CM estimator values with Gaussian priors for a and b: (0.0001684630959802797,
0.7239043147815994)
CM estimator values with Uniform priors for a and b: (0.05778078883340787,
0.9940053250883235)
```

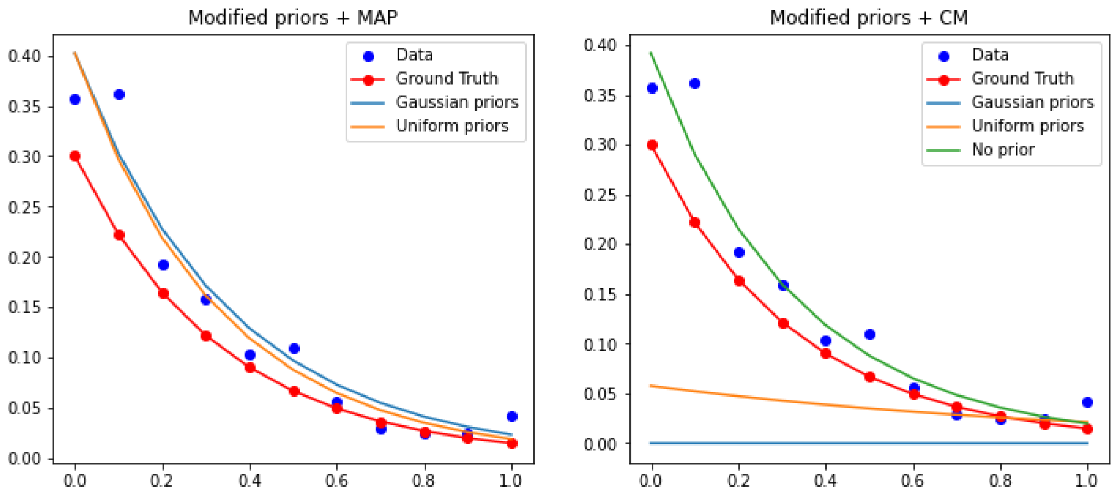
5. Visualization

[55]:
```
exp_decay = lambda a, b: a * np.exp(-b * t)


plt.figure(figsize=(12, 5))
```

```python
plt.subplot(121)
plt.plot(t, y_t, "bo", t, gt, "r-o")
plt.plot(t, exp_decay(optim[0], optim[1]))
plt.legend(["Data", "Ground Truth", "MLE params"])
plt.title("MLE")


plt.subplot(122)
plt.plot(a, G_prior_a(a), b, G_prior_b(b), a, U_prior_a(a), b, U_prior_b(b))
plt.legend(["Gaussian prior a", "Gaussian prior b", "Unif prior a", "Unif prior␣
↪b"])
plt.title("Modified priors")
plt.show()

plt.figure(figsize=(12, 5))
plt.subplot(121)
plt.plot(t, y_t, "bo", t, gt, "r-o")
plt.plot(t, exp_decay(optim_G[0], optim_G[1]), t, exp_decay(optim_U[0],␣
↪optim_U[1]))
plt.legend(["Data", "Ground Truth", "Gaussian priors", "Uniform priors"])
plt.title("Modified priors + MAP")


plt.subplot(122)
plt.plot(t, y_t, "bo", t, gt, "r-o")
plt.plot(t, exp_decay(GCM_a, GCM_b), t, exp_decay(UCM_a, UCM_b), t,␣
↪exp_decay(integral_a[0]/evidence[0], integral_b[0]/evidence[0]))
plt.legend(["Data", "Ground Truth", "Gaussian priors", "Uniform priors", "No␣
↪prior"])
plt.title("Modified priors + CM")
plt.show()
```






Modified priors + MAP
Data
Ground Truth
Gaussian priors
Uniform priors
0.00
0.05
0.10
0.15
0.20
0.25
0.30
0.35
0.40
0.0
0.2
0.4
0.6
0.8
1.0
Modified priors + CM
Data
Ground Truth
Gaussian priors
Uniform priors
No prior