Markov Chain Monte Carlo (MCMC)

In [1]:
```
import numpy as np
import matplotlib.pyplot as plt
plt.rcParams.update({'font.size': 16})
import scipy.stats as stats
import math
import savingfigR as sf
```

1. Use Metropolis-Hastings sampling to randomly draw numbers from a bivariate normal distribution. The two conditional probabilities are: $p(x|y) = \mathcal{N}(\mu_X + \frac{\sigma_X}{\sigma_Y}\rho(y - \mu_Y), (1 - \rho^2)\sigma_X^2)$ and $p(y|x) = \mathcal{N}(\mu_Y + \frac{\sigma_Y}{\sigma_X}\rho(x - \mu_X), (1 - \rho^2)\sigma_Y^2)$. Use the following constants: μ_X = 78.8, σ_X = 3.668, μ_Y = 211, σ_Y = 26.904, and ρ = 0.81 (10 marks).

In [2]:
```
# parameters
muX = 78.8
sigX = 3.668
muY = 211
sigY = 26.904
rho = 0.81
n=10000
# n = 5
```

Gibbs (for comparison)

In [3]:
```
# Gibbs sampler (1: Y, 2: X)
XgY = np.empty(n)
YgX = np.empty(n)
# initialize
XgY[0] = muX

for i in range(1,n):
    # update
    x = XgY[i-1]
    # sample
    YgX[i] = np.random.normal(muY + (sigY/sigX) * rho * (x - muX), np.s
    # update
    y = YgX[i]
    # sample
    XgY[i] = np.random.normal(muX + (sigX/sigY) * rho * (y - muY), np.s
```

a. Make an algorithm to perform Metropolis-Hastings sampling (5 marks).

In [4]:
```
def logp(x):
    if x < 0:
        return 0
    else :
        return np.log(x)
```

In [5]:
```
# Metropolis-Hastings
XgYMH = np.empty(n)
YgXMH = np.empty(n)
# initialize
XgYMH[0] = muX
YgXMH[0] = muY
# iterate
for i in range(1,n):
    # 1. Generate random candidate
    xgy = np.random.normal(XgYMH[i-1], 5)
    ygx = np.random.normal(YgXMH[i-1], 30)

    # 2. Calculate acceptance probability
    num = stats.multivariate_normal.pdf(np.array([xgy, ygx]), np.array(
    denom = stats.multivariate_normal.pdf(np.array([XgYMH[i-1], YgXMH[i
    A = np.min([np.log(1), logp(num/denom)])

    # 3. Accept or reject
    u = np.log(np.random.uniform(low=0, high=1))
    if u <= A: # accept
        YgXMH[i] = ygx
        XgYMH[i] = xgy
    else : # reject
        YgXMH[i] = YgXMH[i-1]
        XgYMH[i] = XgYMH[i-1]
```

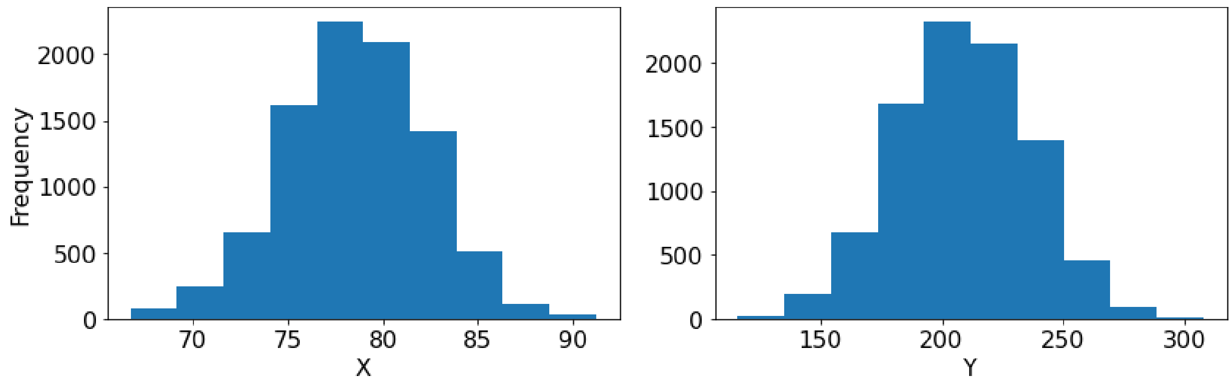
In [6]:
```
acc_rate = (len(np.unique(YgXMH)) / len(YgXMH)) * 100
print(f'Acceptance rate = {acc_rate:.0f}')
```

```
Acceptance rate = 32
```

b. Plot the marginal distributions of X and Y (3 marks).

In [7]:

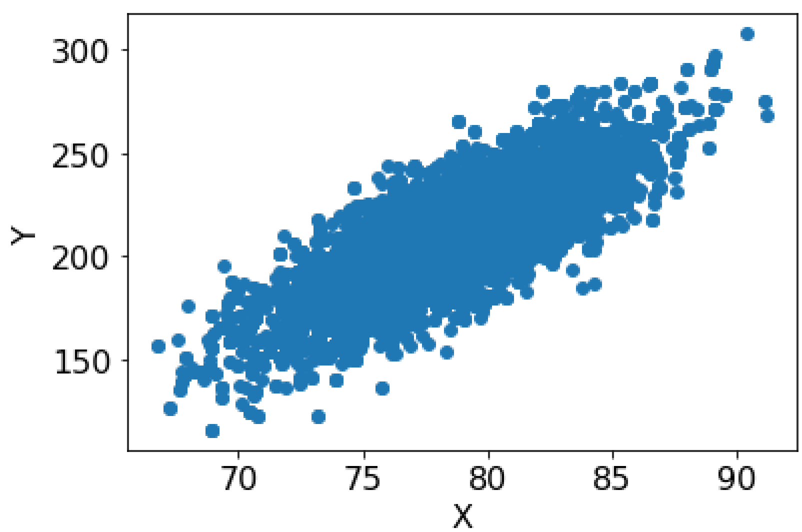
```
fig = plt.figure(figsize=(12,4))
plt.subplot(1,2,1)
plt.hist(XgYMH[1000:]) # 1000 burn in
plt.xlabel('X')
plt.ylabel('Frequency')
plt.subplot(1,2,2)
plt.hist(YgXMH[1000:]) #
plt.xlabel('Y')

plt.tight_layout()
plt.show()

sf.best_save(fig, '1bMH')
```



c. Plot the joint distribution X and Y (2 marks).

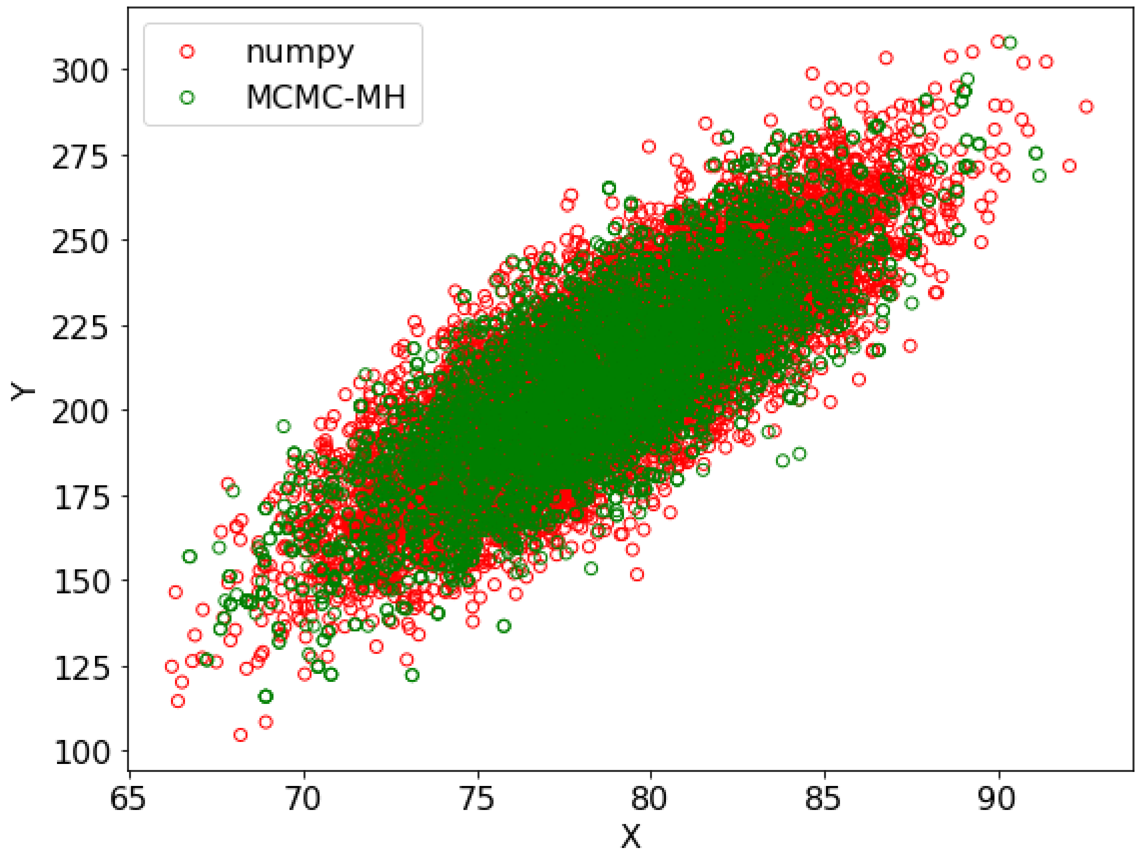
In [8]:

```
fig = plt.figure()
plt.scatter(XgYMH[1000:], YgXMH[1000:])
plt.xlabel('X')
plt.ylabel('Y')
plt.show()

sf.best_save(fig, '1cMH')
```

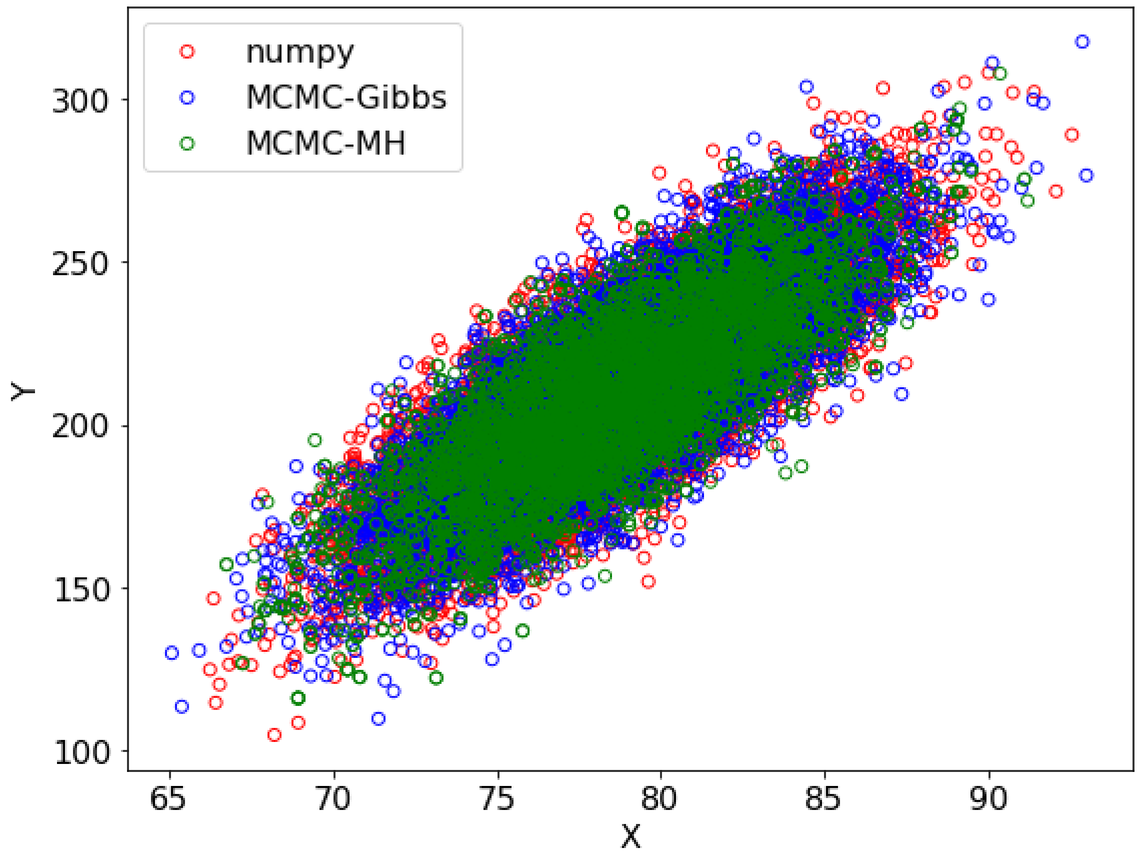


Test via numpy sampler

In [9]:
```
test = np.random.multivariate_normal(np.array([muX, muY]), np.array([[s

fig = plt.figure(figsize=(9,7))
plt.scatter(test[:,0], test[:,1], facecolors='none', edgecolor='r', lab
plt.scatter(XgYMH[1000:], YgXMH[1000:], facecolors='none', edgecolor='g
plt.xlabel('X')
plt.ylabel('Y')
plt.legend(loc=0)
plt.show()

sf.best_save(fig, '1MHvnp')
```



In [10]:
```
# numpy v gibbs v mh
fig = plt.figure(figsize=(9,7))
plt.scatter(test[:,0], test[:,1], facecolors='none', edgecolor='r', lab
plt.scatter(XgY[1000:], YgX[1000:], facecolors='none', edgecolor='b', l
plt.scatter(XgYMH[1000:], YgXMH[1000:], facecolors='none', edgecolor='g
plt.xlabel('X')
plt.ylabel('Y')
plt.legend(loc=0)
plt.show()

sf.best_save(fig, 'npVGibssVMH')
```



Lecture example

Set up

Prior = Beta(α=1, β=1)

Likelihood = Binomial (n=20, k=16)

Posterior = p(w|n,k,α, β) = $\frac{1}{B(\alpha_h,\beta_h)} w^{\alpha_h - 1}(1-w)^{\beta_h - 1}$, s.t.

$\alpha_h = k + \alpha$

$\beta_h = n - k + \beta$

$$p(w|k,n,\alpha,\beta) \propto w^{k+\alpha-1}(1-w^{n-k+\beta-1})$$

Log rules

$$p(w|k,n,\alpha,\beta) \propto (k+\alpha-1) * log(w) + ((n-k+\beta-1) * log(1-w))$$

Propose w from $\mathcal{N}(w_t, 0.4^2)$

Use the common acceptance function.

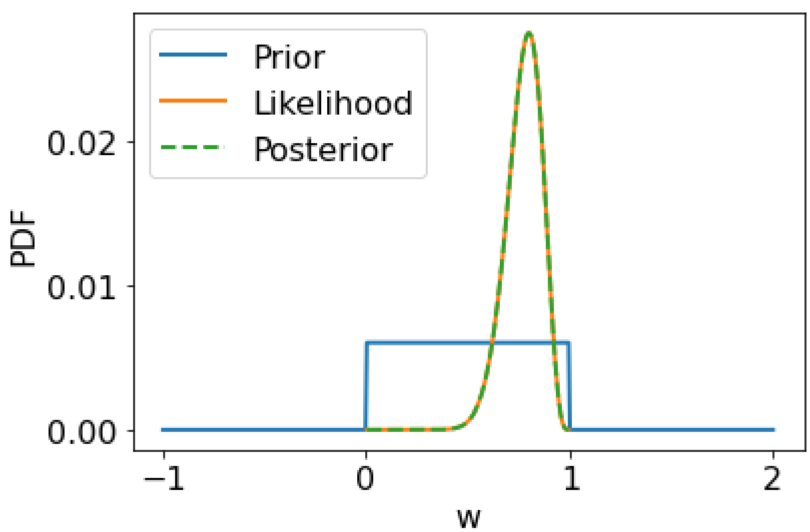
$$A(w', w_t) = \frac{P(w'|k,n,\alpha,\beta)}{P(w_t|k,n,\alpha,\beta)}$$

Don't foget to consider underflow

In [11]:
```
# set up
priorAlpha = 1
priorBeta = 1
likeN = 20
likeK= 16
```

In [12]:

```
x = np.linspace(-1, 2, num=500)
prior = stats.beta.pdf(x, priorAlpha, priorBeta)
like = stats.binom.pmf(likeK, likeN, x)
prior /= np.nansum(prior)
like /= np.nansum(like)
posterior = prior * like
posterior /= np.nansum(posterior)

fig = plt.figure()
plt.plot(x, prior, lw=2, label='Prior')
plt.plot(x, like, lw=2, label='Likelihood')
plt.plot(x, posterior, lw=2, ls='--', label='Posterior')
plt.xlabel('w')
plt.ylabel('PDF')
plt.legend(loc=0)
plt.show()

sf.best_save(fig, 'lMHi')
```



In [13]:

```
# Metropolis-Hastings algorithm

# set up
n = 100000
burn = 1000
w = np.empty(n)
pwgknab = lambda w, k, n, a, b: (k+a-1)*logp(w) + (n-k+b-1)*logp(1-w)

# initialize
w[0] = 0.5

# iterate
for i in range(1,n):

    # generate candidate
    wp = np.random.normal(w[i-1], 0.4)

    # acceptance porbability
    num = pwgknab(wp, likeK, likeN, priorAlpha, priorBeta)
    denom = pwgknab(w[i-1], likeK, likeN, priorAlpha, priorBeta)
    A = np.min([np.log(1), num-denom])

    # accept or reject
    u = np.log(np.random.uniform(low=0, high=1))
    if wp > 1 or wp < 0 : # reject (constrain like this?)
        w[i] = w[i-1]
    elif u <= A: # accept
        w[i] = wp
    else : # reject
        w[i] = w[i-1]
```

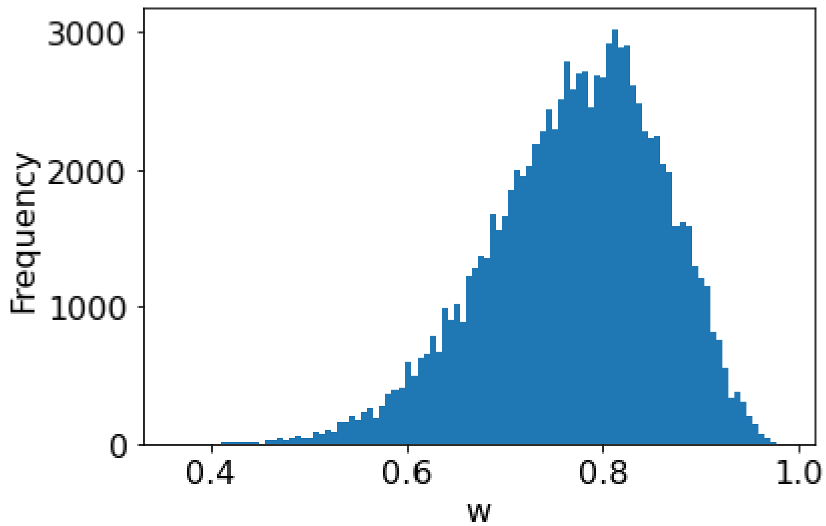
In [14]:

```
acc_rate = (len(np.unique(w)) / len(w)) * 100
print(f'Acceptance rate = {acc_rate:.0f}')
```

```
Acceptance rate = 26
```

In [15]:

```
# visualize
fig = plt.figure()
n, bins, _ = plt.hist(w[burn:], bins=100)
plt.xlabel('w')
plt.ylabel('Frequency')
plt.show()

sf.best_save(fig, 'lMHii')
```

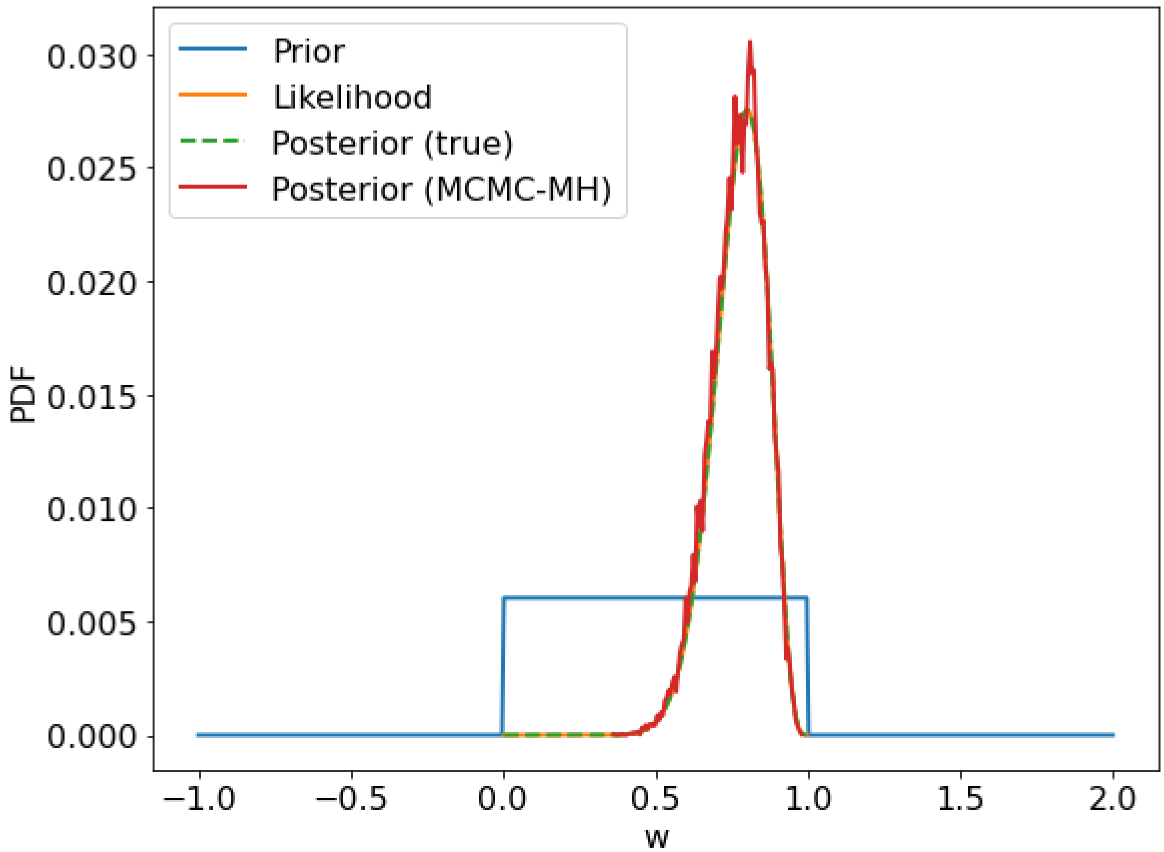


In [16]:

```
# posterior for plotting
xpost = bins[:-1]
ypost = n/sum(n)
print(sum(ypost))
```

```
1.0000000000000002
```

In [17]:
```
fig = plt.figure(figsize=(9,7))
plt.plot(x, prior, lw=2, label='Prior')
plt.plot(x, like, lw=2, label='Likelihood')
plt.plot(x, posterior, lw=2, ls='--', label='Posterior (true)')
plt.plot(xpost, ypost, lw=2, label='Posterior (MCMC-MH)')
plt.legend(loc='upper left')
plt.xlabel('w')
plt.ylabel('PDF')
plt.show()

sf.best_save(fig, 'lMHiii')
```



In [18]:
```
def nll(n, k, p):
    mindiff = -(np.log(math.factorial(n)/(math.factorial(k)*math.factor
    return mindiff
```

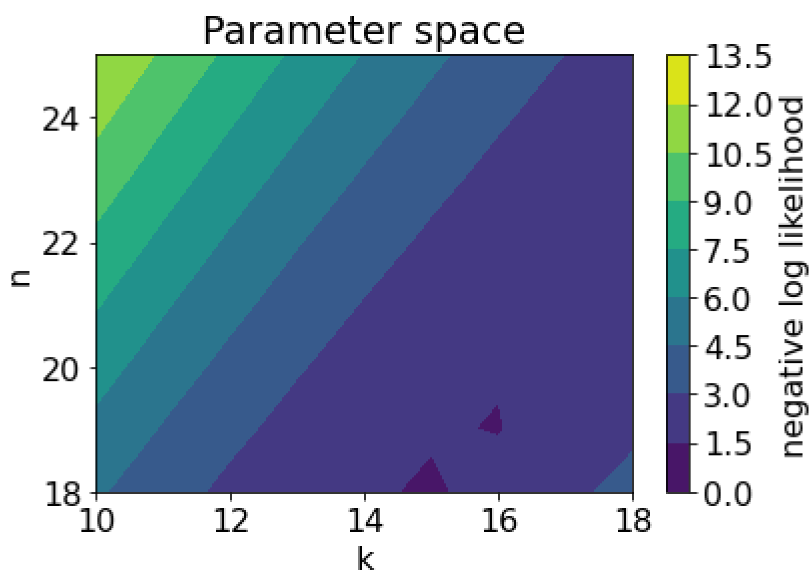
In [19]:
```
# visualize parameter space
n = np.linspace(18,25,8)
k = np.linspace(10,18,9)

NLL = np.empty([len(n),len(k)])
for idx1, N in enumerate(n):
    for idx2, K in enumerate(k):
        NLL[idx1,idx2] = nll(n=int(N), k=int(K), p=xpost[np.argwhere(yp
```

In [20]:
```
minIdx = np.where(NLL == NLL.min())
print(f'$n$ brute force = {np.round(n[minIdx[0][0]]):.3f}')
print(f'$k$ brute force = {np.round(k[minIdx[1][0]]):.3f}')
```

```
$n$ brute force = 18.000
$k$ brute force = 15.000
```

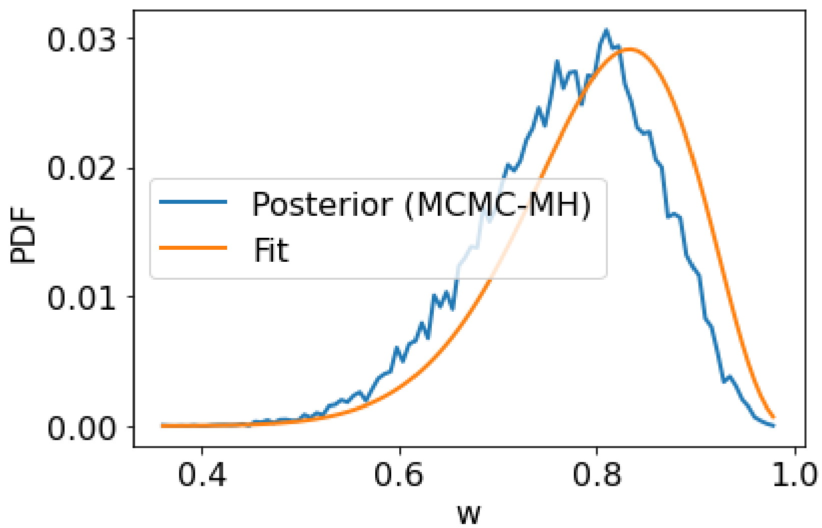
In [21]:
```
# optimizer
# nk = opt.fmin(lambda x: nll(x[0], x[1], p=ypost), np.array((15,19)))
# print(f'$n$ via optimization = {nk[0]:.4f}')
# print(f'$k$ via optimization = {nk[1]:.4f}')
```

In [22]:
```
# visualize
fig = plt.figure()
plt.contourf(k, n, NLL)
plt.colorbar(label='negative log likelihood')
plt.xlabel('k')
plt.ylabel('n')
plt.title('Parameter space')
plt.show()

sf.best_save(fig, 'lMHiv')
```



In [23]:

```
# fit some parameters to the data
fig = plt.figure()
plt.plot(xpost, ypost, lw=2, label='Posterior (MCMC-MH)')
yfit = stats.binom.pmf(k=np.round(k[minIdx[1][0]]), n=np.round(n[minIdx
yfit /= np.nansum(yfit)
plt.plot(xpost, yfit, lw=2, label='Fit')
plt.xlabel('w')
plt.ylabel('PDF')
plt.legend(loc=0)
plt.show()

sf.best_save(fig, 'lMHv')
```

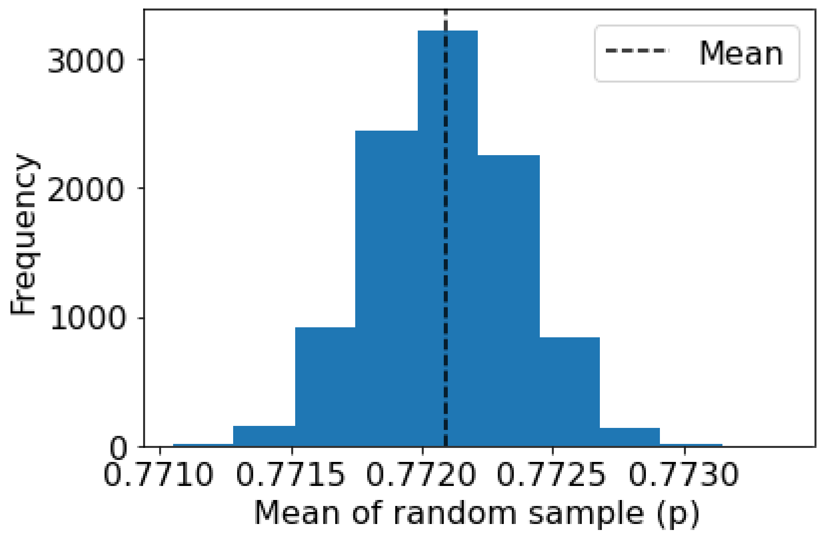


In [24]:

```
# bootstrap the max of the samples to get a better estimate of the true
nBoot = 10000
bootmean = np.empty(nBoot)
for i in range(nBoot):
    samp = np.random.choice(w[burn:], len(w[burn:]))
    bootmean[i] = np.mean(samp)

mumu = np.mean(bootmean)
```

In [25]:

```
# visualize
fig = plt.figure()
plt.hist(bootmean)
plt.axvline(mumu, c='k', ls='--', label='Mean')
plt.xlabel('Mean of random sample (p)')
plt.ylabel('Frequency')
plt.legend(loc=0)
plt.show()

sf.best_save(fig, 'lMHvi')
```



Try again, but with a more accurate mean (p parameter)

In [26]:

```
# visualize parameter space
n = np.linspace(18,25,8)
k = np.linspace(10,18,9)

NLL = np.empty([len(n),len(k)])
for idx1, N in enumerate(n):
    for idx2, K in enumerate(k):
        NLL[idx1,idx2] = nll(n=int(N), k=int(K), p=mumu)
```

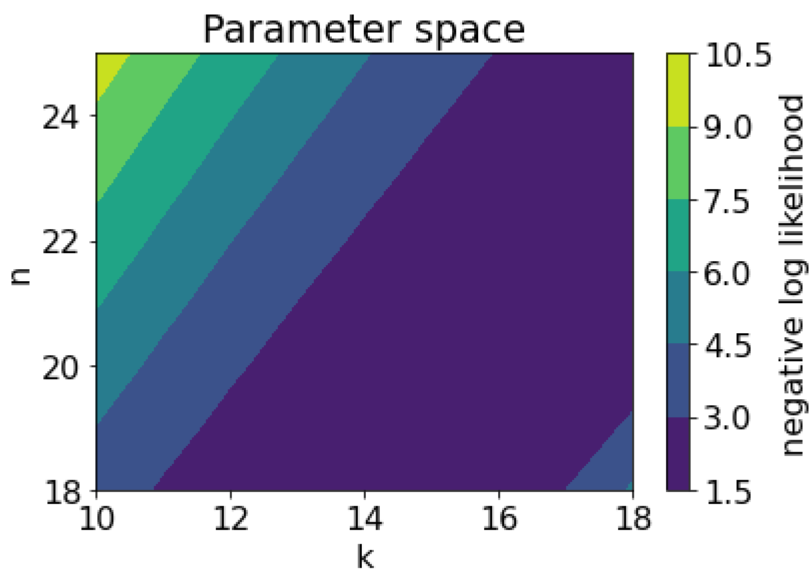
In [27]:

```
minIdx = np.where(NLL == NLL.min())
print(f'$n$ brute force = {np.round(n[minIdx[0][0]]):.3f}')
print(f'$k$ brute force = {np.round(k[minIdx[1][0]]):.3f}')
```

```
$n$ brute force = 18.000
$k$ brute force = 14.000
```

In [28]:

```
# visualize
fig = plt.figure()
plt.contourf(k, n, NLL)
plt.colorbar(label='negative log likelihood')
plt.xlabel('k')
plt.ylabel('n')
plt.title('Parameter space')
plt.show()

sf.best_save(fig, 'lMHvii')
```



In [29]:

```
# fit some parameters to the data
fig = plt.figure()
plt.plot(xpost, ypost, lw=2, label='Posterior (MCMC-MH)')
yfit = stats.binom.pmf(k=np.round(k[minIdx[1][0]]), n=np.round(n[minIdx
yfit /= np.nansum(yfit)
plt.plot(xpost, yfit, lw=2, label='Fit')
plt.xlabel('w')
plt.ylabel('PDF')
plt.legend(loc=0)
plt.show()

sf.best_save(fig, 'lMHviii')
```