

From scratch: Markov chain Monte Carlo (MCMC) - Metropolis Hastings, in python

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Credit: Japan Times.

1 Introduction

In one of the courses during my masters degree, I came across a technique called MCMC, its description was saying something along the lines: Markov chain Monte Carlo, commonly referred to as MCMC, is a class of techniques for sampling from a probability distribution. It can be used to estimate the distribution of parameters, given a set of observations.

Back then, I did not think much of it. I thought, "oh it's just another sampling technique". I decided I'd read on it when I'd practically need it. This need never came up, or maybe it did and I wrongly used something else.

1.1 So why the interest now?

Recently, I have seen a few discussions about MCMC and some of its implementations, specifically the Metropolis-Hastings algorithm and the PyMC3 library. *Markov Chain Monte Carlo in Python – A Complete Real-World Implementation* was the article that caught my attention the most. In it, William Koehrsen explains how he was able to learn the approach by applying it to a real world problem: to estimate the parameters of a logistic function that represents his sleeping patterns.

$$P(\text{sleep}/t, \alpha, \beta) = \frac{1}{1 + e^{\beta t + \alpha}}$$

Mr. Koehrsen uses the PyMC3 implementation of the Metropolis-Hastings algorithm to estimate β and α , thus computing the entire parameter space, and deriving the most likely logistic model.

1.2 So why am I talking about all that?

In this article, I propose to implement from scratch, my own version of the Metropolis-Hastings algorithm to find parameter distributions for a dummy data example and then of a real world problem.

I figured that if I get my hands dirty, I might finally be able to understand it. I will only use numpy to implement the algorithm, and matplotlib to draw pretty things. Alternatively scipy, can be used to compute the density functions, but I will also show how to implement them using numpy.

1.3 Flow of the article:

In part 1, I will introduce Bayesian inference, MCMC-MH and their mathematical components. In part 2, I will explain the algorithm using dummy data. Finally, part 3 will provide a real world application for MCMC-MH.

2 Part 1: Bayesian inference, Markov Chain Monte Carlo, and Metropolis-Hastings

2.1 In order to talk about Bayesian inference and what follows it, I shall first explain what the Bayesian view of probability is, and situate it within its historical context

2.1.1 Frequentist vs Bayesian thinking

There are two major interpretations to probabilities: Bayesian and Frequentist.

From a **Frequentist's** perspective, probabilities represent long term frequencies with which events occur. A frequentist can say that the probability of having tails from a coin toss is equal to 0.5 *on the long run*. Each new experiment, can be considered as one of an infinite sequence of possible repetitions of the same experiment. The idea is that there is *no* belief in a frequentist's view of probability. The probability of event x happening out of n trials is equal to the following frequency: $P(x) = \frac{n_x}{n}$, and the true probability is reached when $n \rightarrow \infty$. Frequentists will never say "I am 45% (0.45) sure that there is lasagna for lunch today", since this does not happen on the long run. Commonly, a frequentist approach is referred to as the *objective* approach since there is no expression of belief and/or prior events in it.

On the other hand, in **Bayesian** thinking, probabilities are treated as an expression of belief. For example, a Bayesian can perfectly say "I am 50% (0.5) sure that there is lasagna for lunch today". By combining *prior* beliefs and current events, the *evidence*, one can compute the *posterior*, the belief that there is lasagna today. The idea behind Bayesian thinking, is to keep updating the beliefs as more evidence is provided. Since this approach deals with belief, it is usually referred to as the *subjective* view on probability.

2.1.2 Bayesian inference

In the philosophy of decision making, Bayesian inference is closely related to Bayesian probability, in the sense that it manipulates priors, evidence, and likelihood to compute the posterior. Given some event B , what is the probability that event A occurs? This is answered by Bayes' famous formula: $P(A/B) = \frac{P(B/A)P(A)}{P(B)}$

- $P(A/B)$ is the **posterior**. What we wish to compute.
- $P(B/A)$ is the **likelihood**. Assuming A occurred, how likely is B .
- $P(A)$ is the **prior**. How likely the event A is regardless of evidence.
- $P(B)$ is the **evidence**. How likely the evidence B is regardless of the event.

In our case, we are mostly interested in the specific formulation of Bayes' formula:

$P(\theta/D) = \frac{P(D/\theta)P(\theta)}{P(D)}$ where, $P(\theta/D)$ is the **posterior**, $P(D/\theta)$ is the **likelihood**, $P(\theta)$ is the **prior** and $P(D)$ is the **evidence**.

We would like to find the most likely distribution of θ , the parameters of the model explaining the data, D .



Thomas Bayes, English statistician, philosopher, and theologian. Image Credit: [Farnam Street](#).

Computing some of these probabilities can be tedious, especially the evidence $P(D)$. Also, other problems can arise such as those of ensuring conjugacy, which I will not dive into in this article. Luckily, some techniques, namely MCMC, allow us to sample from the posterior, and draw distributions over our parameters without having to worry about computing the evidence, nor about conjugacy.

2.1.3 Markov Chain Monte Carlo

MCMC allows us to draw samples from any distribution that we can't sample from directly. It can be used to sample from the posterior distribution over parameters. It has seen much success in many applications, such as computing the distribution of parameters, given a set of observations and some prior belief, and computing high dimensional integrals in physics and in digital communications.

Bottom line: It can be used to compute the distribution over the parameters, given a set of observations and a prior belief.

2.1.4 Metropolis-Hastings

MCMC is a class of methods. Metropolis-Hastings is a specific implementation of MCMC. It works well in high dimensional spaces as opposed to Gibbs sampling and rejection sampling.

This technique requires a simple distribution called the **proposal distribution** (Which for some reason I like to call **transition model**) $Q(\theta'/\theta)$ to help draw samples from an intractable posterior distribution $P(\Theta = \theta/D)$.

Metropolis-Hastings uses Q to randomly walk in the distribution space, accepting or rejecting jumps to new positions based on how likely the sample is. This memoryless random walk is the “Markov Chain” part of MCMC.

The likelihood of each sample is decided by a function f . That’s why f must be proportional to the posterior we want to sample from. In order to ensure proportionality, f is commonly chosen to be the probability density function of the posterior we are trying to sample from.

To get a new position of the parameter, just take our current one θ , and propose a new one θ' , that is a random sample drawn from $Q(\theta'/\theta)$. Often this is a symmetric distribution. For instance, a normal distribution with mean θ and some standard deviation σ : $Q(\theta'/\theta) = \mathcal{N}(\theta, \sigma)$

To decide if θ' is to be accepted or rejected, the following ratio must be computed for each new value of θ' : $\frac{P(\theta'/D)}{P(\theta/D)}$. Using Bayes’ formula this can be easily re-formulated as: $\frac{P(D/\theta')P(\theta')}{P(D/\theta)P(\theta)}$
(The evidence $P(D)$ is simply crossed out during the division). $\frac{P(D/\theta')P(\theta')}{P(D/\theta)P(\theta)}$ is also equivalent to $\frac{\prod_i^n f(d_i/\Theta = \theta')P(\theta')}{\prod_i^n f(d_i/\Theta = \theta)P(\theta)}$

$$P(\text{accept}) = \begin{cases} \frac{\prod_i^n f(d_i/\Theta = \theta')P(\theta')}{\prod_i^n f(d_i/\Theta = \theta)P(\theta)}, & \prod_i^n f(d_i/\Theta = \theta)P(\theta) > \prod_i^n f(d_i/\Theta = \theta')P(\theta') \\ 1, & \prod_i^n f(d_i/\Theta = \theta)P(\theta) \leq \prod_i^n f(d_i/\Theta = \theta')P(\theta') \end{cases}$$

Note: The prior components are often crossed if there is no preference or restrictions on the parameters.

Metropolis-Hastings Algorithm:

- given:
 - f , the PDF of the distribution to sample from
 - Q , the transition model
 - θ_0 , a first guess for θ
 - $\theta = \theta_0$
- for n iterations
 - $p = f(D/\Theta = \theta)P(\theta)$
 - $\theta' = Q(\theta_i)$
 - $p' = f(D/\Theta = \theta')P(\theta')$

- $ratio = \frac{p'}{p}$
- generate a uniform random number r in $[0,1]$
- if $r < ratio$:
 - * set $\theta_i = \theta'$

```
In [41]: import numpy as np
import scipy
import scipy.stats
import matplotlib as mpl
import matplotlib.pyplot as plt
%matplotlib inline
```

3 Part 2: Dummy data example

3.1 Step 1: Data generation

We generate 30,000 samples from a normal distribution with $\mu = 10$, and $\sigma = 3$, but we can only observe 1000 of them.

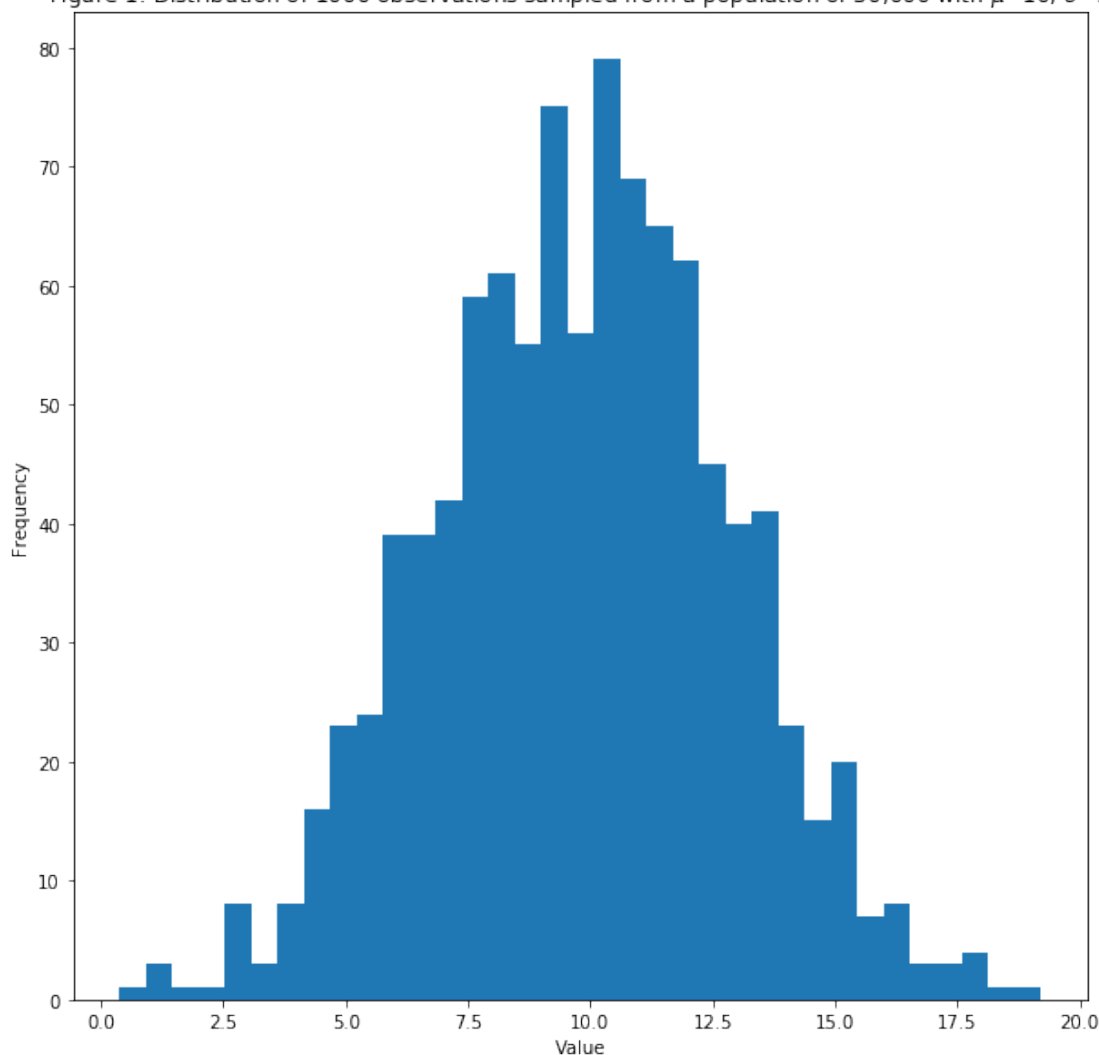
```
In [42]: mod1=lambda t:np.random.normal(10,3,t)

#Form a population of 30,000 individual, with average=10 and scale=3
population = mod1(30000)
#Assume we are only able to observe 1,000 of these individuals.
observation = population[np.random.randint(0, 30000, 1000)]

fig = plt.figure(figsize=(10,10))
ax = fig.add_subplot(1,1,1)
ax.hist( observation,bins=35 ,)
ax.set_xlabel("Value")
ax.set_ylabel("Frequency")
ax.set_title("Figure 1: Distribution of 1000 observations sampled from a
population of 30,000 with  $\mu=10$ ,  $\sigma=3$  ")
mu_obs=observation.mean()
mu_obs
```

```
Out[42]: 9.83685841372828
```


Figure 1: Distribution of 1000 observations sampled from a population of 30,000 with $\mu=10$, $\sigma=3$



3.2 Step 2: What do we want?

We would like to find a distribution for σ_{obs} using the 1000 observed samples. Those of you who are adept at mathematics will say that there is a formula for computing σ ($\sigma = \sqrt{\frac{1}{n} \sum_i^n (x_i - \mu)^2}$)!!!! Why do we want to sample and whatnot?? Well, this is just a dummy data example, the real problem is in part 3, where it's hard to compute the parameters directly. Plus here, we are not trying to find a value for σ , but rather, we are trying to compute a distribution of the possible values of σ .

3.3 Step 3: Define the PDF and the transition model.

From Figure 1, we can see that the data is normally distributed. The mean can be easily computed by taking the average of the values of the 1000 samples. By doing that, we get $\mu_{obs} = 9.8$.(although

on a side note, we could have also assumed σ to be unknown and sampled for it just like we are doing for μ . However, I want to make this starting example simple.)

3.3.1 For the transition model/ proposal distribution:

I have no specific distribution in mind, so I will choose a simple one: the Normal distribution!

$$Q(\sigma_{new}/\sigma_{current}) = N(\mu = \sigma_{current}, \sigma' = 1)$$

Note that σ' is unrelated to σ_{new} and $\sigma_{current}$. It simply specifies the standard deviation of the parameter space. It can be any value desired. It only affects the convergence time of the algorithm.

3.3.2 For the PDF:

We do know that the posterior follows a normal distribution with $\mu_{obs} = 9.8$. f should be its Probability Density Function (PDF) which is in this case:

$$f(x/\mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$

In our case, θ is made up of two values: $[\mu, \sigma]$, and that μ is a constant, $\mu = \mu_{obs}$.

3.4 Step 4: Define when we accept or reject σ_{new} :

We accept σ_{new} if:

$$\frac{Likelihood(\vec{x}/\mu_{obs}, \sigma_{new}) * prior(\mu_{obs}, \sigma_{new})}{Likelihood(\vec{x}/\mu_{obs}, \sigma_{current}) * prior(\mu_{obs}, \sigma_{current})} > 1 \quad (1)$$

If this ratio is smaller or equal to 1, then we compare it to a uniformly generated random number in the closed set $[0,1]$. If the ratio is larger than the random number, we accept σ_{new} , otherwise we reject it.

Note: Since we will be computing this ratio to decide which parameters should be accepted, it is imperative to make sure that the adopted function f is proportional to the posterior itself, $P(\sigma/\vec{x}, \mu)$, which in that case is verified. (f is the PDF of P)

3.5 Step 5: Define the prior and the likelihood:

3.5.1 For the Priors $P(\theta)$ and $P(\theta')$:

We don't have any preferences for the values that σ_{new} and $\sigma_{current}$ can take. The only thing worth noting is that they should be positive. Why? Intuitively, the standard deviation measures dispersion. Dispersion is a distance, and distances cannot be negative. Mathematically,

$\sigma = \sqrt{\frac{1}{n} \sum_i^n (x_i - \mu)^2}$, and the square root of a number cannot be negative. We strictly enforce this in the prior.

3.5.2 For the likelihood :

The total likelihood for a set of observation \vec{x} is:

$$\text{Likelihood}(\vec{x}/\mu_{obs}, \sigma_a) = \prod_i^n f(x_i/\mu_{obs}, \sigma_a), \text{ where } a = \text{new or current}.$$

In our case, we will log both the prior and the likelihood function. Therefore our acceptance condition from equation (1) becomes:

Accept σ_{new} if:

$$\text{Log}(\text{Likelihood}(\vec{x}/\mu_{obs}, \sigma_{new})) + \text{Log}(\text{prior}(\mu_{obs}, \sigma_{new})) - (\text{Log}(\text{Likelihood}(\vec{x}/\mu_{obs}, \sigma_{current})) + \text{Log}(\text{prior}(\mu_{obs}, \sigma_{current}))) > 0$$

Equivalent to:

$$\sum_i^n \text{Log}(f(x_i/\mu_{obs}, \sigma_{new})) + \text{Log}(\text{prior}(\mu_{obs}, \sigma_{new})) - \sum_i^n \text{Log}(f(x_i/\mu_{obs}, \sigma_{current})) - \text{Log}(\text{prior}(\mu_{obs}, \sigma_{current})) > 0$$

Equivalent to:

$$\sum_i^n \text{Log}(f(x_i/\mu_{obs}, \sigma_{new})) + \text{Log}(\text{prior}(\mu_{obs}, \sigma_{new})) > \sum_i^n \text{Log}(f(x_i/\mu_{obs}, \sigma_{current})) + \text{Log}(\text{prior}(\mu_{obs}, \sigma_{current}))$$

Equivalent to:

$$\sum_i^n -n\text{Log}(\sigma_{new}\sqrt{2\pi}) - \frac{(x - \mu_{obs})^2}{2\sigma_{new}^2} + \text{Log}(\text{prior}(\mu_{obs}, \sigma_{new})) > \sum_i^n -n\text{Log}(\sigma_{current}\sqrt{2\pi}) - \frac{(x - \mu_{obs})^2}{2\sigma_{current}^2} + \text{Log}(\text{prior}(\mu_{obs}, \sigma_{current})) \quad (2)$$

This form can be reduced even more by taking the square root and the multiplication out of the log.

In [43]: *#The tranistion model defines how to move from sigma_current to sigma_new*
`transition_model = lambda x: [x[0], np.random.normal(x[1], 0.5, (1,))]`

```
def prior(x):
    #x[0] = mu, x[1]=sigma (new or current)
    #returns 1 for all valid values of sigma. Log(1) =0, so it does not
    #affect the summation.
    #returns 0 for all invalid values of sigma (<=0). Log(0)=-infinity,
    #and Log(negative number) is undefined.
    #It makes the new sigma infinitely unlikely.
    if(x[1] <=0):
        return 0
    return 1
```

#Computes the likelihood of the data given a sigma (new or current)

```

    according to equation (2)
def manual_log_like_normal(x,data):
    #x[0]=mu, x[1]=sigma (new or current)
    #data = the observation
    return np.sum(-np.log(x[1] * np.sqrt(2* np.pi) )-((data-x[0])**2) / (2*x[1]**2))

#Same as manual_log_like_normal(x,data), but using scipy implementation. It's
pretty slow.
def log_lik_normal(x,data):
    #x[0]=mu, x[1]=sigma (new or current)
    #data = the observation
    return np.sum(np.log(scipy.stats.norm(x[0],x[1]).pdf(data)))

#Defines whether to accept or reject the new sample
def acceptance(x, x_new):
    if x_new>x:
        return True
    else:
        accept=np.random.uniform(0,1)
        # Since we did a log likelihood, we need to exponentiate in order
        to compare to the random number
        # less likely x_new are less likely to be accepted
        return (accept < (np.exp(x_new-x)))

def metropolis_hastings(likelihood_computer,prior, transition_model, param_init,
iterations,data,acceptance_rule):
    # likelihood_computer(x,data): returns the likelihood that
    these parameters generated the data
    # transition_model(x): a function that draws a sample from a
    symmetric distribution and returns it
    # param_init: a starting sample
    # iterations: number of accepted to generated
    # data: the data that we wish to model
    # acceptance_rule(x,x_new): decides whether to accept or reject the new sample
    x = param_init
    accepted = []
    rejected = []
    for i in range(iterations):
        x_new = transition_model(x)
        x_lik = likelihood_computer(x,data)
        x_new_lik = likelihood_computer(x_new,data)
        if (acceptance(x_lik + np.log(prior(x)),x_new_lik+np.log(prior(x_new)))):
            x = x_new
            accepted.append(x_new)
        else:
            rejected.append(x_new)

```

```
return np.array(accepted), np.array(rejected)
```

3.6 Step 6: Run the algorithm with initial parameters and collect accepted and rejected samples

```
In [44]: accepted, rejected = metropolis_hastings(manual_log_like_normal,prior,
transition_model,[mu_obs,0.1], 50000,observation,acceptance)
```

3.6.1 The algorithm accepted 8317 samples (which might be different on each new run). The last 10 samples contain the following values for σ :

```
In [45]: accepted[-10:,1]
```

```
Out[45]: array([2.87920187, 3.10388928, 2.94469786, 3.04094103, 2.95522153,
               3.09328088, 3.07361275, 3.08588388, 3.12881964, 3.03651136])
```

```
In [46]: print(accepted.shape)
```

```
(8317, 2)
```

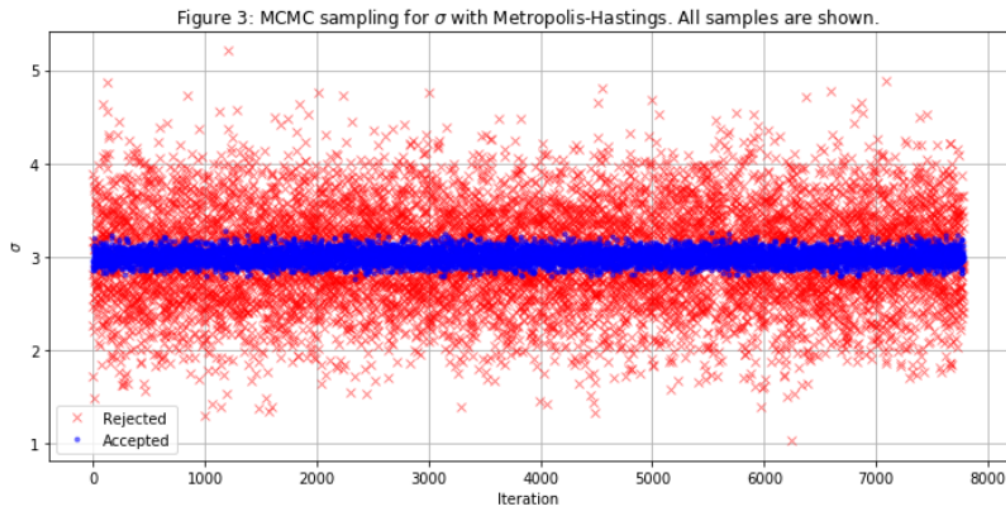
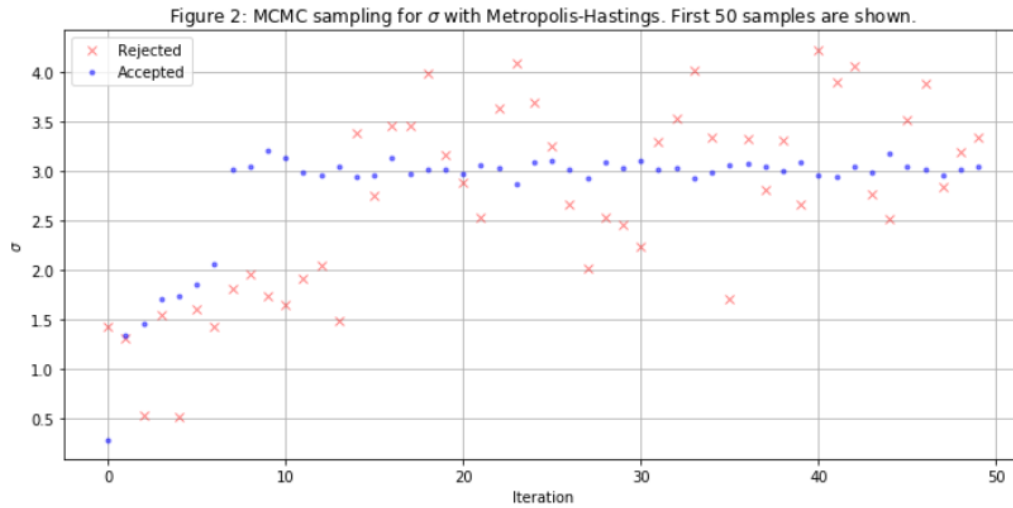
Let's see how the algorithm worked its way to these values:

```
In [47]: fig = plt.figure(figsize=(10,10))
ax = fig.add_subplot(2,1,1)
to_show=-accepted.shape[0]
ax.plot( rejected[0:50,1], 'rx', label='Rejected',alpha=0.5)
ax.plot( accepted[0:50,1], 'b.', label='Accepted',alpha=0.5)
ax.set_xlabel("Value")
ax.set_ylabel("Frequency")
ax.set_title("Figure 2: MCMC sampling for  $\sigma$  with Metropolis-Hastings.
First 50 samples are shown.")
ax.grid()
ax.legend()

ax2 = fig.add_subplot(2,1,2)
to_show=-accepted.shape[0]
ax2.plot( rejected[to_show:,1], 'rx', label='Rejected',alpha=0.5)
ax2.plot( accepted[to_show:,1], 'b.', label='Accepted',alpha=0.5)
ax2.set_xlabel("Value")
ax2.set_ylabel("Frequency")
ax2.set_title("Figure 3: MCMC sampling for  $\sigma$  with Metropolis-Hastings.
All samples are shown.")
ax2.grid()
ax2.legend()
```

```
fig.tight_layout()
accepted.shape
```

Out [47]: (8317, 2)



So, starting from an initial of 0.1, the algorithm converged pretty quickly to the expected value of 3. That said, it's only sampling in a 1D space. so it's not very surprising.

3.6.2 We consider the initial 25% of the values of σ to be "burn-in", so we drop them.

3.6.3 Let's visualize the trace of σ and the histogram of the trace.

```
In [48]: show=int(-0.75*accepted.shape[0])
         hist_show=int(-0.75*accepted.shape[0])

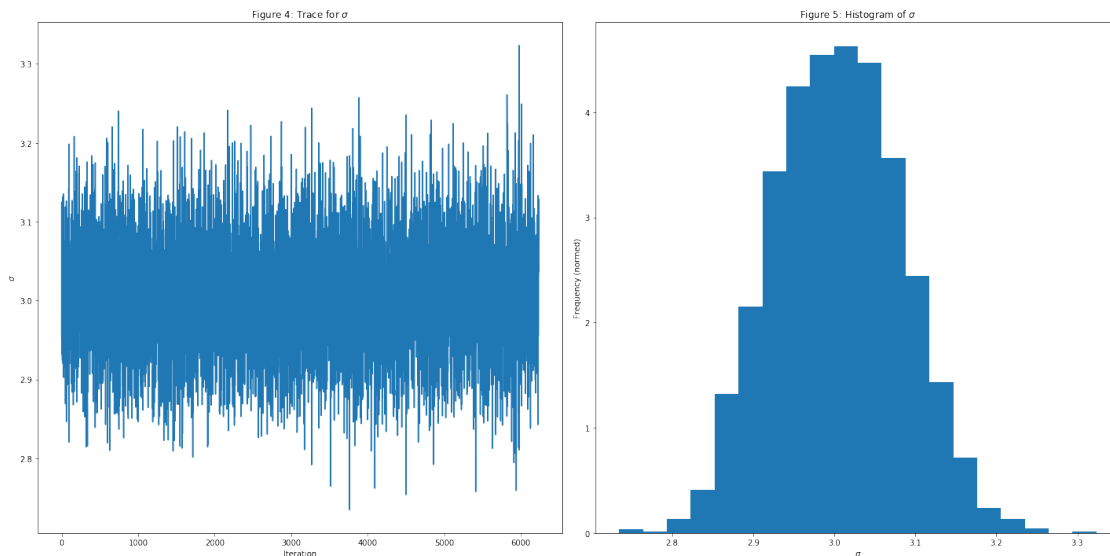
         fig = plt.figure(figsize=(20,10))
```

```

ax = fig.add_subplot(1,2,1)
ax.plot(accepted[show:,1])
ax.set_title("Figure 4: Trace for  $\sigma$ ")
ax.set_ylabel(" $\sigma$ ")
ax.set_xlabel("Iteration")
ax = fig.add_subplot(1,2,2)
ax.hist(accepted[hist_show:,1], bins=20,density=True)
ax.set_ylabel("Frequency (normed)")
ax.set_xlabel(" $\sigma$ ")
ax.set_title("Figure 5: Histogram of  $\sigma$ ")
fig.tight_layout()

ax.grid("off")

```



3.6.4 The most likely for σ is around 3.1. This is a bit more than the original value of 3.0. The difference is due to us observing only 3.33% of the original population (1,000 out of 30,000)

3.6.5 Prediction time rediction time

First, we average the last 75% of accepted samples of μ , and we generate 30,000 random individuals from a normal distribution with $\mu = 9.8$ and $\sigma = 3.05$ (the average of the last 75% of accepted samples) which is actually better than the most likely value of 3.1. And voilà:

```

In [49]: mu=accepted[show:,0].mean()
         sigma=accepted[show:,1].mean()
         print(mu, sigma)
         model = lambda t,mu,sigma:np.random.normal(mu,sigma,t)

```

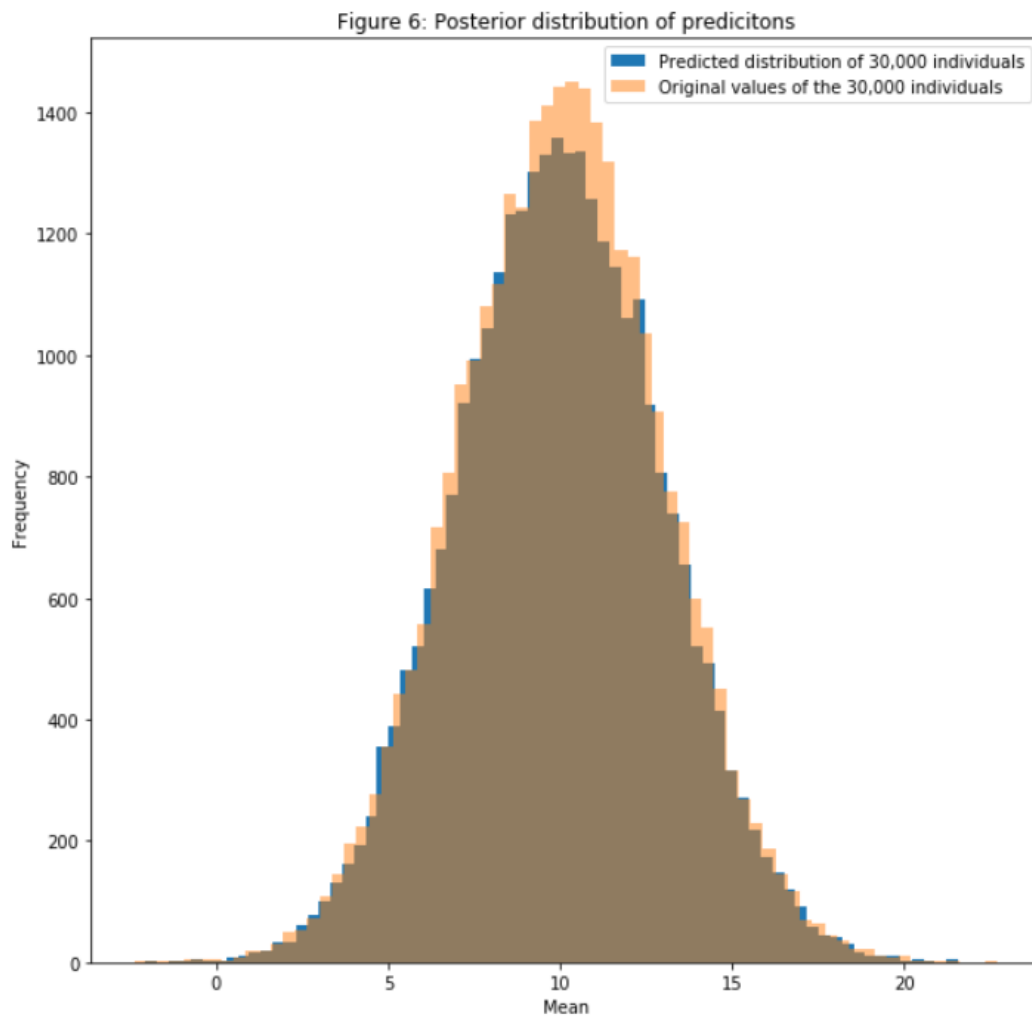
```

observation_gen=model(population.shape[0],mu,sigma)
fig = plt.figure(figsize=(10,10))
ax = fig.add_subplot(1,1,1)
ax.hist( observation_gen,bins=70 ,label="Predicted distribution
of 30,000 individuals")
ax.hist( population,bins=70 ,alpha=0.5, label="Original values of
the 30,000 individuals")
ax.set_xlabel("t")
ax.set_ylabel("Frequency")
ax.set_title("Figure 6: Posterior distribution of predicitions")
ax.legend()

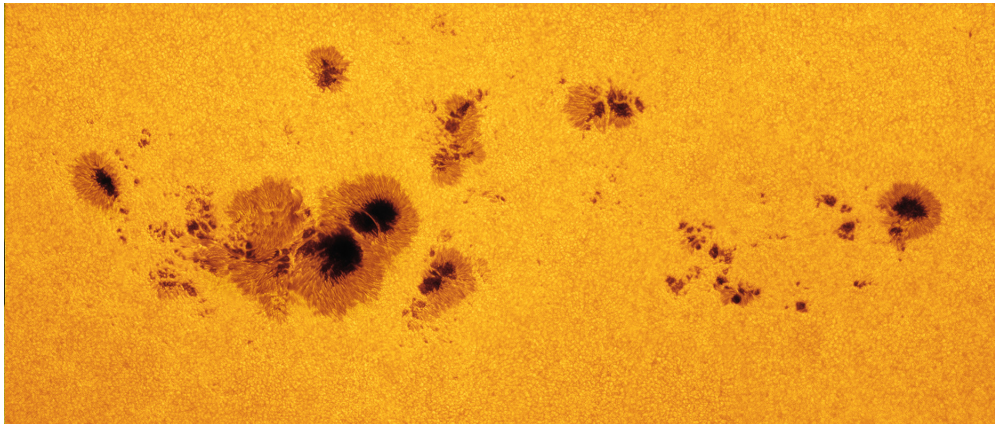
```

9.83685841372828 3.004591127329635

Out[49]: <matplotlib.legend.Legend at 0x1c5f4ef1b38>



4 Part 3: A real world example



Credit: Amateur astronomer Alan Friedman on July 10, 2012.

A sunspot is a region on the Sun's surface (photosphere) that is marked by a lower temperature than its environment. These reduced temperatures are caused by concentrations of magnetic field flux that inhibit convection by an effect similar to [eddy current brakes](#). Sunspots usually appear in pairs of opposite magnetic polarity. Their number varies according to the approximately 11-year solar cycle.

The data we will be working on is the “Monthly mean total sunspot number”, for each month from January 1749 to November 2018. This data collected, curated and made publicly available by the [World Data Center for the production, preservation and dissemination of the international sunspot number](#).

4.1 Let's plot the data over the years to see what the distribution might be like.

```
In [10]: sunspots = np.loadtxt("data/SN_m_tot_V2.0.csv", delimiter=';')
```

```
#years is the third column
years = sunspots[:,2]
#activity is the 4th column
activity = sunspots[:,3] + 0.1
print(years.shape, activity.shape)
fig = plt.figure(figsize=(20,10))
ax = fig.add_subplot(2,1,1)

ax.plot(years, activity, label="Sunspot count")
ax.set_yticks(np.arange(0,500,100))
ax.set_xlabel("Years")
ax.set_ylabel("Monthly mean count of sunspots")
ax.set_title("Figure 7: Sunspots, 1749-2018")
ax.legend()
```



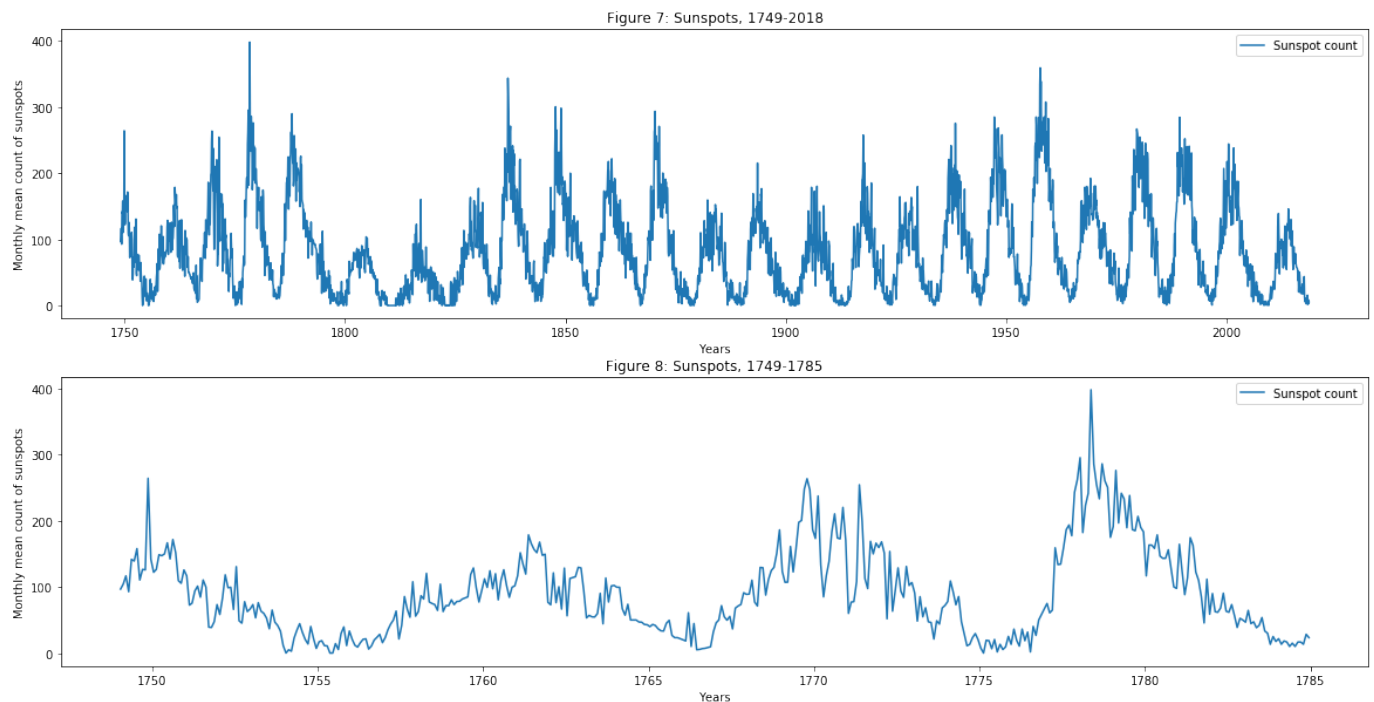
```

ax = fig.add_subplot(2,1,2)
print(years[432])
ax.plot(years[:432], activity[:432], label="Sunspot count")
ax.set_yticks(np.arange(0,500,100))
ax.set_xlabel("Years")
ax.set_ylabel("Monthly mean count of sunspots")
ax.set_title("Figure 8: Sunspots, 1749-1785")
ax.legend()

```

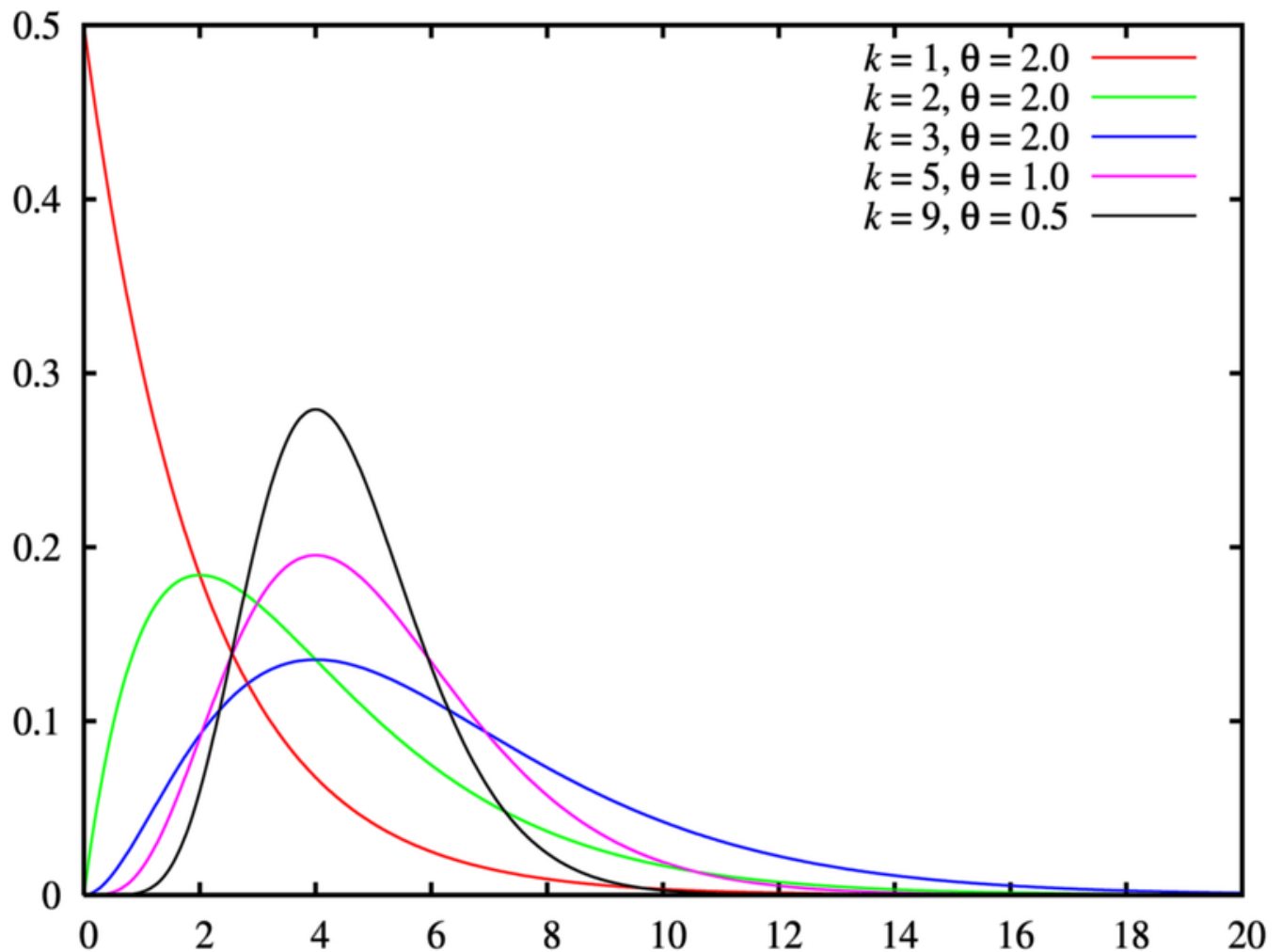
(3238,) (3238,)
1785.042

Out[10]: <matplotlib.legend.Legend at 0x1c5ec0932e8>



4.2 It seems like we could model this phenomenon with a gamma distribution, with a new cycle resetting ever 12 years.

A gamma distribution Γ is a two-parameter family of continuous probability distributions, the parameters are the shape a and the scale b . A random variable X that is gamma-distributed is noted $X \sim \Gamma(a, b)$, and in our case X is the count of sunspots. The two parameters a and b are the unknowns that we would like to calculate distributions for.



For example, in the first cycle, the sunspot counts start from their highest at about 300 at the end of 1749, and fall to their lowest 6 years after, during 1755. Then the number rises up again to its maximum during 1761 and 1762 before falling again during 1766 and so on...

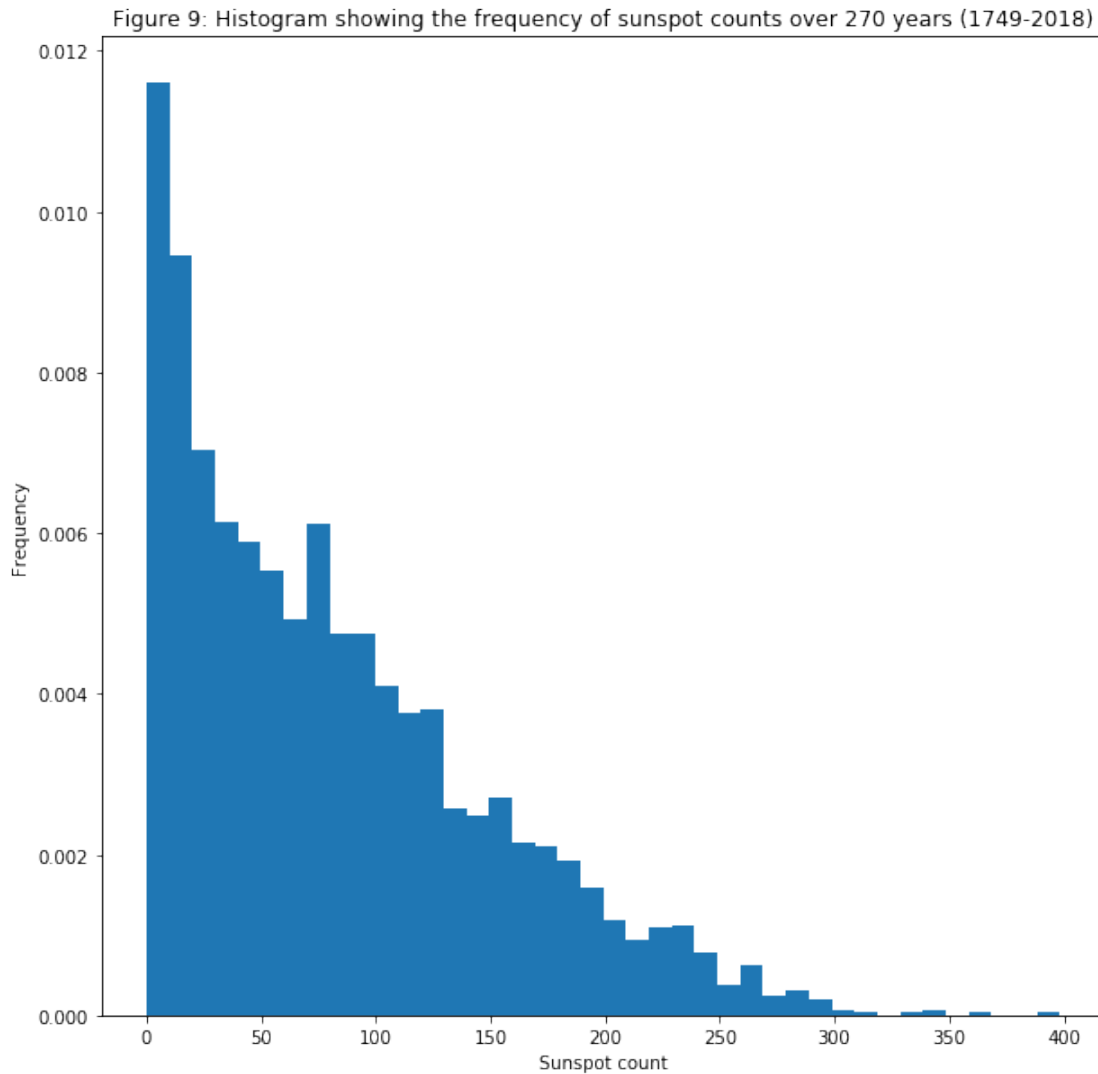
Let's make sure by plotting a histogram of sunspot counts:

```
In [11]: fig = plt.figure(figsize=(10,10))
          ax = fig.add_subplot(1,1,1)
          ax.hist(activity, bins=40, normed=True)
          ax.set_xlabel("Sunspot count")
          ax.set_ylabel("Frequency")
          ax.set_title("Figure 9: Histogram showing the frequency of sunspot
                        counts over 270 years (1749-2018)")
```

D:\Anaconda3\lib\site-packages\matplotlib\axes_axes.py:6510: MatplotlibDeprecationWarning:
The 'normed' kwarg was deprecated in Matplotlib 2.1 and will be removed in 3.1. Use 'density' :

```
alternative="'density'", removal="3.1")
```

Out[11]: Text(0.5, 1.0, 'Figure 9: Histogram showing the frequency of sunspot counts over 270 years (1749-2018)')



4.3 Indeed, it does seem like the frequency of counts follows a gamma distribution

The gamma distribution, has for PDF, $f/f(x; a, b) = \frac{b^a x^{a-1} e^{-ax}}{\Gamma(a)}$ where Γ is the gamma function (not to be confused with the gamma distribution which requires 2 parameters): $\Gamma(a) = (a-1)!$

Following the same procedure as in the dummy data example, we can write down the log likelihood from this pdf (see code below). Alternatively, one could use the

`scipy.stats.gamma(a,b).pdf(x)` function to compute it.

Since a and b must be positive, we enforce this in the prior.

```
In [12]: transition_model = lambda x: np.random.normal(x, [0.05,5], (2,))
import math
def prior(w):
    if(w[0]<=0 or w[1] <=0):
        return 0
    else:
        return 1

def manual_log_lik_gamma(x,data):
    return np.sum((x[0]-1)*np.log(data) - (1/x[1])*data - x[0]*np.log(x[1]) -
        np.log(math.gamma(x[0])))

def log_lik_gamma(x,data):
    return np.sum(np.log(scipy.stats.gamma(a=x[0],scale=x[1],loc=0).pdf(data)))

In [13]: accepted, rejected = metropolis_hastings(manual_log_lik_gamma,prior,
    transition_model,[4, 10], 50000,activity,acceptance)

In [14]: print(accepted.shape)
accepted[-10:]
```

(8561, 2)

```
Out[14]: array([[ 1.0069025 , 81.4658413 ],
 [ 1.00114207, 81.60205149],
 [ 0.99202173, 82.74584913],
 [ 1.01762076, 82.16486545],
 [ 1.01725261, 80.77994436],
 [ 0.95808072, 87.32697333],
 [ 1.01140003, 82.62579073],
 [ 1.00449348, 84.26070321],
 [ 1.01988362, 81.79192804],
 [ 0.98848982, 84.99360422]])
```

Starting from $a=4$, and $b=10$, the algorithm accepted 8561 pairs of samples, the last value for a is 0.98848982 and the last value for b is 84.99360422, which are pretty far off the initial values. As with the dummy data example, let's see how the algorithm worked its way to these values:

```
In [31]: fig = plt.figure(figsize=(10,10))
ax = fig.add_subplot(3,1,1)
ax.plot(accepted[:50,0], accepted[:50,1], label="Path")
ax.plot(accepted[:50,0], accepted[:50,1], 'b.', label='Accepted')
ax.plot(rejected[:50,0], rejected[:50,1], 'rx', label='Rejected')
ax.legend()
```

```
ax.set_title("Figure 10: MCMC sampling for a and b with Metropolis-Hastings.  
First 50 samples are shown.")
```

```
ax = fig.add_subplot(3,1,2)  
ax.plot(accepted[:,0], accepted[:,1], label="Path")  
ax.plot(accepted[:,0], accepted[:,1], 'b.', label='Accepted',alpha=0.3)  
ax.plot(rejected[:,0], rejected[:,1], 'rx', label='Rejected',alpha=0.3)  
ax.legend()  
ax.set_title("Figure 11: MCMC sampling for a and b with Metropolis-Hastings.  
All samples are shown.")
```

```
to_show=50  
ax = fig.add_subplot(3,1,3)  
ax.plot(accepted[-to_show:,0], accepted[-to_show:,1], label="Path")  
ax.plot(accepted[-to_show:,0], accepted[-to_show:,1], 'b.', label='Accepted',  
alpha=0.5)  
ax.plot(rejected[-to_show:,0], rejected[-to_show:,1], 'rx', label='Rejected',  
alpha=0.5)  
ax.legend()  
ax.set_title("Figure 12: MCMC sampling for a and b with Metropolis-Hastings.  
Last 50 samples are shown.")
```

```
Out[31]: Text(0.5, 1.0, 'Figure 12: MCMC sampling for a and b with Metropolis-Hastings.  
Last 50 samples are shown.')
```

Figure 10: MCMC sampling for a and b with Metropolis-Hastings. First 50 samples are shown.

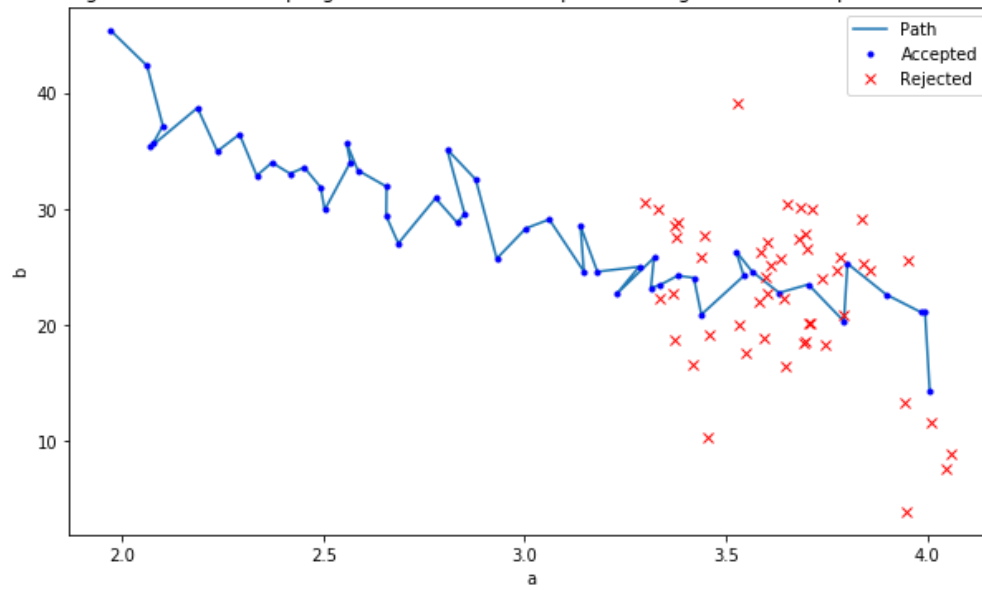


Figure 11: MCMC sampling for a and b with Metropolis-Hastings. All samples are shown.

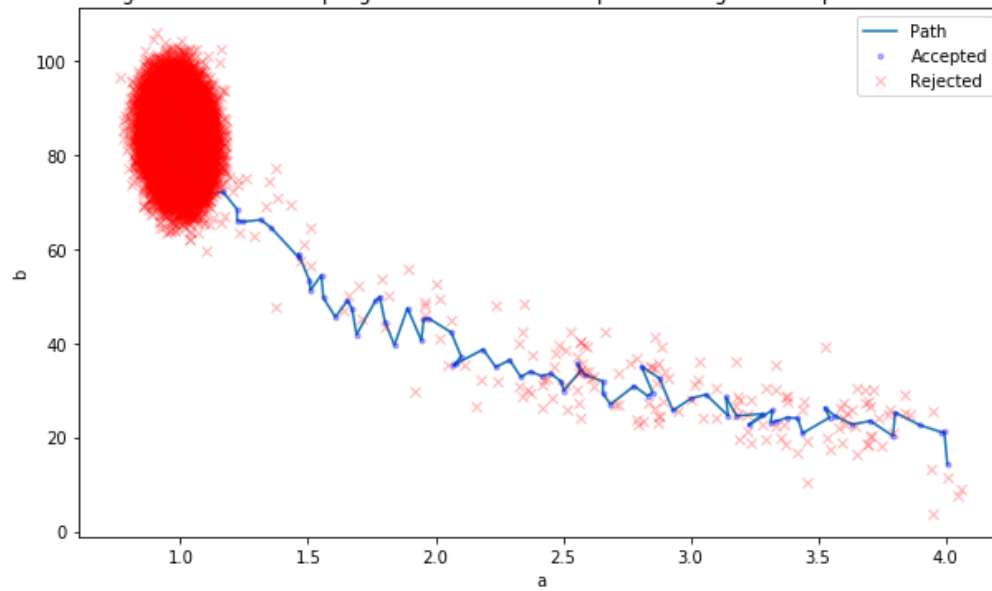
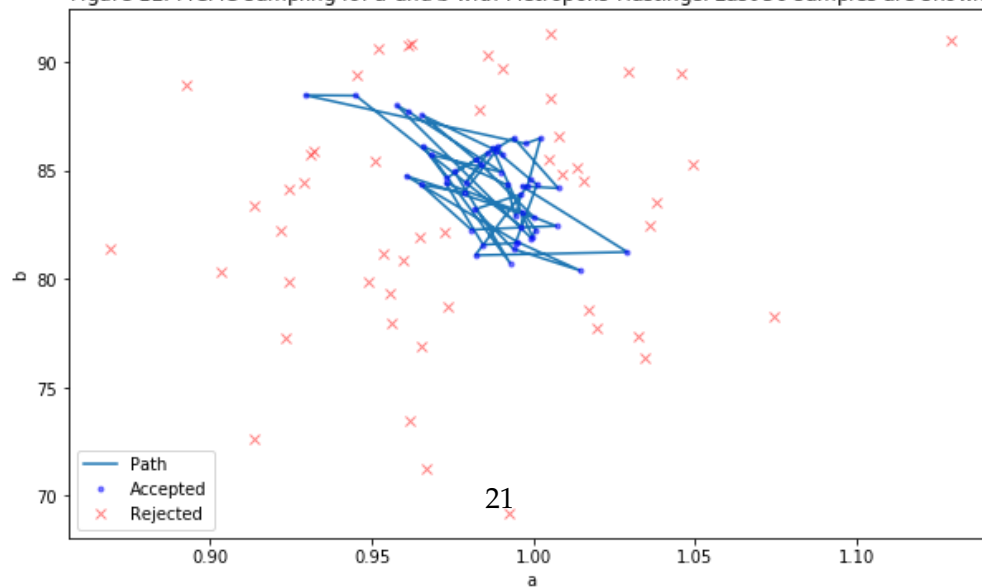


Figure 12: MCMC sampling for a and b with Metropolis-Hastings. Last 50 samples are shown.



As we can see from figures 10, 11, and 12, the algorithm converges quickly to the $[a=1, b=85]$ zone.

Tip: when the algorithm starts to heavily reject samples, that means that we have reached a zone of saturation of the likelihood. Commonly, this can be interpreted as having reached the optimal parameter space from which we can sample, i.e. there is very little reason for the algorithm to accept new values.

4.3.1 We consider the initial 50% of the values of a and b to be “burn-in”, so we drop them.

4.3.2 Let’s visualize the traces of a and b and the histogram of the traces.

```
In [39]: show=int(-0.5*accepted.shape[0])
         hist_show=int(-0.50*accepted.shape[0])

fig = plt.figure(figsize=(15,7))
ax = fig.add_subplot(1,2,1)
ax.plot(accepted[show:,0])
ax.set_title("Figure 13: Trace for a")
ax.set_xlabel("Iteration")
ax.set_ylabel("a")
ax = fig.add_subplot(1,2,2)
ax.hist(accepted[hist_show:,0], bins=20, normed=True)
ax.set_ylabel("Frequency (normed)")
ax.set_xlabel("a")
ax.set_title("Figure 14: Histogram of a")
fig.tight_layout()

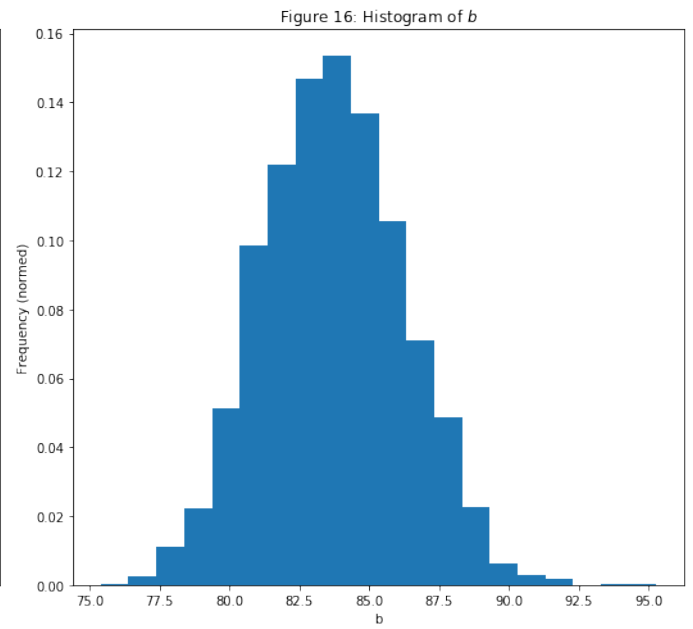
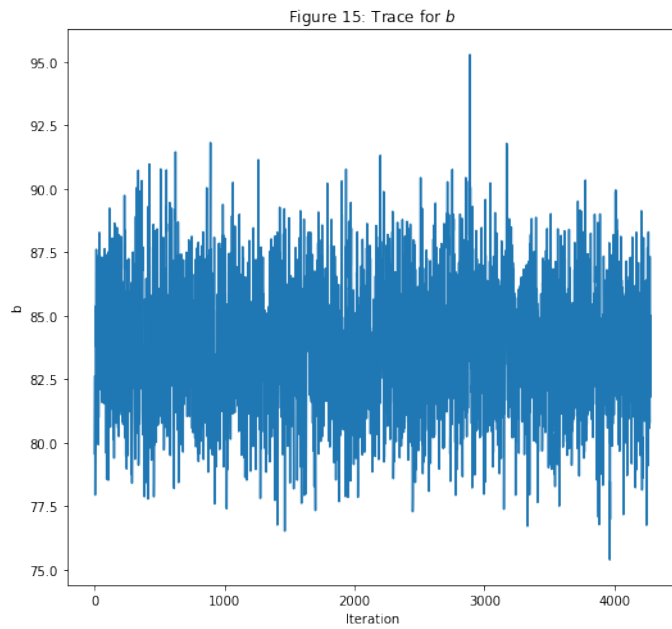
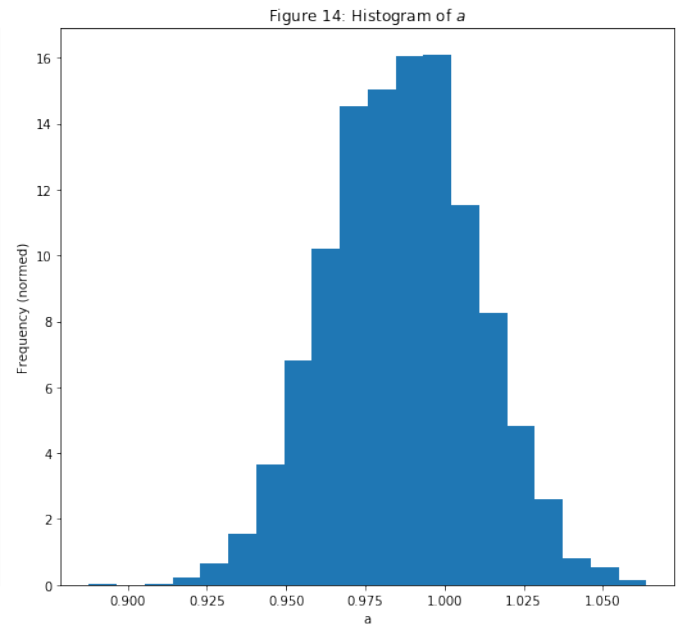
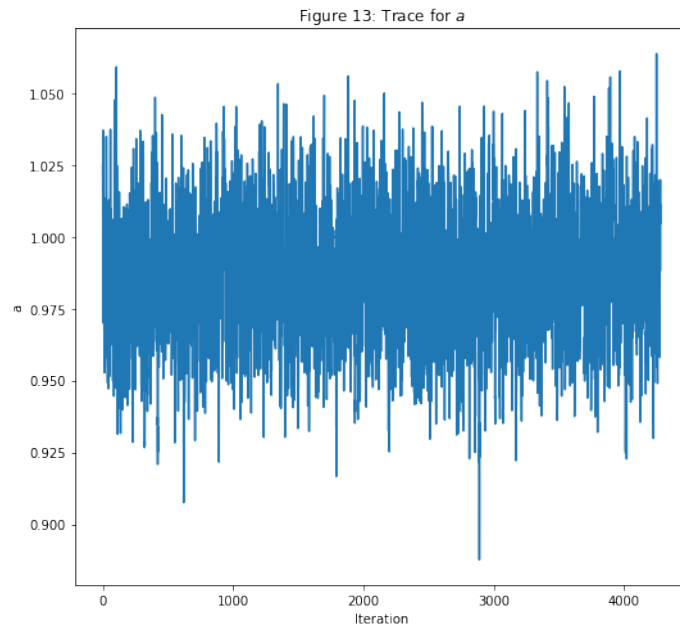
fig = plt.figure(figsize=(15,7))
ax = fig.add_subplot(1,2,1)
ax.plot(accepted[show:,1])
ax.set_title("Figure 15: Trace for b")
ax.set_xlabel("Iteration")
ax.set_ylabel("b")
ax = fig.add_subplot(1,2,2)
ax.hist(accepted[hist_show:,1], bins=20, normed=True)
ax.set_ylabel("Frequency (normed)")
ax.set_xlabel("b")
ax.set_title("Figure 16: Histogram of b")
fig.tight_layout()

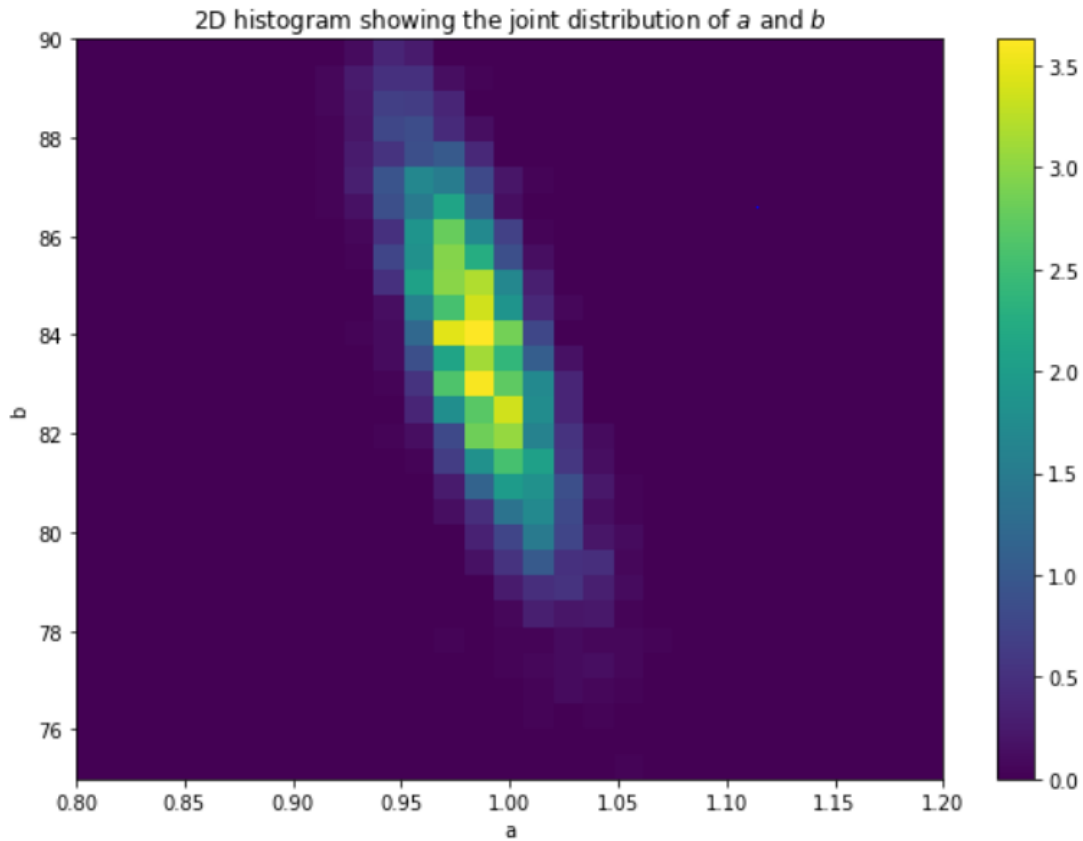
fig = plt.figure(figsize=(10,7))
ax = fig.add_subplot(1,1,1)
xbins, ybins = np.linspace(0.8,1.2,30), np.linspace(75,90,30)
counts, xedges, yedges, im = ax.hist2d(
accepted[hist_show:,0], accepted[hist_show:,1], normed=True, bins=[xbins, ybins])
fig.colorbar(im, ax=ax)
```



```
ax.set_title("2D histogram showing the joint distribution of a and b")
```

```
Out[39]: Text(0.5, 1.0, '2D histogram showing the joint distribution of a and b')
```





4.4 Prediction time

First, we average the last 50% of accepted samples of a and b , and we generate random individuals from a Γ distribution. $a_{average}=0.9866200759935773$ and $b_{average}=83.70749712447888$.

And the predictions:

```
In [32]: show=-int(0.5*accepted.shape[0])

mu=accepted[show:,0].mean()
sigma=accepted[show:,1].mean()
print(mu, sigma)
model = lambda t,mu,sigma:np.random.gamma(mu,sigma,t)
t=np.arange(activity.shape[0])
observation_gen=model(t.shape[0],mu,sigma)
fig = plt.figure(figsize=(10,10))
ax = fig.add_subplot(1,1,1)

ax.hist( observation_gen,bins=np.linspace(0,500,50) ,normed=True,
```

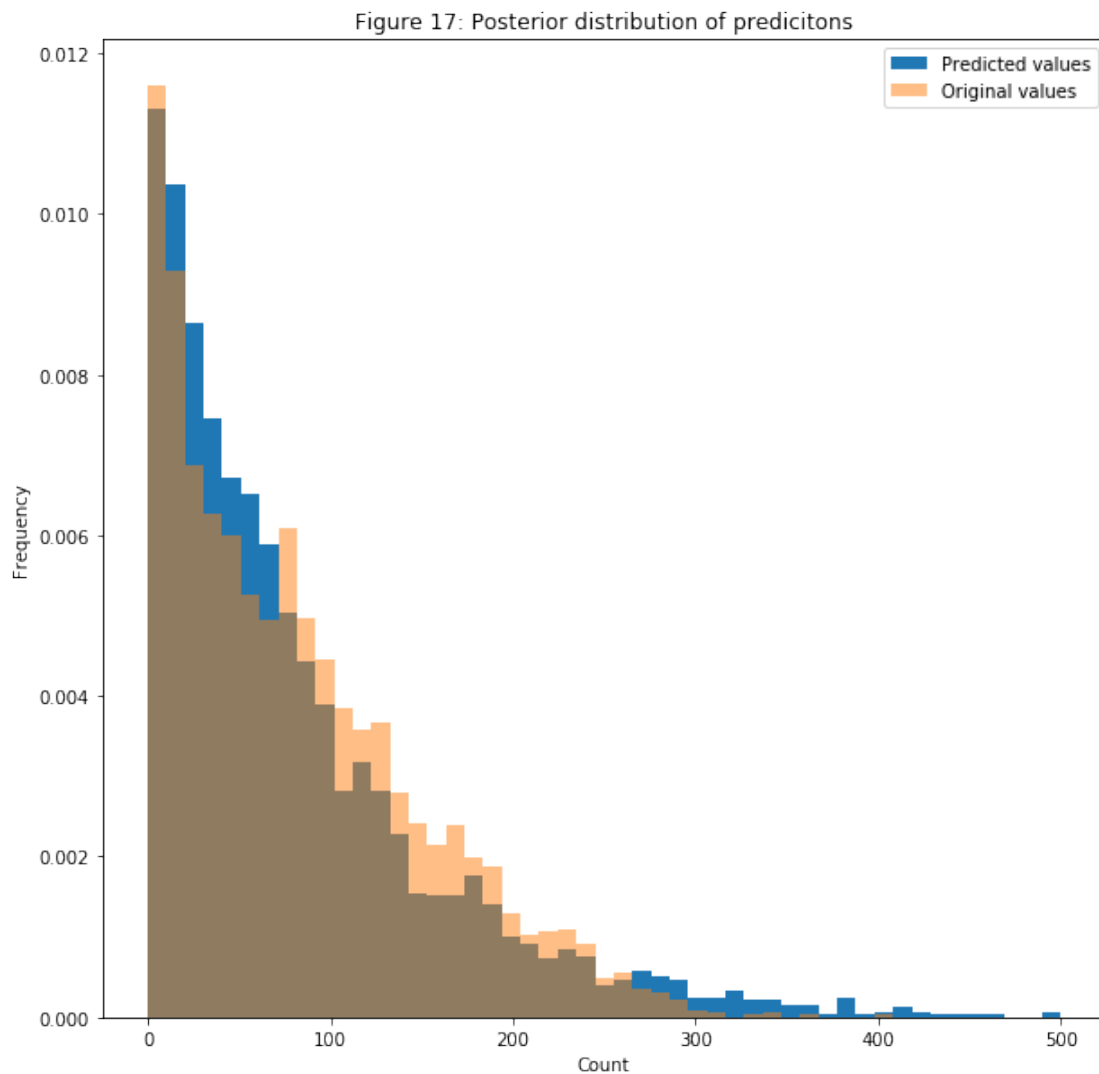
```

label="Predicted values")
ax.hist( activity,bins=np.linspace(0,500,50) ,alpha=0.5,normed=True,
        label="Original values")
ax.set_xlabel("Count")
ax.set_ylabel("Frequency")
ax.set_title("Figure 17: Posterior distribution of predicitions")
ax.legend()

```

0.9866200759935773 83.70749712447888

Out[32]: <matplotlib.legend.Legend at 0x1c5f261ba90>



5 Evaluation

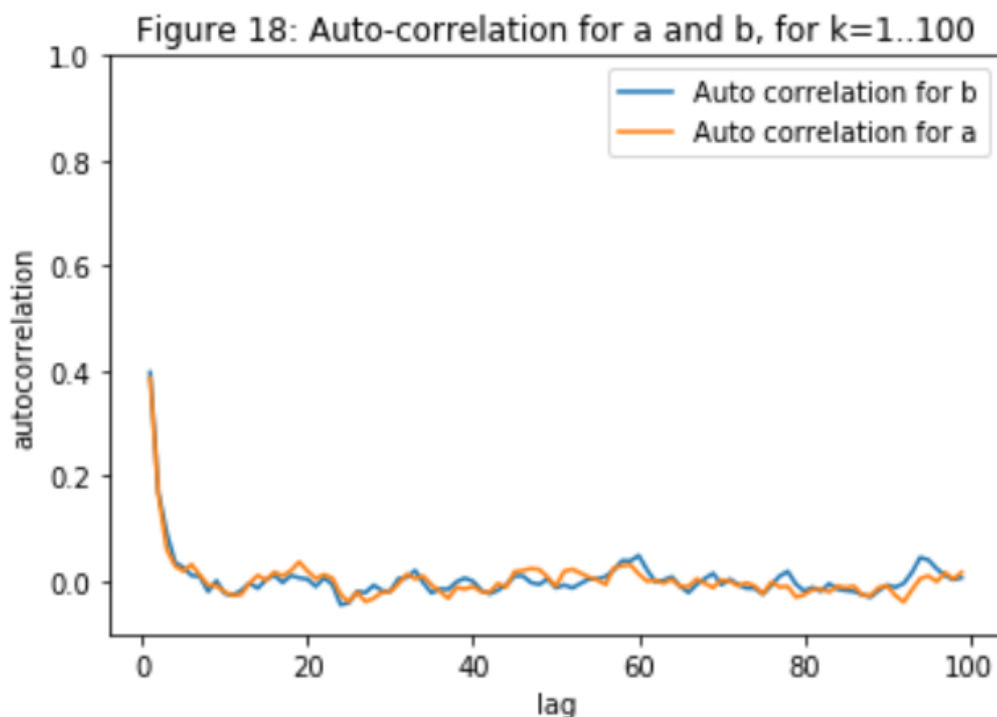
How do we specify the parameters for the distribution Q ? Should we move far from the current sample, or stay relatively close? These questions can be answered by measuring the auto-correlation between accepted samples: we do not want the accepted samples to be too correlated between one another. We don't want distant samples to be too correlated as we are trying to implement a markov chain, i.e. a sample should only depend on its previous sample, and the auto-correlation plot should show a quick, exponential decrease between the correlation of sample i and $i-1, i-2, \dots, i-n$

The auto-correlation is defined by computing the following function for each lag k :

$$r_k = \frac{\sum_{i=1}^{N-k} (Y_i - Y_{avg})(Y_{i+k} - Y_{avg})}{\sum_{i=1}^N (Y_i - Y_{avg})^2}$$

The lag k , is basically the *range* around a sample Y_i in which we would like to measure the correlation.

The plots below show the auto-correlation for a , b for k going from 1 to 100. A lag of $k=1$ means that we are measuring the correlation of a sample with itself, so we expect it to be equal to 1. The higher k goes, the lower that correlation ought to be.



In our case, we are lucky to have a low enough correlation. In general, we might want to setup the parameters of the proposal distribution, Q , automatically, one common method is to keep adjusting the proposal parameters so that more than 50% proposals are rejected. Alternatively, one could use an enhanced version of MCMC called Hamiltonian Monte Carlo, which reduces the correlation between successive sampled states and reaches the stationary distribution quicker.

6 Conclusion

While the abstraction behind this algorithm may seem out of grasp at first, the implementation is actually pretty simple, and gives awesome results.

7 References

Peter Driscoll, "A comparison of least-squares and Bayesian fitting techniques to radial velocity data sets"

Carson Chow, "MCMC and fitting models to data"

John H. Williamson, "Data Fundamentals - Probabilities"

Simon Rogers, "A first course in machine learning"