Lecture 8

Bayesian Stats and Sampling



Today:

- Bayesian Stats recap
- replicative posterior predictives
- Normal-normal Model
- exponential model
- Inverse Transform Sampling
- Rejection Sampling



Last Time

- Entropy
- Maximum Likelihood and Entropy
- Bayesian Stats



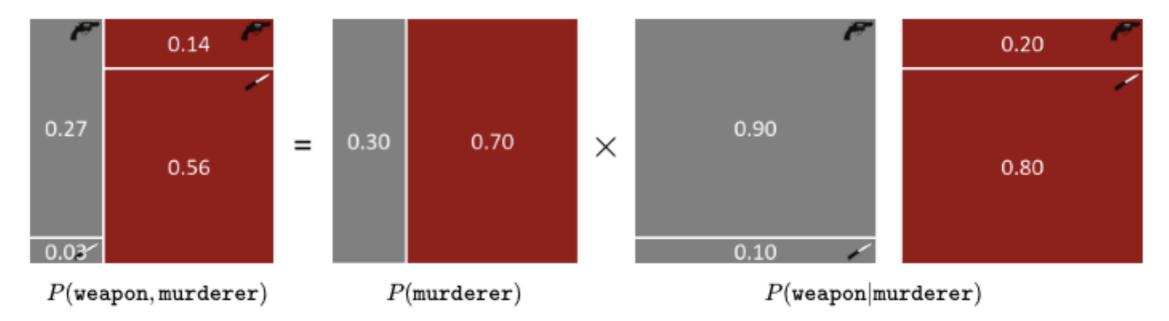
Bayesian Stats

- assume sample IS the data, no stochasticity
- parameters θ are stochastic random variables
- associate the parameter θ with a prior distribution $p(\theta)$
- The prior distribution generally represents our belief on the parameter values when we have not observed any data yet (to be qualified later)
- obtain posterior distributions
- predictive distribution from the posterior



Basic Idea

Get the joint Probability distribution



Now we condition on some random variables and learn the values of others.



Rules

1.
$$P(A, B) = P(A | B)P(B)$$

2. $P(A) = \sum_{B} P(A, B) = \sum_{B} P(A | B)P(B)$

P(A) is called the **marginal** distribution of A, obtained by summing or marginalizing over B.



Posterior

$$p(\theta|D = \{y\}) = rac{p(D|\theta) p(\theta)}{p(D)}$$

Posterior: $p(\theta|D) \propto p(D|\theta) p(\theta)$

Evidence:

$$p(D=\{y\})=\int d heta\,p(heta,D)=\int d heta\,p(D| heta)p(heta).$$



Marginalization

Marginal posterior:
$$p(heta_1|D) = \int d heta_{-1} p(heta|D).$$

Posterior Predictive:

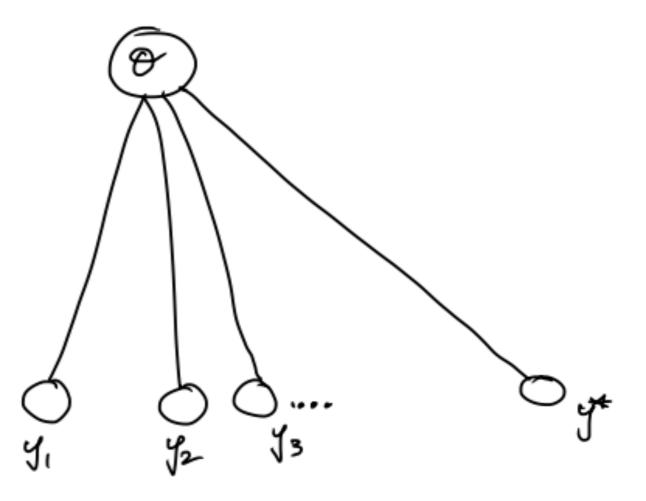
$$p(y^*|D=\{y\})=\int d heta p(y^*, heta|\{y\}).$$



Basic Graph

$$egin{aligned} p(heta,y,y^*) &= p(heta)p(y| heta)p(y)p(y^*| heta) \ &= p(heta|y)p(y)p(y^*| heta) \ &= \int d heta \, p(heta^*,y, heta) \ &= \int d heta \, rac{p(y^*,y, heta)}{p(y)} \end{aligned}$$

$$p(y^*|y) = \int d heta \, p(heta|y) p(y^*| heta)$$





Predictives

The distribution of a future data point y^* :

Posterior predictive:

$$p(y^*|D=\{y\})=\int d heta p(y^*| heta)p(heta|\{y\}).$$

The distribution of a data point *y* from the prior:

Prior predictive:

$$p(y) = \int d heta \, p(heta, y) = \int d heta \, p(y| heta) p(heta).$$



Globe Toss Model

- Seal tosses globe, p is true water fraction
- data WLWWWLWLW
- Modeled using the Binomial Distribution, which is the distribution of a set of Bernoulli random variables.



Griddy Posterior

```
prior_pdf = lambda p: 1
like_pdf = lambda p: binom.pmf(k=6, n=9, p=p)
post_pdf = lambda p: like_pdf(p)*prior_pdf(p)
p_grid = np.linspace(0., 1., 1000)
post_vals = post_pdf(p_grid)
post_vals_normed = post_vals/np.sum(post_vals)
grid_post_samples = np.random.choice(p_grid, size=10000, replace=True, p=post_vals_normed)
```

- create a grid, evaluate posterior on it
- discrete-normalize this posterior to get probabilities
- sample the grid according to these probabilities



Laplace Approximation for p^*

Unnormalized posterior:

$$\log p^*(heta|x) = \log p^*(heta_{MAP}|x) + rac{1}{2}(heta- heta_{MAP})^2 \Big[rac{d^2}{d heta^2} {
m log} p^*(heta|x)\Big]_{ heta= heta_{MAP}} + \ \ldots$$

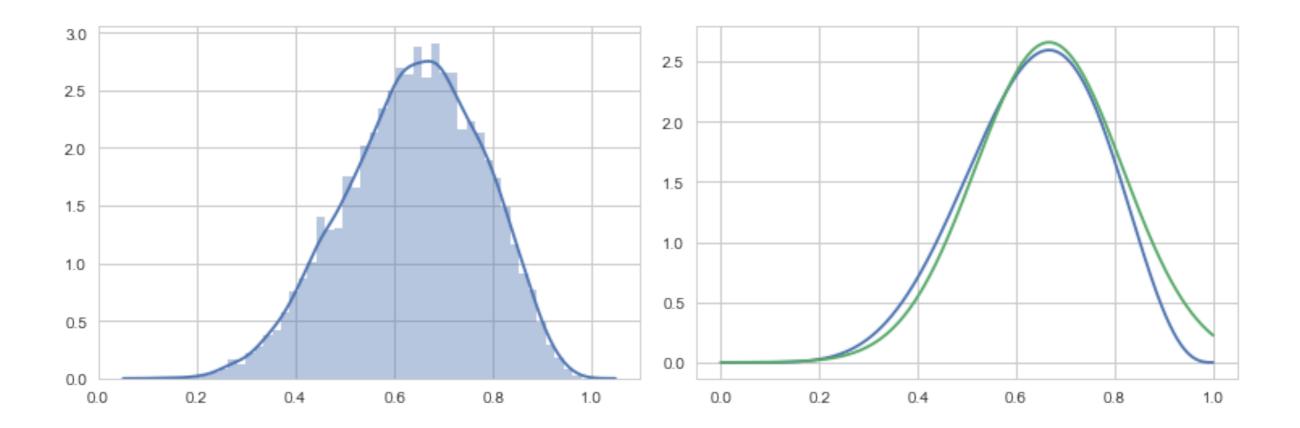
Let $c = -\left[\frac{d^2}{d\theta^2}\log p^*(\theta|x)\right]_{\theta=\theta_{MAP}}$ then we get un-normalized Gaussian:

$$q^*(heta) = p^*(heta_{MAP})e^{-rac{c}{2}(heta- heta_{MAP})^2}$$
 ,

whose normalization $(p^*(\theta_{MAP})\sqrt{\frac{2\pi}{c}})$ we then use to approximate the normalization of p^* .



Griddy and Laplace, together





Conjugate Prior

- A **conjugate prior** is one which, when multiplied with an appropriate likelihood, gives a posterior with the same functional form as the prior.
- Likelihoods in the exponential family have conjugate priors in the same family
- analytical tractability AND interpretability



• The Beta distribution is conjugate to the Binomial distribution

 $p(p|y) \propto p(y|p)P(p) = Binom(n, y, p) \times Beta(\alpha, \beta)$

Because of the conjugacy, this turns out to be:

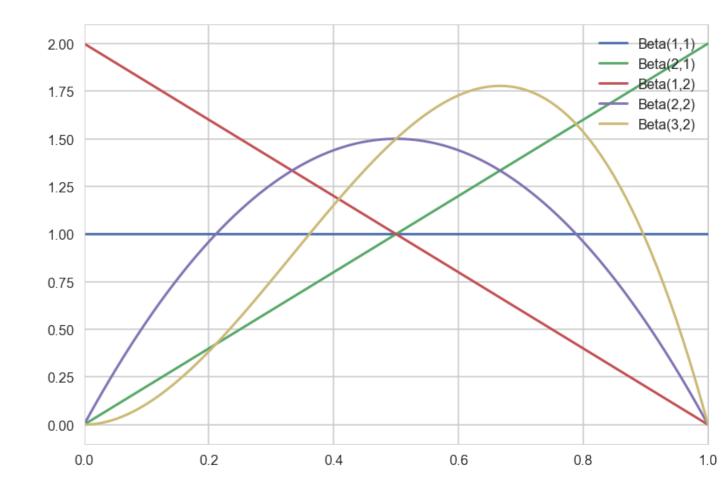
$$Beta(y + \alpha, n - y + \beta)$$

• a *Beta*(1, 1) prior is equivalent to a uniform distribution.



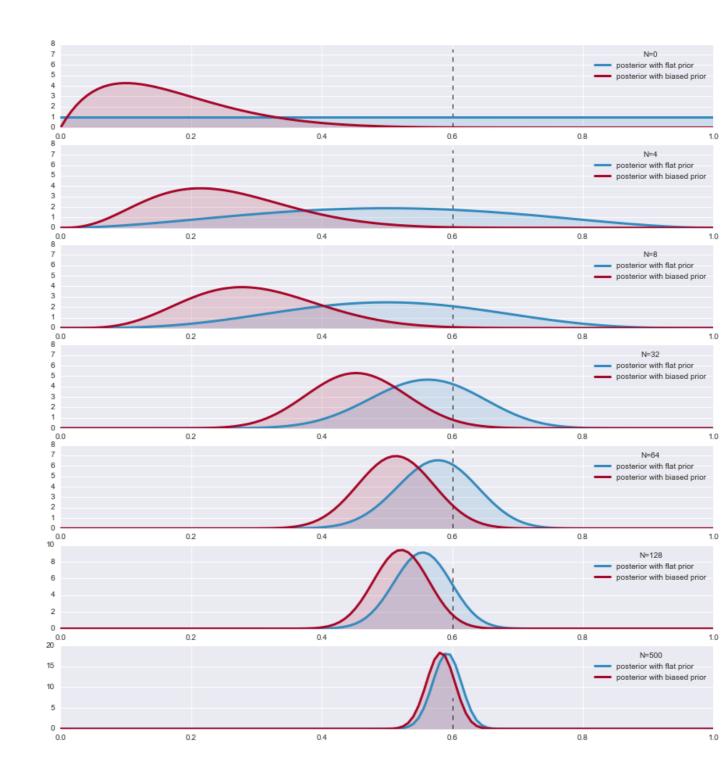
Priors Regularize

- think of a prior as a regularizer.
- Bata(1,1) is an uninformative
 prior. Here the prior adds one heads and one tails to the actual data, providing some
 "towards-center" regularization
- especially useful where in a few tosses you got all heads, clearly at odds with your beliefs.
- a *Beta*(2, 1) prior would bias you to more heads





Data overwhelms prior eventually





Bayesian Updating "on-line"

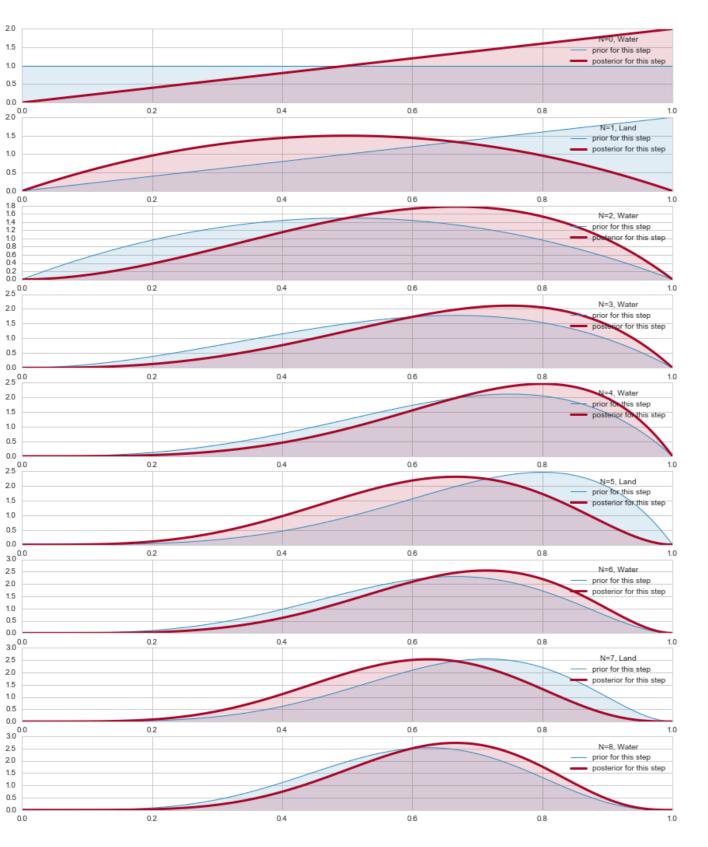
- can update prior to posterior all at once, or one by one
- as each piece of data comes in, you update the prior by multiplying by the one-point likelihood.
- the posterior you get becomes the prior for our next step

$$p(heta \mid \{y_1,\ldots,y_{n+1}\}) \propto p(\{y_{n+1}\} \mid heta) imes p(heta \mid \{y_1,\ldots,y_n\})$$

• the posterior predictive is the distribution of the next data point!

$$p(y_{n+1}|\{y_1,\ldots y_n\}) = E_{p(heta|\{y_1,\ldots y_n\})}[p(y_{n+1}| heta)] = \int d heta\, p(y_{n+1}| heta) p(heta|\{y_1,\ldots y_n\})$$





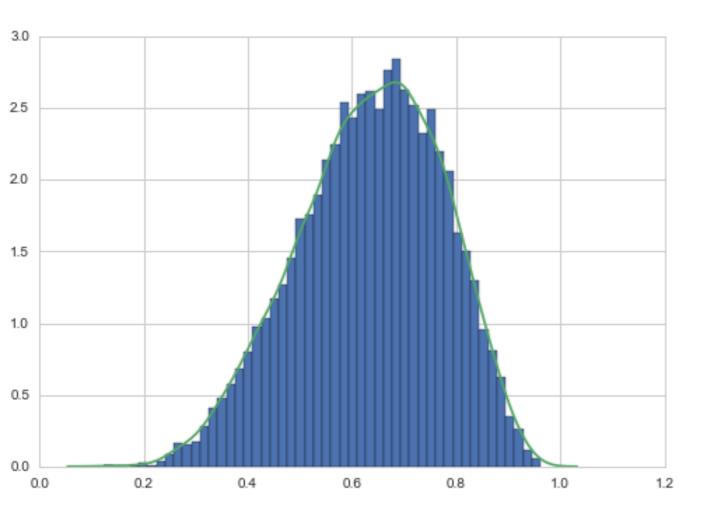
Bayesian Updating of globe

 notice how the posterior shifts left and right depending on new data

At each step:

$$Beta(y+lpha,n-y+eta)$$

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Posterior properties

- The probability that the amount of water is less than 50%: np.mean(samples < 0.5) = 0.173
- Credible Interval: amount of probability mass.
 np.percentile(samples, [10, 90]) = [0.44604094, 0.81516349]
- np.mean(samples), np.median(samples) = (0.63787343440335842, 0.6473143052303143)



Point estimates: MAP

$$egin{aligned} heta_{ ext{MAP}} &= rg\max_{ heta} \, p(heta|D) \ &= rg\max_{ heta} \, rac{\mathcal{L} \, p(heta)}{p(D)} \ &= rg\max_{ heta} \, \mathcal{L} \, p(heta) \end{aligned}$$

sampleshisto = np.histogram(samples, bins=50)
maxcountindex = np.argmax(sampleshisto[0])
mapvalue = sampleshisto[1][maxcountindex]
print(maxcountindex, mapvalue)

31 0.662578641304

OR Optimize!



Point estimates: mean

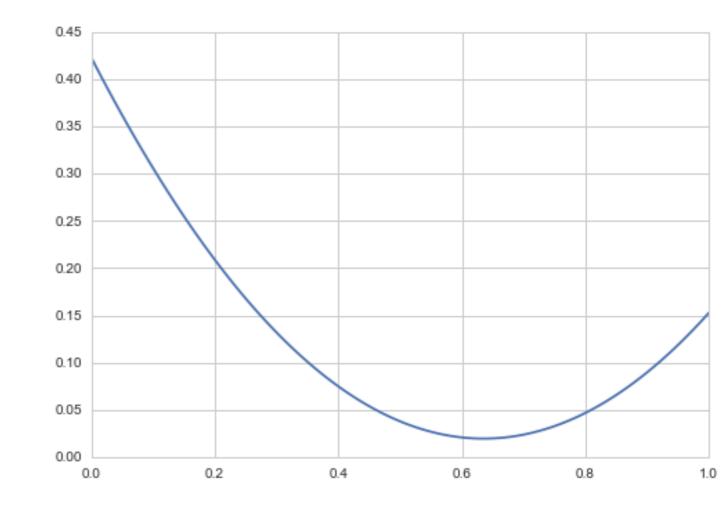
$$R(t)=E_{p(heta|D)}[(heta-t)^2]=\int d heta(heta-t)^2p(heta|D)$$

$$rac{dR(t)}{dt} = 0 \implies t = \int d heta heta p(heta | D)$$

mse = [np.mean((xi-samples)**2) for xi in x]
plt.plot(x, mse);

Mean is at 0.638.

This is **Decision Theory**.





Posterior predictive for globe tosses

$$p(y^*|D) = \int d heta p(y^*| heta) p(heta|D)$$

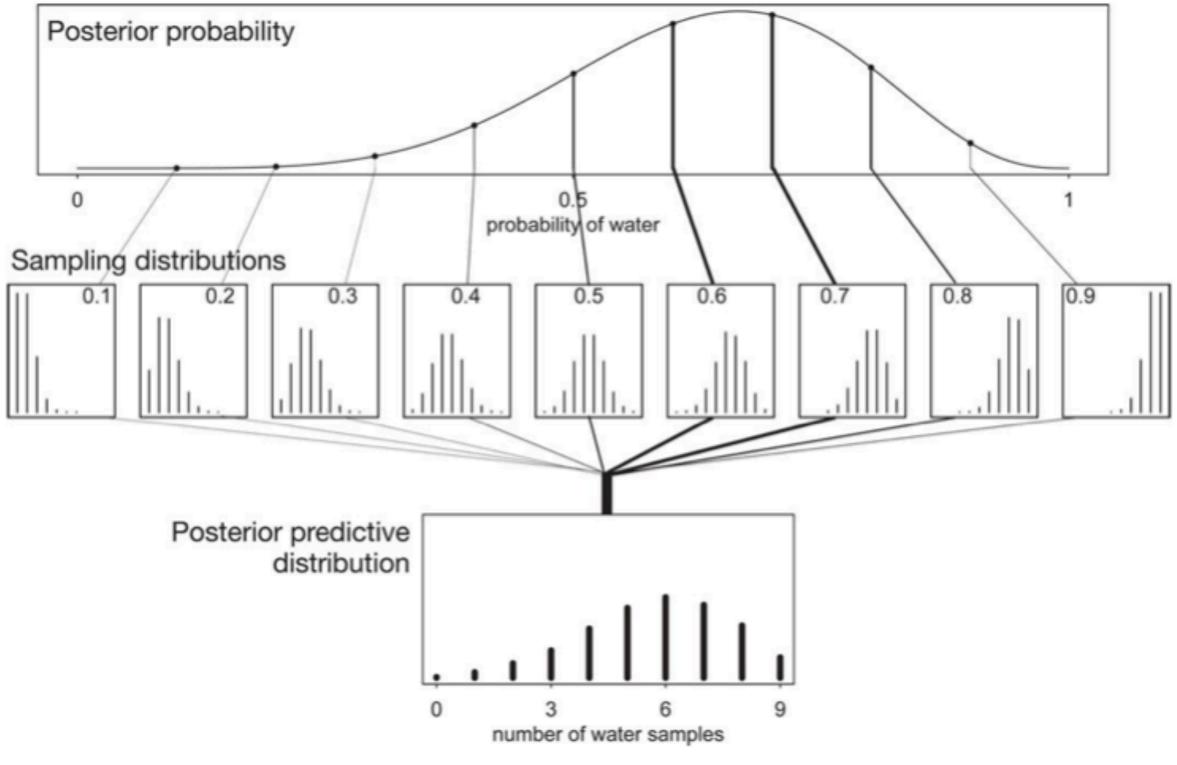
Its a Beta-Binomial distribution.

Can use $p(y^*|D) = p(y^*|\theta_{MAP})$ a sampling distribution.

Underestimates spread.

Sample instead.



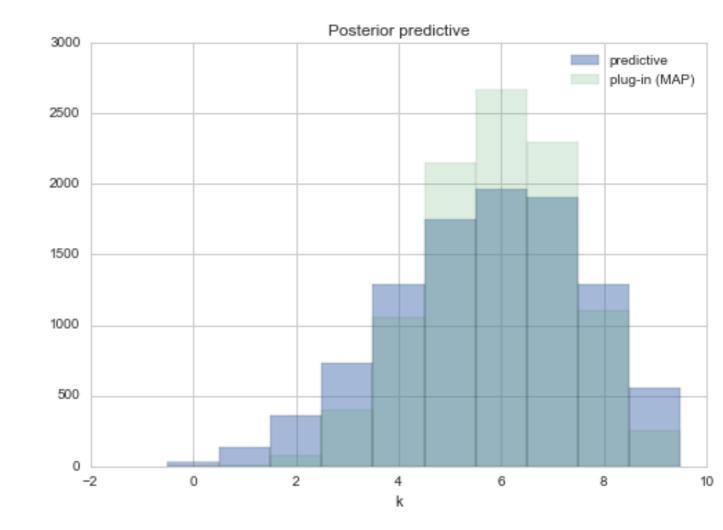




Posterior predictive from sampling

- draw the thetas from posterior
- then draw y's from the sampling distribution
- and histogram it
- these are draws from joint y, θ

postpred = np.random.binomial(n,samples)





Replicative Posterior Predictive

$$p(\{y^*\}) = \int p(\{y^*\}| heta) p(heta|\mathcal{D}) d heta$$
, observed data: $\mathcal{D} = \{y\}$

Replicated Data: $\{y_r\}$: data seen tomorrow if experiment replicated with same model and value of θ producing todays data $\{y\}$.

 $\{y_r\}$ comes from posterior predictive. The idea is to make as many replications as the size of your dataset.



Another way to sample

```
ppc_rep=np.empty((dataset_size, num_samples))
for i in range(dataset_size):
    ppc_rep[i,:] = distrib.rvs(param=posterior_samples)
```

For each data point, sample using the likelihood(sampling distribution) from *S* samples of the posterior. Gives an *S* sized posterior predictive at each "data point".

You can then slice the other way to get a dataset sized posterior-predictive



(sampling-distrib) np y13 912 Yind 911 02 y22 421 J32 Y31 741 451 PS-1 ys1 y 52 453 YSOD JS11 M207mple-ppc

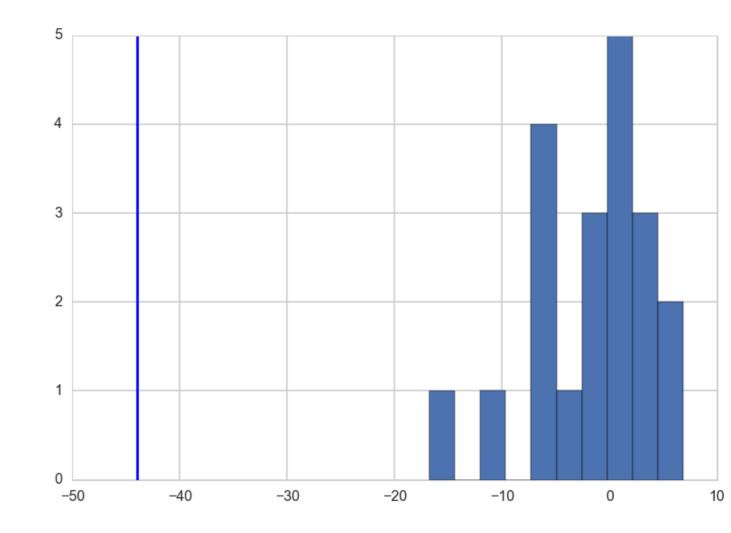
Departure from usual predictive sampling

Sample an entire $\{y_r\}$ at each θ from trace.

This allows to compute distributions from the posterior predictive replications for informal test statistics.

These processes are called **Posterior Predictive Checks**.

Replicative prior predictives are also useful for callibration.





Normal-Normal Model

$$p(\mu,\sigma^2)=p(\mu|\sigma^2)p(\sigma^2)$$

- fixed σ prior: $p(\sigma^2) = \delta(\sigma^2 \sigma_0^2)$
- non-fixed σ prior: Choose a functional form that is mildly informative, e.g., normal, half cauchy, half normal. But NOT CONJUGATE. See Murphy
- μ **prior**: Mildly informative normal with prior mean and wide standard deviation



Marginalization

Marginal posterior:

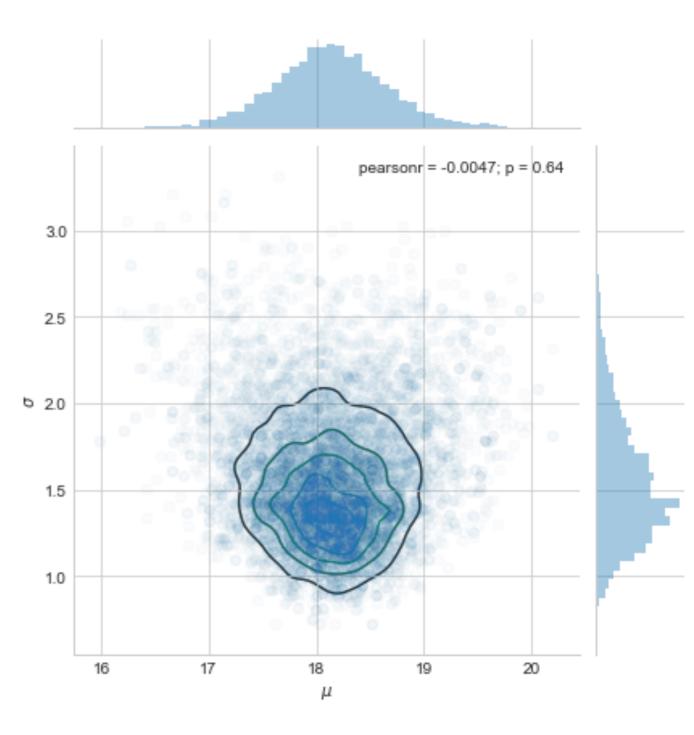
$$p(heta_1|D) = \int d heta_{-1} p(heta|D).$$

samps[20000::,:].shape #(10001, 2)

```
sns.jointplot(
   pd.Series(samps[20000::,0], name="$\mu$"),
   pd.Series(samps[20000::,1], name="$\sigma$"),
    alpha=0.02)
   .plot_joint(
      sns.kdeplot,
   zorder=0, n_levels=6, alpha=1)
```

Marginals are just 1D histograms

plt.hist(samps[20000::,0])





Normal-Normal Model

Posterior for a gaussian likelihood:

$$p(\mu,\sigma^2|y_1,\ldots,y_n,\sigma^2) \propto rac{1}{\sqrt{2\pi\sigma^2}} e^{-rac{1}{2\sigma^2}\sum (y_i-\mu)^2} \, p(\mu,\sigma^2)$$

What is the posterior of μ assuming we know σ^2 ?

Prior for
$$\sigma^2$$
 is $p(\sigma^2) = \delta(\sigma^2 - \sigma_0^2)$



$$p(\mu|y_1,\ldots,y_n,\sigma^2=\sigma_0^2) \propto p(\mu|\sigma^2=\sigma_0^2) \, e^{-rac{1}{2\sigma_0^2}\sum(y_i-\mu)^2}$$

The conjugate of the normal is the normal itself.

Say we have the prior

$$p(\mu|\sigma^2)=\expigg\{-rac{1}{2 au^2}(\hat{\mu}-\mu)^2igg\}$$

posterior: $p(\mu|y_1, \ldots, y_n, \sigma^2) \propto \exp\left\{-\frac{a}{2}(\mu - b/a)^2\right\}$



Here $a = rac{1}{ au^2} + rac{n}{\sigma_0^2}, \quad b = rac{\hat{\mu}}{ au^2} + rac{\sum y_i}{\sigma_0^2}$

Define
$$\kappa = \sigma^2/ au^2$$

$$\mu_p = rac{b}{a} = rac{\kappa}{\kappa+n} \hat{\mu} + rac{n}{\kappa+n} ar{y}$$

which is a weighted average of prior mean and sampling mean.



The variance is

$$au_p^2 = rac{1}{1/ au^2 + n/\sigma^2} \ ext{or better} \ rac{1}{ au_p^2} = rac{1}{ au^2} + rac{n}{ au^2}.$$

as *n* increases, the data dominates the prior and the posterior mean approaches the data mean, with the posterior distribution narrowing...



The variance is

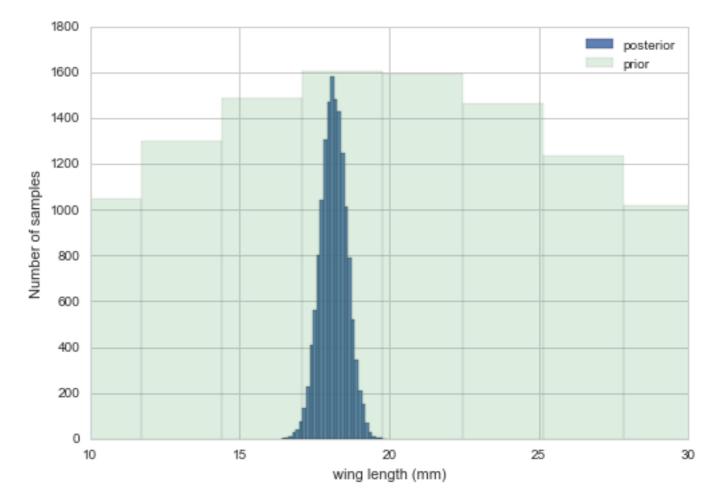
$$au_p^2 = rac{1}{1/ au^2 + n/\sigma^2} \ ext{or better} \ rac{1}{ au_p^2} = rac{1}{ au^2} + rac{n}{ au^2}.$$

as *n* increases, the data dominates the prior and the posterior mean approaches the data mean, with the posterior distribution narrowing...



Moth wing posterior

```
Y = [16.4, 17.0, 17.2, 17.4]
    18.2, 18.2, 18.2, 19.9, 20.8]
# data mean is 18.1
#Data Ouantities
sig = np.std(Y)
# assume that is the value of KNOWN sigma
# (in the likelihood)
mu_data = np.mean(Y)
n = len(Y)
# Prior mean is 19.5
mu_{prior} = 19.5
# prior std
tau = 10
# plug in formulas
kappa = siq^{**2} / tau^{**2}
sig_post =np.sqrt(1./( 1./tau**2 + n/sig**2));
# posterior mean
mu_post = kappa / (kappa + n) *mu_prior
    + n/(kappa+n)* mu_data
#samples
N = 15000
theta_prior = np.random.normal(loc=mu_prior,
    scale=tau, size=N);
theta_post = np.random.normal(loc=mu_post,
    scale=sig post, size=N);
```





Sufficient Statistics and the exponential family

$$p(y_i| heta) = f(y_i)g(heta)e^{\phi(heta)^T u(y_i)}.$$

Likelihood:

$$p(y| heta) = \left(\prod_{i=1}^n f(y_i)
ight)g(heta)^n \; \exp\!\left(\phi(heta)\sum_{i=1}^n u(y_i)
ight)$$

 $\sum_{i=1}^{n} u(y_i)$ is said to be a **sufficient statistic** for heta



Poisson Gamma Example

The data consists of 155 women who were 40 years old. We are interested in the birth rate of women with a college degree and women without. We are told that 111 women without college degrees have 217 children, while 44 women with college degrees have 66 children.

Let $Y_{1,1}, \ldots, Y_{n_1,1}$ children for the n_1 women without college degrees, and $Y_{1,2}, \ldots, Y_{n_2,2}$ for n_2 women with college degrees.



Exchangeability

Lets assume that the number of children of a women in any one of these classes can me modelled as coming from ONE birth rate.

The in-class likelihood for these women is invariant to a permutation of variables.

This is really a statement about what is IID and what is not.

It depends on how much knowledge you have...



Poisson likelihood

$$Y_{i,1} \sim Poisson(heta_1), Y_{i,2} \sim Poisson(heta_2)$$

$$p(Y_{1,1},\ldots,Y_{n_1,1}| heta_1) = \prod_{i=1}^{n_1} p(Y_{i,1}| heta_1) = \prod_{i=1}^{n_1} rac{1}{Y_{i,1}!} heta_1^{Y_{i,1}} e^{- heta_1}$$

$$= c(Y_{1,1}, \dots, Y_{n_1,1}) \; (n_1 heta_1)^{\sum Y_{i,1}} e^{-n_1 heta_1} \sim Poisson(n_1 heta_1)$$

$$Y_{1,2},\ldots,Y_{n_1,2}| heta_2\sim Poisson(n_2 heta_2)$$



Posterior

$$egin{aligned} &c_1(n_1,y_1,\ldots,y_{n_1})\;(n_1 heta_1)^{\sum Y_{i,1}}e^{-n_1 heta_1}\;p(heta_1)\ & imes\; c_2(n_2,y_1,\ldots,y_{n_2})\;(n_2 heta_2)^{\sum Y_{i,2}}e^{-n_2 heta_2}\;p(heta_2) \end{aligned}$$

 $\sum Y_i$, total number of children in each class of mom, is **sufficient statistics**



Conjugate prior

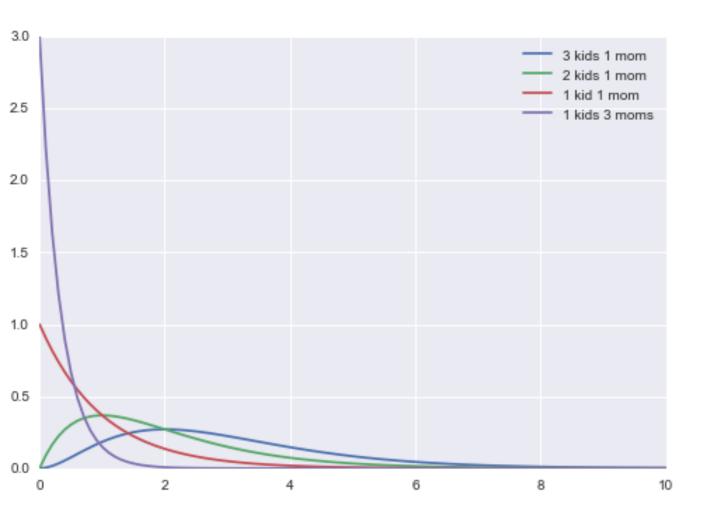
Sampling distribution for θ : $p(Y_1, \ldots, y_n | \theta) \sim \theta^{\sum Y_i} e^{-n\theta}$

Form is of *Gamma*. In shape-rate parametrization (wikipedia)

$$p(heta) = ext{Gamma}(heta, ext{a}, ext{b}) = rac{ ext{b}^{ ext{a}}}{\Gamma(ext{a})} heta^{ ext{a}-1} ext{e}^{- ext{b} heta}$$

Posterior: $p(\theta|Y_1, \dots, Y_n) \propto p(Y_1, \dots, y_n|\theta)p(\theta) \sim \text{Gamma}(\theta, a + \sum Y_i, b + n)$





Priors and Posteriors

We choose 2,1 as our prior.

$$p(heta_1|n_1,\sum_i^{n_1}Y_{i,1})\sim ext{Gamma}(heta_1,219,112)$$

$$p(heta_2|n_2,\sum_i^{n_2}Y_{i,2})\sim ext{Gamma}(heta_2,68,45)$$

Prior mean, variance: $E[\theta] = a/b, var[\theta] = a/b^2.$

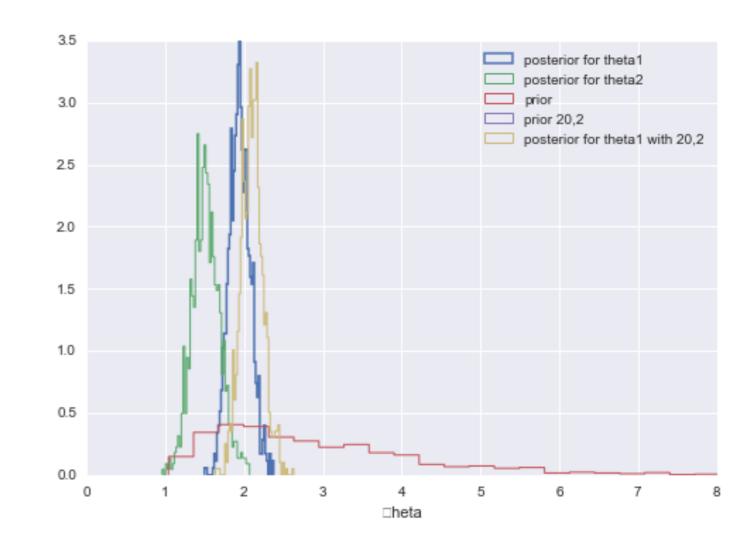


Posteriors

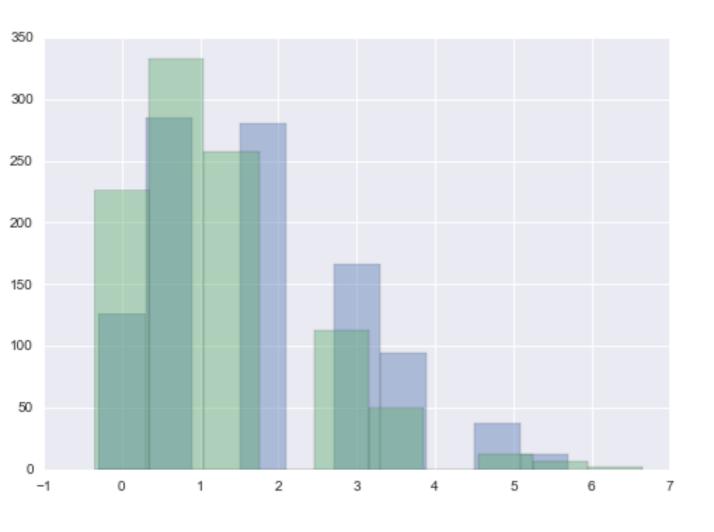
$$E[heta] = (a + \sum y_i)/(b+N)
onumber \ var[heta] = (a + \sum y_i)/(b+N)^2.$$

np.mean(theta1), np.var(theta1) = (1.9516881521791478, 0.018527204185785785)

np.mean(theta2),
np.var(theta2) =
(1.5037252100213609,
0.034220717257786061)







Posterior Predictives

$$p(y^*|D) = \int d heta p(y^*| heta) p(heta|D)$$

Sampling makes it easy:

postpred1 = poisson.rvs(theta1)
postpred2 = poisson.rvs(theta2)

Negative Binomial:

$$E[y^*] = rac{(a+\sum y_i)}{(b+N)}
onumber \ var[y^*] = rac{(a+\sum y_i)}{(b+N)^2} (N+b+1).$$



But see width:

```
np.mean(postpred1),
np.var(postpred1)=(1.976,
1.8554239999999997)
```

Posterior predictive smears out posterior error with sampling distribution

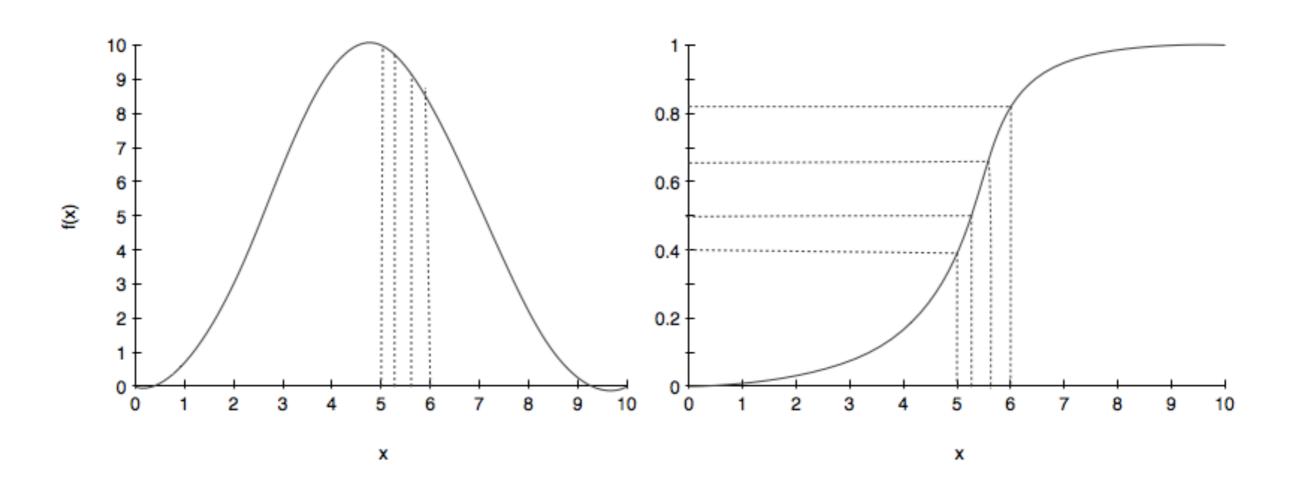


Ok. We need Samples

- to compute expectations, integrals and do statistics, we need samples
- we start that journey today
- inverse transform
- rejection sampling
- importance sampling: a direct, low-variance way to do integrals and expectations



Inverse transform





algorithm

The CDF *F* must be invertible!

- 1. get a uniform sample u from Unif(0, 1)
- 2. solve for x yielding a new equation $x = F^{-1}(u)$ where F is the CDF of the distribution we desire.
- 3. repeat.



Why does it work?

 $F^{-1}(u) =$ smallest x such that F(x) >= u

What distribution does random variable $y = F^{-1}(u)$ follow?

The CDF of y is $p(y \le x)$. Since F is monotonic:

p(y <= x) = p(F(y) <= F(x)) = p(u <= F(x)) = F(x)

F is the CDF of y, thus f is the pdf.



Example: exponential

pdf:
$$f(x) = rac{1}{\lambda} e^{-x/\lambda}$$
 for $x \ge 0$ and $f(x) = 0$ otherwise.

$$u=\int_{0}^{x}rac{1}{\lambda}e^{-x'/\lambda}dx'=1-e^{-x/\lambda}$$

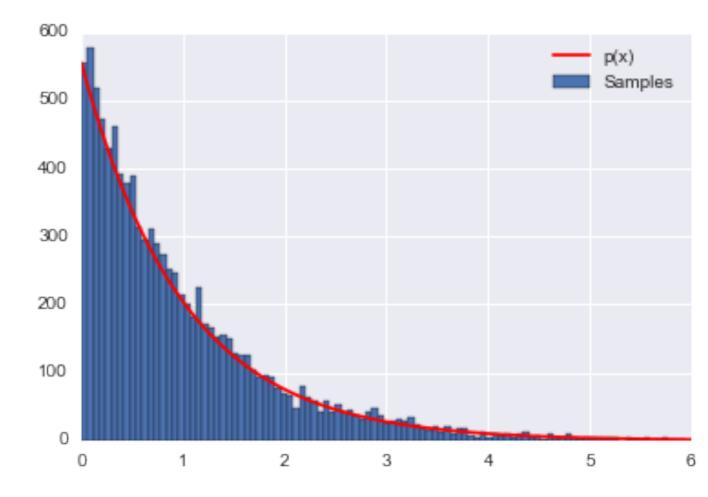
Solving for x

$$x = -\lambda \ln(1-u)$$



code

p = lambda x: np.exp(-x)CDF = lambda x: 1-np.exp(-x)invCDF = lambda r: -np.log(1-r) # invert the CDF xmin = 0 # the lower limit of our domain xmax = 6 # the upper limit of our domain rmin = CDF(xmin) rmax = CDF(xmax)N = 10000# generate uniform samples in our range then invert the CDF # to get samples of our target distribution R = np.random.uniform(rmin, rmax, N) X = invCDF(R)hinfo = np.histogram(X, 100)plt.hist(X,bins=100, label=u'Samples'); # plot our (normalized) function xvals=np.linspace(xmin, xmax, 1000) plt.plot(xvals, hinfo[0][0]*p(xvals), 'r', label=u'p(x)') plt.legend()







Rejection Sampling

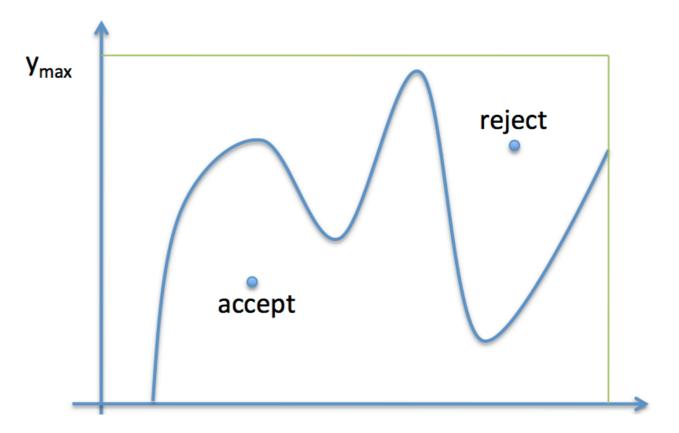
- Generate samples from a uniform distribution with support on the rectangle
- See how many fall below y(x) at a specific x.



h

Algorithm

- 1. Draw x uniformly from $[x_{min}, x_{max}]$
- 2. Draw y uniformly from $[0, y_{max}]$
- 3. if y < f(x), accept the sample
- 4. otherwise reject it
- 5. repeat

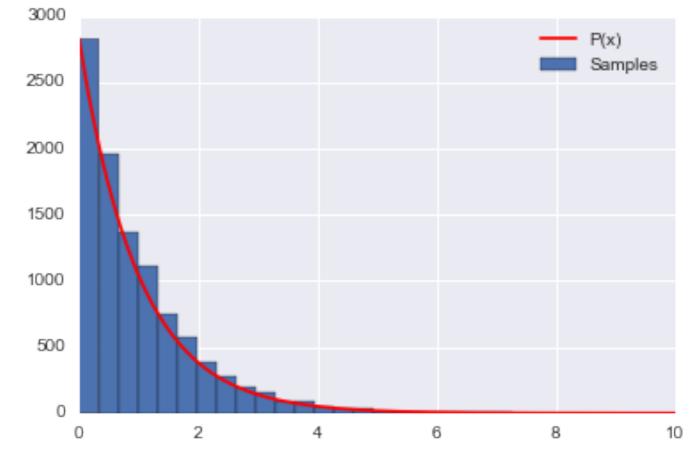




example

P = lambda x: np.exp(-x)xmin = 0 # the lower limit of our domain xmax = 10 # the upper limit of our domain vmax = 1#you might have to do an optimization to find this. N = 10000 # the total of samples we wish to generate accepted = 0 # the number of accepted samples samples = np.zeros(N)count = 0 # the total count of proposals while (accepted < N): # pick a uniform number on [xmin, xmax) (e.g. 0...10) x = np.random.uniform(xmin, xmax) # pick a uniform number on [0, ymax]y = np.random.uniform(0, ymax) # Do the accept/reject comparison if y < P(x): samples[accepted] = xaccepted += 1count +=1 print("Count", count, "Accepted", accepted) hinfo = np.histogram(samples, 30) plt.hist(samples,bins=30, label=u'Samples'); xvals=np.linspace(xmin, xmax, 1000) plt.plot(xvals, hinfo[0][0]*P(xvals), 'r', label=u'P(x)')

Count 100294 Accepted 10000





plt.legend()

problems

- determining the supremum may be costly
- the functional form may be complex for comparison
- even if you find a tight bound for the supremum, basic rejection sampling is very inefficient: low acceptance probability
- infinite support



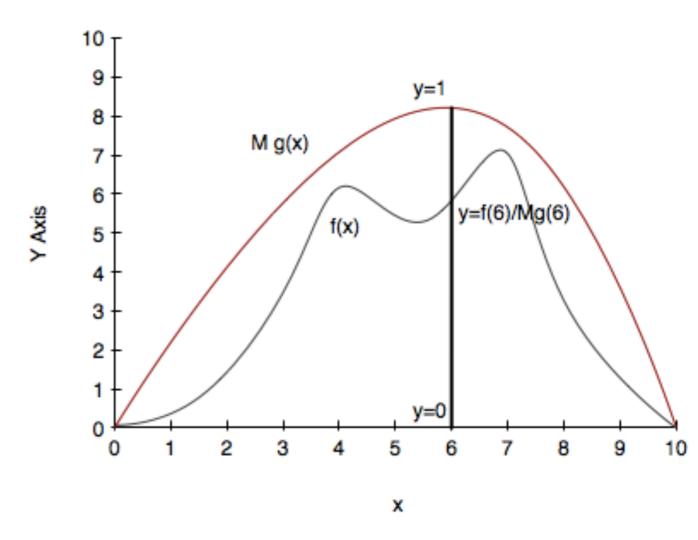
Variance Reduction



Rejection on steroids

Introduce a **proposal density** g(x).

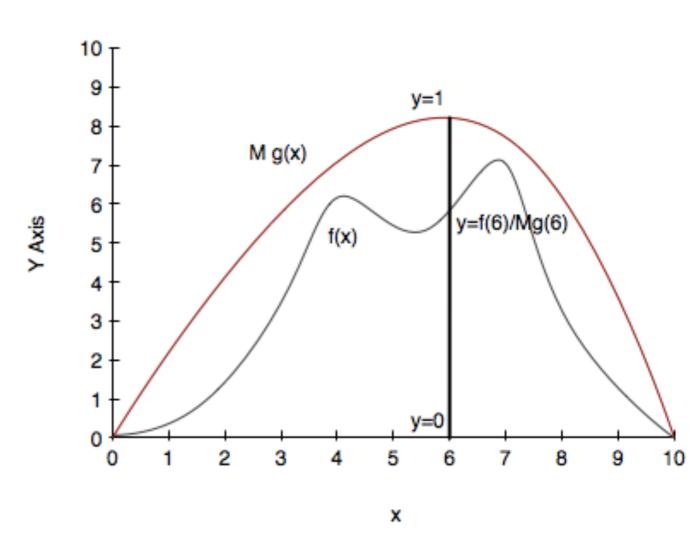
- g(x) is easy to sample from and (calculate the pdf)
- Some M exists so that M g(x) > f(x) in your entire domain of interest
- ideally g(x) will be somewhat close to f
- optimal value for M is the supremum over your domain





Algorithm

- 1. Draw x from your proposal distribution g(x)
- 2. Draw *y* uniformly from [0,1]
- 3. if y < f(x)/M g(x), accept the sample
- 4. otherwise reject it
- 5. repeat



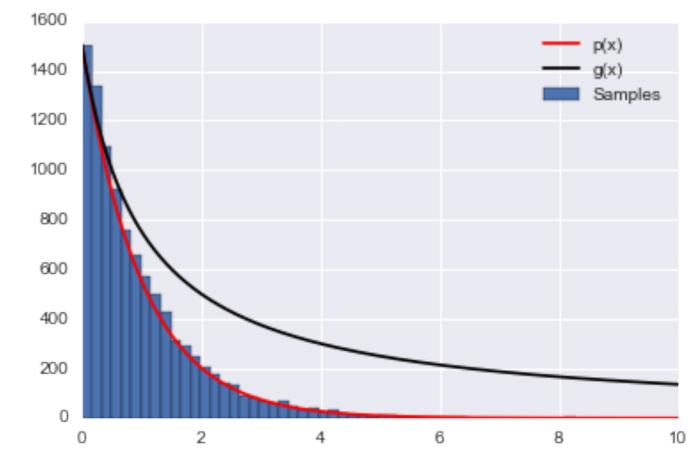


Example

<pre>p = lambda x: np.exp(-x) # our distribution g = lambda x: 1/(x+1) # our proposal pdf (we're thus choosing M to be 1) invCDFg = lambda x: np.log(x +1) # generates our proposal using inverse sampling xmin = 0 # the lower limit of our domain xmax = 10 # the upper limit of our domain # range limits for inverse sampling umin = invCDFg(xmin) umax = invCDFg(xmax) N = 10000 # the total of samples we wish to generate accepted = 0 # the number of accepted samples complete = nm memory (N)</pre>
<pre>samples = np.zeros(N) count = 0 # the total count of proposals</pre>
count - 0 # the total count of proposats
while (accepted < N):
<pre># Sample from g using inverse sampling u = np.random.uniform(umin, umax) xproposal = np.exp(u) - 1</pre>
<pre># pick a uniform number on [0, 1) y = np.random.uniform(0,1)</pre>
<pre># Do the accept/reject comparison if y < p(xproposal)/g(xproposal): samples[accepted] = xproposal accepted += 1</pre>
count +=1

```
print("Count", count, "Accepted", accepted)
# get the histogram info
hinfo = np.histogram(samples,50)
plt.hist(samples,bins=50, label=u'Samples');
xvals=np.linspace(xmin, xmax, 1000)
plt.plot(xvals, hinfo[0][0]*p(xvals), 'r', label=u'p(x)')
plt.plot(xvals, hinfo[0][0]*g(xvals), 'k', label=u'g(x)')
plt.legend()
```

Count 23809 Accepted 10000





Importance sampling

The basic idea behind importance sampling is that we want to draw more samples where h(x), a function whose integral or expectation we desire, is large. In the case we are doing an expectation, it would indeed be even better to draw more samples where h(x)f(x) is large, where f(x) is the pdf we are calculating the integral with respect to.

Unlike rejection sampling we use all samples!!



$$E_f[h] = \int_V f(x)h(x)dx.$$

Choosing a proposal distribution g(x):

$$E_f[h] = \int h(x) g(x) rac{f(x)}{g(x)} dV$$

$$E_f[h] = \lim_{N o \infty} rac{1}{N} \sum_{x_i \sim g(.)} h(x_i) rac{f(x_i)}{g(x_i)}$$

If
$$w(x_i) = f(x_i)/g(x_i)$$
:

$$E_f[h] = \lim_{N o \infty} rac{1}{N} \sum_{x_i \sim g(.)} w(x_i) h(x_i)$$

