Lecture 9

Bayesian Stats and Sampling



Last Time

- Bayesian Stats in detail
- Posterior, Posterior predictive
- Bayesian Stats



Today:

- Exchangeability and the exponential model
- Prior predictive
- Bayesian Regression
- Logistic Regression
- Inverse Transform Sampling
- Rejection Sampling



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

$$p(heta|D=\{x,y\})=rac{p(\{y\}| heta,\{x\})\,p(heta)}{p(\{y\}\mid\{x\})}$$

Posterior: $p(\theta|D) \propto p(\{y\}|\theta, \{x\}) p(\theta)$

Evidence:

$$p(\{y\} \mid \{x\}) = \int d heta \, p(heta, D) = \int d heta \, p(\{y\} ert heta, \{x\}) p(heta).$$



Marginalization

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

Posterior Predictive:

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





Replicative Posterior Predictive

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

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 y12 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.





Sufficient Statistics and the exponential family

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

Likelihood:

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

 $\sum_{i=1}^{n} u(y_i)$ 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: $p(\theta|Y_1, \dots, Y_n) \propto p(Y_1, \dots, y_n|\theta)p(\theta) \sim \text{Gamma}(\theta, a + \sum Y_i, b + n)$



Complete Posterior

Multiplies the 2 posteriors





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



Box's loop



REVISE MODEL



(from @ericnovik) Bayesian Workflow







Howell's data

- These are census data for the Dobe area !Kung San people
- Nancy Howell conducted detailed quantitative studies of this Kalahari foraging population in the 1960s.

| | height | weight | age | male |
|---|---------|-----------|------|------|
| 0 | 151.765 | 47.825606 | 63.0 | 1 |
| 1 | 139.700 | 36.485807 | 63.0 | 0 |
| 2 | 136.525 | 31.864838 | 65.0 | 0 |
| 3 | 156.845 | 53.041915 | 41.0 | 1 |
| 4 | 145.415 | 41.276872 | 51.0 | 0 |



Model

$$h \sim N(\mu, \sigma) \ \mu \sim Normal(148, 20) \ \sigma = samplestd$$



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...



Normal-Normal Posterior Predictive

So the posterior is

$$p(\mu \mid \{y\}, \sigma^2) = N(\mu_p, au_p^2)$$

The corresponding posterior predictive is:

$$p(y^* \mid \{y\}) = N(\mu_p, au_p^2 + \sigma^2)$$

Predictive variance is uncertainty due to the obsv. noise plus uncertainty due to the parameters.







Bayesian Formulation of Regression

Data $D = \{(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), \dots, (\mathbf{x}_n, y_n)\}$

All data points are combined into a $D \times n$ matrix X.

Model:

$$egin{aligned} y &= \mathbf{x^T}\mathbf{w} + \epsilon \ \epsilon &\sim N(0, \sigma_n^2) \end{aligned}$$





Likelihood

The likelihood is, because we assume independency, the product

$$\begin{aligned} \mathcal{L} &= p(\mathbf{y} | \mathbf{X}, \mathbf{w}) = \prod_{i=1}^{n} p(\mathbf{y}_{i} | \mathbf{X}_{i}, \mathbf{w}) = \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi}\sigma_{n}} \exp\left(-\frac{(\mathbf{y}_{i} - \mathbf{X}_{i}^{\mathrm{T}} \mathbf{w})^{2}}{2\sigma_{n}^{2}}\right) \\ &\propto \exp\left(-\frac{|\mathbf{y} - \mathbf{X}^{\mathrm{T}} \mathbf{w}|^{2}}{2\sigma_{n}^{2}}\right) \propto N(X^{T} \mathbf{w}, \sigma_{n}^{2} \mathbf{I}) \end{aligned}$$





Prior
$$\mathbf{w} \sim \mathbf{N}(\mathbf{w}_0, \boldsymbol{\Sigma})$$

 $\mathbf{w} \sim \mathbf{N}(\mathbf{w_0}, au^2 \mathbf{I})$





Posterior

$$p(\mathbf{w}|\mathbf{y}, \mathbf{X}) \propto p(\mathbf{y}|\mathbf{X}, \mathbf{w}) \mathbf{p}(\mathbf{w})$$

 $\propto \exp\left(-\frac{1}{2\sigma_n^2}(\mathbf{y} - \mathbf{X}^T \mathbf{w})^T(\mathbf{y} - \mathbf{X}^T \mathbf{w})\right) \exp\left(-\frac{1}{2}\mathbf{w}^T \mathbf{\Sigma}^{-1} \mathbf{w}\right)$

$$p(\mathbf{w}|\mathbf{y}, \mathbf{X}) \propto \exp\left(-rac{1}{2}(\mathbf{w}-ar{\mathbf{w}})^{\mathrm{T}}(rac{1}{\sigma_{\mathrm{n}}^{2}}\mathbf{X}\mathbf{X}^{\mathrm{T}}+\mathbf{\Sigma}^{-1})(\mathbf{w}-ar{\mathbf{w}})
ight)$$

Inverse covariance $A = \sigma_n^{-2} X X^T + \Sigma^{-1}$

where the new mean is $\bar{\mathbf{w}} = A^{-1} \Sigma^{-1} \mathbf{w_0} + \sigma_n^{-2} (A^{-1} X^T \mathbf{y})$





Bayesian updating

def update(x,y,likelihoodPrecision,priorMu,priorCovariance):
 postCovInv = np.linalg.inv(priorCovariance) +
 likelihoodPrecision*np.outer(x.T,x)
 postCovariance = np.linalg.inv(postCovInv)
 postMu =
 np.dot(
 np.dot(postCovariance,
 np.linalg.inv(priorCovariance)
),
 priorMu)
 +likelihoodPrecision*
 np.dot(postCovariance,np.outer(x.T,y)).flatten()
 postW = lambda w: multivariate_normal.pdf(
 w, postMu, postCovariance)
 return postW, postMu, postCovariance

Posterior Predictive

$$p(y^*|x^*,\mathbf{x},\mathbf{y}) =$$

$$\int p(\mathbf{y}^*|\mathbf{x}^*,\mathbf{w})p(\mathbf{w}|\mathbf{X},\mathbf{y})\mathbf{dw}$$

$$= \mathcal{N}\left(y|ar{\mathbf{w}}^Tx^*, \sigma_n^2 + x^{*^T}A^{-1}x^*
ight)$$





priorPrecision/likelihoodPrecision

4.0

This ratio is the ridge α .

M 207

Regression, adding a predictor, weight

$$egin{aligned} &h\sim N(\mu,\sigma)\ &\mu=intercept+slope imes weight\ intercept\sim N(150,100)\ &slope\sim N(0,10)\ &\sigma=std.\,dev \end{aligned}$$

Priors

Posteriors

Posterior at weight 55

DO INTERCEPT SLOPE, AND WEIGHT 55

Posteriors on a grid

Why so tight?

Predictives on grid

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

M 207

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)')

plt.legend()

Count 100294 Accepted 10000

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 samples = np.zeros(N) count = 0 # the total count of proposals</pre> | | | |
|---|--|--|--|
| 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

MLE for Logistic Regression

- example of a Generalized Linear Model (GLM)
- "Squeeze" linear regression through a Sigmoid function
- this bounds the output to be a probability
- What is the sampling Distribution?

Sigmoid function

This function is plotted below:

h = lambda z: 1./(1+np.exp(-z))
zs=np.arange(-5,5,0.1)
plt.plot(zs, h(zs), alpha=0.5);

Identify: $z = \mathbf{w} \cdot \mathbf{x}$ and $h(\mathbf{w} \cdot \mathbf{x})$ with the probability that the sample is a '1' (y = 1).

Then, the conditional probabilities of y = 1 or y = 0 given a particular sample's features **x** are:

$$egin{aligned} P(y=1|\mathbf{x}) &= h(\mathbf{w}\cdot\mathbf{x}) \ P(y=0|\mathbf{x}) &= 1-h(\mathbf{w}\cdot\mathbf{x}). \end{aligned}$$

These two can be written together as

$$P(y|\mathbf{x},\mathbf{w}) = h(\mathbf{w}\cdot\mathbf{x})^y(1-h(\mathbf{w}\cdot\mathbf{x}))^{(1-y)}$$

BERNOULLI!!

Multiplying over the samples we get:

$$P(y|\mathbf{x},\mathbf{w}) = P(\{y_i\}|\{\mathbf{x}_i\},\mathbf{w}) = \prod_{y_i\in\mathcal{D}} P(y_i|\mathbf{x}_i,\mathbf{w}) = \prod_{y_i\in\mathcal{D}} h(\mathbf{w}\cdot\mathbf{x}_i)^{y_i}(1-h(\mathbf{w}\cdot\mathbf{x}_i))^{(1-y_i)}$$

A noisy y is to imagine that our data \mathcal{D} was generated from a joint probability distribution P(x, y). Thus we need to model y at a given x, written as $P(y \mid x)$, and since P(x) is also a probability distribution, we have:

$$P(x,y) = P(y \mid x)P(x),$$

Indeed its important to realize that a particular sample can be thought of as a draw from some "true" probability distribution.

maximum likelihood estimation maximises the likelihood of the sample y,

$$\mathcal{L} = P(y \mid \mathbf{x}, \mathbf{w}).$$

Again, we can equivalently maximize

$$\ell = log(P(y \mid \mathbf{x}, \mathbf{w}))$$

Thus

$$egin{aligned} \ell &= log \left(\prod_{y_i \in \mathcal{D}} h(\mathbf{w} \cdot \mathbf{x}_i)^{y_i} (1 - h(\mathbf{w} \cdot \mathbf{x}_i))^{(1-y_i)}
ight) \ &= \sum_{y_i \in \mathcal{D}} log \left(h(\mathbf{w} \cdot \mathbf{x}_i)^{y_i} (1 - h(\mathbf{w} \cdot \mathbf{x}_i))^{(1-y_i)}
ight) \ &= \sum_{y_i \in \mathcal{D}} log h(\mathbf{w} \cdot \mathbf{x}_i)^{y_i} + log (1 - h(\mathbf{w} \cdot \mathbf{x}_i))^{(1-y_i)} \ &= \sum_{y_i \in \mathcal{D}} (y_i log(h(\mathbf{w} \cdot \mathbf{x})) + (1 - y_i) log(1 - h(\mathbf{w} \cdot \mathbf{x})))) \end{aligned}$$

