The Clever Machine

Topics in Computational Neuroscience & Machine Learning

MCMC: The Metropolis Sampler

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Posted by **dustinstansbury**

As discussed in an earlier post (https://theclevermachine.wordpress.com/2012/09/24/a-brief-introduction-to-markov-chains/), we can use a Markov chain to sample from some ***target probability distribution*** $p(x)$ from which drawing samples directly is difficult. To do so, it is necessary to design a transition operator for the Markov chain which makes the chain's stationary distribution match the target distribution. The Metropolis sampling algorithm (and the more general Metropolis-Hastings sampling algorithm) uses simple heuristics to implement such a transition operator.

Metropolis Sampling

Starting from some random initial state $x^{(0)} \sim \pi^{(0)}$, the algorithm first draws a possible sample x^* from a ***proposal distribution*** $q(x|x^{(t-1)})$. Much like a conventional transition operator for a Markov chain, the proposal distribution depends only on the previous state in the chain. However, the transition operator for the Metropolis algorithm has an additional step that assesses whether or not the target distribution has a sufficiently large density near the proposed state to warrant accepting the proposed state as a sample and setting it to the next state in the chain. If the density of $p(x)$ is low near the proposed state, then it is likely (but not guaranteed) that it will be rejected. The criterion for accepting or rejecting a proposed state are defined by the following heuristics:

1. If $p(x^*) \geq p(x^{(t-1)})$, the proposed state is kept x^* as a sample and is set as the next state in the chain (i.e. move the chain's state to a location where $p(x)$ has equal or greater density).
2. If $p(x^*) < p(x^{(t-1)})$–indicating that $p(x)$ has low density near x^*–then the proposed state may still be accepted, but only randomly, and with a probability $\frac{p(x^*)}{p(x^{(t-1)})}$

These heuristics can be instantiated by calculating the ***acceptance probability*** for the proposed state.

$$\alpha = \min\left(1, \frac{p(x^*)}{p(x^{(t-1)})}\right)$$

Having the acceptance probability in hand, the transition operator for the metropolis algorithm

works like this: if a random uniform number u is less than or equal to α, then the state x^* is accepted (as in (1) above), if not, it is rejected and another state is proposed (as in (2) above). In order to collect M samples using Metropolis sampling we run the following algorithm:

1. set t = 0
2. generate an initial state $x^{(0)}$ from a prior distribution $\pi^{(0)}$ over initial states
3. repeat until $t = M$

set $t = t + 1$

generate a proposal state x^* from $q(x|x^{(t-1)})$

calculate the acceptance probability $\alpha = \min\left(1, \frac{p(x^*)}{p(x^{(t-1)})}\right)$

draw a random number u from $\text{Unif}(0, 1)$

if $u \leq \alpha$, accept the proposal and set $x^{(t)} = x^*$

else set $x^{(t)} = x^{(t-1)}$

Example: Using the Metropolis algorithm to sample from an unknown distribution

Say that we have some mysterious function

$$p(x) = (1 + x^2)^{-1}$$

from which we would like to draw samples. To do so using Metropolis sampling we need to define two things: (1) the prior distribution $\pi^{(0)}$ over the initial state of the Markov chain, and (2) the proposal distribution $q(x|x^{(t-1)})$. For this example we define:

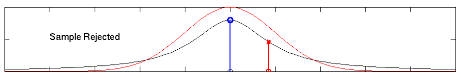
$$\pi^{(0)} \sim \mathcal{N}(0, 1)$$

$$q(x|x^{(t-1)}) \sim \mathcal{N}(x^{(t-1)}, 1),$$

both of which are simply a Normal distribution, one centered at zero, the other centered at previous state of the chain. The following chunk of MATLAB code runs the Metropolis sampler with this proposal distribution and prior.

```
% METROPOLIS SAMPLING EXAMPLE
randn('seed',12345);

% DEFINE THE TARGET DISTRIBUTION
p = inline('(1 + x.^2).^-1','x')

% SOME CONSTANTS
nSamples = 5000;
burnIn = 500;
nDisplay = 30;
sigma = 1;
minn = -20; maxx = 20;
xx = 3*minn:.1:3*maxx;

target = p(xx);
pauseDur = .8;

% INITIALZE SAMPLER
x = zeros(1 ,nSamples);
x(1) = randn;
t = 1;

% RUN SAMPLER
while t < nSamples
    t = t+1;

    % SAMPLE FROM PROPOSAL
    xStar = normrnd(x(t-1) ,sigma);
    proposal = normpdf(xx,x(t-1),sigma);

    % CALCULATE THE ACCEPTANCE PROBABILITY
    alpha = min([1, p(xStar)/p(x(t-1))]);

    % ACCEPT OR REJECT?
    u = rand;
    if u < alpha
        x(t) = xStar;
        str = 'Accepted';
    else
        x(t) = x(t-1);
        str = 'Rejected';
    end

    % DISPLAY SAMPLING DYNAMICS
    if t < nDisplay + 1
        figure(1);
        subplot(211);
        cla
        plot(xx,target,'k');
        hold on;
        plot(xx,proposal,'r');
        line([x(t-1),x(t-1)],[0 p(x(t-1))],'color','b','linewidth',2)
        scatter(xStar,0,'ro','Linewidth',2)
        line([xStar,xStar],[0 p(xStar)],'color','r','Linewidth',2)
        plot(x(1:t),zeros(1,t),'ko')
        legend({'Target','Proposal','p(x^{(t-1)})','x^*','p(x^*)','Kept Sa

        switch str
            case 'Rejected'
```

```
                scatter(xStar,p(xStar),'rx','Linewidth',3)
            case 'Accepted'
                scatter(xStar,p(xStar),'rs','Linewidth',3)
        end
            scatter(x(t-1),p(x(t-1)),'bo','Linewidth',3)
        title(sprintf('Sample % d %s',t,str))
        xlim([minn,maxx])
        subplot(212);
        hist(x(1:t),50); colormap hot;
        xlim([minn,maxx])
        title(['Sample ',str]);
        drawnow
        pause(pauseDur);
    end
end

% DISPLAY MARKOV CHAIN
figure(1); clf
subplot(211);
stairs(x(1:t),1:t, 'k');
hold on;
hb = plot([-10 10],[burnIn burnIn],'b--')
ylabel('t'); xlabel('samples, x');
set(gca , 'YDir', 'reverse');
ylim([0 t])
axis tight;
xlim([-10 10]);
title('Markov Chain Path');
legend(hb,'Burnin');

% DISPLAY SAMPLES
subplot(212);
nBins = 200;
sampleBins = linspace(minn,maxx,nBins);
counts = hist(x(burnIn:end), sampleBins);
bar(sampleBins, counts/sum(counts), 'k');
xlabel('samples, x' ); ylabel( 'p(x)' );
title('Samples');

% OVERLAY ANALYTIC DENSITY OF STUDENT T
nu = 1;
y = tpdf(sampleBins,nu)
hold on;
plot(sampleBins, y/sum(y) , 'r-', 'LineWidth', 2);
legend('Samples',sprintf('Theoretic\nStudent''s t'))
axis tight
xlim([-10 10]);
```



(https://theclevermachine.files.wordpress.com/2012/10/metropolis2.gif)
Using the Metropolis algorithm to sample from a continuous distribution (black)

In the figure above, we visualize the first 50 iterations of the Metropolis sampler.The black curve represents the target distribution $p(x)$. The red curve that is bouncing about the x-axis is the proposal distribution $q(x|x^{(t-1)})$ (if the figure is not animated, just click on it). The vertical blue line (about which the bouncing proposal distribution is centered) represents the quantity $p(x^{(t-1)})$, and the vertical red line represents the quantity $p(x^*)$, for a proposal state x^* sampled according to the red curve. At every iteration, if the vertical red line is longer than the blue line, then the sample x^* is accepted, and the proposal distribution becomes centered about the newly accepted sample. If the blue line is longer, the sample is randomly rejected or accepted.

But why randomly keep "bad" proposal samples? It turns out that doing this allows the Markov chain to every-so-often visit states of low probability under the target distribution. This is a desirable property if we want the chain to adequately sample the entire target distribution, including any tails.

An attractive property of the Metropolis algorithm is that the target distribution $p(x)$ does not have to be a properly normalized probability distribution. This is due to the fact that the acceptance probability is based on the ratio of two values of the target distribution. I'll show you what I mean. If $p(x)$ is an unnormalized distribution and

$$p^*(x) = \frac{p(x)}{Z}$$

is a properly normalized probability distribution with normalizing constant Z, then

$$p(x) = Zp^*(x)$$

and a ratio like that used in calculating the acceptance probability α is

$$\frac{p(a)}{p(b)} = \frac{Zp^*(a)}{Zp^*(b)} = \frac{p^*(a)}{p^*(b)}$$

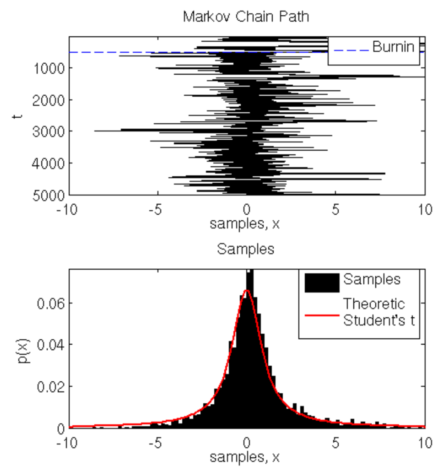
The normalizing constants Z cancel! This attractive property is quite useful in the context of Bayesian methods, where determining the normalizing constant for a distribution may be impractical to calculate directly. This property is demonstrated in current example. It turns out that the "mystery" distribution that we sampled from using the Metropolis algorithm is an unnormalized form of the Student's-t distribution with one degree of freedom. Comparing $p(x)$ to the definition of the definition Student's-t

$$Student(x,\nu) = \frac{\Gamma\left(\frac{\nu+1}{2}\right)}{\sqrt{\nu\pi}\Gamma\left(\frac{\nu}{2}\right)}\left(1+\frac{x^2}{\nu}\right)^{-\frac{\nu+1}{2}} = \frac{(1+x^2)^{-1}}{Z} = \frac{p(x)}{Z}$$

we see that $p(x)$ is a Student's-t distribution with degrees of freedom $\nu = 1$, but missing the normalizing constant

$$Z = \left(\frac{\Gamma\left(\frac{\nu+1}{2}\right)}{\sqrt{\nu\pi}\Gamma\left(\frac{\nu}{2}\right)}\right)^{-1}$$

Below is additional output from the code above showing that the samples from Metropolis sampler draws samples that follow a *normalized* Student's-t distribution, even though $p(x)$ is not normalized.



(https://theclevermachine.files.wordpress.com/2012/10/metropolisstudentst2.png)
Metropolis samples from an unnormalized t-distribution follow the normalized distribution

The upper plot shows the progression of the Markov chain's progression from state $x^{(0)}$ (top) to state $x^{(5000)}$ (bottom). The burn in period for this chain was chosen to be 500 transitions, and is indicated by the dashed blue line (for more on burnin see this previous post (https://theclevermachine.wordpress.com/2012/09/24/a-brief-introduction-to-markov-chains/)).

The bottom plot shows samples from the Markov chain in black (with burn in samples removed). The theoretical curve for the Student's-t with one degree of freedom is overlayed in red. We see that the states kept by the Metropolis sampler transition operator sample from values that follow the Student's-t, even though the function $p(x)$ used in the transition operator was not a properly normalized probability distribution.

Reversibility of the transition operator

It turns out that there is a theoretical constraint on the Markov chain the transition operator in order for it settle into a stationary distribution (i.e. a target distribution we care about). The constraint states that the probability of the transition $x^{(t)} \to x^{(t+1)}$ must be equal to the probability of the reverse transition $x^{(t+1)} \to x^{(t)}$. This reversibility property is often referred to as ***detailed balance***. Using the Metropolis algorithm transition operator, reversibility is assured if the proposal distribution

$q(x|x^{(t-1)})$ is symmetric. Such symmetric proposal distributions are the Normal, Cauchy, Student's-t, and Uniform distributions.

However, using a symmetric proposal distribution may not be reasonable to adequately or efficiently sample all possible target distributions. For instance if a target distribution is bounded on the positive numbers $0 < x \leq \infty$, we would like to use a proposal distribution that has the same support, and will thus be assymetric. This is where the ***Metropolis-Hastings*** sampling algorithm comes in. We will discuss in a later post how the Metropolis-Hastings sampler uses a simple change to the calculation of the acceptance probability which allows us to use non-symmetric proposal distributions.

About dustinstansbury

I recently received my PhD from UC Berkeley where I studied computational neuroscience and machine learning.

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Posted on October 5, 2012, in Algorithms, Sampling Methods, Statistics and tagged Acceptance Probability, Detailed Balance, Markov Chain Monte Carlo, MCMC, Metropolis sampling, Metropolis-Hastings Sampling, Proposal Distribution, Reversibility, Target Distribution. Bookmark the permalink. 3 Comments.

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Aparna Sen | July 21, 2018 at 10:01 pm
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