Why M-H algorithm works. Basic "all-out-once" M-H: use détailed balance argument. Need: $T(n) \times (x, y) = T(y) \times (y, x)$ i.e., $\pi(x) = \pi(x,y) \times (x,y) = \pi(y) = \pi(y) = \pi(y,x) \times (y,x)$ If x=y, Atrivially satisfied. Assume w.l.o.g. that T(y) q(y,x) >T(x) q(x,y) then LHS of \mathfrak{G} is $\overline{T(n)} \ q(n,y) + \min \ \{1, \frac{\overline{T(y)} \ q(n,y)}{\overline{T(n)} \ q(n,y)} \}$ $=\pi(\pi)$ $q(\pi,y)$. 1 PHS of * is $T(y) q(y,x) \cdot \min \left\{1, \frac{T(y)}{T(y)} \frac{q(x,y)}{q(y,x)}\right\}$ = T(y)q(y,x). T(x)q(x,y) = RHS.

Hence détailed balance is satisfied.

Sufficient conditions for M. chain SLLN to hold:

(A) It g(x,y)=0 tx,y=1, M.C. is trivally invednible every set A can be reached in 1 step.

(B) If, P(TIX) g(n,y) = TI(y) g(y,x)) = 1 then M.C. has positive prob of staying at x. M.C. is strongly aperiodic. Why: $\alpha(x,y) = 1$ where $\alpha(x,y)$

Hene, positive probability of staying et x.

(c) Destacted balance is satisfied w.r.t. To.

satisfied, M.C. is Hamic eyodic ω / II D, B, O Tt. Thm. 1 (SLLN) applies. 19.273 stationary distr. Robert & Casella

Why Variable-at-a-time M-H works

Consider transition kernel of M.C. to be the product of transition kernels for each block. For e.g. two blocks, $\chi = (\pi_1, \chi_2)$ Transition kernel of chain, $\chi = (\pi_1, \chi_2)$ $= \chi_1 = (\chi_1, \chi_2), (\chi_1, \chi_2), (\chi_1, \chi_2), (\chi_1, \chi_2)$ $= \chi_1 = (\chi_1, \chi_2), (\chi_1, \chi_2), (\chi_1, \chi_2), (\chi_1, \chi_2)$ update

Also: see this as composition of kernels, preserving stationarity

Hong Har works: Can show trans. Keened K has
It as its Actionery dostr. $\int \int \underbrace{K_{1/2}(x_1,y_1|x_1)}_{K_{1/2}(x_1,y_2|x_1)} \underbrace{K_{2/1}(x_2,y_2|y_1)}_{K(x_1,y_2)} \underbrace{\pi(x_1,x_2)}_{\pi(x_1)} dx, dx_1$ = [[(* 27/2 / 91) [[] (x , 9, | x2) [[x | +2) dx] [(x) dx2 (: Kilz bos is frans kerned by w) = JK211 (x2194491) TI12 (4/1X2) tr/x1) dx2 Antoney distr. Tils = [Kill (x2, y2/y1) The (x2/y1) th, (y1) dx2 = Th.(yi) [Ky, (xz, yz/y,) Tz/, (xz/y) dxz = Th(y1) The (y2/y1) = TC(y)So, $\int_{x \in X} K(x,y) \pi(x) dx = \pi(y)$ of Tis stationary distr. of K. Can similarly show such a result for VMH W/ an arbitrary # of blocks > 2.

Elegant proof regulars Mark-at-atime Met-Hashigs is generally

Note: M. S. Ferom Mark-at-atime not reverible . However, can easily make it reverible by randomizing order of update of the blocker, or ung palindrome updater K12,3 K2/1,3 K3/1,2 K2/1,3 K7/2,3

KA KA KA KA KA KA

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Rev. 12x Pel for many Newhol results (north New monerer.)

Total variational distance between two distributions TI, and The is defined $\|T_{i}-T_{i}\|_{Tr} = \sup_{A \in \mathcal{B}(\mathcal{H})} |T_{i}(A)-T_{i}(A)|$ where $TT_{r}(A) = \int_{A}^{A} TT_{r}(x) dx$ when TT_{r}, TT_{r} are densities $TT_{r}(A) = \int_{A}^{A} TT_{r}(x) dx$ Thm 2: If {Xn} is a Harris egodic M.C. in/
stationary distr. To and nestep transition kernel k"(y|x) $\lim_{x\to 2} \|P_n(x,\cdot) - \pi(\cdot)\| = 0$ where $P^n(x, A) = \int_A k^n(y|x) dy$ i.e, P"(x,A)= P(Xim GA) Xi=x)

Implication: regardless et stanting value, Harris-ergodic M.C. w/ stationary distr. It will produce values that look like draws from Tt, after the M.C. has been running for a long time.

in total-vouisitional distance: Kates of conveyence

 $\|P^n(x,\cdot)-\pi(\cdot)\|_{L^p}\leq M(x)\frac{t^n}{20}$ and M(x) is extended red-value ometric ergodicity: above holds $y|t\in I$, M(x) is extended red-value inform ergodicity: above holds $y|t\in I$ and $M(x)\in M^{\frac{1}{p}}<\infty$. Geometric ergodicity: above Uniform eyodicity: above

WITML

A rough guide to writing an MCMC algorithm

Here is a rough guide for constructing an MCMC algorithm. Each step describes some of the decisions that need to be made at each stage along with associated tradeoffs.

- 1. Derive $h(\Theta)$, the unnormalized joint distribution of interest, which is proportion to the target $\propto \pi(\Theta)$ where $\Theta = (\theta_1, \dots, \theta_p)$.
- 2. Identify blocks or components of Θ that would be relatively easy to simulate 'all-at-once'. This is a very difficult decision to make in general and will typically require some trial and error though, sometimes, the structure of the problem may suggest a blocking strategy. A basic principle to follow is to look for blocks that appear to be highly correlated, as updating these jointly in a sensible fashion will typically make the sampler more efficient. The tradeoff will often be as follows: updating large blocks of parameters will allow the sampler to move around the distribution more efficiently but designing good proposals for large blocks can be difficult and updating large blocks of parameters may be computationally more demanding (due to matrix operations that may be involved in the proposal and accept-reject steps of the algorithm.)
- 3. Derive full conditional distributions for each block based on the decision made in Step 2.
- 4. Identify any blocks with full conditionals that have a known form. Use Gibbs updates for these full conditionals. Please note, however, that this is only the first approach to take if the sampler works poorly, you may even decide to use a Metropolis-Hastings update instead of a Gibbs update.
- 5. Construct Metropolis-Hastings updates for the remaining blocks. There are a large number of possibilities when it comes to determining what M-H update to use. The first M-H update to try is a simple Metropolis update with a symmetric proposal. It may also be useful to try transformations. For example, if θ_i has positive support, try $\phi_k = \log(\theta_i)$ instead. ϕ_i 's full conditional distribution may be easier to deal with and it is easy to transform the sampled value back to θ_i .

- 6. Run the M-H algorithm for short trial runs, printing out lots of intermediate results:
 - (a) This can help you make sure there are no obvious errors with your algebra or your programming.
 - (b) You can see if you need to make changes to your algorithm. For example: If some of the parameters seem to be highly correlated, you may decide to sample them in a block. If Metropolis updates seem to result in highly autocorrelated samples, try changing the tuning parameters.
 - (c) Save the last draw of each of your trial runs and use it to start your next run. This is a great way to obtain reasonable starting values. Any value you would not mind having in your sample is a reasonable value to start the sampler at (Geyer 2000).
- 7. Once obvious problems have been fixed and you have fine tuned your algorithm, run the chain for as long as possible. If the Monte Carlo standard errors for the estimates of expectations of interest are acceptable, you can stop the chain. There are many estimates of Monte Carlo standard error. We recommend the consistent batch means estimate ((3)). Of course, be aware that this approach works well only when the sampler is working reasonably well. If the Markov chain sampler is poor (slow mixing) and unable to find multiple modes of a multimodal distribution, all methods for deciding when to stop the chain will be ineffective.
- 8. Report your final estimates, along with any estimates of error associated with them. It is useful to also indicate (for future reference) the length of the chain used and what algorithm you finally ended up using.

An important general computing principle is to always do calculations on the log scale as far as possible. For instance, for the Metropolis-Hastings accept-reject step, instead of simulating $U \sim \text{Unif}(0,1)$ and checking if

$$U < \frac{\pi(\theta_i^*|\Theta_{-i})q(\theta_i^*, \theta_i)}{\pi(\theta_i|\Theta_{-i})q(\theta_i, \theta_i^*)},$$

check whether:

$$\log(U) < \log(\pi(\theta_i^*|\Theta_{-i})) + \log(q(\theta_i^*, \theta_i)) - \log(\pi(\theta_i|\Theta_{-i})) - \log(q(\theta_i, \theta_i^*)).$$

Of course, this is the same principle that was applied to classical Monte Carlo approaches, leading to much more stable and accurate computations.

Burn-in, subsampling, and multiple chains

Burn-in: Since the Markov chain is typically not started with a value from the stationary distribution, the estimates based on the samples are biased. Unfortunately, there is no way to know how much bias is being removed (if any) by discarding some initial draws. The only thing we know for sure is that the variability of the estimate has been increased! For more on this, read the thoughtful (and entertaining) discussion on MCMC diagnostics by C.I. Gever (http://www.stat.umn_edu/achara.) (http://www.stat.umn.edu/~charlie/mcmc/diag.html). To quote Geyer (2000) "Any value you do not mind having in your sample is a reasonable starting value." A useful recommendation is to simply start the chain off at the last sample from the previous MCMC run. Since there is often a fair amount of tuning involved in developing an effective Metropolis-Hastings algorithm, these tuning runs can be helpful in providing the initial value for the final run of the sampler.

(hek

Gui 62: effect of Lins & n while effect of serious & In Subsampling: Many MCMC users are troubled by heavy autocorrelation in their samples, as they should be. One way to deal with this issue is to simply subsample the chain, i.e., pick off every kth sample. For k large enough, this would result in a much less autocorrelated sample. From basic Markov chain theory, the subsampled Markov chain inherits the important properties of the original Markov chain (crucially, it has the same stationary distribution.) If samples are easy to produce and expensive to process, subsampling can be a simple but useful approach. For example: If it takes very little time to generate samples from a 10,000 dimensional distribution, and the draws are heavily autocorrelated, it may be worth subsampling the chain just to reduce the burden on storage and processing the samples (computing estimates of different kinds based on the samples.) The flipside is that if it is expensive to generate samples, and the cost of processing them is not very high, subsampling is wasteful. Using fewer samples, even if the samples are fairly dependent, is usually going to result in greater variability (reduced accuracy) of the estimates — the Monte Carlo standard errors are going to

on X1, X2, ... for large b (we are ilour' to T). increase.

Multiple chains: Starting the sampler off at a few different values is a reasonable way to make sure that nothing eggregiously wrong is happening with the sampler. This is primarily useful for diagnosing coding errors and can be helpful (if we are lucky) with figuring out obvious multimodalities in the distribution. Luck comes into the picture because we will need to have chosen starting points that are located appropriately near the different modes to detect them, something that users typically cannot do. Much more important is the idea of running the chain for as long as feasible, since a long run is likely to eventually pick up unusual features of the target distribution.

Being very coneful

- () Construct two different M-Hay, both resulting in same distr. Similar results?
- 1) Plot maginal densities : overlagy after M2 and after N Similar ?
- (3) Run chain for very long
- (4) MCse = smell value, Ess for each component > 5.000.
- (5) Try a few fairly different starting values Similar?
- To compare alg: look at act plots.

| Terminology Notes: |
|---|
| Metropolis-Hastings alg: (V-MH): |
| Produce Havis egodic M.C. w/ stationary |
| Produce Harris ergodic M.C. w/ stationary distr. The by using M-H update for each |
| "block" of variables. |
| M-H update suppose target distr. is $T(\theta_1,,\theta_p)$. |
| MH Update of Ok: propose Ok ~ g(Ok, Ok Ok) |
| MH Update of O_R : propose $O_R^* \sim g(O_R, O_R^* O_{-R})$ Accept w/ prob. $\times (O_R, O_R^*) = \min\{1, \frac{\pi(O_R^* O_{-R})}{\pi(O_R O_{-R})} \frac{g(O_R, O_R)}{g(O_R, O_R^* O_{-R})}\}$ The Size is a cases: |
| It Special cases: Metropolis update of O_R : $q(O_R, O_R^+ O_{-R}) = q(O_R^+, O_R^-)O_{-R}$ so it is symmetric; in its argume eg. nandam wilk in Normal proper |
| 50 it is summetric in the answer eg. namelan wilk wi Normal proper |
| Accept w/ prob. $\propto (\theta_{k}, \theta_{k}^{\dagger}) = \min \left\{ 1, \frac{\pi(\theta_{k} \theta_{-k})}{\pi(\theta_{k} \theta_{-k})} \right\}$ |
| Gibbs update of Ox: II(Ox TOx)= q(On,Ox/Ox)= TI(Ox/Ox) |
| that is, simulate proposal directly from full could! distr. |
| That is, simulate proposal directly from full condth. distr. Accept ω prob ω ($O_{\mathbf{k}}, \mathbf{k}^*$)= $\min \left\{ 1, \frac{\pi(o_{\mathbf{k}} o_{-\mathbf{k}})}{\pi(o_{\mathbf{k}} o_{-\mathbf{k}})} \frac{\pi(o_{\mathbf{k}} o_{-\mathbf{k}})}{\pi(o_{\mathbf{k}} o_{-\mathbf{k}})} \right\}$ $= 1. Always accept.$ |
| = 1. Always accept. |
| M-H algorithm allows for combination of all these |
| Rinds of updates. |
| Gibbs sampler => M-H algorithm where in your |
| M-H algorithm allows for combination of all these kinds of updates. Gibbs sampler => M-H algorithm where all updates are Gibbs updates. |
| |

McMc 24 Ca)

Note: Data arguentation: also falls under M-H algorithms in Situations where adding roudon variables (augmentation of target distr.) makes things easier. e.g. missing data problems—treating missing data are additional random variables to be sampled. e.g. mixture models, classification problems, survival analysis.

No need for terminology tike Metropolis walken Gibbs, 'Hybrid M-H' etc.

Reminder of distinction between notions of variability in frequentist (classical) and Bayesian interence: Frequentist: variability of estimates - if more random samples are obtained (of the same size as the observations), from same dist. brow would this charge the estimate? Sampling variability of estimates estimates estimates estimates estimates theory, bootstrap parametric or non-parametric Bayesian: Suppose we quartity our knowledge about a parameter via a prob. distr. (prior distr") and we now observe data that informs us about the param. (via a prob. undel plikelihood fr.). What is our knowledge of the parameter now (condtl on data)? Posterier div. of

parameter. estimate via: asymptetic Meory, Monte Carlo /mcMc.

Monte Carlo seemen Versus [posterior] standard derivation = fixed Mcse is an estimate of the quality of your estimate 'simulation evar'. E.g. estimate of [posterior mean], $E_{\pi}(\beta) = 2.5$ W/ Mcse of 0.0003 est. of [posterior variance]. En {(B-En(B))}=1.2 w/ Mise of 0.004 (If Benya) sider = [ET {(p3-ET(p3))}]

(if Benya)

est. w/ posterior siderication. For inference: case abt. parterior man, sider. To ensure estimates, are accurate: care about MCse.

Central Limit Thm. & servous for MCMC I.i.d. Case: If $Var_{i}(g(x_i)) = \infty$ Vn (Mn-M) -> N(0, 62) where $\sigma^2 = Var_{\mathcal{K}} g(X_i)$ and $Var(\hat{M}_n) = \frac{\sigma^2}{n}$ Easy to estimate or from Xi,..., Xn 21d TI 22 = S2 = sample variance et X1, ..., Xn. S_0 , $\hat{\mathcal{M}}_n \sim \mathcal{N}(\mathcal{M}_n, \frac{\hat{\mathcal{M}}_n}{n})$ and, $\mathcal{V}_{\mathcal{M}}(\hat{\mathcal{M}}_n) \approx \frac{\hat{\mathcal{M}}_n}{n}$ Which can be used to estimate CI's. (1) Vary g(xi) <0 does not control Mether a CIT McMc can: 2 Vac $(\hat{n}_n) = \frac{1}{n^2} \underbrace{Z}_{i=1}^n Cov (g(x_i), g(x_j))$

since g(xi): me not iid.

eg, batch meens Imak.

Need to estimate covariances.

(skip delails)

There are many different sets of sufficient Conditions for a Markov Chain CLT. two of the more intuitive sufficient Here are If {Xn} is a Harris-egodic Markor chain, w/ stationams dich or E 2. 7×13 is geometrically ergodic, reversible and 3. $\{X_n\}_{s}$ is uniformly engodic and $E_n(g(x)^2) < \infty$ then, for any initial distr.,

hon , In (Mn-M) -> N(O, 52)

2700

More détails: see Jones'04 and Roberts & Rosenthal .'04.

Monte Carlo seur for MCMC (MCMCse) Need to estimete asymptotic variance, or MCMCse = 0/5n ienerally, I is not easy to estimate. One approach: botch meens. Idea: Run M. chain for n = ab length.

Define $Y_k = \underbrace{\sum_{i=(k-i)b+1}^{kb} g(X_i)}_{h}$, k = 1, ..., a= M.C. estimate of M= ISLX) T(X) dx based on k" batch" $\hat{\mathcal{T}}' = \frac{b}{a-1} \left[\left(\frac{1}{2} \left(\frac{1}{2} \hat{\mathcal{H}}_{k} - \hat{\mathcal{H}}_{k} \right)^{2} \right] \right] \qquad M(se = \frac{c}{2})$ Above: Van (Yk) = 2 (Yk-h)/(a-1), and Van (Mn) = b Van (Yk)
b batch size should large enough so we can treat I'm as approximately independent "Consistent botch meens", $b = \sqrt{n}$, so $a = \sqrt{n}$.

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Simulation studies as Monte Carlo

Examples: Companing two estimators

Studying Natidating asymptotic results in finite samples

Studying coverage prob. If a C.I.

E.S.1. My estimator is better than theirs. Investigate a scenario.

Sim. 1:
$$(y_{10}, -y_{10}) = y_1$$
: $\hat{\phi}_1$: $\hat{\psi}_1$: $\hat{\psi}_2$: $\hat{\psi}_2$: $\hat{\psi}_2$: $\hat{\psi}_2$: $\hat{\psi}_3$: $\hat{\psi}_4$: $\hat{\psi}_4$: $\hat{\psi}_5$: $\hat{\psi}_6$:

Sim. B: $\hat{\psi}_6$: $\hat{\psi}_7$: $\hat{\psi}_8$: $\hat{$

MSE of $\hat{\Psi} = E_{\sigma}(\hat{\Psi} - \theta)^{2}$, our expectation!

est. by $\frac{Z}{S}(\hat{\Psi} - \theta)^{2}$, $\hat{\Psi}_{mse}$

Compare: Donse I 2 serior to Vonne I 2 serior

M.c. man

Hapefully my estimator is better! (significantly smaller MSE)

Of course this may change w/ scenario.

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E.g. Does my method for constructing a CI have the right coverage, ie, does my 95% C.I. A have $P(O \in A) = 0.95$ Sim 1. Y, A, I(OGA) Sim B YB AB I(OEAB) M.C. estimate = $\frac{B}{E} I(\Theta \in A_b)$ = $\frac{\widehat{corg}(A)}{B}$ Again, use M.Cs. euron as a gride to determine Note: easy to get, estimate for cong (A): \(\frac{\cong}{B} \)

m/m/ 28

Monte Callo (or MCMC) Maximum Likelihood Suppose F= 3 fo: OE 囲了 is a family of normalized densities Now suppose $f_{\theta}(x) = \frac{h_{\theta}(x)}{c(\theta)}$ and you only now ho(n) c(0) is normalizing function. This can happen when using flexible models

for complicated problems. e.g. $h_{\phi}(x) = e^{-(x)}$ (enponential family) t(x) is vector valued state. σ is parameter (unknown). God: Want MLE for O, &= argmax fo(x)
Problem: Don't know C(0)! MCML solution: Pick some 4E 1 s.t. $h_{\psi}(x)=0$ = 7 $h_{\theta}(x)=0$ for (almost) all x Now, $\frac{C(\theta)}{C(4)} = \frac{1}{C(4)} \int h_{\theta}(x) dx = \int \frac{h_{\theta}(n)}{C(4)} dx$ $=\int \frac{h_{\theta}(x)}{h_{\psi}(x)/f_{\psi}(x)} dx = \int \frac{h_{\theta}(x)}{h_{\psi}(x)} f_{\psi}(x) dx$ $= E_{f_{\psi}} \left\{ \frac{h_{\sigma}(\pi)}{h_{\psi}(\pi)} \right\}$ Can simulate 1,..., Ym ~ for by rejsampling, M-Wete.

and extinate $\frac{C(0)}{C(V)}$ by $\frac{M}{J-1}$ $\frac{h_0(V_j)}{h_V(V_j)}$ /M

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McML 1

Goal: agmax $f_0(x) = \underset{\varphi \in \mathbb{B}}{\operatorname{argmax}} \frac{f_0(x)}{f_{\psi}(x)} \leftarrow \underset{\text{w.r.t.} \theta}{\operatorname{constant}}$ $=) \hat{\Theta} = \underset{\Phi \in \bigoplus}{\operatorname{argmax}} \underset{f_{\Psi}(\pi)}{\operatorname{fo}(\pi)} = \underset{\Phi \in \bigoplus}{\operatorname{argmax}} \underset{h}{\operatorname{log}}, say$ Now, $l(\theta) = log \left(\frac{h_{\theta}(\pi)}{c(\theta)} \right) - log \left(\frac{h_{\pi}(\pi)}{c(\pi)} \right)$ = log [hor(x)] - log [c(v)]

hor(x)] $=) \hat{l}(\theta) = log \left(\frac{h_{\theta}(x)}{h_{\eta}(x)}\right) - log \frac{m}{h_{\eta}(x)} \frac{h_{\theta}(x)}{h_{\eta}(x)}\right)$ completely known Monte Carlo estronate $\tilde{\Theta}$ that maximizes $\hat{l}(\theta)$ is estimate of M2E.

MCM(33

Overniew of Prob., Stats., Stock Proc. L. Monte Calo

Modani
Ch. 3, 4, 5, 6, Sim. bru on P.P.,

Probability M. H. on image analysis Contactive
Michael for etc.

Stockastic
Model (Data)
Generality Process

Stat. Int.

Bayerian int., likelhood int.

(me mc Mickelhood)