STA3431 (Monte Carlo Methods) Lecture Notes, Sept–Dec 2017

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Note: I will update these notes regularly (on the course web page). However, they are just rough, point-form notes, with no guarantee of completeness or accuracy. They should in no way be regarded as a substitute for attending the lectures, doing the homework exercises, studying for the test, or reading the reference books.

INTRODUCTION:

- Introduction to course, handout, references, prerequisites, etc.
  - Course web page: probability.ca/sta3431
  - Sidney Smith Hall room 2120, Mondays 10:10–12:00.
  - If not Stat Dept grad student, must REQUEST enrolment (by e-mail); need advanced undergraduate probability/statistics background, plus basic computer programming experience.
  - Conversely, if you already know lots about MCMC etc., then this course might not be right for you since it's an INTRODUCTION to these topics.
  - How many of you are stat grad students? undergrads? math? computer science? physics? economics? management? engineering? other? Auditing??
- Theme of the course: use (pseudo)randomness on a computer to simulate (and hence estimate) important/interesting quantities.
- Example: Suppose want to estimate $m := \mathbf{E}[Z^4 \cos(Z)]$, where $Z \sim \text{Normal}(0, 1)$.
  - "Classical" Monte Carlo solution: replicate a large number $z_1, \ldots, z_n$ of Normal(0,1) random variables, and let $x_i = z_i^4 \cos(z_i)$.
  - Their mean $\overline{x} \equiv \frac{1}{n} \sum_{i=1}^n x_i$ is an (unbiased) estimate of $\mathbf{E}[X] \equiv \mathbf{E}[Z^4 \cos(Z)]$.
  - R: Z = rnorm(100); X = Z∧4 ∗ cos(Z); mean(X) [file "RMC"]
  - unstable ... but if replace "100" with "1000000" then $\overline{x}$ close to -1.213 ...
  - Variability??
  - Well, can estimate standard deviation of $\overline{x}$ by the (estimated) "standard error" of $\overline{x}$, which is:

$$se \;=\; n^{-1/2}\,\text{sd}(x) \;\approx\; n^{-1/2}\sqrt{\text{var}(x)} \;=\; n^{-1/2}\sqrt{\frac{1}{n-1}\sum_{i=1}^{n}(x_i - \overline{x})^2}\,.$$

[file "RMCse"]

- Then what is, say, a 95% confidence interval for m?
- Well, by central limit theorem (CLT), for large n, have $\overline{x} \approx N(m, v) \approx N(m, se^2)$.
  - (Strictly speaking, should use "t" distribution, not normal distribution ... but if n large that doesn't really matter – ignore it for now.)
  - So $\frac{m-\overline{x}}{se} \approx N(0,1)$.
  - So, $\mathbf{P}(-1.96 < \frac{m-\overline{x}}{se} < 1.96) \approx 0.95$.
  - So, $\mathbf{P}(\overline{x} - 1.96\, se\ < m < \overline{x} + 1.96\, se\,) \approx 0.95$.
  - i.e., approximate 95% confidence interval is [file "RMCci"]

$$(\overline{x} - 1.96\, se,\ \overline{x} + 1.96\, se)\,.$$

- Alternatively, could compute expectation as

$$\int_{-\infty}^{\infty} z^4 \cos(z)\, \frac{e^{-z^2/2}}{\sqrt{2\pi}}\, dz\,.$$

Analytic? Numerical? Better? Worse? [file "RMCcomp": -1.213]

- (Aside: In fact, by considering it as the real part of $\mathbf{E}(Z^4 e^{iZ})$, this can be computed exactly, to be $-2/\sqrt{e} \doteq -1.213061$. But what about an even harder example?)
- What about higher-dimensional versions? (Can't do numerical integration!)
- Note: In this course we will often use R to automatically sample from simple distributions like Normal, Uniform, Exponential, etc.
  - But how does it work? (See below.)
- What if distribution too complicated to sample from?
  - (MCMC! ... Metropolis, Gibbs, tempered, trans-dimensional, ...)

HISTORICAL EXAMPLE – BUFFON'S NEEDLE:

- Have series of parallel lines ... line spacing w, needle length $\ell \le w$ (say $\ell = w$) ... what is prob that needle lands touching line? [http://www.metablake.com/pi.swf]
- Let θ be angle counter-clockwise from line direction, and h distance of top end above nearest line.
- Then $h \sim \text{Uniform}[0, w]$ and $\theta \sim \text{Uniform}[0, \pi]$, independent.
- Touches line iff $h < \ell \sin(\theta)$.
- So, prob $= \frac{1}{\pi} \int_0^\pi \frac{1}{w} \int_0^w \mathbf{1}_{h<\ell \sin(\theta)}\, dh\, d\theta = \frac{1}{\pi} \int_0^\pi \frac{1}{w} \ell \sin(\theta)\, d\theta = 2\ell/w\pi$.

- Hence, by LLN, if throw needle n times, of which it touches a line m times, then for n large, $m/n \approx 2\ell/w\pi$, so $\pi \approx 2n\ell/mw = 2n/m$ (if $\ell = w$).
- [e.g. recuperating English Captain O.C. Fox, 1864: $\ell = 3$, $w = 4$, $n = 530$, $m = 253$, so $\pi \approx 2n\ell/mw \doteq 3.1423$.]
- But for modern simulations, use computer. How to randomise??

PSEUDORANDOM NUMBERS:

- Goal: generate an i.i.d. sequence $U_1, U_2, U_3, \ldots \sim \text{Uniform}[0,1]$.
- One method: LINEAR CONGRUENTIAL GENERATOR (LCG).
  - Choose (large) positive integers m, a, and b.
  - Start with a "seed" value, x_0. (e.g., the current time in milliseconds)
  - Then, recursively, $x_n = (ax_{n-1} + b) \bmod m$, i.e. $x_n =$ remainder when $ax_{n-1} + b$ is divided by m.
  - So, $0 \le x_n \le m - 1$.
  - Then let $U_n = x_n/m$.
  - Then $\{U_n\}$ will "seem" to be approximately i.i.d. $\sim$ Uniform$[0,1]$. (file "Rrng")
- Choice of m, a, and b?
- Many issues:
  - need m large (so many possible values);
  - need a large enough that no obvious "pattern" between U_{n-1} and U_n.
  - need b to avoid short "cycles" of numbers.
  - many statistical tests, to try to see which choices provide good randomness, avoid correlations, etc. (e.g. "diehard tests", "dieharder": www.phy.duke.edu/~rgb/General/dieharder.php)
  - One common "good" choice: $m = 2^{32}$, $a = 69,069$, $b = 23,606,797$.
- Theorem: the LCG has full period (m) if and only if both (i) $\gcd(b, m) = 1$, and (ii) every "prime or 4" divisor of m also divides $a - 1$.
  - So, if $m = 2^{32}$, then if b odd and $a - 1$ is a multiple of 4, then the LCG has full period $m = 2^{32} \doteq 4.3 \times 10^9$; good.
  - Many other choices, e.g. C programming language (glibc) uses $m = 2^{32}$, $a = 1,103,515,245$, $b = 12,345$.
  - One bad choice: $m = 2^{31}$, $a = 65539 = 2^{16} + 3$, $b = 0$ ("RANDU") ... used for many years (esp. early 1970s) ... but then $x_{n+2} = 6x_{n+1} - 9x_n \bmod m$ ... too much serial correlation. [Proof: $x_{n+2} = (2^{16}+3)^2 x_n = (2^{32} + 6(2^{16}) + 9)x_n \equiv (0 + 6(2^{16}+3) - 9)x_n \pmod{2^{31}} = 6x_{n+1} - 9x_n$.]

  - (Microsoft Excel pre-2003: period $< 10^6$, too small ... Excel 2003 used floating-point “version” of LCG, which sometimes gave negative numbers – bad!)

- Not “really” random, just “pseudorandom” ...
  - Can cause problems!
  - Will fail certain statistical tests ...
  - Some implementations also use external randomness, e.g. current temperature of computer’s CPU / entropy of kernel (e.g. Linux’s “urandom”).
  - Or the randomness of *quantum mechanics*, e.g. www.fourmilab.ch/hotbits
  - Or of atmospheric noise, e.g. random.org.
  - But for most purposes, standard pseudorandom numbers are pretty good ...

- We’ll consider LCG’s “good enough for now”, but:
  - Other generators include “Multiply-with-Carry” [$x_n = (ax_{n-r} + b_{n-1}) \bmod m$ where $b_n = \lfloor (ax_{n-r} + b_{n-1})/m \rfloor$; and ‘Kiss” [$y_n = (x_n + J_n + K_n) \bmod 2^{32}$, where x_n as above, and J_n and K_n are “shift register generators”, given in bit form by $J_{n+1} = (I + L^{15})(I + R^{17})J_n \bmod 2^{32}$, and $K_{n+1} = (I + L^{13})(I + R^{18})K_n \bmod 2^{31}$]; and “Mersenne Twister” [$x_{n+k} = x_{n+s} \oplus (x_n^{(\text{upper})} | x_{n+1}^{(\text{lower})})A$, where $1 \leq s < k$ where $2^{kw-r} - 1$ is Mersenne prime, and A is $w \times w$ (e.g. 32×32) with $(w-1) \times (w-1)$ identity in upper-right, with matrix mult. done bit-wise mod 2], and many others too.
  - (R implementation: see “?.Random.seed” ... default is Mersenne Twister.)

- So, just need computer to do <u>simple arithmetic</u>. No problem, right?

LIMITATIONS OF COMPUTER ARITHMETIC:

- Consider the following computations in R:

  -
    ```
    > 2 + 1 - 2
    [1] 1
    > 2∧10 + 1 - 2∧10
    > 2∧100 + 1 - 2∧100
    ```

- Why??

- Homework question: for what values of n does:
  ```
  > 2∧n + 1 - 2∧n
  ```
  give 0 instead of 1??

- (Similarly in many other computer languages too, e.g. C (powertest.c), Java (powertest.java) ... and Python with floating numbers ... but not Python with *integer* variables (powertest.py), because it then does dynamic memory allocation ...)

- So, numerical computations are just approximations, with their own errors!

- We'll usually ignore this, but MUST BE CAREFUL!
  - Then can simulate uniform random variables.
  - What about other random variables?

SIMULATING OTHER DISTRIBUTIONS:

- Once we have $U_1, U_2, \ldots$ i.i.d. $\sim$ Uniform$[0,1]$ (at least approximately), how do we generate other distributions?

- With transformations, using "change-of-variable" theorem!

- e.g. to make $X \sim$ Uniform$[L, R]$, set $X = (R-L)U_1 + L$.

- e.g. to make $X \sim$ Bernoulli(p), set

$$X = \begin{cases} 1, & U_1 \le p \\ 0, & U_1 > p \end{cases}$$

- e.g. to make $Y \sim$ Binomial(n, p), either set $Y = X_1 + \ldots + X_n$ where

$$X_i \;=\; \begin{cases} 1, & U_i \le p \\ 0, & U_i > p \end{cases},$$

  or set

$$Y \;=\; \max\Big\{j \;:\; \sum_{k=0}^{j-1} \binom{n}{k} p^k (1-p)^{n-k} \;\le\; U_1\Big\}$$

  (where by convention $\sum_{k=0}^{-1}(\cdots) = 0$). ("Inverse CDF method")

- More generally, to make $\mathbf{P}(Y = x_i) = p_i$ for some $x_1 < x_2 < x_3 < \ldots$, where $p_i \ge 0$ and $\sum_i p_i = 1$, simply set

$$Y \;=\; \max\{x_j\,;\; \sum_{k=1}^{j-1} p_k \;\le\; U_1\}\,.$$

- e.g. to make $Z \sim$ Exponential(1), set $Z = -\log(U_1)$.
  - Then $\mathbf{P}(Z > x) = \mathbf{P}(-\log(U_1) > x) = \mathbf{P}(\log(U_1) < -x) = \mathbf{P}(U_1 < e^{-x}) = e^{-x}$.
  - Then, to make $W \sim$ Exponential(λ), set $W = Z/\lambda = -\log(U_1)/\lambda$.

- What if want X to have density $6\,x^5 \mathbf{1}_{0<x<1}$.

  - Let $X = U_1^{1/6}$.
  - Then for $0 < x < 1$, $\mathbf{P}(X \le x) = \mathbf{P}(U_1^{1/6} \le x) = \mathbf{P}(U_1 \le x^6) = x^6$.
  - Hence, $f_X(x) = \frac{d}{dx}\Big[\mathbf{P}(X \le x)\Big] = \frac{d}{dx} x^6 = 6\, x^5$ for $0 < x < 1$.
  - More generally, for $r > 1$, if $X = U_1^{1/r}$, then $f_X(x) = r\, x^{r-1}$ for $0 < x < 1$. [CHECK!]

- What about normal dist.? Fact: If

$$X \;=\; \sqrt{2\,\log(1/U_1)}\;\cos(2\pi U_2)\,,$$

$$Y \;=\; \sqrt{2\,\log(1/U_1)}\;\sin(2\pi U_2)\,,$$

  then $X, Y \sim N(0,1)$ (independent!). ["Box-Muller transformation": Ann Math Stat 1958, 29, 610-611]

  - Proof: By multidimensional change-of-variable theorem, if $(x,y) = h(u_1,u_2)$ and $(u_1,u_2) = h^{-1}(x,y)$, then $f_{X,Y}(x,y) = f_{U_1,U_2}(h^{-1}(x,y))\,/\,|J(h^{-1}(x,y))|$. Here $f_{U_1,U_2}(u_1,u_2) = 1$ for $0 < u_1, u_2 < 1$ (otherwise 0), and

$$J(u_1,u_2) \;=\; \det\begin{pmatrix} \frac{\partial x}{\partial u_1} & \frac{\partial x}{\partial u_2} \\ \frac{\partial y}{\partial u_1} & \frac{\partial y}{\partial u_2} \end{pmatrix}$$

$$=\; \det\begin{pmatrix} -\cos(2\pi u_2)\,/\,u_1\sqrt{2\log(1/u_1)} & -2\pi\sin(2\pi u2)\sqrt{2\log(1/u_1)} \\ -\sin(2\pi u_2)\,/\,u_1\sqrt{2\log(1/u_1)} & 2\pi\cos(2\pi u2)\sqrt{2\log(1/u_1)} \end{pmatrix}$$

$$=\; -2\pi\,/\,u_1\,.$$

    But $u_1 = e^{-(x^2+y^2)/2}$, so density of (X,Y) is

$$f_{X,Y}(x,y) \;=\; 1/|J(h^{-1}(x,y))| \;=\; 1/|-2\pi\,/\,e^{-(x^2+y^2)/2}| \;=\; e^{-(x^2+y^2)/2}/2\pi$$

$$=\; \Big(\frac{1}{\sqrt{2\pi}}e^{-x^2/2}\Big)\Big(\frac{1}{\sqrt{2\pi}}e^{-y^2/2}\Big)\,,$$

    i.e. $X \sim N(0,1)$ and $Y \sim N(0,1)$ are independent.

- Another approach: "INVERSE CDF METHOD":
  - Suppose <u>want</u> $\mathbf{P}(X \le x) = F(x)$. ("CDF")
  - For $0 < t < 1$, set $F^{-1}(t) \;=\; \min\{x\,;\; F(x) \ge t\}$. ("inverse CDF")
  - Then set $X = F^{-1}(U_1)$.
  - Then $X \le x$ if and only if $U_1 \le F(x)$. [Subtle; see e.g. Rosenthal, *A First Look at Rigorous Probability Theory*, 2nd ed., Lemma 7.1.2.]
  - So, $\mathbf{P}(X \le x) \;=\; \mathbf{P}(U_1 \le F(x)) \;=\; F(x)$.
  - Very general, but computing $F^{-1}(t)$ could be difficult ...

- So, generating (pseudo)random numbers for most "standard" one-dimensional distributions is pretty easy ...

  - So, can get Monte Carlo estimates of expectations involving standard one-dimensional distributions, e.g. $\mathbf{E}[Z^4 \cos(Z)]$ where $Z \sim \text{Normal}(0,1)$.

- But what if distribution is complicated, multidimensional, etc.? Simulate!

SIMULATION EXAMPLE: QUEUEING THEORY:

  - $Q(t)$ = number of people in queue at time $t \geq 0$.

- Suppose service times $\sim$ Exponential(μ) [mean $1/\mu$], and interarrival times $\sim$ Exponential(λ) ("M/M/1 queue"), so $\{Q(t)\}$ Markovian. Then well known [e.g. STA447/2006]:
  - If $\mu \leq \lambda$, then $Q(t) \to \infty$ as $t \to \infty$.
  - If $\mu > \lambda$, then $Q(t)$ converges in distribution as $t \to \infty$:
  - $\mathbf{P}(Q(t) = i) \to (1 - \frac{\lambda}{\mu})(\frac{\lambda}{\mu})^i$, for $i = 0, 1, 2, \ldots$.
  - Easy! (e.g. $\mu = 3$, $\lambda = 2$, $t = 1000$) [file "Rqueue"]

- Now suppose instead that service times $\sim$ Uniform$[0,1]$, and interarrival times have distribution of $|Z|$ where $Z \sim \text{Normal}(0,1)$. Limits not easily computed. Now what?
  - Simulate it! [file "Rqueue2"]

- Or, to make the means the same as the first example, suppose service times $\sim$ Uniform$[0, 2/3]$, and interarrival times have distribution of $Z^2/2$ where $Z \sim \text{Normal}(0,1)$. Now what? [file "Rqueue3"]

EXAMPLE – CODE BREAKING:

- Try it out: "decipherdemo". [uses file "decipher.c"]

- Data is the coded message text: $s_1 s_2 s_3 \ldots s_N$, where $s_i \in \mathcal{A} = \{A, B, C, \ldots, Z, \text{space}\}$.

- State space $\mathcal{X}$ is set of all bijections (for now) of $\mathcal{A}$, i.e. one-to-one onto mappings $f : \mathcal{A} \to \mathcal{A}$, subject to $f(\text{space}) = \text{space}$.
  - ["substitution cipher"]

- Use a reference text (e.g. "War and Peace") to get matrix $M(x,y) = 1+$ number of times y follows x, for $x, y \in \mathcal{A}$.

- Then for $f \in \mathcal{X}$, let $\pi(f) = \prod_{i=1}^{N-1} M\Big(f(s_i), f(s_{i+1})\Big)$.
  - (Or raise this all to a power, e.g. 0.25.)

- Idea: if $\pi(f)$ is larger, then f leads to pair frequencies which more closely match the reference text, so f is a "better" choice.

- Would like to find the choice of f which <u>maximises</u> $\pi(f)$.

- To do this, run a Metropolis algorithm for π:
  - Choose $a, b \in \mathcal{A} \setminus \{\text{space}\}$, uniformly at random.

  - Propose to replace f by g, where $g(a) = f(b)$, $g(b) = f(a)$, and $g(x) = f(x)$ for all $x \neq a, b$.
  - Accept with probability $\min\left(1, \frac{\pi(g)}{\pi(f)}\right)$.

- Easily seen to be an irreducible, aperiodic, reversible Markov chain [later!].
- So, converges (quickly!) to correct answer, breaking the code.
- References: S. Conner (2003), "Simulation and solving substitution codes". P. Diaconis (2008), "The Markov Chain Monte Carlo Revolution".
- We later extended this, to transposition ciphers and more: J. Chen and J.S. Rosenthal (2010), "Decrypting Classical Cipher Text Using Markov Chain Monte Carlo" (*Statistics and Computing* **22(2)**, 397–413, 2011).

END WEEK #1

EXAMPLE – PATTERN DETECTION:

- Try it out: faces.html
- Data is an image, given in terms of a grid of pixels (each "on" or "off").
- Want to "find" the face in the image.
  - (Harder for computers than for humans!)
- Define the face location by a vector θ of various parameters (face center, eye width, nose height, etc.).
- Then define a score function $S(\theta)$ indicating how well the image agrees with having a face in the location corresponding to the parameters θ.
- Then run a "mixed" Monte Carlo search (sometimes updating by small RWM moves, sometimes starting fresh from a random vector) over the entire parameter space, searching for $\text{argmax}_\theta\, S(\theta)$, i.e. for the parameter values which maximise the score function.
  - Keep track of the best θ so far – this allows for greater flexibility in trying different search moves without needing to preserve a stationary distribution.
  - Works pretty well, and fast! ("faces.html" Java applet)
  - For details, see Java applet source code file "faces.java", or the paper J.S. Rosenthal, Optimising Monte Carlo Search Strategies for Automated Pattern Detection. F. E. J. Math. Sci. 2009.
- In both of these examples, wanted to MAXIMISE (i.e., OPTIMISE) π, rather than SAMPLE from π.
  - General method? Simulated Annealing – later.

MONTE CARLO INTEGRATION:

- How to compute an integral with Monte Carlo?
  - Re-write it as an expectation!
- EXAMPLE: Want to compute $\int_0^1 \int_0^1 g(x,y)\, dx\, dy$.
  - Regard this as $\mathbf{E}[g(X,Y)]$, where X, Y i.i.d. $\sim$ Uniform$[0,1]$.
  - e.g. $g(x,y) = \cos(\sqrt{xy}\,)$. (file "RMCint") Easy!
  - Get about 0.88 ± 0.003 ... Mathematica gives 0.879544.
- e.g. estimate $I = \int_0^5 \int_0^4 g(x,y)\, dy\, dx$, where $g(x,y) = \cos(\sqrt{xy}\,)$.
  - Here

    $$\int_0^5 \int_0^4 g(x,y)\, dy\, dx \;=\; \int_0^5 \int_0^4 5{\cdot}4{\cdot}g(x,y)\,(1/4)dy\,(1/5)dx \;=\; \mathbf{E}[5{\cdot}4{\cdot}g(X,Y)]\,,$$

    where $X \sim$ Uniform$[0,5]$ and $Y \sim$ Uniform$[0,4]$.
  - So, let $X_i \sim$ Uniform$[0,5]$, and $Y_i \sim$ Uniform$[0,4]$ (all independent).
  - Estimate I by $\frac{1}{M}\sum_{i=1}^M (5 \cdot 4 \cdot g(X_i, Y_i))$. (file "RMCint2")
  - Standard error: $se = M^{-1/2}\, sd(5 \cdot 4 \cdot g(X_1,Y_1),\, \ldots,\, 5 \cdot 4 \cdot g(X_M, Y_M))$.
  - With $M = 10^6$, get about -4.11 ± 0.01 ... Mathematica gives -4.11692.
- e.g. estimate $\int_0^1 \int_0^\infty h(x,y)\, dy\, dx$, where $h(x,y) = e^{-y^2} \cos(\sqrt{xy}\,)$.
  - (Can't use "Uniform" expectations.)
  - Instead, write this as $\int_0^1 \int_0^\infty (e^y\, h(x,y))\, e^{-y}\, dy\, dx$.
  - This is the same as $\mathbf{E}[e^Y\, h(X,Y)]$, where $X \sim$ Uniform$[0,1]$ and $Y \sim$ Exponential(1) are independent.
  - So, estimate it by $\frac{1}{M}\sum_{i=1}^M e^{Y_i} h(X_i, Y_i)$, where $X_i \sim$ Uniform$[0,1]$ and $Y_i \sim$ Exponential(1) (i.i.d.). (file "RMCint3")
  - With $M = 10^6$ get about 0.767 ± 0.0004 ... Small error! Mathematica: 0.767211.
- Alternatively, could write this as $\int_0^1 \int_0^\infty (\frac{1}{5}\, e^{5y}\, h(x,y))\, (5\, e^{-5y})\, dy\, dx = \mathbf{E}[\frac{1}{5} e^{5Y} h(X,Y)]$ where $X \sim$ Uniform$[0,1]$ and $Y \sim$ Exponential(5) (indep.).
  - Then, estimate it by $\frac{1}{M}\sum_{i=1}^M \frac{1}{5} e^{5y_i} h(x_i, y_i)$, where $x_i \sim$ Uniform$[0,1]$ and $y_i \sim$ Exponential(5) (i.i.d.).
  - With $M = 10^6$, get about 0.767 ± 0.0016 ... larger standard error ... (file "RMCint4").
  - If replace 5 by 1/5, get about 0.767 ± 0.0015 ... about the same.
- So which choice is best?
  - Whichever one minimises the standard error! ($\lambda \approx 1.5$, $se \approx 0.00025$?)

- In general, to evaluate $I \equiv \mathbf{E}[h(Y)] = \int h(y)\,\pi(y)\,dy$, where Y has density π, could instead re-write this as $I = \int h(x)\,\frac{\pi(x)}{f(x)}\,f(x)\,dx$, where f is easily sampled from, with $f(x) > 0$ whenever $\pi(x) > 0$.
  - Then $I = \mathbf{E}\left(h(X)\,\frac{\pi(X)}{f(X)}\right)$, where X has density f.
  - ("Importance Sampling")
  - Can then do classical (iid) Monte Carlo integration, get standard errors etc.
  - Good if easier to sample from f than π, and/or if the function $h(x)\,\frac{\pi(x)}{f(x)}$ is less variable than h itself.

- In general, best to make $h(x)\,\frac{\pi(x)}{f(x)}$ approximately constant.
  - e.g. extreme case: if $I = \int_0^\infty e^{-3x}\,dx$, then $I = \int_0^\infty (1/3)(3e^{-3x})dx = \mathbf{E}[1/3]$ where $X \sim$ Exponential(3), so $I = 1/3$ (error $= 0$, no MC needed).

UNNORMALISED DENSITIES:

- Suppose now that $\pi(y) = c\,g(y)$, where we know g but <u>don't</u> know c or π. ("Unnormalised density", e.g. Bayesian posterior.)
  - Obviously, $c = \frac{1}{\int g(y)\,dy}$, but this might be hard to compute.
  - Still, $I = \int h(x)\,\pi(x)\,dx = \int h(x)\,c\,g(x)\,dx = \frac{\int h(x)\,g(x)\,dx}{\int g(x)\,dx}$.
  - If sample $\{x_i\} \sim f$ (i.i.d.), then $\int h(x)\,g(x)\,dx = \int \Big(h(x)\,g(x)\,/\,f(x)\Big) f(x)\,dx = \mathbf{E}[h(X)\,g(X)\,/\,f(X)]$ where $X \sim f$.
  - So, $\int h(x)\,g(x)\,dx \approx \frac{1}{M}\sum_{i=1}^M \Big(h(x_i)\,g(x_i)\,/\,f(x_i)\Big)$.
  - Similarly, $\int g(x)\,dx \approx \frac{1}{M}\sum_{i=1}^M \Big(g(x_i)\,/\,f(x_i)\Big)$.
  - So, $I \approx \frac{\sum_{i=1}^M \Big(h(x_i)\,g(x_i)\,/\,f(x_i)\Big)}{\sum_{i=1}^M \Big(g(x_i)\,/\,f(x_i)\Big)}$. ("Importance Sampling": weighted average)
  - (Because we are taking <u>ratios</u> of (unbiased) estimates, the resulting estimate is <u>not</u> unbiased, and its standard errors are less clear – but it is still consistent as $M \to \infty$.)
  - (Good to use <u>same</u> sample $\{x_i\}$ for both numerator and denominator: easier computationally, and leads to smaller variance.)

- Example: compute $I \equiv \mathbf{E}(Y^2)$ where Y has density $c\,y^3\sin(y^4)\cos(y^5)\,\mathbf{1}_{0<y<1}$, where $c > 0$ unknown (and hard to compute!).
  - Here $g(y) = y^3\sin(y^4)\cos(y^5)\,\mathbf{1}_{0<y<1}$, and $h(y) = y^2$.
  - Let $f(y) = 6\,y^5\mathbf{1}_{0<y<1}$. [Recall: if $U \sim$ Uniform$[0,1]$, then $X \equiv U^{1/6} \sim f$.]

- Then $I \approx \frac{\sum_{i=1}^{M} \big(h(x_i)\, g(x_i) \,/\, f(x_i)\big)}{\sum_{i=1}^{M} \big(g(x_i) \,/\, f(x_i)\big)} = \frac{\sum_{i=1}^{M} \big(\sin(x_i^4)\, \cos(x_i^5)\big)}{\sum_{i=1}^{M} \big(\sin(x_i^4)\, \cos(x_i^5) \,/\, x_i^2\big)}$. (file "Rimp" ... get about 0.766 ...)
- Or, let $f(y) = 4\,y^3 \mathbf{1}_{0<y<1}$. [Then if $U \sim$ Uniform$[0,1]$, then $U^{1/4} \sim f$.]
- Then $I \approx \frac{\sum_{i=1}^{M} \big(h(x_i)\, g(x_i) \,/\, f(x_i)\big)}{\sum_{i=1}^{M} \big(g(x_i) \,/\, f(x_i)\big)} = \frac{\sum_{i=1}^{M} \big(\sin(x_i^4)\, \cos(x_i^5)\; x_i^2\big)}{\sum_{i=1}^{M} \big(\sin(x_i^4)\, \cos(x_i^5)\big)}$. (file "Rimp")

- With importance sampling, is it important to use the same samples $\{x_i\}$ in both numerator and denominator?
  - What if independent samples are used instead?
  - Let's try it! (file "Rimpind")
  - Both ways work, but usually the same samples work better.

- What other methods are available to iid sample from π?

REJECTION SAMPLER:

- Assume $\pi(x) = c\, g(x)$, with π and c unknown, g known but hard to sample from.

- Want to sample $X \sim \pi$.
  - Then if $X_1, X_2, \ldots, X_M \sim \pi$ iid, then can estimate $\mathbf{E}_\pi(h)$ by $\frac{1}{M}\sum_{i=1}^{M} h(X_i)$, etc.

- Find some other, easily-sampled density f, and known $K > 0$, such that $K\, f(x) \ge g(x)$ for all x. (i.e., $K\, f(x) \ge \pi(x) \,/\, c$, i.e. $c\, K\, f(x) \ge \pi(x)$)

- Sample $X \sim f$, and $U \sim$ Uniform$[0,1]$ (indep.).
  - If $U \le \frac{g(X)}{K f(X)}$, then accept X (as a draw from π).
  - Otherwise, reject X and start over again.

- Now, since $0 \le \frac{g(x)}{K f(x)} \le 1$, therefore $\mathbf{P}(U \le \frac{g(X)}{K f(X)} \,|\, X = x) = \frac{g(x)}{K f(x)}$.
  - Hence, $\mathbf{P}\Big(U \le \frac{g(X)}{K f(X)}\Big) = \mathbf{E}\Big[\mathbf{P}\Big(U \le \frac{g(X)}{K f(X)}\Big| X\Big)\Big] = \mathbf{E}\Big[\frac{g(X)}{K f(X)}\Big] = \int_{-\infty}^{\infty} \frac{g(x)}{K f(x)}\, f(x)\, dx = \frac{1}{K}\int_{-\infty}^{\infty} g(x)\, dx$.
  - Similarly, for any $y \in \mathbf{R}$, $\mathbf{P}\Big(X \le y,\; U \le \frac{g(X)}{K f(X)}\Big) = \mathbf{E}\Big[\mathbf{1}_{X \le y} \mathbf{P}\Big(U \le \frac{g(X)}{K f(X)}\Big| X\Big)\Big] = \mathbf{E}\Big[\mathbf{1}_{X \le y} \frac{g(X)}{K f(X)}\Big] = \int_{-\infty}^{y} \frac{g(x)}{K f(x)}\, f(x)\, dx = \frac{1}{K}\int_{-\infty}^{y} g(x)\, dx$.
  - So, conditional on accepting, we have for any $y \in \mathbf{R}$ that

$$\mathbf{P}\Big(X \le y \,\Big|\, U \le \frac{g(X)}{K f(X)}\Big) = \frac{\mathbf{P}\Big(X \le y,\;\; U \le \frac{g(X)}{K f(X)}\Big)}{\mathbf{P}\Big(U \le \frac{g(X)}{K f(X)}\Big)}$$

$$= \frac{\int_{-\infty}^{y} \frac{g(x)}{K f(x)}\, f(x)\, dx}{\int_{-\infty}^{\infty} \frac{g(x)}{K f(x)}\, f(x)\, dx} = \frac{\int_{-\infty}^{y} g(x)\, dx}{\int_{-\infty}^{\infty} g(x)\, dx} = \int_{-\infty}^{y} \pi(x)\, dx\,.$$

  - So, conditional on accepting, $X \sim \pi$. Good! iid!

- However, prob. of accepting may be very small.
- If so, then get very few samples – bad.

END WEEK #2

- Example: $\pi = N(0,1)$, i.e. $g(x) = \pi(x) = (2\pi)^{-1/2} \exp(-x^2/2)$.
  - Want: $\mathbf{E}_\pi(X^4)$, i.e. $h(x) = x^4$. (Should be 3.)
  - Let f be double-exponential (Laplace) distribution, i.e. $f(x) = \frac{1}{2} e^{-|x|}$.
- If $K = 8$, then:
  - For $|x| \leq 2$, $K f(x) = 8 \frac{1}{2} \exp(-|x|) \geq 8 \frac{1}{2} \exp(-2) \geq (2\pi)^{-1/2} \geq \pi(x) = g(x)$.
  - For $|x| \geq 2$, $K f(x) = 8 \frac{1}{2} \exp(-|x|) \geq 8 \frac{1}{2} \exp(-x^2/2) \geq (2\pi)^{-1/2} \exp(-x^2/2) = \pi(x) = g(x)$.
  - See graph: file “Rrejgraph”.
- So, can apply rejection sampler with this f and K, to get samples, estimate of $\mathbf{E}[X]$, estimate of $\mathbf{E}[h(X)]$, estimate of $\mathbf{P}[X < -1]$, etc.
  - Try it: file “Rrej”
- For Rejection Sampler, $P(\text{accept}) = \mathbf{E}[P(\text{accept}|X)] = \mathbf{E}[\frac{g(X)}{Kf(X)}] = \int \frac{g(x)}{Kf(x)} f(x)\,dx = \frac{1}{K} \int g(x)\,dx = \frac{1}{cK}$. (Only depends on K, not f.)
  - So, in M attempts, get about M/cK iid samples.
  - (“Rrej” example: $c = 1$, $K = 8$, $M = 10{,}000$, so get about $M/8 = 1250$ samples.)
  - Since c fixed, try to minimise K.
  - Extreme case: $f(x) = \pi(x)$, so $g(x) = \pi(x)/c = f(x)/c$, and can take $K = 1/c$, whence $P(\text{accept}) = 1$, iid sampling: optimal.
- Note: these algorithms all work in discrete case too.
  - Can let π, f, etc. be “probability functions”, i.e. probability densities with respect to counting measure.
  - Then the algorithms proceed exactly as before.

AUXILIARY VARIABLE APPROACH:

- (related: “slice sampler”)
- Suppose $\pi(x) = c\, g(x)$, and (X, Y) chosen uniformly under graph of g.
  - i.e., $(X, Y) \sim \text{Uniform}\{(x, y) \in \mathbf{R}^2 : 0 \leq y \leq g(x)\}$.
  - Then $X \sim \pi$, i.e. we have sampled from π.

- Why? For $a < b$, $\mathbf{P}(a < X < b) = \frac{\text{area with } a<X<b}{\text{total area}} = \frac{\int_a^b g(x)\,dx}{\int_{-\infty}^{\infty} g(x)\,dx} = \int_a^b \pi(x)\,dx$.
- So, if repeat, get i.i.d. samples from π, can estimate $\mathbf{E}_\pi(h)$ etc.

- Auxiliary Variable rejection sampler:
  - If support of g contained in $[L,R]$, and $|g(x)| \le K$, then can first sample $(X,Y) \sim \text{Uniform}([L,R] \times [0,K])$, then reject if $Y > g(X)$, otherwise accept as sample with $(X,Y) \sim \text{Uniform}\{(x,y) : 0 \le y \le g(x)\}$, hence $X \sim \pi$.

- Example: $g(y) = y^3 \sin(y^4) \cos(y^5)\, \mathbf{1}_{0<y<1}$.
  - Then $L = 0$, $R = 1$, $K = 1$.
  - So, sample $X, Y \sim \text{Uniform}[0,1]$, then keep X iff $Y \le g(X)$.
  - If $h(y) = y^2$, could compute e.g. $\mathbf{E}_\pi(h)$ as the mean of the squares of the accepted samples. (file "Raux")

- Can iid / importance / rejection / auxiliary sampling solve all problems? No!
  - Many challenging cases arise, e.g. from Bayesian statistics (later).
  - Some are high-dimensional, and the above algorithms fail.
  - Alternative algorithm: MCMC!

MARKOV CHAIN MONTE CARLO (MCMC):

- Suppose have complicated, high-dimensional density $\pi = c\,g$.
- Want samples $X_1, X_2, \ldots \sim \pi$. (Then can do Monte Carlo.)
- Define a Markov chain (dependent random process) $X_0, X_1, X_2, \ldots$ in such a way that for large enough n, $X_n \approx \pi$.
- METROPOLIS ALGORITHM (1953):
  - Choose some initial value X_0 (perhaps random).
  - Then, given X_{n-1}, choose a proposal move $Y_n \sim MVN(X_{n-1}, \sigma^2 I)$ (say).
  - Let $A_n = \pi(Y_n) / \pi(X_{n-1}) = g(Y_n) / g(X_{n-1})$, and $U_n \sim \text{Uniform}[0,1]$.
  - Then, if $U_n < A_n$, set $X_n = Y_n$ ("accept"), otherwise set $X_n = X_{n-1}$ ("reject").
  - Repeat, for $n = 1, 2, 3, \ldots, M$.
  - (Note: only need to compute $\pi(Y_n) / \pi(X_{n-1})$, so multiplicative constants cancel.)
  - Try it: "www.probability.ca/rwm.html" Java applet.

- Fact: Then, for large n, have $X_n \approx \pi$. (Markov chain theory: later.)
- Then can estimate $\mathbf{E}_\pi(h) \equiv \int h(x)\,\pi(x)\,dx$ by:

$$\mathbf{E}_\pi(h) \;\approx\; \frac{1}{M-B} \sum_{i=B+1}^{M} h(X_i)\,,$$

  where B ("burn-in") chosen large enough so $X_B \approx \pi$, and M chosen large enough to get good Monte Carlo estimates.

- Note: This is called "random walk Metropolis" (RWM). Why? Because the proposals (if we always accepted them) would form a random walk.
- How large B? Difficult to say! Some theory (later) … usually just use trial-and-error / statistical analysis of output, and hope for the best …
- What initial value X_0?
  - Virtually any one will do, but "central" ones best.
  - Can also use an "overdispersed starting distribution": choose X_0 randomly from some distribution that "covers" the "important" parts of the state space. Good for checking consistency …
- EXAMPLE: $g(y) = y^3 \sin(y^4) \cos(y^5)\, \mathbf{1}_{0<y<1}$.
  - Want to compute (again!) $\mathbf{E}_\pi(h)$ where $h(y) = y^2$.
  - Use Metropolis algorithm with proposal $Y \sim N(X, 1)$. [file "Rmet"]
  - Works pretty well, but lots of variability!
  - Plot: appears to have "good mixing" …
  - acf: has some serial autocorrelation. Important! (Soon.)
  - What if we change σ? How does that affect estimate? plot? acf?
- EXAMPLE: $\pi(x_1, x_2) \;=\; C\,|\cos(\sqrt{x_1\,x_2}\,)|\; I(0 \le x_1 \le 5,\; 0 \le x_2 \le 4)$.
  - Want to compute $\mathbf{E}_\pi(h)$, where $h(x_1, x_2) = e^{x_1} + (x_2)^2$.
  - Metropolis algorithm (file "Rmet2") … works, but large uncertainty.
  - Gets between about 34 and 44 … (Mathematica gets 38.7044)
  - Individual plots appear to have "good mixing" …
  - Joint plot shows fewer samples where $x_1 x_2 \approx (\pi/2)^2 \doteq 2.5$ …
- OPTIMAL SCALING:
  - Can change proposal distribution to $Y_n \sim MVN(X_{n-1},\, \sigma^2 I)$ for any choice of $\sigma > 0$. Which is best?
  - If σ too small, then usually accept, but chain won't move much.
  - If σ too large, then will usually reject proposals, so chain still won't move much.

- Optimal: need σ "just right" to avoid both extremes. ("Goldilocks Principle")
- Can experiment ... ("rwm.html" applet, files "Rmet", "Rmet2") ...
- Some theory ... limited ... active area of research ...
- General principle: the acceptance rate should be far from 0 and far from 1.
- In a certain idealised high-dimensional limit, optimal acceptance rate is 0.234 (!). [Roberts et al., Ann Appl Prob 1997; Roberts and Rosenthal, Stat Sci 2001]

MCMC STANDARD ERROR:

- What about standard error, i.e. uncertainty?
  - It's usually larger than in iid case (due to correlations), and harder to quantify.
- Simplest: re-run the chain many times, with same M and B, with different initial values drawn from some overdispersed starting distribution, and compute standard error of the sequence of estimates.
  - Then can analyse the estimates obtained as iid ...
- But how to estimate standard error from a single run?
- i.e., how to estimate $v \equiv \text{Var}\left(\frac{1}{M-B}\sum_{i=B+1}^{M} h(X_i)\right)$?
  - Let $\overline{h}(x) = h(x) - \mathbf{E}_\pi(h)$, so $\mathbf{E}_\pi(\overline{h}) = 0$.
  - And, assume B large enough that $X_i \approx \pi$ for $i > B$.
  - Then, for large $M - B$,

$$v \approx \mathbf{E}_\pi\Big[\Big(\Big(\frac{1}{M-B}\sum_{i=B+1}^{M} h(X_i)\Big) - \mathbf{E}_\pi(h)\Big)^2\Big] = \mathbf{E}_\pi\Big[\Big(\frac{1}{M-B}\sum_{i=B+1}^{M} \overline{h}(X_i)\Big)^2\Big]$$

END WEEK #3

$$= \frac{1}{(M-B)^2}\Big[(M-B)\mathbf{E}_\pi(\overline{h}(X_i)^2) + 2(M-B-1)\mathbf{E}_\pi(\overline{h}(X_i)\overline{h}(X_{i+1}))$$

$$+2(M-B-2)\mathbf{E}_\pi(\overline{h}(X_i)\overline{h}(X_{i+2})) + \dots\Big]$$

$$\approx \frac{1}{M-B}\Big(\mathbf{E}_\pi(\overline{h}(X_i)^2) + 2\,\mathbf{E}_\pi(\overline{h}(X_i)\overline{h}(X_{i+1})) + 2\,\mathbf{E}_\pi(\overline{h}(X_i)\overline{h}(X_{i+2})) + \dots\Big)$$

$$= \frac{1}{M-B}\Big(\text{Var}_\pi(h) + 2\,\text{Cov}_\pi(h(X_i)h(X_{i+1})) + 2\,\text{Cov}_\pi(h(X_i)h(X_{i+2})) + \dots\Big)$$

$$= \frac{1}{M-B}\,\mathrm{Var}_\pi(h)\Big(1+2\,\mathrm{Corr}_\pi(h(X_i),h(X_{i+1}))+2\,\mathrm{Corr}_\pi(h(X_i),h(X_{i+2}))+\ldots\Big)$$

$$\equiv \frac{1}{M-B}\,\mathrm{Var}_\pi(h)(\mathrm{varfact}) \;=\; (\mathrm{iid\ variance})\,(\mathrm{varfact})\,,$$

where

$$\mathrm{varfact} \;=\; 1+2\sum_{k=1}^{\infty}\mathrm{Corr}_\pi\Big(h(X_0),h(X_k)\Big) \;\equiv\; 1+2\sum_{k=1}^{\infty}\rho_k \;=\; \sum_{k=-\infty}^{\infty}\rho_k$$

(also called "integrated auto-correlation time" or "ACT").

- Note that $\rho_0 = 1$ and $\rho_{-k} = \rho_k$, so also varfact $= 2\,(\sum_{k=0}^{\infty}\rho_k) - 1$.
- Then can estimate both iid variance, and varfact, from the sample run, as usual.
- Note: to compute varfact, don't sum over all k, just e.g. until, say, $|\rho_k| < 0.05$ or $\rho_k < 0$ or ...
- (Can use R's built-in "acf" function, or can write your own – better.)
- Then standard error $= se = \sqrt{v} = (iid\text{-}se)\,\sqrt{\mathrm{varfact}}$.

- e.g. the files Rmet and Rmet2. (Recall: true answers are about 0.766 and 38.7, respectively.)
  - Usually varfact $\gg 1$; try to get "better" chains so varfact smaller.
  - Sometimes even try to design chain to get varfact < 1 ("antithetic").

CONFIDENCE INTERVALS:

- Suppose we estimate $u \equiv \mathbf{E}_\pi(h)$ by the quantity $e = \frac{1}{M-B}\sum_{i=B+1}^{M} h(X_i)$, and obtain an estimate e and an approximate variance (as above) v.
- Then what is, say, a 95% confidence interval for u?
- Well, if have central limit theorem (CLT), then for large $M-B$, $e \approx N(u,v)$.
  - So $(e-u)\,v^{-1/2} \approx N(0,1)$.
  - So, $\mathbf{P}(-1.96 < (e-u)\,v^{-1/2} < 1.96) \approx 0.95$.
  - So, $\mathbf{P}(-1.96\,\sqrt{v} < e-u < 1.96\,\sqrt{v}\,) \approx 0.95$.
  - i.e., with prob 95%, the interval $(e-1.96\,\sqrt{v},\; e+1.96\,\sqrt{v})$ will contain u.
  - (Again, strictly speaking, should use "t" distribution, not normal distribution ... but if $M-B$ large that doesn't really matter – ignore it for now.)
- e.g. the files Rmet and Rmet2. (Recall: true answers are about 0.766 and 38.7, respectively.)
- But does a CLT even hold??

  - Does not follow from classical i.i.d. CLT. Does not always hold. But often does.
  - For example, CLT holds if chain is "geometrically ergodic" (later!) and $\mathbf{E}_\pi(|h|^{2+\delta}) < \infty$ for some $\delta > 0$.
  - (If chain also reversible then don't need δ: Roberts and Rosenthal, "Geometric ergodicity and hybrid Markov chains", ECP 1997.)

- So MCMC is more complicated than standard Monte Carlo.
  - Why should we bother?
  - Some problems too challenging for other methods! (e.g. Bayesian – later) In fact, need other MCMC algorithms too. For example . . .

METROPOLIS-HASTINGS ALGORITHM:

- (Hastings [Canadian!], Biometrika 1970; see www.probability.ca/hastings)
- Previous Metropolis algorithm works provided proposal distribution is symmetric, i.e. $q(x, y) = q(y, x)$. But what if it isn't?
- FACT: if we replace "$A_n = \pi(Y_n) / \pi(X_{n-1})$" by $A_n = \frac{\pi(Y_n)\, q(Y_n, X_{n-1})}{\pi(X_{n-1})\, q(X_{n-1}, Y_n)}$, then it's still valid (justification later); everything else remains the same.
  - i.e., still accept if $U_n < A_n$, otherwise reject.
  - (Intuition: if $q(x, y) >> q(y, x)$, then Metropolis chain would spend too much time at y and not enough at x, so need to accept fewer moves $x \to y$.)
  - Do require that $q(x, y) > 0$ iff $q(y, x) > 0$.
- EXAMPLE: again $\pi(x_1, x_2) = C\, |\cos(\sqrt{x_1 x_2}\,)|\ I(0 \le x_1 \le 5,\ 0 \le x_2 \le 4)$, and $h(x_1, x_2) = e^{x_1} + (x_2)^2$. (Recall: Mathematica gives $\mathbf{E}_\pi(h) \doteq 38.7044$.)
  - Proposal distribution: $Y_n \sim MVN(X_{n-1},\ \sigma^2\,(1 + |X_{n-1}|^2)^2\, I)$.
  - (Intuition: larger proposal variance if farther from center.)
  - So, $q(x, y) = C\,(1 + |x|^2)^{-2}\, \exp(-|y - x|^2 \,/\, 2\,\sigma^2 (1 + |x|^2)^2)$.
  - So, can run Metropolis-Hastings algorithm for this example. (file "RMH")
  - Usually get between 34 and 43, with claimed standard error ≈ 2. (Recall: Mathematica gets 38.7044.)

LANGEVIN ALGORITHM:

  - Special case of Metropolis-Hastings algorithm.
  - $Y_n \sim MVN(X_{n-1} + \frac{1}{2}\,\sigma^2\, \nabla \log \pi(X_{n-1}),\ \sigma^2 I)$.
  - Intuition: tries to move in direction where π increasing.

  - Based on discrete approximation to "Langevin diffusion".
  - Usually more efficient, but requires knowledge and computation of $\nabla \log \pi$. (Hard. Homework?)
  - For theory, see e.g. Roberts & Tweedie, Bernoulli **2(4)**, 341–363, 1996; Roberts & Rosenthal, JRSSB **60**, 255–268, 1998.

INDEPENDENCE SAMPLER:

- Propose $\{Y_n\} \sim q(\cdot)$, i.e. the $\{Y_n\}$ are i.i.d. from some fixed density q, independent of X_{n-1}. (e.g. $Y_n \sim MVN(0, I_d)$)
  - Then accept if $U_n < A_n$ where $U_n \sim \text{Uniform}[0,1]$ and $A_n = \frac{\pi(Y_n)\,q(X_{n-1})}{\pi(X_{n-1})\,q(Y_n)}$.
  - Special case of the Metropolis-Hastings algorithm, where $Y_n \sim q(X_{n-1}, \cdot)$, and $A_n = \frac{\pi(Y_n)\,q(Y_n, X_{n-1})}{\pi(X_{n-1})\,q(X_{n-1}, Y_n)}$.
  - Very special case: if $q(y) \equiv \pi(y)$, i.e. propose exactly from target density π, then $A_n \equiv 1$, i.e. make great proposals, and always accept them (iid).
- e.g. independence sampler with $\pi(x) = e^{-x}$ and $q(y) = ke^{-ky}$ for $x > 0$.
  - Then if $X_{n-1} = x$ and $Y_n = y$, then $A_n = \frac{e^{-y}\,ke^{-kx}}{e^{-x}\,ke^{-ky}} = e^{(k-1)(y-x)}$. (file "Rind")
  - $k = 1$: iid sampling (great).
  - $k = 0.01$: proposals way too large (so-so).
  - $k = 5$: proposals somewhat too small (terrible).
  - And with $k = 5$, confidence intervals often miss 1. (file "Rind2")
  - Why is large k so much worse than small k?

VARIABLE-AT-A-TIME MCMC:

- Propose to move just one coordinate at a time, leaving all the other coordinates fixed (since changing all coordinates at once may be difficult).
  - e.g. proposal Y_n has $Y_{n,i} \sim N(X_{n-1,i}, \sigma^2)$, with $Y_{n,j} = X_{n-1,j}$ for $j \neq i$.
  - (Here $Y_{n,i}$ is the i^{th} coordinate of Y_n.)
- Then accept/reject with usual Metropolis rule (symmetric case: "Metropolis-within-Gibbs", or "Componentwise Metropolis") or Metropolis-Hastings rule (general case: "Metropolis-Hastings-within-Gibbs", or "Componentwise Metropolis-Hastings").
- Need to choose which coordinate to update each time ...
  - Could choose coordinates in sequence $1, 2, \ldots, d, 1, 2, \ldots$ ("systematic-scan").
  - Or, choose coordinate $\sim \text{Uniform}\{1, 2, \ldots, d\}$ each time ("random-scan").

- Note: one systematic-scan iteration corresponds to d random-scan ones …

- EXAMPLE: again $\pi(x_1, x_2) = C\,|\cos(\sqrt{x_1\,x_2}\,)|\;I(0 \le x_1 \le 5,\, 0 \le x_2 \le 4)$, and $h(x_1, x_2) = e^{x_1} + (x_2)^2$. (Recall: Mathematica gives $\mathbf{E}_\pi(h) \doteq 38.7044$.)
  - Works with systematic-scan (file "Rmwg") or random-scan (file "Rmwg2").

- So, lots of MCMC algorithms to choose from.
  - Why do we need them all?
  - To compute with complicated models! For example …

BAYESIAN STATISTICS:

- Have unknown parameter(s) θ, and a statistical model (likelihood function) for how the distribution of the data Y depends on θ: $\mathcal{L}(Y \,|\, \theta)$.

- Have a <u>prior</u> distribution, representing our "initial" (subjective?) probabilities for θ: $\mathcal{L}(\theta)$.

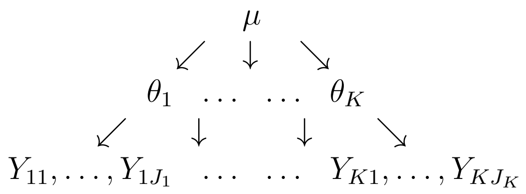
- Combining these gives a full joint distribution for θ and Y, i.e. $\mathcal{L}(\theta, Y)$.

- Then <u>posterior</u> distribution of θ, $\pi(\theta)$, is then the <u>conditional</u> distribution of θ, <u>conditioned</u> on the observed data y, i.e. $\pi(\theta) = \mathcal{L}(\theta \,|\, Y = y)$.
  - In terms of densities, if have prior density $f_\theta(\theta)$, and likelihood $f_{Y|\theta}(y, \theta)$, then joint density is $f_{\theta,Y}(\theta, y) = f_\theta(\theta)\; f_{Y|\theta}(y, \theta)$, and posterior density is

$$\pi(\theta) \;=\; \frac{f_{\theta,Y}(\theta, y)}{f_Y(y)} \;=\; C\, f_{\theta,Y}(\theta, y) \;=\; C\, f_\theta(\theta)\; f_{Y|\theta}(y, \theta)\,.$$

END WEEK #4

- Bayesian Statistics Example: VARIANCE COMPONENTS MODEL (a.k.a. "random effects model"):


μ
θ_1 … … θ_K
$Y_{11}, \ldots, Y_{1J_1}$ … … $Y_{K1}, \ldots, Y_{KJ_K}$

$\theta_i \sim N(\mu, V)$

$Y_{ij} \sim N(\theta_i, W)$ [observed]

  - Suppose some population has overall mean μ (unknown).
  - Population consists of K groups.
  - Observe $Y_{i1}, \ldots, Y_{iJ_i}$ from group i, for $1 \le i \le K$.
  - Assume $Y_{ij} \sim N(\theta_i, W)$ (cond. ind.), where θ_i and W unknown.

- Assume the different θ_i are "linked" by $\theta_i \sim N(\mu, V)$ (cond. ind.), with μ and V also unknown.
- Want to estimate some or all of $V, W, \mu, \theta_1, \ldots, \theta_K$.
- Bayesian approach: use prior distributions, e.g. ("conjugate"):

$$V \sim IG(a_1, b_1); \qquad W \sim IG(a_2, b_2); \qquad \mu \sim N(a_3, b_3)\,,$$

  where a_i, b_i known constants, and $IG(a,b)$ is the "inverse gamma" distribution, with density $\frac{b^a}{\Gamma(a)}\, e^{-b/x}\, x^{-a-1}$ for $x > 0$.

- Combining the above dependencies, we see that the joint density is (for $V, W > 0$):

$$\begin{aligned}
&f(V, W, \mu, \theta_1, \ldots, \theta_K, Y_{11}, Y_{12}, \ldots, Y_{KJ_K}) \\
&= \left(\frac{b_1^{a_1}}{\Gamma(a_1)} e^{-b_1/V} V^{-a_1-1}\right) \left(\frac{b_2^{a_2}}{\Gamma(a_2)} e^{-b_2/W} W^{-a_2-1}\right) \left(\frac{1}{\sqrt{2\pi b_3}} e^{-(\mu-a_3)^2/2b_3}\right) \times \\
&\qquad \times \left(\prod_{i=1}^{K} \frac{1}{\sqrt{2\pi V}} e^{-(\theta_i-\mu)^2/2V}\right) \left(\prod_{i=1}^{K}\prod_{j=1}^{J_i} \frac{1}{\sqrt{2\pi W}} e^{-(Y_{ij}-\theta_i)^2/2W}\right) \\
&= C_2\, e^{-b_1/V} V^{-a_1-1} e^{-b_2/W} W^{-a_2-1} e^{-(\mu-a_3)^2/2b_3} V^{-K/2} W^{-\frac{1}{2}\sum_{i=1}^{K} J_i} \times \\
&\qquad \times \ \exp\left[-\sum_{i=1}^{K}(\theta_i-\mu)^2/2V\right] \ \exp\left[-\sum_{i=1}^{K}\sum_{j=1}^{J_i}(Y_{ij}-\theta_i)^2/2W\right].
\end{aligned}$$

- Then

$$\begin{aligned}
&\pi(V, W, \mu, \theta_1, \ldots, \theta_K) \\
&= f(V, W, \mu, \theta_1, \ldots, \theta_K, Y_{11}, Y_{12}, \ldots, Y_{KJ_K}) \;/\; f_Y(Y_{11}, Y_{12}, \ldots, Y_{KJ_K}) \\
&\propto f(V, W, \mu, \theta_1, \ldots, \theta_K, Y_{11}, Y_{12}, \ldots, Y_{KJ_K}) \\
&= C_3\, e^{-b_1/V} V^{-a_1-1} e^{-b_2/W} W^{-a_2-1} e^{-(\mu-a_3)^2/2b_3} V^{-K/2} W^{-\frac{1}{2}\sum_{i=1}^{K} J_i} \times \\
&\qquad \times \ \exp\left[-\sum_{i=1}^{K}(\theta_i-\mu)^2/2V\right] \ \exp\left[-\sum_{i=1}^{K}\sum_{j=1}^{J_i}(Y_{ij}-\theta_i)^2/2W\right].
\end{aligned}$$

- NOTE: Many applications of variance components model, e.g.:
  - Predicting success at law school (D. Rubin, JASA 1980), $K = 82$ schools.
  - Melanoma (skin cancer) recurrence (),
    with $K = 19$ different patient categories.
  - Comparing baseball home-run hitters (J. Albert, The American Statistician 1992), $K = 12$ players.
  - Analysing fabric dyes (Davies 1967; Box/Tiao 1973; Gelfand/Smith JASA 1990), $K = 6$ batches of dyestuff. (data in file "Rdye")

- Here, the dimension is $d = K + 3$, e.g. $K = 19$, $d = 22$. High!
- How to compute/estimate, say, $\mathbf{E}_\pi(W/V)$, or the effect of changing b_1?
  - Numerical integration? No, too high-dimensional!
  - Importance sampling? Perhaps, but what "f"? Too inefficient!
  - Rejection sampling? What "f"? What "K"? Virtually no samples!
  - Perhaps MCMC can work!
  - But need clever, useful MCMC algorithms!
  - Perhaps Metropolis, or ...
- ASIDE: For big complicated π, often better to work with logarithms, e.g. accept iff $\log(U_n) < \log(A_n) = \log(\pi(Y_n)) - \log(\pi(X_{n-1}))$.
  - Then only need to compute $\log(\pi(x))$, which might work better.
  - So, better to program on log scale: $\log \pi(V, W, \mu, \theta_1, \ldots, \theta_K) = \ldots$.
  - Can avoid "overflow" problems.
  - Also sometimes simpler, e.g. if $\pi(x) = \exp\left(\sum_{i<j} |x_j - x_i|\right)$, then $\log(\pi(x)) = \sum_{i<j} |x_j - x_i|$. (Best to type in the log formula directly.)

GIBBS SAMPLER:

- (Special case of Metropolis-Hastings-within-Gibbs.)
- Proposal distribution for i^{th} coordinate is equal to the conditional distribution of that coordinate (according to π), conditional on the current values of all the other coordinates.
  - Then, always accept. (Reason later.)
  - Can use either systematic or random scan, just like above.
- EXAMPLE: Variance Components Model:
  - Update of μ (say) should be from conditional density of μ, conditional on current values of all the other coordinates: $\mathcal{L}(\mu \,|\, V, W, \theta_1, \ldots, \theta_K, Y_{11}, \ldots, Y_{J_K K})$.
  - This conditional density is proportional to the full joint density, but with all variables besides μ treated as constant.
  - Recall: full joint density is:

$$= C_3 e^{-b_1/V} V^{-a_1-1} e^{-b_2/W} W^{-a_2-1} e^{-(\mu-a_3)^2/2b_3} V^{-K/2} W^{-\frac{1}{2}\sum_{i=1}^K J_i} \times$$

$$\times \exp\left[-\sum_{i=1}^K (\theta_i - \mu)^2/2V\right] \exp\left[-\sum_{i=1}^K \sum_{j=1}^{J_i} (Y_{ij} - \theta_i)^2/2W\right].$$

  - So, combining "constants", the conditional density of μ is

$$C_4\, e^{-(\mu-a_3)^2/2b_3} \exp\left[-\sum_{i=1}^K (\theta_i - \mu)^2/2V\right].$$

  - This equals (verify this! HW?)

$$C_5 \exp\Big(-\mu^2(\frac{1}{2b_3}+\frac{K}{2V})+\mu(\frac{a_3}{b_3}+\frac{1}{V}\sum_{i=1}^{K}\theta_i)\Big)\,.$$

  - Side calculation: if $\mu \sim N(m,v)$, then density $\propto e^{-(\mu-m)^2/2v} \propto e^{-\mu^2(1/2v)+\mu(m/v)}$.
  - Hence, here $\mu \sim N(m,v)$, where $1/2v = \frac{1}{2b_3}+\frac{K}{2V}$ and $m/v = \frac{a_3}{b_3}+\frac{1}{V}\sum_{i=1}^{K}\theta_i$.
  - Solve: $v = b_3V/(V+Kb_3)$, and $m = (a_3V + b_3\sum_{i=1}^{K}\theta_i)\,/\,(V+Kb_3)$.
  - So, in Gibbs Sampler, each time μ is updated, we sample it from $N(m,v)$ for this m and v (and always accept).

- Similarly (HW?), conditional distribution for V is:

$$C_6 e^{-b_1/V} V^{-a_1-1} V^{-K/2} \exp\left[-\sum_{i=1}^{K}(\theta_i-\mu)^2/2V\right], \qquad V>0\,.$$

  - Recall that "$IG(r,s)$" has density $\frac{s^r}{\Gamma(r)}\, e^{-s/x}\, x^{-r-1}$ for $x>0$.
  - So, conditional distribution for V equals $IG(a_1+K/2,\ b_1+\frac{1}{2}\sum_{i=1}^{K}(\theta_i-\mu)^2)$.

- Can similar compute conditional distributions for W and θ_i (HW?).

- The systematic-scan Gibbs sampler then proceeds (HW?) by:
  - Update V from its conditional distribution $IG(\ldots,\ldots)$.
  - Update W from its conditional distribution $IG(\ldots,\ldots)$.
  - Update μ from its conditional distribution $N(\ldots,\ldots)$.
  - Update θ_i from its conditional distribution $N(\ldots,\ldots)$, for $i=1,2,\ldots,K$.
  - Repeat all of the above M times.

- Or, the random-scan Gibbs sampler proceeds by choosing one of $V, W, \mu, \theta_1, \ldots, \theta_K$ uniformly at random, and then updating that coordinate from its corresponding conditional distribution.
  - Then repeat this step M times [or $M(K+3)$ times?].
  - How well does it work? HW?

MCMC CONVERGENCE RATES THEORY:

- $\{X_n\}$: Markov chain on $\mathcal{X}$, with stationary distribution $\Pi(\cdot)$.
- Let $P^n(x,S) = \mathbf{P}[X_n \in S \,|\, X_0 = x]$.
  - Hope that for large n, $P^n(x,S) \approx \Pi(S)$.
- Let $D(x,n) = \|P^n(x,\cdot)-\Pi(\cdot)\| \equiv \sup_{S\subseteq\mathcal{X}} |P^n(x,S)-\Pi(S)|$.

- DEFN: chain is ergodic if $\lim_{n\to\infty} D(x,n) = 0$, for Π-a.e. $x \in \mathcal{X}$.

- DEFN: chain is geometrically ergodic if there is $\rho < 1$, and $M : \mathcal{X} \to [0,\infty]$ which is Π-a.e. finite, such that $D(x,n) \le M(x)\,\rho^n$ for all $x \in \mathcal{X}$ and $n \in \mathbf{N}$.

- DEFN: a quantitative bound on convergence is an actual number n^* such that $D(x,n^*) < 0.01$ (say). [Then sometimes say chain "converges in n^* iterations".]

- Quantitative bounds often difficult (though I've worked on them a lot, see e.g. Rosenthal, "Quantitative convergence rates of Markov chains: A simple account", Elec Comm Prob 2002 and the references therein), but "geometric ergodicity" is often easier to verify.

- Fact (mentioned earlier): CLT holds for $\frac{1}{n}\sum_{i=1}^{n} h(X_i)$ if chain is geometrically ergodic and $\mathbf{E}_\pi(|h|^{2+\delta}) < \infty$ for some $\delta > 0$.
  - (If chain also reversible then don't need δ: Roberts and Rosenthal, "Geometric ergodicity and hybrid Markov chains", ECP 1997.)
  - If CLT holds, then (as before) have 95% confidence interval $(e - 1.96\sqrt{v},\ e + 1.96\sqrt{v})$.

- First Question: What do we know about ergodicity?
  - Theorem (later): if chain is irreducible and aperiodic and $\Pi(\cdot)$ is stationary, then chain is ergodic.

- But what about convergence rates?

- Special Case: INDEPENDENCE SAMPLER.
  - By Thm, independence sampler is ergodic provided $q(x) > 0$ whenever $\pi(x) > 0$.
  - But is that sufficient?
  - No, e.g. previous "Rind" example with $k = 5$: ergodic (of course), but performs terribly.
  - FACT: independence sampler is geometrically ergodic IF AND ONLY IF there is $\delta > 0$ such that $q(x) \ge \delta\pi(x)$ for π-a.e. $x \in \mathcal{X}$, in which case $D(x,n) \le (1-\delta)^n$ for π-a.e. $x \in \mathcal{X}$.

- EXAMPLE: Independence sampler with $\pi(x) = e^{-x}$ and $q(x) = ke^{-kx}$ for $x > 0$.
  - If $0 < k \le 1$, then setting $\delta = k$, we have that $q(x) = ke^{-kx} \ge ke^{-x} = k\pi(x) = \delta\pi(x)$ for all $x > 0$, so it's geometrically ergodic, and furthermore $D(x,n) \le (1-k)^n$.
  - e.g. if $k = 0.01$, then $D(x, 459) \le (0.99)^{459} \doteq 0.0099 < 0.01$ for all $x > 0$, i.e. "converges after 459 iterations".

  - But if $k > 1$, then cannot find any $\delta > 0$ such that $q(x) \geq \delta\pi(x)$ for all x, so it is not geometrically ergodic.
  - If $k > 2$, then no CLT (Roberts, J. Appl. Prob. **36**, 1210–1217, 1999).
  - So, if $k = 5$ (as in "Rind"), then not geometrically ergodic, and CLT does not hold. Indeed, confidence intervals often miss 1. (file "Rind2")
  - Fact: if $k = 5$, then $D(0, n) > 0.01$ for all $n \leq 4{,}000{,}000$, while $D(0, n) < 0.01$ for all $n \geq 14{,}000{,}000$, i.e. "convergence" takes between 4 million and 14 million iterations. Slow! [Roberts and Rosenthal, "Quantitative Non-Geometric Convergence Bounds for Independence Samplers", MCAP 2011.]

- What about other chains (besides independence sampler)?

- FACT: if state space is finite, and chain is irreducible and aperiodic, then always geometrically ergodic. (See e.g. J.S. Rosenthal, SIAM Review 37:387-405, 1995.)

- What about for the "random-walk Metropolis algorithm" (RWM), i.e. where $\{Y_n - X_{n-1}\} \sim q$ (i.i.d.) for some fixed symmetric density q?
  - e.g. $Y_n \sim N(X_{n-1}, \sigma^2 I)$, or $Y_n \sim \text{Uniform}[X_{n-1} - \delta,\, X_{n-1} + \delta]$.

- FACT: RWM is geometrically ergodic essentially if and only if π has exponentially light tails, i.e. there are $a, b, c > 0$ such that $\pi(x) \leq a e^{-b|x|}$ whenever $|x| > c$. (Requires a few technical conditions: π and q continuous and positive; q has finite first moment; and π non-increasing in the tails, with (in higher dims) bounded Gaussian curvature.) [Mengersen and Tweedie, Ann Stat 1996; Roberts and Tweedie, Biometrika 1996]

- EXAMPLES: RWM on $\mathbf{R}$ with usual proposals: $Y_n \sim N(X_{n-1},\, \sigma^2)$.
  - CASE #1: $\Pi = N(5, 4^2)$, and functional $h(y) = y^2$, so $\mathbf{E}_\pi(h) = 5^2 + 4^2 = 41$. (file "Rnorm" … $\sigma = 1$ v. $\sigma = 4$ v. $\sigma = 16$)
  - Does CLT hold? Yes! (geometrically ergodic, and $\mathbf{E}_\pi(|h|^p) < \infty$ for all p.)
  - Indeed, confidence intervals "usually" contain 41. (file "Rnorm2")
  - CASE #2: $\pi(y) = c\,\frac{1}{(1+y^4)}$, and functional $h(y) = y^2$ (file "Rheavy"), so

$$\mathbf{E}_\pi(h) \;=\; \frac{\int_{-\infty}^{\infty} y^2\,\frac{1}{(1+y^4)}\,dy}{\int_{-\infty}^{\infty} \frac{1}{(1+y^4)}\,dy} \;=\; \frac{\pi/\sqrt{2}}{\pi/\sqrt{2}} \;=\; 1\,.$$

  - Not exponentially light tails, so no CLT; estimates less stable, confidence intervals often miss 1.
  - CASE #3: $\pi(y) = \frac{1}{\pi(1+y^2)}$ (Cauchy), and functional $h(y) = \mathbf{1}_{-10<y<10}$, so $\mathbf{E}_\pi(h) = \Pi(|X| < 10) = 2\arctan(10)/\pi = 0.93655$. [$\Pi(0 < X < x) = \arctan(x)/\pi$] (file "Rcauchy")

  - Not geometrically ergodic.
  - Confidence intervals often miss 0.93655.
  - CASE #4: $\pi(y) = \frac{1}{\pi(1+y^2)}$ (Cauchy), and functional $h(y) = \min(y^2, 100)$. [Numerical integration: $\mathbf{E}_\pi(h) \doteq 11.77$] (file "Rcauchy2")
  - Again, not geometrically ergodic, and 95% CI often miss 11.77, though iid MC does better.

- NOTE: Even when CLT holds, it can be rather unstable, e.g. it requires that chain has converged to Π, so it might underestimate v.
  - Estimate of v is very important! And "varfact" is not always reliable!
  - Repeated runs?
  - Another approach is "batch means", whereby chain is broken into m large "batches", which are assumed to be approximately i.i.d.

END WEEK #5

JUSTIFICATION: WHY DOES METROPOLIS ALG WORK?:

- (Uses Markov chain theory ... e.g. STA447/2006 ... already know?)
- Basic fact: if a Markov chain is "irreducible" and "aperiodic", with "stationarity distribution" π, then $\mathcal{L}(X_n) \to \pi$ as $n \to \infty$. More precisely:
- THEOREM: If Markov chain is irreducible, with stationarity probability density π, then for π-a.e. initial value $X_0 = x$,
(a) if $\mathbf{E}_\pi(|h|) < \infty$, then $\lim_{n\to\infty} \frac{1}{n} \sum_{i=1}^n h(X_i) = \mathbf{E}_\pi(h) \equiv \int h(x)\,\pi(x)\,dx$; and
(b) if chain aperiodic, then also $\lim_{n\to\infty} \mathbf{P}(X_n \in S) = \int_S \pi(x)\,dx$ for all $S \subseteq \mathcal{X}$.
  - Let's figure out what this all means ...
  - Notation: $P(i,j) = \mathbf{P}(X_{n+1} = j \,|\, X_n = i)$ (discrete case), or $P(x, A) = \mathbf{P}(X_{n+1} \in A \,|\, X_n = x)$ (general case). Also $\Pi(A) = \int_A \pi(x)\,dx$.
- Well, irreducible means that you have positive probability of eventually getting from anywhere to anywhere else.
  - Discrete case: for all $i, j \in \mathcal{X}$ (the state space), there is $n \in \mathbf{N}$ such that $P(X_n = j \,|\, X_0 = i) > 0$.
  - Actually, we only need to require this for states j such that $\pi(j) > 0$.
  - General case: for all $x \in \mathcal{X}$, and for all $A \subseteq \mathcal{X}$ with $\Pi(A) > 0$, there is $n \in \mathbf{N}$ such that $P(X_n \in A \,|\, X_0 = x) > 0$. ("$\pi$-irreducible")
  - (Since usually $P(X_n = y \,|\, X_0 = x) = 0$ for all y.)
  - Irreducibility is usually satisfied for MCMC.

- And, aperiodic means there are no forced cycles, i.e. there do not exist disjoint non-empty subsets $\mathcal{X}_1, \mathcal{X}_2, \ldots, \mathcal{X}_d$ for $d \geq 2$, such that $P(x, \mathcal{X}_{i+1}) = 1$ for all $x \in \mathcal{X}_i$ ($1 \leq i \leq d-1$), and $P(x, \mathcal{X}_1) = 1$ for all $x \in \mathcal{X}_d$. [Diagram.]
  - This is true for virtually any Metropolis algorithm, e.g. it's true if $P(x, \{x\}) > 0$ for any one state $x \in \mathcal{X}$, e.g. if positive prob of rejection.
  - Also true if $P(x, \cdot)$ has positive density throughout S, for all $x \in S$, for some $S \subseteq \mathcal{X}$ with $\Pi(S) > 0$. (e.g. Normal proposals)
  - Not quite guaranteed, e.g. $\mathcal{X} = \{0, 1, 2, 3\}$, and π uniform on $\mathcal{X}$, and $Y_n = X_{n-1} \pm 1 \pmod 4$. [Diagram.] But almost always holds.
- What about Π being a stationary distribution?
- Begin with DISCRETE CASE (e.g. rwm.html).
- Assume for simplicity that $\pi(x) > 0$ for all $x \in \mathcal{X}$.
  - Let $q(x, y) = \mathbf{P}(Y_n = y \,|\, X_{n-1} = x)$ be proposal distribution, e.g. $q(x, x+1) = q(x, x-1) = 1/2$. Assume symmetric, i.e. $q(x, y) = q(y, x)$ for all $x, y \in \mathcal{X}$.
  - Let $\alpha(x, y)$ be probability of accepting a proposed move from x to y, i.e.

$$\alpha(x,y) = \mathbf{P}(U_n < A_n \,|\, X_{n-1} = x,\, Y_n = y) \;=\; \mathbf{P}(U_n < \frac{\pi(y)}{\pi(x)}) \;=\; \min[1,\, \frac{\pi(y)}{\pi(x)}]\,.$$

  - State space is $\mathcal{X}$, e.g. $\mathcal{X} \equiv \{1, 2, 3, 4, 5, 6\}$.
- Then, for $i, j \in \mathcal{X}$ with $i \neq j$,

$$P(i,j) \;=\; q(i,j)\; \alpha(i,j) \;=\; q(i,j)\; \min(1,\, \frac{\pi(j)}{\pi(i)})\,.$$

- Follows that chain is "(time) reversible": for all $i, j \in \mathcal{X}$, by symmetry,

$$\pi(i)\, P(i,j) \;=\; q(i,j)\, \min(\pi(i),\, \pi(j)) \;=\; q(j,i)\, \min(\pi(i),\, \pi(j)) \;=\; \pi(j)\, P(j,i)\,.$$

  - (Case $i \neq j$ is proved above, and case $i = j$ is trivial.)
  - (Intuition: if $X_0 \sim \pi$, i.e. $\mathbf{P}(X_0 = i) = \pi(i)$ for all $i \in \mathcal{X}$, then $\mathbf{P}(X_0 = i,\; X_1 = j) = \pi(i)\, P(i,j) = \mathbf{P}(X_0 = j,\; X_1 = i)\; \ldots$)
- We then compute that if $X_0 \sim \pi$, i.e. that $\mathbf{P}(X_0 = i) = \pi(i)$ for all $i \in \mathcal{X}$, then:

$$\mathbf{P}(X_1 = j) \;=\; \sum_{i \in \mathcal{X}} \mathbf{P}(X_0 = i)\, P(i,j) \;=\; \sum_{i \in \mathcal{X}} \pi(i)\, P(i,j) \;=\; \sum_{i \in \mathcal{X}} \pi(j)\, P(j,i)$$

$$=\; \pi(j) \sum_{i \in \mathcal{X}} P(j,i) \;=\; \pi(j)\,,$$

i.e. $X_1 \sim \pi$ too!

  - So, the Markov chain "preserves" π, i.e. π is a stationary distribution.
  - This is true for any Metropolis algorithm!

- It then follows from the Theorem (i.e., "Basic Fact") that as $n \to \infty$, $\mathcal{L}(X_n) \to \pi$, i.e. $\lim_{n\to\infty} P(X_n = i) = \pi(i)$ for all $i \in \mathcal{X}$. (applet "rwm.html")
  - Also follows that if $\mathbf{E}_\pi(|h|) < \infty$, then $\lim\limits_{n\to\infty} \frac{1}{n} \sum_{i=1}^{n} h(X_i) = \mathbf{E}_\pi(h) \equiv \int h(x)\,\pi(x)\,dx$. ("LLN")

JUSTIFICATION: GENERAL CONTINUOUS CASE:

- Some notation:
  - Let $\mathcal{X}$ be the state space of all possible values. (Usually $\mathcal{X} \subseteq \mathbf{R}^d$, e.g. for Variance Components Model, $\mathcal{X} = (0,\infty) \times (0,\infty) \times \mathbf{R} \times \mathbf{R}^K \subseteq \mathbf{R}^{K+3}$.)
  - Let $q(x,y)$ be the proposal density for y given x. (e.g. $q(x,y) = (2\pi\sigma)^{-d/2} \exp\big(-\sum_{i=1}^{d}(y_i - x_i)^2/2\sigma^2\big)$.) Symmetric: $q(x,y) = q(y,x)$.
  - Let $\alpha(x,y) = \min[1,\ \frac{\pi(y)}{\pi(x)}]$ be probability of accepting a proposed move from x to y.
  - Let $P(x,S) = \mathbf{P}(X_1 \in S \,|\, X_0 = x)$ be the transition probabilities.
  - (Don't use $P(x,y)$ since that is usually 0.)

- Then if $x \notin S$, then

$$P(x,S) \;=\; \mathbf{P}(Y_1 \in S,\ U_1 < A_1 \,|\, X_0 = x) \;=\; \int_S q(x,y)\ \min[1,\ \pi(y)/\pi(x)]\,dy\,.$$

  - Shorthand: for $x \neq y$, $P(x,dy) = q(x,y)\ \min[1,\ \pi(y)/\pi(x)]\,dy$.
  - Then for $x \neq y$, $P(x,dy)\,\pi(x)\,dx \;=\; q(x,y)\ \min[1,\ \pi(y)/\pi(x)]\,dy\,\pi(x)\,dx \;=\; q(x,y)\ \min[\pi(x),\ \pi(y)]\,dy\,dx \;=\; P(y,dx)\,\pi(y)\,dy$. (symmetric)
  - Follows that $P(x,dy)\,\pi(x)\,dx \;=\; P(y,dx)\,\pi(y)\,dy$ for all $x,y \in \mathcal{X}$. ("reversible")
  - Shorthand: $P(x,dy)\,\Pi(dx) = P(y,dx)\,\Pi(dy)$.

- How does "reversible" help? Just like for discrete chains!

- Indeed, suppose $X_0 \sim \Pi$, i.e. we "start in stationarity". Then

$$\mathbf{P}(X_1 \in S) \;=\; \int_{x\in\mathcal{X}} \mathbf{P}(X_1 \in S \,|\, X_0 = x)\,\pi(x)\,dx \;=\; \int_{x\in\mathcal{X}} \int_{y\in S} P(x,dy)\,\pi(x)\,dx$$

$$=\; \int_{x\in\mathcal{X}} \int_{y\in S} P(y,dx)\,\pi(y)\,dy \;=\; \int_{y\in S} \pi(y)\,dy \;\equiv\; \Pi(S)\,,$$

so also $X_1 \sim \Pi$. So, chain "preserves" Π, i.e. Π is stationary distribution.

- So, again, the Theorem applies.

- Note: key facts about $q(x,y)$ are symmetry, and irreducibility.

JUSTIFICATION OF METROPOLIS-HASTINGS:

- Previous Metropolis algorithm works provided proposal distribution is symmetric, i.e. $q(x,y) = q(y,x)$. But what if it isn't?
- For Metropolis, key was that $q(x,y)\,\alpha(x,y)\,\pi(x)$ was symmetric (to make the Markov chain be reversible).
- If instead $A_n = \frac{\pi(Y_n)\,q(Y_n,X_{n-1})}{\pi(X_{n-1})\,q(X_{n-1},Y_n)}$, i.e. acceptance prob. $\equiv \alpha(x,y) = \min\left[1,\ \frac{\pi(y)\,q(y,x)}{\pi(x)\,q(x,y)}\right]$, then:

$$q(x,y)\,\alpha(x,y)\,\pi(x) \;=\; q(x,y)\ \min\left[1,\ \frac{\pi(y)\,q(y,x)}{\pi(x)\,q(x,y)}\right]\ \pi(x)$$

$$=\ \min\Big[\pi(x)\,q(x,y),\ \pi(y)\,q(y,x)\Big]\,.$$

  So, still symmetric, even if q wasn't.

  - So, for Metropolis-Hastings algorithm, replace "$A_n = \pi(Y_n)\,/\,\pi(X_{n-1})$" by $A_n = \frac{\pi(Y_n)\,q(Y_n,X_{n-1})}{\pi(X_{n-1})\,q(X_{n-1},Y_n)}$, then still reversible, and everything else remains the same: still accept if $U_n < A_n$, otherwise reject.
  - We require only that $q(x,y) > 0$ iff $q(y,x) > 0$.

- INDEPENDENCE SAMPLER (mentioned earlier):
  - Proposals $\{Y_n\}$ i.i.d. from some fixed distribution (say, $Y_n \sim MVN(0,\,I)$).
  - Another special case of Metropolis-Hastings algorithm.
  - Then $q(x,y) = q(y)$, depends only on y.
  - So, now $A_n = \frac{\pi(Y_n)\,q(X_{n-1})}{\pi(X_{n-1})\,q(Y_n)}$. (files "Rind", "Rind2" from before)

- VARIABLE-AT-A-TIME: The exact same justification works if we update the variables one-at-a-time (e.g. Metropolis-within-Gibbs, Metropolis-Hastings-within-Gibbs, etc.); each individual step is still reversible (for the same reason), so π is still stationary.

JUSTIFICATION OF GIBBS SAMPLER:

- Special case of Metropolis-Hastings-within-Gibbs.
- Proposal distribution for i^{th} coordinate is equal to the conditional distribution of that coordinate (according to π), conditional on the current values of all the other coordinates.
  - That is, $q_i(x,y) = C(x^{(-i)})\,\pi(y)$ whenever $x^{(-i)} = y^{(-i)}$, where $x^{(-i)}$ means all coordinates except the i^{th} one.
  - Here $C(x^{(-i)})$ is the appropriate normalising constant (which depends on $x^{(-i)}$). (So $C(x^{(-i)}) = C(y^{(-i)})$.)

  - Then $A_n = \frac{\pi(Y_n)\, q_i(Y_n, X_{n-1})}{\pi(X_{n-1})\, q_i(X_{n-1}, Y_n)} = \frac{\pi(Y_n)\, C(Y_n^{(-i)})\, \pi(X_{n-1})}{\pi(X_{n-1})\, C(X_{n-1}^{(-i)})\, \pi(Y_n)} = 1$.
  - So, always accept (i.e., can ignore the accept-reject step).
  - (Intuition: if start in stationary distribution, then update one coordinate from its conditional stationary distribution (and always accept), then the distribution remains the same, i.e. stationarity is preserved.)

EXAMPLES RE WHY DOES MCMC WORK:

- EXAMPLE #1: Metropolis algorithm where $\mathcal{X} = \mathbf{Z}$, $\pi(x) = 2^{-|x|}/3$, and $q(x, y) = \frac{1}{2}$ if $|x - y| = 1$, otherwise 0.
  - Reversible? Yes, it's a Metropolis algorithm!
  - π stationary? Yes, follows from reversibility!
  - Aperiodic? Yes, since $P(x, \{x\}) > 0$!
  - Irreducible? Yes: $\pi(x) > 0$ for all $x \in \mathcal{X}$, so can get from x to y in $|x - y|$ steps.
  - So, by theorem, probabilities and expectations converge to those of π – good.
- EXAMPLE #2: Same as #1, except now $\pi(x) = 2^{-|x|-1}$ for $x \neq 0$, with $\pi(0) = 0$.
  - Still reversible, π stationary, aperiodic, same as before.
  - Irreducible? No – can't go from positive to negative!
- EXAMPLE #3: Same as #2, except now $q(x, y) = \frac{1}{4}$ if $1 \leq |x - y| \leq 2$, otherwise 0.
  - Still reversible, π stationary, aperiodic, same as before.
  - Irreducible? Yes – can "jump over 0" to get from positive to negative, and back!
- EXAMPLE #4: Metropolis algorithm with $\mathcal{X} = \mathbf{R}$, and $\pi(x) = C\, e^{-x^6}$, and proposals $Y_n \sim \text{Uniform}[X_{n-1} - 1, X_{n-1} + 1]$.
  - Reversible? Yes since it's Metropolis, and $q(x, y)$ still symmetric.
  - π stationary? Yes since reversible!
  - Irreducible? Yes, since the n-step transitions $P^n(x, dy)$ have positive density whenever $|y - x| < n$.
  - Aperiodic? Yes since if periodic, then if e.g. $\mathcal{X}_1 \cap [0, 1]$ has positive measure, then possible to go from $\mathcal{X}_1$ directly to $\mathcal{X}_1$, i.e. if $x \in \mathcal{X}_1 \cap [0, 1]$, then $P(x, \mathcal{X}_1) > 0$. (Or, even simpler: since $P(x, \{x\}) > 0$ for all $x \in \mathcal{X}$.)
  - So, by theorem, probabilities and expectations converge to those of π – good.

- EXAMPLE #5: Same as #4, except now $\pi(x) = C_1\, e^{-x^6}(\mathbf{1}_{x<2} + \mathbf{1}_{x>4})$.
  - Still reversible and stationary and aperiodic, same as before.
  - But no longer irreducible: cannot jump from $[4, \infty)$ to $(-\infty, 2]$ or back.
  - So, does <u>not</u> converge.
- EXAMPLE #6: Same as #5, except now proposals are $Y_n \sim \text{Uniform}[X_{n-1} - 5, X_{n-1} + 5]$.
  - Still reversible and stationary and aperiodic, same as before.
  - And now irreducible, too: now <u>can</u> jump from $[4, \infty)$ to $(-\infty, 2]$ or back.
- EXAMPLE #7: Same as #6, except now $Y_n \sim \text{Uniform}[X_{n-1} - 5, X_{n-1} + 10]$.
  - Makes no sense – proposals not symmetric, so not a Metropolis algorithm! (Not even symmetrically zero, for a Metropolis-Hastings algorithm, e.g. have positive density 3 → 9 but not 9 → 3.)
- ASIDE: Why does Theorem say "π-a.e." $X_0 = x$?
- Example: $\mathcal{X} = \{1, 2, 3, \ldots\}$, and $P(1, \{1\}) = 1$, and for $x \geq 2$, $P(x, \{1\}) = 1/x^2$ and $P(x, \{x + 1\}) = 1 - (1/x^2)$.
  - Stationary distribution: $\Pi(\cdot) = \delta_1(\cdot)$, i.e. $\Pi(S) = \mathbf{1}_{1 \in S}$ for $S \subseteq \mathcal{X}$.
  - Irreducible, since if $\Pi(S) > 0$ then $1 \in S$ so $P(x, S) \geq P(x, \{1\}) > 0$ for all $x \in \mathcal{X}$.
  - Aperiodic since $P(1, \{1\}) > 0$.
  - So, by Theorem, for π-a.e. X_0, have $\lim_{n\to\infty} \mathbf{P}(X_n \in S) = \Pi(S)$, i.e. $\lim_{n\to\infty} \mathbf{P}(X_n = 1) = 1$.
  - But if $X_0 = x \geq 2$, then $\mathbf{P}[X_n = x + n \text{ for all } n] = \prod_{j=x}^{\infty}(1 - (1/j^2)) > 0$ (since $\sum_{j=x}^{\infty}(1/j^2) < \infty$), so $\lim_{n\to\infty} \mathbf{P}(X_n = 1) \neq 1$.
  - Convergence holds if $X_0 = 1$, which is π-a.e. since $\Pi(1) = 1$, but not from $X_0 = x \geq 2$.
- So, convergence subtle. But <u>usually</u> holds from <u>any</u> $x \in \mathcal{X}$. ("Harris recurrent", see e.g. http://probability.ca/jeff/ftpdir/harris.pdf)

END WEEK #6

MONTE CARLO IN FINANCE [brief]:

- X_t = stock price at time t
- Assume that $X_0 = a > 0$, and $dX_t = bX_t dt + \sigma X_t dB_t$, where $\{B_t\}$ is Brownian motion.

- i.e., for small $h > 0$,

  $$(X_{t+h} - X_t \mid X_t) \;\approx\; bX_t(t+h-t) + \sigma X_t(B_{t+h} - B_t) \;\sim\; bX_t(t+h-t) + \sigma X_t \, N(0,h)\,,$$

  so

  $$(X_{t+h} \mid X_t) \;\sim\; N\left(X_t + bX_t h,\; \sigma^2 (X_t)^2 h\right)\,. \qquad (*)$$

- A "European call option" is the option to purchase one share of the stock at a fixed time $T > 0$ for a fixed price $q > 0$.

- Question: what is a fair <u>price</u> for this option?
  - At time T, its value is $\max(0,\ X_T - q)$.
  - So, at time 0, its value is $e^{-rT}\ \max(0,\ X_T - q)$, where r is the "risk-free interest rate".
  - But at time 0, X_T is unknown! So, what is fair price??

- FACT: the fair price is equal to $\mathbf{E}(e^{-rT} \max(0,\ X_T - q))$, but only after replacing b by r.
  - (Proof: transform to risk-neutral martingale measure . . .)
  - Intuition: if b very large, might as well just buy stock itself.

- If σ and r constant, then there's a <u>formula</u> ("Black-Scholes eqn") for this price, in terms of Φ = cdf of $N(0,1)$:

  $$a\,\Phi\left(\frac{1}{\sigma\sqrt{T}}\Big(\log(a/q) + T(r + \frac{1}{2}\sigma^2)\Big)\right) - qe^{-rT}\Phi\left(\frac{1}{\sigma\sqrt{T}}\Big(\log(a/q) + T(r - \frac{1}{2}\sigma^2)\Big)\right)$$

- But we can also estimate it through (iid) Monte Carlo!
  - Use $(*)$ above (for fixed small $h > 0$, e.g. $h = 0.05$) to generate samples from the difusion.
  - Any <u>one</u> run is highly variable. (file "RBS", with $M = 1$)
  - But <u>many</u> runs give good estimate. (file "RBS", with $M = 1000$)
  - Note that it's iid replications, so varfact $\equiv 1$.

- An "Asian call option" is similar, but with X_T replaced by $\overline{X}_{k,t} \equiv \frac{1}{k}\sum_{i=1}^{k} X_{iT/k}$, for some fixed positive integer k (e.g., $k = 8$).
  - Above "FACT" still holds (again with X_T replaced by $\overline{X}_{k,t}$).
  - Now there is no simple formula . . . but can still simulate! (file "RAO")

MONTE CARLO OPTIMISATION – Simulated Annealing:

- General method to find highest <u>mode</u> of π.

- Idea: mode of π is same as mode of a <u>flatter</u> or a <u>more peaked</u> version π_τ, for any $\tau > 0$.

  - e.g. $\pi_\tau \equiv \pi^{1/\tau}$. Flatter if $\tau > 1$, more peaked if $\tau < 1$. ("tempered")
  - For large τ, MCMC explores a lot; good at beginning of search.
  - For small τ, MCMC narrows in on local mode; good at end of search.

- So, use tempered MCMC, but where $\tau = \tau_n \searrow 0$, so π_{τ_n} becomes more and more concentrated at mode as $n \to \infty$.

- Need to choose $\{\tau_n\}$, the "cooling schedule".
  - e.g. geometric ($\tau_n = \tau_0\, r^n$ for some $r < 1$).
  - or linear ($\tau_n = \tau_0 - dn$ for some $d > 0$, chosen so $\tau_M = \tau_0 - dM \geq 0$).
  - or logarithmic ($\tau_n = \tau_0 / \log(1 + n)$).
  - or ...
  - Theorem:: if $c \geq \sup \pi$, then simulated annealing with $\tau_n = c/\log(1+n)$ will converge to the global maximum as $n \to \infty$. (But very slow.)

- EXAMPLE: $\Pi_\tau = 0.3\, N(0, \tau^2) + 0.7\, N(20, \tau^2)$. (file "Rsimann")
  - Highest mode is at 20 (for any τ).
  - If run usual Metropolis algorithm, it will either jump forever between modes (if τ large), or get stuck in one mode or the other with equal probability (if τ small) – bad.
  - But if $\tau_n \searrow 0$ slowly, then can usually find the highest mode (20) – good.
  - Try both geometric and linear (better?) cooling ... (file "Rsimann")

OPTIMAL RWM PROPOSALS:

- Consider RWM on $\mathcal{X} = \mathbf{R}^d$, where $Y_n \sim MVN(X_{n-1},\, \Sigma)$ for some $d \times d$ proposal covariance matrix Σ.

- What is best choice of Σ?
  - Usually we take $\Sigma = \sigma^2 I_d$ for some $\sigma > 0$, and then choose σ so acceptance rate not too small, not too large (e.g. 0.234).
  - But can we do better?

- Suppose for now that $\Pi = MVN(\mu_0,\, \Sigma_0)$ for some fixed μ_0 and Σ_0, in dim=5. Try RWM with various proposal distributions (file "Ropt"):
  - first version: $Y_n \sim MVN(X_{n-1},\, I_d)$. ($acc \approx 0.06$; $varfact \approx 220$)
  - second version: $Y_n \sim MVN(X_{n-1},\ 0.1\, I_d)$. ($acc \approx 0.234$; $varfact \approx 300$)
  - third version: $Y_n \sim MVN(X_{n-1},\, \Sigma_0)$. ($acc \approx 0.31$; $varfact \approx 15$)
  - fourth version: $Y_n \sim MVN(X_{n-1},\ 1.4\, \Sigma_0)$. ($acc \approx 0.234$; $varfact \approx 7$)

- Or in dim=20 (file "Ropt2", with file "Rtarg20"):
  - $Y_n \sim MVN(X_{n-1}, 0.025\, I_d)$. $(acc \approx 0.234; \quad varfact \approx 400$ or more)
  - $Y_n \sim MVN(X_{n-1}, 0.283\, \Sigma_0)$. $(acc \approx 0.234; \quad varfact \approx 50)$
- Conclusion: acceptance rates near 0.234 are better.
- But also, proposals shaped like the target are better.
  - Indeed, best is when proposal covariance $= ((2.38)^2/d)\Sigma_0$.
  - This has been proved for targets which are orthogonal transformations of independent components (Roberts et al., Ann Appl Prob 1997; Roberts and Rosenthal, Stat Sci 2001 ; Bédard, Ann Appl Prob 2007).
  - And it's "approximately" true for most unimodal targets ...
- Problem: Σ_0 would usually be unknown; then what?
  - Can perhaps "adapt"!

ADAPTIVE MCMC:

- What if target covariance Σ_0 is unknown??
- Can estimate target covariance based on run so far, to get empirical covariance Σ_n.
- Then update proposal covariance "on the fly".
- "Learn as you go": see e.g. the Java applet "adapt.html"

END WEEK #7

- For Adaptive MCMC, could use proposal $Y_n \sim MVN(X_{n-1},\ ((2.38)^2/d)\Sigma_n)$.
  - Hope that for large n, $\Sigma_n \approx \Sigma_0$, so proposals "nearly" optimal.
  - (Usually also add ϵI_d to proposal covariance, to improve stability, e.g. $\epsilon = 0.05$.)
- Try R version, for the same MVN example as in Ropt (file "Radapt"):
  - Need much longer burn-in, e.g. $B = 20,000$, for adaption to work.
  - Get varfact of last 4000 iterations of about 18 ... "competitive" with Ropt optimal ...
  - The longer the run, the more benefit from adaptation.
  - Can also compute "slow-down factor", $s_n \equiv d \left(\sum_{i=1}^{d} \lambda_{in}^{-2} \,/\, (\sum_{i=1}^{d} \lambda_{in}^{-1})^2\right)$, where $\{\lambda_{in}\}$ eigenvals of $\Sigma_n^{1/2}\, \Sigma_0^{-1/2}$. Starts large, should converge to 1. [Motivation: if $\Sigma_n = \Sigma_0$, then $\lambda_{in} \equiv 1$, so $s_n = d(d/d^2) \equiv 1$.] See Roberts and Rosenthal, Examples of Adaptive MCMC, JCGS 2009.
- Higher dimensions: figure "RplotAMx200.png" (dim=200). (beautiful!)

  - Works well, but it takes many iterations before the adaption is helpful.

- BUT IS "ADAPTIVE MCMC" A VALID ALGORITHM??

- Not in general: see e.g. "adapt.html"

- Algorithm now non-Markovian, doesn't preserve stationarity at each step.

- However, still guaranteed to converge to Π under various technical conditions.

- For example, it suffices (see Roberts & Rosenthal, "Coupling and Convergence of Adaptive MCMC" (J. Appl. Prob. 2007)) that the adaption satisfies:
  - (a) Diminishing Adaptation: Adapt less and less as the algorithm proceeds. Formally, $\sup_{x \in \mathcal{X}} \|P_{\Gamma_{n+1}}(x, \cdot) - P_{\Gamma_n}(x, \cdot)\| \to 0$ in prob. [Can always be made to hold, since adaption is user controlled.]
  - (b) Containment: For all $\epsilon > 0$, the time to converge to within ϵ of stationary from $x = X_n$, if fix $\gamma = \Gamma_n$, remain bounded in probability as $n \to \infty$. [Technical condition, to avoid "escape to infinity". Holds if e.g. the state space and adaption spaces are both compact, etc. And always seems to hold in practice.]
  - (This also guarantees WLLN for bounded functionals. Various other results about LLN / CLT under stronger assumptions.)
  - There are various "checkable" sufficient conditions which guarantee Containment, e.g. Y. Bai, G.O. Roberts, and J.S. Rosenthal, Adv. Appl. Stat. 2011 and Craiu, Gray, Latusynski, Madras, Roberts, and Rosenthal, Ann. Appl. Prob. 2015 and J.S. Rosenthal and J. Yang, Ergodicity of Combocontinuous Adaptive MCMC Algorithms, MCAP, to appear.

- So, some "reasonable" theory, but you have to be careful!

TEMPERED MCMC:

- Suppose $\Pi(\cdot)$ is multi-modal, i.e. has distinct "parts" (e.g., $\Pi = \frac{1}{2} N(0,1) + \frac{1}{2} N(20,1)$)

- Usual RWM with $Y_n \sim N(X_{n-1}, 1)$ (say) can explore well within each mode, but how to get from one mode to the other?

- Idea: if $\Pi(\cdot)$ were flatter, e.g. $\frac{1}{2} N(0, 10^2) + \frac{1}{2} N(20, 10^2)$, then much easier to get between modes.

- So: define a sequence $\Pi_1, \Pi_2, \ldots, \Pi_m$ where $\Pi_1 = \Pi$ ("cold"), and Π_τ is flatter for larger τ ("hot"). (e.g. $\Pi_\tau = \frac{1}{2} N(0, \tau^2) + \frac{1}{2} N(20, \tau^2)$; file "Rtempered")

- In the end, only "count" those samples where $\tau = 1$.

- Proceed by defining a joint Markov chain (x, τ) on $\mathcal{X} \times \{1, 2, \ldots, m\}$, with stationary distribution $\overline{\Pi}$ defined by $\overline{\Pi}(S \times \{\tau\}) = \frac{1}{m}\,\Pi_\tau(S)$.
  - (Can also use other weights besides $\frac{1}{m}$.)
- The Markov chain should have both spatial moves (change x) and temperature moves (change τ).
  - e.g. perhaps chain alternates between:
    (a) propose $x' \sim N(x, 1)$, accept with prob $\min\Big(1,\ \frac{\overline{\pi}(x',\tau)}{\overline{\pi}(x,\tau)}\Big) = \min\Big(1,\ \frac{\pi_\tau(x')}{\pi_\tau(x)}\Big)$.

    (b) propose $\tau' = \tau \pm 1$ (prob $\frac{1}{2}$ each), accept with prob
    $\min\Big(1,\ \frac{\overline{\pi}(x,\tau')}{\overline{\pi}(x,\tau)}\Big) = \min\Big(1,\ \frac{\pi_{\tau'}(x)}{\pi_\tau(x)}\Big)$.
- Chain should converge to $\overline{\Pi}$.
- Then, as above, only "count" those samples where $\tau = 1$. (red)
- EXAMPLE: $\Pi = \frac{1}{2}\,N(0,1) + \frac{1}{2}\,N(20,1)$
  - Assume proposals are $Y_n \sim N(X_{n-1}, 1)$.
  - Mixing for Π: terrible! (file "Rtempered" with dotempering=FALSE and temp=1; note the small claimed standard error!)
  - Define $\Pi_\tau = \frac{1}{2}\,N(0,\tau^2) + \frac{1}{2}\,N(20,\tau^2)$, for $\tau = 1, 2, \ldots, 10$.
  - Mixing better for larger τ! (file "Rtempered" with dotempering=FALSE and temp=1,2,3,4,...,10)
  - (Compare graphs of π_1 and π_8: plot commands at bottom of "Rtempered" …)
  - So, use above "(a)–(b)" algorithm; converges fairly well to $\overline{\Pi}$. (file "Rtempered", with dotempering=TRUE)
  - So, conditional on $\tau = 1$, converges to Π. ("points" command at end of file "Rtempered")
  - So, average of those $h(x)$ with $\tau = 1$ gives good estimate of $\mathbf{E}_\pi(h)$.
- HOW TO FIND THE TEMPERED DENSITIES π_τ?
- Usually won't "know" about e.g. $\Pi_\tau = \frac{1}{2}\,N(0,\tau^2) + \frac{1}{2}\,N(20,\tau^2)$.
- Instead, can e.g. let $\pi_\tau(x) = c_\tau\,(\pi(x))^{1/\tau}$. (Sometimes write $\beta = 1/\tau$.)
  - Then $\Pi_1 = \Pi$, and π_τ flatter for larger τ – good.
  - (e.g. if $\pi(x)$ density of $N(\mu, \sigma^2)$, then $c_\tau(\pi(x))^{1/\tau}$ density of $N(\mu, \tau\sigma^2)$.)
  - Then temperature acceptance probability is:

$$\min\Big(1,\ \frac{\pi_{\tau'}(x)}{\pi_\tau(x)}\Big) \ = \ \min\Big(1,\ \frac{c_{\tau'}}{c_\tau}(\pi(x))^{(1/\tau')-(1/\tau)}\Big)\,.$$

  - This depends on the c_τ, which are usually unknown – bad.

- What to do?

PARALLEL TEMPERING:

- (a.k.a. Metropolis-Coupled MCMC, or MCMCMC: Geyer, 1991)
- Alternative to tempered MCMC.
- Instead, use state space $\mathcal{X}^m$, with m chains, i.e. one chain for each temperature.
- So, state at time n is $X_n = (X_{n1}, X_{n2}, \ldots, X_{nm})$, where $X_{n\tau}$ is "at" temperature τ.
- Stationary distribution is now $\overline{\Pi} = \Pi_1 \times \Pi_2 \times \ldots \times \Pi_m$, i.e. $\overline{\Pi}(X_1 \in S_1,\ X_2 \in S_2,\ \ldots, X_m \in S_m) = \Pi_1(S_1)\ \Pi_2(S_2)\ \ldots\ \Pi_m(S_m)$.
- Then, can update the chain $X_{n-1,\tau}$ at temperature τ (for each $1 \le \tau \le m$), by proposing e.g. $Y_{n,\tau} \sim N(X_{n-1,\tau},\ 1)$, and accepting with probability $\min\left(1,\ \frac{\pi_\tau(Y_{n,\tau})}{\pi_\tau(X_{n-1,\tau})}\right)$.
- And, can also choose temperatures τ and τ' (e.g., at random), and propose to "swap" the values $X_{n,\tau}$ and $X_{n,\tau'}$, and accept this with probability $\min\left(1,\ \frac{\pi_\tau(X_{n,\tau'})\,\pi_{\tau'}(X_{n,\tau})}{\pi_\tau(X_{n,\tau})\,\pi_{\tau'}(X_{n,\tau'})}\right)$.
  - Now, normalising constants cancel, e.g. if $\pi_\tau(x) = c_\tau\,(\pi(x))^{1/\tau}$, then acceptance probability is:

    $$\min\left(1,\ \frac{c_\tau \pi(X_{n,\tau'})^{1/\tau}\ c_{\tau'}\pi(X_{n,\tau})^{1/\tau'}}{c_\tau \pi(X_{n,\tau})^{1/\tau}\ c_{\tau'}\pi(X_{n,\tau'})^{1/\tau'}}\right) = \min\left(1,\ \frac{\pi(X_{n,\tau'})^{1/\tau}\ \pi(X_{n,\tau})^{1/\tau'}}{\pi(X_{n,\tau})^{1/\tau}\ \pi(X_{n,\tau'})^{1/\tau'}}\right),$$

    so c_τ and $c_{\tau'}$ are not required.
- EXAMPLE: suppose again that $\Pi_\tau = \frac{1}{2}\,N(0,\tau^2) + \frac{1}{2}\,N(20,\tau^2)$, for $\tau = 1, 2, \ldots, 10$.
  - Can run parallel tempering … works pretty well. (file "Rpara")

TRANSDIMENSIONAL MCMC:

- (a.k.a. "reversible-jump MCMC": Green, Biometrika 1995)
- What if the state space is a union of parts of different dimension?
  - Can we still apply Metropolis-Hastings then??
- (EXAMPLE: autoregressive process: suppose $Y_n = a_1 Y_{n-1} + a_2 Y_{n-2} + \ldots + a_k Y_{n-k}$, but we don't know what k should be.)
- OUR EXAMPLE: suppose $\{y_j\}_{j=1}^J$ are known data which are assumed to come from a mixture distribution: $\frac{1}{k}(N(a_1, 1) + N(a_2, 1) + \ldots + N(a_k, 1))$.
- Want to estimate the unknown $k, a_1, \ldots, a_k$.

  - Here the number of parameters is also unknown, i.e. the dimension is unknown and variable, which makes MCMC more challenging!

- The state space is $\mathcal{X} = \{(k, a) : k \in \mathbf{N},\ a \in \mathbf{R}^k\}$.

- Prior distributions: $k - 1 \sim \text{Poisson}(2)$, and $a|k \sim MVN(0, I_k)$ (say).

- Define a reference measure λ by: $\lambda(\{k\} \times A) = \lambda_k(A)$ for $k \in \mathbf{N}$ and (measurable) $A \subseteq \mathbf{R}^k$, where λ_k is Lebesgue measure on $\mathbf{R}^k$.
  - i.e., $\lambda = \delta_1 \times \lambda_1 + \delta_2 \times \lambda_2 + \delta_3 \times \lambda_3 + \ldots$

- Then in our mixture example, posterior density (with respect to λ) is:

$$\pi(k, a) \;=\; C\, \frac{e^{-2} 2^{k-1}}{(k-1)!} (2\pi)^{-k/2} \exp\Big(-\frac{1}{2} \sum_{i=1}^{k} a_i^2\Big)\, (2\pi)^{-J/2} \prod_{j=1}^{J} \Big(\sum_{i=1}^{k} \frac{1}{k} \exp\Big(-\frac{1}{2}(y_j - a_i)^2\Big)\Big)\,.$$

- So, on a log scale,

$$\log \pi(k, a) \;=\; \log C + \log \frac{e^{-2} 2^{k-1}}{(k-1)!} - \frac{k}{2} \log(2\pi) - \frac{1}{2} \sum_{i=1}^{k} a_i^2 - \frac{J}{2} \log(2\pi) +$$

$$\sum_{j=1}^{J} \log\Big(\sum_{i=1}^{k} \frac{1}{k} \exp\Big(-\frac{1}{2}(y_j - a_i)^2\Big)\Big)\,.$$

  (Can ignore $\log C$ and $\frac{J}{2}\log(2\pi)$, but not $\frac{k}{2}\log(2\pi)$.)

- How to "explore" this posterior distribution??

- For fixed k, can move around $\mathbf{R}^k$ in usual way with RWM (say).

- But how to change k?

- Can propose to replace k with, say, $k' = k \pm 1$ (prob $\frac{1}{2}$ each).

- Then have to correspondingly change a. One possibility:
  - If $k' = k+1$, then $a' = (a_1, \ldots, a_k, Z)$ where $Z \sim N(0, 1)$ ("elongate").
  - If $k' = k - 1$, then $a' = (a_1, \ldots, a_{k-1})$ ("truncate").

- Then accept with usual probability, $\min\Big(1,\ \frac{\pi(k',a')\, q\big((k',a'),(k,a)\big)}{\pi(k,a)\, q\big((k,a),(k',a')\big)}\Big)$.
  - Here if $k' = k + 1$, then $q((k', a'), (k, a)) = \frac{1}{2}$, while $q((k, a), (k', a')) = \frac{1}{2} \frac{1}{\sqrt{2\pi}} e^{-(a'_{k'})^2/2}$.
  - Or, if $k' = k - 1$, then $q((k, a), (k', a')) = \frac{1}{2}$, while $q((k', a'), (k, a)) = \frac{1}{2} \frac{1}{\sqrt{2\pi}} e^{-(a_k)^2/2}$.

- Seems to work okay; final k usually between 5 and 9 ... (file "Rtrans")

- (NOTE: We didn't really have time to cover the remaining material in detail. So, I still hope you read it, but you don't need it for the test.)

- ALTERNATIVE method for the "correspondingly change a" step:

- If $k' = k+1$, then $a' = (a_1, \ldots, a_{k-1}, a_k - Z, a_k + Z)$ where $Z \sim N(0,1)$ ("split").
- If $k' = k-1$, then $a' = (a_1, \ldots, a_{k-2}, \frac{1}{2}(a_{k-1} + a_k))$ ("merge").
- What about the densities $q((k', a'), (k, a))$?
- Well, if $k' = k+1$, then $q((k', a'), (k, a)) = \frac{1}{2}$, while roughly speaking,

$$q((k,a),(k',a')) \;=\; \frac{1}{2}\,\frac{1}{\sqrt{2\pi}} e^{-z^2/2} \;=\; \frac{1}{2}\,\frac{1}{\sqrt{2\pi}} e^{-(\frac{1}{2}(a'_{k'} - a'_k))^2/2}\,.$$

- One subtle additional point: The map $(a, Z) \mapsto a' = (a_1, \ldots, a_{k-1}, a_k - Z, a_k + Z)$ has "Jacobian" term:

$$\det\left(\frac{\partial a'}{\partial(a,Z)}\right) \;=\; \det\begin{pmatrix} I_{k-1} & 0 & 0 \\ 0 & 1 & -1 \\ 0 & 1 & 1 \end{pmatrix} \;=\; 1 - (-1) \;=\; 2\,,$$

  i.e. the split moves "spread out" the mass by a factor of 2.
- So by Change-of-Variable Thm, actually

$$q((k,a),(k',a')) \;=\; \frac{1}{2}\,\frac{1}{\sqrt{2\pi}} e^{-(\frac{1}{2}(a'_{k'} - a'_k))^2/2} \Big/ 2\,.$$

- Similarly, if $k' = k-1$, then $q((k,a),(k',a')) = \frac{1}{2}$, while

$$q((k',a'),(k,a)) \;=\; \frac{1}{2}\,\frac{1}{\sqrt{2\pi}} e^{-(\frac{1}{2}(a_k - a_{k'}))^2/2} \Big/ 2\,.$$

- Algorithm still seems to work okay ... (file "Rtrans2")

- For more complicated transformations, need to include more complicated "Jacobian" term (but above it equals 1 or 2).

- Check: if we start the algorithms with, say, $k = 24$, then they don't manage to reduce k enough!
  - They might be trying to remove the "wrong" a_i.

- So, try another MODIFICATION, this time where any coordinate can be added/removed, not just the last one.
  - While we're at it, change "new a_i distribution" from $Z \sim N(0,1)$ to $Z \sim \text{Uniform}(-20, 30)$, with corresponding change to the $q((k,a),(k',a'))$ formulae.
  - file "Rtrans3" – now works well even if started with $k = 24$.
  - Seems to settle on $k = 6$ regardless of starting value.
  - This seems to indicate rapid mixing – good!

- FINAL SUMMARY: Monte Carlo can be used for nearly everything!