Joachim Vandekerckhove

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"Now that we have these data, what are the likely values of the generating parameters?"

What is the probability distribution of a, assuming that

$$\forall i: \left\{ \begin{array}{ll} \theta_i^f & = & \frac{f_i}{N} \\ \theta_i^h & = & \Phi\left(a + \Phi^{-1}(\theta_i^f)\right) \\ f_i & \sim & \text{Bin}\left(\theta_i^f, N\right) \\ h_i & \sim & \text{Bin}\left(\theta_i^h, S\right) \end{array} \right.$$

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In other words, what is p(a|D)?

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$$S(a|D) = \sqrt{E(a^2|D) - [E(a|D)]^2}$$

Numerical integration methods

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- Draw random samples that fall under the curve
- Characterize the curve with summary statistics of the sample

A very convenient approximation to the expectation integral is

$$E(a|D) = \int_{-\infty}^{+\infty} a \, p(a|D) \, da$$

$$\approx \frac{1}{R} \sum_{r=1}^{R} a_r \text{ where } \forall r : a_r \stackrel{iid}{\sim} p(a|D)$$

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It follows that in order to characterize an arbitrary distribution, it suffices to be able to draw random samples from it.

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- Their initial development in 1947 almost immediately followed the completion of ENIAC, the first general-purpose digital computer, in 1945.
- There are many MC methods, but the most common ones are Markov chain Monte Carlo (MCMC) methods.

Metropolis sampler

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- In the algorithm, we will randomly generate candidate samples from some simple distribution, and then decide to accept or reject the candidate.
- Metropolis algorithms need some customization and fine-tuning to be most efficient.

Given a target function $f(\theta) \propto p(\theta|D)$ and a symmetric candidate generating distribution Q(x|y) = Q(y|x), a Metropolis sampling algorithm proceeds as follows:

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- 6 Set $i \leftarrow i+1$. If $i \leq R$, return to Step 3, otherwise halt

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- Q() will often be something that's easy to sample, like a normal distribution.
- $p(\theta|D)$ will often be our posterior distribution.
- Often, for computational stability, we will deal with $\log (p(\theta|D))$, in which case we come the log of the acceptance probability $\log(\alpha) = \log (p(\theta^c|D)) \log (p(\theta^{(i-1)}|D))$ and compare it to the log of a uniform variate, $\log(u)$.

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- That way, more samples can be accepted and the algorithm can be more efficient.
- We will tune the sampler so that it accepts approximately 40% of all proposed samples.
- During the adaptation phase, we will "warm up" the
 algorithm but the samples drawn during this phase are not yet
 samples from the target distribution, so we discard them.

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- A simple rule to update the standard deviation is

$$\sigma_{\sf new} = \sigma_{\sf old} \times \left(\frac{r_{\sf target}}{r_k}\right)^{1.1}$$

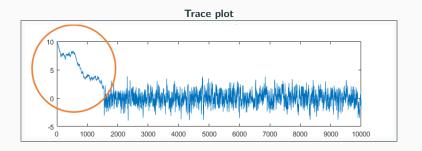
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How much to fine-tune depends on the specific case.

Metropolis sampler: Post-processing

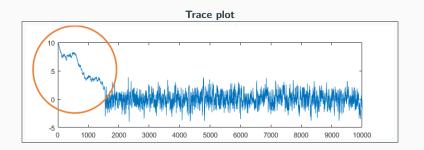
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Metropolis sampler: Post-processing

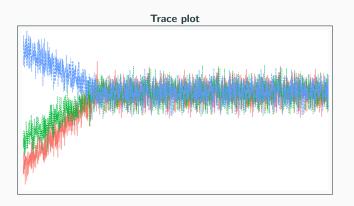
- We have to make sure the chain has converged to a stationary sampling state before using the samples for inference.
- Often, we will discard a number of initial samples known as the burn-in:

$$\hat{a} = \frac{1}{R - B} \sum_{i=B+1}^{R} a^{(i)}$$



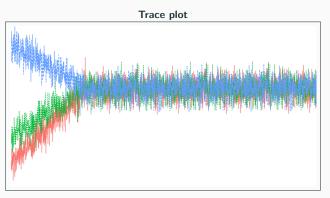
Metropolis sampler: Diagnostics

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Metropolis sampler: Diagnostics

- We usually also repeat the procedure a few times with different values for $\theta^{(0)}$ to ensure that the algorithm converges to the same stationary distribution.
- Several convergence statistics exist, with Geweke's and Gelman's \hat{R} being the most popular.



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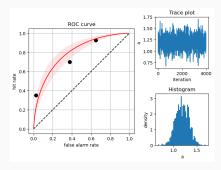
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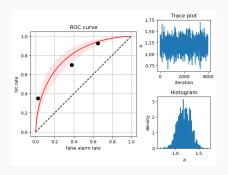
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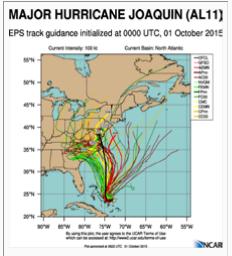
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- Figures can also be summary statistics!
 - You could draw a curve to visualize your data and then draw a distribution of synthetic curves using your sampled parameters

Metropolis sampler: Inference

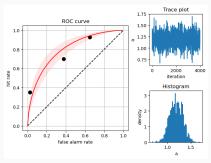


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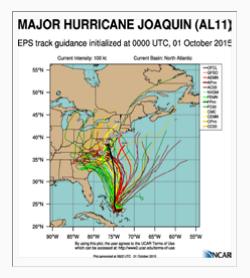




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Typical steps of a Metropolis analysis are thus:

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- 5. Diagnose: Visualize chains and calculate convergence statistics
- 6. Inference: Calculate summary statistics of interest

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- The development of computers and numerical algorithms in the 20th century greatly expanded the range of problems that could be solved using numerical integration. They are partly responsible for the Bayesian revolution in the 21st century.

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