Numerical integration

Joachim Vandekerckhove

Motivating application

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

Motivating application: Signal detection

What is the probability distribution of a, assuming that

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

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In other words, what is $p\left(a|D\right)$?

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We can actually work out that distribution:

$$p\left(a|D\right) = \frac{p\left(D|a\right)p\left(a\right)}{p\left(D\right)} \propto p\left(D|a\right)p\left(a\right)$$

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

Numerical integration methods

Some basic methods

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

Monte Carlo methods

Numerical integration

A very convenient approximation to the expectation integral is

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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.

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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.

Metropolis sampler: Pseudocode

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:

1 `Set` $i \leftarrow 1$ and `choose` sample size R

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

Metropolis sampler: Common choices

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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 $\log(\alpha) = \log(p(\theta^c|D)) - \log\left(p(\theta^{(i-1)}|D)\right)$ and compare it to the log of a uniform variate, $\log(u)$.

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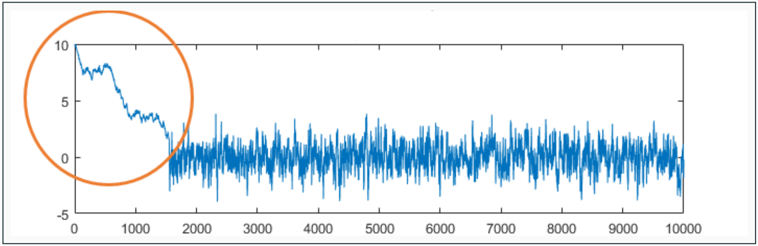
- How much to fine-tune depends on the specific case.

Metropolis sampler: Post-processing

- We have to make sure the chain has converged to a stationary sampling state before using the samples for inference.

Trace plot



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- Often, we will discard a number of initial samples known as the burn-in:

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

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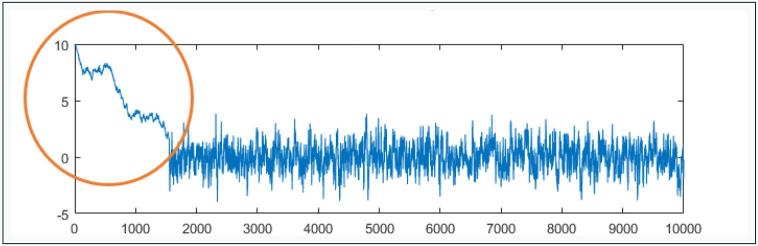

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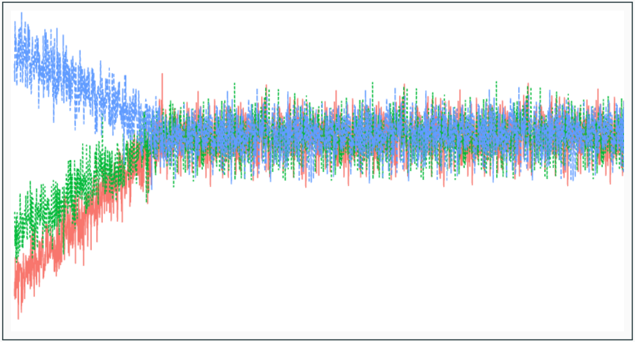

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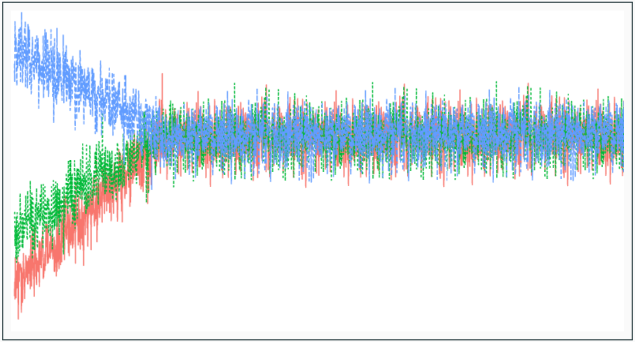

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    - You could draw a curve to visualize your data and then draw a distribution of synthetic curves using your sampled parameters

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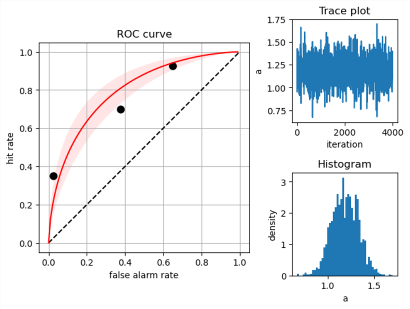

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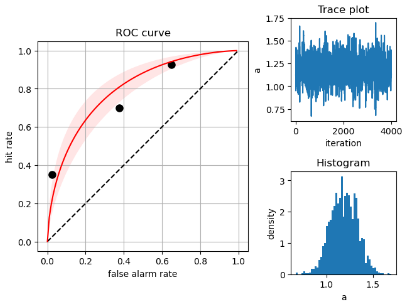

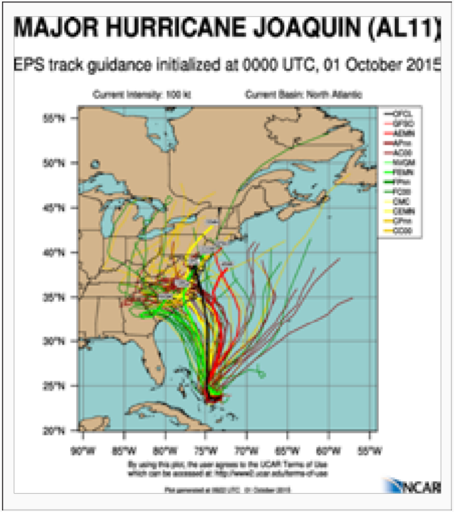

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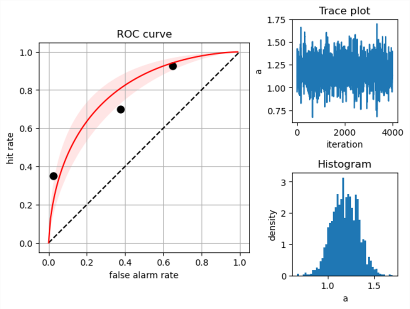

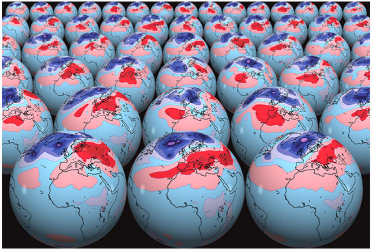

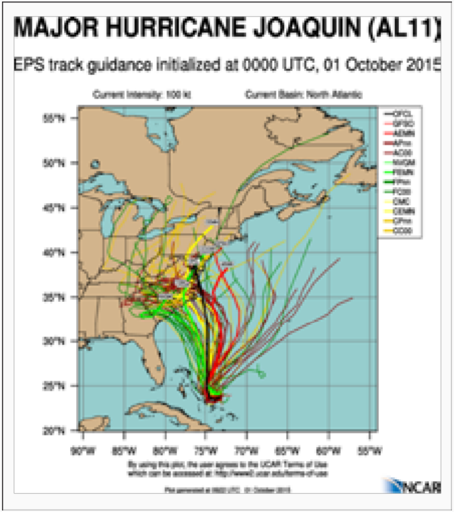

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5. Diagnose: Visualize chains and calculate convergence statistics

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4. Post-process: Burn samples before convergence
5. Diagnose: Visualize chains and calculate convergence statistics
6. Inference: Calculate summary statistics of interest

Numerical integration

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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.

Numerical integration

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