An introduction to bayesian data analysis with PyMC3

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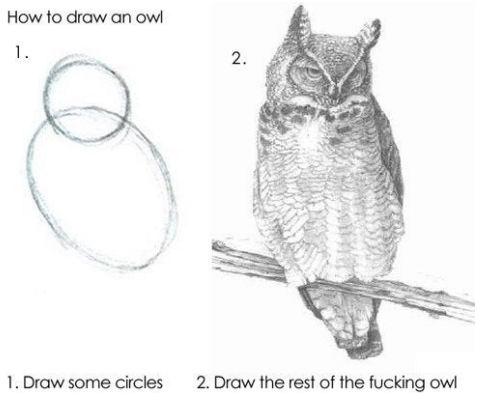
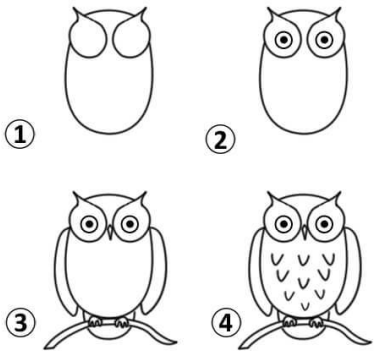
inmeta

17. februar 2020

Googling bayesian analysis vs this presentation





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Road map

1. Theory
   (a) The basics of Bayesianism
   (b) Markov chain Monte Carlo methods (MCMC)
2. Practice
   (a) Probabilistic programming with PyMC3

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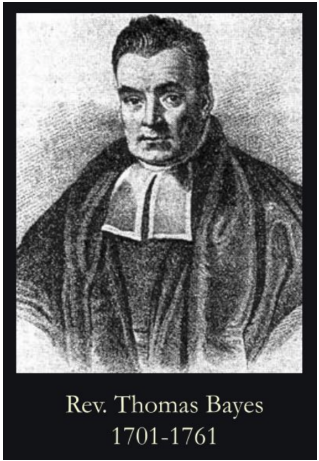
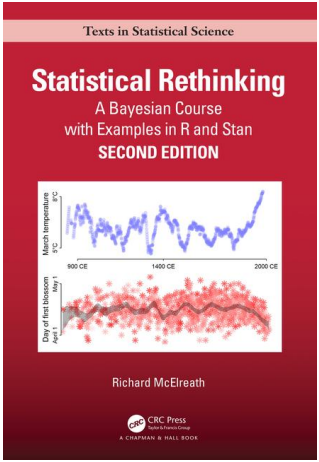
What is Bayesian data analysis?

"A Bayesian is one who, vaguely expecting a horse, and catching a glimpse of a donkey, strongly believes he has seen a mule."



It's just counting!

- Richard McElreath: "Bayesian inference is just counting."
- Count all the ways observed data could have arisen according to assumptions
- Assumptions that can arise in more ways are more consistent with the data, and therefore more plausible

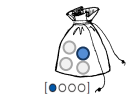


The Garden of Forking Data

Counting possibilities

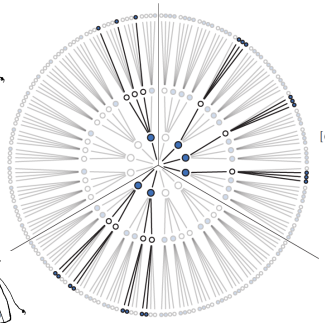
Evidence (i.e. data)**:**

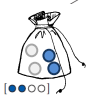
Draw 3 marbles from the bag (with replacement)



3 paths

9 paths





8 paths

Conjecture	Ways to produce ●○●
[○○○○]	$0 \times 4 \times 0 = 0$
[●○○○]	$1 \times 3 \times 1 = 3$
[●●○○]	$2 \times 2 \times 2 = 8$
[●●●○]	$3 \times 1 \times 3 = 9$
[●●●●]	$4 \times 0 \times 4 = 0$

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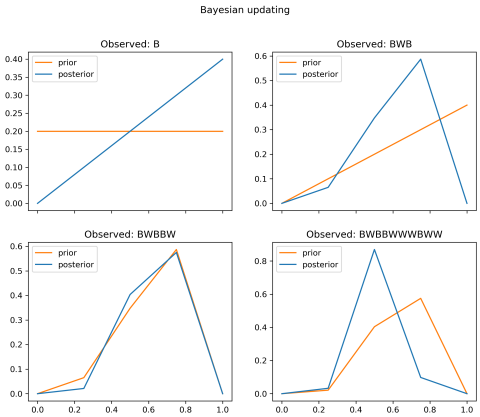
Priors, posteriors and likelihoods

Prior $p(\theta)$: Encodes assumptions about θ
Likelihood $p(y|\theta)$: How were the observed data generated?
Posterior $p(\theta|y)$: Assumptions about θ consistent with data

$$p(\theta|y) = \frac{p(\theta)p(y|\theta)}{\int p(y|\theta)p(\theta)\,d\theta} \propto p(\theta)p(y|\theta)$$

posterior $\propto$ *prior* $\cdot$ *likelihood*



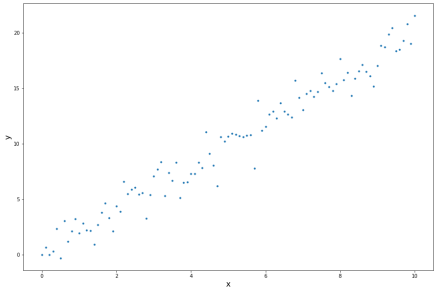
Model

- In the Bayesian analysis we are trying to describe the process that generated the data.
- We assume that the process can be expressed as a parametic model

$$M(input, \theta)$$

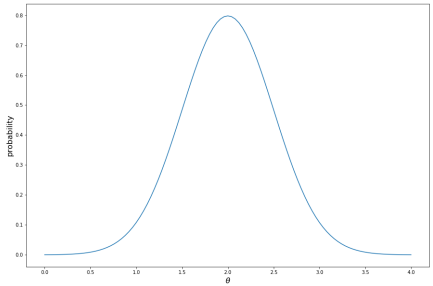
Example

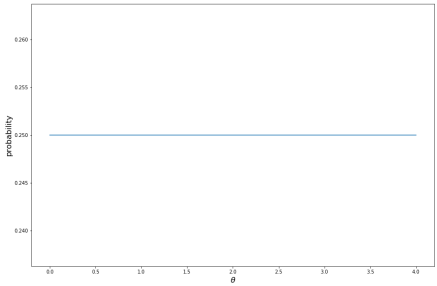
The oh so boring linear regression example....



Model: $y_i = \theta x_i + \varepsilon_i, \quad \varepsilon \sim N(0, \sigma^2)$

Example: Priors

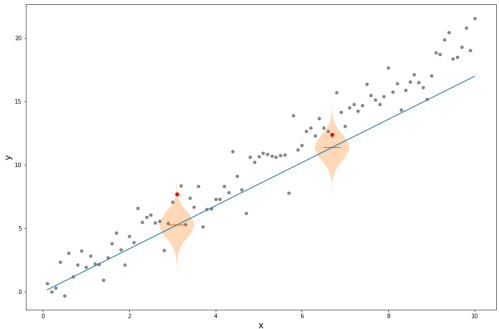




Example: Likelihood

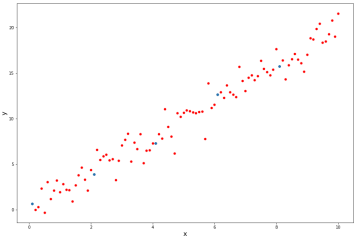
$$p(y|\theta) = \prod_{i=1}^{n} p(y_i|\theta)$$

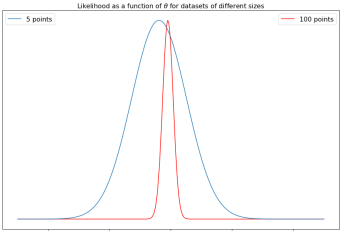
$$p(y_i|\theta) = N(y_i|\theta x_i, \sigma^2)$$

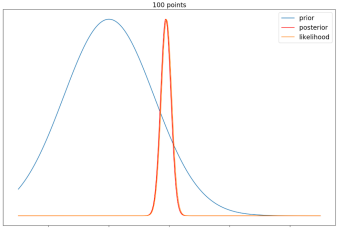


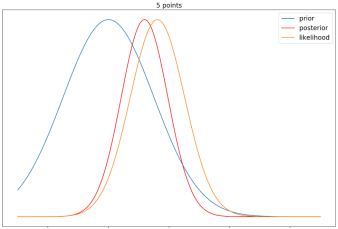
What is the probability of my data given the model and parameters I've chosen?

Example: Size of dataset









Towards a Bayesian workflow

1. Design the model (tell the data story)
   (a) Describe data generating process:
   $p(y|\theta) = \theta^{\sum_i \mathbf{1}(y_i=1)}(1-\theta)^{\sum_i \mathbf{1}(y_i\neq 1)}$
   (b) Encode assumptions about parameters: $p(\theta) = \frac{1}{5}$
2. Condition on the data (update step)
   (a) $p(\theta|y) \propto p(\theta)p(y|\theta)$
3. Evaluate the model (critique), and either
   (a) be happy, it worked as planned, or
   (b) return to step 1

The Garden of Forking Data, revisited

```python
import numpy as np

## Observed data
data = np.array([1, 0, 1])

## Conjectures (possible values for theta)
# array([0., 0.25, 0.5, 0.75, 1.])
theta = np.linspace(0, 1, num=5)

# Prior distribution over theta
# array([0.2, 0.2, 0.2, 0.2, 0.2])
uniform_prior = np.repeat(0.2, repeats=5)

# Likelihood function
def likelihood(data, theta):
    num_blue = data.sum()
    num_white = len(data) - num_blue
    return theta**num_blue * (1 - theta)**num_white

# Unnormalised posterior over theta
# array([0., 0.009375, 0.025, 0.028125, 0.])
unnormalised_posterior = uniform_prior * likelihood(data, theta)

# Posterior distribution over theta
# array([0., 0.15, 0.4, 0.45, 0.])
posterior = unnormalised_posterior / unnormalised_posterior.sum()
```

The Garden of Forking Data, revisited

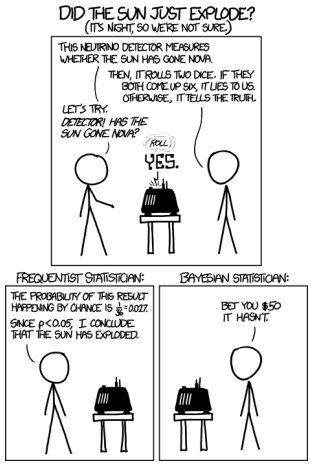
```
import numpy as np

# Number of paths consistent with conjectures
forking_data = np.array([0, 3, 8, 9, 0])

# array([0., 0.15, 0.4, 0.45, 0.]
forking_data / forking_data.sum()
```

The Frequentist vs. Bayesian debacle

- Frequentist statistics
  - Probability = limiting frequency
  - Uncertainty arises from sampling variation
- Bayesian statistics
  - Frequency ≠ probability
  - Uncertainty arises from ignorance ¡¡¡¡¡¡¡ HEAD
- Principled way to represent and take into account uncertainty =======
- Intuitive way to represent and take into account uncertainty ¿¿¿¿¿¿¿ updates
- Easily incorporates prior information



But priors are subjective! Buu! Hiss!

- Non-informative vs. informative priors
  - Forking data example: $Uniform(0, 1)$ vs. $Uniform(\frac{1}{4}, \frac{3}{4})$
- Test your assumptions, e.g. using prior predictive checks
- More about priors:
  - Gelman et al. (2017): `https://arxiv.org/abs/1708.07487`
  - Bayesian Methods for Hackers: `https://tinyurl.com/v2yzyqv`
- For more Bayesian challenges, see e.g. Gelman and Yao (2020): `https://tinyurl.com/sbr2tev`

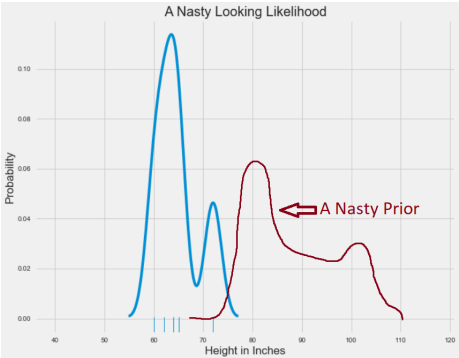
Telling the data story

“ People think in terms of stories - thus the unreasonable power of the anecdote to drive decision-making, well-founded or not. Existing analytics largely fails to provide this kind of story; instead, numbers seemingly appear out of thin air.”

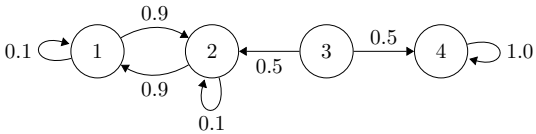
Beau Cronin, *Why Probabilistic Programming Matters (2013)*

How to sample from intractable posteriors?

- In textbooks, nice, we can sample directly from well-behaved, analytical posteriors
- In the real world, often impossible to sample directly from $p(\theta|y)$
- A general class of algorithms called **Markov chain Monte Carlo** let us approximately sample from posterior



Markov chains



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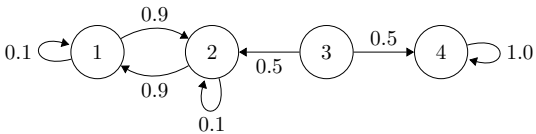
- A Markov chain defines a joint probability distribution over sequences
- Used to model events in discrete and continuous time (manufacturing processes, queuing systems, etc.)
- Typically interested in the long-term distribution of being in a certain state =======
- A Markov chain defines a joint probability distribution over a sequence of events
- Used to model events in discrete and continuous time

Properties of a Markov chain



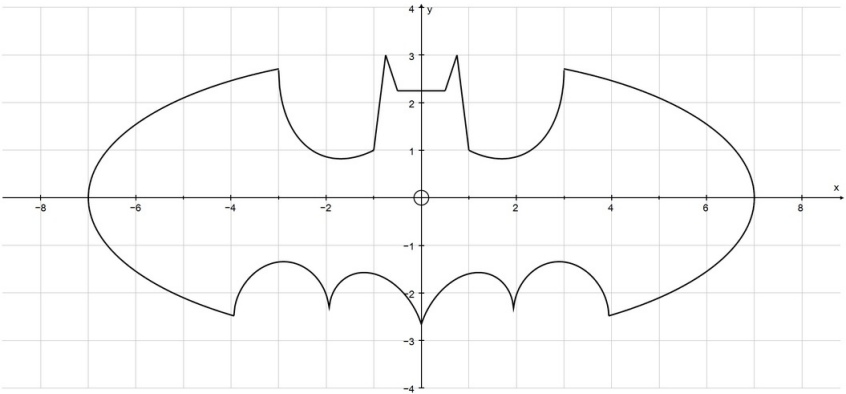
- Memoryless (Markov property):
  $P(X_t \mid X_{t-1}, X_{t-2}, \ldots, X_1) = P(X_t \mid X_{t-1})$
- Under certain conditions, guaranteed to have a unique, limiting distribution (aka. stationary distribution)
  - Long run proportion of time spent in each state
  - For more details, check
    `https://github.com/smu095/presentations/`

Monte Carlo simulations

- Monte Carlo (MC) simulations are just a way to approximate numerical results using repeated random sampling
- Main idea:
  - Generate N samples $x_1, \ldots, x_N$ from $p(x)$, approximate f using the empirical distribution of $\{f(x_n)\}_{n=1}^{N}$
  - $\mathbb{E}[f] = \int f(x)p(x)\,dx \approx \frac{1}{N}\sum_{n=1}^{N} f(x_n) = \hat{f}$
- MC estimates converge thanks to Law of Large Numbers
  - $(\hat{f} - \mathbb{E}[f]) \to \mathcal{N}\left(0, \frac{Var[f]}{N_{eff}}\right)$ as $N \to \infty$

Application: Evaluate integrals

- Calculate difficult integrals, such as the area of the Batman sign



Application: Evaluate integrals

- Repeatedly sample $(u_1, u_2) \sim \text{Uniform}(-\frac{1}{2}, \frac{1}{2})$
- Calculate area A of Batman sign as $A = \text{area of rectangle} \times \frac{\text{green dots}}{\text{all dots}}$

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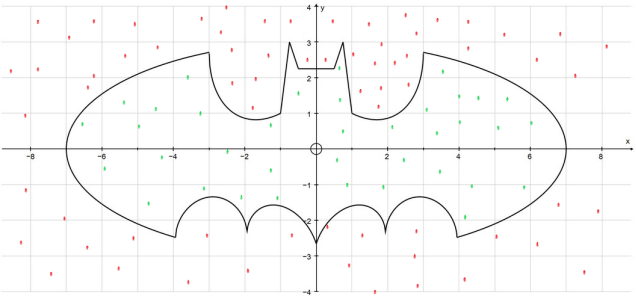

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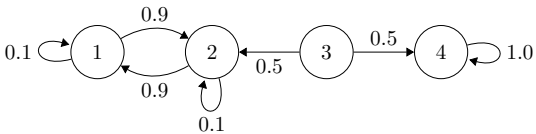

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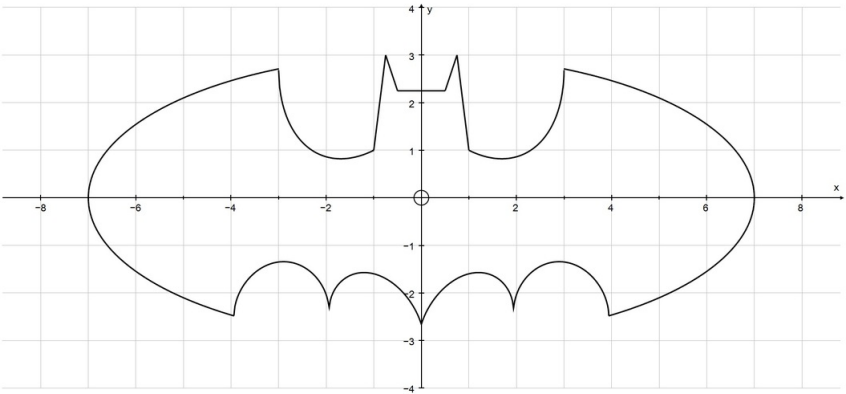

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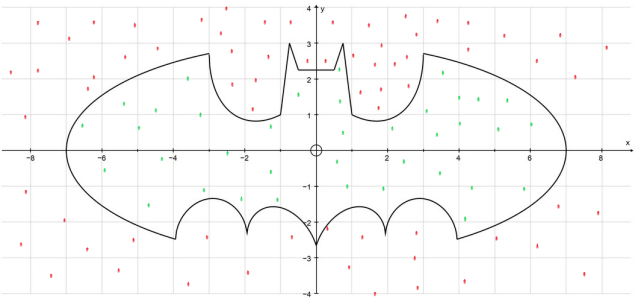

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Markov chain Monte Carlo methods

- **Main idea:** Construct a Markov chain over the parameter space where the stationary distribution is the posterior $p(\theta \mid y)$
  - For more details, check
    `https://github.com/smu095/presentations/`
- Randomly move around the parameter space such that the fraction of time spent at each randomly sampled parameter value is proportional to the true target density $p(\theta \mid y)$.
- Use the sequence of parameters generated by Markov chain to calculate MC approximations of any quantity of interest

Algorithmic view of MCMC

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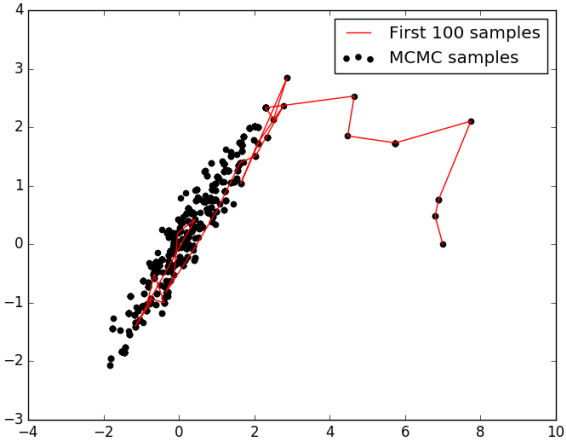
1. Start at current position.
2. Propose new position.
3. Accept/reject new position based on position's adherence to data and prior distributions.
   (a) If reject: Remain in your current position, return to step 1.
   (b) If accept: Move to the new position, return to step 1.
4. After large number of iterations, return sequence of accepted positions.

Metropolis algorithm

1. Start at some initial parameter value θ_0
2. for $t = 1$ to T:
   (a) Sample θ^* from a proposal distribution $q(\theta^* \mid \theta_{t-1})$
   (b) Evaluate $\alpha_{\theta^*} = \dfrac{p(\theta^* \mid y)}{p(\theta_{t-1} \mid y)}$.
   (c) Set acceptance probability to $r_{\theta^*} = \min(1, \alpha_{\theta^*})$.
   (d) Draw $u \sim \mathit{Uniform}(0,1)$
   (e) Set $\theta_t = \begin{cases} \theta^*, & \text{if } u < r \\ \theta_{t-1}, & \text{o.w.} \end{cases}$ =======
3. Start with current parameter values
4. Propose new parameter values.

MCMC illustration



Metropolis algorithm

1. Start at some initial parameter value θ_0
2. For $t = 1$ to T:

(a) Sample θ^* from a proposal distribution $q(\theta^* \mid \theta_{t-1})$

$\theta^* = \theta_{t-i} + \mathcal{N}(0, \text{jump scale})$

(b) Evaluate $\alpha_{\theta^*} = \dfrac{p(\theta^* \mid y)}{p(\theta_{t-1} \mid y)}$.

(c) Accept/reject θ^*

If $\alpha_{\theta^*} \geq 1$ set $\theta_t = \theta^*$

Else draw $u \sim \mathit{Uniform}(0,1)$ set $\theta_t = \begin{cases} \theta^*, & \text{if } u < \alpha_{\theta^*} \\ \theta_{t-1}, & \text{o.w.} \end{cases}$

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Metropolis in Python

```
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"""Metropolis sampling from posterior of mean"""
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import numpy as np

# Marbles data
data = np.array([1, 0, 1])

def log_p(theta, x):
    N = len(x)
    k = np.sum(x)
    logprior = np.repeat(0.2, len(x))
    loglik = k*np.log(theta + 10e-8) + (N - k)*np.log(1 - theta + 10e-8)
    return np.sum(logprior + loglik)

# Initial value for theta
theta = 0.5
=======
import numpy as np
data = np.array([1, 0, 1]) # Observations

def log_p(theta, x): # Proportional log posterior
    N, k = len(x), np.sum(x)
    logprior = np.repeat(0.2, N)
    loglik = k*np.log(theta + 10e-8) + (N - k)*np.log(1 - theta + 10e-8)
    return np.sum(logprior + loglik)
```

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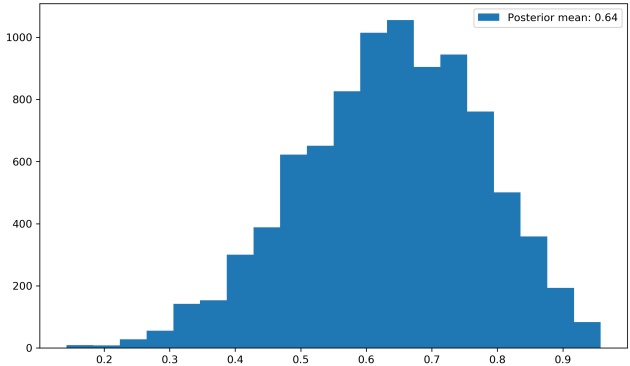

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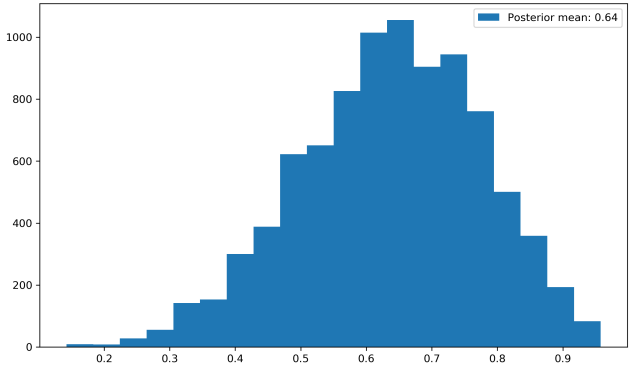
```

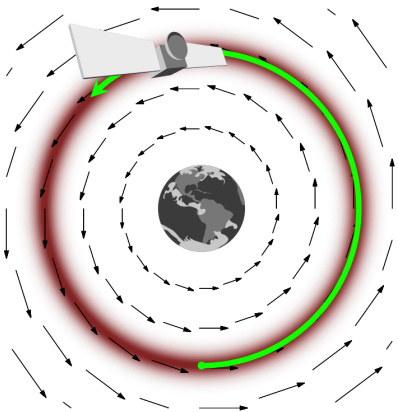
Metropolis in Python



¿¿¿¿¿¿¿ updates

Sampling algorithms

- Many different sampling algorithms exist
- Currently, the state-of-the-art is Hamiltonian Monte Carlo (HMC)
  - See e.g. Betancourt (2017): `https://arxiv.org/abs/1701.0`



Probabilistic programming in Python

- PyStan
- PyMC3
- Pyro
- TensorFlow Probability

PyMC3

- Python package for for fitting Bayesian models using modern methods (MCMC, variational inference, etc.)
- Well-documented, large suite of statistical models
- Highly flexible, but easy to use
- Uses Theano-backend (not good)
- PyMC4 in development, uses TensorFlow Probability-backend