Bayesian data analysis with TensorFlow Probability

www.tweag.io

Your hosts

Simeon will give the presentation

- background in computational biology
- Data Scientist at Tweag since 2019

Dorran will happily answer questions

- previous positions in geophysics
- Data Scientist at Tweag since 2019

Tweag I/O

TODO

Tweag I/O is a software innovation lab and consultancy based in Paris with employees all around the world.

We specialize in

- software engineering, with a focus on functional programming
- DevOps, with a focus on reproducible software systems and builds
- data science

What you're in for

This tutorial consists of alternating blocks of

- theory / example slides
- practical examples on either external websites or Google Colab notebooks. Links are provided at `https://github.com/tweag/tutorial-dsc-2020/`

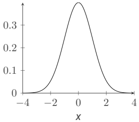
Requirements:

- a Google account (for the practical exercises)
- elementary knowledge in probability theory and statistics

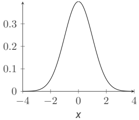
Reminder: Probabilities

Probability distributions can be...

discrete: $\mathrm{Ber(k; b)} = b^k(1-b)^{1-k}$



continuous: $\mathcal{N}(\mathrm{x}; \mu, \sigma) = \frac{1}{\sqrt{2\pi\sigma^2}} \, \mathrm{exp}(-\frac{1}{2\sigma^2}(x-\mu)^2)$



Important concepts:

Conditional probability

$p(A|B)$: probability that A is true, given B is true

Joint probability

$p(A,B)$: probability that both A and B are true

Conditional joint probability

$p(A,B|C)$: probability that both A and B are true, given C is true

Bayesian vs frequentist probabilities

Example: fair coin flip with $p(\text{head}) = p(\text{tail}) = \frac{1}{2}$

Frequentist probability

$p(\text{"flip results in head"}|b = \frac{1}{2}) = \frac{1}{2}$:

$\frac{\text{\# of heads}}{\text{\# total flips}}$ for ∞ many fair coin flips

Bayesian probability

$p(\text{"flip results in head"}|b = \frac{1}{2}) = \frac{1}{2}$:

measure of *belief* in the statement "flip results in head" given single fair coin flip

TODO: this slide looks complicated and is aesthetically offputting

Prior beliefs

Assume: unknown bias b

Prior probability

Encodes prior belief in b *before* flipping the coin

What is known about b?

- b is a probability: $0 \leq b \leq 1$
- most coins are fair

$\rightarrow$ choose prior distribution defined between 0 and 1, with maximum at and symmetric around $b = \frac{1}{2}$

Example:

$$b \sim \text{Beta}(\alpha = 2, \beta = 2)$$

with

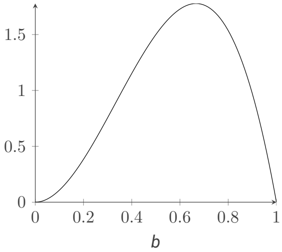
$$\text{Beta}(x; \alpha, \beta) \propto x^{\alpha-1}(1-x)^{\beta-1}$$

Posterior belief

Now: flip coin one time, result: head

Posterior belief

$p(b|\text{head})$: updated prior belief after obtaining new data



Update rule

Bayes' theorem

$$p(A|B) = \frac{p(B|A) \times p(A)}{p(B)}$$

(easily derived from rules for conditional probabilities)

In data analysis:

$$\underbrace{p(x|D,I)}_{\text{posterior}} = \underbrace{p(D|x,I)}_{\text{likelihood}} \times \underbrace{p(x|I)}_{\text{prior}} \,/\, \underbrace{p(D|I)}_{\text{evidence}}$$

x: model parameter

D: data

I: prior information (often not made explicit)

Likelihood

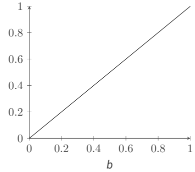
$p(D|x)$: probability of the data given fixed model parameters
$\rightarrow$ models data-generating process

In our case:

$$p(k|b) = b^k(1-b)^{k-1} = \mathrm{Ber}(k; b)$$

with

$$k = \begin{cases} 0: & \text{tail} \\ 1: & \text{head} \end{cases}$$



Evidence

$p(D) = \int \mathrm{d}x\, p(D|x)p(x)$:

normalization constant (long story...)

In our case:

$$
\begin{aligned}
p(k=1) &= \int_0^1 \mathrm{d}b\, L(k=1|b)p(b) \\
&= \int_0^1 \mathrm{d}b\;\; \mathrm{Ber}(k;b) \times \mathrm{Beta}(k;\alpha=2,\beta=2)\big|_{k=1} \\
&= \int_0^1 \mathrm{d}b\;\; b^k(1-b)^{k-1}b(1-b)\Big|_{k=1} \\
&\vdots \\
&= \frac{1}{12}
\end{aligned}
$$

Evidence

$p(D) = \int \mathrm{d}x \; p(D|x)p(x)$:

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In our case:

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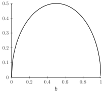
&= \int_0^1 \mathrm{d}b \;\; b^k(1-b)^{k-1} b(1-b)\Big|_{k=1} \\
&\;\vdots \\
&= \frac{1}{12}
\end{aligned}
$$

YIKES

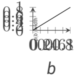
Update rule

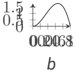
In our coin flip example:

prior: $$p(b) = \text{Beta}(b; \alpha = 2, \beta = 2) \propto b(1-b)$$



likelihood: $$p(D|b) = \text{Ber}(k = 1; b) = b$$





posterior: $$p(b|D) \propto p(D|b) \times p(b)/p(D) = \text{Beta}(b; \alpha = 3, \beta = 2) \propto b^2(1-b)$$

$L(D|b)$

– no slides for interactive stuff –

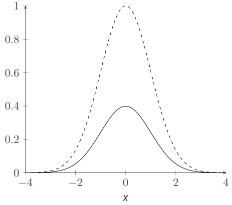
Real-world Bayesian data analysis

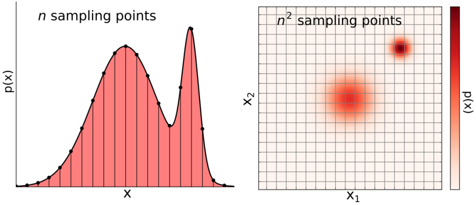
In the real world, probability distributions often

- are multidimensional
- are known only up to a normalization constant (intractability)
- have highly correlated random variables

Consequences:

- analytical evaluation of expectation values is impossible
- naïve sampling approaches are inefficient (curse of dimensionality)





Approximation workhorse: Metropolis-Hastings

Markov chain

Random process with

$$p(x_{i+1}|x_i, x_{i-1}, \ldots, x_1) = p(x_{i+1}|x_i)$$

$\rightarrow$ a Markov chain has no "memory"

In some conditions: converges to a unique invariant distribution $\pi(x)$

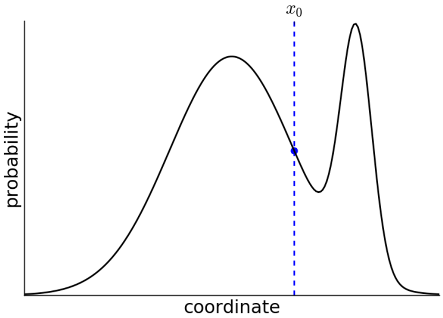
Metropolis-Hastings algorithm

Construct Markov chain with invariant distribution $\pi(x) = p(x)$:

1. starting at state, x_i, propose a new state x_i^* from $q(x_i^*|x_i)$
2. calculate acceptance probability p_{acc}
3. draw $u \sim \mathcal{U}(0, 1)$
4. if $u < p_{\mathrm{acc}}$: $x_{i+1} = x_i^*$, else $x_{i+1} = x_i$

Metropolis(-Hastings)

Initialize with any state x_0



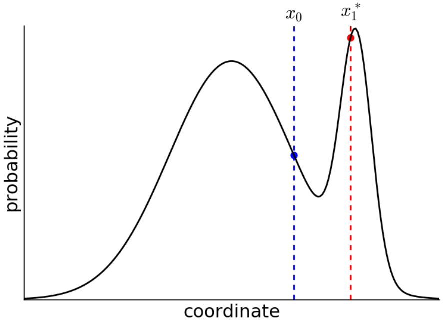
Sequence of states:
(x_0)

Metropolis et al., J. Chem. Phys (1953); Hastings, Biometrika (1970)

Metropolis(-Hastings)

Initial state: x_0

1. calculate a proposal state x_0^* by randomly perturbing x_0



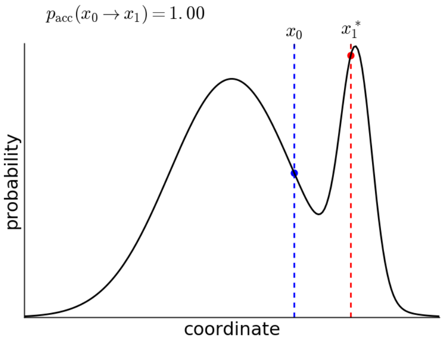
Metropolis et al., J. Chem. Phys (1953); Hastings, Biometrika (1970)

Metropolis(-Hastings)

Initial state: x_0

1. calculate a proposal state x_0^* by randomly perturbing x_0
2. calculate acceptance probability

$$p_{\text{acc}} = \min\left(1, \frac{p(x_0^*)}{p(x_0)}\right)$$



Metropolis et al., J. Chem. Phys (1953); Hastings, Biometrika (1970)

Metropolis(-Hastings)

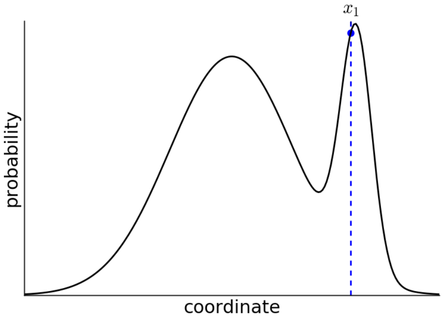
Initial state: x_0

1. calculate a proposal state x_0^* by randomly perturbing x_0
2. calculate acceptance probability

$$p_{\text{acc}} = \min\left(1, \frac{p(x_0^*)}{p(x_0)}\right)$$

3. with probability p_{acc}, accept proposal state x_0^* as the next state x_1, else copy x_0

Sequence of states:
(x_0, x_1)

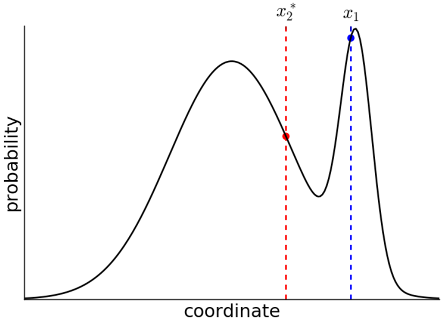


Metropolis et al., J. Chem. Phys (1953); Hastings, Biometrika (1970)

Metropolis(-Hastings)

Current state: x_1

1. calculate a proposal state x_1^* by randomly perturbing x_1



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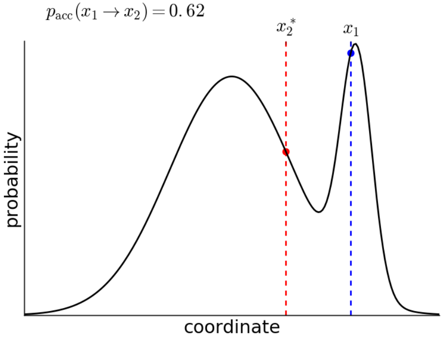

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Metropolis(-Hastings)

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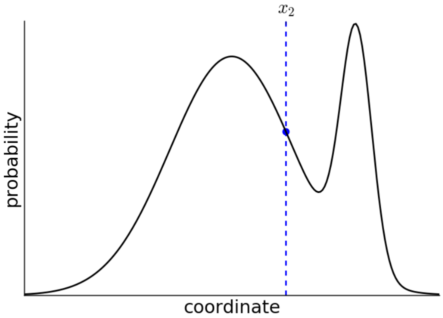
3. with probability p_{acc}, accept proposal state x_1^* as the next state x_2, else copy x_1

Sequence of states:
(x_0, x_1, x_2)



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Metropolis(-Hastings)

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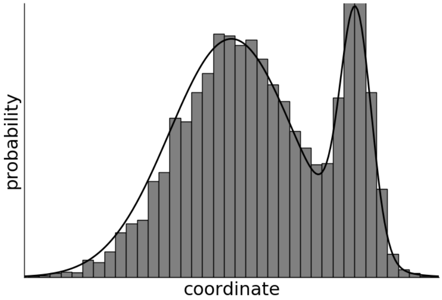
$$p_{\mathrm{acc}} = \min\left(1, \frac{p(x_1^*)}{p(x_1)}\right)$$

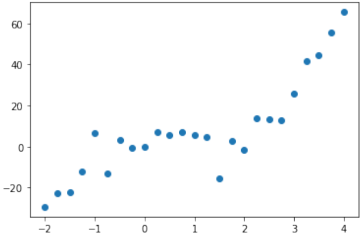
3. with probability p_{acc}, accept proposal state x_1^* as the next state x_2, else copy x_1

Sequence of states:
$(x_0, x_1, x_2, \ldots, x_n)$



Metropolis et al., J. Chem. Phys (1953); Hastings, Biometrika (1970)

Realistic application



Often: measured data = idealized data + noise

Guess:

idealized data: $\hat{f}(x; a, b, c, d) = a + bx + cx^2 + dx^3$

noise: normally distributed

Likelihood:

$$p(y_i | a, b, c, d, \sigma) = \mathcal{N}(\hat{f}(x_i; a, b, c, d), \sigma) \quad \textit{(single data point)}$$

$$p(D | a, b, c, d, \sigma) = \prod_{i=1}^{N} p(y_i | a, b, c, d, \sigma) \quad \textit{(all data points)}$$

Prior:

$$p(a) = p(b) = p(c) = p(d) = \mathcal{N}(0, 5)$$

$$p(\sigma) = \text{Lognormal}(2, 0.5) \text{ (has positive support)}$$