Monte Carlo methods

Nordic Probabilistic AI School

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Outline:

- Aim and scope of Monte Carlo methods
- Markov chain Monte Carlo
- Application: Bayesian linear regression
- Application: Disease transmission model
- Importance sampling and model comparison
- Discussion

Remark: This is a course on effectively applying Monte Carlo methods, rather than developing them from scratch.

However, principled use of MC methods requires a rigorous understanding of how they are implemented. So we need to talk about theory and low-level implementation—all whilst remaining pragmatic.

Code for exercises:

- We'll use `R` scripts and the probabilistic programming language `Stan` .
- This is not a course on coding in `R`: the methods apply generally and `Stan` can be interfaced with other languages, including `Python` and `Julia`.
- Code for the exercises at `https://github.com/charlesm93/stanTutorial/tree/main/Nordic_Prob_AI`

I
Aim and scope of Monte Carlo methods

Goal: compute an intractable expectation value with respect to $\pi(\theta)$.

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- Statistical physics

$$\pi(\theta) \propto \exp\left(-E(\theta)\right)$$

- Bayesian inference

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- Variational inference

$$\pi(\theta) = q(\theta)$$

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What might we want to learn about these distributions?

- Expectation, variance, and quantiles of $f(\theta)$ with respect to π.
- **Monte Carlo:** draw samples and construct sample estimators,

$$\theta^{(1)}, \theta^{(2)}, \cdots, \theta^{(N)} \sim \pi(\theta).$$

- When no exact simulation is possible, use Markov chain Monte Carlo, or importance sampling.

II

Markov chain Monte Carlo

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Can get a sample estimator for mean, variance and quantiles.

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If $\theta^{(1)}, \theta^{(2)}, \cdots, \theta^{(N)}$ are i.i.d,

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We also have a *central limit theorem*, i.e. for large N

$$\widehat{\mathbb{E}}[f(\theta)] \overset{\text{approx}}{\sim} \text{normal}\left(\mathbb{E}f(\theta), \sqrt{\frac{\text{Var}[f(\theta)]}{N}}\right).$$

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- The first samples suffer from a large bias.
- Discard these samples during a burn-in or *warmup* phase.

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3. Return the chain $(\theta^{(1)}, \theta^{(2)}, ..., \theta^{(N)})$.

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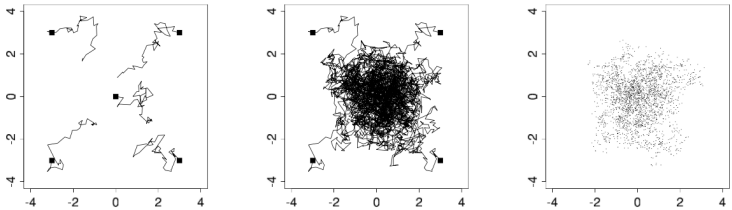

Figure from [Gelman et al., 2013].

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Benefits:

- Only requires evaluating $p(\theta, y) = p(\theta)p(y \mid \theta)$.
- Asymptotically, the algorithm samples from $p(\theta \mid y)$.

Drawbacks:

- In the finite regime, the samples are **biased**.
- The samples are not independent; there are correlated, which **increases the variance** of our Monte Carlo estimators.

Example: Continuous diffusion process

In the limit where we take infinitesimally small steps, many MCMC algorithms can be approximated by a random diffusion process [Gelman et al., 1997, Roberts and Rosenthal, 1998].

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Then after time T,

$$\theta^{(T)} \sim \text{normal}\left[(\mu_0 - \mu)e^{-T} + \mu, \quad \left(\sigma_0^2 - \sigma^2\right) e^{-2T} + \sigma^2\right].$$

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For T large enough, the bias becomes negligible.

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$$\frac{1}{N}\sum_i f(\theta^{(n)}) \overset{\text{approx}}{\sim} \text{Normal}\left(\mathbb{E}[f(\theta)], \frac{\text{Var} f(\theta)}{N_{\text{eff}}}\right)$$

  where N_{eff} is the **effective sample size (ESS)**.

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- $$N_{\text{eff}} = \frac{N}{1 + 2\sum_{t=1}^{\infty} \rho_t}.$$

  ρ_t is the chain's autocorrelation between $\theta^{(i)}$ and $\theta^{(i+t)}$.

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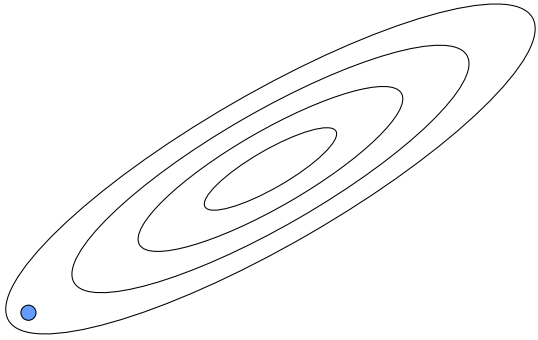
Warmup phase: We run the process for several steps for the bias to become negligible but don't use any of those samples in our Monte Carlo estimator.

Sampling phase: Collect enough samples to have a large ESS and reduce the variance of the Monte Carlo estimator.

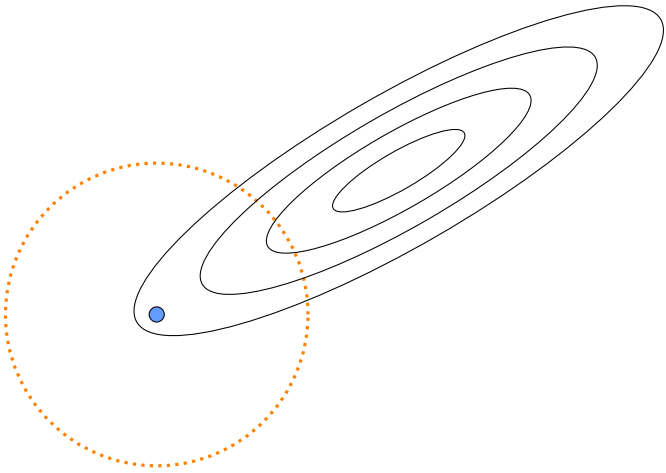
Question: Which transition kernel should we choose? Many choices!

Metropolis, Gibbs, Metropolis-adjusted Langevin approximation, Hamiltonian Monte Carlo,...

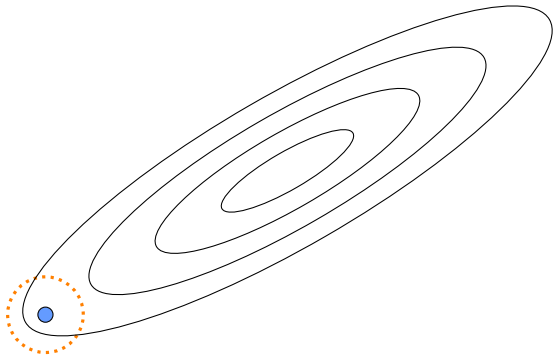
Example: ill-conditioned Gaussian



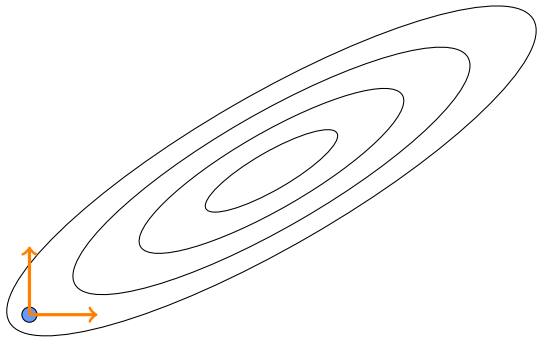
Kernel: Metropolis-Hastings proposal (low acceptance probability)



Kernel: Metropolis-Hastings proposal (small step)



Kernel: Gibbs sampler (moves one coordinate at a time)



Hamiltonian Monte Carlo

- Treat the Markov chain as a physical particle, which evolves over $\mathbb{R}^D$, subject to a *potential*:

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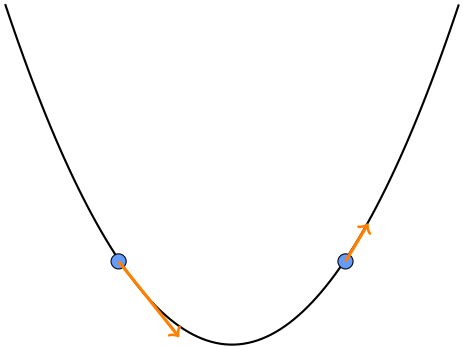
$$\xi_0 \sim \text{normal}(0, M)$$

- Simulate a the laws of classical mechanics for a time T,

$$(\theta_0, \xi_0) \to (\theta_T, \xi_T).$$

$$\frac{\mathrm{d}\theta}{\mathrm{d}t} = M^{-1}\xi, \quad \frac{\mathrm{d}\xi}{\mathrm{d}t} = \nabla_\theta \log p(\theta \mid y).$$

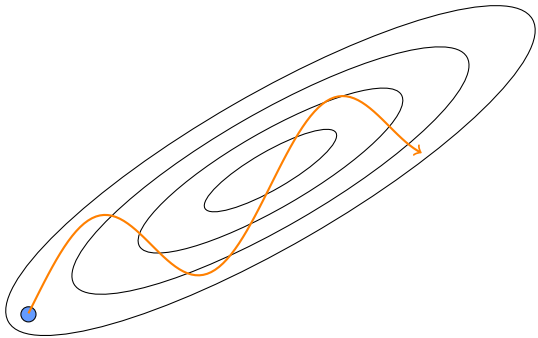


A particle accelerates when $U(\theta) = -\log p(\theta \mid y)$ decreases.

It decelerates when $U(\theta) = -\log p(\theta \mid y)$ increases.

This is based on $\nabla_\theta \log p(\theta \mid y)$.

Kernel: Hamiltonian Monte Carlo



Some challenges in implementing HMC:

- Need to compute $\nabla_\theta \log p(\theta \mid y) \rightarrow$ automatic differentiation
- Tuning parameters:
  - The length of the Hamiltonian trajectory
  - The precision with which we solve Hamilton's equations of motion (step size)
  - The mass matrix of the fictitious particle

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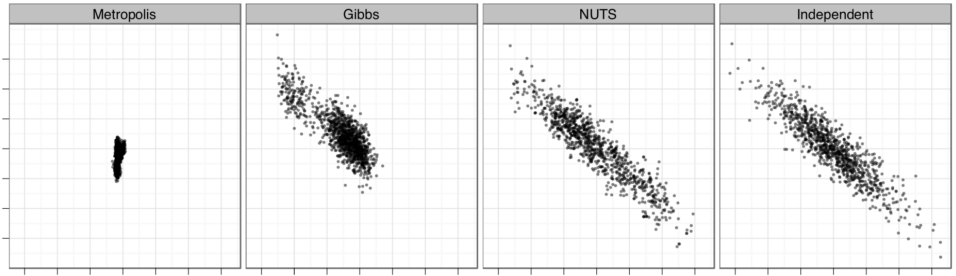
- `Stan` implements autodiff and the No-U-Turn Sampler (NUTS) [Hoffman and Gelman, 2014].
  - Adaptive setting of trajectory length to avoid U-Turns
  - Adaptive tuning of step size and mass matrix during warmup



- Figure from [Hoffman and Gelman, 2014].
- Geometric structures are common in complex models and arise naturally in high dimensions.
- `Stan` implements an improved NUTS sampler [Betancourt, 2018]. I highly recommends Betancourt's paper on HMC for those who want to dive deeper!

III
Application: Bayesian Linear Regression
(warmup example)

How Stan works

- The Stan file specifies the joint distribution

$$p(\theta, y) = p(y|\theta)p(\theta) \propto p(\theta \mid y)$$

- The input includes:
  - the data, y
  - tuning parameters for the algorithm

- The output can include:
  - an approximate sample from the posterior distribution
  - summaries of the run which can help us diagnose problems.

Inference algorithms in `Stan`

- Hamiltonian Monte Carlo (HMC)
- No-U Turn Sampler (NUTS)
- Automatic differentiation variational inference (ADVI)
- Pathfinder Variational Inference
- ...

We can manage the Stan file, the input, and the output using a scripting language, such as:

- `R`
- `Python`
- `Julia`
- The command line
- . . .

The Stan documentation is your friend:
https://mc-stan.org/users/documentation/!!

And so is its community: https://discourse.mc-stan.org/.

Example: Bayesian linear regression

The data generating process is:

$$\begin{aligned} p(\beta) &= \text{Normal}(2, 1) \\ p(\sigma) &= \text{Normal}^{+}(1, 1) \\ p(y \mid \beta, \sigma) &= \text{Normal}\left(\beta x, \sigma\right) \end{aligned}$$

Our goal is to estimate $\theta = (\beta, \sigma)$, based on the observation $z = (x, y)$ and prior knowledge we have of β and σ.

Writing the Stan file

Stan retains certain C++ features:

- Variables need to be declared.
- Each statement must end with a semi-colon.

For example:

```
real x;
real y = 2 * x;
int N;
vector[N] v;
```

Writing the Stan file

```
data {
 Declare the data that will be given as an input.
}

parameters {
 Declare the parameters we want to sample.
}

model {
 Compute the log joint distribution.
}
```

code demo

Convergence diagnostic

Are the chains still biased by their initializations?

Proposition: Start multiple chains at a different locations and check that they all converge to the same distribution.

Examine:

1. the trace plots
2. the density plots
3. the $\widehat{R}$ statistic

$$\widehat{R} := \frac{\text{Standard deviation across all chains}}{\text{Standard deviation within chain}}$$

- If the chains sample from the same target, expect $\widehat{R} \approx 1$.
- If the chains are disagreement, $\widehat{R} \gg 1$.

code demo

A more in-depth look at $\widehat{R}$

Let $\theta^{(nm)}$ be the n^{th} sample from the m^{th} chain.

Let $f : \Theta \to \mathbb{R}$ be some function of interest.

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Can write $\widehat{R}$ as

$$\widehat{R} = \sqrt{\frac{N-1}{N} + \frac{\widehat{B}}{\widehat{W}}},$$

where

- $\widehat{B}$ is the sample variance of $\bar{f}\left(\theta^{(\cdot m)}\right)$.
- $\widehat{W}$ is the (average) within-chain variance.

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$\widehat{R} \leq 1 + \epsilon \iff \widehat{B} \lessapprox 2\epsilon\widehat{W} + \mathcal{O}(\epsilon^2)$.

Want to make sure $\text{Var}\left[f\left(\bar{\theta}^{(\cdot m)}\right)\right]$ is small.

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Question. What can Var $\left[f\left(\bar{\theta}^{(\cdot m)}\right)\right]$ teach us about convergence and bias decay?

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The nonstationary variance measures how well the chains forget their starting points.

As we warmup the chains, both the nonstationary variance and squared bias decay to 0, and so $\widehat{R}$ acts as a "proxy clock" for bias.

A more in-depth look at $\widehat{R}$

- What quantity does $\widehat{R}$ measure and how close to 1 should it be?
  - [Vehtari et al., 2021] propose checking that $\widehat{R} \leq 1.01$.
  - [Margossian et al., 2024] examine $\widehat{R}$ for nonstationary chains and propose a more direct measure of the nonstationary variance.

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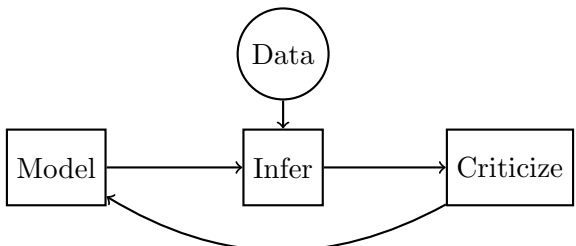
- ESS_{tail} quantifies information for tail estimates [Vehtari et al., 2021].
- Median, $M(\theta)$ and Median Absolute Deviation (MAD),

$$M(|\theta^{(i)} - M(\theta)|)$$

  can be helpful when the first moments are not finite.

Posterior predictive checks

- Recall Box's loop (from *Bayesian Workflow*)!
- Does our model accurately describe the data?



Posterior predictive checks ("check trained model")

Proposition:

Each time we draw a sample, $\theta^{(i)} = \left(\beta^{(i)}, \sigma^{(i)}\right)$, we will also simulate data, according to:

$$y_{\text{pred}}^{(i)} \sim \text{Normal}\left(x\beta^{(i)}, \sigma^{(i)}\right)$$

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Want to study the posterior predictive distribution,

$$p(y_{\text{pred}} \mid y) = \int_{\Theta} p(y_{\text{pred}} \mid \theta) p(\theta \mid y) \mathrm{d}\theta.$$

code demo

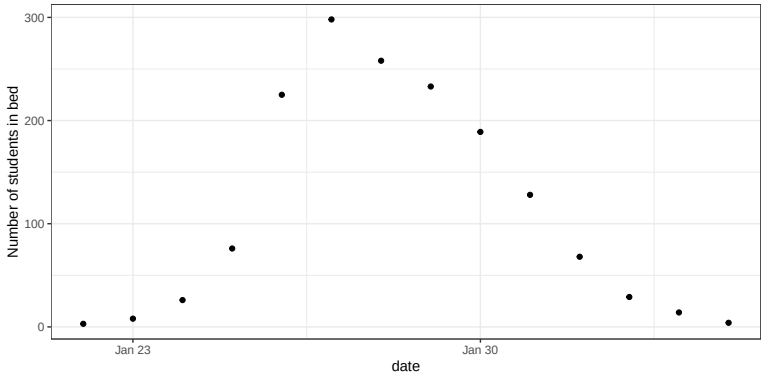
Improving the model

- The ppc suggest our model can improve with an intercept parameter.
- *Exercise: repeat the above procedure, but this time add an intercept parameter* β_0*. Check that the inference is reliable and perform new posterior predictive checks.*

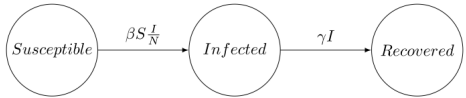
III
Disease transmission model

1978 influenza outbreak in a British boarding school.

Data: daily number of students in bed.



Susceptible-Infected-Recovered (SIR) model



N: total number of individuals,
$N = S + I + R$.

$$\begin{aligned} \dot{S} &= -\beta SI/N \\ \dot{I} &= \beta SI/N - \gamma I \\ \dot{R} &= \gamma I \end{aligned}$$

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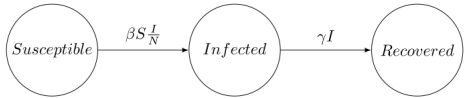

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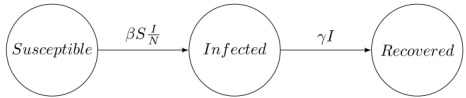

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N: total number of individuals, $N = S + I + R$.

β: transmission rate.

γ: rate of recovery of infected individuals.

- I/N: the proportion of infectious individuals.
- $\beta(I/N)$: the probability that a single susceptible individual becomes infected in one day.

Which measurement model should we use?

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1. *Poisson* likelihood parameterized by $\lambda(t) = I(t)$.
   - Then $\mathbb{E}(y(t)) = I(t)$ and $\text{Var}\,(y(t)) = I(t)$.
   - `array[n_days] vector[3] y = ode_rk45(sir, y0, t0, ts, beta,gamma,N);`
   - `cases` $\sim$ `poisson(y[, 2])`;

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   - Then $\mathbb{E}(y(t)) = I(t)$ and $\text{Var}\,(y(t)) = I(t) + \frac{I(t)^2}{\phi}$.
   - In Stan use `neg_binomial_2`.
   - Define in `parameters` block ϕ^{-1}.
   - `real phi = 1 ./ phi_inv;`
   - `cases` $\sim$ `neg_binomial_2(y[,2], phi);`

Which prior should we use?

- $p(\beta) = \text{normal}^+(2, 1)$: restricts β to be positive and $p(\beta < 4) = 0.975$.
- $p(\gamma) = \text{normal}^+(0.4, 0.5)$: restricts γ to be positive and $p(\gamma < 1) = 0.9$, i.e. 90% of the time, we expect the average time spent in bed to be less than 1 day).
- $p(\phi^{-1}) = \text{exponential}(5)$, see [Grinsztajn et al., 2021].

code demo

Additional controls for the MCMC sampler.

- Number of (parallel) chains
- Number of warmup iterations
- Number of sampling iterations

Exercise: *Write and fit an SIR model for the 1978 influenza outbreak.*

- *Check the standard diagnostics ($\widehat{R}$ and ESS) and examine the density and trace plots. Is the inference reliable?*
- *Do posterior predictive checks: does the model accurately describe the data?*
- *Report β, γ, $R_0 = \beta/\gamma$ and the recovery time $T = 1/\gamma$.*
- *How precise are your estimates of T? Should you run longer Markov chains? Shorter ones?*
- *Compare the two proposed measurement models: Poisson and negative binomial.*

For more about this model (e.g. choice of priors), see [Grinsztajn et al., 2021].

For discussion on length of Markov chains, see [Margossian and Gelman, 2024].

IV
Model Comparison

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  - **Training set:** The data y_{train} used to learn the parameters, and on which we condition the posterior,
    $$p(\theta \mid y_{\text{train}}).$$
  - **Validation set:** The data y_{val} we use to "test" the model's predictions.

    Example: At $t = 12$, the model predicts $\tilde{y}(t = 12)$. Compute the *prediction error*,
    $$\text{Err} = \left(\tilde{y}(t = 12) - y_{\text{val}}(t = 12)\right)^2.$$

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Suppose we have a normal likelihood, with point estimates for the learned parameters,

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and $\hat{\sigma}$ is unaccounted for!

Instead, let's evaluate the *point-estimate log predictive density*,

$$\begin{aligned} \text{p-lpd} &= \log p(y_{\text{val}}(t) \mid \hat{\mu}, \hat{\sigma}) \\ &= \text{const.} - \log \hat{\sigma} - \frac{1}{2\hat{\sigma}^2}(y_{\text{val}}(t) - \hat{\mu}(t))^2. \end{aligned}$$

Testing *uncertainty calibration* in (point) predictions

Suppose we have a Bernoulli likelihood, with point estimates for the learned parameters,

$$\text{Bernoulli}(\hat{\pi}(t)).$$

Our "best" prediction is $\tilde{y}(t) = \mathbb{I}[\hat{\pi}(t) > 0.5]$.

Then the prediction error is

$$\text{Err} = \mathbb{I}[\tilde{y}(t) = y_{\text{val}}(t)].$$

Instead, let's evaluate the *point-estimate log predictive density*,

$$\begin{aligned} \text{p-lpd} &= \log p(y_{\text{val}}(t) \mid \hat{\pi}(t)) \\ &= y_{\text{val}}(t) \log \hat{\pi}(t) + (1 - y_{\text{val}}(t)) \log(1 - \hat{\pi}(t)). \end{aligned}$$

Testing *uncertainty calibration* in Bayesian predictions

We have a general strategy which accounts for uncertainty in the likelihood for a fixed θ,

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In a Bayesian framework, we integrate with respect to the posterior and obtain the *expected log predictive density*,

$$\begin{aligned} \text{elpd} &= \log p(y_{\text{val}}(t) \mid y_{\text{train}}) \\ &= \log \int_{\Theta} p(y_{\text{val}}(t) \mid \theta) p(\theta \mid y_{\text{train}}) \mathrm{d}\theta. \end{aligned}$$

How do we split the data (t, y) into a training and a test set?

Proposition: Do *leave-one-out cross validation* and compute

$$\text{elpd}_{\text{loo}} = \sum_{i=1}^{N} \log p(y_i \mid y_{-i}),$$

where

$$p(y_i \mid y_{-i}) = \int_{\Theta} p(y_i \mid \theta) p(\theta \mid y_{-i}) \mathrm{d}\theta.$$

Recap.

Prediction error based on "best" prediction, $(y_{\text{val}} - \tilde{y})^2$

$\rightarrow$ point-wise log predictive score, p-lpd $= \log p(y_{\text{val}} \mid \hat{\theta})$

$\rightarrow$ expected log predictive score, elpd $= \log p(y_{\text{val}} \mid y_{\text{train}})$

$\rightarrow$ loo CV, $\text{elpd}_{\text{loo}} = \sum_{i=1}^{N} \log p(y_i \mid y_{-i})$

How do we estimate elpd_{loo} efficiently?

Importance Sampling

- **Idea:** Suppose we need to estimate an expectation with respect to $\ell(\theta)$,

$$\int_{\Theta} f(\theta)\ell(\theta)\mathrm{d}\theta,$$

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$$\widehat{\mathbb{E}}f(\theta) = \frac{1}{S}\sum_{s=1}^{S} f(\theta^{(s)})\frac{\ell(\theta^{(s)})}{q(\theta^{(s)})}.$$

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Proposition

When the y_j's are independent conditioned on θ, the importance sampling Monte Carlo estimator is

$$\widehat{p}(y_i \mid y_{-i}) = \frac{1}{\sum_{s=1}^{S} \frac{1}{p(y_i|\theta^{(s)})}},$$

where $\theta^{(s)} \sim p(\theta \mid y)$.

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- The R package `loo` computes PSIS.
- In Stan 's `generated quantities`, need to compute `log_lik`, where

```
log_lik[i] = log p(cases[i] | theta);
```

Exercise: *Compare the predictive scores of the SIR models.*

- *Evaluate in* `generated quantities` *the log probability mass functions using* `poisson_lpmf` *and* `neg_binomial_2_lpmf`*.*
- *In R, use the* `loo` *package to compute the PSIS estimates of the* elpd_{loo}*.*
- *Check* $\hat{k}$ *to see if the IS estimators are reliable.*
- *Which likelihood achieves the best predictive score?*

V
Concluding Remarks

Where does Stan fit in the Bayesian modeler's toolkit?

Historical contribution:

- Stan was born around 2012.
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Several algorithms were developed as part of Stan 's development:

- Adaptive Hamiltonian Monte Carlo [Hoffman and Gelman, 2014, Betancourt, 2018]
- ADVI: a black box variational inference [Kucukelbir et al., 2017]
- PathFinder: an improved variational inference [Zhang et al., 2022].

- Adjoint-differentiated Laplace approximation [Margossian et al., 2020]
- Delayed rejection HMC [Modi et al., 2023]
- GIST sampler [Bou-Rabee et al., 2024]

Stan by the people, for the people

- Stan is open source: https://github.com/stan-dev
- Contributing new functions to Stan : https://github.com/stan-dev/stan/wiki/Contributing-New-Functions-to-Stan

- Straightforward to interface Stan with your own gradient-based algorithm (written in your language of choice), via BridgeStan: https://roualdes.github.io/bridgestan/latest/.

StanCon 2024

Conference on Stan programming and Bayesian Modeling

Oxford University, UK. September 2024

https://mc-stan.org/events/stancon2024/

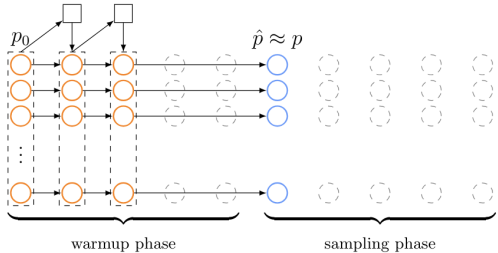

Figure 5: *Many-short-chains regime using cross-chain adaptation. Using many chains reduces the length of the sampling phase required to achieve a target precision. Cross-chain adaptation pools information between the chains to tune the sampler during the warmup phase. For some problems, the improved adaptation means we achieve an acceptable bias with fewer warmup iterations per chain.*

- A lot of other probabilistic programming languages out there: `PyMC`, `Turing`, `TensorFlow Probability`, `PyTorch`, etc.
- Ongoing work with the TFP team to build GPU-friendly samplers. See [Lao et al., 2020, Margossian and Gelman, 2024].

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(a high-level comparison)

Markov chain Monte Carlo

Variational inference

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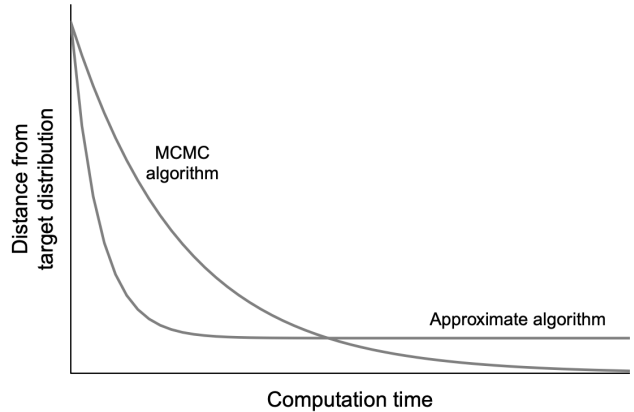

Figure from [Gelman et al., 2020].

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