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 <u>not</u> 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
$$\pi(\theta) = p(\theta \mid y) \propto p(\theta)p(y \mid \theta)$$
- 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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Markov chain Monte Carlo:

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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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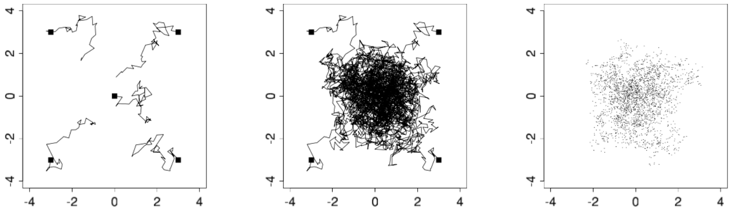

Figure from [Gelman et al., 2013].

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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 <u>not</u> 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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$$\frac{1}{N}\sum_i f(\theta^{(n)}) \overset{\text{approx}}{\sim} \text{Normal}\left(\mathbb{E}[f(\theta)], \frac{\text{Var} f(\theta)}{N_{\text{eff}}}\right)$$

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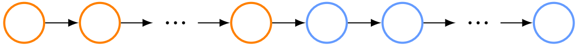
- $$N_{\text{eff}} = \frac{N}{1 + 2\sum_{t=1}^{\infty} \rho_t}.$$

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

Handling the error of MCMC



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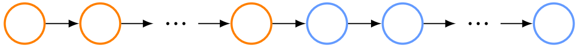

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Warmup phase: We run the process for several steps for the bias to become negligible but don't use any of those samples in our Monte Carlo estimator.

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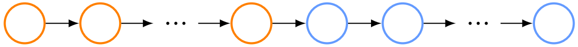


In practice, MCMC proceeds in two phases:

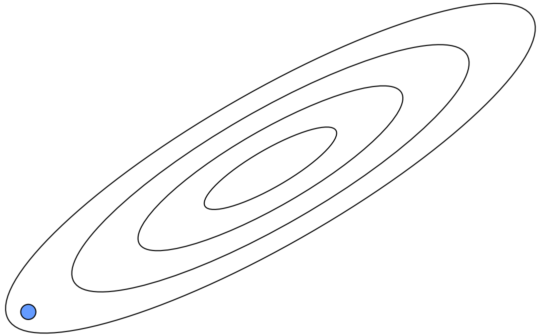
Warmup phase: We run the process for several steps for the bias to become negligible but don't use any of those samples in our Monte Carlo estimator.

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

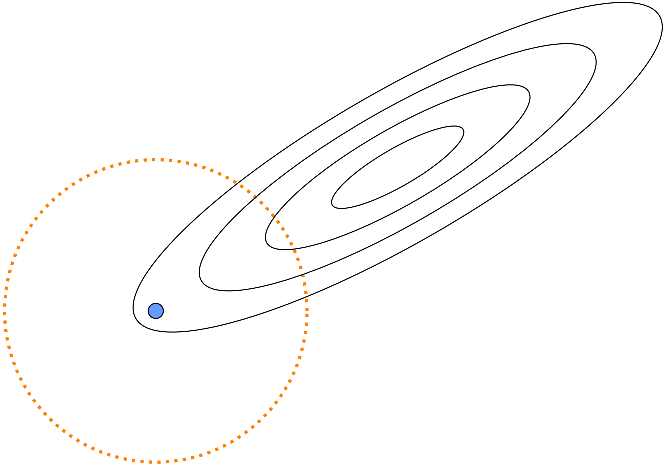
Question: Which transition kernel should we choose? Many choices!

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

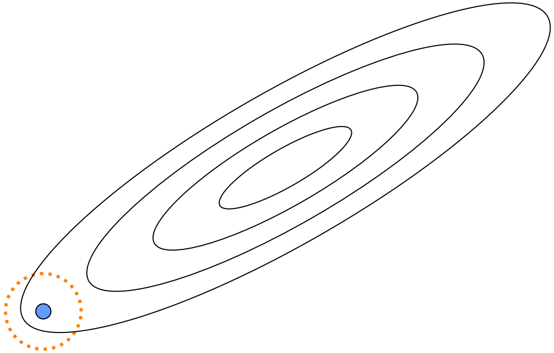
Example: ill-conditioned Gaussian



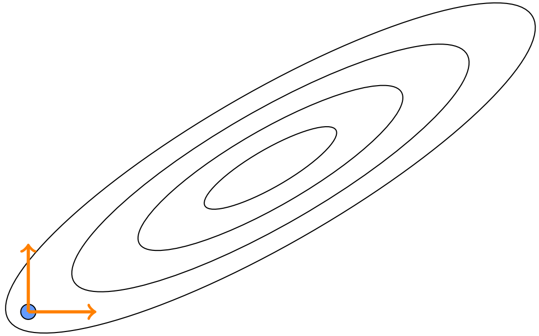
Kernel: Metropolis-Hastings proposal (low acceptance probability)



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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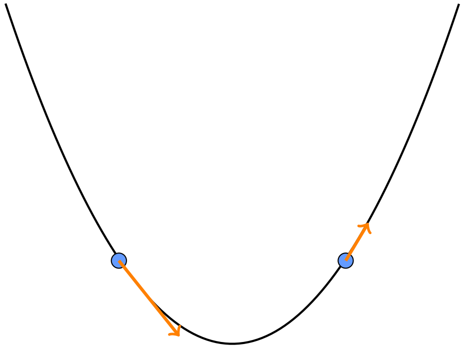
$$\xi_0 \sim \text{normal}(0, M)$$
- Simulate a the laws of classical mechanics for a time T,
$$(\theta_0, \xi_0) \to (\theta_T, \xi_T).$$

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

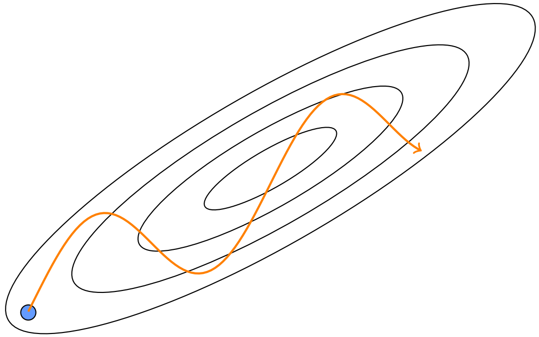


A particle <u>accelerates</u> when $U(\theta) = -\log p(\theta \mid y)$ decreases.

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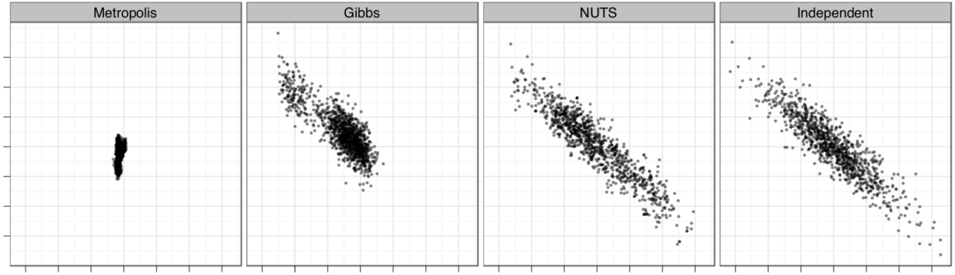
- `Stan` implements autodiff and the No-U-Turn Sampler (NUTS) [Hoffman and Gelman, 2014].
    - Adaptive setting of trajectory length to avoid U-Turns
    - Adaptive tuning of step size and mass matrix during warmup



- 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;
```

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 $\bar{f}\left(\theta^{(\cdot m)}\right)$.
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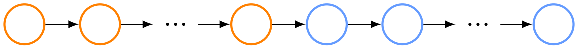
$\widehat{R} \leq 1 + \epsilon \iff \widehat{B} \lessapprox 2\epsilon\widehat{W} + \mathcal{O}(\epsilon^2)$.

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

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



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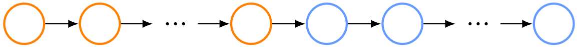

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$$\text{Var}\left(\bar{f}^{(\cdot m)}\right) = \text{Var}\left(\mathbb{E}\left(\bar{f}^{(\cdot m)} \mid f^{(0)}\right)\right) + \mathbb{E}\left(\text{Var}\left(\bar{f}^{(\cdot m)} \mid f^{(0)}\right)\right).$$

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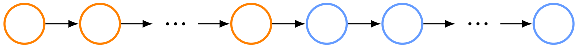

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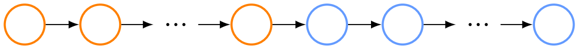

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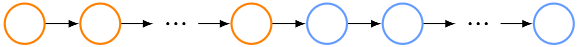
As we warmup the chains, both the nonstationary variance and squared bias decay to 0, and so $\widehat{R}$ acts as a “proxy clock” for bias.

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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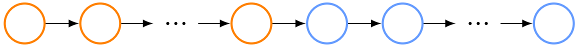

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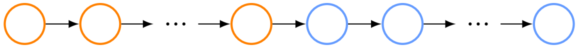

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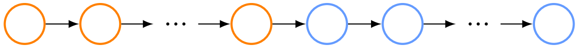

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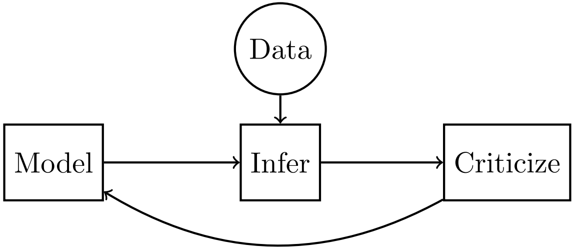
- ESS_{tail} quantifies information for tail estimates [Vehtari et al., 2021].
- Median, $M(\theta)$ and Median Absolute Deviation (MAD),

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

  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:

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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

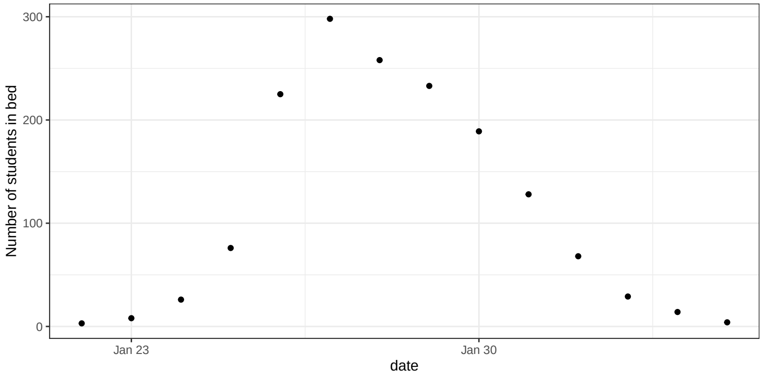
Improving the model

- 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

$$\begin{tikzcd}
\mathit{Susceptible} \arrow[r, "\beta S \frac{I}{N}"] & \mathit{Infected} \arrow[r, "\gamma I"] & \mathit{Recovered}
\end{tikzcd}$$

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
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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 $\operatorname{Var}(y(t)) = I(t)$.

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   - In `Stan` use `neg_binomial_2`.
   - Define in `parameters` block ϕ^{-1}.

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 discussion about this model (e.g. choice of priors, sensitivity tests), see [Grinsztajn et al., 2021].

For more discussion about the length of Markov chains, see [**?**].

IV
Model Comparison

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

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

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

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*,

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

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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

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

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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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].

- Delayed rejection HMC [Modi et al., 2023]
- Adjoint-differentiated Laplace approximation [Margossian et al., 2020]
- 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/`.

- A lot of other probabilistic programming languages out there: `PyMC`, `Turing`, `TensorFlow Probability`, `PyTorch`, etc.

Where do Monte Carlo methods fit in the probabilistic modeling toolkit?
(a high-level comparison)

Markov chain Monte Carlo

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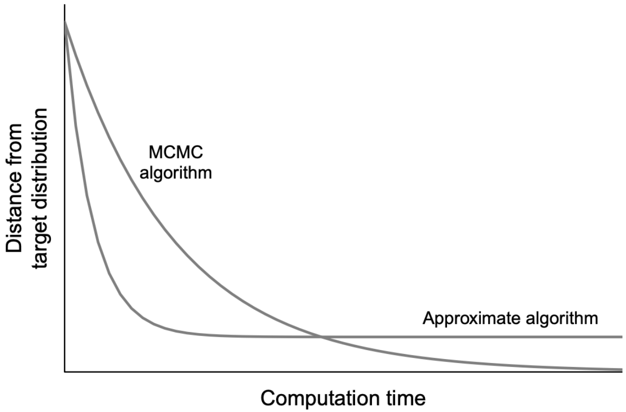

Figure from [Gelman et al., 2020].

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