Approximate Posterior Sampling via Stochastic Optimisation

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- It is useful to understand parameter uncertainty using Bayesian inference
- Usually simulate the Bayesian posterior using Markov Chain Monte Carlo (MCMC) sampling algorithms
- Stochastic gradient MCMC methods combine stochastic optimisation methods with MCMC to reduce computation time

Notation

In the Bayesian approach, the unknown parameter θ is treated as a random variable.

The Bayesian posterior distribution $\pi(\theta|\boldsymbol{x})$ has the form:

$$\pi(\theta|\boldsymbol{x}) \propto p(\theta)\ell(\boldsymbol{x}|\theta) = p(\theta)\prod_{i=1}^{N}\ell(x_i|\theta),$$

where:

- $p(\theta)$ is the prior distribution
- $\ell(x_i|\theta)$ is the likelihood associated with observation i
- N is the size of the dataset

In particular, gradient-based MCMC algorithms use the log posterior $f(\theta)$ to propose moves:

$$f(\theta) = k + f_0(\theta) + \sum_{i=1}^{N} f_i(\theta) \equiv k + \log p(\theta) + \sum_{i=1}^{N} \log \ell(x_i|\theta)$$

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3. Set $\theta_{t+1} = \theta_t + \epsilon_t \nabla \hat{f}(\theta_t) + \gamma(\theta_t - \theta_{t-1})$

There are many ways of speeding up convergence, such as adding in a momentum term.

Stochastic Optimisation

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  If $\sum_{t=1}^{\infty} \epsilon_t = \infty$ and $\sum_{t=1}^{\infty} \epsilon_t^2 < \infty$, then θ_t will converge to a local maximum

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- Usually set $\epsilon_t = (\alpha t + \beta)^{-\gamma}$ with $\gamma \in (0.5, 1]$
- These algorithms only converge to a point estimate of the posterior mode

MCMC

Many problems for which Bayesian inference would be useful involve non-standard distributions and a large number of parameters, making exact inference challenging.

MCMC algorithms aim to generate random samples from the posterior. These samplers construct a Markov chain, often a random walk, which converges to the desired stationary distribution.

Metropolis-Adjusted Langevin Algorithm (MALA)

The Langevin diffusion describes dynamics which converge to $\pi(\theta)$:

$$d\theta(t) = \frac{1}{2}\nabla f(\theta(t)) + db(t)$$

MALA uses the following discretisation to propose samples:

$$\theta_{t+1} = \theta_t + \frac{\sigma^2}{2}\nabla f(\theta_t) + \sigma\eta_t$$

A Metropolis-Hastings accept/reject step is then used to correct discretisation errors, ensuring convergence to the desired stationary distribution.

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2. Accept and set $\theta_{t+1} = \theta^*$ with probability $a(\theta^*, \theta_t) = \min\left\{1, \frac{\pi(\theta^*)q(\theta_t|\theta^*)}{\pi(\theta_t)q(\theta^*|\theta_t)}\right\}$, where $q(x|y) = P(\theta^* = x|\theta_t = y)$

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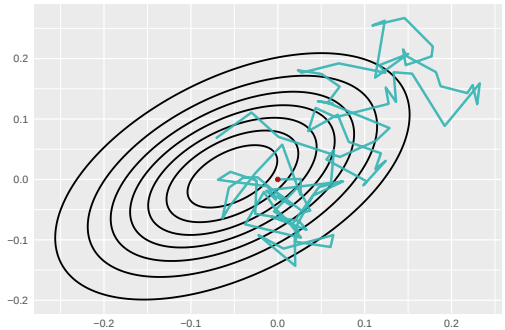
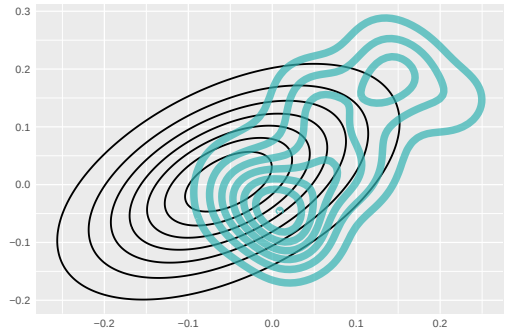
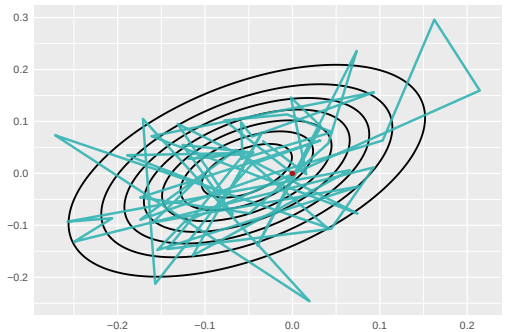
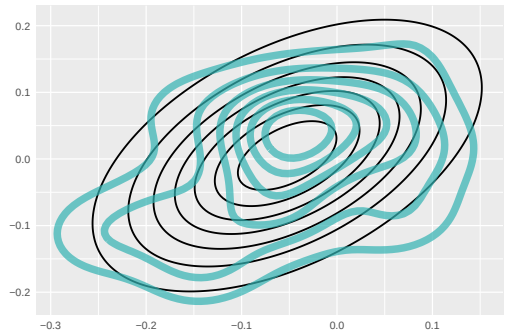
3. If rejected, set $\theta_{t+1} = \theta_t$

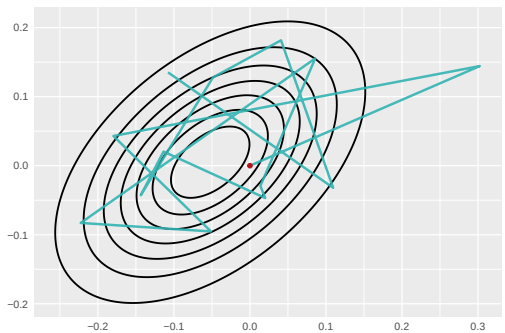
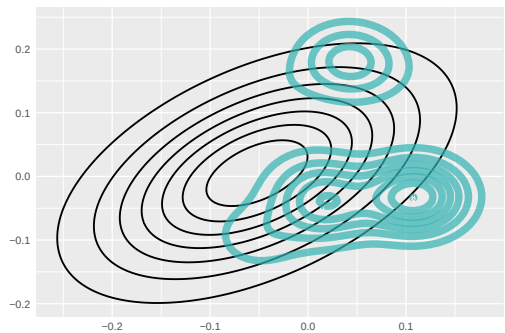
$\sigma = 0.03$ $a = 0.99$

$\sigma = 0.13$ $a = 0.57$

$\sigma = 0.20$ $a = 0.13$

Stochastic Gradient Langevin Dynamics (SGLD)

SGLD aims to reduce the computational cost of MALA by replacing the full gradient calculation in the proposal with the stochastic approximation $\nabla \hat{f}(\theta)$:

$$\theta_{t+1} = \theta_t + \frac{\epsilon_t}{2} \nabla \hat{f}(\theta_t) + \sqrt{\epsilon_t} \eta_t$$

Here, the ϵ_t are decreasing to 0 as in SGA.

Since the Metropolis-Hastings acceptance rate tends to 1 as the step size decreases, the costly accept/reject step is ignored.

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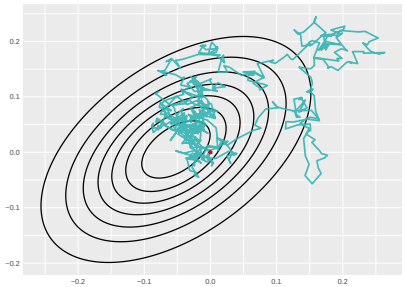
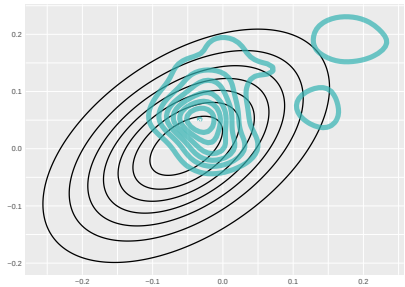
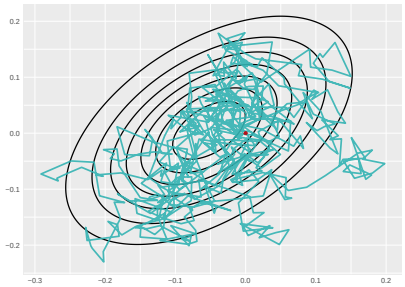
In practice, a fixed step size often works and is far easier to tune.

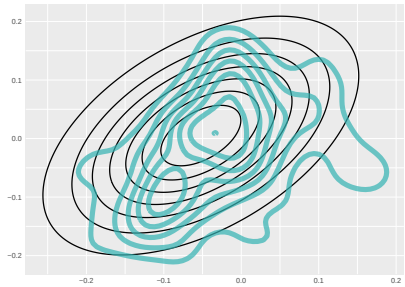
$\epsilon = 0.0001$



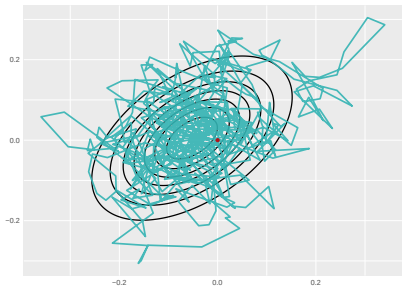


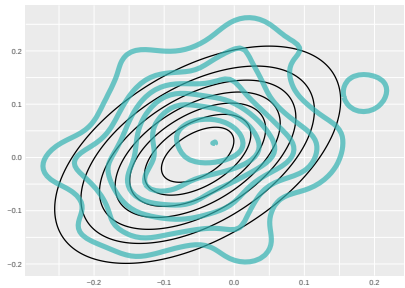
$\epsilon = 0.0005$



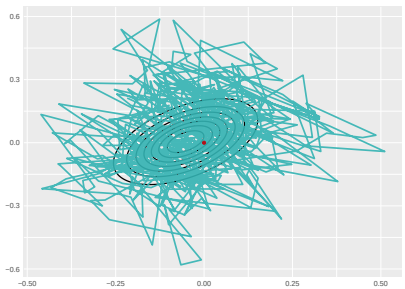


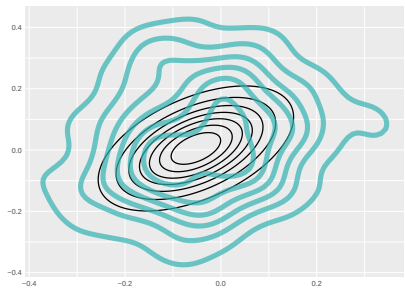
$\epsilon = 0.0013$





$\epsilon = 0.0050$





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- The variance of the gradient estimator can be reduced using control variates
- This is achieved by finding $\hat{\theta}$, a value of θ close to the mode, called the centering value. The gradient estimates in the sampler will condition on $\hat{\theta}$

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In full our new estimate $\nabla \tilde{f}$ is:

$$\nabla f(\hat{\theta}) + \left[\nabla f_0(\theta_t) - \nabla f_0(\hat{\theta})\right] + \frac{N}{n} \sum_{x_i \in S_t} \left[\nabla f_i(\theta_t) - \nabla f_i(\hat{\theta})\right]$$

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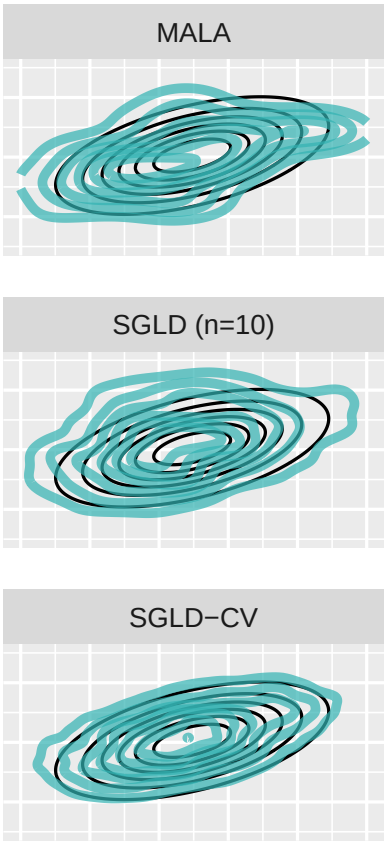
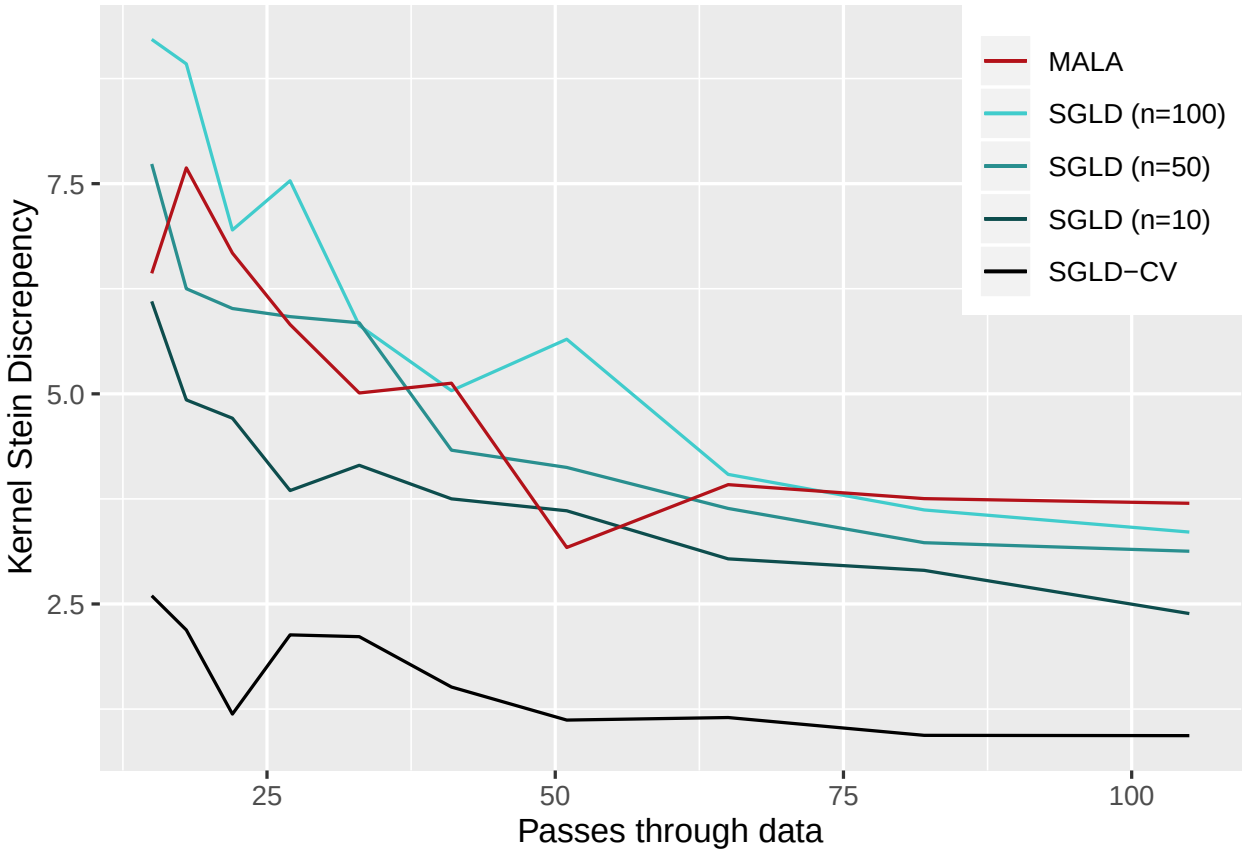
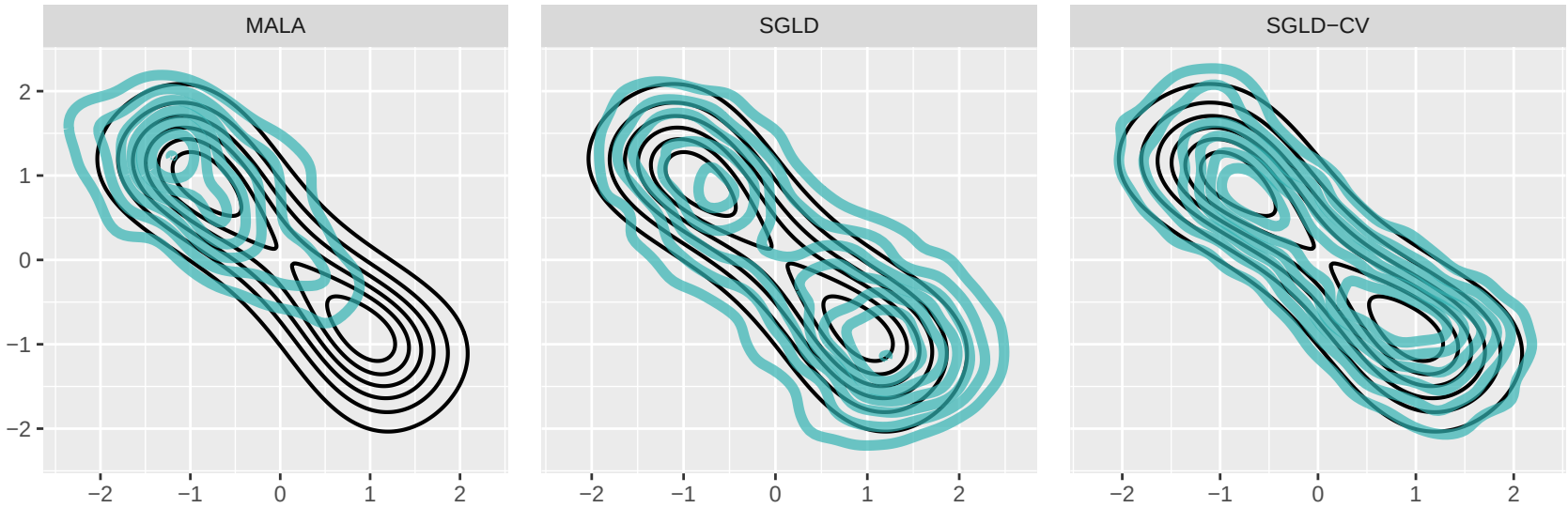

MALA
SGLD (n=10)
SGLD−CV


MALA
SGLD (n=100)
SGLD (n=50)
SGLD (n=10)
SGLD−CV
Kernel Stein Discrepency
7.5
5.0
2.5
25
50
75
100
Passes through data



- Comparison of the samplers for a more complicated multimodal target distribution
- Data distribution: $\boldsymbol{x} \sim \frac{1}{2}N(\mu_1, \sigma) + \frac{1}{2}N(\mu_2, \sigma)$
- Each sampler was given 500 passes through the data and 20 passes of burn-in or optimisation

The Covertype Dataset

The sampling algorithms discussed above were used to fit a binary logistic regression model to the **covertype** dataset.
The aim was to predict the class of tree cover from 54 forest terrain factors.

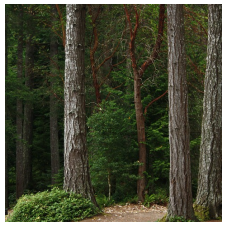
Elevation (m)
Aspect (degrees azimuth)
Slope (degrees)
Horizontal distance to nearest surface water (m)
Vertical distance to nearest surface water (m)
Horizontal distance to nearest roadway (m)
Hillshade 9am (0-255)
Hillshade Noon (0-255)
Hillshade 3pm (0-255)
Horizontal distance to wildfire ignition points (m)
Wilderness area designation x4 (binary)
Soil type x40 (binary)

Class (1-7)

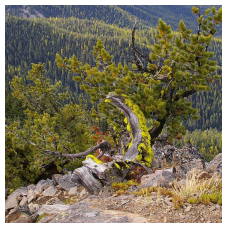

1: Spruce/Fir

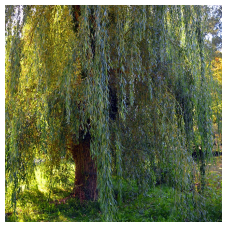

5: Aspen


2: Lodgepole Pine


6: Douglas Fir


3: Ponderosa Pine


7: Krummholz


4: Willow/
Cottonwood

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- Instead of class, used the response variable y where:

$$y_i = \begin{cases} 1, & \text{if class}(\boldsymbol{x}_i) = 2 \\ 0, & \text{else} \end{cases}$$

$$P(y_i = 1|\boldsymbol{x}_i) = \sigma(\beta_0 + \beta^T \boldsymbol{x}_i) \equiv \frac{1}{1 + \exp\left[-(\beta_0 + \beta^T \boldsymbol{x}_i)\right]}$$

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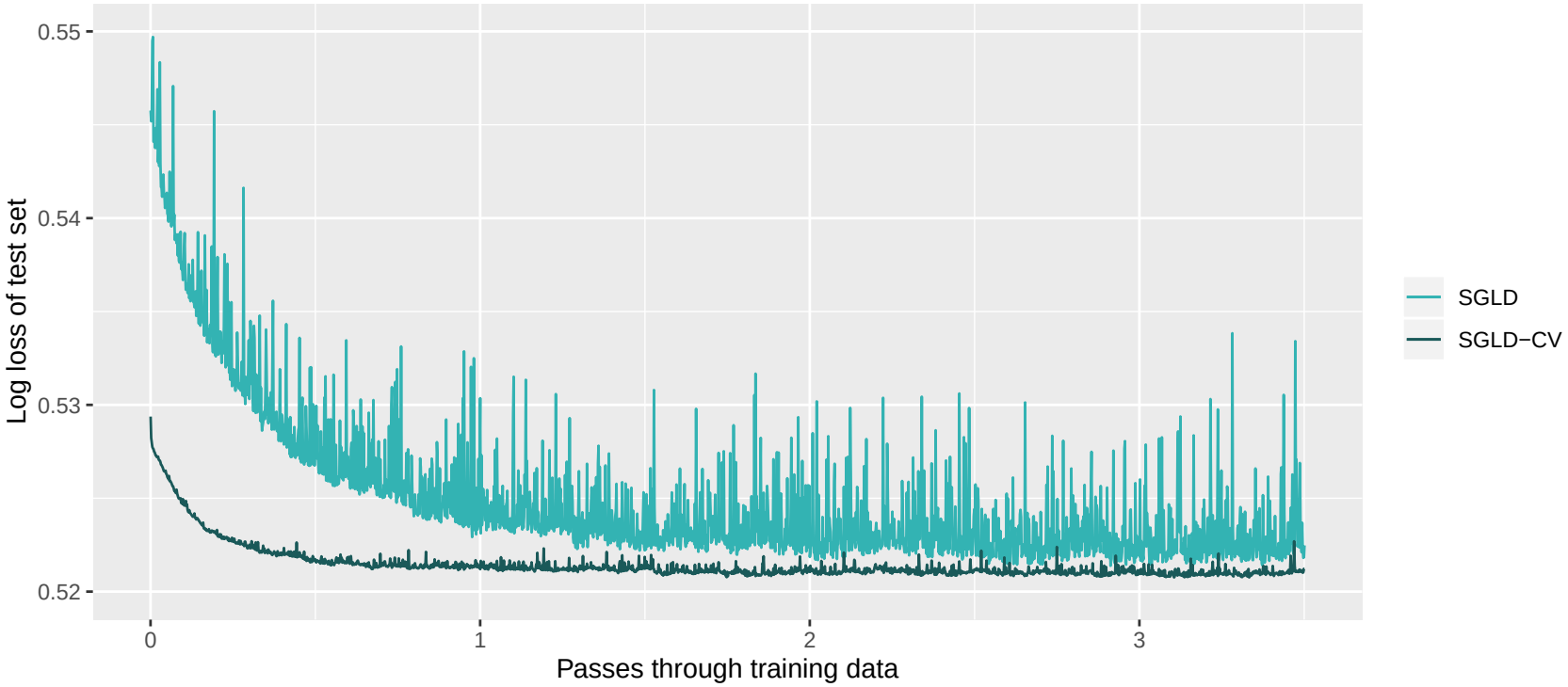
- The training dataset had 570 000 observations and an additional 10 000 were used to test the model



Performance measure: log loss

$$\frac{1}{|T|} \sum_{y_i \in T} [y_i \log(\hat{p}_i) + (1 - y_i) \log(1 - \hat{p}_i)]$$

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- Tuning SGLD is very difficult - have to test a wide range of stepsizes and use a metric like KSD to assess performance
- SGLD-CV also has a high tuning burden, since both the optimisation and the sampling stages have to be tuned
- Gradient calculations had to be done by hand, making it difficult to implement more complicated models
  - It is more practical to use numerical differentiation for this (e.g. sgmcmc for R)

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Any Questions?