02477 – Bayesian Machine Learning: Lecture 9

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Outline

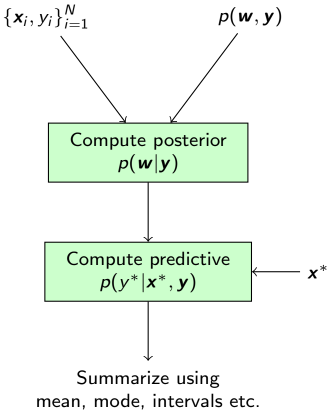
Markov chain Monte Carlo

Bayesian inference and probabilistic modelling

- Bayesian supervised learning in general:
  1. Joint model of data $\boldsymbol{y}$ and parameters $\boldsymbol{w}$.
  2. Summarize knowledge of $\boldsymbol{w}$ given data $\boldsymbol{y}$.
  3. Compute posterior predictive distribution.

- Goal: separate modelling from inference:
  1. Build models reflecting domain knowledge.
  2. Push "inference button" and get results.

- Inference methods:
  1. Laplace approximations.
  2. Markov chain Monte Carlo.
  3. Variational approximations.



Monte Carlo: Posterior inference using samples

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- We can compute expectations wrt. p using the *Monte Carlo estimator*

$$\bar{f} = \mathbb{E}_p\left[f(\boldsymbol{z})\right] = \int f(\boldsymbol{z})p(\boldsymbol{z})\mathrm{d}\boldsymbol{z} \approx \frac{1}{S}\sum_{i=1}^{S} f(\boldsymbol{z}^i) \equiv \hat{f},$$

where $\boldsymbol{z}^i \sim p(\boldsymbol{z})$ for $i = 1, \ldots, S$

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- We showed last time that ...
  1. the Monte Carlo estimator $\hat{f}$ is *unbiased*
  2. the variance of $\hat{f}$ decreases with $1/S$ when the samples are *i.i.d.*

A zoo of sampling-based methods

- Simple sampling methods
  1. Rejection sampling
  2. Ancestral sampling
  3. Importance sampling
  4. Transformation methods
  5. Inverse transform sampling
  6. ...
- MCMC methods
  1. Metropolis-Hastings
  2. Gibbs Sampling
  3. Slice sampling
  4. Hamiltonian Monte Carlo
  5. ...

MCMC using the Metropolis-Hastings algorithm

- We can use the MH to generate samples from a distribution of interest $p(\boldsymbol{z})$.

The Metropolis-Hastings algorithm

- Start from some initial value $\boldsymbol{z}^1$ (e.g., a sample from the prior).
- Repeat for $k = 1$ to K:
  1. Given last value $\boldsymbol{z}^{k-1}$, generate *candidate sample* using proposal distribution
  $$\boldsymbol{z}^\star \sim q(\boldsymbol{z}^\star|\boldsymbol{z}^{k-1}).$$
  2. Compute *acceptance probability* A_k as follows
  $$A_k = \min\left(1, \frac{p(\boldsymbol{z}^\star)q(\boldsymbol{z}^{k-1}|\boldsymbol{z}^\star)}{p(\boldsymbol{z}^{k-1})q(\boldsymbol{z}^\star|\boldsymbol{z}^{k-1})}\right).$$
  3. Simulate $u_k \sim \mathcal{U}(0,1)$ and define $\boldsymbol{z}^k$ as
  $$\boldsymbol{z}^{k+1} = \begin{cases} \boldsymbol{z}^\star & \text{if } u_k < A_k \\ \boldsymbol{z}^{k-1} & \text{otherwise} \end{cases}$$

- What do we need in order to implement MH for a given model?

Markov chain Monte Carlo theory I

- Metropolis-Hastings defines a chain of samples $\boldsymbol{z}^0, \boldsymbol{z}^1, \boldsymbol{z}^2, \dots$ with a *Markov property*

$$p(\boldsymbol{z}^{k+1}|\boldsymbol{z}^1, \boldsymbol{z}^2, .., \boldsymbol{z}^k) = p(\boldsymbol{z}^{k+1}|\boldsymbol{z}^k)$$

- The *transition kernel* tells us how to iterate the chain

$$T(\boldsymbol{z}^{k+1}|\boldsymbol{z}^k) \equiv p(\boldsymbol{z}^{k+1}|\boldsymbol{z}^k)$$

- The distribution of $\boldsymbol{z}^{k+1}$ is given by *sum rule*

$$p(\boldsymbol{z}^{k+1}) = \int T(\boldsymbol{z}^{k+1}|\boldsymbol{z}^k)p(\boldsymbol{z}^k)\mathrm{d}\boldsymbol{z}^k$$

- A distribution $p^*(\boldsymbol{z})$ is said to be *invariant* or *stationary* wrt. the Markov chain if each step does not change the distribution

$$p^*(\boldsymbol{z}) = \int T(\boldsymbol{z}|\boldsymbol{z}')p^*(\boldsymbol{z}')\mathrm{d}\boldsymbol{z}'$$

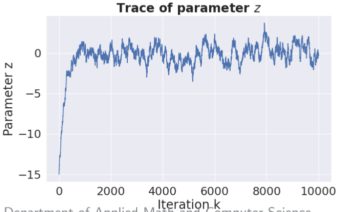
- We require $p^*(\boldsymbol{z})$ to be a limiting distribution of the chain *(independent of the initial distribution)*.

$$p(\boldsymbol{z}^k) \quad \to \quad p^*(\boldsymbol{z}) \qquad \text{for} \qquad k \to \infty$$

Transistion kernel for Metropolis-Hastings

- Recall the acceptance probability for Metropolis-Hastings

$$A(\boldsymbol{z}^\star|\boldsymbol{z}^k) = \min\left[1, \frac{p(\boldsymbol{z}^\star)q(\boldsymbol{z}^k|\boldsymbol{z}^\star)}{p(\boldsymbol{z}^k)q(\boldsymbol{z}^\star|\boldsymbol{z}^k)}\right]$$



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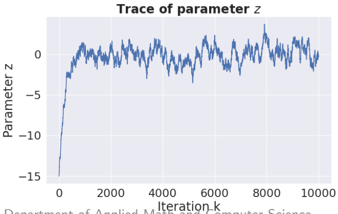

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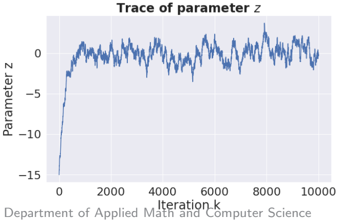
- The big picture

1. We initialize $\boldsymbol{z}^1$.
2. We iterate $\boldsymbol{z}^{k+1}|\boldsymbol{z}^k \sim T(\boldsymbol{z}^{k+1}|\boldsymbol{z}^k)$ (*warm-up phase*).
3. Eventually the distribution of $\boldsymbol{z}^k$ will converge to the target distribution p^* (*sampling phase*).



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- Conditions required for a Markov chain to have a limiting distribution equal to the unique stationary distribution:

(A1) *Irreducible*: all states $\boldsymbol{z}$ can be reached.

$$\text{Counter example:} \quad z^{k+1} = z^k + |e_k|, \quad \text{where} \quad e_k \sim \mathcal{N}(0, 1)$$

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(A3) *Positive recurrent*: the chain has positive probability of returning to any given state (+ finite expected return-time).

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- A chain that satisfies *(A1)–(A3)* is said to be *ergodic* and ensures $p(\boldsymbol{z}^k) \rightarrow p^*(\boldsymbol{z})$.

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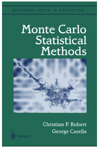
- For example, all (non-degenerate) Gaussian proposals lead to detailed balance, but convergence time may vary drastically depending on the proposal variance.
- More theory and details: Monte Carlo Statistical Methods by Robert and Casella.



Pros and cons of Metropolis-Hastings

Pros

- Strong mathematical guarantees: If we sample long enough, the iterates $\boldsymbol{z}^k$ will converge to the exact target distribution

$$p(\boldsymbol{z}^k) \quad \to \quad p^*(\boldsymbol{z}) \qquad \text{for} \qquad k \to \infty$$

- Easy to implement.
- Easy to prototype and evaluate different models.

Cons

- May have to sample "infinitely" long for difficult distributions.
- Acceptance ratio can be low.
- Slow for large datasets.
- Proposal distribution may require tuning.

Questions: True or false?

Quiz via DTU Learn:

Lecture 9: Metropolis-Hastings (12 questions)

Check you knowledge

Gibbs sampling

Gibbs sampling

- When using Metropolis-Hastings,

  1. we have to choose a proposal distribution (and sometimes tune it), and
  2. it may suffer from low acceptance rates.

- *Gibbs sampling* works by iteratively updating each coordinate of $\boldsymbol{z}$ by sampling from the posterior conditionals $p(z_i|\boldsymbol{z}_{-i})$ ($\boldsymbol{z}_{-i}$ means the entire vector except index i).

The Gibbs Sampler

- Initialize all parameter values $\left\{z_i^0\right\}_{i=1}^D$
- Repeat for $k = 1$ to K:
  - Sample $z_1^k \sim p(z_1|z_2^{k-1}, z_3^{k-1}, \ldots, z_D^{k-1})$.
  - Sample $z_2^k \sim p(z_2|z_1^k, z_3^{k-1}, \ldots, z_D^{k-1})$.
  - Sample $z_3^k \sim p(z_3|z_1^k, z_2^k, z_4^{k-1}, \ldots, z_D^{k-1})$
  - Sample ...
  - Sample $z_D^k \sim p(z_D|z_1^k, z_2^k, z_3^k, \ldots, z_{D-1}^k)$.

Example: Gaussian linear model I

- Suppose we want to derive a Gibbs sampler for the following target distribution

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\begin{aligned}
y|w &\sim \mathcal{N}(y|w_1x_1 + w_2x_2, \sigma^2)\\
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- The posterior distribution is proportional to the joint density $p(y, w_1, w_2)$

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- *General technique* for identifying $p(w_i|y, \boldsymbol{w}_{-i})$:
  1. Write up the log joint density.
  2. Identify all quantities that depends on w_i and ignore the rest.
  3. Identify the distribution $p(w_i|y, \boldsymbol{w}_{-i})$ from its *functional form*.

Example: Gaussian linear model II

- Write out the logarithm of the joint density

$$p(w_1, w_2|y) \propto \mathcal{N}(t|w_1x_1 + w_2x_2, \sigma^2)\mathcal{N}(w_1|0, \kappa^2)\mathcal{N}(w_2|0, \kappa^2)$$

- Recall the expression for a Gaussian density

$$\mathcal{N}(x|m, v) = \frac{1}{\sqrt{2\pi v}} \exp\left(-\frac{(x-m)^2}{2v}\right)$$

- Let's write it out the log density and identify all terms that depend on w_1 or w_2

$\log p(w_1, w_2|y) =$

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$$\begin{aligned}\log p(w_1, w_2|y) = & -\frac{1}{2}\log(2\pi\sigma^2) - \frac{1}{2\sigma^2}(y - w_1x_1 - w_2x_2)^2 + \\ & -\frac{1}{2}\log(2\pi\kappa^2) - \frac{1}{2\kappa^2}w_1^2 - \frac{1}{2}\log(2\pi\kappa^2) - \frac{1}{2\kappa^2}w_2^2 + K\end{aligned}$$

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=& -\frac{1}{2\sigma^2}(y^2 + (w_1 x_1 + w_2 x_2)^2 - 2y(w_1 x_1 - w_2 x_2)) - \frac{1}{2\kappa^2}w_1^2 - \frac{1}{2\kappa^2}w_2^2 + K'
\end{aligned}$$

Example: Gaussian linear model II

- Write out the logarithm of the joint density

$$p(w_1, w_2|y) \propto \mathcal{N}(t|w_1x_1 + w_2x_2, \sigma^2)\mathcal{N}(w_1|0, \kappa^2)\mathcal{N}(w_2|0, \kappa^2)$$

- Recall the expression for a Gaussian density

$$\mathcal{N}(x|m, v) = \frac{1}{\sqrt{2\pi v}} \exp\left(-\frac{(x-m)^2}{2v}\right)$$

- Let's write it out the log density and identify all terms that depend on w_1 or w_2

$$\begin{aligned}
\log p(w_1, w_2|y) = & -\frac{1}{2}\log(2\pi\sigma^2) - \frac{1}{2\sigma^2}(y - w_1x_1 - w_2x_2)^2 + \\
& -\frac{1}{2}\log(2\pi\kappa^2) - \frac{1}{2\kappa^2}w_1^2 - \frac{1}{2}\log(2\pi\kappa^2) - \frac{1}{2\kappa^2}w_2^2 + K \\
= & -\frac{1}{2\sigma^2}(y - w_1x_1 - w_2x_2)^2 - \frac{1}{2\kappa^2}w_1^2 - \frac{1}{2\kappa^2}w_2^2 + K' \\
= & -\frac{1}{2\sigma^2}(y^2 + (w_1x_1 + w_2x_2)^2 - 2y(w_1x_1 - w_2x_2)) - \frac{1}{2\kappa^2}w_1^2 - \frac{1}{2\kappa^2}w_2^2 + K' \\
= & -\frac{1}{2\sigma^2}(w_1x_1 + w_2x_2)^2 + \frac{1}{\sigma^2}y(w_1x_1 - w_2x_2) - \frac{1}{2\kappa^2}w_1^2 - \frac{1}{2\kappa^2}w_2^2 + K''
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\log p(w_1, w_2|y) = & -\frac{1}{2}\log(2\pi\sigma^2) - \frac{1}{2\sigma^2}(y - w_1 x_1 - w_2 x_2)^2 + \\
& -\frac{1}{2}\log(2\pi\kappa^2) - \frac{1}{2\kappa^2}w_1^2 - \frac{1}{2}\log(2\pi\kappa^2) - \frac{1}{2\kappa^2}w_2^2 + K \\
= & -\frac{1}{2\sigma^2}(y - w_1 x_1 - w_2 x_2)^2 - \frac{1}{2\kappa^2}w_1^2 - \frac{1}{2\kappa^2}w_2^2 + K' \\
= & -\frac{1}{2\sigma^2}(y^2 + (w_1 x_1 + w_2 x_2)^2 - 2y(w_1 x_1 - w_2 x_2)) - \frac{1}{2\kappa^2}w_1^2 - \frac{1}{2\kappa^2}w_2^2 + K' \\
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\end{aligned}$$

Example: Gaussian linear model III

- We just arrived at

$$\log p(w_1, w_2|y) = -\frac{1}{2\sigma^2}(w_1^2 x_1^2 + w_2^2 x_2^2 + 2w_1 x_1 w_2 x_2) + \frac{1}{\sigma^2} y(w_1 x_1 - w_2 x_2) - \frac{1}{2\kappa^2} w_1^2 - \frac{1}{2\kappa^2} w_2^2 + K''$$

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- Let's compare that to a generic Gaussian distribution:

$$\begin{aligned}\log \mathcal{N}(w_1|m, v) &= -\frac{1}{2}\log(2\pi v) - \frac{1}{2v}(w_1 - m)^2 \\ &= -\frac{1}{2}\log(2\pi v) - \frac{1}{2v}(w_1^2 + m^2 - 2w_1 m) = -\frac{1}{2v} w_1^2 + \frac{1}{v} m w_1 + C\end{aligned}$$

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$$\log p(w_1, w_2|y) = -\frac{1}{2\sigma^2}(w_1^2x_1^2 + w_2^2x_2^2 + 2w_1x_1w_2x_2) + \frac{1}{\sigma^2}y(w_1x_1 - w_2x_2) - \frac{1}{2\kappa^2}w_1^2 - \frac{1}{2\kappa^2}w_2^2 + K''$$

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- Recall: *The functional form* of the logarithm of a Gaussian density is a quadratic function.

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$$\log p(w_1|y, w_2) = -\frac{1}{2\sigma^2}(w_1^2 x_1^2 + w_2^2 x_2^2 + 2w_1 x_1 w_2 x_2) + \frac{1}{\sigma^2} y(w_1 x_1 - w_2 x_2) - \frac{1}{2\kappa^2} w_1^2 - \frac{1}{2\kappa^2} w_2^2 + K''$$

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$$\log p(w_1, w_2|y) = -\frac{1}{2\sigma^2}(w_1^2 x_1^2 + w_2^2 x_2^2 + 2w_1x_1w_2x_2) + \frac{1}{\sigma^2}y(w_1x_1 - w_2x_2) - \frac{1}{2\kappa^2}w_1^2 - \frac{1}{2\kappa^2}w_2^2 + K''$$

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- We conclude that the distribution $\log p(w_1|y, w_2)$ must be a Gaussian, because *its functional form is quadratic wrt. w_1*.

Example: Gaussian linear model IV

- A generic Gaussian distribution

$$\ln \mathcal{N}(w_1|m, v) = -\frac{1}{2v} w_1^2 + \frac{1}{v} m w_1 + C$$

- We know $p(w_1|y, w_2) = \mathcal{N}(w_1|m_1, v_1)$ is Gaussian, so all we need is a mean and variance

$$\log p(w_1|y, w_2) = -\frac{1}{2}\left(\frac{1}{\sigma^2} x_1^2 + \frac{1}{\kappa^2}\right) w_1^2 + \left(\frac{1}{\sigma^2} y x_1 - \frac{1}{\sigma^2} x_1 w_2 x_2\right) w_1 + K'''$$

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- *Comparing the coefficients* for the *second order term* w_1^2, we get the variance

$$v_1 = \left(\frac{1}{\sigma^2}x_1^2 + \frac{1}{\kappa^2}\right)^{-1}$$

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- *Comparing the coefficients* for the *second order term* w_1^2, we get the variance

$$v_1 = \left(\frac{1}{\sigma^2} x_1^2 + \frac{1}{\kappa^2}\right)^{-1}$$

- and by comparing coefficients for the *first order* term w_1, we get the mean

$$\frac{m_1}{v_1} = \left(\frac{1}{\sigma^2} y x_1 - \frac{1}{\sigma^2} x_1 w_2 x_2\right) \iff m_1 = \frac{v_1}{\sigma^2}\left(y x_1 - x_1 w_2 x_2\right)$$

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- A generic Gaussian distribution

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$$\log p(w_1|y, w_2) = -\frac{1}{2}\left(\frac{1}{\sigma^2}x_1^2 + \frac{1}{\kappa^2}\right) w_1^2 + \left(\frac{1}{\sigma^2} y x_1 - \frac{1}{\sigma^2} x_1 w_2 x_2\right) w_1 + K'''$$

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- *By symmetry*, we get $p(w_2|y, w_1) = \mathcal{N}(w_2|m_2, v_2)$

$$v_2 = \left(\frac{1}{\sigma^2}x_1^1 + \frac{1}{\kappa^2}\right)^{-1} \iff m_2 = \frac{v_2}{\sigma^2}\left(y x_2 - x_2 w_1 x_1\right)$$

Example: Gaussian linear model V

- Initialize w_1 and w_2.

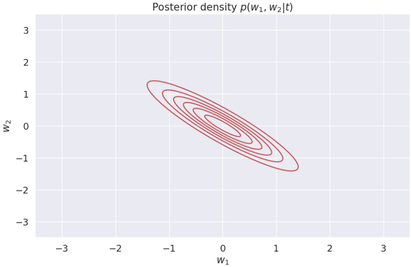
1. Sample w_1 conditioned w_2,

$$w_1 \sim p(w_1|y, w_2) = \mathcal{N}(w_1|m_1, v_1).$$

2. Sample w_2 conditioned w_1,

$$w_2 \sim p(w_2|y, w_1) = \mathcal{N}(w_2|m_2, v_2).$$

3. Repeat.



Example: Gaussian linear model V

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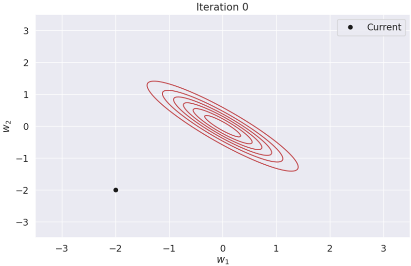

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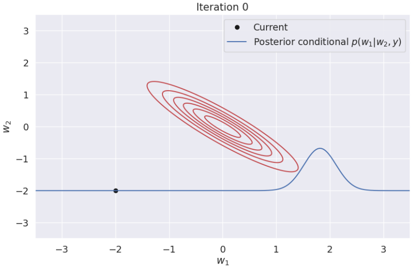

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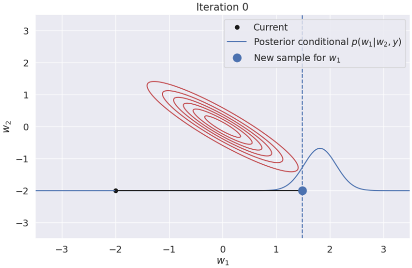

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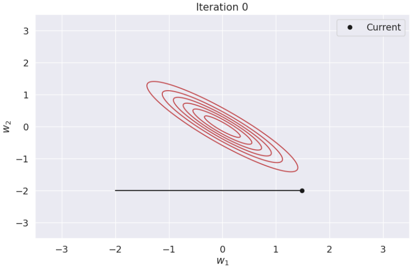

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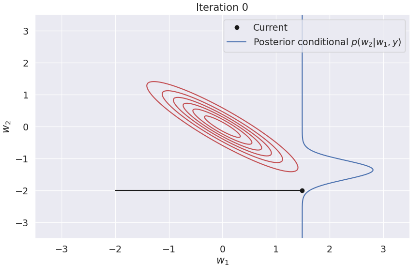

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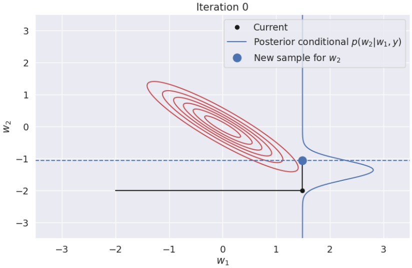

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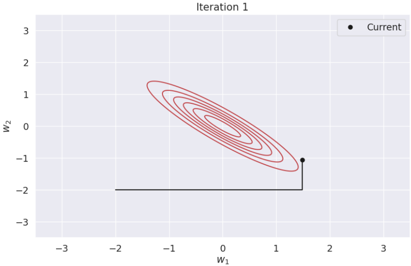

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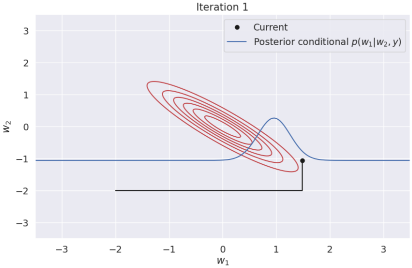

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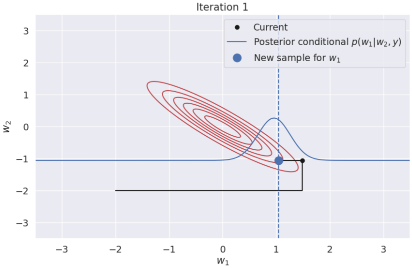

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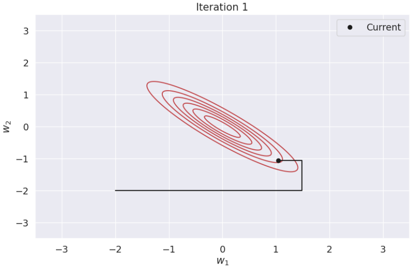

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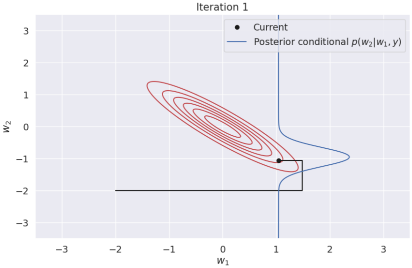

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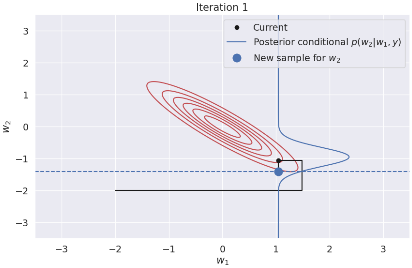

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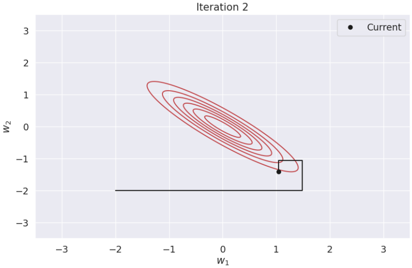

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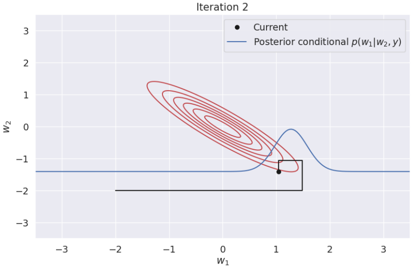

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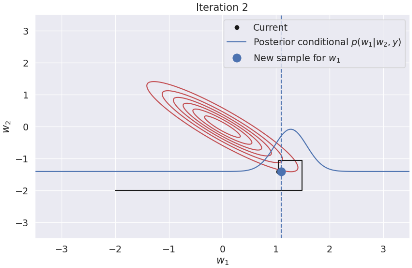

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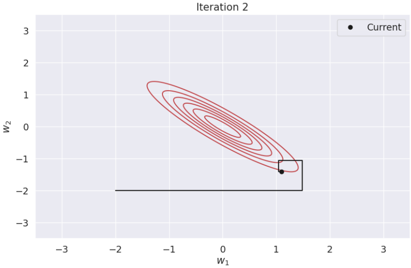

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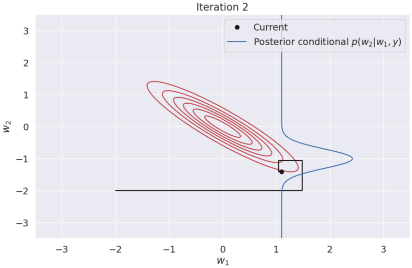

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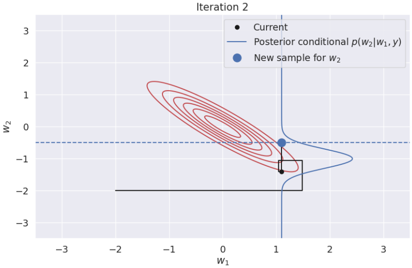

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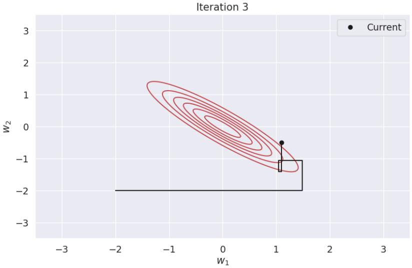

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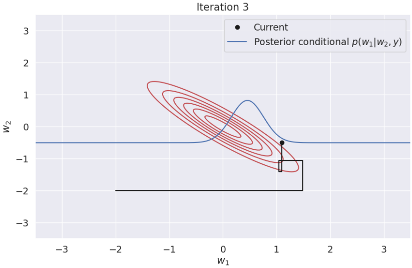

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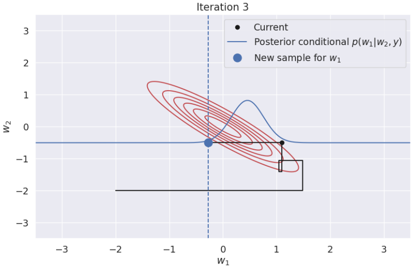

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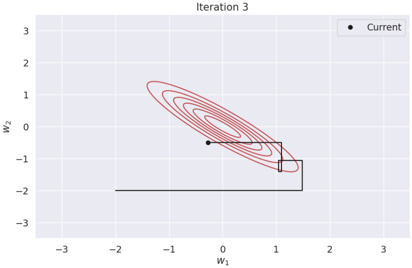

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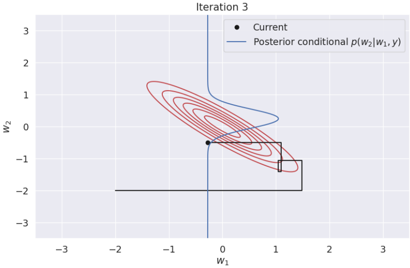

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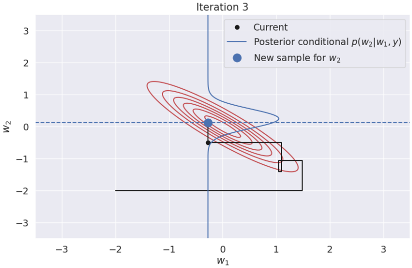

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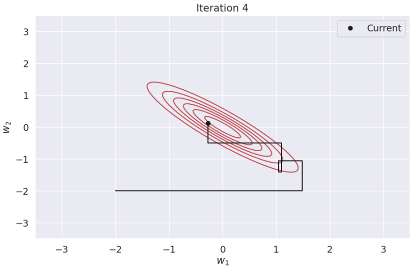

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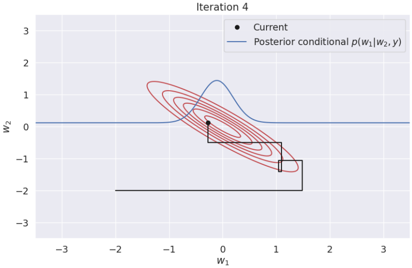

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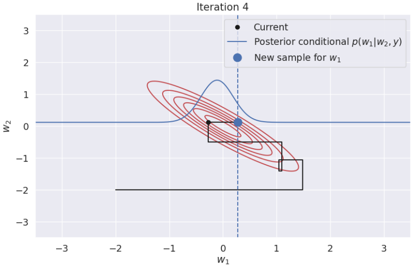

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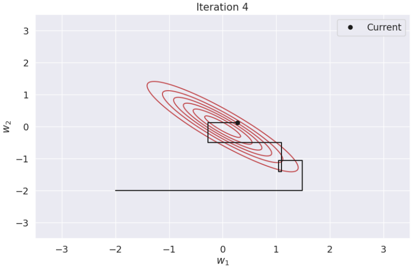

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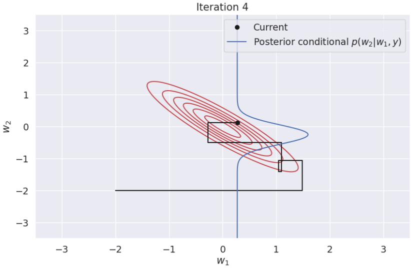

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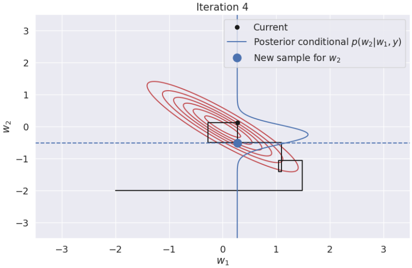

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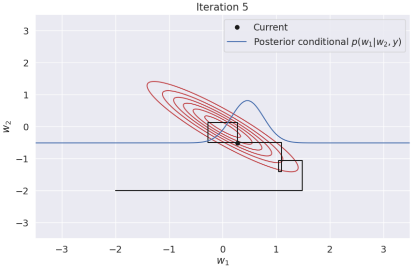

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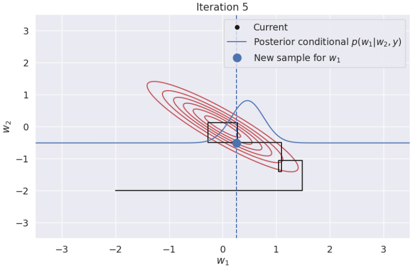

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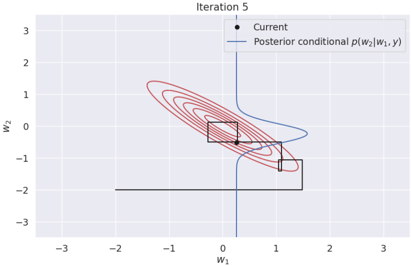

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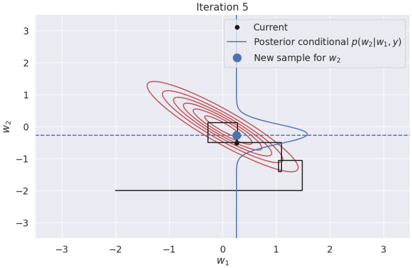

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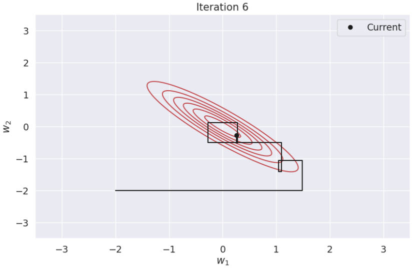

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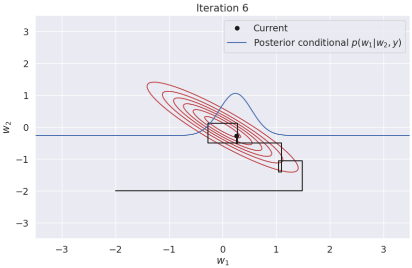

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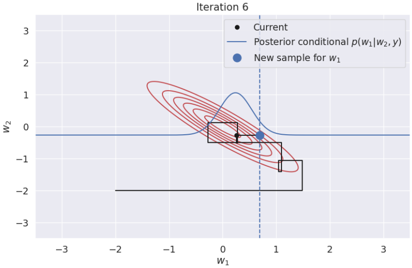

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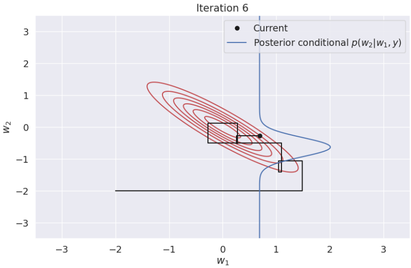

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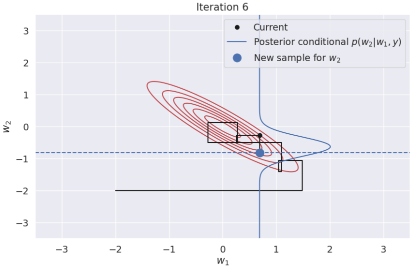

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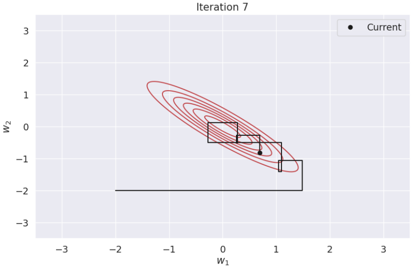

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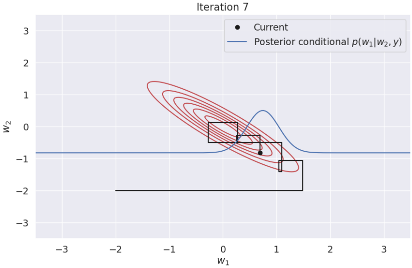

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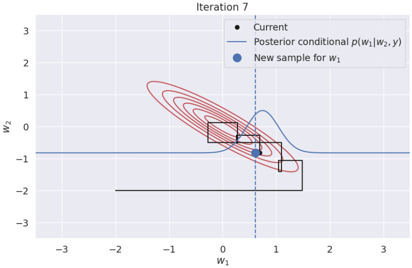

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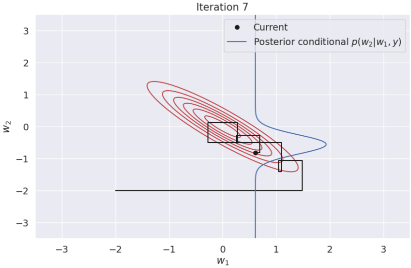

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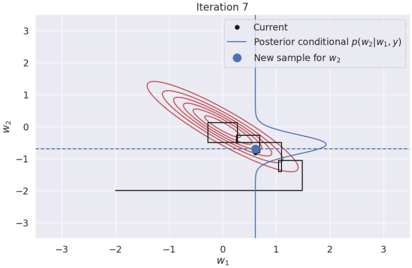

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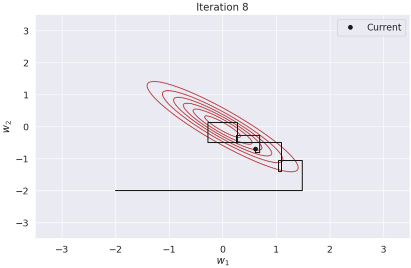

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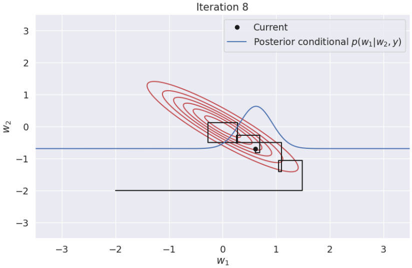

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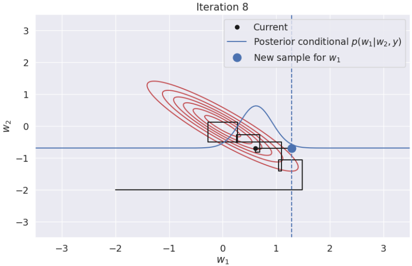

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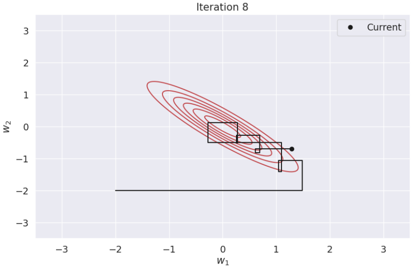

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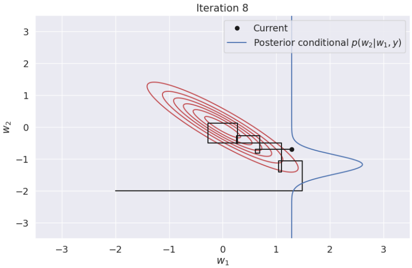

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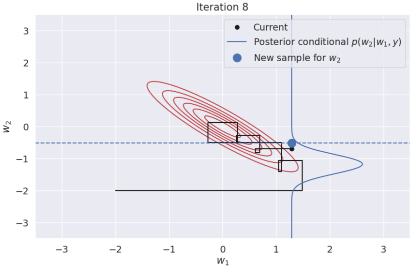

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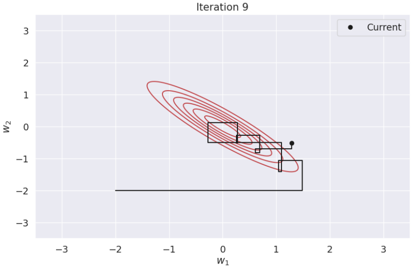

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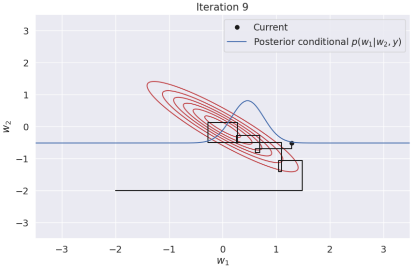

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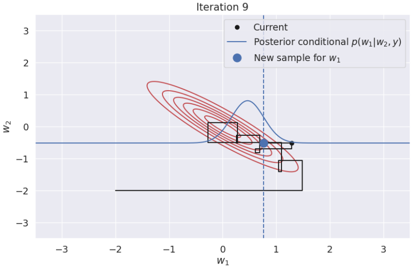

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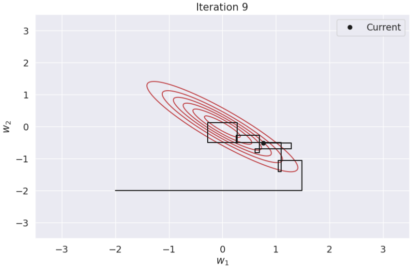

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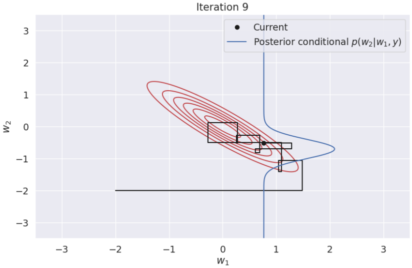

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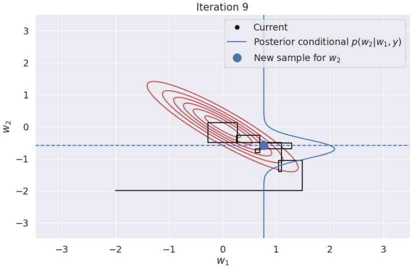

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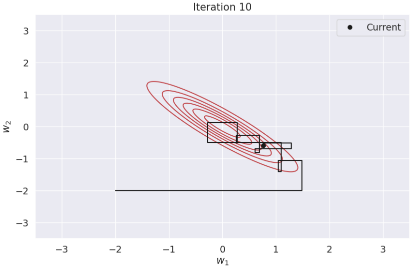

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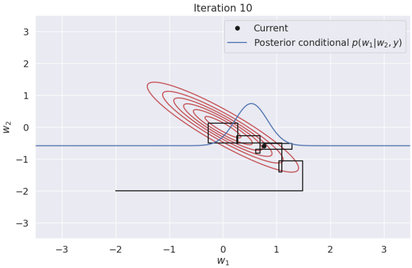

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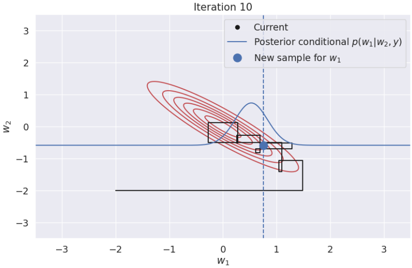

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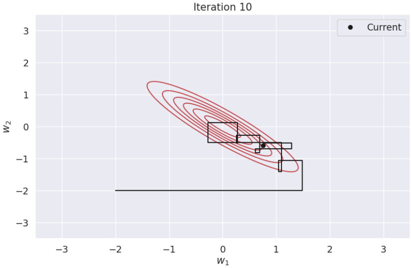

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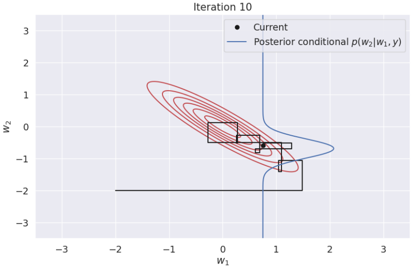

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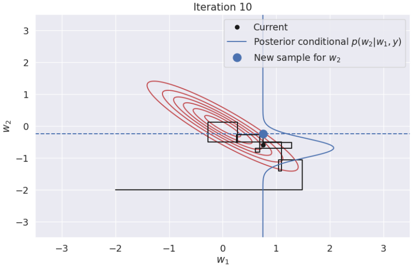

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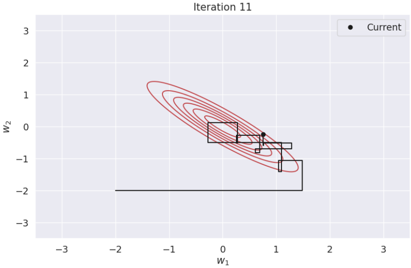

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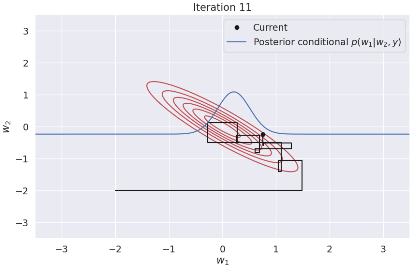

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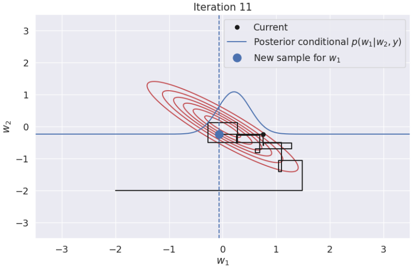

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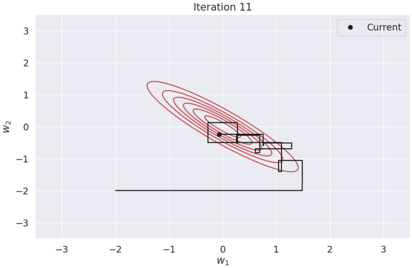

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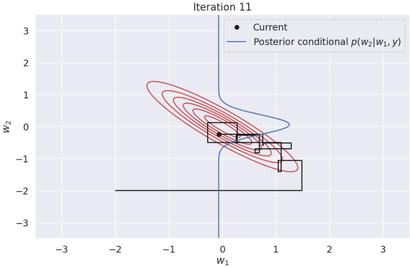

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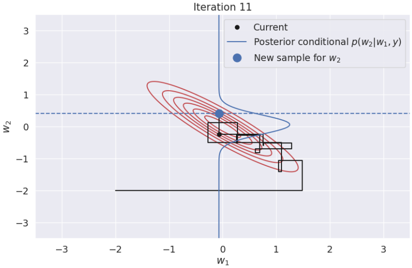

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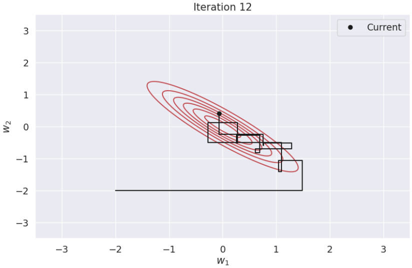

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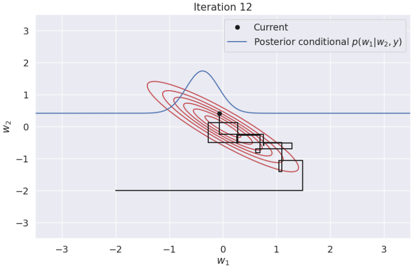

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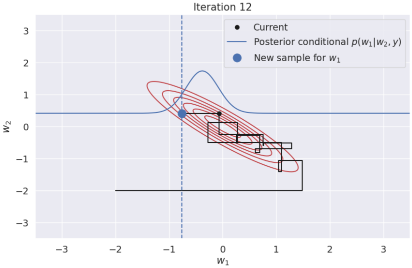

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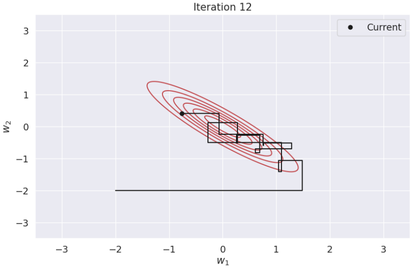

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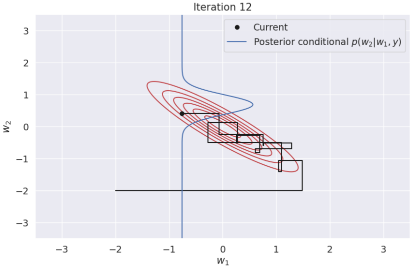

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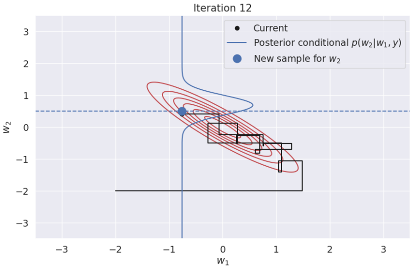

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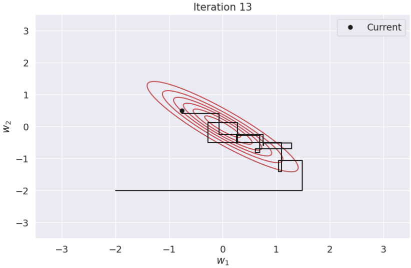

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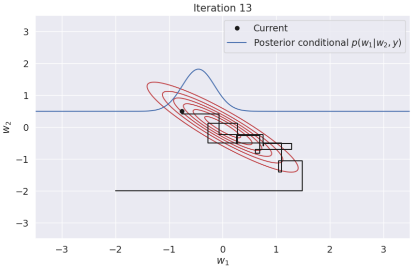

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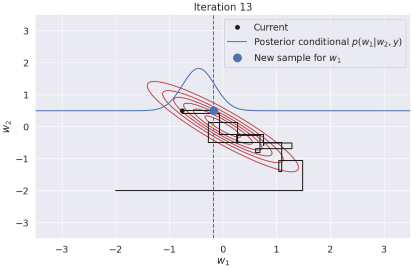

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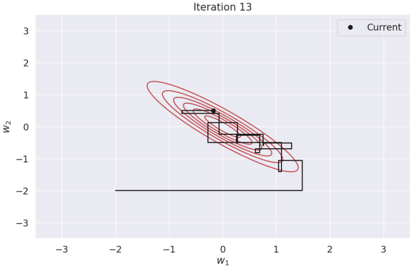

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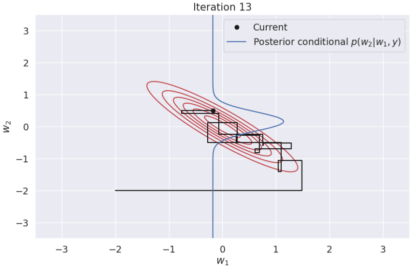

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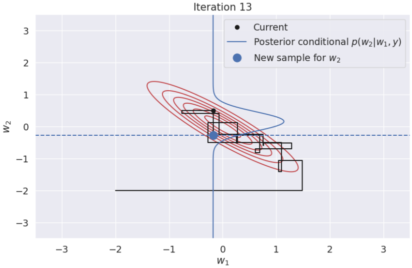

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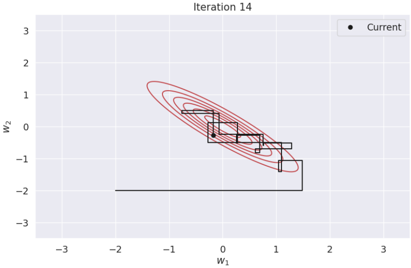

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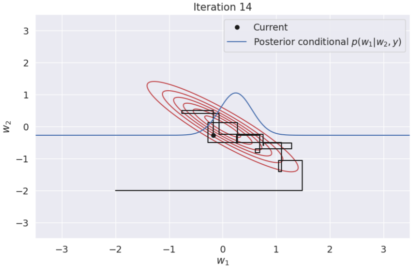

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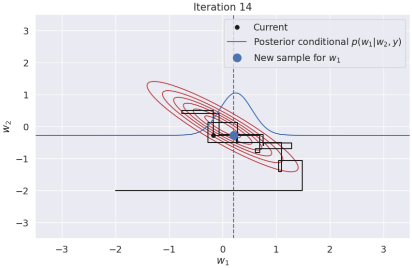

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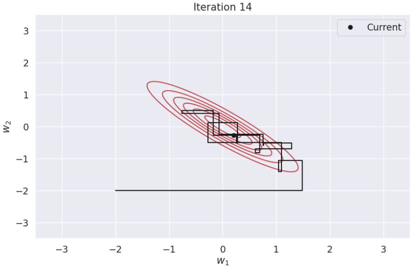

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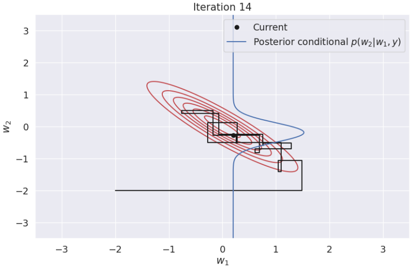

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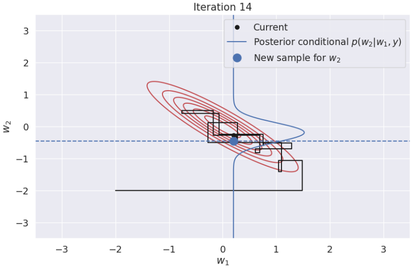

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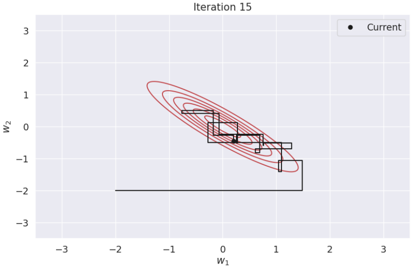

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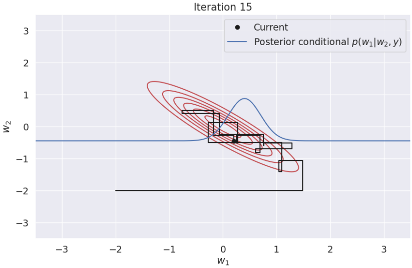

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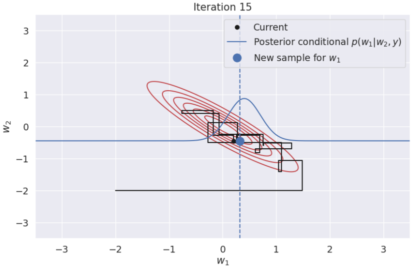

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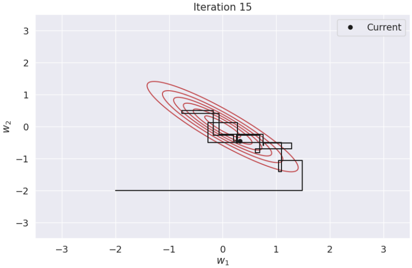

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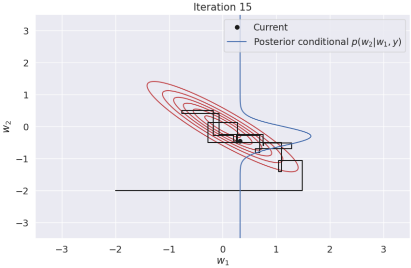

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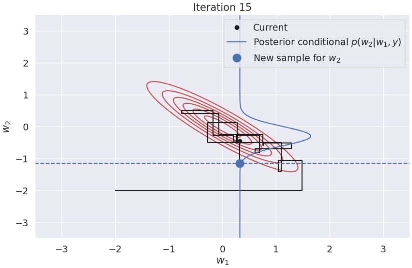

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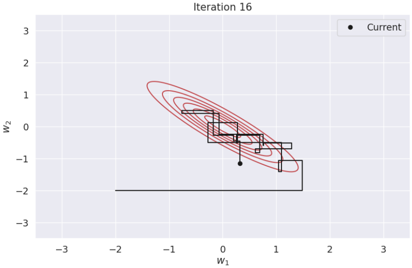

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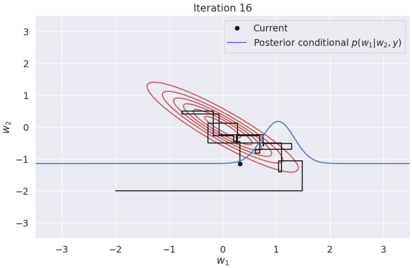

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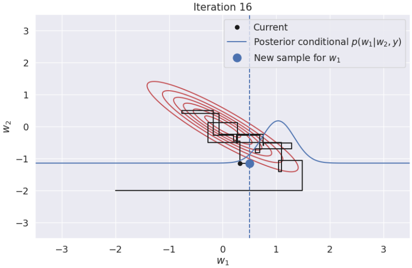

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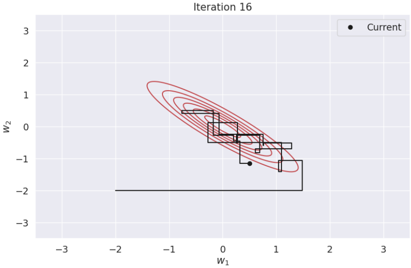

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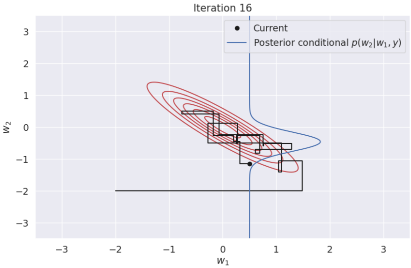

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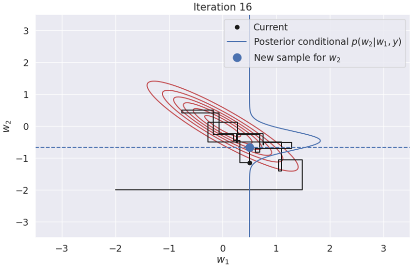

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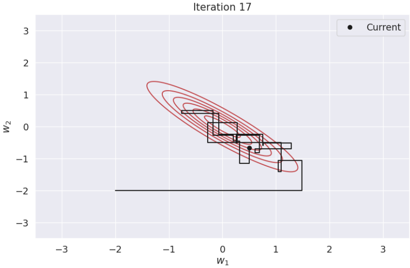

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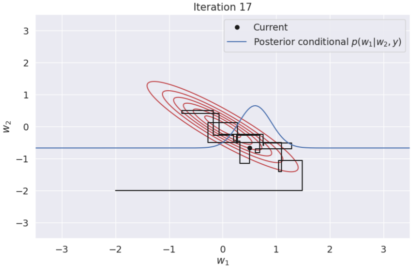

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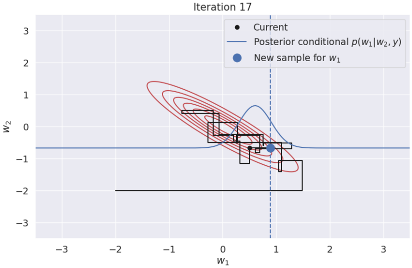

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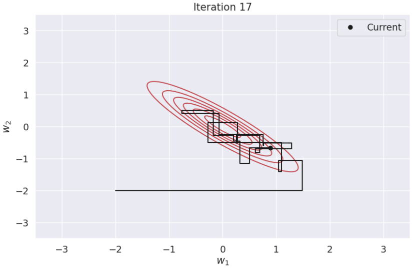

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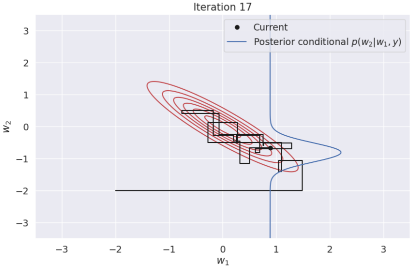

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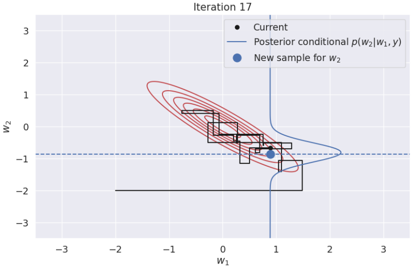

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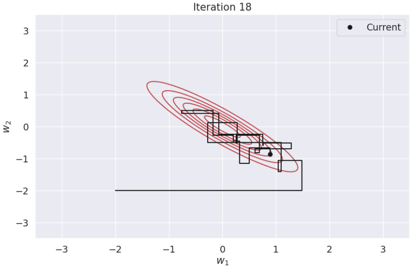

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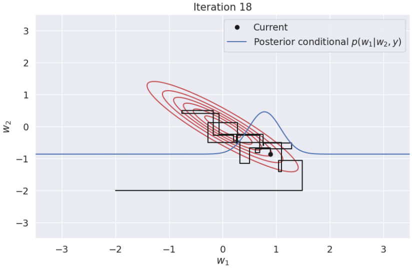

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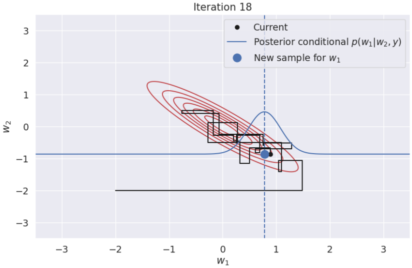

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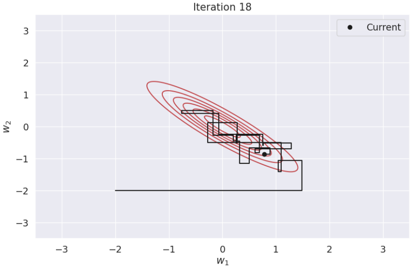

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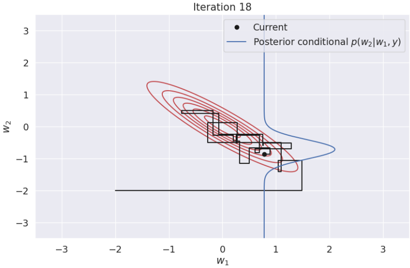

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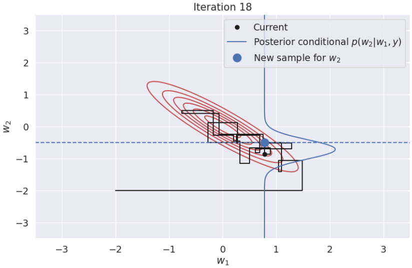

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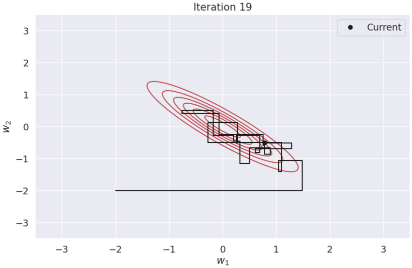

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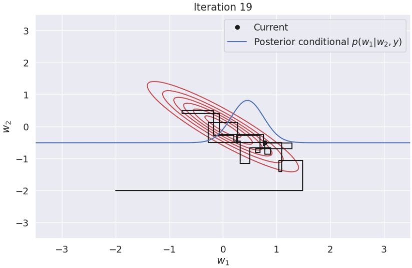

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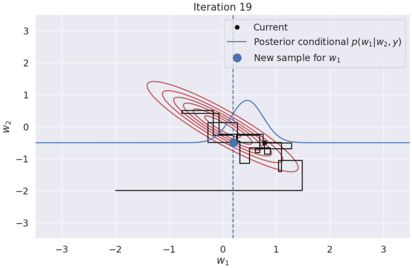

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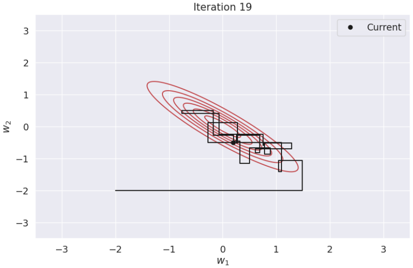

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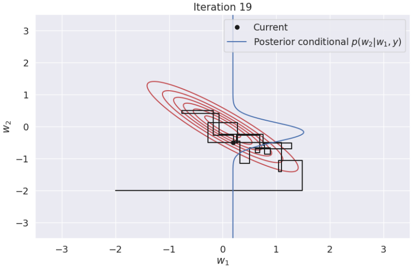

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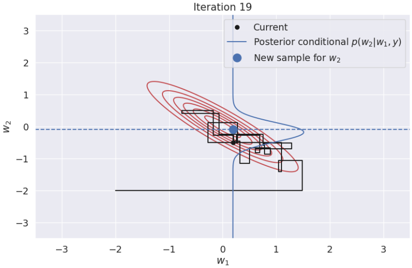

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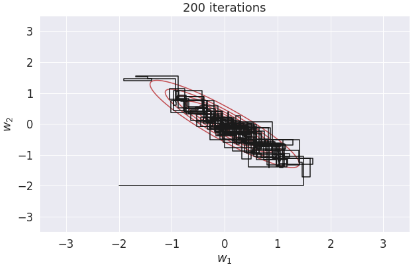

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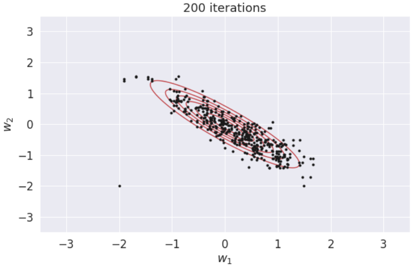

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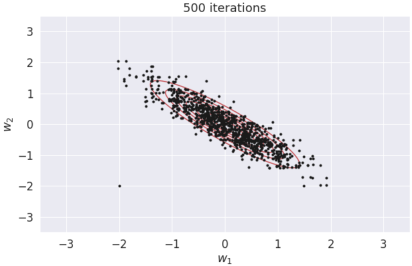

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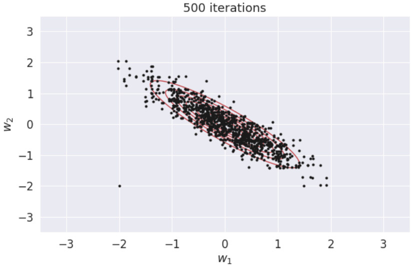

- Example shows typical *staircase behavior* of Gibbs samplers due sampling from the *posterior conditionals*

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- A Gibbs sampler is a special case of MH, where the proposed candidate is always accepted.

Questions: True or false?

Quiz via DTU Learn:

Lecture 9: Gibbs (5 questions)

Check you knowledge

Convergence diagnostics

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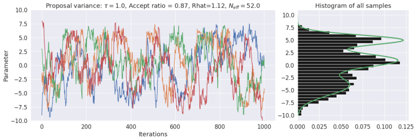

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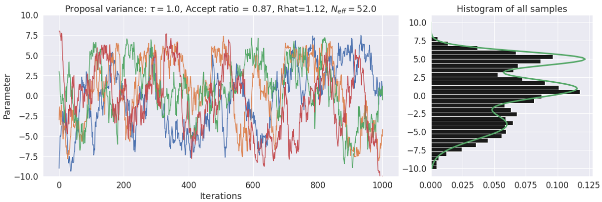

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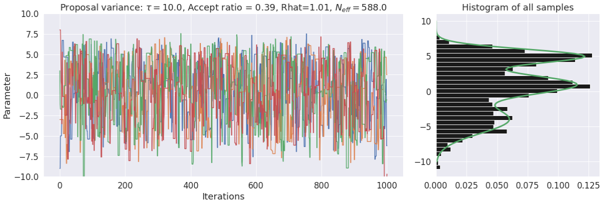

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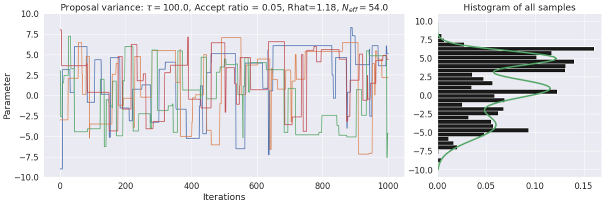
- Next week

  1. A few words on Hamiltonian Monte Carlo
  2. We will do a short discussion on pros and cons of MCMC in practice
  3. Start discussing variational inference.



Hierarchical models

Revisiting the Poisson regression

- "*Being Bayesian*" usually refers to treating quantities of interest as *random variable* and reason using the rules of *probability theory*
- When we talked about "*fully Bayesian*" inference, we refer the setting, where we have *prior distributions on all parameters, including hyperparameters*
- Before the holidays, we worked with a fully Bayesian Poisson regression model via MCMC

$$
\begin{aligned}
y_n|\mu_n &\sim \text{Poisson}(\mu_n), \\
\mu_n &= \exp(f_n) \\
f_n &= \mathbf{w}^T \mathbf{x}_n \\
\mathbf{w}|\kappa &= \mathcal{N}(0, \kappa^2 \mathbf{I}) \\
\kappa &\sim \mathcal{N}_+(0, 1)
\end{aligned}
$$

  with the following joint distribution

$$
p(\mathbf{y}, \mathbf{w}, \kappa) = \prod_{n=1}^{N} p(y_n|\mathbf{w}) p(\mathbf{w}|\kappa) p(\kappa),
$$

- This is an example of a *hierarchical model*

Hierarchical modelling

- *Hierarchical* or *multi-level* models are one of the key strength of the Bayesian framework

- Suppose we have a model $p(\mathcal{D}|\boldsymbol{\theta})$ with data $\mathcal{D}$, parameters $\boldsymbol{\theta}$ and hyperparameters $\boldsymbol{\xi}$

$$\boldsymbol{\xi} \longrightarrow \boldsymbol{\theta} \longrightarrow \mathcal{D}$$

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$$p(\mathcal{D}, \boldsymbol{\theta}, \boldsymbol{\xi}) \propto p(\mathcal{D}|\boldsymbol{\theta})p(\boldsymbol{\theta}|\boldsymbol{\xi})p(\boldsymbol{\xi})$$

- Useful when you want to
  1. make inference more robust
  2. reason probabilistically about data, parameters and hyperparameters
  3. model hierarchical structure in data (random effects models)
  4. squeeze out every bit of predictive performance of a model/dataset

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Full Bayes	$p(\boldsymbol{\theta}, \boldsymbol{\xi}\|\mathcal{D}) \propto p(\mathcal{D}\|\boldsymbol{\theta})p(\boldsymbol{\theta})p(\boldsymbol{\xi})$

Example

- Recall the model for Bayesian linear regression

$$p(\boldsymbol{w}|\alpha) = \mathcal{N}(\boldsymbol{w}|0, \alpha^{-1}\boldsymbol{I}) \qquad (\textit{prior})$$

$$p(\boldsymbol{y}|\boldsymbol{w}, \beta) = \mathcal{N}(\boldsymbol{y}|\boldsymbol{\Phi}\boldsymbol{w}, \beta^{-1}\boldsymbol{I}) \qquad (\textit{likelihood})$$

$$p(\boldsymbol{w}|\boldsymbol{y}, \alpha, \beta) = \mathcal{N}(\boldsymbol{w}|\boldsymbol{m}, \boldsymbol{S}) \qquad (\textit{posterior})$$

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- Fully Bayesian inference on the full joint distribution

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- Making predictions via MCMC

$$p(y^*|\mathbf{y}) = \mathbb{E}_{p(\alpha,\beta|\mathbf{y})}\left[p(y^*|\boldsymbol{y}, \alpha, \beta)\right] \approx \frac{1}{S}\sum_{i=1}^{S} p(y^*|\boldsymbol{y}, \alpha^{(i)}, \beta^{(i)})$$

for $\alpha^{(i)}, \beta^{(i)} \sim p(\alpha, \beta|\mathbf{y})$

Fully Bayesian Gaussian process regression: Example

- Example with $N = 20$ data points and additive Gaussian noise
- Gaussian process regression with squared exponential kernel
- We impose a *weakly informative* prior on the lengthscale to
  1. rule out really short length scales (smaller than the grid size)
  2. rule out really long length scales (larger than span data of data)
- Joint distribution

$$p(\mathbf{y}, \mathbf{f}, \ell, \sigma, \kappa) = p(\mathbf{y}|\mathbf{f}, \sigma)p(\boldsymbol{f}|\ell, \kappa)p(\kappa)p(\ell)$$

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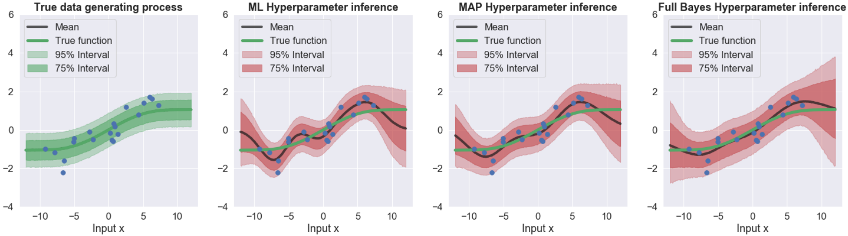

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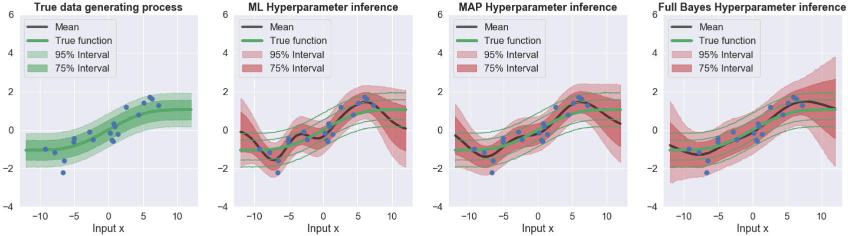

Medical example

- Suppose you work for a medical company and are asked to analyze data from a drug evaluation on rats prior to human trials
- Suppose the drug was administered to N rats, where y rats ended up developing tumors.
- We could use a Beta-Binomial model to estimate the probability of developing tumors θ

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- *Bayesian hierarchical models* allows us to borrow statistical strength from groups with lots of data to help groups with less data

Medical example cont.

- Let $\boldsymbol{y} = \{y_j\}_{j=1}^{J}$ and $\boldsymbol{\theta} = \{\theta_j\}_{j=1}^{J}$, then

$$p(\boldsymbol{y}, \boldsymbol{\theta}, \alpha, \beta) = \prod_{j=1}^{J} \text{Bin}(y_j|N_j, \theta_j) \prod_{j=1}^{J} \text{Beta}(\theta_j|\alpha, \beta) p(\alpha, \beta)$$

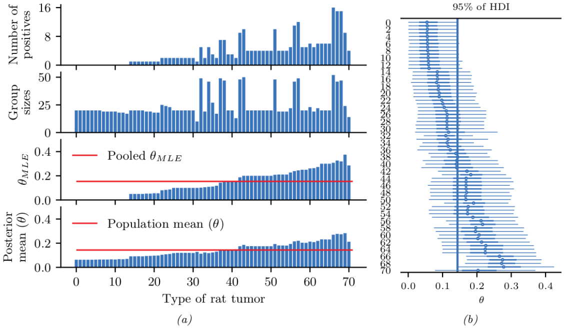

Figure 3.15: Data and inferences for the hierarchical binomial model fit using HMC. Generated by hierarchical_binom_rats.ipynb.

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- The transition kernel for Metropolis-Hasting

$$T(\mathbf{z}'|\mathbf{z}) = \begin{cases} q(\mathbf{z}'|\mathbf{z})A(\mathbf{z}'|\mathbf{z}) & \text{if} \quad \mathbf{z}' \neq \mathbf{z} \\ q(\mathbf{z}|\mathbf{z})A(\mathbf{z}|\mathbf{z}) + \int q(\mathbf{z}''|\mathbf{z})\left[1 - A(\mathbf{z}''|\mathbf{z})\right]\mathrm{d}\mathbf{z}'' & \text{if} \quad \mathbf{z}' = \mathbf{z} \end{cases}$$

The detailed balance condition II

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$$T(\mathbf{z}^\star|\mathbf{z}^k) = q(\mathbf{z}^\star|\mathbf{z}^k)A(\mathbf{z}^\star|\mathbf{z}^k) = q(\mathbf{z}^\star|\mathbf{z}^k)\frac{p(\mathbf{z}^\star)q(\mathbf{z}^k|\mathbf{z}^\star)}{p(\mathbf{z}^k)q(\mathbf{z}^\star|\mathbf{z}^k)} = \frac{p(\mathbf{z}^\star)q(\mathbf{z}^k|\mathbf{z}^\star)}{p(\mathbf{z}^k)}$$

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- If $p(\mathbf{z}^k)q(\mathbf{z}^\star|\mathbf{z}^k) > p(\mathbf{z}^\star)q(\mathbf{z}^k|\mathbf{z}^\star)$, then $A(\mathbf{z}^\star|\mathbf{z}^k) < 1$ and $A(\mathbf{z}^k|\mathbf{z}^\star) = 1$

- To jump from $\mathbf{z}^k$ to $\mathbf{z}^\star$, we first need to propose it and then accept it

$$T(\mathbf{z}^\star|\mathbf{z}^k) = q(\mathbf{z}^\star|\mathbf{z}^k)A(\mathbf{z}^\star|\mathbf{z}^k) = q(\mathbf{z}^\star|\mathbf{z}^k)\frac{p(\mathbf{z}^\star)q(\mathbf{z}^k|\mathbf{z}^\star)}{p(\mathbf{z}^k)q(\mathbf{z}^\star|\mathbf{z}^k)} = \frac{p(\mathbf{z}^\star)q(\mathbf{z}^k|\mathbf{z}^\star)}{p(\mathbf{z}^k)}$$

- It follows

$$p(\mathbf{z}^k)T(\mathbf{z}^\star|\mathbf{z}) = p(\mathbf{z}^\star)q(\mathbf{z}^k|\mathbf{z}^\star)$$

The detailed balance condition III

- We just arrived at

$$p(\boldsymbol{z}^k)T(\boldsymbol{z}^\star|\boldsymbol{z}^k) = p(\boldsymbol{z}^\star)q(\boldsymbol{z}^k|\boldsymbol{z}^\star)$$

- What about the opposite direction?

$$T(\boldsymbol{z}^k|\boldsymbol{z}^\star) = q(\boldsymbol{z}^k|\boldsymbol{z}^\star)A(\boldsymbol{z}^k|\boldsymbol{z}^\star) = q(\boldsymbol{z}^k|\boldsymbol{z}^\star)$$

The detailed balance condition III

- We just arrived at

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- What about the opposite direction?

$$T(\boldsymbol{z}^k|\boldsymbol{z}^\star) = q(\boldsymbol{z}^k|\boldsymbol{z}^\star)A(\boldsymbol{z}^k|\boldsymbol{z}^\star) = q(\boldsymbol{z}^k|\boldsymbol{z}^\star)$$

- Combining the two and we are done

$$p(\boldsymbol{z}^k)T(\boldsymbol{z}^\star|\boldsymbol{z}^k) = p(\boldsymbol{z}^\star)T(\boldsymbol{z}^k|\boldsymbol{z}^\star)$$