Chapter 1

Conjugate Bayesian Linear Q learning

In an attempt to find a better balance between exploration and exploitation this thesis investigates the use of bayesian methods to allow for Thompson sampling. This chapter builds and compares bayesian methods in a linear model context to investigate what models to use and what factors are important in a reinforcement learning setting.

1.1 Linear Q learning

In linear Q learning the goal is to create a regression model that maps the state and action to a Q-value, $Q(s, a)$. Let x_t denote the state and action at timestep t. X then denotes the design matrix containing these features and Q the vector of corresponding Q-values. The regression model for a single action can then be defined as

$$Q(X, a) = X\beta + \varepsilon \quad \text{where} \quad \varepsilon \sim N(0, \sigma^2)$$

with the response value defined as

$$Q(s, a) = r_t + \arg\max_{a'} Q(s', a'). \tag{1.1}$$

The ordinary least squares solution to the β coefficients can then be found using the normal equation which in matrix form is

$$\beta = [X^T X]^{-1} X^T Q$$

Given this model the agent can take an action by acting greedily over the models $Q(s, a)$ values in a given state. Since this is purely an exploitation strategy, it is often coupled with the ε-greedy policy.

1.2 Bayesian Linear Q learning

To extend linear Q learning methods to Thompson sampling a bayesian perspective is required. To do this a prior distribution is placed over the regression parameters. Using bayes rule the posterior distribution of the parameters can be calculated and used to calculate the marginal distribution over Q.

$$p(\theta|Q, \mathcal{F}) \propto p(Q|\theta, \mathcal{F})p(\theta)$$
$$p(Q) = \int p(Q|\theta, \mathcal{F})p(\theta)d\theta$$

Q is a vector of all Q-values given the state X_t, θ denotes all parameters and $\mathcal{F}$ denotes all previous transitions. Since this is only used for Thompson sampling the value of the integral is not of interest. Instead it is the samples from $p(Q|\theta, \mathcal{F})$ that will be used to drive exploration.

1.3 Conjugate Bayesian Linear Q learning

TODO:Emphasize the assumptions in this chapter

The calculation of an arbitrary posterior can be computationally heavy which is ill-suited to the already long running reinforcement learning methods. In order to keep computation costs low to this thesis will consider conjugate priors which have an analytical solution.

1.3.1 Gaussian Prior with Known noise

There are multiple ways to setup a bayesian regression model using conjugate priors. First consider the case used in Azizzadenesheli et al. (2019) which creates one model per action and assumes the noise variance is known. The known noise variance is then treated as a hyperparameter. In this case the posterior can be expressed as

$$p(\beta_a|Q_a, \sigma_{\varepsilon_a}, \mathcal{F}) \propto p(Q_a|\beta_a, \sigma_{\varepsilon_a}, \mathcal{F})p(\beta_a)$$
$$p(Q_a|\sigma_{\varepsilon_a}, \mathcal{F}) = \int p(Q_a|\beta_a, \sigma_{\varepsilon_a}, \mathcal{F})p(\beta_a)d\beta_a$$

In literature it is common to use a gaussian prior for β

$$p(\beta) = \mathrm{N}(\mu, \sigma_\varepsilon \Lambda^{-1})$$

where Λ is the precision matrix. This results in the following posterior update

TODO:Add the development of these posterior updates to the appendix

$$\begin{aligned} \Lambda_n &= X^T X + \Lambda_0 \\ \mu_n &= \Lambda_n^{-1}(\Lambda_0 \mu_0 + X^T Q_a) \end{aligned} \tag{1.2}$$

Actions are picked by Thompson sampling. To sample However when calculating the target Q-value Azizzadenesheli et al. (2019) uses the MAP estimate of β instead. In this case the MAP estimate is μ.

1.3.2 Propagating Variance

Using the MAP estimate means that the targets are calculated by

$$y = r_t + \max_a X_{t+1} \mu_a.$$

This does not correctly encorporate the target variance. To see why recall the definition of the Q-value

$$\begin{aligned} Q_t &= \mathbb{E}[G_t] = \mathbb{E}[r_t + r_{t+1} + \dots] \\ &= \mathbb{E}[r_t + Q_{t+1}] = \mathbb{E}[r_t + Q_{t+1}] \end{aligned}$$

This results in the regression problem $\mathbb{E}[r_t + Q_{t+1}] = X\beta_a$. However, since the expected reward is unknown this cannot be used. Instead one has access to the sample rewards from the environment. Asymptotically the mean of the samples approaches the expected value so this can be treated as a regression task with a noise term

$$\begin{aligned} \mathbb{E}[r_t + Q_{t+1}] &= X\beta_a \\ r_t + Q_{t+1} &= X\beta_a + \varepsilon \end{aligned}$$

where ε accounts for the difference between the sample and the mean, $r_t - \mathbb{E}[r_t] + Q_{t+1} - \mathbb{E}[Q_{t+1}]$. This implies that the target used must be a sample from the posterior of Q_t not its expected value $X\mu_a$ as used in Azizzadenesheli et al. (2019).

The result of this is that the known noise model only includes the variance in the reward process through r. It does not convey the variance in the Q-value estimate of the next state. Even in a deterministic environment the policy shifts during training mean that

there is an uncertainty in the Q-value of the next state. Quoting Moerland et al. (2017), "... repeatedly visiting a state-action pair should not makes us certain about its value if we are still uncertain about what to do next."

Based on the above a better choice of target is

$$y = r_t + \max_a (X_{t+1}\beta + \varepsilon)$$

where β is sampled from its posterior and ε from the gaussian noise distribution. However the variance of β, as seen in equation 1.2, is independent of the target. One way to include a variance term that is dependent on the target is to include σ_ε as an unknown parameter.

1.3.3 Normal Prior with Unknown noise

Including σ_ε as an unknown parameter resuts in the following:

$$p(\beta_a, \sigma_{\varepsilon_a} | Q_a, \mathcal{F}) \propto p(Q_a | \beta_a, \sigma_{\varepsilon_a}, \mathcal{F}) p(\theta)$$
$$p(Q_a | \mathcal{F}) = \int p(Q_a | \beta_a, \sigma_{\varepsilon_a}, \mathcal{F}) p(\beta_a, \sigma_{\varepsilon_a}) d\beta_a d\sigma_{\varepsilon_a}$$

The conjugate priors for this setup are

$$p(\sigma^2) = \text{InvGamma}(\alpha, b)$$
$$p(\beta | \sigma^2) = \text{N}(\mu, \sigma^2 \Sigma)$$

with the posterior update

$$\Lambda_n = (X^T X + \Lambda_0)$$
$$\mu_n = \Lambda_n^{-1}(\Lambda_0 \mu_0 + X^T Q)$$
$$\alpha_n = \alpha_0 + \frac{n}{2}$$
$$b_n = b_0 + (Q^T Q + \mu^T \Lambda_0 \mu_0 - \mu_n^T \Lambda_n \mu_n)$$

TODO:Add the development of these posterior updates to the appendix

1.3.4 Testing Variance Propagation

To ensure that this method is propagating uncertainty consider a simple example from Osband et al. (2018). Consider a MPD with two states. The initial state allows only one

action that deterministicly leads to state 2 with no reward. State 2 is a terminal state with a known posterior distribution. If a RL method properly propagates uncertainty the posterior distribution of state 1 should match state 2 as long as $\gamma = 1$.

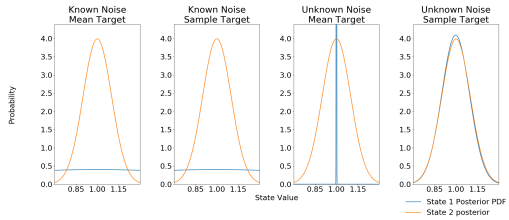
Both models were tested with both MAP and sample targets. The priors for the known noise models were set to

$$\begin{aligned} \beta &\sim N(0, 10^3) \\ \sigma^2 &= 1 \end{aligned}$$

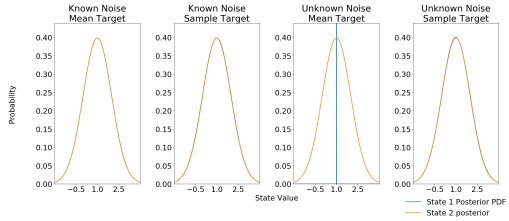
and the priors for the unknown noise models were set to

$$\begin{aligned} \beta &\sim N(0, 10^3) \\ \sigma^2 &\sim InvGamma(1, 1). \end{aligned}$$

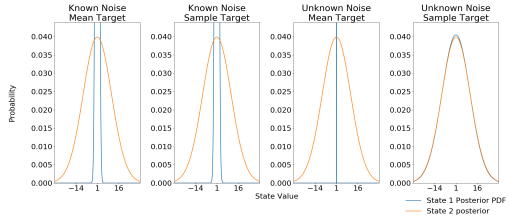
Three MDP's were set up with a known posterior of $N(1, 0.1), N(1, 1)$ and $N(1, 10)$ respectively. The results are seen in figure 1.1.



(a) $N(1, 0.1^2)$



(b) $N(1, 1^2)$



(c) $N(1, 10^2)$

Figure 1.1: Variance Propagation On 2 State Toy Example: The blue lines show the models Q-value posterior distribution while the orange lines show the target posterior distribution. Only the unknown noise model with sample targets is able to correctly estimate the target in all cases.

The results summarized in figure 1.1 showed that all models were able to correctly estimate the mean. However the target variance was only correctly estimated by the the unknown noise model with sample targets. The unknown noise model with the MAP target leads to the correct mean but dramatically understimates the variance. This would be an expected result if the model is approximating $\mathbb{E}[Q]$ instead of Q. The known noise model is only correct for both the mean and sample target if the hyperparameter ε is set to the correct variance. In an unknown and more complex environment this is unlikely to be possible. However with enough hyperparameter tuning one could argue that this can lead to good results which might explain the results achieved in Azizzadenesheli et al. (2019).

Based on these results further developments are focused on the unknown noise model with sampled targets.

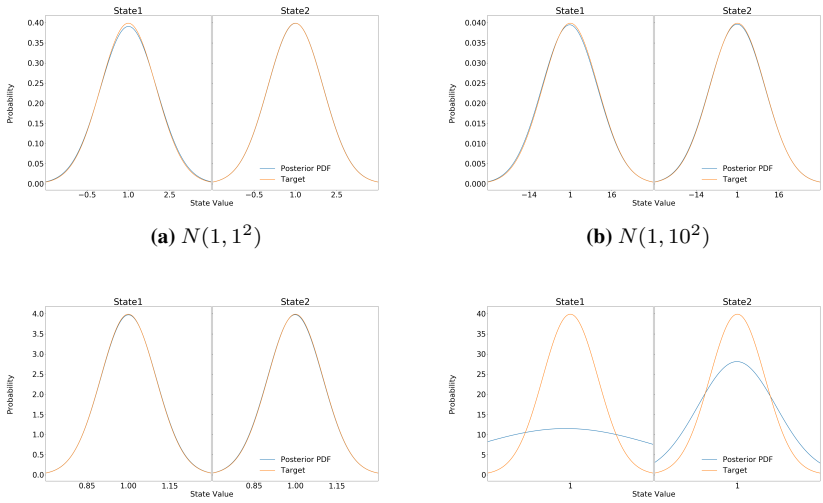
1.4 Variance Propagation

1.4.1 Over Multiple States

The setting above is in essence a regular regression setting. In a RL setting this variance needs to be propagated to further states. To test that this is still the case with the unknown noise model consider a modification to the environment where an extra state is placed between the initial and terminal state. This state has the same dynamics as earlier. It deterministically transitions to the next state with zero reward over the transition. The correct posterior for each state is then the target posterior in the terminal state.

The same priors as earlier are used on 4 different target posteriors. The results are summarised in figure 1.2.

TODO:Add details around these experiments in the appendix



(a) $N(1, 1^2)$ **(b)** $N(1, 10^2)$

(c) $N(1, 0.1^2)$ **(d)** $N(1, 0.01^2)$

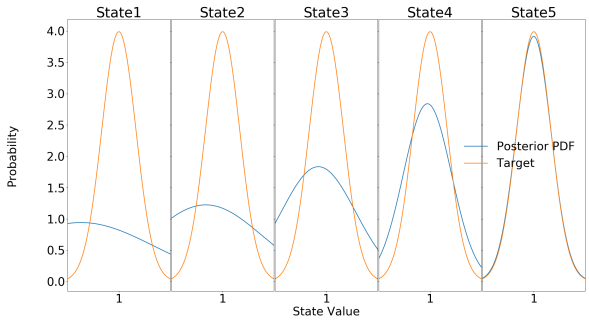
Figure 1.2: Variance Propagation On 3 State Toy Example: The models posterior estimate for the two first states are shown. The third state is the terminal state that returns a sample from the target distribution.

Figure 1.2 shows that for larger variance targets the propagation correctly updates the state 1 variance. However the low variance targets results in an overestimation over the variance in state 1. Running this experiment for more iterations does lead to a better approximation implying that the problem lies in the the convergence rate for different posteriors.

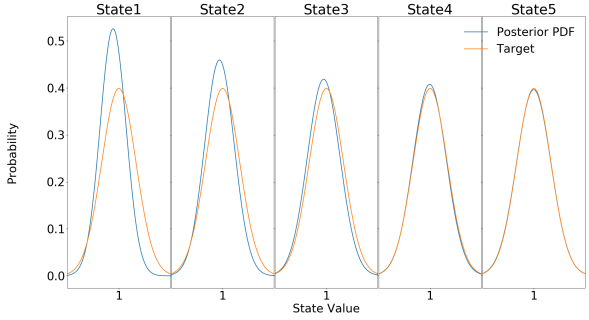
One possible reason for this is that the posterior representing the 0.01 standard deviation posterior is more sensitive to small changes in in its parameters than the larger variance posteriors. In other words small changes in the parameters for a distribution with low

variance leads to large changes in the variance of the posterior. Since the learning is happening in an online fashion the first estimates of the posterior will likely have large error. This effect is amplified for state 1 since it is training on the large error state 2 posterior. (TODO:: Confirm/source that this is actually the case)

By extending the toy example to even more states as in figure 1.3 one can see that this problem increases the further the variance needs to be propagated. Even large variance targets will fail to correctly propagate given enough states.



(a) 6 States with $N(0.1, 1^2)$



(b) 6 States with $N(1, 1^2)$ target

Figure 1.3: Failure of variance propagation over many states: (**a**) shows that the error in estimation close to the terminal state leads to failure in the estimation of the posterior of the initial states. In (**b**) the seemingly correct estimation close to the terminal state still does not prevent errors Closer to the initial state.

This issue will be refered to as the speed of propagation. It encompasses the problem of quickly propagating variance estimates from downstream states back to states which are far from the environments reward.

TODO:: Define speed of propagation. Maybe a seperate subsection that plots how the error changes with length of chain. How do we measure the error between two distributions?

KL Divergence?

1.4.2 Speed of propagation

Inorder to improve the speed of propagation insight is required into what causes the issue. In this section two causes and methods for counteracting them are discussed. However these are not necessarily the only two causes of slow propagation.

TODO:These argumentations are weak and require sources or ”proof”.

The first cause is best explained using an example. Consider the 3 state toy example. State 1 can only converge to the correct distribution once State 2 has converged. If more states are added, State 1 will converge once all the states between it and the terminal state have converged. The longer the chain is, the more iterations are required for state 1 to converge. This issue is the same issue faced with the expected Q value in regular RL which is dealt with through a bias-variance trade-off (TODO:Include n-step in theory). Similarly extending the 1-step update to an n-step update one will increase the speed of variance propagtation with the downside of introducing more variance to the σ_ε estimate.

The second cause is a result of no longer using a step size when updating the Q-values using bayesian updates. In regular Q-learning the step size can be viewed as the weighting of new data relative to the current model. This effect is also found in the bayesian setting in the posterior update that combines the prior and the new data. However, in regular Q-learning the step size also leads to the model forgetting old data(Sutton and Barto (2018)TODO:find this page). This does not happen in the bayesian regression setting that has been used.

In the bayesian regression setting described the prior is always the previous posterior. In simple terms the model assumes all data to be equally important. Recalling that the prior used is the previous posterior, a prior based on many datapoints will have a bigger impact on the posterior than a single new datapoint. This is a problem since a reinforcement learning problem is almost always non-stationary. With this weighting scheme the new data points which are more relevant to the current target are weighted the same as a datapoint collected based on the initial priors.

1.5 Performance on Linear RL Problem

1.6 Bayesian Deep Q Network

TODO:this section assumes DQN has been explained

The predominant issue with bayesian methods in deep reinforcement learning is using bayesian methods with neural networks. This thesis will address the linear layer method (TODO:Actual name for method), a simple and computationally efficient method that comes at the cost of accuracy.

The final layer in a DQN is a linear layer. Since bayesian regression is also a linear combination one can replace the final layer with a bayesian regression model per action.

This is equivalent to rewriting the regression task to

$$Q = \phi(X)\beta + \varepsilon \quad \text{where} \quad \varepsilon \sim N(0, \sigma^2)$$

where $\phi(X)$ is the neural networks output given an input X. Note that this means the bayesian regression no longer incorporates all the uncertainty since the above assumes no uncertainty in the $\phi(X)$ encoding.

Training the model now needs to be split into two processes. Firstly the bayesian regression is trained using the posterior update shown above. The neural network is trained using a similar loss function as the DQN. However the networks Q-value estimate is replaced by the MAP estimate of β resulting in

$$\theta = \theta - \alpha \nabla_\theta \big(Q_t - [\mu_n^T \phi_\theta(x_t)]\big)^2.$$

Note that these do not have to happen sequentially. In Azizzadenesheli et al. (2019) and this implementation the bayesian regression is updated less often than the neural network.

Finally to deal with the fact that reinforcement learning is a non-stationary problem the the bayesian regression is trained for scratch each time it is updated.

Bibliography

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