WEEK 2 SUMMARY

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- 1. Summary. Last week's experiments indicated that the original parameterization, treating u, τ, α as the variables, would not converge even after 100,000 iterations. However, there was a mistake in the prior distribution of τ , and later there is a discussion on fixing the error and getting working simulations. First, we explain the different parameterization that we tried this week. We decided to try a different parameterization which treats ξ, τ, α as variables to sample, and we compare results between this and the old parameterization.
 - 2. Learning τ and α with non-centered parameterization.
- **2.1. Algorithm.** In the centered parameterization, the prior was $u|\tau, \alpha \sim N(0, C(\tau, \alpha))$, τ, α distributed independently and uniformly over intervals. We would take the posterior by Bayes' theorem to be

$$f(u,\tau,\alpha) \propto \exp\left(-\Phi(u) - \frac{1}{2}\langle u, C(\tau,\alpha)^{-1}u\rangle - \frac{1}{2}\log(\det(C(\tau,\alpha))) + \log(\pi_0(\tau,\alpha))\right)$$

In the new parameterization, we sample $\xi \sim N(0,I)$ and τ,α on uniform intervals as before. ξ is related to u by $T(\xi,\tau,\alpha)=u=\sum_{j=0}^{M}(\lambda_j+\tau^2)^{-\alpha/2}\xi_jq_j$. Recall that we are taking M=N-1. The new joint posterior becomes:

$$g(\xi, \tau, \alpha) \propto \exp\left(-\Phi(T(\xi, \tau, \alpha)) - \frac{1}{2}\langle u, u \rangle + \log(\pi_0(\tau, \alpha))\right)$$

This algorithm works as follows:

Algorithm 1 Non-centered parameterization: sampling ξ, τ, α

Choose $\xi^{(0)} \in \mathbb{R}^N$, $\alpha^{(0)}$, $\tau^{(0)} > 0$, $\beta \in (0, 1]$ and $\epsilon_1, \epsilon_2 > 0$.

for k = 0 to S do

Propose $\hat{\xi}^{(k)} = (1 - \beta^2)\xi^{(k)} + \beta\zeta^{(k)}, \, \zeta^{(k)} \sim N(0, I)$

Make transition $\xi^{(k+1)} \to \hat{\xi}^{(k)}$ with probability

$$A(\xi^{(k)} \to \hat{\xi}^{(k)}) = \min\{1, \frac{g(\hat{\xi}^{(k)}, \tau^{(k)}, \alpha^{(k)})}{g(\xi^{(k)}, \tau^{(k)}, \alpha^{(k)})}\}$$

Propose $\hat{\tau}^{(k)} = \tau^{(k)} + \epsilon_1 \rho^{(k)}, \rho^{(k)} \sim N(0, I)$ Make transition $\tau^{(k+1)} \to \hat{\tau}^{(k)}$ with probability

$$A(\tau^{(k)} \to \hat{\tau}^{(k)}) = \min\{1, \frac{g(\xi^{(k+1)}, \hat{\tau}^{(k)}, \alpha^{(k)})}{g(\xi^{(k+1)}, \tau^{(k)}, \alpha^{(k)})}\}$$

Propose $\hat{\alpha}^{(k)} = \alpha^{(k)} + \epsilon_2 \sigma^{(k)}, \sigma^{(k)} \sim N(0, I)$ Make transition $\alpha^{(k+1)} \to \hat{\alpha}^{(k)}$ with probability

$$A(\alpha^{(k)} \to \hat{\alpha}^{(k)}) = \min\{1, \frac{g(\xi^{(k+1)}, \tau^{(k+1)}, \hat{\alpha}^{(k)})}{g(\xi^{(k+1)}, \tau^{(k+1)}, \alpha^{(k)})}\}$$

end for return $\{T(\xi^{(k)}, \tau^{(k)}, \alpha^{(k)}), \tau^{(k)}, \alpha^k\}$

2.2. Simulation results. The relevant figures are Figure 1, Figure 2, Figure 3, Figure 4, Figure 5, Figure 6. The parameters used are as follows:

Iterations	100000
Burn in period	1000
Laplacian	self-tuning, unnormalized
β	0.1
γ	0.0001
Labeled +1	280 - 290
Labeled -1	20 - 30
ϵ_{lpha}	1
$\epsilon_{ au}$	1
Initial τ	30
Initial α	5
au range	[0, 60]
α range	[0, 100]
Average τ	3.74
Average α	63.5
Percent of correct classification	0.864407
Time elapsed	183.21 s

Fig. 1. α acceptance probability

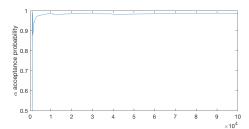


Fig. 2. α trace

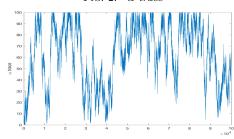


Fig. 3. τ acceptance probability

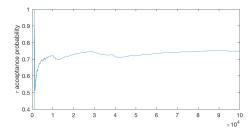


Fig. 4. τ trace

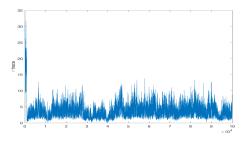


Fig. 5. ξ acceptance probability

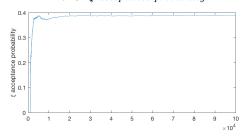
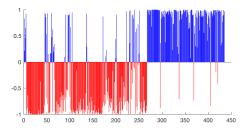


Fig. 6. u final average



3. Revisiting the centered parameterization. After trying new prior intervals for τ, α in the old parameterization, I found that the MCMC could actually converge quickly and accurately. I allowed τ and α to be sampled from (0,60]. Last week, forcing τ to be in (0,1] proved to be too small of an interval. β was adjusted to obtain a reasonable acceptance probability for $u^{(k)}$. The parameters that worked are:

Iterations	10000
Burn in period	500
Laplacian	unnormalized
Weight function parameters (p, q, l)	(2, 2, 1)
β	0.2
γ	0.0001
Labeled +1	280 - 283
Labeled -1	25 - 28
ϵ_{lpha}	0.1
$\epsilon_ au$	0.5
Initial τ	40
Initial α	30
τ range	[0, 60]
α range	[0, 60]
Average τ	1.31
Average α	22.76
Percent of correct classification	0.826698
Time elapsed	105.56 s

The initial τ does not have a large effect on the final average τ , subtracting the burn-in period. Initializing τ at 20 resulted in an average τ of around 1.2, while initializing at 0.1 resulted in an average of 0.99. I made a video with the traces of $(u^{(k)}, \tau^{(k)}, \alpha^{(k)})$. Diagrams: Figure 7, Figure 8, Figure 9, Figure 10, Figure 11, Figure 12.

Fig. 7. α acceptance probability

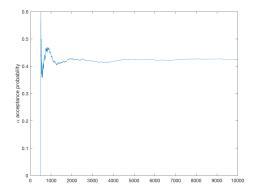
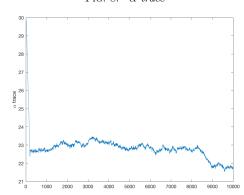
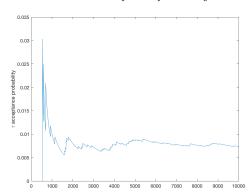


Fig. 8. α trace



4. Two moons data. The non-centered parameterization with the unnormalized Laplacian does not perform well on the two moons data set. One possibility is that the first eigenvector in the unnormalized Laplacian is constant and is throwing off the classification.

Fig. 9. τ acceptance probability



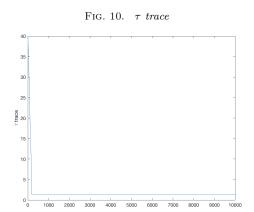


Fig. 11. u acceptance probability

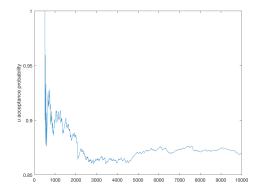


Fig. 12. u final average

