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Recap

We have setup a mocked up task based on cheap docking data for a different task (docking to D4 Dopamine receptor). In our mocked up task this cheap docking data counts as the ground truth.

To create results from cheap docking/expensive docking/FEP oracles for our mocked up task we are adding the outputs of randomly initialized NNs (after tuning so that they have suitable variances) to our "ground truth" values.

This allows us to check the BayesOpt pipeline before using it on the more complicated task.

Bayes Model

Implementing a Bayesian Linear Regression from fingerprints to dopamine score — just to ensure that it gets calibrated uncertainties and get an idea of how much data it needs to train.

In particular we want to make sure that the inference scheme which we are using works and whether we need to setup any hyperpriors etc.

The weirdness at 1000 training points is probably related to the fact that the fingerprints are 1000 dimensional?

Bayes Model

Name	Training set size	` '	Avg Loglikelihood (†)
Dummy Gaussian (var=1)	10	19.85	-10.84
Linear Regression/w Gaussian likelihood (var=1)	10	19.93	-10.89
Bayesian Regression	10	19.88	-2.98
Sklearn Bayesian Ridge Regression	10	19.43	-2.91
Bayesian Regression with the sklearn learnt precisions (weights: 1534.742,noise:0.058)	10	19.43	-2.91
Dummy Gaussian (var=1)	20	19.77	-10.80
Linear Regression/w Gaussian likelihood (var=1)	20	18.08	-9.96
Bayesian Regression	20	18.08	-2.94
Sklearn Bayesian Ridge Regression	20	19.40	-2.92
Bayesian Regression with the sklearn learnt precisions (weights: 248.117,noise:0.065)	20	19.40	-2.92
Dummy Gaussian (var=1)	50	19.46	-10.65
Linear Regression/w Gaussian likelihood (var=1)	50	15.46	-8.65
Bayesian Regression	50	15.44	-2.87
Sklearn Bayesian Ridge Regression	50	15.48	-4.03
Bayesian Regression with the sklearn learnt precisions (weights: 2.445,noise:0.380)	50	15.48	-2.79
Dummy Gaussian (var=1)	100	19.51	-10.67
Linear Regression/w Gaussian likelihood (var=1)	100	15.21	-8.52
Bayesian Regression	100	15.07	-2.83
Sklearn Bayesian Ridge Regression	100	14.66	-3.56
Bayesian Regression with the sklearn learnt precisions (weights: 2.555,noise:0.330)	100	14.66	-2.77
Dummy Gaussian (var=1)	500	19.53	-10.68

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Linear Regression/w Gaussian likelihood (var=1)	500	20.88	-11.36
Bayesian Regression	500	17.84	-2.93
Sklearn Bayesian Ridge Regression	500	12.21	-2.68
Bayesian Regression with the sklearn	500	12.21	-2.67
learnt precisions (weights: 3.421, noise:0.135)			
Dummy Gaussian (var=1)	1000	19.43	-10.64
Linear Regression/w Gaussian likelihood (var=1)	1000	367.00	-184.42
Bayesian Regression	1000	24.10	-4.26
Sklearn Bayesian Ridge Regression	1000	11.22	-2.63
Bayesian Regression with the sklearn	1000	11.22	-2.63
learnt precisions (weights: 4.101, noise:0.119)			
Dummy Gaussian (var=1)	2500	19.42	-10.63
Linear Regression/w Gaussian likelihood (var=1)	2500	14.44	-8.14
Bayesian Regression	2500	13.64	-5.29
Sklearn Bayesian Ridge Regression	2500	10.26	-2.58
Bayesian Regression with the sklearn	2500	10.26	-2.58
learnt precisions (weights: 5.372, noise:0.110)			
Dummy Gaussian (var=1)	5000	19.42	-10.63
Linear Regression/w Gaussian likelihood (var=1)	5000	11.23	-6.54
Bayesian Regression	5000	11.12	-5.46
Sklearn Bayesian Ridge Regression	5000	9.83	-2.56
Bayesian Regression with the sklearn	5000	9.83	-2.56
learnt precisions (weights: 5.978, noise:0.111)			
Dummy Gaussian (var=1)	7500	19.42	-10.63
Linear Regression/w Gaussian likelihood (var=1)	7500	10.26	-6.05
Bayesian Regression	7500	10.21	-5.39
Sklearn Bayesian Ridge Regression	7500	9.50	-2.54
Bayesian Regression with the sklearn	7500	9.50	-2.54
learnt precisions (weights: 6.127, noise:0.112)			
Dummy Gaussian (var=1)	10000	19.42	-10.63
Linear Regression/w Gaussian likelihood (var=1)	10000	9.72	-5.78
Bayesian Regression	10000	9.70	-5.32
Sklearn Bayesian Ridge Regression	10000	9.27	-2.53
Bayesian Regression with the sklearn	10000	9.27	-2.53
learnt precisions (weights: 6.242, noise:0.114)	10000	0121	2.00

[⇒] Seems a Bayesian linear model does not that work well unless we put hyperpriors on the weight variance and noise variance parameters. How is it best to do?

BayesOpt vs Traditional VS baseline

Running the Bayesian model in a VS pipeline to compare against not using it and instead just filtering on the previous results.

Note that this model is not currently taking in the cheaper docking scores as input, just the molecular fingerprints

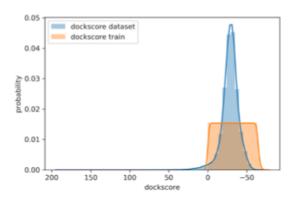
Full Dataset -9.79673 -9.74911 -9.74911 -9.56339	-9.43006
BayesVS -9.6253 -9.45149 -9.44911 -8.9872	-8.62768
PlainVS -9.6253 -9.56339 -9.45149 -9.32768	-8.90863

[⇒] Very preliminary — need to actually implement Bayesian model properly (ie give it good feats and use actually sensible priors)

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Misc Notes

- changed it to a minimization problem.
- this subset of data we are operating on (~250k in size) has been preprocessed to uniformly sample over dockscores, this means that it may be an easier task to do well randomly on than the original data...?
 - 4. Here is the plot blue is the original distribution, yellow is the sampled distribution



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