$\underbrace{\log P(\alpha|F_1, ..., F_n)}_{Posterior} = -\sum_i \frac{1}{2}\frac{1}{\sigma_i^2}\langle\rangle_\alpha$

1 Introduction

Here we derive a number of analytical results to use as unit tests of FitEnsemble.

2 Reweighting a 1D Gaussian

$$\Delta U(x;\alpha) = \sum_i^n \alpha_i f_i(x)$$

$$\pi_j(\alpha) = \frac{1}{\sum_k \exp[-\Delta U(x_k;\alpha)]} \exp[-\Delta U(x_j;\alpha)]$$

Suppose $x = N(0,1)$.

$$P_0(x) = \frac{1}{\sqrt{2\pi}} \exp(-\frac{1}{2}x^2)$$

Suppose we reweight with BELT:

$$P_1(x) \propto \exp(-\frac{1}{2}x^2 - \alpha x)$$

Completing the square shows that

$$x' \sim N(-\alpha, 1)$$

3 Reweighting a 2D Gaussian

In the case of multiple dimensions, the same result should hold but with vectors:

$$x' \sim N(-\alpha, 1)$$

4 1D Gaussian BELT

Suppose the $P(\alpha) \sim 1$. Then

$$LP(\alpha|F) = -\frac{1}{2\sigma_i^2}(\langle f_i(x)\rangle_\alpha - F_i)^2 + LP(\alpha)$$

Because $x' \sim N(-\alpha, 1)$, we know that

$$\langle f_i(x)\rangle_\alpha = -\alpha$$

If $LP(\alpha)$ is constant, it follows that the

$$P(\alpha|F) \sim N(-F, \sigma_i)$$

It appears that this test is difficult to run because the MCMC sampler occasionally gets stuck in a local minimum, leading to slowly converging chains with a larger than expected standard deviation. We therefore chose to test things with a non-zero prior.

5 1D Gaussian BELT with Maxent Prior

According to Wikipedia, the relative entropy of two normal distributions with unit variance is given by:

$$\frac{1}{2}(\mu_1 - \mu_0)^2$$

$$\mu_0 = 0$$

$$LP(\alpha|F) = -\frac{1}{2\sigma_i^2}(\langle f_i(x)\rangle_\alpha - F_i)^2 - \frac{\lambda}{2}(\mu_1)^2$$

Because $x' \sim N(-\alpha, 1)$, we know that

$$\langle f_i(x)\rangle_\alpha = -\alpha$$

$$\mu_1 = -\alpha$$

We have

$$-\frac{1}{2}\frac{1}{\sigma^2}(\alpha+F)^2-\frac{\lambda}{2}\alpha^2$$

Let's let $\sigma = 1$.

$$-\frac{1}{2}(\alpha+F)^2-\frac{\lambda}{2}\alpha^2$$

$$-\frac{1}{2}(\alpha^2(1+\lambda)+2\alpha F+F^2)$$

Let $\rho = (1+\lambda)^{-1/2}$
Then

$$-\frac{1}{2\rho^2}(\alpha^2+2\alpha F\rho^2+F^2\rho^2)$$

Then we have

$$-\frac{1}{2\rho^2}(\alpha+F\rho^2)^2+[...]$$

Thus, we have

$$\alpha \sim N(F\rho^2, \rho^2)$$

6 1D Gaussian BELT with MVN prior

Suppose that x is a multivariate standard normal.

$$LP(\alpha|F) = -\frac{1}{2}\sum_i \frac{1}{\sigma_i^2}(\langle f_i(x)\rangle_\alpha - F_i)^2 + LP(\alpha)$$

$$LP(\alpha|F) = -\frac{1}{2}\sum_i \frac{1}{\sigma_i^2}(\alpha + F_i)^2 + LP(\alpha)$$

Because α is MVN,

$$LP(\alpha|F) = -\frac{1}{2}\sum_i \frac{1}{\sigma_i^2}(\alpha_i + F_i)^2 - \frac{\lambda}{2}\sum_i \alpha_i^2$$

7 Uniform RV on [0,1]

Suppose $x \sim U(0,1)$.

$$P^0(x) = 1$$

$$P^1(x) = \frac{1}{Z}\exp(-\alpha x)$$

$$Z = \frac{1}{\alpha}(1 - \exp(-\alpha))$$

$$< x >_\alpha = \frac{1}{\alpha} - (\exp(\alpha) - 1)^{-1}$$

8 Exponential RV

Let

$$P^0(x) = k\exp(-kx)$$

Then

$$P^1(x) = (k+\alpha)\exp(-(k+\alpha)x)$$

9 Summary:

If

$$x^0 \sim N(0,1)$$

Then

$$x^1 \sim N(-\alpha,1)$$

If $x^0 \sim N(0,1)$ and α has a Maxent or MVN prior, and F is our measurement, then

$$\alpha \sim N(F\rho^2, \rho^2)$$

Let $\rho = (1+\lambda)^{-1/2}$