



## Maximum Likelihood with Tree Normals

### 1 Why

What if we use the principle of maximum likelihood to select the maximum likelihood normal density which factors according to a tree?

### 2 Definition

A *maximum likelihood tree normal* of a dataset in  $\mathbf{R}^d$  is a multivariate normal density that factors according to a tree and maximizes the likelihood of the dataset.

### 3 Results

**Proposition 1.** *Let  $D = (x^1, \dots, x^n)$  be a dataset in  $\mathbf{R}^d$ . A normal density is a maximum likelihood tree normal of  $D$  if and only if it is an optimal tree approximator of the empirical normal density of  $D$ .*

*Proof.* First, let  $f : \mathbf{R}^d \rightarrow \mathbf{R}$  be a normal density.

First, express the log likelihood of  $f$  on a record  $x^k$  by

$$\log f(x^k) = -\frac{1}{2}(x^k - \mu)^\top \Sigma^{-1}(x^k - \mu) - \frac{1}{2} \log \mathbf{det} \Sigma - \frac{d}{2} \log 2\pi.$$

Second, use the trace to rewrite the quadratic form

$$-\frac{1}{2} \mathbf{tr} \left( \Sigma^{-1}(x^k - \mu)(x^k - \mu)^\top \right).$$

Third, use these two, and the linearity of trace to express the average negative log likelihood by

$$-\frac{1}{n} \sum_{k=1}^n \log f(x^k) = \frac{1}{2} \mathbf{tr} \left( \Sigma^{-1} \left( \frac{1}{n} \sum_{i=1}^n (x^k - \mu)(x^k - \mu)^\top \right) \right) + \frac{1}{2} \log \mathbf{det} \Sigma + \frac{d}{2} \log 2\pi.$$

Fourth, use matrix calculus (or the derivation in Proposition 1 of Multivariate Normal Maximum Likelihood) to see that, for a minimizer of the negative average log likelihood, the mean must be  $\frac{1}{n} \sum_{i=1}^n x^k$ .

Fifth, recognize the empirical covariance matrix  $\frac{1}{n} \sum_{k=1}^n (x^k - \mu)(x^k - \mu)^\top$ ; denote it by  $S$ .

Sixth, change variables with  $P = \Sigma^{-1}$  and express

$$\log(\mathbf{det}(\Sigma)) = \log(\mathbf{det}(P^{-1})) = \log((\mathbf{det} P)^{-1}) = -\log(\mathbf{det}(P))$$

Seventh, write the likelihood in simplified form (using circulant property of trace)

$$\frac{1}{2} \mathbf{tr}(SP) - \frac{1}{2} \log \mathbf{det} P - \frac{d}{2} \log 2\pi$$

Eighth, drop the constant and prefactors:

$$\mathbf{tr}(SP) - \log \mathbf{det} P$$

Ninth, if  $g$  is a normal with then the tree density approximation objective is the same equivalent to

$$d(g, f) = h(g, f) - h(f) \sim h(g, f) = - \int_{\mathbf{R}^d} g \log f.$$

TODO: Extra, the let  $g$  be normal and  $f$  be normal. The tree normal approximation problem

$$d(g, f) \sim h(g, f) = - \int_{R^d} g \log f.$$

The log of  $f$  is

$$-\frac{1}{2} \mathbf{tr} \left( \Sigma_f \int_{\mathbf{R}^d} (x - \mu_f)(x - \mu_f)^\top dx \right) - \frac{1}{2} \log \mathbf{det} \Sigma_f^{-1} - \frac{d}{2} \log 2\pi$$

Since the set of optimal solutions for both optimization is contained in the set of normal densities which match on the mean we can assume that  $\mu_f = \mu_g$ . So the approximation objective is equivalent to

$$\mathbf{tr} P_f \Sigma_g - \log \mathbf{det} P_f,$$

which is exactly the maximum likelihood objective.

Thus, a solution is a maximum likelihood tree normal of a dataset if and only if it is an optimal tree approximator of the empirical normal density of the dataset.

□