

## MAXIMUM LIKELIHOOD TREE NORMALS

## Why

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

## Definition

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

## Results

**Prop. 1.** Let  $D = (x^1, ..., x^n)$  be a dataset in  $\mathbb{R}^d$ . 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  $f: \mathbf{R}^d \to \mathbf{R}$  be a normal density.

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

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

Second, use the trace to rewrite the quadratic form

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

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

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

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

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

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

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

Eighth, drop the constant and prefactors:

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

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

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

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

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

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.

