Weibull - Mixed Weibull - Cox Proportional Hazards Model relpy new statistical features

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1 Weibull fitting

1.1 PDF

Weibull PDF f^W:

$$f^W(x,\Theta=(\beta,\eta)) = \frac{\beta}{\eta}\left(\frac{x}{\eta}\right)^{\beta-1} e^{-(\frac{x}{\eta})^\beta}$$

1.2 Likelihood

$$L(\Theta) = \sum_{i=1}^{f} ln\left(\frac{\beta}{\eta}(\frac{x_i}{\eta})^{\beta-1}\right) - \sum_{i=1}^{n}\left(\frac{x_i}{\eta}\right)^\beta$$

where f is the number of failure points (indeces from 1 to f: failures, from $f+1$ to n: suspensions).

1.3 MLE

Let's take a look at the gradient of the Log-likelihood:

$$\nabla L(\Theta) = \begin{cases} \frac{f}{\beta} + \sum\limits_{i=1}^{f} \ln\left(\frac{x_i}{\eta}\right) - \sum\limits_{i=1}^{n}\left(\frac{x_i}{\eta}\right)^\beta \ln\left(\frac{x_i}{\eta}\right) \\ -\frac{f\beta}{\eta} + \frac{\beta}{\eta}\sum\limits_{i=1}^{n}\left(\frac{x_i}{\eta}\right)^\beta \end{cases} = 0$$

The second equation gives us a relation between η and β:

$$\eta = \left(\frac{\sum\limits_{i=1}^{n} x_i^\beta}{f}\right)^{1/\beta}$$

Reinjecting this formula into the likelihood, we get a new objective function

$$\begin{aligned} f(\beta) &= L(\beta,\eta(\beta)) \\ &= f ln(\beta) - f ln\left(\sum_{i=1}^{n} x_i^\beta\right) + (\beta-1)\sum_{i=1}^{f} ln(x_i) + \text{cst} \end{aligned}$$

Deriving it, we obtain a new equation:

$$\nabla f(\beta) = \frac{f}{\beta} - \frac{f \sum\limits_{i=1}^{n} ln(x_i) x_i^{\beta}}{\sum\limits_{i=1}^{n} x_i^{\beta}} + \sum_{i=1}^{f} ln(x_i)$$
$$= 0$$

$$\frac{1}{\beta} - \frac{\sum\limits_{i=1}^{n} ln(x_i) x_i^{\beta}}{\sum\limits_{i=1}^{n} x_i^{\beta}} + \frac{1}{f} \sum_{i=1}^{f} ln(x_i) = 0$$

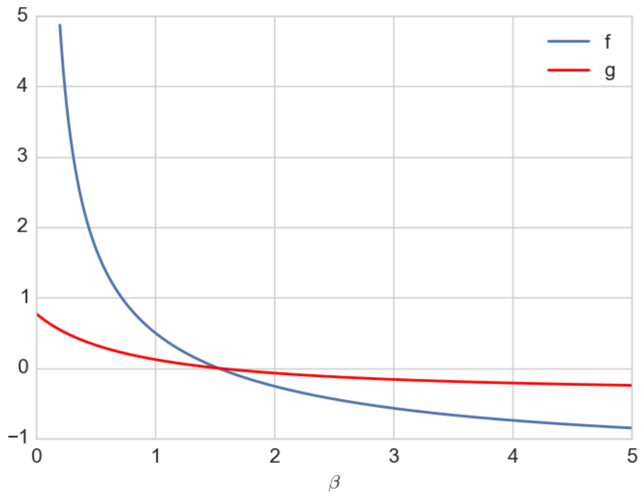
Solving it would give us the optimal β.

To solve it, we need to apply the Newton descent method on either of these 2 functions:

$$f(\beta) = \frac{1}{\beta} - \frac{\sum\limits_{i=1}^{n} ln(x_i) x_i^{\beta}}{\sum\limits_{i=1}^{n} x_i^{\beta}} + \frac{1}{f} \sum_{i=1}^{f} ln(x_i)$$

$$g(\beta) = \frac{\sum\limits_{i=1}^{n} x_i^{\beta}}{\sum\limits_{i=1}^{n} ln(x_i) x_i^{\beta}} - \frac{\beta}{1 + \beta \frac{1}{f} \sum_{i=1}^{f} ln(x_i)}$$

f vs. g Let's look at an example plot of f and g:



f goes to infinity in 0, so if close to 0, Newton will be really unefficient. Also, complicated to find a reliable starting point.

On the other hand, g is globally way flatter, and 0 is finite, so good match for a starting point.

We apply Newton to g:

$$g'(\beta) = 1 - \frac{\sum\limits_{i=1}^{n} ln(x_i)^2 x_i^{\beta} \sum\limits_{i=1}^{n} x_i^{\beta}}{\left(\sum\limits_{i=1}^{n} ln(x_i) x_i^{\beta}\right)^2} - \frac{1}{\left(1 + \frac{\beta}{f} \sum\limits_{i=1}^{n} ln(x_i)\right)^2}$$

2 Mixed Weibull fitting

2.1 Mixed Weibull probability distribution

See: The Mixed Weibull Distribution

Mixed Weibull PDF f^{MW}:

$$f^{MW}(x,\Theta) = \sum_{j=i}^{S} \frac{N_j}{N} \frac{\beta_j}{\eta_j} \left(\frac{x}{\eta_j}\right)^{\beta_j - 1} e^{-(\frac{x}{\eta_j})^{\beta_j}}$$

where :

- S is the number of subpopulationss
- N_i is the cardinal of subpopulation number i
- N is the total size of the sample
- Θ is the set of parameters: $\{\beta_1, \beta_2, \cdots, \beta_S, \eta_1, \cdots, \eta_S, N_1, \cdots, N_S\}$

We can see this Mixed Weibull PDF as a sum of Weibull distributions weighted by the shares of each subpopoulation $\pi_j = \frac{N_j}{N}$, where $\sum \pi_j = 1$.

The PDF becomes:

$$f^{MW}(x,\Theta) = \sum_{j=i}^{S} \pi_j f^W(x, \theta_j)$$

2.2 Log-likelihood

Given an input data vector of size n $X = (x_1, \cdots, x_n)$, the likelihood of the Mixed Weibull is:

$$\begin{aligned}
L(\Theta) &= \sum_{i=1}^{n} ln(f^{MW}(x,\Theta)) \\
&= \sum_{i=1}^{n} ln\left(\sum_{j=i}^{S} \pi_j f^W(x_i, \theta_j)\right) \\
&= \sum_{i=1}^{n} ln\left(\sum_{j=i}^{S} \pi_j \frac{\beta_j}{\eta_j} \left(\frac{x_i}{\eta_j}\right)^{\beta_j - 1} e^{-(\frac{x_i}{\eta_j})^{\beta_j}}\right)
\end{aligned}$$

2.3 MLE

The problem becomes: find Θ^* such that

$$\Theta^* = \underset{\Theta}{\operatorname{argmax}}\, L(\Theta) = \underset{\pi_1,\beta_1,\eta_1,\cdots,\pi_S,\beta_S,\eta_S}{\operatorname{argmax}} \sum_{i=1}^{n} ln\left(\sum_{j=i}^{S} \pi_j \frac{\beta_j}{\eta_j} \left(\frac{x_i}{\eta_j}\right)^{\beta_j - 1} e^{-(\frac{x_i}{\eta_j})^{\beta_j}}\right)$$

Under constraint: $\sum_{j=1}^{S} \pi_j = 1$

2.4 Dealing with supension data

In case the data shows suspension, we need to tweak the objective function, the same way we would do for a Weibull distribution.

If we have f failures, $n-f$ suspensions, the log-likelihood becomes:

$$L(\Theta) = \sum_{i=1}^{f} ln\left(\sum_{j=i}^{S} \pi_j \frac{\beta_j}{\eta_j}\left(\frac{x_i}{\eta_j}\right)^{\beta_j - 1} e^{-(\frac{x_i}{\eta_j})^{\beta_j}}\right) + \sum_{i=f+1}^{n} ln\left(\sum_{j=i}^{S} \pi_j e^{-(\frac{x_i}{\eta_j})^{\beta_j}}\right)$$

To keep it simple, I'll keep using f^W in the equations, but the form above is the right one to use.

2.5 Expectation Maximization Algorithm

We are using the MLE to find the parameters. In order to maximize the Log-Likelihood, we are using the Expectation-Maximization algorithm.

Basically, read wikipedia article: Expectation Maximization Algorithm

French article with a nice example: Algorithme esperance-maximisation

We define the set of random variables $Z = \{z_{ij} \in \{0,1\}, \quad i \in [\![1,n]\!], j \in [\![1,S]\!]\}$ as:

$$z_{ij} = \begin{cases} 1 & \text{if } x_i \text{ belongs to population j} \\ 0 & \text{otherwise} \end{cases}$$

The Log-likelihood then becomes:

$$L(\Theta) = \sum_{i=1}^{n} \sum_{j=i}^{S} z_{ij} ln(\pi_j f^W(x_i, \theta_j))$$

We don't have acess to z_{ij}, we can only estimate it with its expectation (expectation step) and then refine this estimation at each iteration.

The problem of finding Θ comes down to iterating the sequence $\left\{\Theta^k\right\}$ which converges to Θ^*, the desired set of parameters:

$$\Theta^{k+1} = \underset{\Theta}{\operatorname{argmax}} F(\Theta, \Theta^k) = \sum_{i=1}^{n} \sum_{j=i}^{S} E\left(z_{ij} | x, \Theta^k\right) \ln\left(\pi_j f^W(x_i, \theta_j)\right)$$

The algorithm includes 2 steps at each iteration:

- the Expectation (step E): the value of the expectation at iterate k is estimated using Bayes' theorem
$$a_{ij}^k = E\left(z_{ij} | x, \Theta^k\right) = \frac{\pi_j^k f^W(x_i, \theta_j^k)}{\sum_{l=1}^{S} \pi_l^k f^W(x_i, \theta_l^k)}$$

- the Maximization (step M): computes $\left\{\Theta^{k+1}\right\}$ solving the optimization subproblem under constraint $\sum \pi_j = 1$.

$$\Theta^{k+1} = \underset{\Theta}{\operatorname{argmax}} \left\{ \sum_{i=1}^{n} \sum_{j=i}^{S} a_{ij}^k \ln\left(\pi_j f^W(x_i, \theta_j)\right) \right\}$$

Thanks to the separability properties[1] of the objective function:

$$
\begin{aligned}
\max_{\Theta}\left\{\sum_{i=1}^{n}\sum_{j=i}^{S}a_{ij}^{k}\ln\left(\pi_j f^{W}(x_i,\theta_j)\right)\right\} &= \max_{\Theta}\left\{\sum_{j=i}^{S}\sum_{i=1}^{n}\left(a_{ij}^{k}\ln\left(\pi_j\right)+a_{ij}^{k}\ln\left(f^{W}(x_i,\theta_j)\right)\right)\right\}\\
&= \max_{\Pi}\left\{\sum_{j=i}^{S}\sum_{i=1}^{n}a_{ij}^{k}\ln\left(\pi_j\right)\right\}+\max_{\theta_j}\left\{\sum_{j=i}^{S}\sum_{i=1}^{n}a_{ij}^{k}\ln\left(f^{W}(x_i,\theta_j)\right)\right\}\\
&= \max_{\Pi}\left\{\sum_{j=i}^{S}\sum_{i=1}^{n}a_{ij}^{k}\ln\left(\pi_j\right)\right\}+\sum_{j=i}^{S}\left\{\max_{\theta_j}\sum_{i=1}^{n}a_{ij}^{k}\ln\left(f^{W}(x_i,\theta_j)\right)\right\}
\end{aligned}
$$

where Π is the set of parameters $\Pi = \{\pi_1, \cdots, \pi_S\}$.

It results in 2 optimization sub(sub)problems:

Sspb 1:

$$
\begin{cases}
\max_{\Pi}\sum_i\sum_j a_{ij}^{k} ln(\pi_j)\\
s.t. \sum_j \pi_j = 1
\end{cases}
$$

Sspb 2: $\forall j$,

$$
\max_{\theta_j}\sum_{i=1}^{n}a_{ij}^{k}\ln\left(f^{W}(x_i,\theta_j)\right)
$$

2.6 First subproblem

Let's write the Langrangian l of the problem:

$$
l(\Pi,\lambda) = \sum_j\left(ln(\pi_j)\sum_i a_{ij}^{k}\right)+\lambda\left(\sum_j \pi_j - 1\right)
$$

According to the KKT conditions, the solution couple (Π^*, λ^*) verifies:

$$\lambda^* > 0$$

$$\nabla l(\Pi^*, \lambda^*) = 0$$

resulting in :

$$
\begin{pmatrix}
\frac{\sum_i a_{i1}^{k}}{\pi_1^*} - \lambda^*\\
\vdots\\
\frac{\sum_i a_{iS}^{k}}{\pi_S^*} - \lambda^*
\end{pmatrix} = 0
$$

[1] **Separability property** in a nutshell: Given a function f of 2 independant sets of variables X and Y, if there exist 2 functions g and h such that:

$$f(X,Y) = g(X) + h(Y)$$

then:

$$\max_{X,Y} f(X,Y) = \max_{X} g(X) + \max_{Y} g(Y)$$

Finally, we obtain that $\forall j$,

$$\pi_j^* = \lambda^* \sum_i a_{ij}^k$$

And thanks to the constraint condition:

$$\lambda^* = \frac{1}{\sum_i \sum_j a_{ij}} = \frac{1}{n}$$

Therefore, $\forall j$,

$$\pi_j^{(k+1)*} = \frac{1}{n} \sum_i a_{ij}^k$$

2.7 Second subproblem

We can notice that the quantity $\sum_{i=1}^n a_{ij}^k \ln\left(f^W(x_i,\theta_j)\right)$ is almost the same as the the log-likelihood function of the Weibull: $L(x,\theta) = \sum_{i=1}^n \ln\left(f^W(x_i,\theta_j)\right)$ up to a constant multiplier for each term.

We can use a slightly modified version of fitWeibull to solve it, using the Newton algorithm.

Equation to solve for Weibull:

$$\frac{1}{\beta} - \frac{\sum_{i=1}^n \ln(x_i) x_i^\beta}{\sum_{i=1}^n x_i^\beta} + \frac{\sum_{i=1}^r \ln(x_i)}{r} = 0$$

Equation to solve for Mixed Weibull:

$$\forall j, \quad \frac{1}{\beta} - \frac{\sum_{i=1}^n a_{ij} \ln(x_i) x_i^\beta}{\sum_{i=1}^n a_{ij} x_i^\beta} + \frac{\sum_{i=1}^r a_{ij} \ln(x_i)}{\sum_{i=1}^r a_{ij}} = 0$$

3 Cox-Proportional Hazards model

3.1 Definition of the model

See: Relia-Wiki

The model is defined thanks to the instantaneous failure rate λ. Given:

- a failure time t
- a set of covariates $X = [x_1, \cdots, x_m]$
- a set of weights $A = [a_1, \cdots, a_m]$
- a baseline failure rate λ_0,

the instantaneous failure rate in the Cox-Proportional hazard model is defined as:

$$\lambda(t,X) = \frac{f(t,X)}{R(t,X)} = \lambda_0(t) e^{\sum a_j x_j}$$

where f is the PDF of the distribution and R is the reliability function.

The baseline failure rate λ_0 determines the underlying distribution that is going to be used.

For the Weibull distribution, it is:

$$\lambda_0(t) = \frac{\beta}{\eta}\left(\frac{t}{\eta}\right)^{\beta-1}$$

3.2 Log-likelihood

$$L(\Theta) = \sum_{i=1}^{f} ln(\beta t_i^{\beta-1} e^{\sum_{j=0}^{m} a_j x_{ij}}) - \sum_{i=1}^{n} t_i^{\beta} e^{\sum_{j=0}^{m} a_j x_{ij}}$$

Here, we are adding a new constant covariate equal to 1 $x_0 = [x_{10}, \cdots, x_{n0}] = [1, \cdots, 1]$ to go with a new weight a_0 so that we can include η in the sum:

$$a_0 = -\beta ln(\eta)$$

3.3 MLE

Solving for a_0:

$$\frac{\partial L}{\partial a_0} = f - e^{a_0} \sum_{i=1}^{n} t_i^{\beta} e^{\sum_{j=1} a_j x_{ij}} = 0$$

This equation gives us a_0 function of the other parameters:

$$a_0 = ln\left(\frac{f}{\sum t_i^{\beta} e^{\sum a_j x_{ij}}}\right)$$

New objective function obtained by reinjecting this expression into the Likelihood:

$$L(\beta, A) = f ln(\beta) + (\beta - 1) \sum_{i=1}^{f} ln(t_i) - f ln(\sum_{i=1}^{n} t_i^{\beta} e^{\sum a_j x_{ij}}) + \sum_{i=1}^{n} \sum_{j} a_j x_{ij}$$

Gradient:

$$\frac{\partial L}{\partial \beta} = \frac{f}{\beta} + \sum_{i=1}^{f} ln(t_i) - \frac{f \sum_{i=1}^{n} ln(t_i) t_i^{\beta} e^{\sum a_j x_{ij}})}{\sum_{i=1}^{n} t_i^{\beta} e^{\sum a_j x_{ij}}}$$

$$\frac{\partial L}{\partial a_j} = \sum_{i=1}^{n} x_{ij} - \frac{f \sum_{i=1}^{n} x_{ij} t_i^{\beta} e^{\sum a_j x_{ij}})}{\sum_{i=1}^{n} t_i^{\beta} e^{\sum a_j x_{ij}}}$$

Hessian (you can do the calculations yourself and check in the code ;)):

$$\frac{\partial^2 L}{\partial \beta^2} = \cdots$$

$$\frac{\partial^2 L}{\partial a_j^2} = \cdots$$

$$\frac{\partial^2 L}{\partial \beta \partial a_j} = \cdots$$