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Approximating Dendrochronology Smoothing Splines Using Conventional Techniques

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ABSTRACT. Dendrochronologists study tree rings to reconstruct past climatic conditions. To do so, non-climatic influences are separated from climatic trends typically by fitting cubic smoothing splines, which are weighted, piece-wise polynomials used in many fields. In dendrochronology, the standard approach is to use a method developed by Cook and Peters to select the smoothing parameter of the spline (1981). The Cook and Peters method (CP Method) is unique to dendrochronology; other, more conventional smoothing parameter selection methods are not used in dendrochronology. Connecting the CP Method with a traditional approach would provide more insight into the CP Method and allow access to the robust set of techniques available with conventional splines. Our research finds a direct equivalence between traditional splines and the CP Method by setting the degrees of freedom (df) for the spline, which can produce approximately equal splines to the CP Method. The root mean squared differences between the CP Method and the closest df approach were values less than 10^{-5}. Further, correlations that modeled the CP Method's smoothing parameter against the df-approach's smoothing parameters were greater than 0.999.

1. Introduction

For many species of trees, a tree adds a new layer of growth around its perimeter each year creating a new tree ring. The growth of these rings is dependent on many factors, with climate being an important driver. For instance, under warm and wet conditions, a tree may grow faster, causing thicker rings. Conversely, a tree may grow more slowly under cold and dry conditions, causing thinner rings. Because climate creates variation in tree-ring width over time, dendrochronologists can use tree-ring sequences to reconstruct past climatic conditions (Cook and Kairiukstis, 1989; Fritts, 1976).

However, climate is not the only factor that influences ring growth. To create a proxy climate record from tree rings, non-climatic influences (e.g., stand dynamics) need to be separated from climatic trends. Stand dynamics occur in closed-canopy forests where the trees are in close proximity to each other – examples include forests in Northeast America and Europe. The closeness of the trees creates competition for resources such as water and sunlight. An example of stand dynamics is a large mature tree blocking the sunlight from smaller trees around it. The growth of the smaller trees is suppressed due to the lack of access to sunlight. When the larger tree dies, the trees around it have a sudden increase in access to sunlight causing an increase in growth.

Due to stand dynamics, trees in closed-canopy forests often have complex growth trends with peaks and valleys that cannot be adequately modeled with simpler models. A method for modeling these complex trends was developed by Cook and Peters in 1981 and is still widely used today (Cook and Peters, 1981). This method, based on spline theory from Reinsch (1967) and the use of

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splines as frequency filters from Horowitz (1974), uses a flexible model called smoothing splines that can adequately fit complex growth trends.

Since Cook and Peters developed their approach to smoothing splines in the early 1980s, much research and development has been done with smoothing splines from a statistical and theoretical perspective (e.g., Wahba (1990)). Sections 1.1 and 1.2 provide the background conventional smoothing splines and the typical dendrochronological approach, respectively. In this current paper, a connection between conventional smoothing splines and the Cook and Peters splines is developed. The data (publicly available tree-ring datasets) and methodology used for analysis is described in Section 2. Results for numerical approximations (Section 3.1) and a linear transformation (Section 3.2) are provided that allow researchers to translate one version of the splines to the other. Finally, the results are discussed in Section 3.3.

1.1. Conventional Smoothing Splines

Smoothing splines, popularized by Reinsch (1967), are a method for interpolating data that follow complex patterns. In traditional smoothing splines, the goal is to minimize the following expression:

$$\sum_{i=0}^{n-1}[g(x_i) - y_i]^2 + \lambda \int_{x_o}^{x_{n-1}} [g''(x)]^2 dx, \tag{1.1}$$

where $g(\cdot)$ is the spline function, x_i is the independent data, y_i is the dependent data, and n is the total number of data points. The first half of the expression calculates the sum of squared residuals between the data and the model. If the second term were excluded, then the expression would be the standard linear regression model. The second term of the expression can be thought of as an aggregate measure of the “curviness” of the model. If this term were minimized without the first part of the expression, $g(x)$ would closely fit the raw data, forming what is called an interpolating spline.

The important element of the minimization expression for our research is the smoothing parameter, λ. By weighting the linear regression and the interpolation portions, the smoothing parameter balances how smooth the model is. Due to the nature of minimization, λ acts as a penalty to interpolation. A larger λ leads to a more linear and regression-like model (e.g., the blue dot-dash line in Figure 1.1). Conversely, a smaller λ makes the model more interpolating (e.g., the black solid line in Figure 1.1).

Selecting an appropriate smoothing parameter has been the focus of much research in statistics and has led to multiple ways for choosing λ (e.g., generalized cross-validation). Our research focuses on the use of degrees of freedom. Contrary to traditional regression models where the degrees of freedom are equal to the number of parameters, smoothing splines do not carry this direct equivalence (Helwig, 2021). As such, the degrees of freedom are commonly called the effective degrees of freedom (EDF); however, we use “degrees of freedom” in this manuscript for simplicity.

Regardless, selecting the degrees of freedom of a smoothing spline is analogous to selecting the smoothing parameter. More degrees of freedom creates a more interpolating spline. Conversely, fewer degrees of freedom creates a more linear relationship, with $df = 2$ typically resembling a linear regression. The equation for degrees of freedom, df, is defined as

$$df = tr(S_\lambda), \tag{1.2}$$

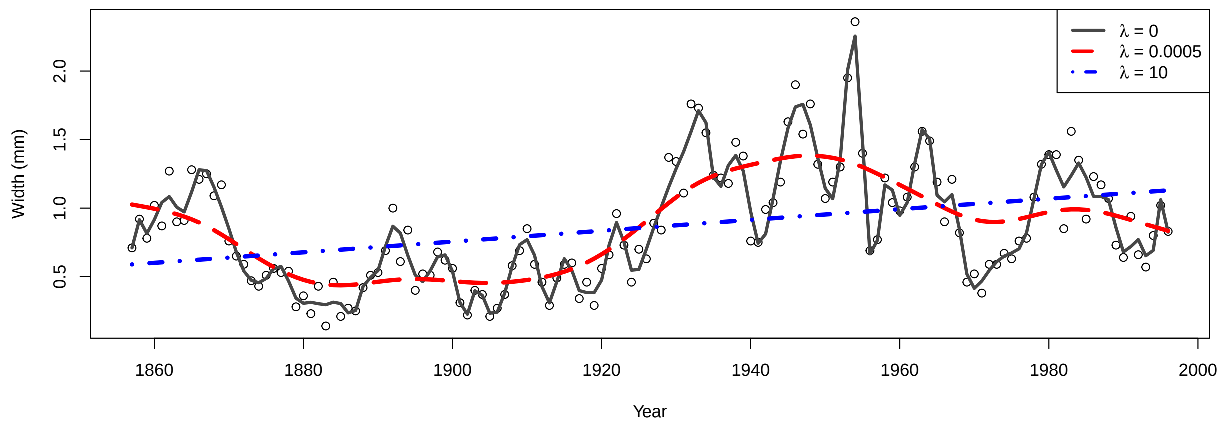

FIGURE 1.1. Three splines with varying λ values fit to tree-core HBTH0059 from the Swed320 dataset from Stockholm, Sweden (Linderholm, 2008).

where S_λ is an $n \times n$ smoother matrix, also known as the hat matrix. The form for S_λ can be found in McLeod (2018) or Wang (2011).

1.2. Smoothing Splines in Dendrochronology

In 1981, Cook and Peters applied smoothing splines to tree-ring processing in the field of dendrochronology. Smoothing splines allowed the complex growth trends in closed canopy forests to be better modeled. Their approach, which we denote simply in this paper as the CP Method, uses a reconfiguration of the typical smoothing spline expression. In the CP Method, the smoothing parameter, notated as p in their version, is placed on the summation (Expression 1.3) in contrast to the parameter λ on the integral term (Expression 1.1). It is important to note that this does not change the spline fit, but simply reconfigures the expression so that the smoothing parameter penalizes the regression term instead of the interpolation term.

$$2p \sum_{i=0}^{n-1} [g(x_i) - y_i]^2 + \int_{x_o}^{x_{n-1}} [g^{''}(x)]^2 dx \tag{1.3}$$

The primary difference in the CP Method and conventional smoothing splines is the smoothing parameter selection process. The CP Method uses Fourier transformations to decompose the data into different frequencies, which allows certain frequencies to be filtered out (e.g., short-term fluctuations in the data). In the CP Method, a frequency of interest is identified and then a smoothing parameter is found that reduces the corresponding amplitude (also known as the frequency response in tree-ring literature) by 50%. Since climate signals are typically low frequencies and disturbances are higher frequencies, reducing the frequency response aims to remove the high frequency disturbances while preserving the low frequency climate data.

To choose the smoothing parameter, Cook and Peters (1981) derived the following equation:

$$u(f) = 1 - \frac{1}{1 + \frac{p(cos(2\pi f)+2)}{6(cos(2\pi f)-1)^2}} \tag{1.4}$$

where p is the smoothing parameter, $u(f)$ is the frequency response as a proportion, and f is the target frequency to be filtered. To choose the smoothing parameter, dendrochronologists set the target frequency, f, using what is called the $\%n$ criterion (Cook and Peters, 1981). Given a tree-ring sequence's length n (i.e., the number of years in the sequence), the target frequency will correspond to a period of a certain percentage of n, where the period is the inverse of the frequency. Percentages range between 30% and 75% of the series length, but the most common choice is $67\%n$ (Cook and Kairiukstis, 1989).

What remains is to set how much of the amplitude to reduce the target frequency. The most common choice of the frequency response is 50%, or $u(f) = 0.50$. Using this choice, Equation 3 can be simplified to the following form to solve for the smoothing parameter given a target frequency (Cook and Peters, 1981):

$$p = \frac{6(cos(2\pi f) - 1)^2}{cos(2\pi f) + 2} \tag{1.5}$$

2. Data and Methods

Tree-ring data were sourced from the International Tree-Ring Data Bank (ITRDB). Each dataset provides the width of tree rings with the corresponding year for all tree cores sampled in a stand. Three different stands were used for analysis, coded ARGE010, SWED320, and ZIMB001 (Holmes and Ambrose, 1996; Linderholm, 2008; Stahle et al., 2005). However, for simplicity, our analyses primarily use the SWED320 dataset, which is a closed canopy tree core data set collected from Stockholm, Sweden (Linderholm, 2008). Analyses performed with other datasets showed similar results to the SWED320 data.

Analyses were performed using R version 4.2.1 (R Core Team, 2021). In addition to base R functions (e.g., the smooth.spline function to create smoothing splines using the conventional techniques), the R packages dplR (Bunn et al., 2021) and dplyr were used (Wickham et al., 2022). The dendrochronology dplR package was used for the functions read.rwl and detrend. Read.rwl imports uniquely formatted dendrochronology data sets. Detrend creates spline fits using the CP Method. The dplyr package was used for data wrangling. All code is available on the Github repository: `https://github.com/nbussberg/Tree_Ring_Spline_Approx`.

The CP Method's smoothing splines were compared against conventional splines whose smoothing parameter was chosen by setting the degrees of freedom of the spline. We denote this degrees of freedom approach as the *df* method for simplicity. For the CP Method, we used a $67\%n$ criterion to choose the target frequency. Though we focused on the common choice of frequency response ($u(f)$) of 0.5, we also analyzed comparisons with $u(f)$ between 0 and 1. For the *df* method, we analyzed smoothing spline fits for *df* integer values between 2 and 9. The CP Method and *df* method splines were compared graphically and numerically using the root mean squared difference (RMSD) to quantify how similar the splines were.

3. Results and Discussion

We present two ways to use degrees of freedom to create smoothing splines equivalent to those produced by the CP Method. The first relies on numerical approximations that equate particular degrees of freedom with a desired frequency response. The second uses a linear regression equation to convert a smoothing parameter calculated by R's built-in smooth.spline function. This equation

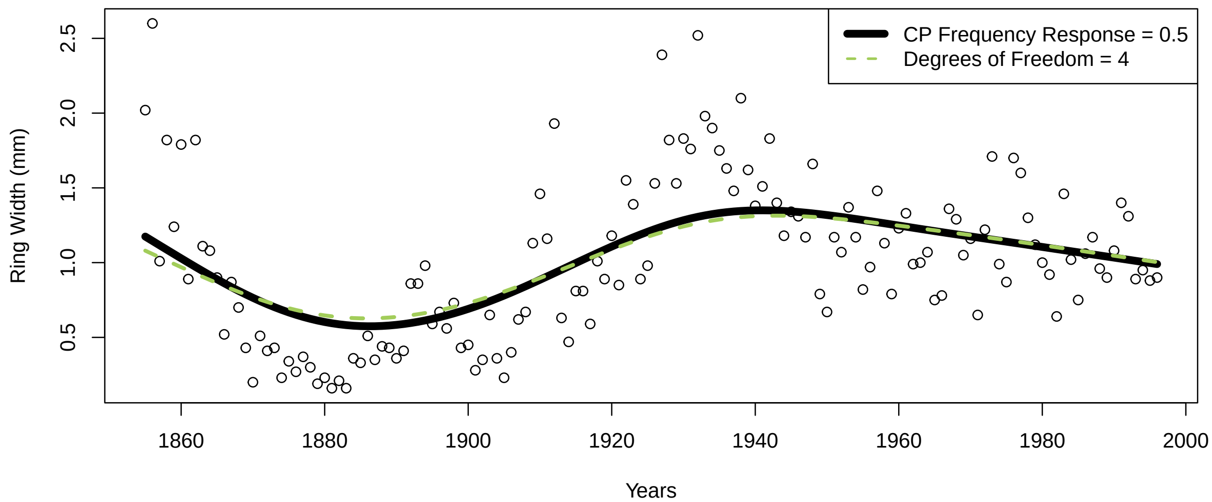

FIGURE 3.1. CP Method spline with a frequency response of 0.5 and the spline created by R's smooth.spline function with $df = 4$. The tree-ring data is core HBHT0089 from the SWED320 dataset (Linderholm, 2008).

directly connects the CP Method's smoothing parameter with the smoothing parameter produced by degrees of freedom in traditional smoothing splines.

3.1. Numerical Approximation of CP Splines using Degrees of Freedom

Setting the degrees of freedom using R's smooth.spline function can create approximately equivalent smoothing splines to the CP Method. For example, a commonly desired frequency response for the CP Method is 0.5. Using smooth.spline with degrees of freedom set to 4 creates a close approximation of the CP Method with a frequency response of 0.5. The root mean squared difference (RMSD) between the smoothing splines with four degrees of freedom and the CP method using a frequency response of 0.5 was on average 2.54×10^{-4}, supporting that the two methods' smoothing splines are nearly identical. All tree-ring sequences in the SWED320 dataset had small RMSD values; the highest RMSD observed was 1.11×10^{-3}, which is still small for the scale of tree-ring widths. This can be seen visually in Figure 3.1, which plots the CP Method's spline against the $df = 4$ spline. Though minor differences exist between these two approaches, the splines fit the data similarly.

The equivalency between the CP Method and the *df* approach can be extended to other *df* and frequency responses (Table 3.1). In the table, each *df* corresponds to a range of frequency responses in the CP Method. To use these numerical results, first note what frequency response is desired for the CP Method (i.e., what is entered in dplR package's detrend function's frequency response argument). Then, match the range that captures this frequency response to its corresponding degrees of freedom. For example, to most closely approximate the CP Method spline

TABLE 3.1. Numerical equivalencies between CP Method's frequency responses (fr range) and degrees of freedom (df). The 'fr range' indicates the range of frequency responses that are best approximated by each df. The 'closest fr' is the frequency response that generates a CP Method spline with the smallest RMSD for the given df spline. 'Mean RMSD' represents the average performance of the degrees of freedom method vs. the CP Method for all tree cores tested. Values were calculated using the SWED320 dataset (Linderholm, 2008).

df	fr range	closest fr	Mean RMSD
2	0.01 - 0.03	0.01	4.68×10^{-5}
3	0.04 - 0.25	0.11	4.92×10^{-7}
4	0.26 - 0.54	0.40	2.25×10^{-7}
5	0.55 - 0.76	0.68	1.01×10^{-6}
6	0.77 - 0.87	0.84	2.07×10^{-6}
7	0.88 - 0.93	0.91	2.41×10^{-6}
8	0.94 - 0.96	0.95	9.05×10^{-7}
9	0.97 - 0.99	0.97	1.11×10^{-6}

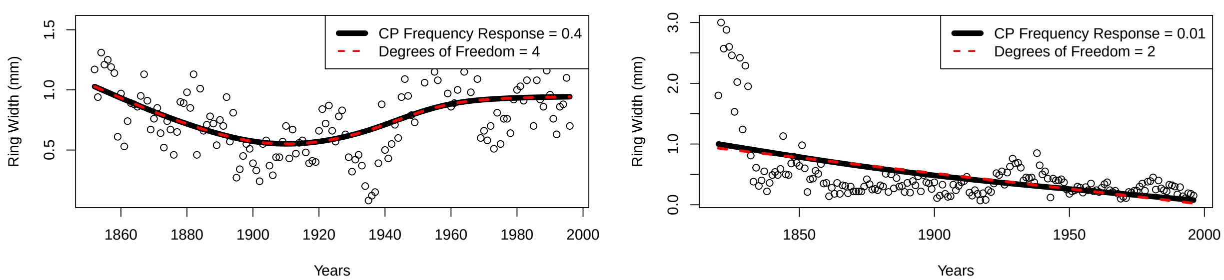

FIGURE 3.2. The closest frequency response (fr) matches for $df = 4$ (left) and $df = 2$ (right). The left graph shows the lowest (best) average RMSD between the CP Method and the df method (produced with core HMFB0059). The right graph shows the highest (worst) RMSD between the CP Method and the df method (core HBHT0119). Values were calculated using the SWED320 dataset (Linderholm, 2008).

with a frequency response of 0.85, the associated degrees of freedom for the built-in smooth.spline function would be 6.

The highest and lowest RMSDs comparing the CP Method against the df method for the SWED320 data are shown visually in Figure 3.2. The df spline fit with the lowest RMSD (when $df = 4$) is a very precise match to its corresponding CP Method spline fit. The spline fit with the highest RMSD (when $df = 2$) deviates slightly, but it is still a close match to its corresponding CP Method spline. Note that the highest RMSD used a $df = 2$, which approximates a linear relationship. While there

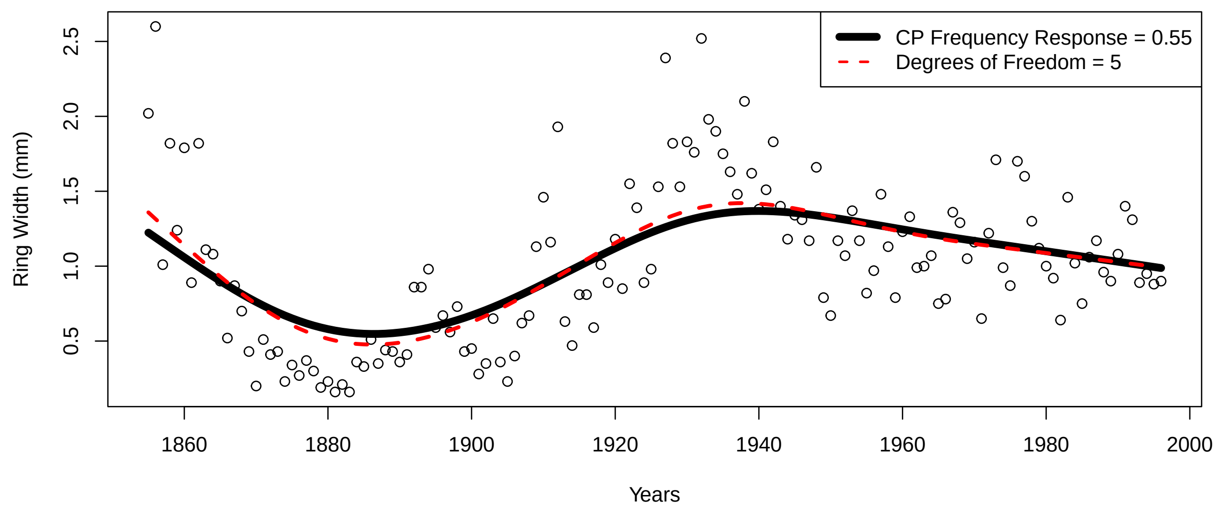

FIGURE 3.3. CP Method spline with frequency response of 0.55 (at the bottom of the fr range, see Table 3.1 for details) graphed against the spline created by its suggested df method spline. Values were calculated using the SWED320 dataset (Linderholm, 2008).

is some variability in the degrees of freedom method, even the worst performing spline fits are adequate substitutes for their corresponding CP spline fits.

It should be noted that the degrees of freedom can only be set to integers. Thus, this parameter has a broader scale relative to setting the CP Method smoothing parameter, which is a continuous variable. Table 3.1 indicates the range of frequency responses that would be best approximated by a choice of df. However, even at the edges of these ranges, the df method still produces a good approximation of the corresponding CP Method spline (e.g., Figure 3.3).

Additionally, note that for the ranges specified in Table 3.1, the frequency response values tested were between 0 and 1 with iterations of 0.01. Iterations of 0.01 provided sufficient resolution for the current research, but a finer scale could provide more detail at the bounds of each range. Frequency response values that fall between two ranges will be denoted here as intermediate fr values. For example, Figure 3.4 shows spline fit comparisons for intermediate fr values for two cores. Because the fr values fall between two choices of df, both choices are shown in the graphs. Either choice of df results in a small RMSD between the df method spline and the CP Method spline. Core HBHT0119 produces fits with RMSD of 3.70×10^{-3} and 2.63×10^{-3} for $df = 3$ and 4, respectively. Similarly, core HBHT0089 produces fits with an RMSD of 3.33×10^{-4} and 5.13×10^{-4} for $df = 6$ and 7, respectively.

3.2. Relationship between df Method's and CP Method's Smoothing Parameters

For many practical applications, the numerical approximations provided in Section 3.1 will be sufficient to change the df method's smoothing parameter to the CP Method's and vice versa.

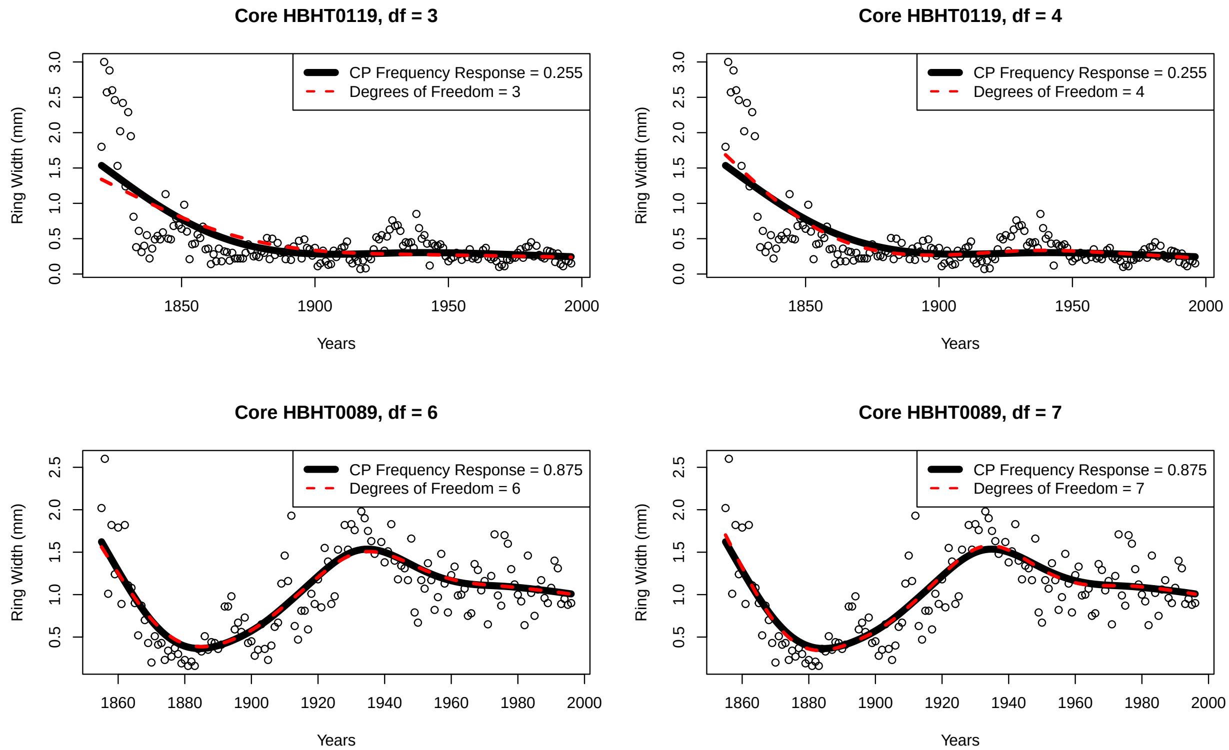

FIGURE 3.4. CP Method splines with intermediate frequency responses (see Table 3.1 for frequency response ranges) compared against the corresponding two choices of df method splines. Both graphs on the top are for core HBHT0119; the bottom two graphs are for core HBHT0089. Values were calculated using the SWED320 dataset (Linderholm, 2008)

However, there is a more direct relationship between the two methods that can more precisely perform the conversion.

The relationship between λ_d (the CP Method λ chosen with dplR's detrend function) and λ_{s4} (the corresponding λ to a spline with $df = 4$ chosen with the function smooth.spline) is

$$\lambda_d = (781\lambda_{s4} - 0.431)^4. \tag{3.1}$$

Note, $\lambda_d = \frac{1}{p}$, where p is the CP smoothing parameter, based on expression 1.3. This relationship was obtained numerically using all three datasets in our study (Holmes and Ambrose, 1996; Linderholm, 2008; Stahle et al., 2005). The correlation coefficient of the relationship was greater than 0.999 (Figure 3.5), indicating a very strong fit.

For other choices of df, similar equations may be able to be constructed. Table 3.2 shows some relationships for varying degrees of freedom. The relatively high correlations (> 0.999 for $df > 2$) indicate strong relationships for each. Based on the equations, it is apparent that the coefficient associated with λ_s increases at an increasing rate with increasing df. In future work, this relationship could be more clearly outlined. Additionally, it is important to note the correlation outlier ($r = -0.885$) for $df = 2$. Because $df = 2$ approximates a linear relationship (see Figure 3.2), this outlier is likely the result of the poor fit for the data.

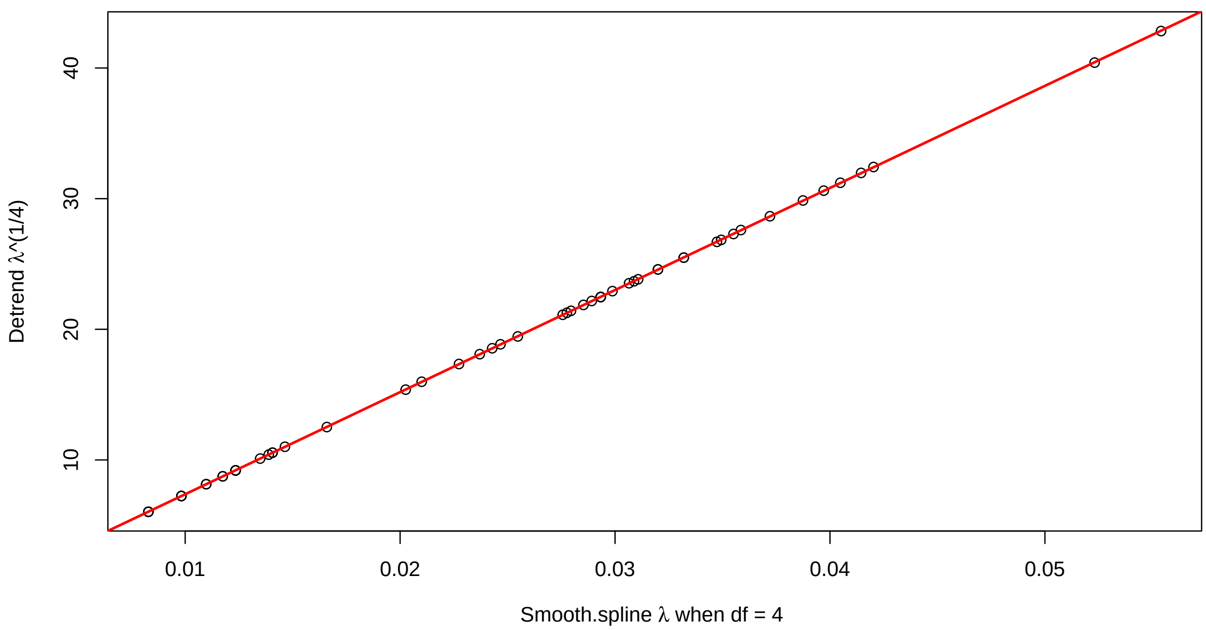

FIGURE 3.5. The relationship between λ_d (notated Detrend λ) and λ_{s4} (Smooth.spline λ). The red line follows the equation $\lambda_d = (781.28\lambda_{s4} - 0.431)^4$. Relationship computed with values from the SWED320, ARGE010, and ZIMB001 datasets (Linderholm, 2008; Holmes and Ambrose, 1996; Stahle et al., 2005).

TABLE 3.2. Relationships between $\lambda_{df,4}$ (the corresponding λ to a spline with *df* chosen with the function smooth.spline) and λ_d (the CP Method λ chosen with dplR's detrend function) for varying degrees of freedom. Relationships computed with values from the SWED320, ARGE010, and ZIMB001 datasets (Linderholm, 2008; Holmes and Ambrose, 1996; Stahle et al., 2005).

df	Equation	Correlation
2	$\lambda_d = (-0.09\lambda_{s2} + 40.134)^4$	-0.885
3	$\lambda_d = (153.63\lambda_{s3} - 0.403)^4$	> 0.999
4	$\lambda_d = (781.28\lambda_{s4} - 0.431)^4$	> 0.999
5	$\lambda_d = (2473.74\lambda_{s5} - 0.473)^4$	> 0.999
6	$\lambda_d = (6020.96\lambda_{s6} - 0.386)^4$	> 0.999

The equations in Table 3.2 are specific to the case where $fr = 0.5$. If a different choice of fr is desired, a slight change to the equation can be made. Let $\lambda_d(fr)$ denote the function to calculate the CP Method's λ given some frequency response, fr. Then, the relationship becomes

$$\lambda_d(fr) = \left(\frac{1}{1 - fr} - 1\right)(781\lambda_{s4} - 0.431)^4. \tag{3.2}$$

Equation 3.2 can be used to obtain any CP Method $\lambda_d(fr)$ from λ_{s4}. This relationship could naturally be expanding to other choices of degrees of freedom similar to Table 3.2.

3.3. Discussion

The spline method proposed by Cook and Peters (1981) revolutionized the way tree-ring data were processed. Their method is still one of, if not the, most common ways to process tree rings. In the time since Cook and Peters developed their approach for tree-ring analysis, statistical theory and methods for smoothing splines have been greatly expanded (see, for example, Wahba (1990)) for a wide range of applications. Traditional smoothing spline methods are now included in standard statistical packages: for example, the smooth.spline function in base R. The accessibility of these methods means that more researchers from different disciplines can use them in applications and engage in improving them. For example, dendrochronologists could use the base R smooth.spline function that could provide more insight into tree-ring processing itself.

Our research proposed two relationships between the CP Method and traditional smoothing splines. Both of our solutions rely on the connection between setting the degrees of freedom for a standard smoothing spline and choosing the smoothing parameter in the CP Method. The first approach supplies numerical approximations for converting degrees of freedom to the CP smoothing parameter. The second approach establishes a linear relationship between the two. Particularly for the second method, the strong correlation based on real data demonstrates that there are indeed approaches to translate a CP Method smoothing parameter to a traditional smoothing parameter (via degrees of freedom in our research) and vice versa. This should allow dendrochronologists to more easily access the wide array of smoothing spline techniques developed for other applications, and it could allow non-tree-ring researchers the ability to contribute to the growing methodology in the tree-ring community if desired.

Due to the strength of the correlation showed in Section 3.2, it appears likely that an analytical relationship could be derived. One direction could be to explore the terms associated with λ_s in Table 3.2, as there appears to be an exponential relationship as the df increase. An exact solution would bypass the need for numerical approximations and further strengthen the conclusions and recommendations of this manuscript. For example, a simple R package could be developed and published for users to easily convert CP Method parameters to traditional spline parameters.

Further work should also investigate the relationship between the CP Method and traditional splines for different $\%n$ criteria. Our research used $67\%n$ for all CP smoothing parameter calculations as it is a common assumption in dendrochronology. Although $67\%n$ is a common choice, dendrochronologists typically select between $30\%n$ and $75\%n$. Examining the relationship between the CP Method and the df method for varying $\%n$ would expand the utility of the df method. Different forms of splines like polynomial regression splines (e.g., Acharjee and Das (2022)) could also help modeling these relationships.

Lastly, further work could be done to connect the degrees of freedom method with the complete version of the Cook and Peters method as derived in Bussberg et al. (2020). The complete solution provided by Bussberg et al. yields different smoothing parameter choices given the same conditions than the original CP method. This research focused on the original CP Method for simplicity, but could be extended to the complete CP Method.

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