

The data obtained through various experimental measurements are easily compared with a time series, as they typically show some quantity measured all along the depth of an ice core. This depth is often, at short intervals, treated as a regular linear time series thus making it possible to use some of the known signal analysis methods. Of course, when considering the entirety of an ice core, the linearity disappears as thinning and compression makes the depth series non linear. But when considering short lengths of core it is possible to estimate a linearity, assuming conformity in this specific layer.

0.1 Back Diffusion

Due to diffusion in firn and ice, some of the water isotopic signal is lost. Some of this signal can be restored by investigating the diffusion process, and through filtering and deconvolution techniques(REFERENCES). For the data of this thesis two different restoration techniques are presented: a spectral method, determining the effect of mixing and diffusion as a spectral filter(REFERENCES), and a kernel restoration method much like the ones used to restore pixel resolution in images (REFERENCES).

0.1.1 Spectral Analysis

Power Spectral Densities

A very useful tool for analyzing signals exhibiting oscillatory effects is analysis of the signals power spectrum. Instead of considering the signal in time, it is transformed to the spectral domain, where it is possible to obtain an estimate of both the signal and the underlying noise. This is crucial for enhancing the signal and filtering away noise. But to be able to examine these effects, first the data must be transformed. A range of different methods may be used to compute the frequency transform of the depth series, here I present the three I have been working with. Since the data are discrete and experimental, I will be presenting the discrete and applicable mathematical models.

When considering a signal, it may be of interest to investigate how the energy of said signal is distributed with frequency. The total power is defined as:

$$\text{Total Power} = \int_{-\infty}^{\infty} |X(\tau)|^2 d\tau. \quad (1)$$

Using Parseval's theorem (REFERENCE) (assuming that the signal has a finite total energy), the power of the signal can alternatively be written as

$$\int_{-\infty}^{\infty} |X(\tau)|^2 d\tau = \int_{-\infty}^{\infty} |\tilde{X}(\tau)|^2 df \quad (2)$$

where $\tilde{X}(f)$ is the spectral (Fourier) transform of the signal, from time to frequency domain, defined as:

$$\tilde{X}(f) = \int_{-\infty}^{\infty} X(\tau) e^{2\pi i f \tau} d\tau \quad (3)$$

and the inverse spectral (Fourier) transform, from frequency to time domain, defined as:

$$X(t) = \int_{-\infty}^{\infty} \tilde{X}(f) e^{-2\pi i f \tau} df. \quad (4)$$

Both $X(t)$ and $\tilde{X}(f)$ represent the same function, just in different variable domains. Often, the angular frequency ω is used instead, with the relation between ω and f being $\omega \equiv 2\pi f$, giving the Fourier and inverse Fourier transforms as:

$$\begin{aligned} \tilde{X}(\omega) &= \int_{-\infty}^{\infty} X(t) e^{i\omega\tau} d\tau \\ X(\tau) &= \int_{-\infty}^{\infty} \tilde{X}(\omega) e^{-i\omega\tau} d\omega \end{aligned} \quad (5)$$

From Equation 2 we can interpret the integrand on the right hand side $|\tilde{X}(f)|^2$ as a density function, describing the energy per unit frequency. This is a property which is able to reveal much information about the considered signal, and it is useful to define this as the (one-sided) Power Spectral Density:

$$P_X(f) \equiv |\tilde{X}(f)|^2 + |\tilde{X}(-f)|^2 \quad 0 \leq f < \infty \quad (6)$$

This entity ensures that the total power is found just by integrating over $P_X(f)$ from 0 to ∞ . When the function is purely real, the PSD reduces to $P_X(f) = 2|\tilde{X}(f)|^2$.

In the above the transform used to define the PSD was presented as the Fourier transform. When working with discrete data, as is very common when analyzing real world data, there are a number of different ways of estimating the PSD. In the following three different methods will be presented, all used in this thesis.

RETHINK THIS PART. DO NOT USE TIME ON ALL THE CALCULATIONS. WRITE THE GENERAL IDEAS

OF THE METHODS AND STATE HOW TO CALCULATE/COMPUTE. SMALL CODE SNIP TO GIVE GENERAL IDEA.

Discrete and Fast Fourier Transform

The definition of the continuous Fourier transform and its inverse was presented in the above. The Fourier transform is as seen a way of representing the function under consideration as an infinite sum of periodic components. When the function is discrete, so will the Fourier transform be, and the integral is replaced with a sum. This gives us the Discrete Fourier Transform (DFT) which transforms the signal into a sum of separate components contributing at different frequencies. The DFT is dependent on the sampling interval, Δ , and we can describe our discrete signal X as a function of N discrete time steps $t_k = k \cdot \Delta$, where $k = 0, 1, \dots, N - 1$:

$$X_k \equiv X(t_k) \quad (7)$$

This sample size is supposed to be representative for the entire discrete function, if the function continues beyond the N sampled points. When sampling discretely at interval Δ , there will be a special frequency, the Nyquist critical frequency, defined through the sampling size as:

$$f_{NQ} \equiv \frac{1}{2\Delta}. \quad (8)$$

This frequency is of great importance in transformation of discrete signals. If the continuous signal is sampled at an interval Δ is bandwidth limited to frequencies smaller in magnitude than f_{NQ} , $\tilde{X}(f) = 0$ for $|f| \geq f_{NQ}$ - i.e. the transformed function has only non-zero values inside the Nyquist interval, $\tilde{X}(-f_{NQ}), \dots, \tilde{X}(f), \dots, \tilde{X}(f_{NQ})$. This means that the function is completely determined since we have all information about the signal contained in our available frequency space.

On the other hand, which is much more likely, if the continuous signal consists of frequencies both inside and outside the Nyquist interval, then all spectral information outside of this range will be falsely interpreted as being inside this range. Thus a wave inside the interval with a frequency of f_n will have a number of wave siblings outside of the interval, with frequencies of $k \cdot \frac{1}{\Delta} f_n$, k being integers, which will be aliased into the Nyquist interval and give rise to an increased power at the frequency f_n .

When analyzing an already measured discrete signal, this might give rise to

some headache. What can be done is to assume that the signal has been sampled competently and then assume that the Fourier transform is zero outside of the Nyquist interval. After the analysis it will then be possible to determine if the signal was indeed competently sampled, as the Fourier series will go to zero at f_{NQ} given a correct assumption, and go to a fixed value, if the sampling was not done competently.

Now with the basics of understanding the limits of frequency transform of a discretely sampled signal, it is possible to estimate the DFT of the signal $X_k \equiv X(t_k)$. Since the Fourier transform is a symmetric transformation it is easiest to assume that N is even.

Since the input information is of size N we should expect only to sample the frequency transform $\tilde{X}(f)$ at only discrete values of f in the range between the upper and lower critical Nyquist frequencies, $-f_{NQ}$ to f_{NQ} :

$$f_n \equiv \frac{n}{N\Delta}, \quad n = -\frac{N}{2}, \dots, \frac{N}{2} \quad (9)$$

This will indeed actually give rise to $N + 1$ values, since 0 will be in the interval as well, but the limit frequencies are actually not independent, but all frequencies between are, which reduces it to N samples.

Now the integral from Equation 3 needs to be estimated as a sum:

$$\tilde{X}(f_n) = \int_{-\infty}^{\infty} X(\tau) e^{2\pi i f_n \tau} d\tau \approx \sum_{k=0}^{N-1} X_k e^{2\pi i f_n t_k} \Delta = \Delta \sum_{k=0}^{N-1} X_k e^{2\pi i k \frac{n}{N}} \quad (10)$$

The Discrete Fourier Transform is thus defined as:

$$\tilde{X}_n \equiv \sum_{k=0}^{N-1} X_k e^{2\pi i k \frac{n}{N}} \quad (11)$$

This gives the approximate relation between the DFT estimate and the continuous Fourier transform $\tilde{X}(f)$ when sampling at size Δ as:

$$\tilde{X}(f_n) \approx \Delta \tilde{X}_n \quad (12)$$

The inverse DFT is given as:

$$X_n \equiv \frac{1}{N} \sum_{n=0}^{N-1} X \tilde{X}_n e^{-2\pi i k \frac{n}{N}} \quad (13)$$

Computation of the DFT can be very slow and tiresome, since it involves complex multiplication between a number of vectors and matrices. If we write

Equation 11 as $\tilde{X}_n = \sum_{k=0}^{N-1} W^{nk} X_k$, where W is a complex number $W \equiv e^{2\pi i/N}$. This shows that the vector X_k must be multiplied with a complex matrix which (n,k)th component consists of the constant W to the power of nk . This matrix multiplication evidently leads to a process of $O(N^2)$. Fortunately, a number of different algorithms(REFERENCES) have been developed for fast and efficient computation of the discrete Fourier transform. One of these is called the Fast Fourier Transform (FFT), which can reduce the computations to just $O(N \log_2 N)$! In this thesis the FFT used is the one implemented in the numpy.fft Python package(REFERENCES) which is based on the works of (REFERENCES). See said article for implementation details. One important thing about this specific algorithm is that for the algorithm to function most efficiently, the number of points computed in the frequency space must be of a power of 2, following the use of base \log_2

Discrete Cosine Transform

The DFT is generally defined for complex inputs and outputs, where the sine components of the transform describe the complex part and the cosine describes the real part.

Since the data analyzed in this thesis is purely real, it makes sense, for computational speed, to only work with the cosine parts of the transform. This leads to the Discrete Cosine Transform (DCT) which transforms real inputs to real outputs.

0.1.2 Spectral Filtering

Wiener Filtering

Through spectral analysis it is possible to treat the noise of the signal consistently. The goal is to create spectral filters which enhances the signal while minimizing the effect of the noise, thus increasing the signal-to-noise ratio (SNR).

Theoretically, without any diffusion, the change in isotopic concentration would be described through a step function, going from one constant concentration to another. This step function can be described by the Heaviside function:

$$D(t) = \begin{cases} 0, & t < 0 \\ 1, & t \geq 0 \end{cases} \quad (14)$$

In reality, a number of different mixing processes change this step function, and the measured signal will be a smooth curve, $s(t)$, which corresponds to

the convolution of $S(t)$ with the mixing response function $M(\tau)$

$$d(t) = \int_{-\infty}^{\infty} D(\tau) \cdot M(t - \tau) d\tau \quad (15)$$

0.1.3 Signal Restoration by Optimal Diffusion Length

Kernel Estimation

As is well known, in the spectral domain, convolution is multiplication and the mixing is described as the multiplication between the Fourier transform of S and M :

$$\tilde{d} = \tilde{D} \cdot \tilde{M} \quad (16)$$

By differentiation with respect to time, the mixing filter M is unaffected, and differentiation of the measured system response, the Heaviside function, S' is a delta function, which Fourier transformed is unity, leading to:

$$\tilde{d}' = \tilde{D}' \cdot \tilde{M} = \tilde{M} \quad (17)$$

The mixing filter can thus be determined by measuring the system response to a step function, differentiating performing Fourier transform of the result d' .

After determination of the mixing filter \tilde{M} , the unmixed signal D can be estimated in theory by inverse Fourier transform of

$$\tilde{D} = \tilde{d} \cdot \tilde{M}^{-1} \quad (18)$$

During the mixing, cycles with short wavelengths are heavily washed out, and through the restoration in Eq. 18, the amplitudes corresponding to these wavelengths are heavily amplified by the filter. This method though has a drawback, which is that when the measurements contain noise, the restored signal will be dominated by high-frequency noise, greatly amplified by the mixing filter. Thus it is a problem of retaining as much (short wavelength) signal as possible while simultaneously attempting to amplify the high-frequency noise as little as possible. This optimal trade-off can be found by creating an optimum filter for the considered measured isotopic signal:

$$\delta_M(z) = \delta_m(z) + \eta(z) \quad (19)$$

This optimal (Wiener) filter \tilde{F} , defined for each wave number $k = 2\pi\omega$, is presented as the ratio between pure signal and pure signal plus noise described

in Power Spectral Densities as:

$$\tilde{F}(k) = \frac{|\tilde{\delta}_m(\omega)|^2}{|\tilde{\delta}_m(\omega)|^2 + |\tilde{\eta}(\omega)|^2} \quad (20)$$

In this work, the power spectral densities of the signal and the noise, respectively, are determined through analysis of the power spectral density of the combined signal/noise PSD.

The PSD of the noise free measured signal, $|\tilde{\delta}_m(\omega)|^2$, is assumed describe as

$$|\tilde{\delta}_m(\omega)|^2 = P_0 e^{-k^2 \sigma_{\text{tot}}^2} \quad (21)$$

where σ_{tot}^2 describes the total estimated diffusion length of the mixing.

The noise is assumed to be red noise, described by an autoregressive process of first order, AR1:

$$|\tilde{\eta}(\omega)|^2 = \frac{\sigma_\eta^2 \Delta z}{|1 + a_1 \exp(-2\pi i \omega \Delta z)|^2} \quad (22)$$

where σ_η^2 is the variance of the red noise, a_1 is the AR1 coefficient and Δz is the resolution of the time/depth data. It is then possible to estimate the parameters P_0 , σ_{tot}^2 , σ_η^2 and a_1 by curve fitting, separately, the two expressions in Eq. 21 and 22 to the data. The estimated parameters are varied to find the optimal guess to use for the filter.

0.2 Enhanced Resolution and Peak Detection

0.2.1 B Spline Multipolynomial Interpolation

0.2.2 Detrending and Standardising

0.2.3 Cycle Length Estimation of Detrended Signal