Principles of Wavelet Denoising for ESR

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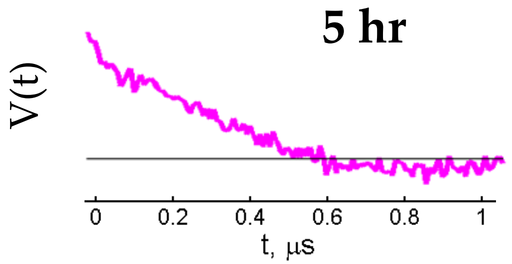
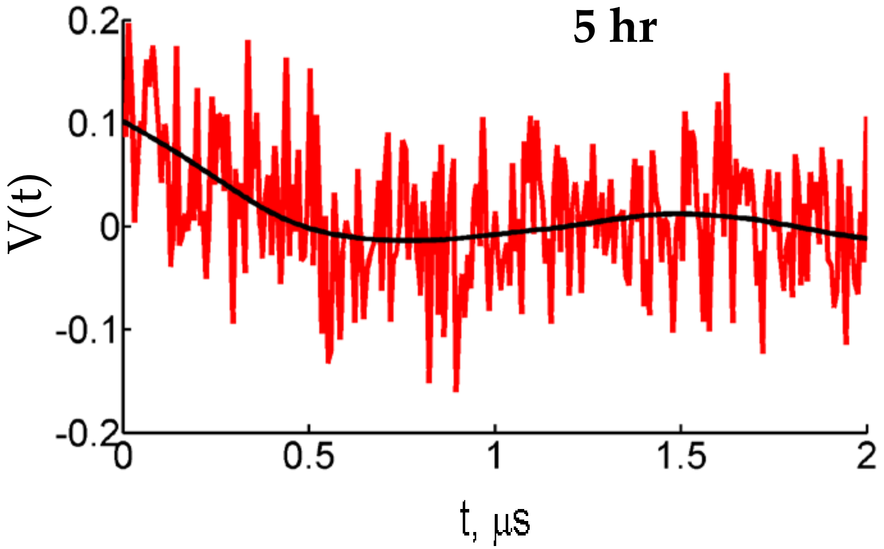
- Madhur Srivastava

Challenge: Real-world Example Shows That While Higher Experimental Sensitivity is Deemed Necessary, There are Options

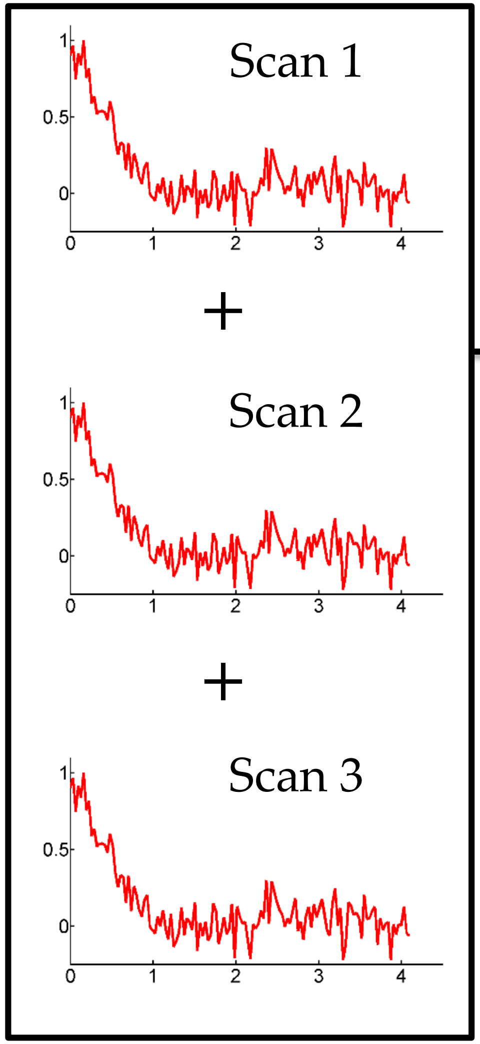


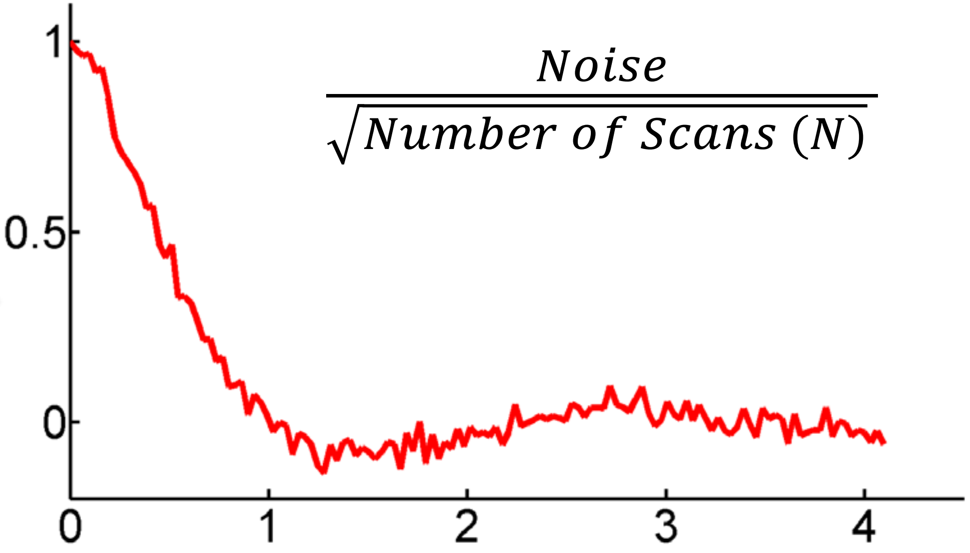


17 GHz DQC data for two anion radicals from flavin cofactors of a membrane receptor. Phase-memory time is ~1μs and radical yield is relatively low.

The DQC signal (in black), buried under overwhelming noise, was extracted by de-noising and its first half coincides with a better signal (magenta) obtained using a half of the sampling period.

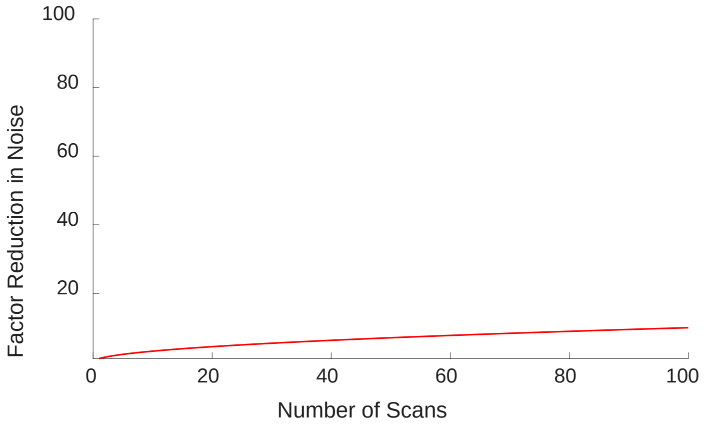
Standard Noise Reduction Method: *Signal Averaging*





$$\frac{Noise}{\sqrt{Number\ of\ Scans\ (N)}}$$

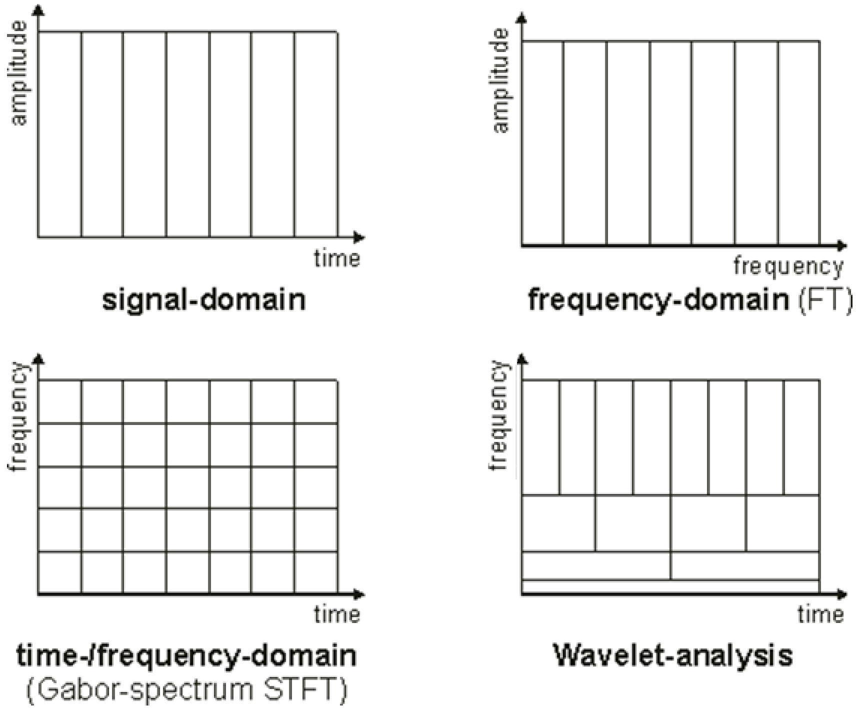
Noise Reduction Rate in Signal Averaging



Disadvantages:

- Long Acquisition Times
- Sample Breakdown
- High Sample Concentration Needed
- Instrument Drifts and Malfunction
- Inability to Acquire Signals from Unstable Samples

Comparison of Fourier Transform (FT), Short Time Fourier Transform (STFT), Wavelet Transform (WT)



FT $$F(\omega) = \int_{-\infty}^{+\infty} f(t) e^{-i\omega t} dt$$

STFT $$F(\tau,\omega) = \int_{-\infty}^{+\infty} f(t) w(t-\tau) e^{-i\omega t} dt$$

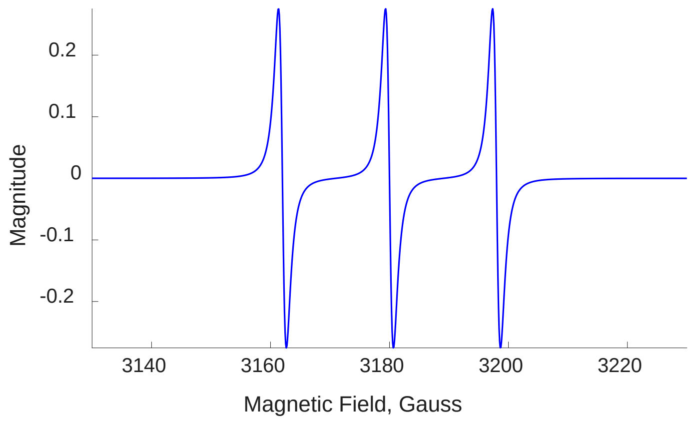
WT $$F(a,b) = \frac{1}{\sqrt{a}} \int_{-\infty}^{+\infty} f(t)\, \psi^* \left(\frac{t-b}{a}\right) dt$$

Inverse Frequency (a) Time Displacement (b)

Fourier Transform

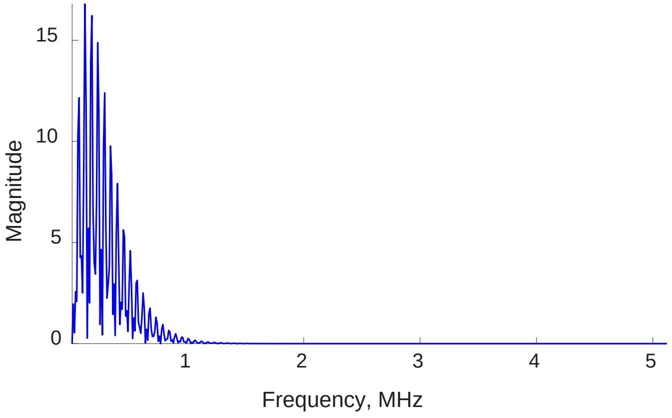
cw-ESR Spectra

a



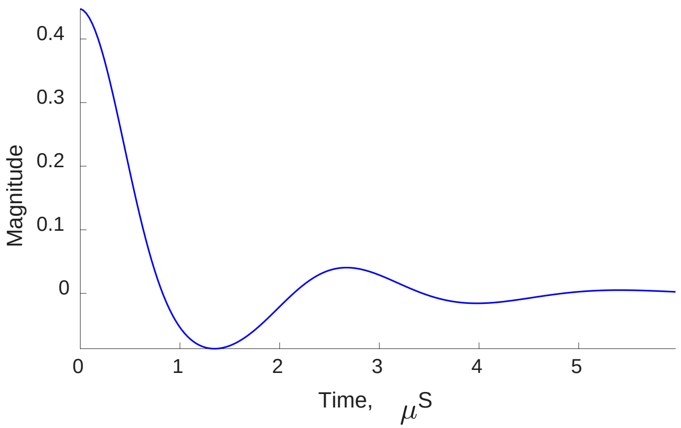
Fourier Transform

b Frequency Information



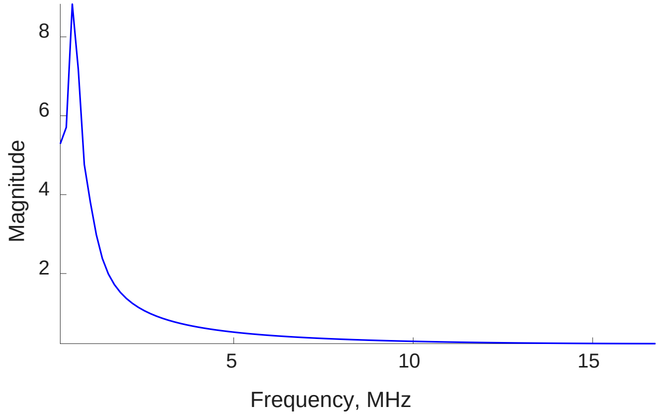
Pulsed Dipolar Signal

a

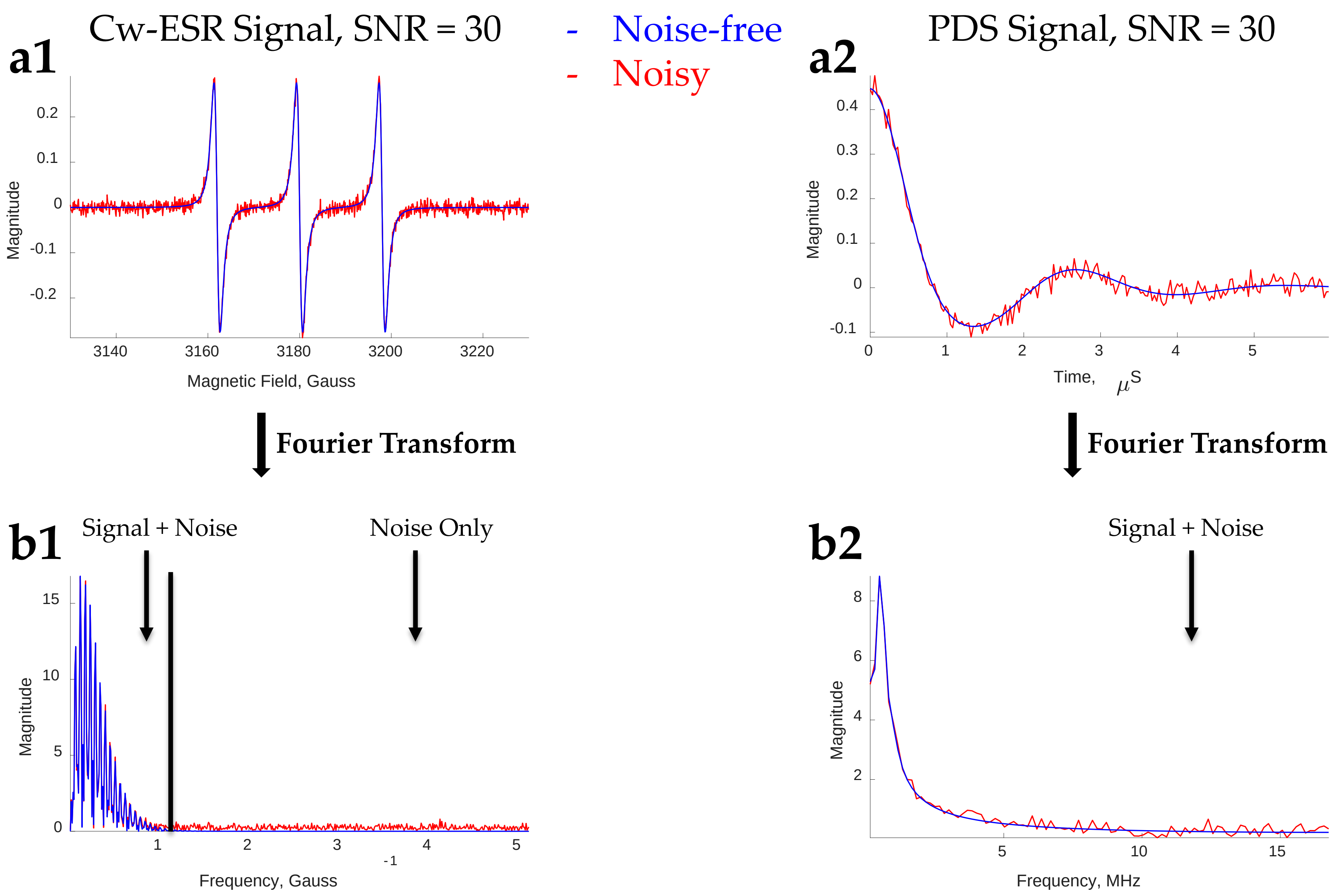


Fourier Transform

b Frequency Information



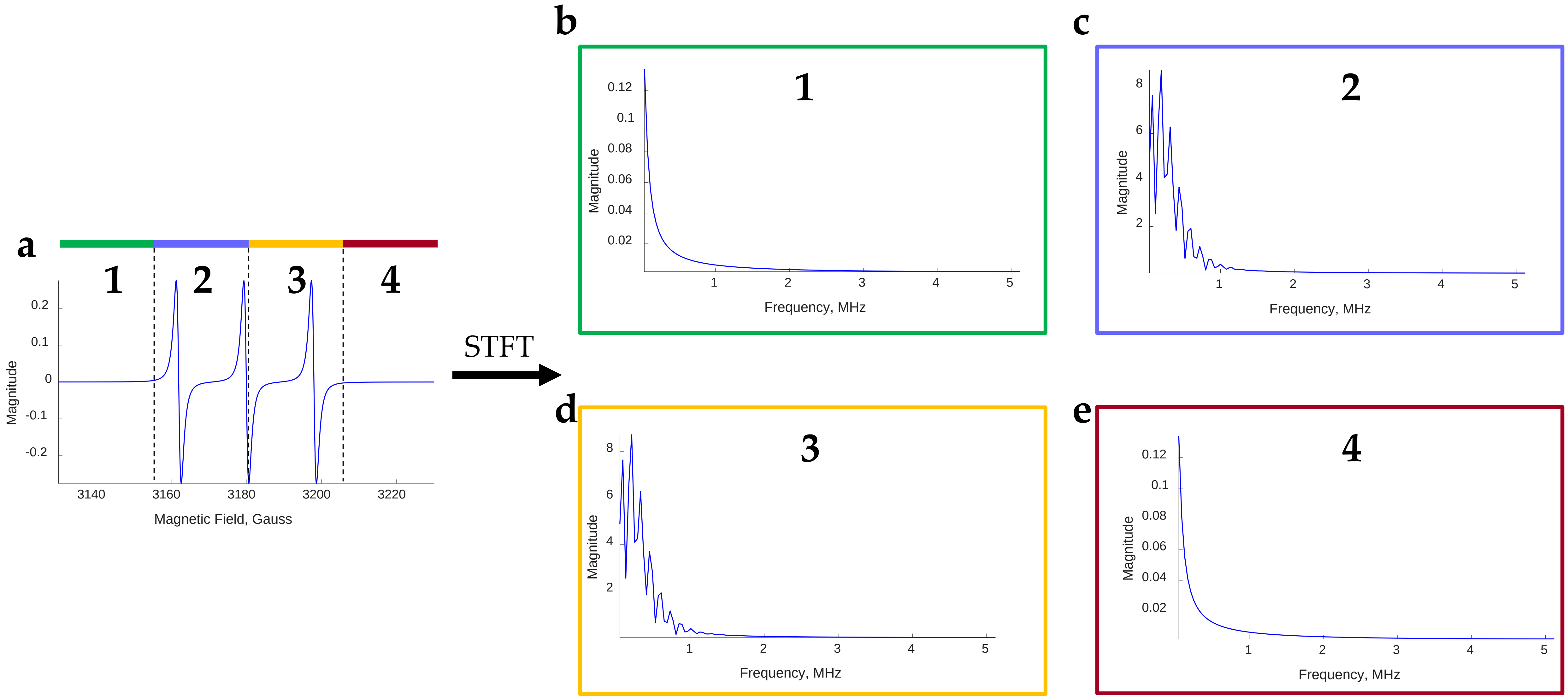
Effects of Noise in Frequency Domain



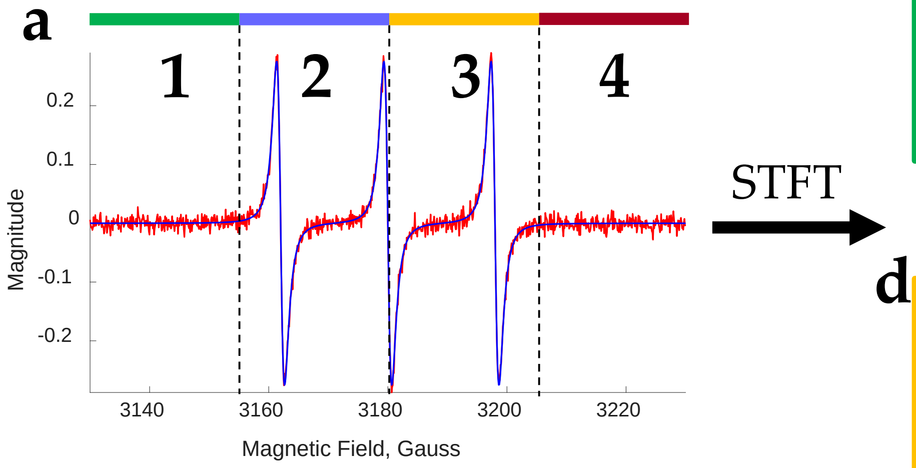
Disadvantages: Limits Fourier Filtering

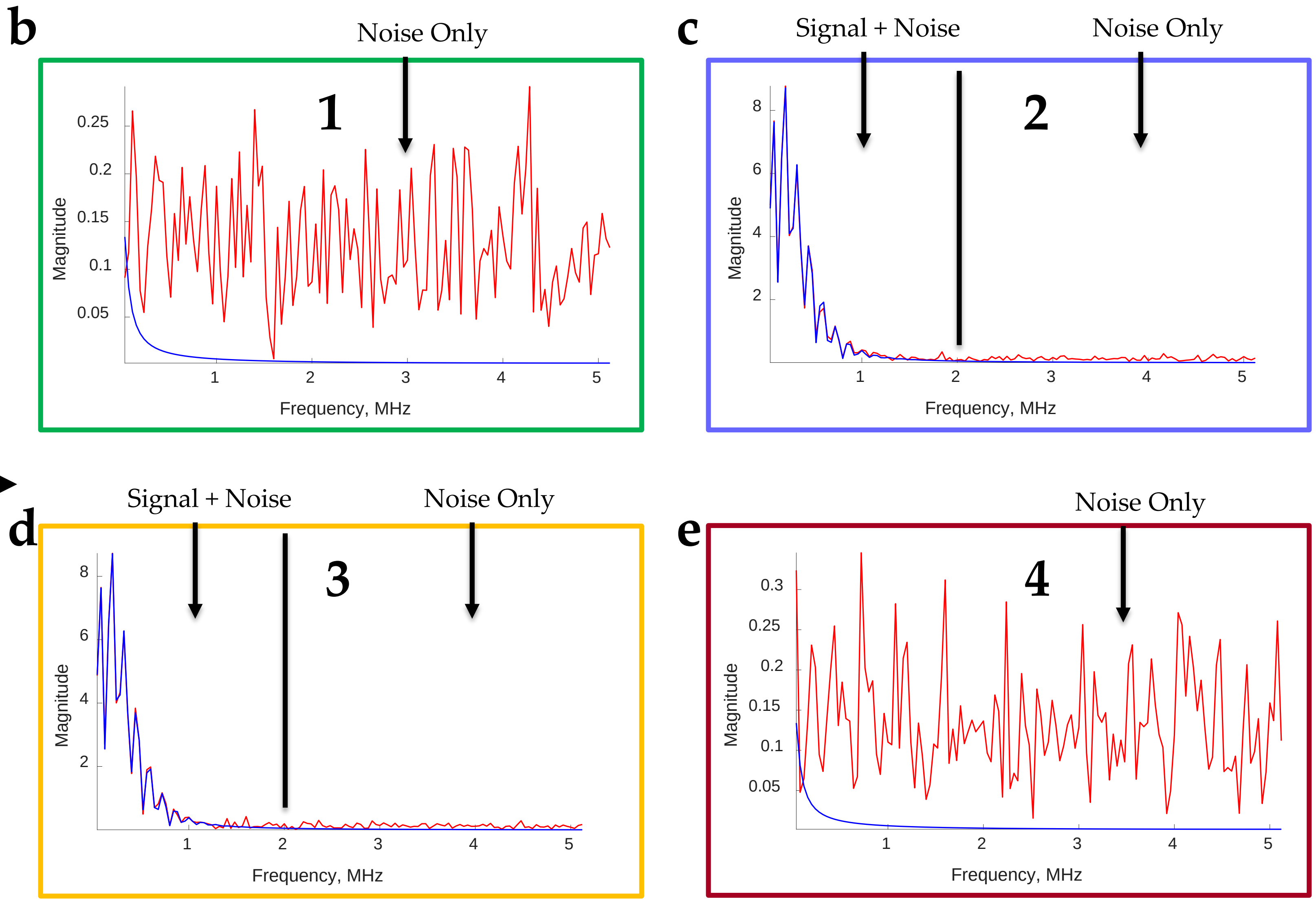
- Cannot Separate Noise and Signal Frequencies
- Cannot Identify Noise Only Frequencies

Short Time Fourier Transform



Short Time Fourier Transform: Noise and its Effects in cw-ESR

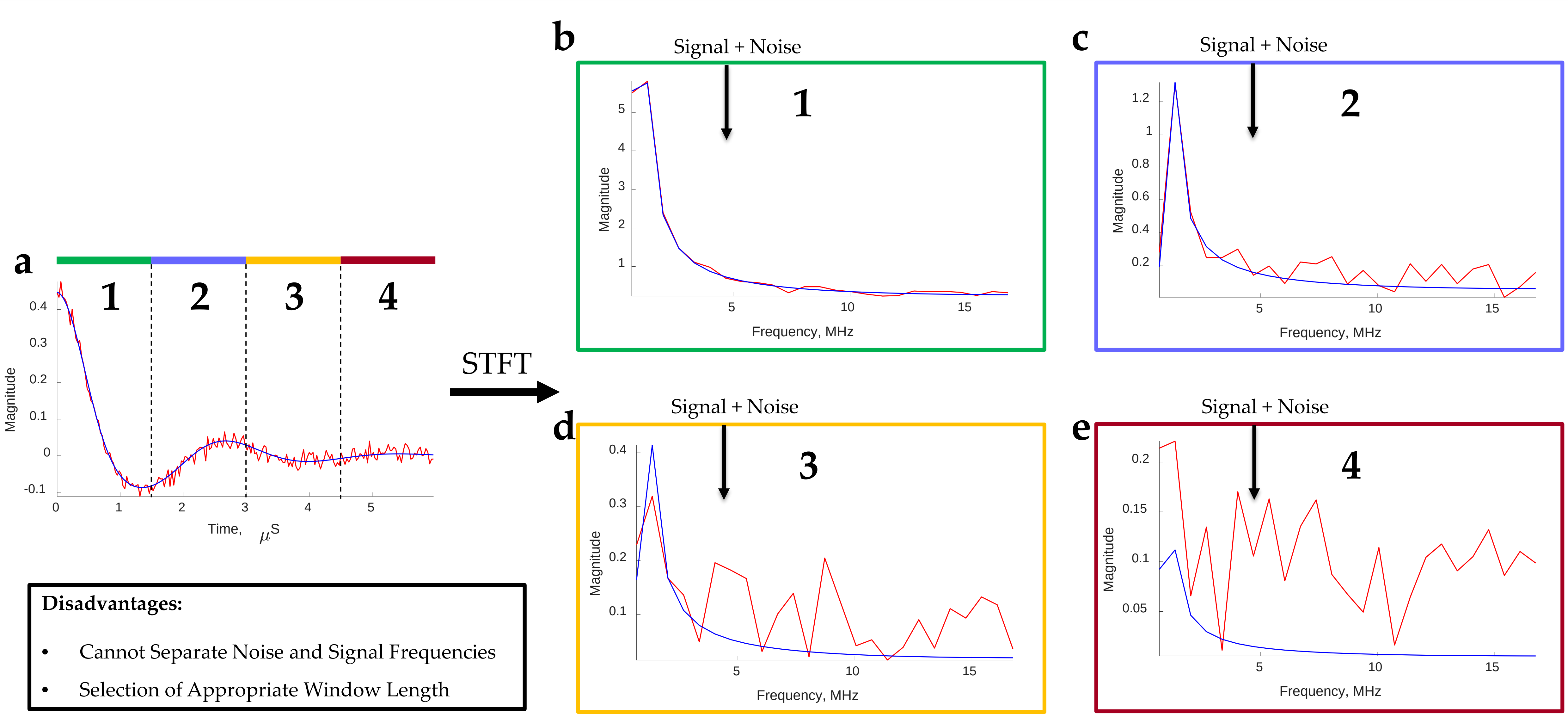




Disadvantages:

- Cannot Separate Noise and Signal Frequencies
- Cannot Identify Noise Only Frequencies
- Selection of Appropriate Window Length

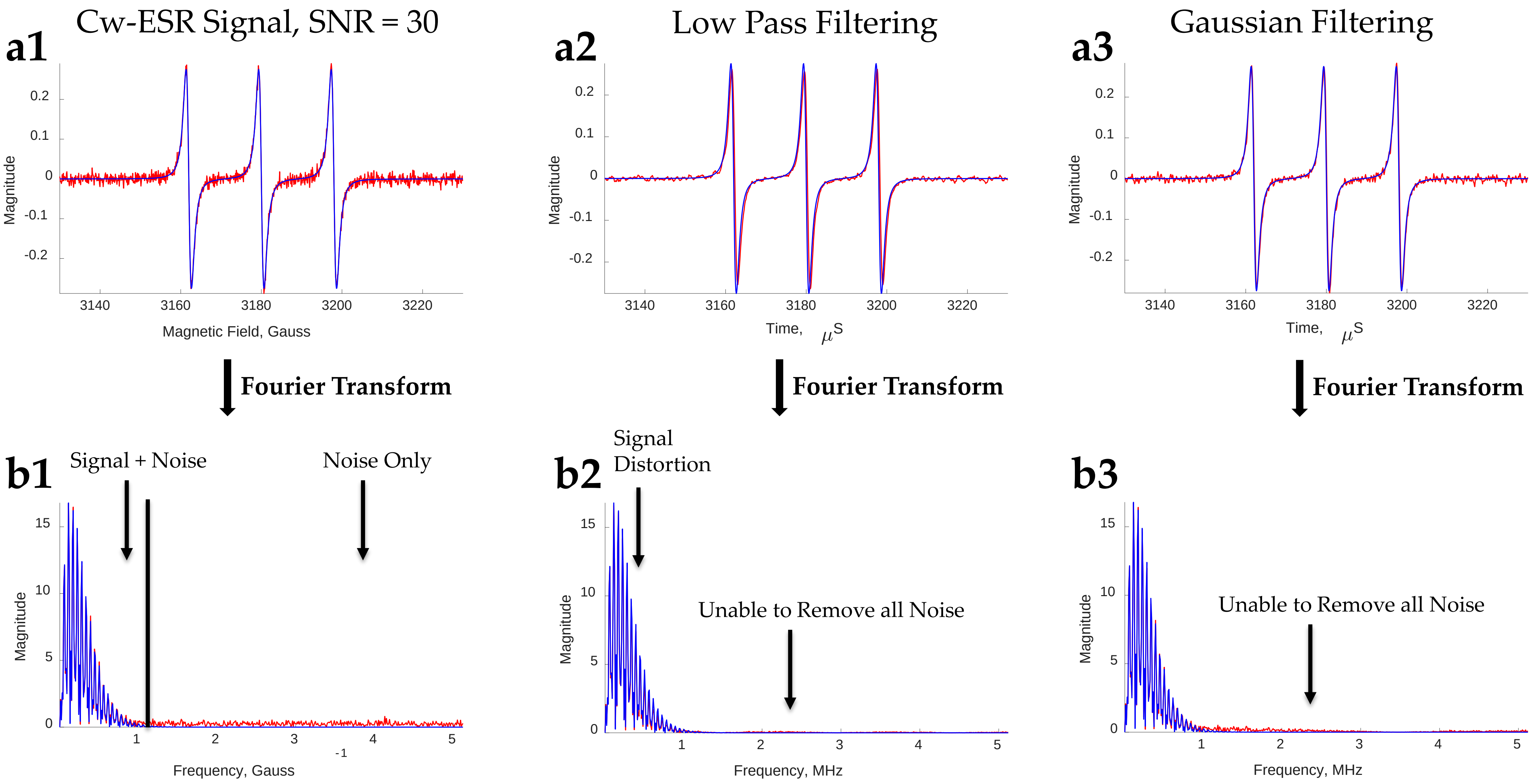
Short Time Fourier Transform: Noise and Effects in PDS



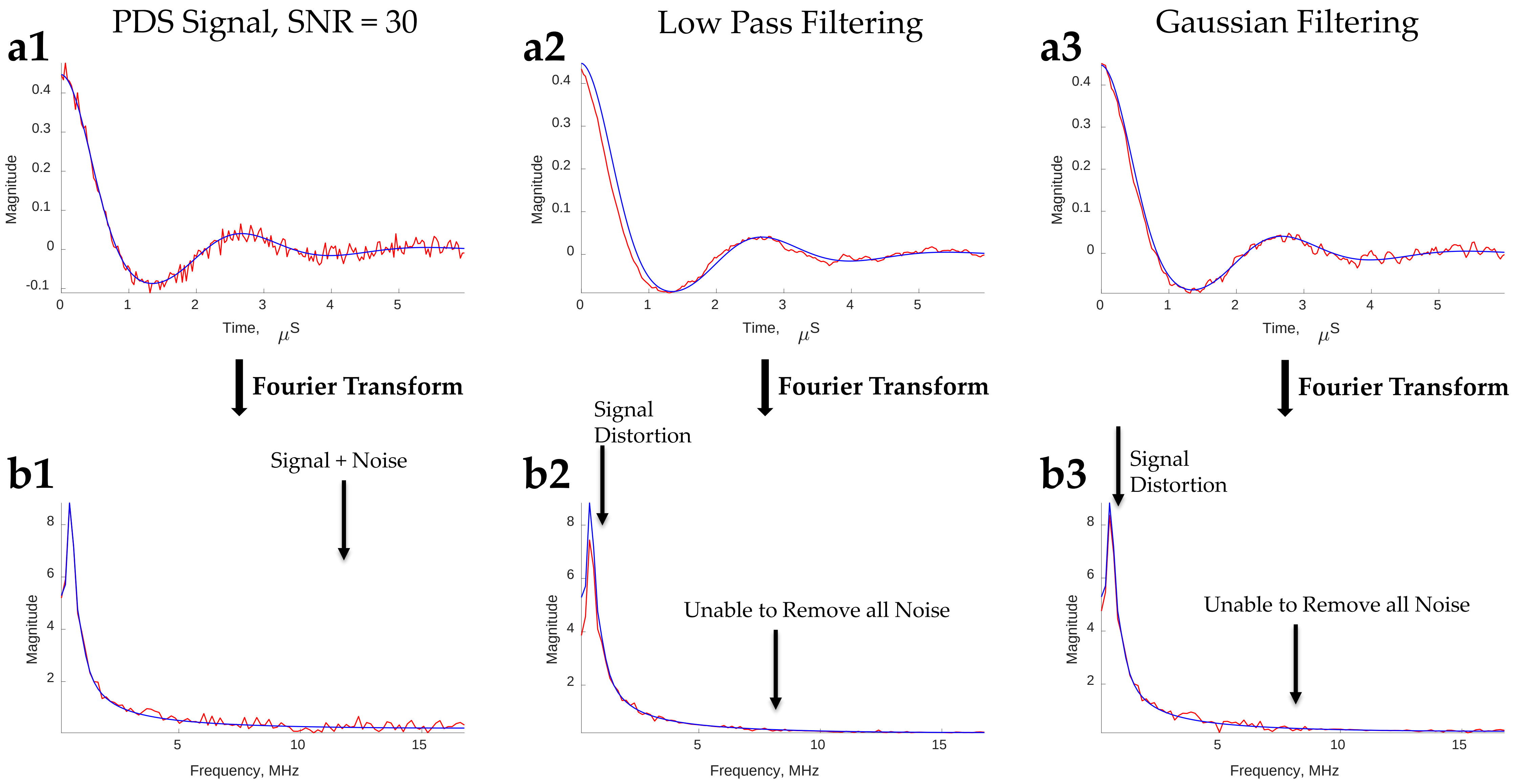
Disadvantages:

- Cannot Separate Noise and Signal Frequencies
- Selection of Appropriate Window Length

Low Pass and Gaussian Noise Filtering Methods in cw-ESR



Low Pass and Gaussian Noise Filtering Methods in PDS



Need a method that can provide signal and its frequency information simultaneously

Wavelet Transform

Continuous Wavelet Transform (CWT)

$$F(a,b) = \frac{1}{\sqrt{a}} \int_{-\infty}^{+\infty} f(t)\, \psi^* \left(\frac{t-b}{a}\right) dt$$

Discrete Wavelet Transform (DWT)

$$D[a,b] = \frac{1}{\sqrt{a}} \sum_{m=1}^{p} f[t_m]\, \psi \left(\frac{t_m - b}{a}\right)$$

Logarithmic Discretization

$$D_j[k] = \frac{1}{\sqrt{a_0^j}} \sum_{m=1}^{p} f[t_m]\, \psi \left(\frac{t_m - k b_0 a_0^j}{a_0^j}\right)$$

Dyadic Discretization

$$D_j[k] = \frac{1}{\sqrt{2^j}} \sum_{m=1}^{p} f[t_m]\, \psi \left(\frac{t_m - k2^j}{2^j}\right)$$

D = Detail or Wavelet Component

j = Decomposition level: positive integers

k = Translation parameter: positive integers

t_m = Discrete signal at integer time or location m

p = Length of discrete input signal $f[t_m]$

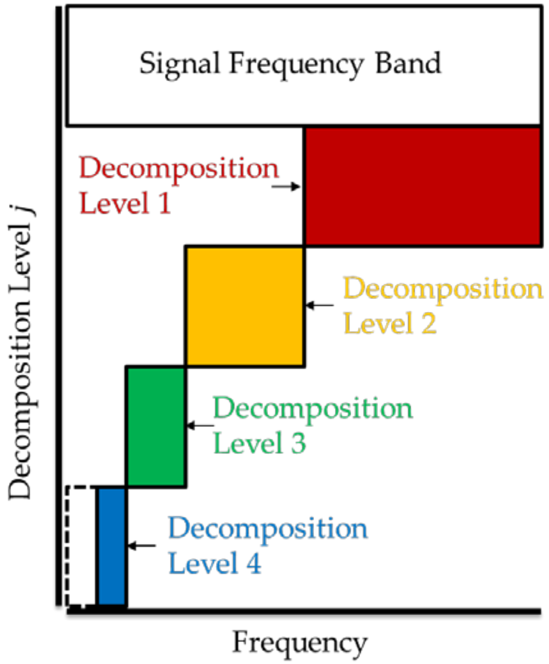
ϕ = Scaling function

ψ = Wavelet function

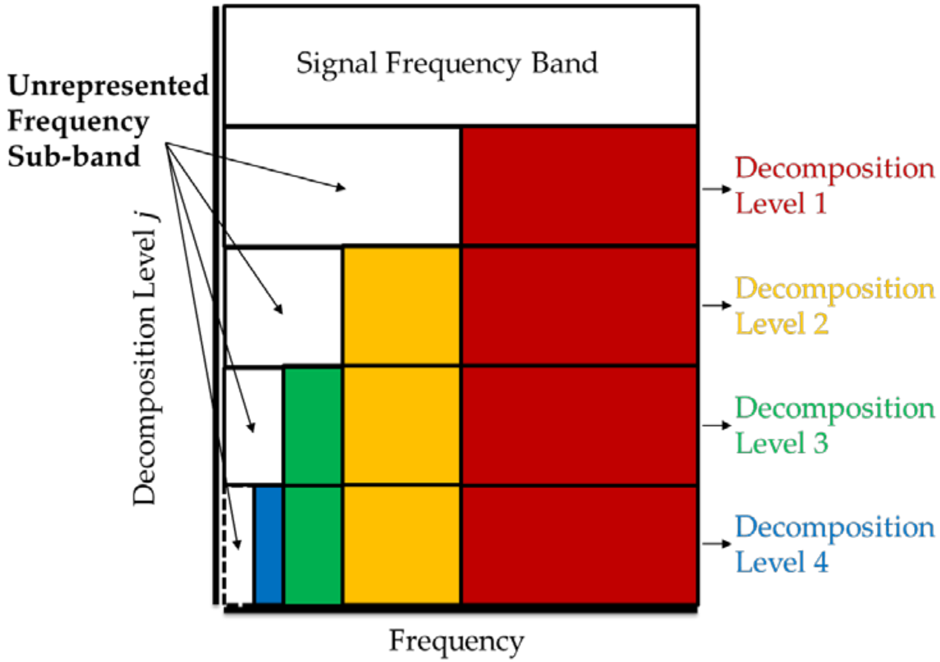
Dyadic Discretization: $b = k2^j$, $a = 2^j$

Frequency Sub-band Representation of Signal in Wavelet Domain

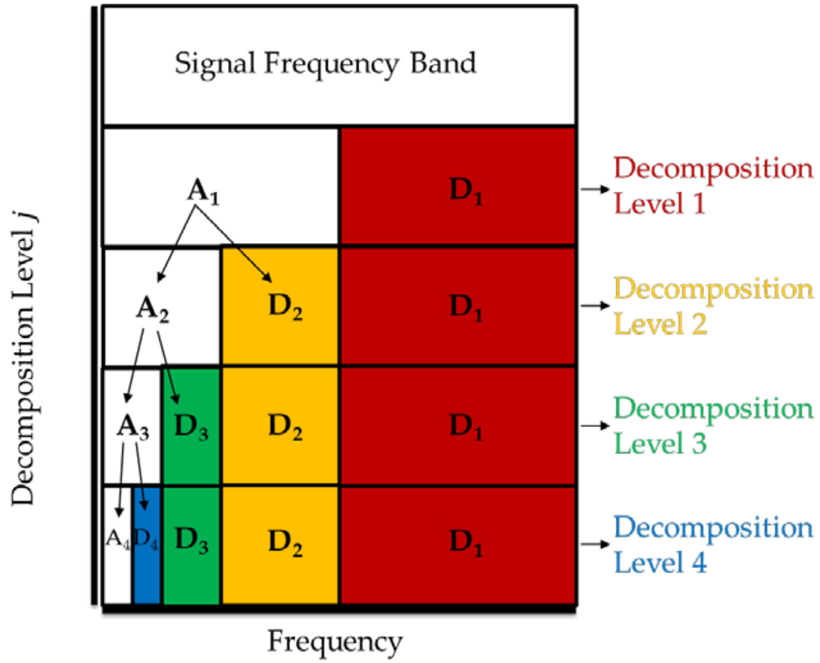
Frequency Sub-band Division in Wavelet Domain



Frequency Sub-band Representation at Each Decomposition Level



Detail and Approximation Component Representation



Scaling Function

Scaling Function

$$\phi(t_m) = (-1)^k c_k \, \psi(2t_m - k)$$

Approximation Component

$$A_j[k] = \frac{1}{\sqrt{2^j}} \sum_{m=1}^{p} f[t_m] \, \phi\left(\frac{t_m - k2^j}{2^j}\right)$$

A = Approximation or Residual Component

j = Decomposition level: positive integers

k = Translation parameter: positive integers

t_m = Discrete signal at integer time or location m

p = Length of discrete input signal $f[t_m]$

ϕ = Scaling function

ψ = Wavelet function

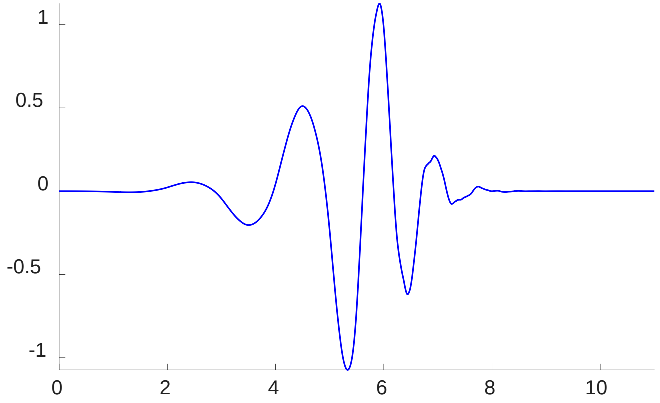
c_k = Coefficients of wavelet function

Dyadic Discretization:

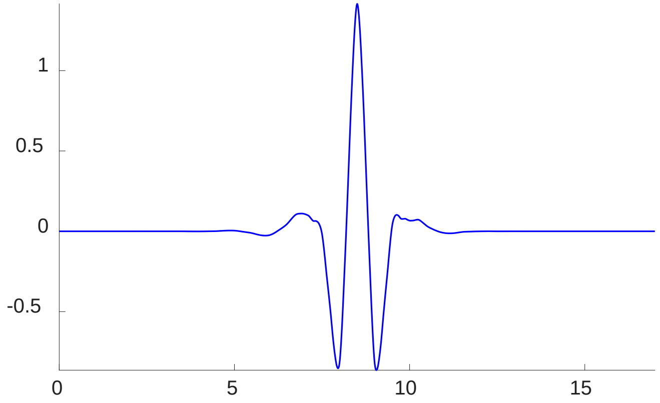
$$b = k2^j$$
$$a = 2^j$$

Different Wavelets

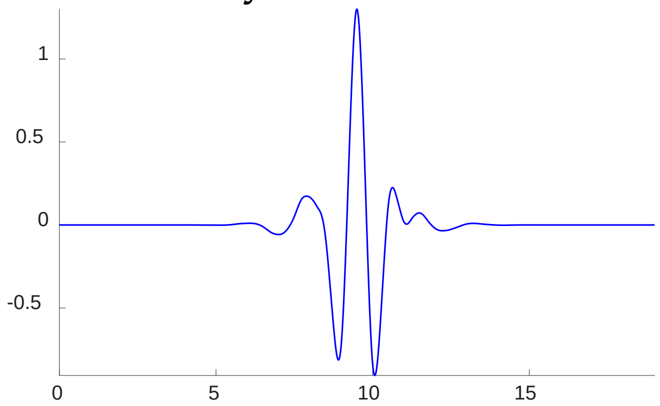
a Daubechies Wavelet



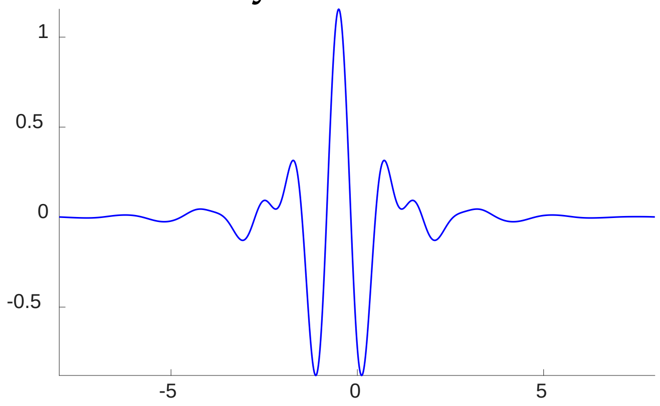
b Coiflet Wavelet



c Symlet Wavelet



d Meyer Wavelet



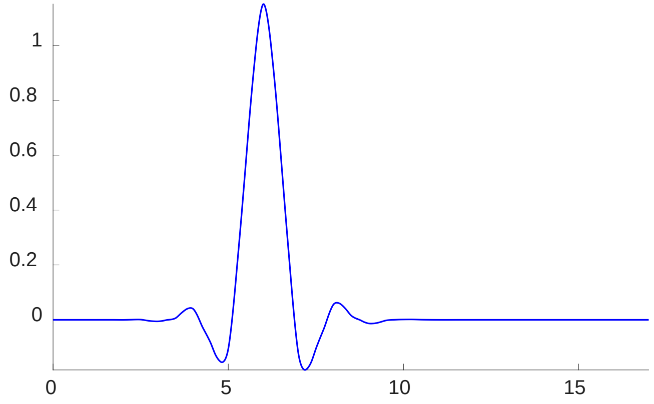
<u>Low Computational Complexity</u>

$O(p)$, where p is discrete signal length. 10ms for data length 4096 on a 64-bit operating system with 16 GB RAM and a 3.30 GHz processor

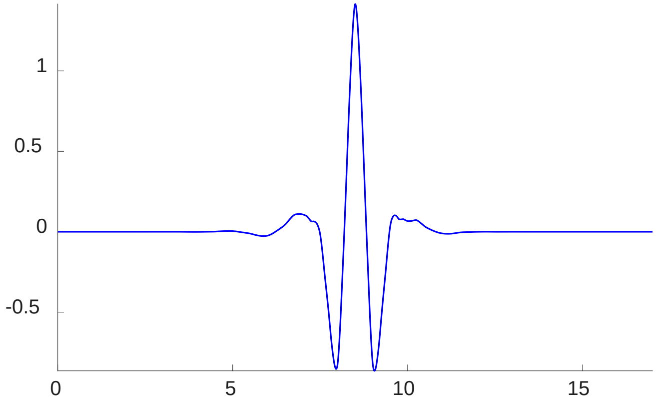
FFT: $O(p \log p)$

Scaling and Wavelet Functions

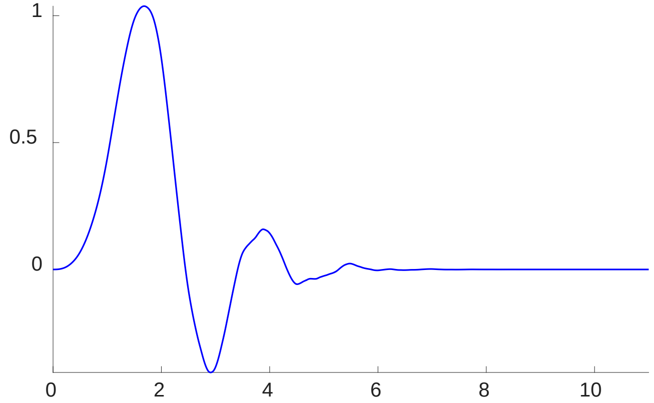
a Coif-3: Scaling Function



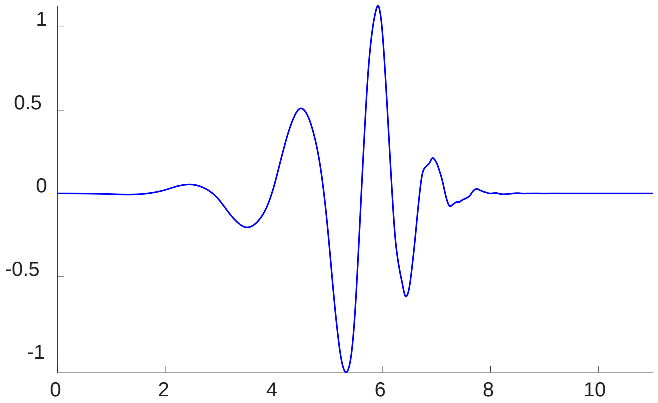
b Coif-3: Wavelet Function



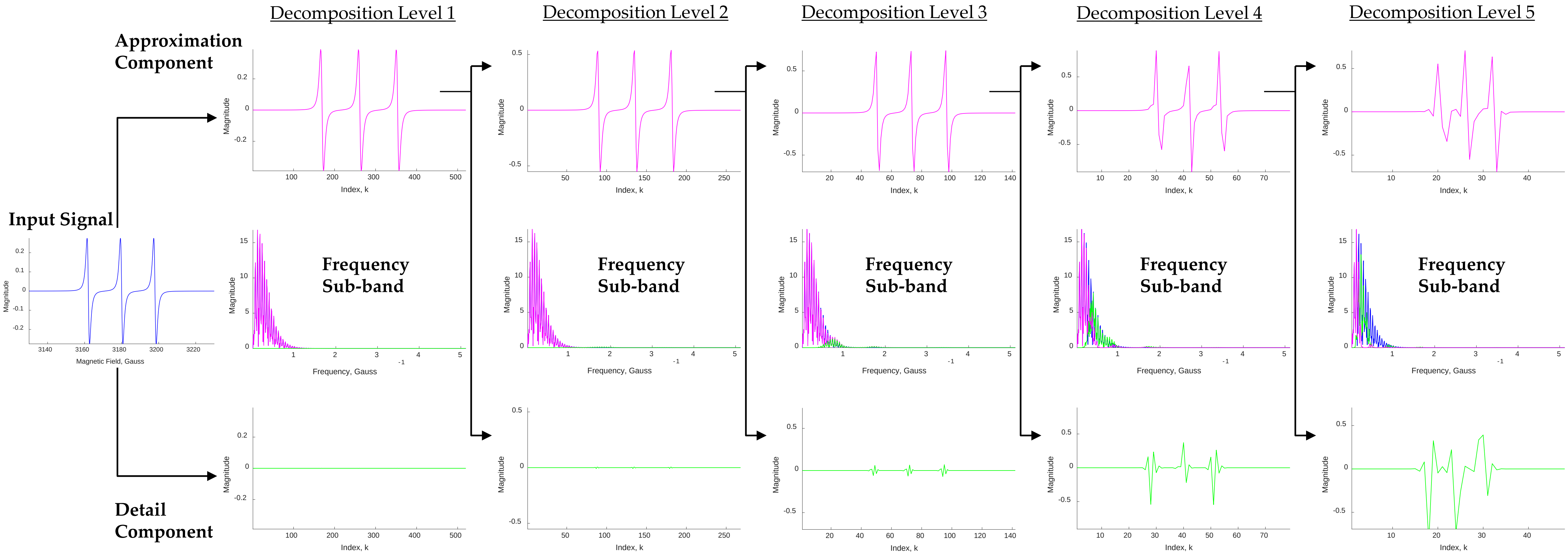
c db-6: Scaling Function



d db-6: Wavelet Function



Wavelet Transforms



Signal Displacement (Field Sweep)

$$F(a,b) = \frac{1}{\sqrt{a}} \int_{-\infty}^{+\infty} f(t)\, \psi^{*}\left(\frac{t-b}{a}\right) dt$$

Inverse Frequency

Detail Component is always centered around 0 because it represents non-zero frequency, i.e. relative change

Mallat (2009) *A Wavelet Tour of Signal Processing*

Inverse DWT and Orthonormality

Inverse Discrete Wavelet Transform (IDWT)

$$f[t_m] = \sum_{k=1}^{p_j} A_{j_0}[k]\phi\left(\frac{t_m - k2^{j_0}}{2^N}\right) + \sum_{j=1}^{j_0}\sum_{k=1}^{p_j} D_j[k]\,\psi\left(\frac{t_m - k2^j}{2^j}\right)$$

Orthonormality of the DWT

$$\sum_{t=1}^{L}\psi\left(\frac{t_m - k2^j}{2^j}\right)\phi\left(\frac{t_m - k2^{j'}}{2^{j'}}\right) = 0, \qquad \forall\, j \leq j'$$

$$\sum_{t=1}^{L}\psi\left(\frac{t_m - k2^j}{2^j}\right)\psi\left(\frac{t_m - k'2^{j'}}{2^{j'}}\right) = \begin{cases} 1, & if\ j = j'and\ k = k' \\ 0, & otherwise \end{cases}$$

Relationship Between Wavelet and Scaling Function

$$|\Phi(\omega)|^2 = \sum_{j=j'+1}^{\infty}\frac{\left|\Psi(2^{-j}\omega)\right|^2}{2^{-j}}$$

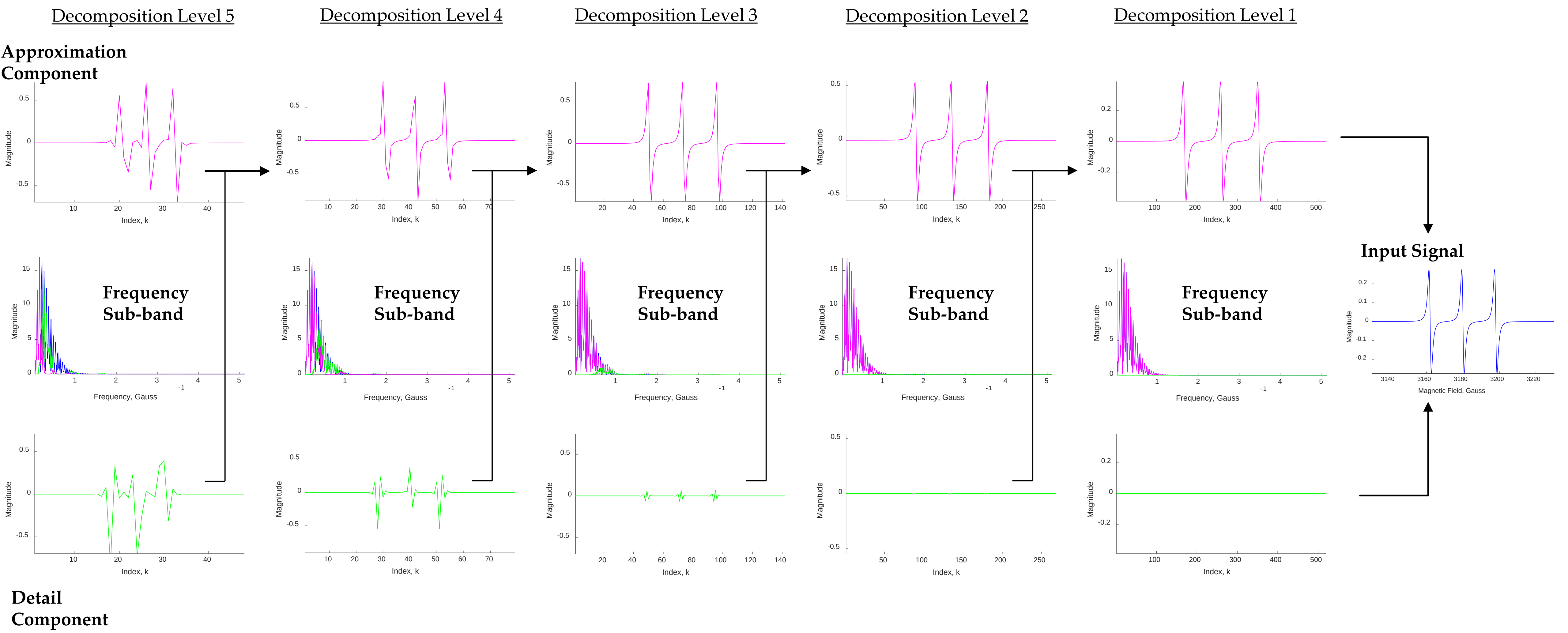
p_j= Length of the j^{th} Detail/ Approximation component.

L = Discrete length of the wavelet and scaling functions.

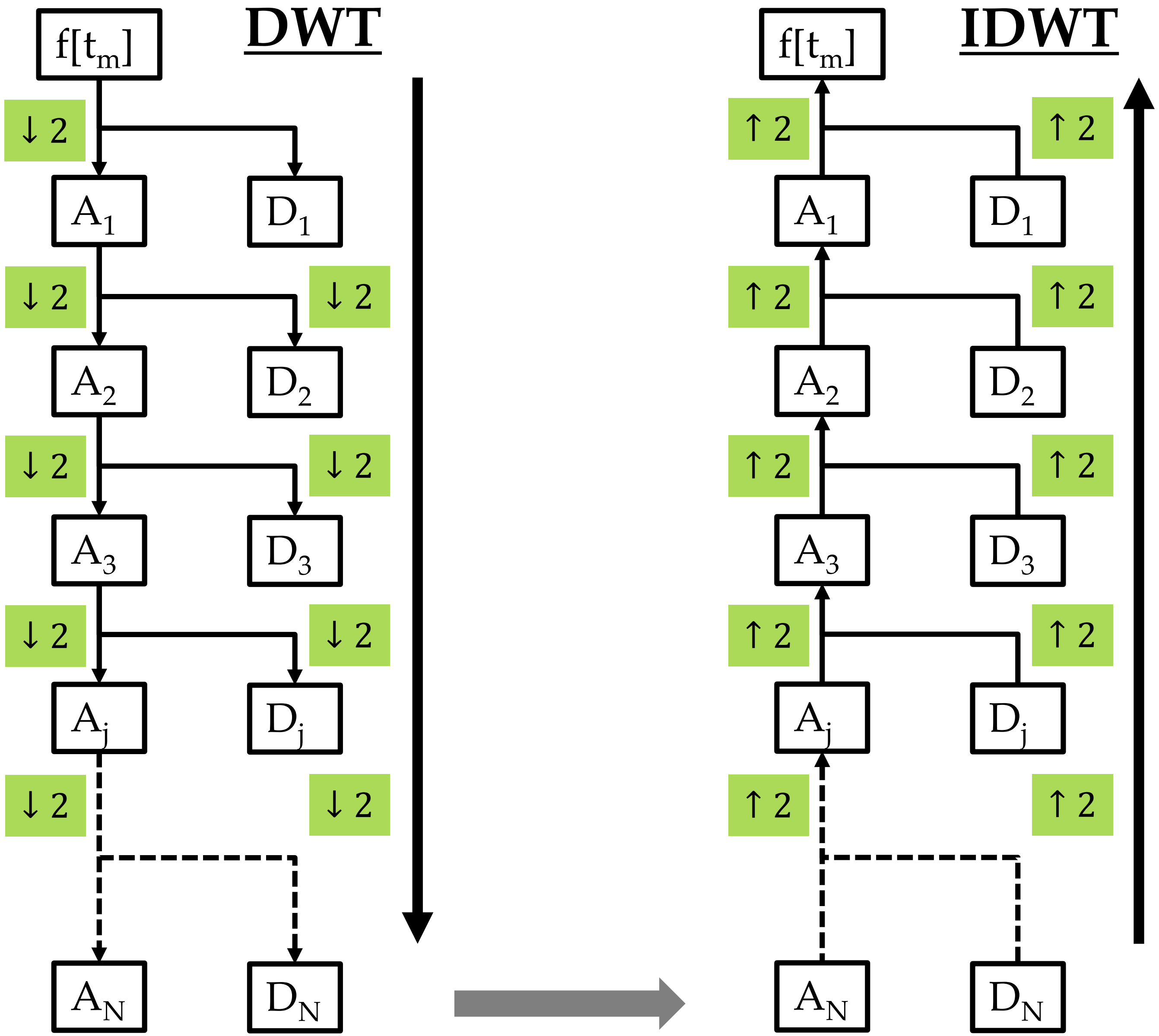
N = Maximum number of decomposition levels, $\lfloor log_2\, p \rfloor$

j_0 = Arbitrary decomposition level where $1 \leq j_0 \leq N$

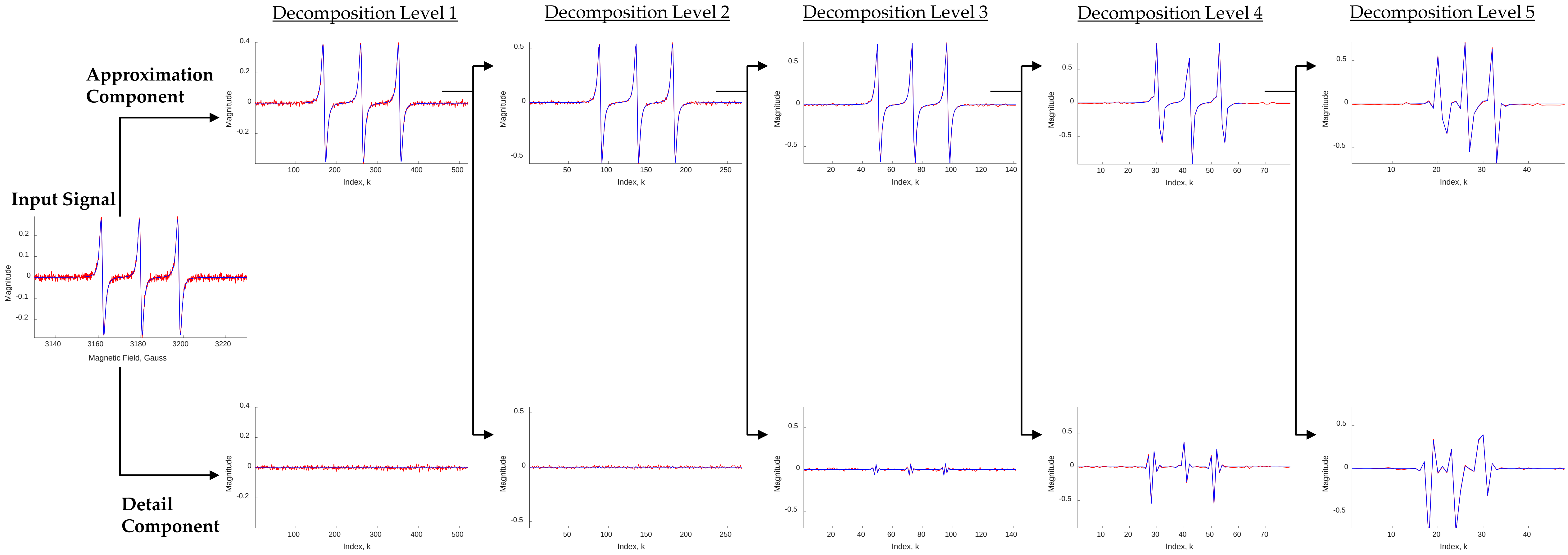
IFWT Process



Decimated DWT and IDWT



Effects of Noise in Wavelet Components

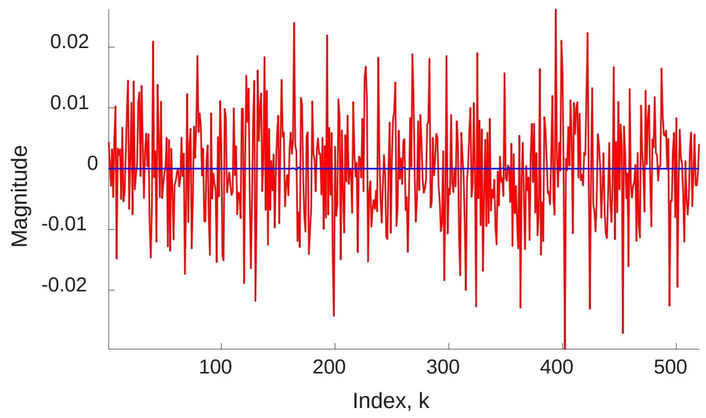


- Signal Magnitude is larger than noise magnitude
- Contribution of Each Detail Component Varies with respect to Input Signal

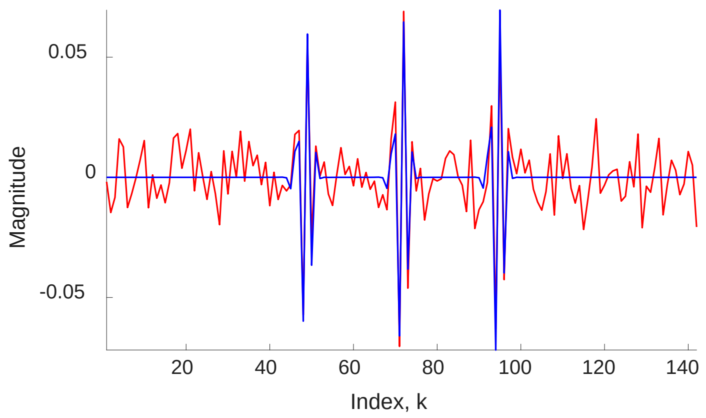
Signal Domain-Frequency Representation in Wavelet Domain

- Noise-free
- Noisy

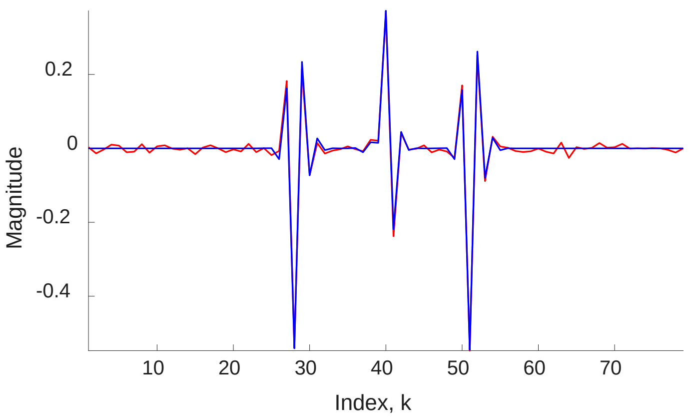
Detail Component with All Noise



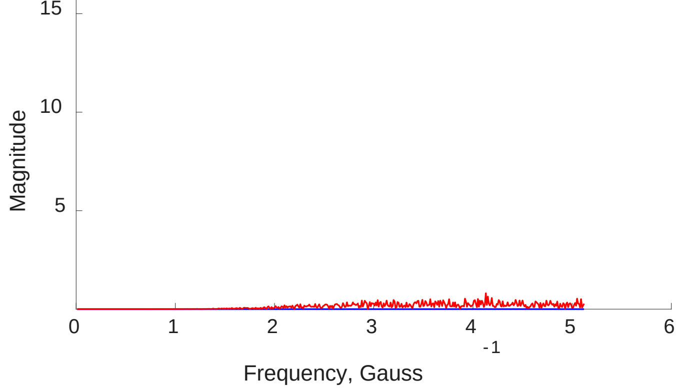
Detail Component with Heavy Noise



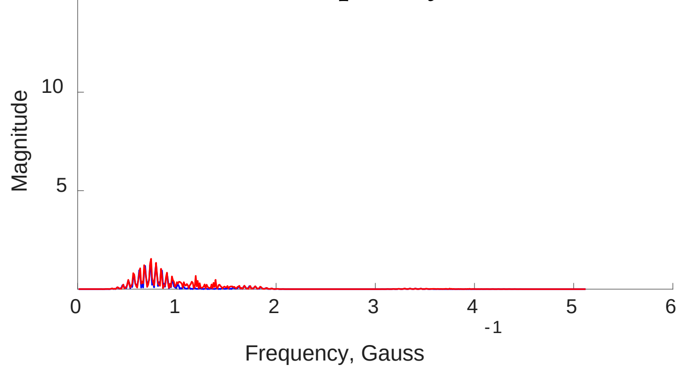
Detail Component with Little Noise



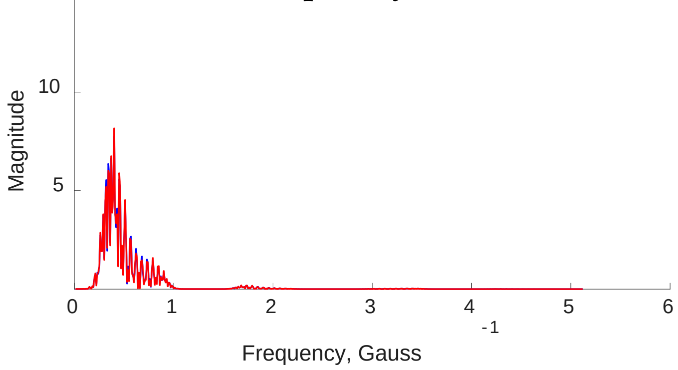
Noise Only Frequency



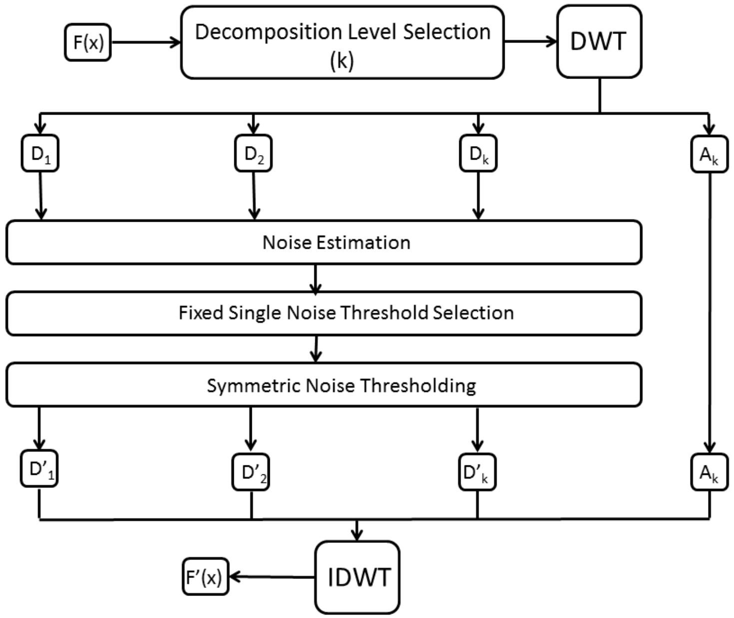
Noise and Signal Frequency Overall



Noise and Signal Frequency Overall



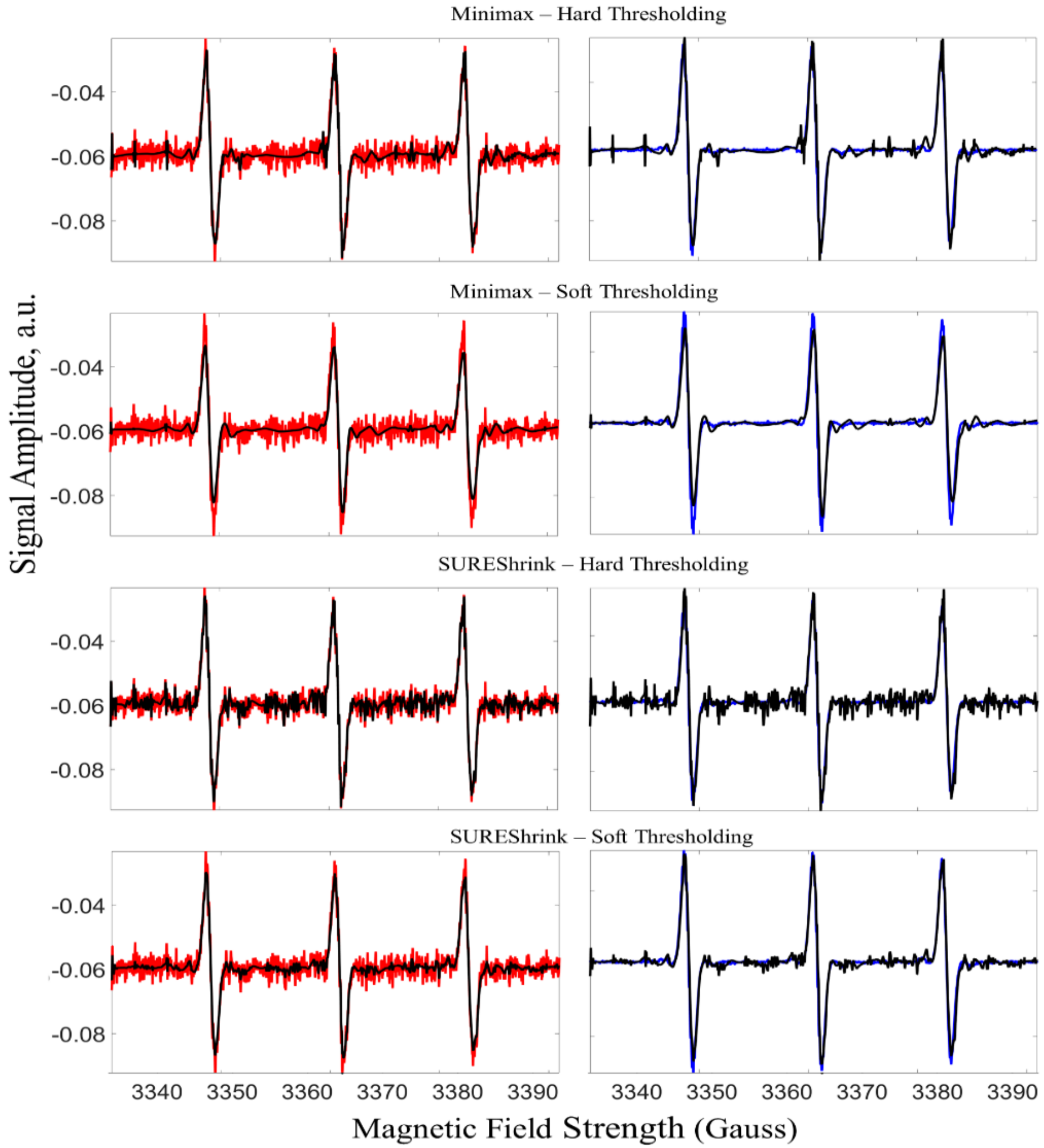
Wavelet Shrinkage Methods



Sequential Steps:

1. Select a wavelet.
2. Select Detail components to denoise.
3. Estimate noise in each Detail component.
4. Calculate noise threshold at each Detail component.
5. Apply noise thresholding.
6. Take IDWT

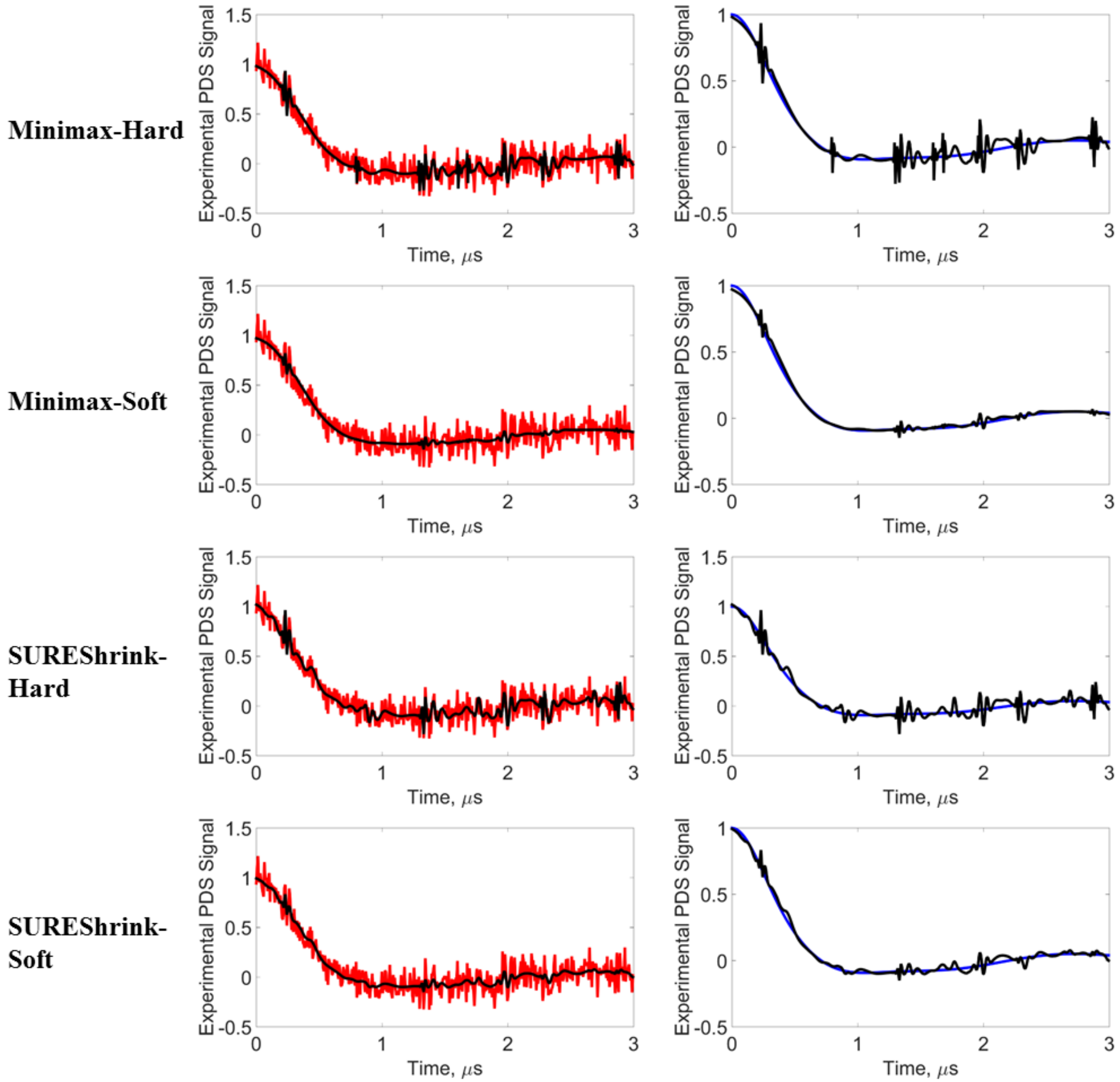
Standard Wavelet Denoising: cw-ESR Example



- Reference (500 scans)
- Denoised (4 scans)
- Noisy (4 scans)

Srivastava, Anderson, Freed (2016) *IEEE Access*

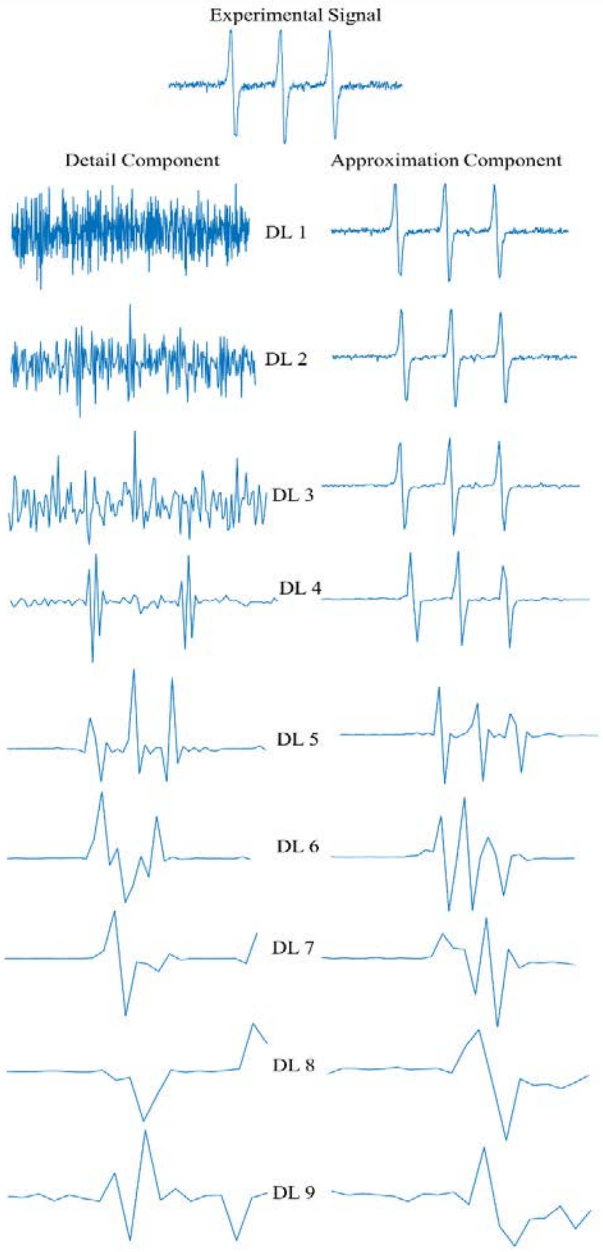
Standard Wavelet Denoising: PDS Example



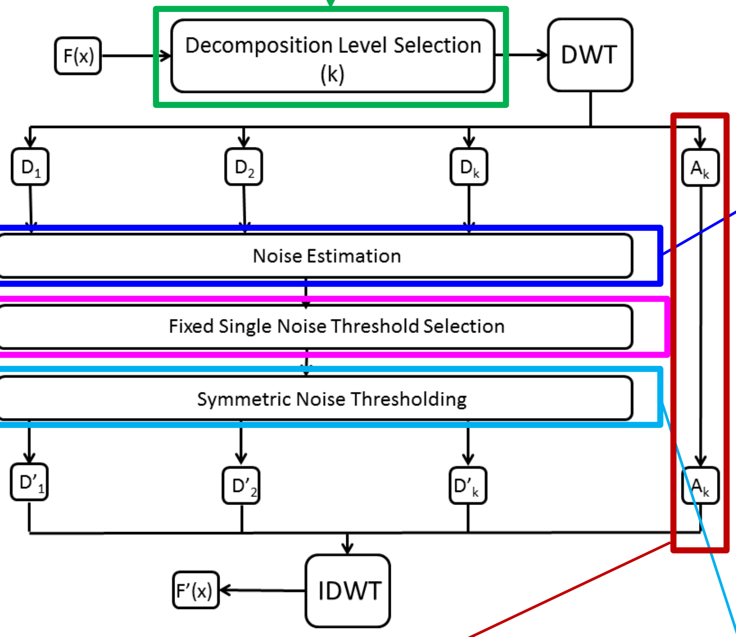
- Model
- Denoised
- Noisy

*Srivastava, Georgieva, Freed (2017) *J. Phys. Chem. A*

Summary of Limitations



No criteria: Arbitrary selection of decomposition level for denoising, influencing the outcome.



Single threshold for negative and positive coefficients. Assumes no bias.

Noise thresholds are not based on information in Detail components, but on its length.

Non-adjustable thresholds to remove coherent noise or to separate weak signal coefficient from nearby strong noise coefficient.

$$\lambda_j = \eta_j \sqrt{2 \log_2 p_j}$$

No definitive way to estimate noise; different noise estimates yield different noise thresholds.

Different noise levels can have same median absolute deviation.

$$\eta_j = \frac{MAD(|D_j|)}{0.6745}$$

$$\eta_j = \frac{MAD(|D_1|)}{0.6745}$$

Relies on single threshold to remove noise for positive and negative coefficients, resulting in keeping noise coefficients and/or distortion signal.

Soft-thresholding:

$$D'_j[i] = \begin{cases} sgn(D_j[i])\,(|D_j[i]| - \lambda_j) & : |D_j[i]| \geq \lambda_j \\ 0 & : |D_j[i]| < \lambda_j \end{cases}$$

Hard-thresholding:

$$D'_j[i] = \begin{cases} D_j[i] & : |D_j[i]| \geq \lambda_j \\ 0 & : |D_j[i]| < \lambda_j \end{cases}$$

Not removing low frequency noise

Srivastava, Anderson, Freed (2016) *IEEE Access*

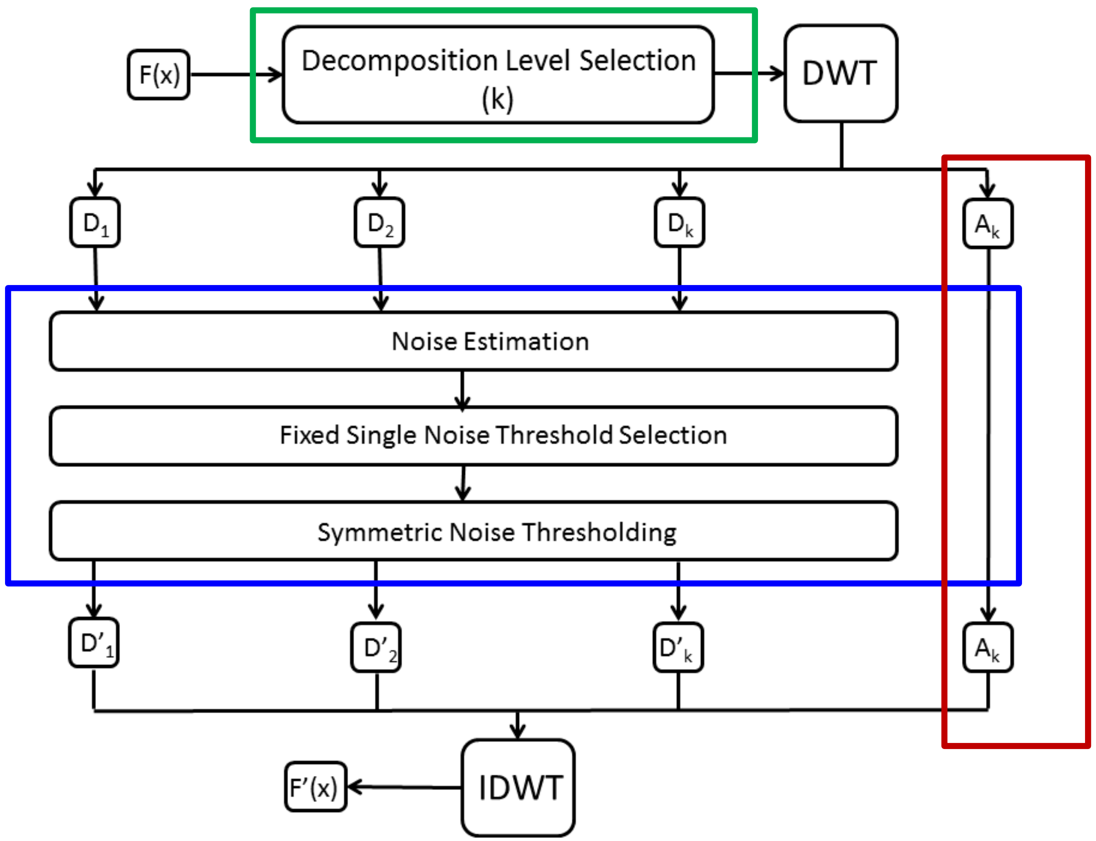
Donoho et al. (1994), Biometrika;
Donoho et al. (1995), J. American Stat. Assoc.;
Johnstone et al. (1997), J. Roy. Stat. Soc.

New Wavelet Denoising Method

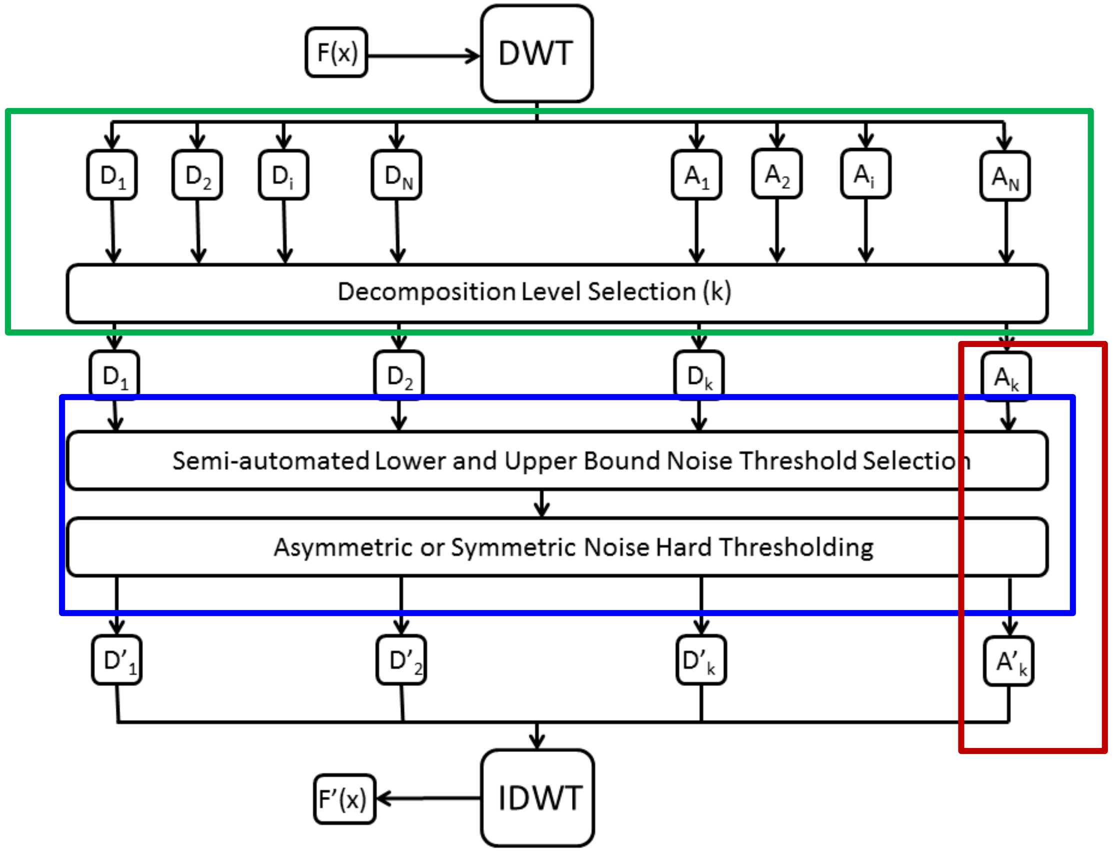
- Provides a method to select the number of decomposition levels to denoise
- Uses a new formula to calculate noise thresholds that does not require noise estimation
- Uses separate noise thresholds for positive and negative wavelet coefficients
- Applies denoising to the approximation component
- Allows flexibility for adjusting the noise thresholds

New Wavelet Denoising Method

Standard Method



New Method*

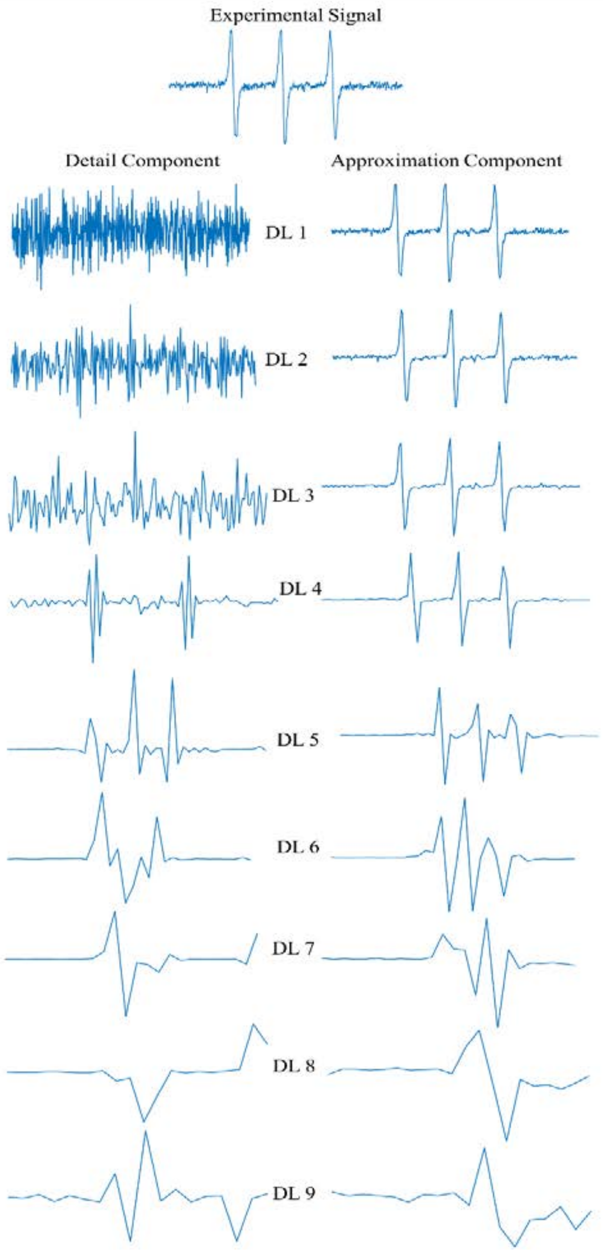


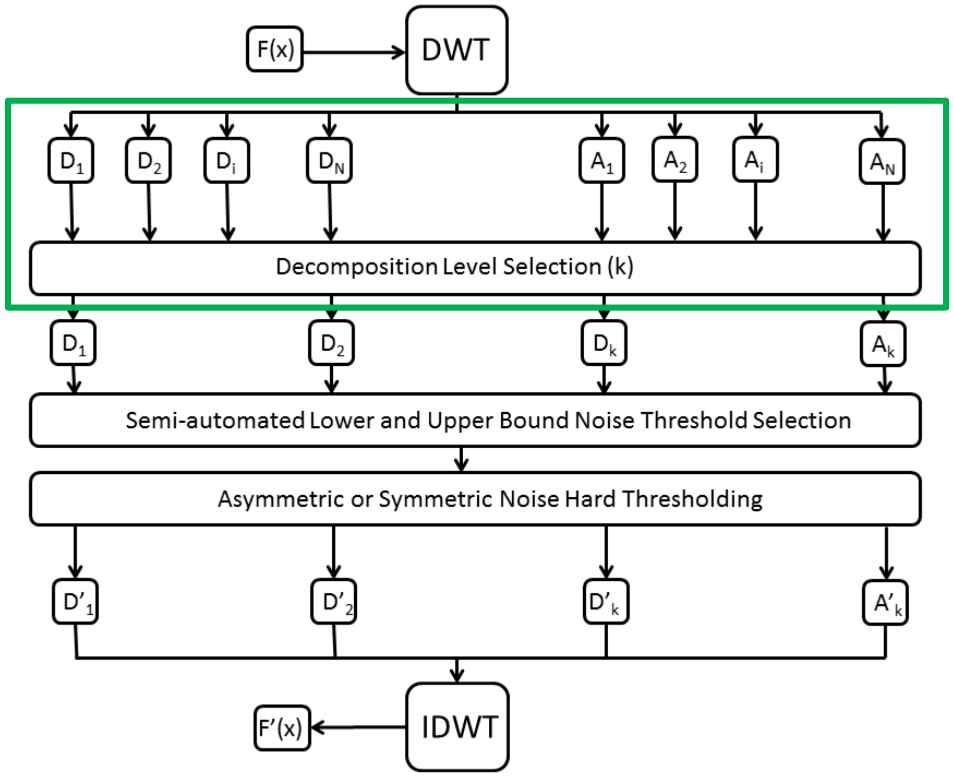
1. Decomposition Level Selection Criteria
2. New Noise Threshold Procedure
3. Removing Low Frequency Noise

*USPTO Patent Application # 62/334,626;

Srivastava, Anderson, Freed (2016) *IEEE Access*

Decomposition Level Selection





1) Subjective Method:

Examine Detail components!

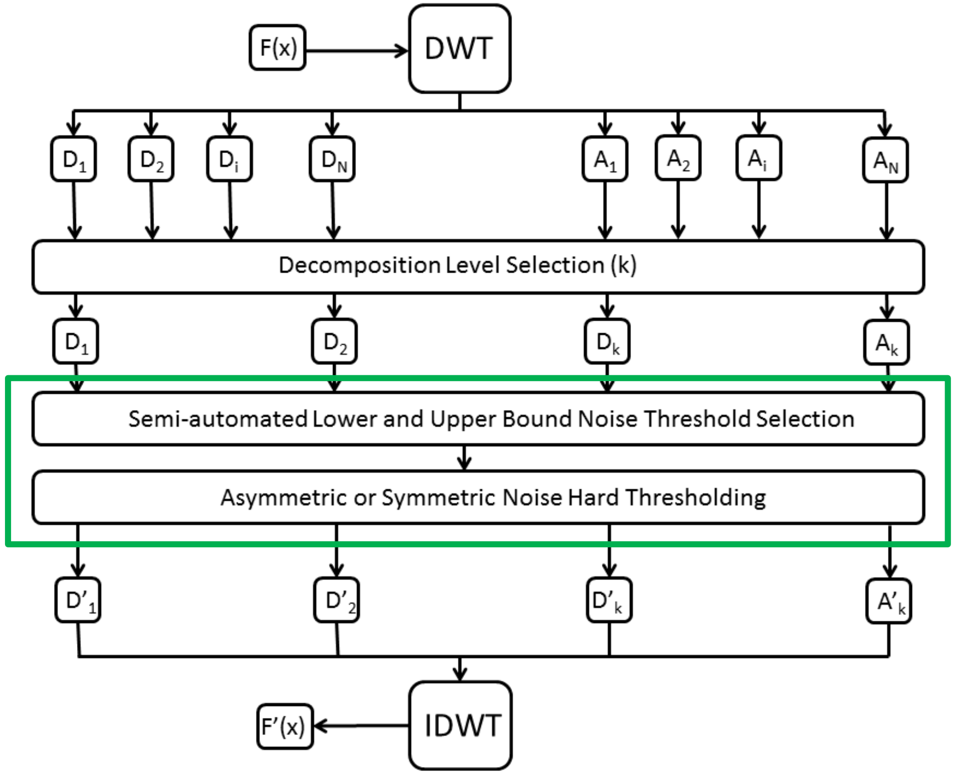
2) Objective Method:

$$S_j = \frac{max(|D_j[i]|)}{\sum_{k=1}^{p_j} |D_j[i]|}$$

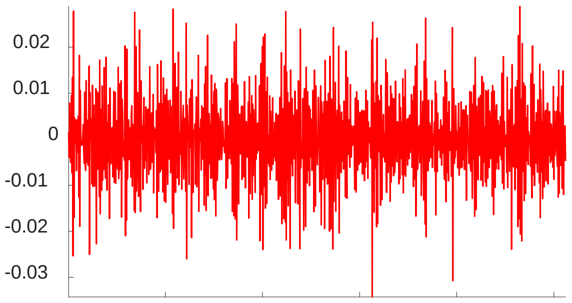
S_j reflects the **sparsity of a wavelet component** allowing the **assessment of noise presence.**

Srivastava, Anderson, Freed (2016) *IEEE Access*

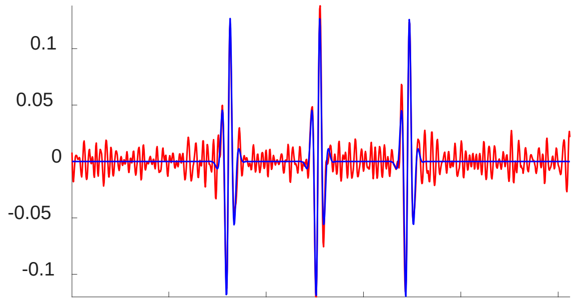
Noise Thresholds and Thresholding



Noise-Only Components (D)



Signal Components with Noise Presence (D)



<u>Noise Threshold Selection</u>

$$\lambda_{j,L} = \mu_j - \kappa_{j,L}\sigma_j$$

$$\lambda_{j,H} = \mu_j + \kappa_{j,H}\sigma_j$$

Two noise thresholds compared to single noise threshold in standard method which distinguishes **positive and negative** noise components.

<u>Noise Thresholding:</u>

$$D'_j[i] = \begin{cases} 0, & \lambda_{j,L} \le D_j[i] \le \lambda_{j,H} \\ D_j[i], & otherwise \end{cases}$$

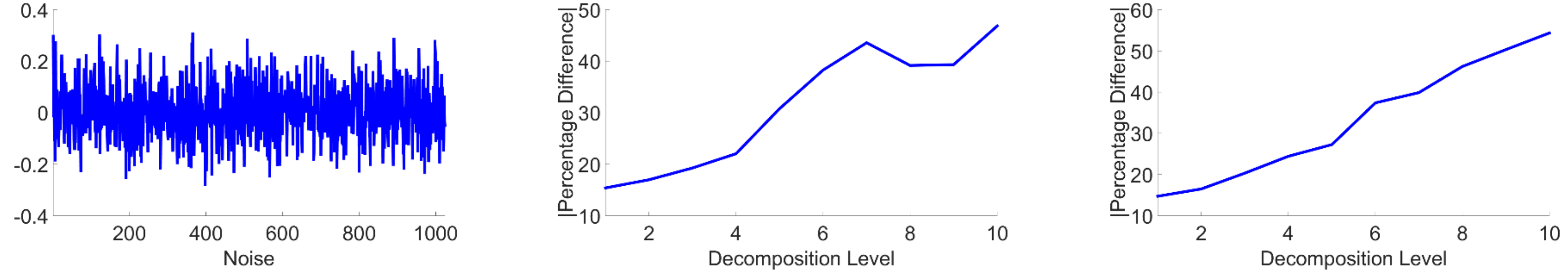
Hard thresholding over soft thresholding used in standard method.

Srivastava, Anderson, Freed (2016) *IEEE Access*

Positive or negative bias in Gaussian noise

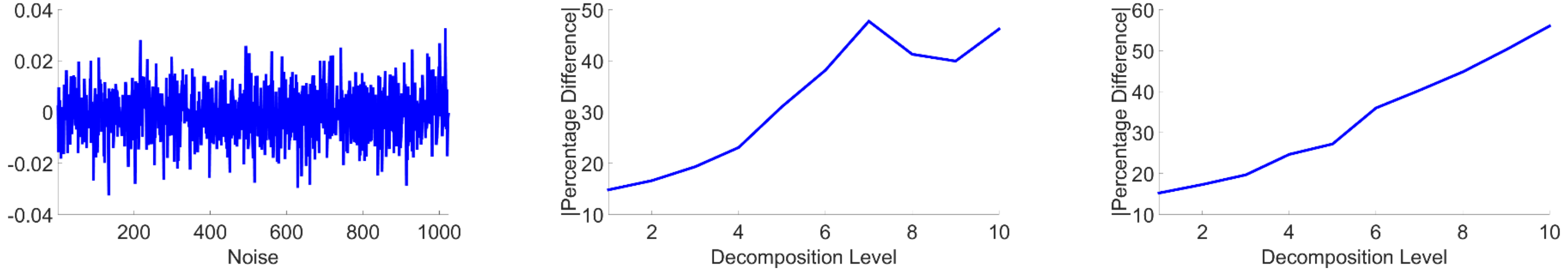
SNR 10

coif 3 db6



SNR 100

coif 3 db6



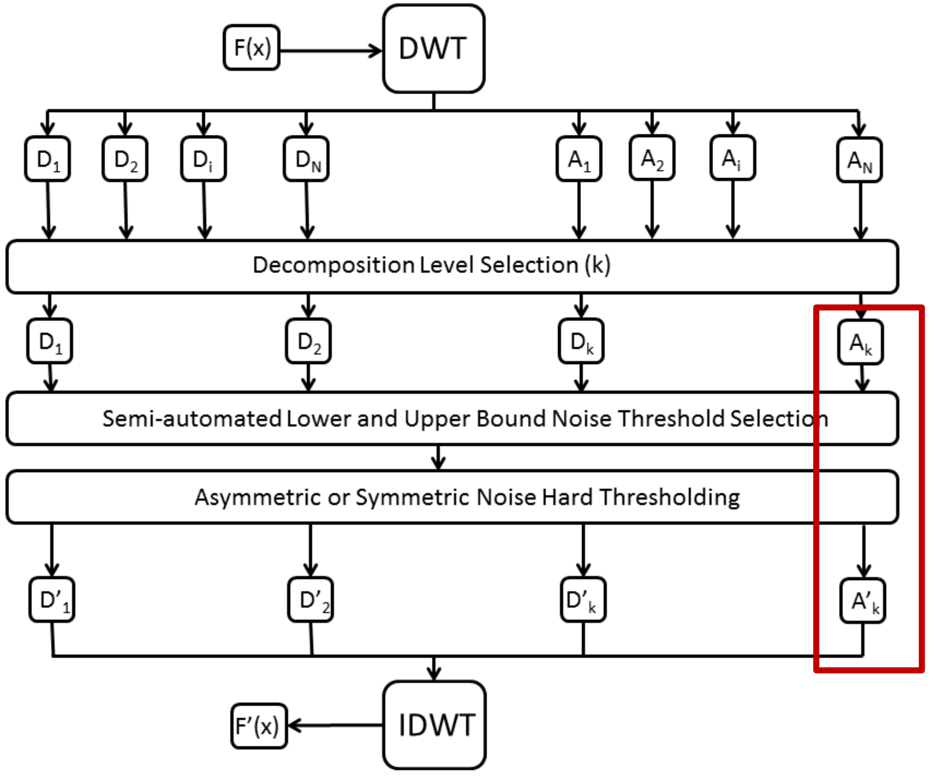
5000 simulations average

Non-Gaussian after WT because of separating Gaussian sub-bands

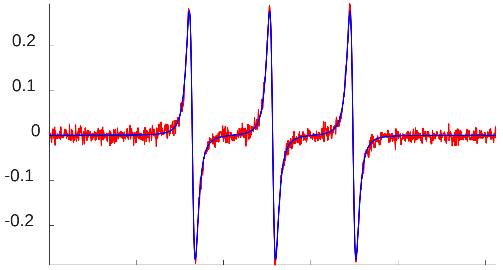
Srivastava, Anderson, Freed (2016) *IEEE Access*

Noise Thresholding Approximation Component

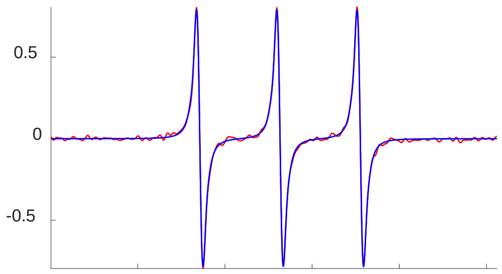
- Noise-free
- Noisy



Noisy Signal at SNR 30



Approximation Component (A_k)



Noise Threshold Selection

$$\lambda_{j,L} = \mu_j - \kappa_{j,L}\sigma_j$$

$$\lambda_{j,H} = \mu_j + \kappa_{j,H}\sigma_j$$

Two noise thresholds

Noise Thresholding:

$$A'_j[i] = \begin{cases} 0, & \lambda_{j,L} \le A_j[i] \le \lambda_{j,H} \\ A_j[i], & otherwise \end{cases}$$

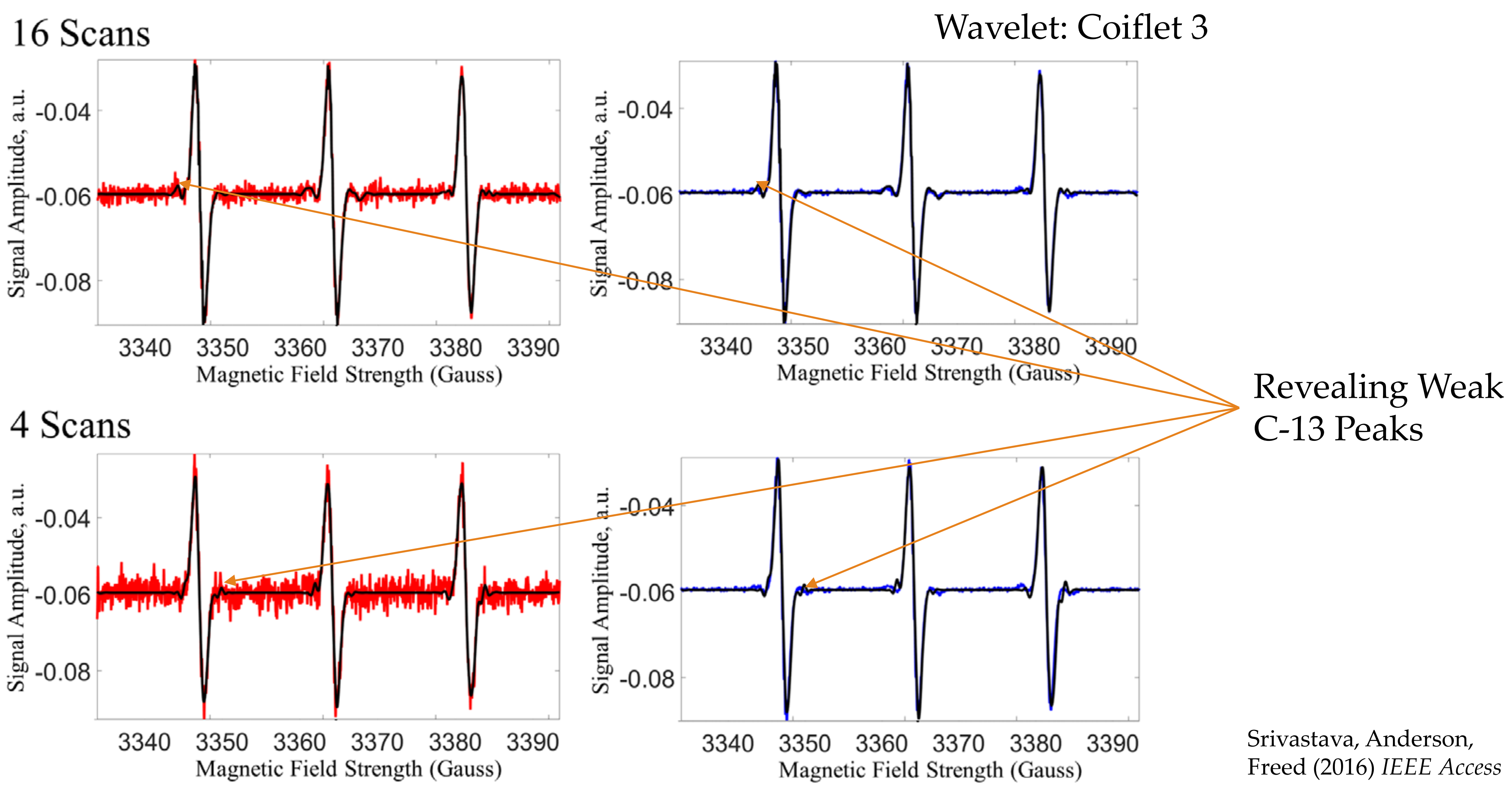
Hard thresholding over soft thresholding used in standard method.

Srivastava, Anderson, Freed (2016) *IEEE Access*

Wavelet Denoising Results: cw-ESR

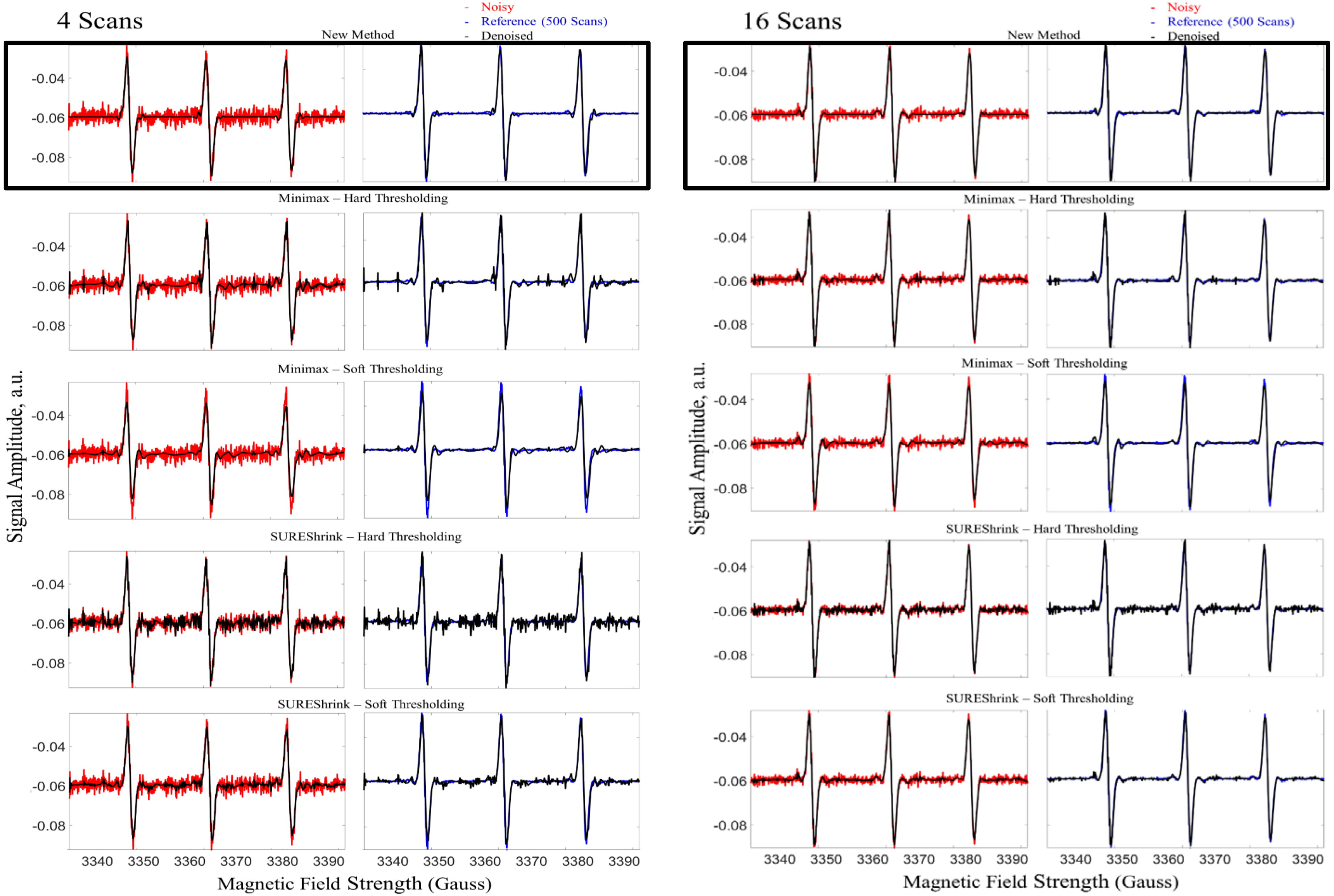
Sample: Tempol, 0.1mM in water at room temperature. X-Band 9.4GHz cw-ESR.

- Noisy
- Reference (500 scans)
- Denoised



Srivastava, Anderson, Freed (2016) *IEEE Access*

Wavelet Denoising Results: Cw-ESR



- **Noisy**
- **Reference (500 scans)**
- **Denoised**

Sample: Tempol, 0.1mM in water at room temperature. X-Band 9.4GHz cw-ESR.

Srivastava, Anderson, Freed (2016) *IEEE Access*

Wavelet Denoising: Comparison using Objective Measures

Method	4 scans				16 scans			
	SNR	SSIM	DL	CT(s)	SNR	SSIM	DL	CT(s)
Noisy	**14**	**0.9684**	**-**	**-**	**30**	**0.9903**	**-**	**-**
Minimax-Hard	40	0.9880	7	0.0834	73	0.9959	7	0.0804
Minimax-Soft	57	0.9890	12	0.0788	100	0.9954	7	0.0807
SUREShrink-Hard	20	0.9779	9	0.0878	41	0.9938	9	0.0853
SUREShrink-Soft	39	0.9905	12	0.0866	79	0.9966	7	0.0873
Zhao	40	0.9790	6	0.0864	104	0.9821	6	0.0864
Poornachandra	36	0.9803	6	0.0849	84	0.9825	6	0.0857
Zhang	40	0.9778	6	0.0855	105	0.9821	6	0.0858
Lin	39	0.9800	6	0.0852	134	0.9825	6	0.0867
New Method	***784***	***0.9957***	***6***	***0.0140***	***2220***	***0.9969***	***6***	***0.0131***

$$SSIM(X,Y) = \frac{(2\mu_X\mu_Y + c_1)(2\sigma_{XY} + c_2)}{(\mu_X^2 + \mu_Y^2 + c_1)(\sigma_X^2 + \sigma_Y^2 + c_2)}$$

μ_X = mean of signal X
μ_Y = mean of signal Y
σ_X^2 = variance of X
σ_Y^2 = variance of Y
σ_{XY} = co-variance of X and Y
c_1, c_2 = constant terms

* For standard methods, DL that resulted in maximum SNR was selected.

- Hard and Soft is hard and soft thresholding
- SSIM is structural similarity index measure
- DL is decomposition level
- CT is computation time

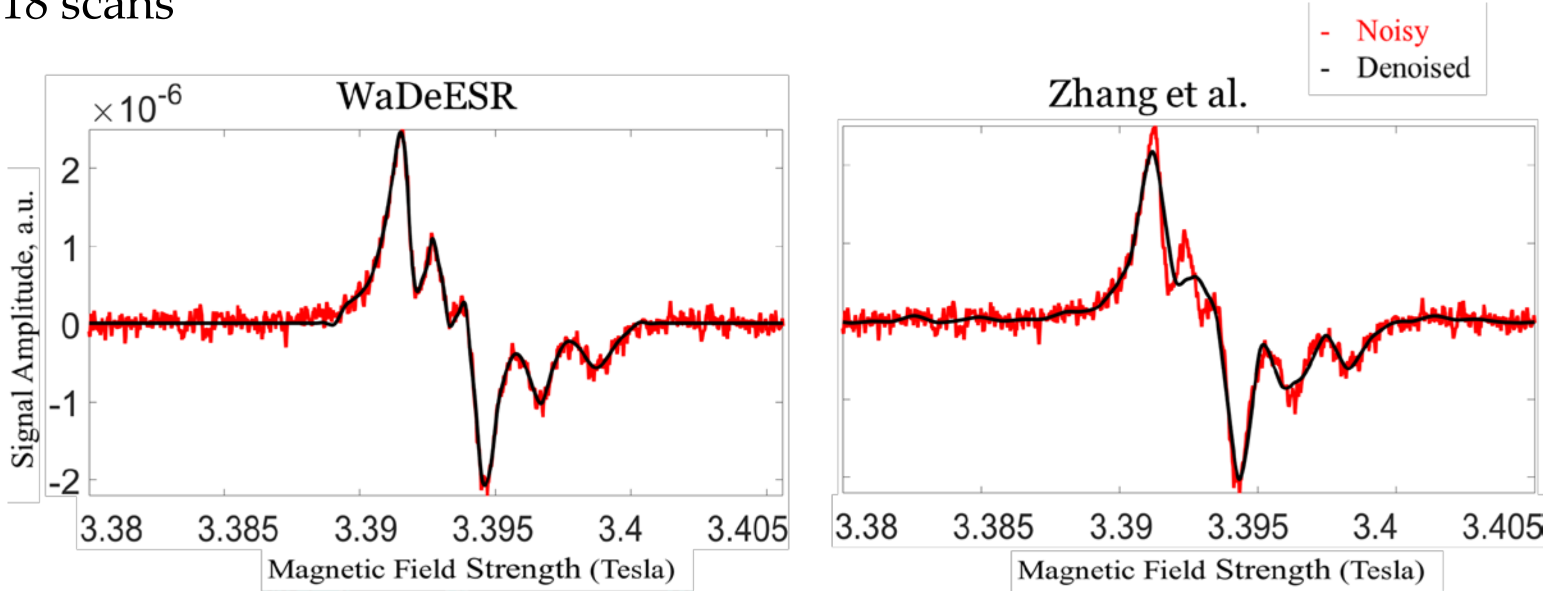
Srivastava, Anderson, Freed (2016) *IEEE Access*

WaDeESR: Experimental Slow Motion cw-ESR Denoising

Sample: 0.5% lipid spin label 16-PC in lipid vesicles at room temperature. W-band 95 GHz cw-ESR

18 scans

Wavelet: Coiflet 3



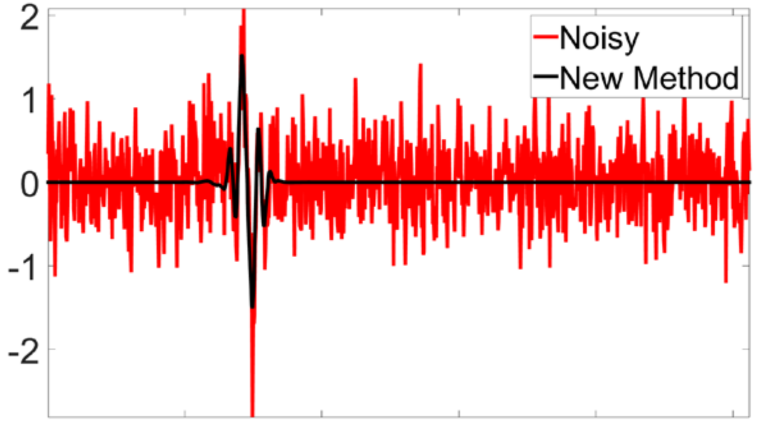
Method	***SNR***	***DL***
Noisy	49	-
Minimax-Hard	81	10
Minimax-Soft	149	6
SUREShrink-Hard	76	7
SUREShrink-Soft	115	9
Zhang et al.	167	6
WaDeESR	***$191*10^6$***	***4***

Srivastava, Anderson, Freed, IEEE Access, 2016

Spin Echo Signal Denoising to Further Improve Sensitivity

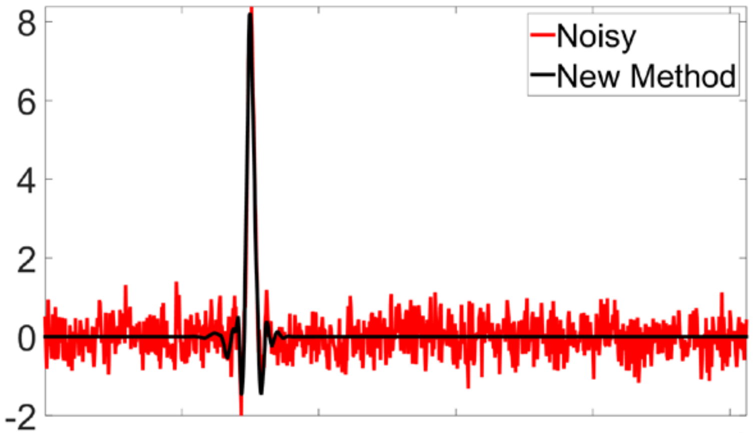
Wavelet: Coiflet 3

Dispersion



SNR Noisy: 4
SNR Denoised: 1.69 x 10^7

Absorption



SNR Noisy: 19
SNR Denoised: 8.96 x 10^6

Sample: 20 μM of a biradical, i.e. 40 μM nitroxide spins in the rigid limit. The $\pi/2$ pulses were 2 ns providing full coverage. The signal was phased to find the real part of the signal in the I channel.

Srivastava, Georgieva, Freed (2017) *J. Phys. Chem. A*

Noise Elimination and Reduction via Denoising (NERD)

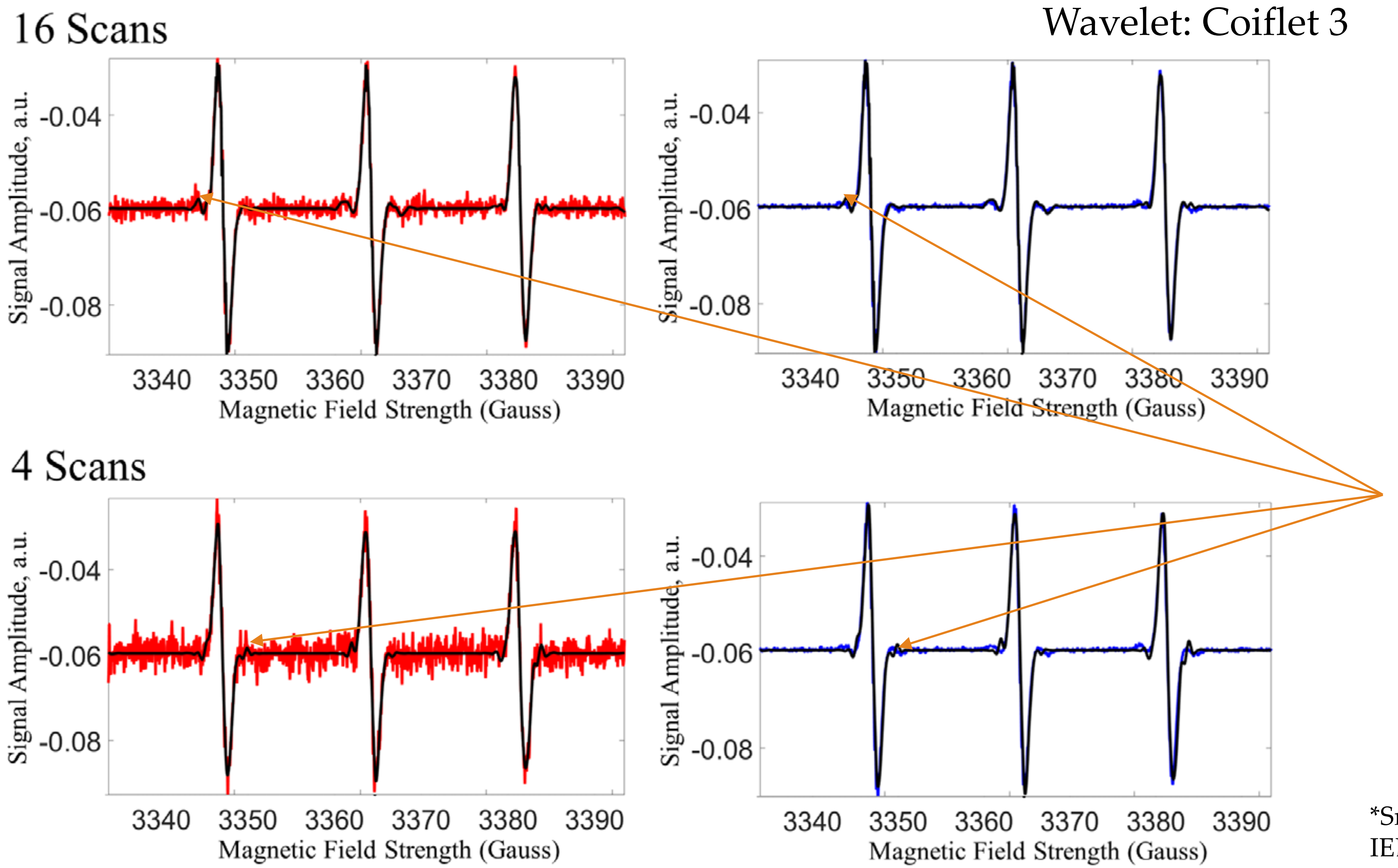
cw-ESR and Other Spectroscopies

NERD: 1) Replace Decimated by Undecimated Discrete Wavelet Transform
2) Signal Localization during Noise Thresholding

Problem: DWT Limits the Signal Resolution

Sample: Tempol, 0.1mM in water at room temperature. X-Band 9.4GHz cw-ESR.

- Noisy
- Reference (500 scans)
- Denoised

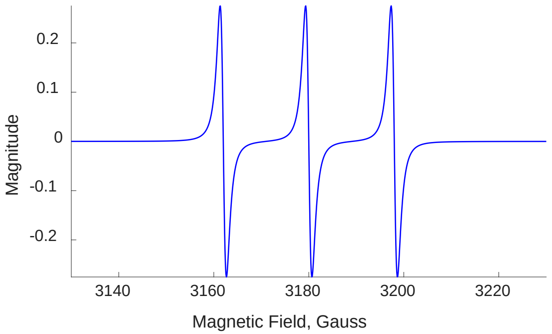


Revealing Weak C-13 Peaks, **but needs better resolution**

*Srivastava, Anderson, Freed, IEEE Access, 2016

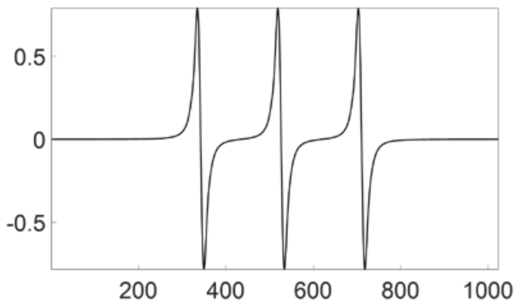
Undecimated vs Decimated Approximation Components

Input Signal

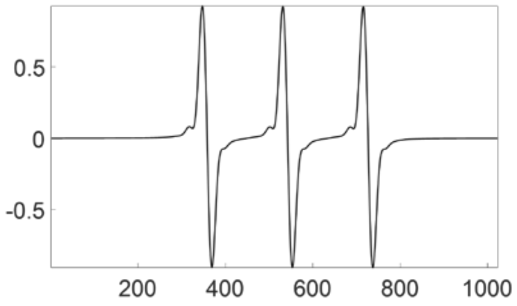


Undecimated DWT

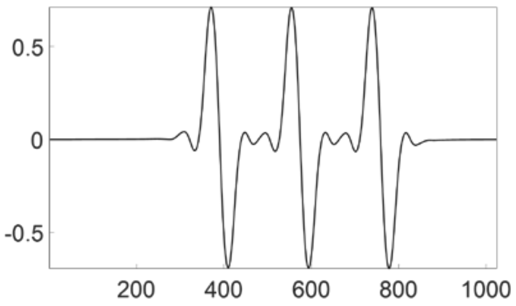
Decomposition Level 3



Decomposition Level 4

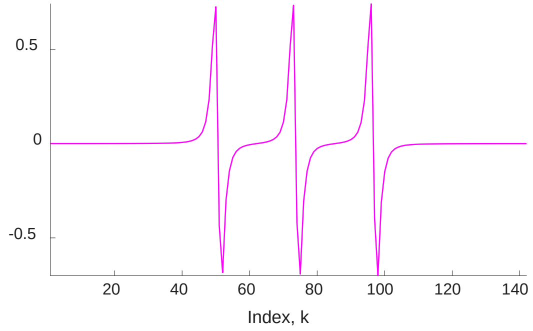


Decomposition Level 5

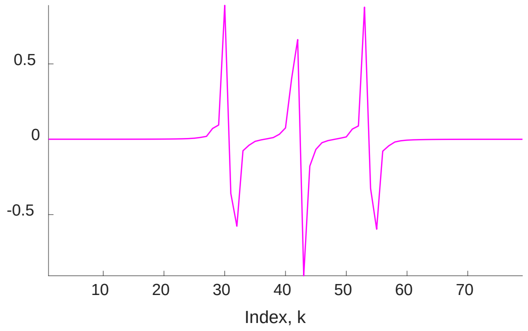


Decimated DWT

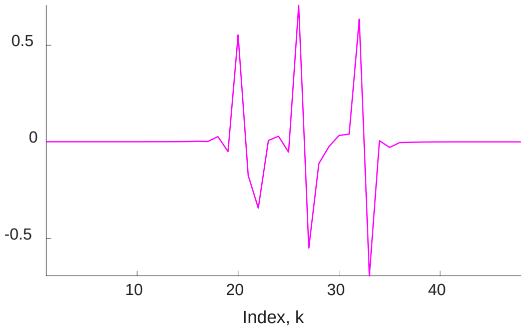
Decomposition Level 3



Decomposition Level 4

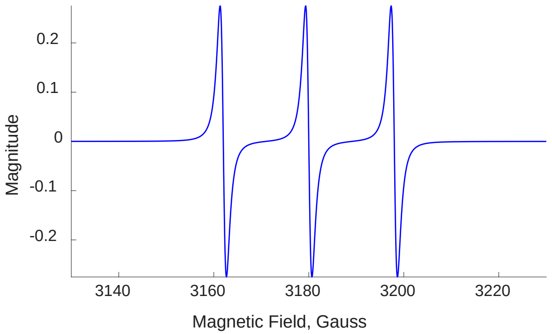


Decomposition Level 5



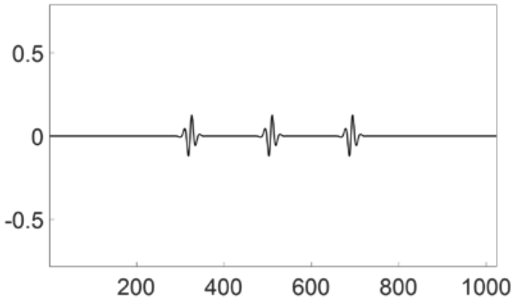
Undecimated vs Decimated Detail Components

Input Signal

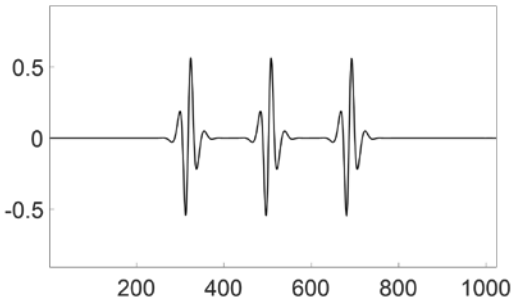


Undecimated DWT

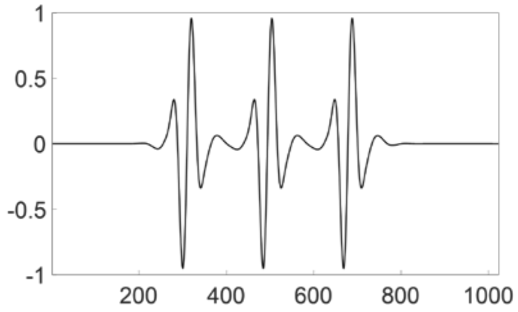
Decomposition Level 3



Decomposition Level 4

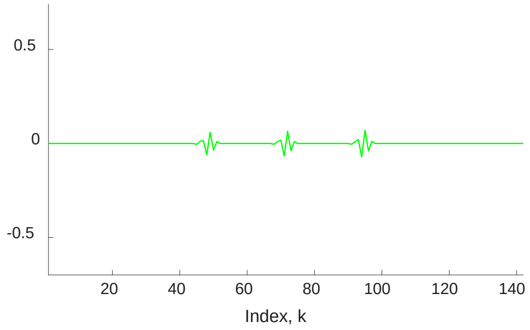


Decomposition Level 5

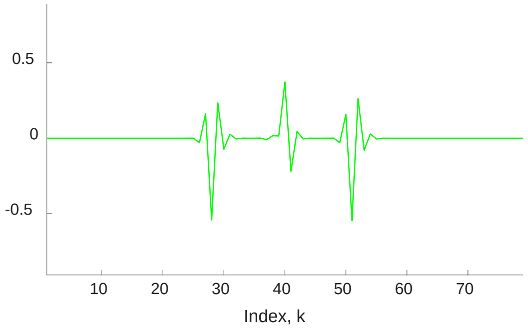


Decimated DWT

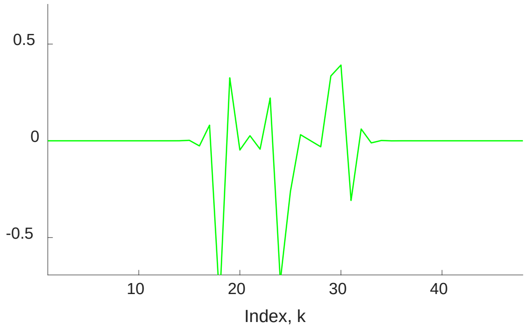
Decomposition Level 3



Decomposition Level 4

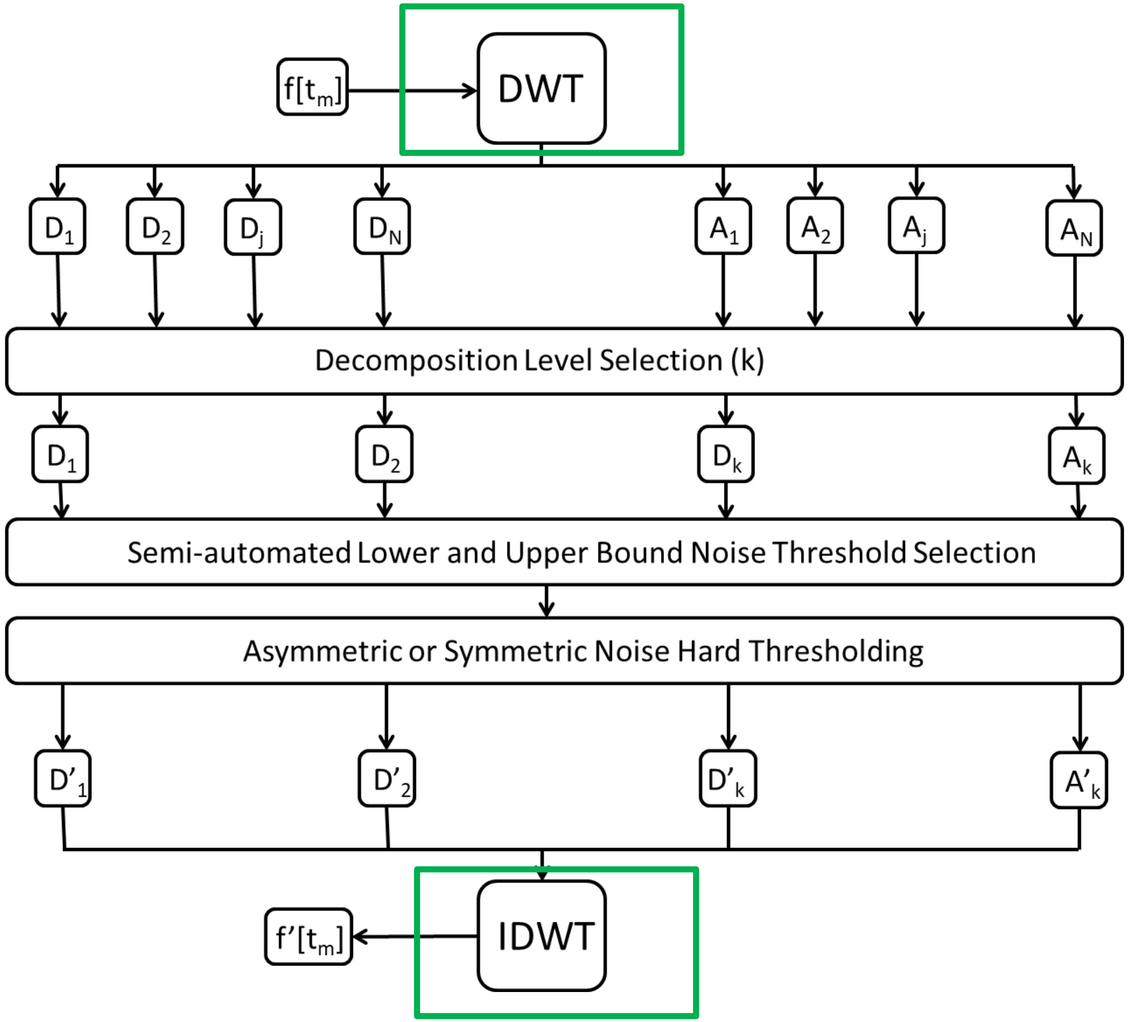


Decomposition Level 5

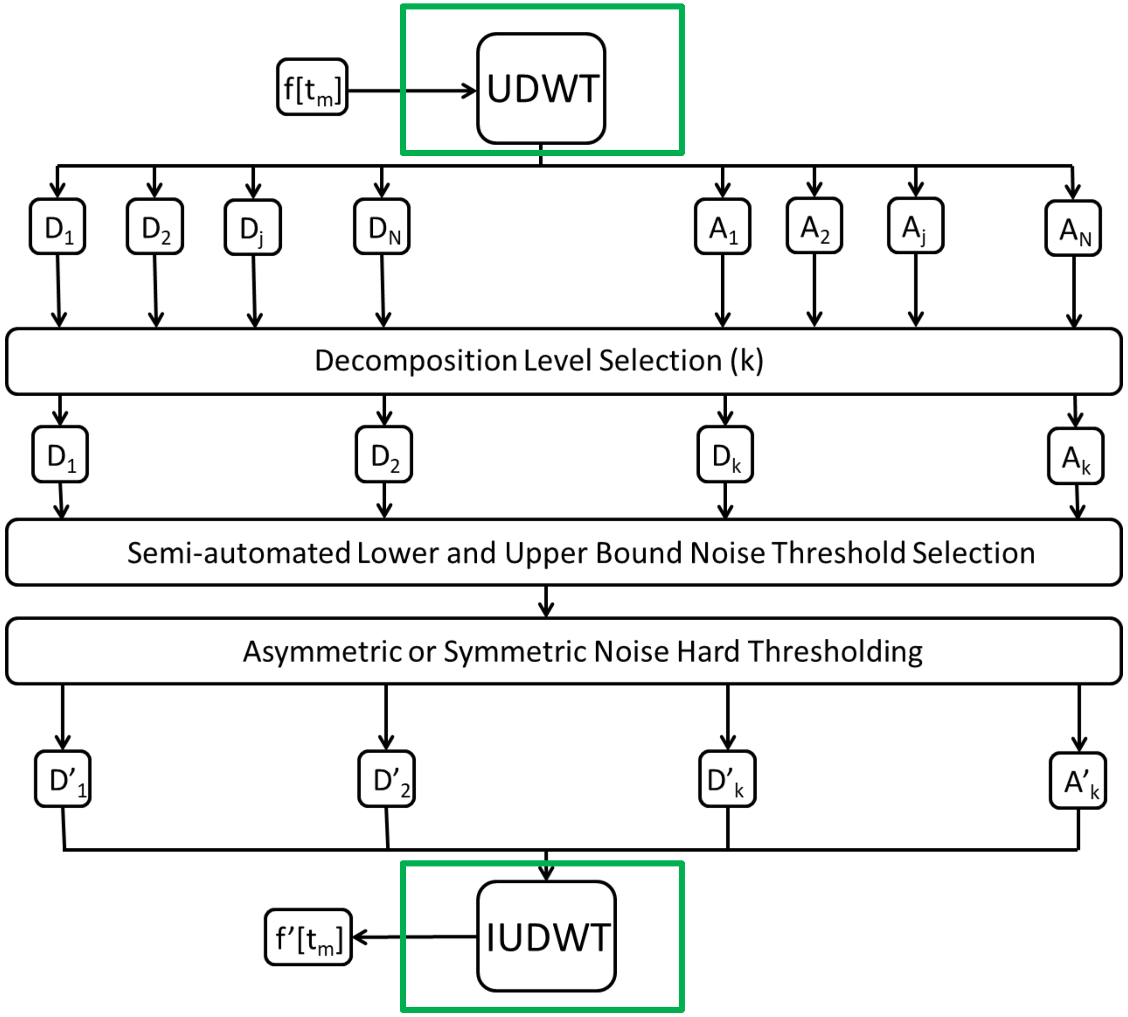


NERD Method

New Method (IEEE Paper):



NERD

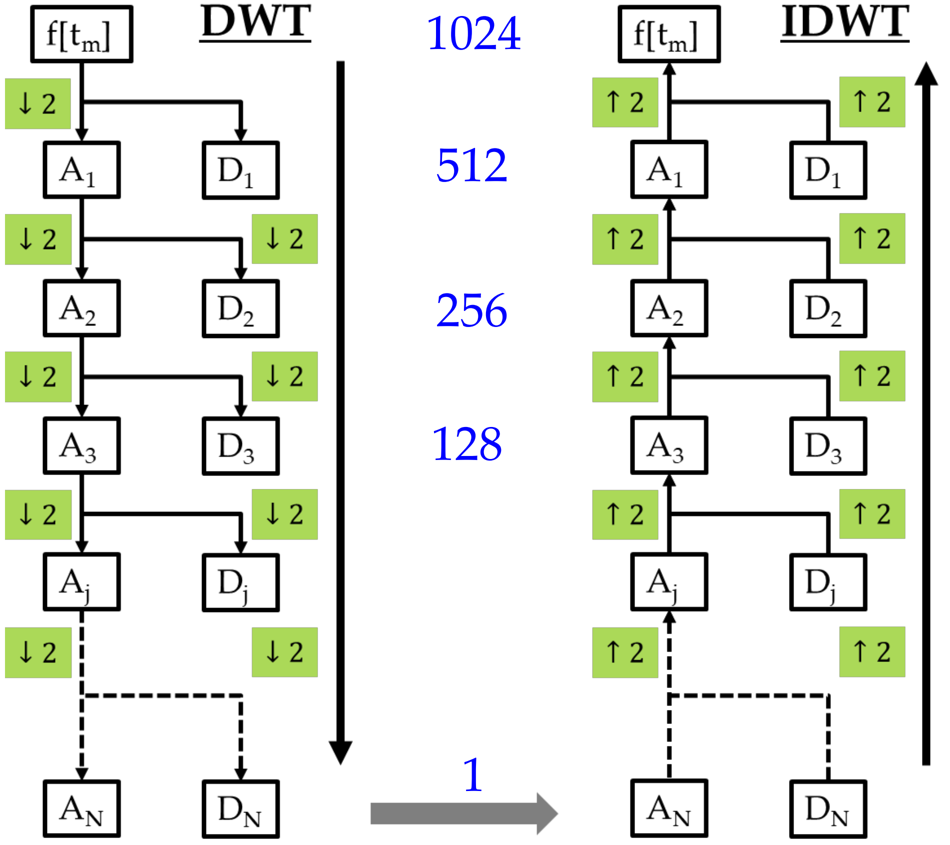


NERD uses Undecimated Discrete Wavelet Transform to improve signal resolution for denoising

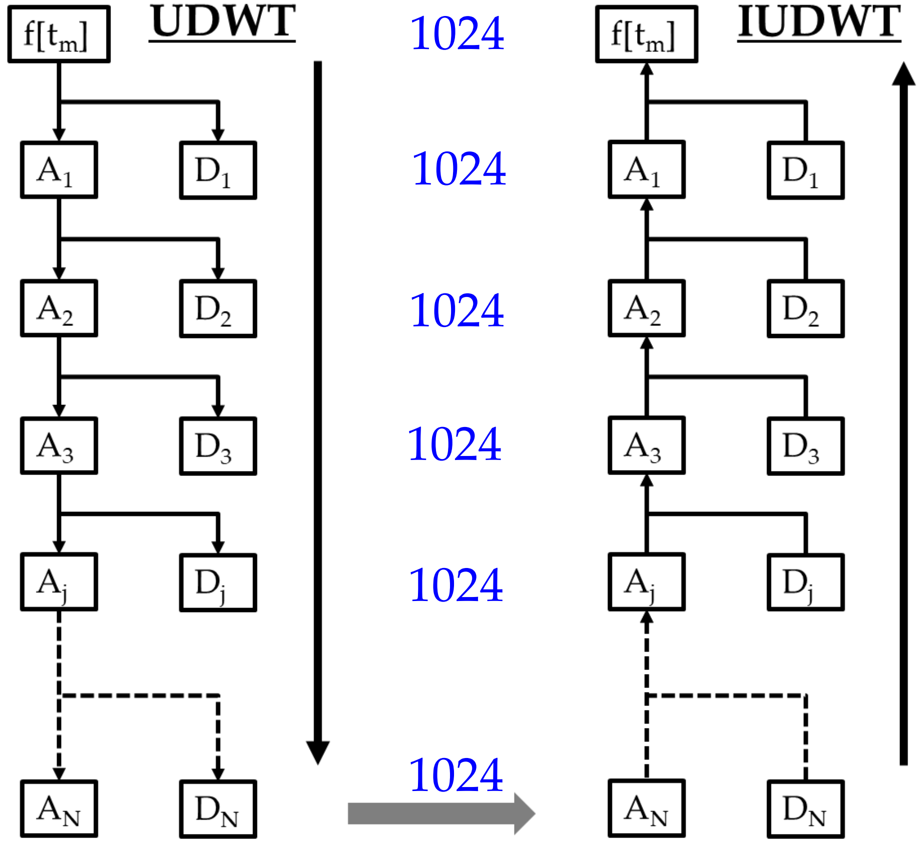
*Srivastava, Dzikovski, Freed (in preparation)

DWT vs UDWT

Decimated DWT and IDWT



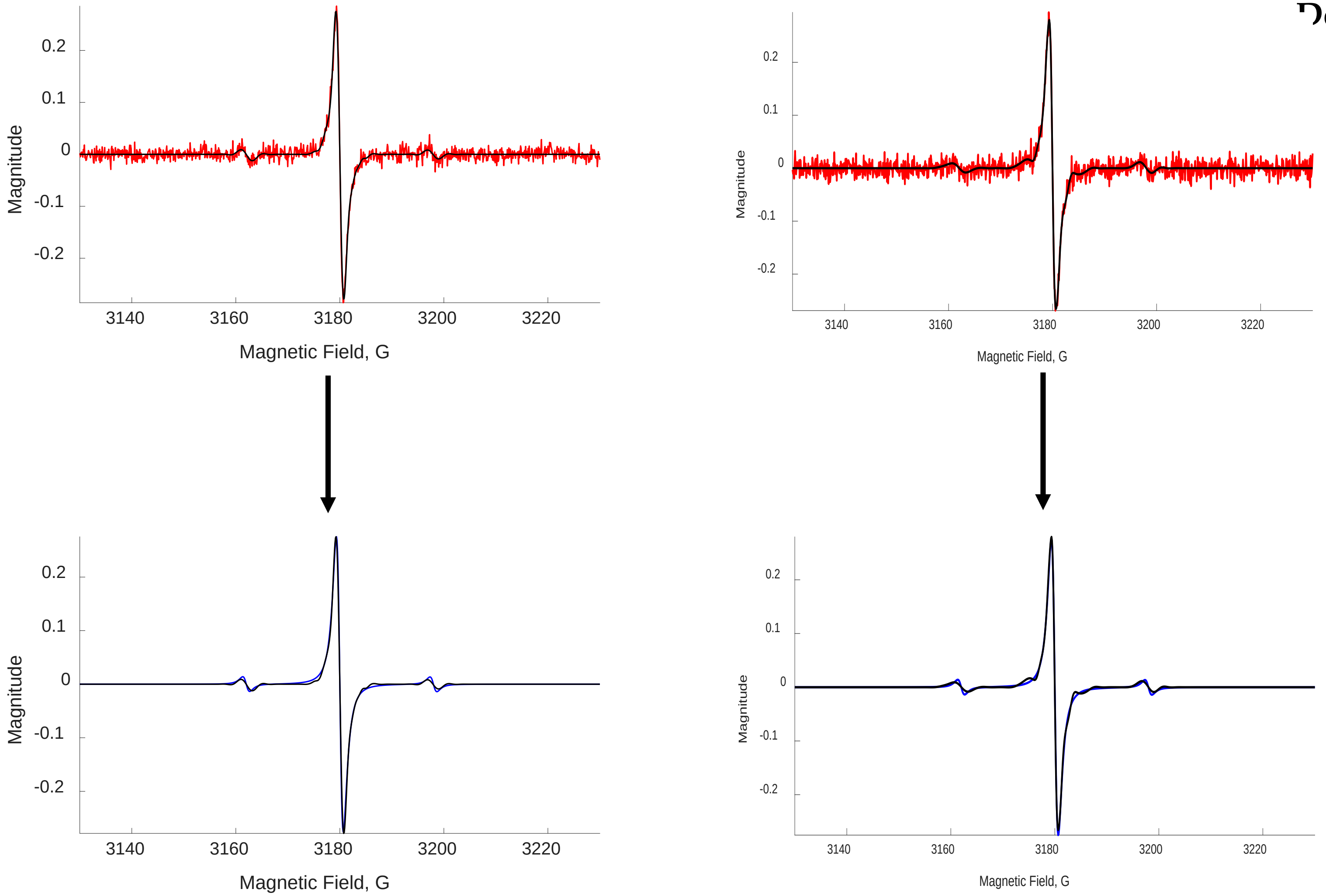
Undecimated DWT and IDWT



$$N = \log_2(Signal_{Length})$$

NERD Results: Model cw-ESR

- Noisy
- Reference (500 scans)
- Denoised



Signal		Noisy SNR	Denoised SNR
Case 1	Main Signal	30	**4.36 x 10^6**
	Weak Signal	3	**1.91 x 10^5**
Case 2	Main Signal	10	**1.99 x 10^5**
	Weak Signal	1	**4.70 x 10^3**

*Srivastava, Dzikovski, Freed (in preparation)

NERD Results: Experimental cw-ESR Data 1

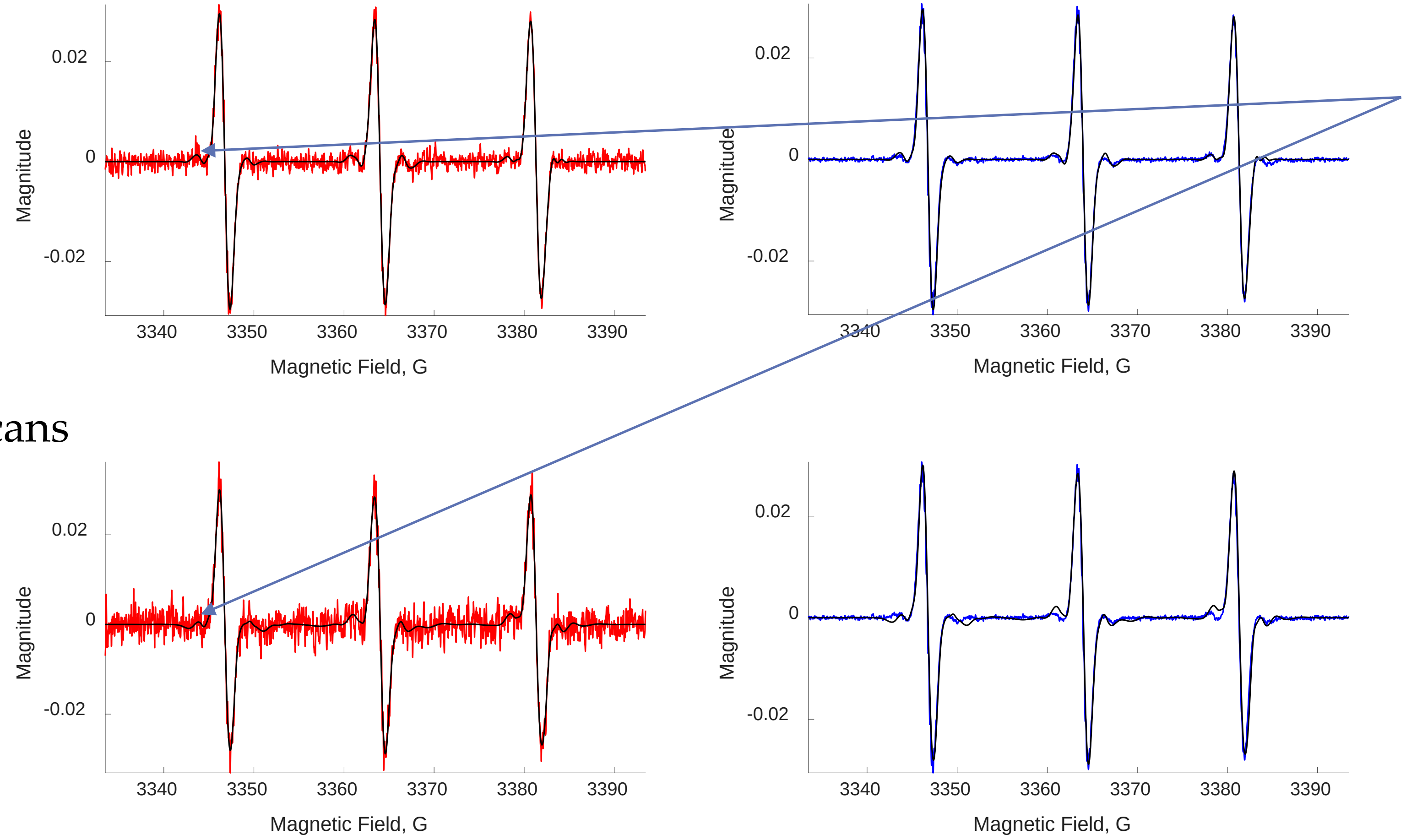
Sample: Tempol, 0.1mM in water at room temperature. X-Band 9.4GHz cw-ESR.

- Noisy
- Reference (500 scans)
- Denoised

Wavelet: Coiflet 3

16 Scans

4 Scans

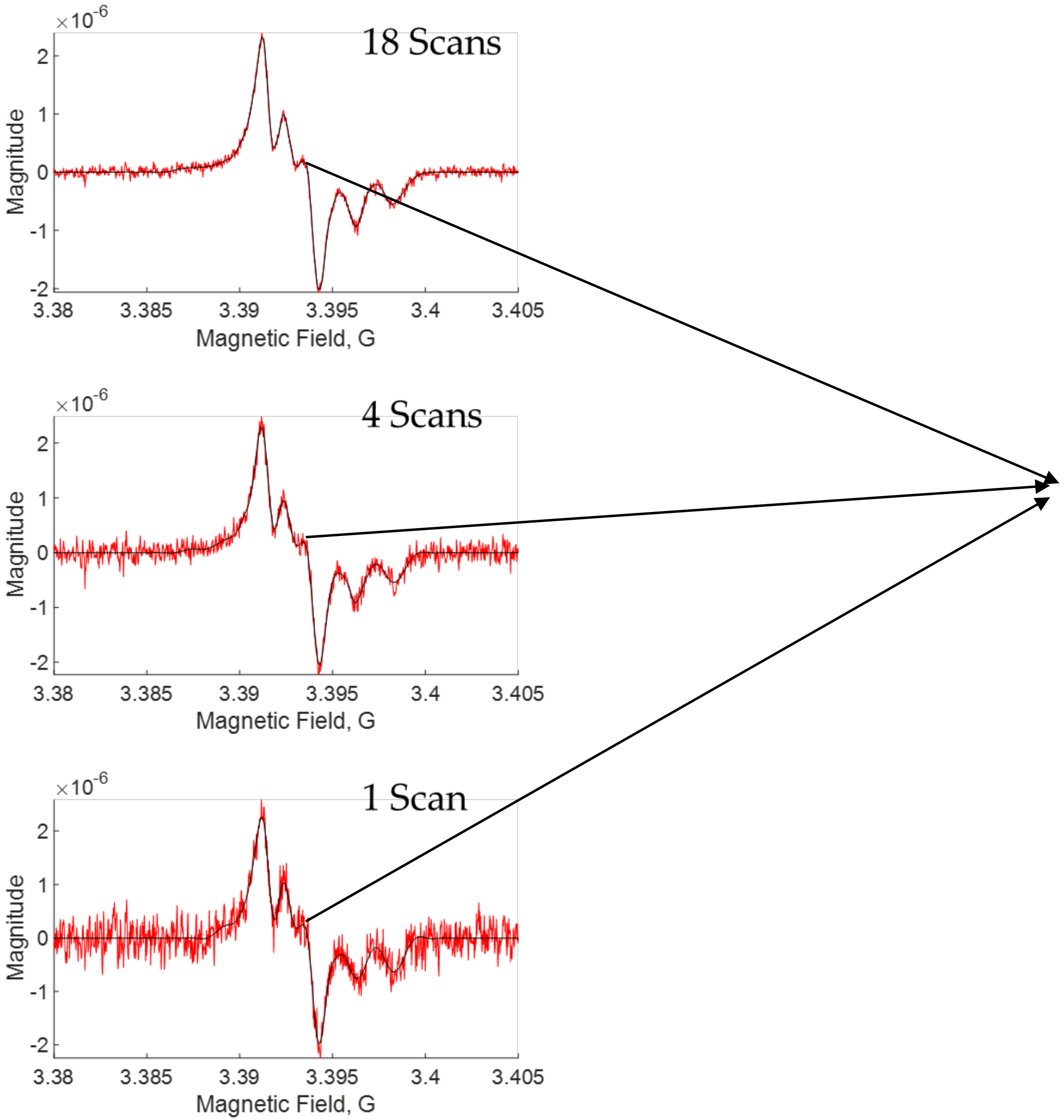


Revealing Weak C-13 Peaks

Signal		Noisy SNR	Denoised SNR
16 Scans	Main Signal	30	**46416**
	Weak Signal	1.5	**1613**
4 Scans	Main Signal	14	**2435**
	Weak Signal	0.5	**85**

*Srivastava, Dzikovski, Freed (in preparation)

NERD Results: Experimental cw-ESR Data 2



Hidden Peaks Extracted

Wavelet: Coiflet 3

Sample: 0.5% lipid spin label 16-PC in lipid vesicles at room temperature. W-band 95 GHz cw-ESR

Signal	**Noisy SNR**	**Denoised SNR**
18 Scans	39	**6×10^7**
4 Scans	19	**7×10^4**
1 Scan	10	**4×10^3**

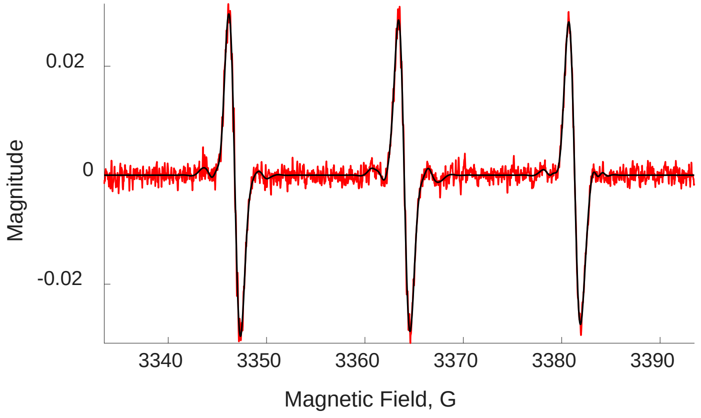
*Srivastava, Dzikovski, Freed (in preparation)

Results: Decimated vs Undecimated DWT

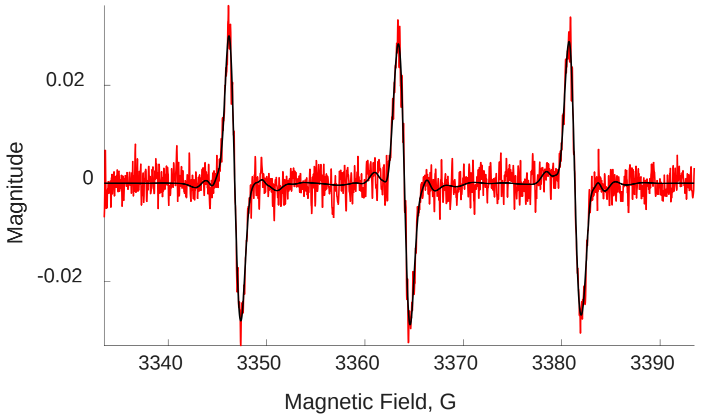
Sample: Tempol, 0.1mM in water at room temperature. X-Band 9.4GHz cw-ESR.

Undecimated DWT

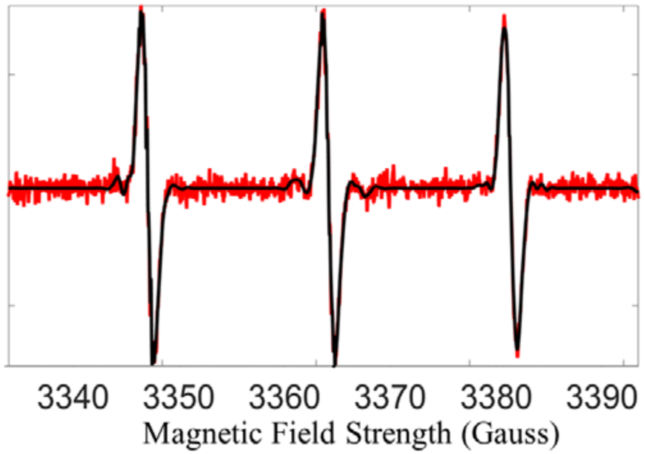
16 Scans

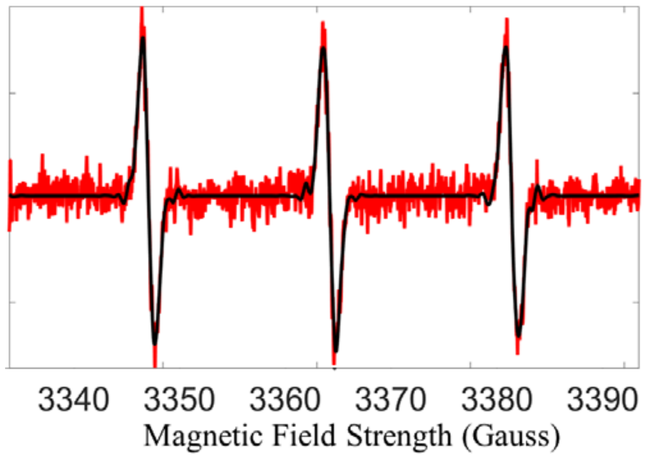


4 Scans



Decimated DWT





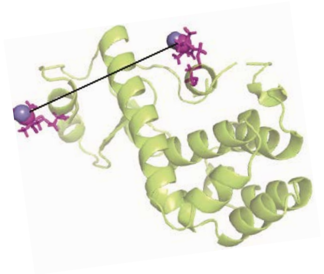
Signal		**Noisy SNR**	**Denoised SNR**
16 Scans	NERD	30	**46416**
	New Method	30	**2220**
4 Scans	NERD	14	**2435**
	New Method	14	**784**

*Srivastava, Dzikovski, Freed (in preparation)

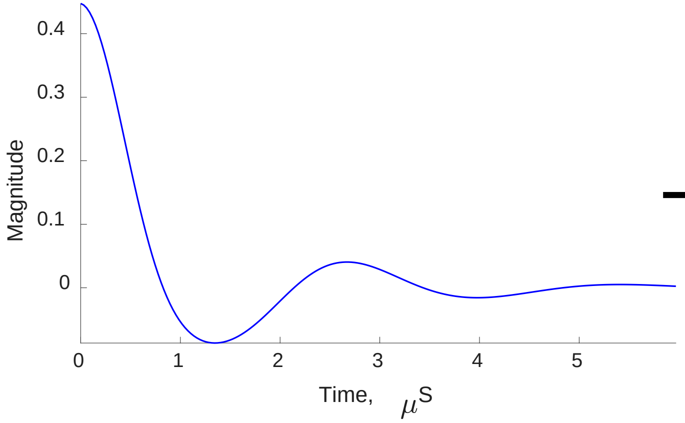
Wavelet Denoising for Pulsed Dipolar Spectroscopy (WavPDS)

Pulsed Dipolar Spectroscopy (PDS)

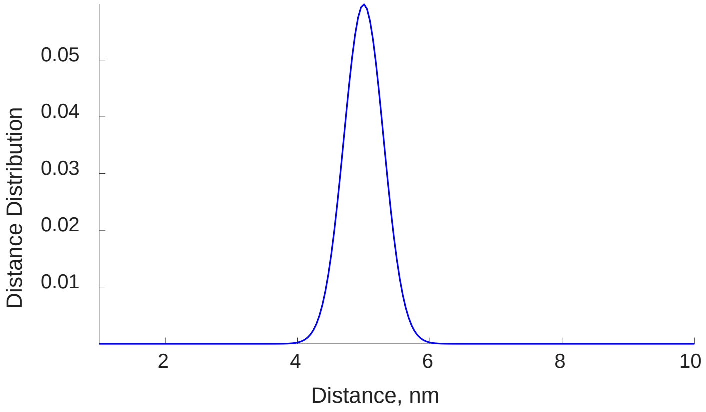
Sample



Dipolar Signal (S)



Distance Distribution (P)



Mathematical Formulation:

$$S(t) = \int_{R_{min}}^{R_{max}} K(r,t)P(r)\, dr$$

$S(t)$ - the experimental time-domain signal from spin pairs.

$P(r)$ - the distance distribution in pairs defined on the interval $[R_{min}, R_{max}]$.

$K(r,t)$ - the kernel for the Fredholm equation & can be of more complex form, if necessary.

Discrete Form:

$$KP = S$$

Matrix Inversion:

$$P = K^{-1}S$$ ✖

P cannot have single unique solution because K is singular, but see later.

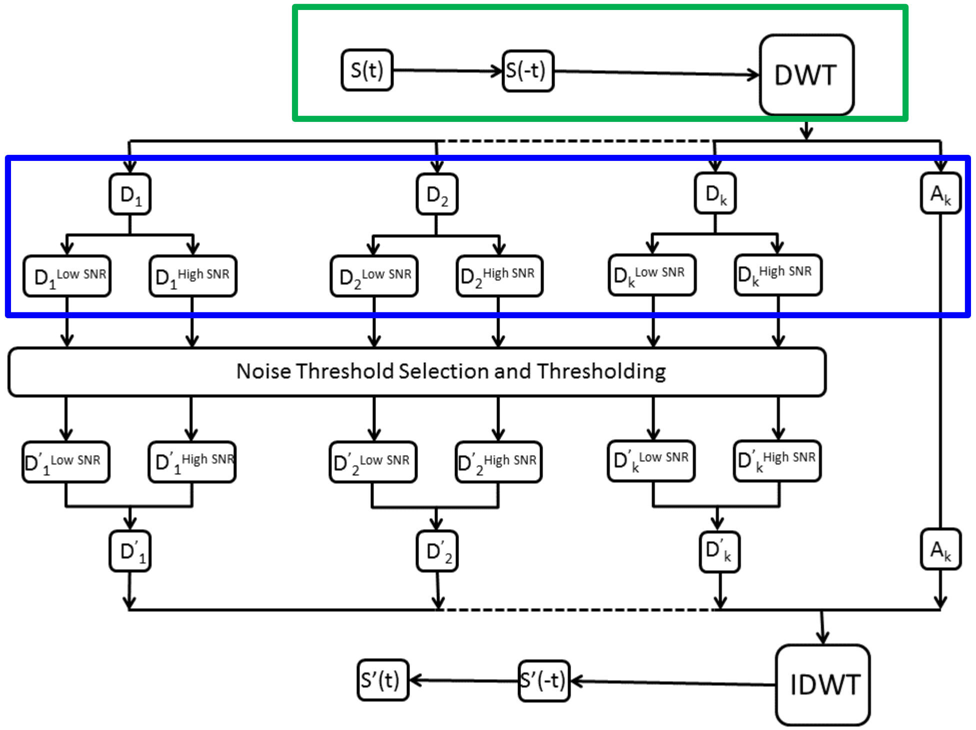
Tikhonov Regularization:

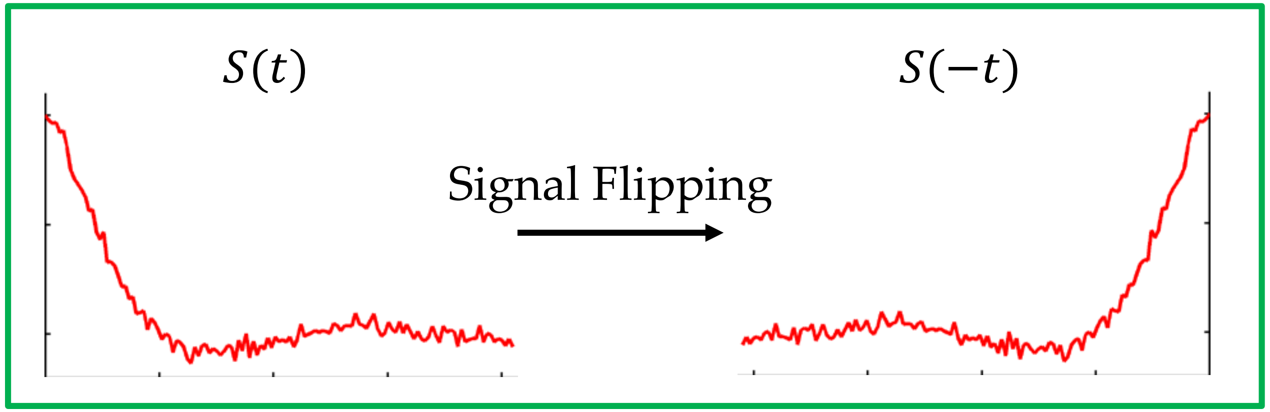
$$\phi_{TIKR}[P] \equiv \min \|KP - S\|^2 + \lambda^2\|LP\|^2$$

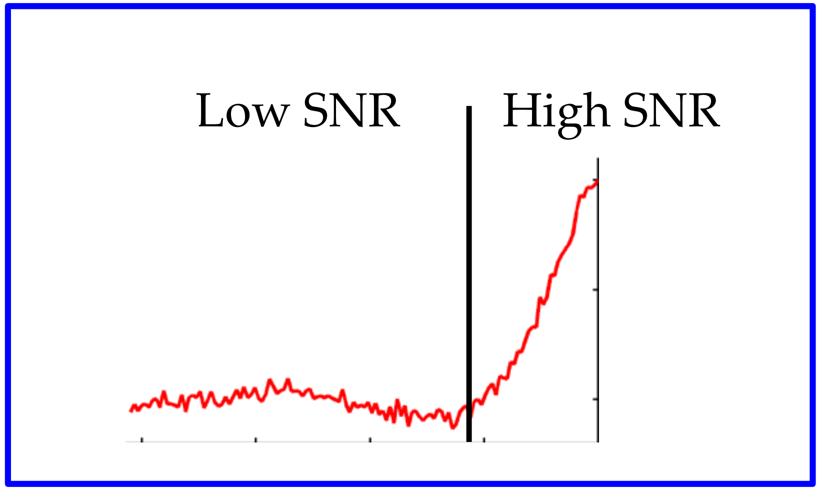
Regularization is used to obtain P

WavPDS Method

WavPDS





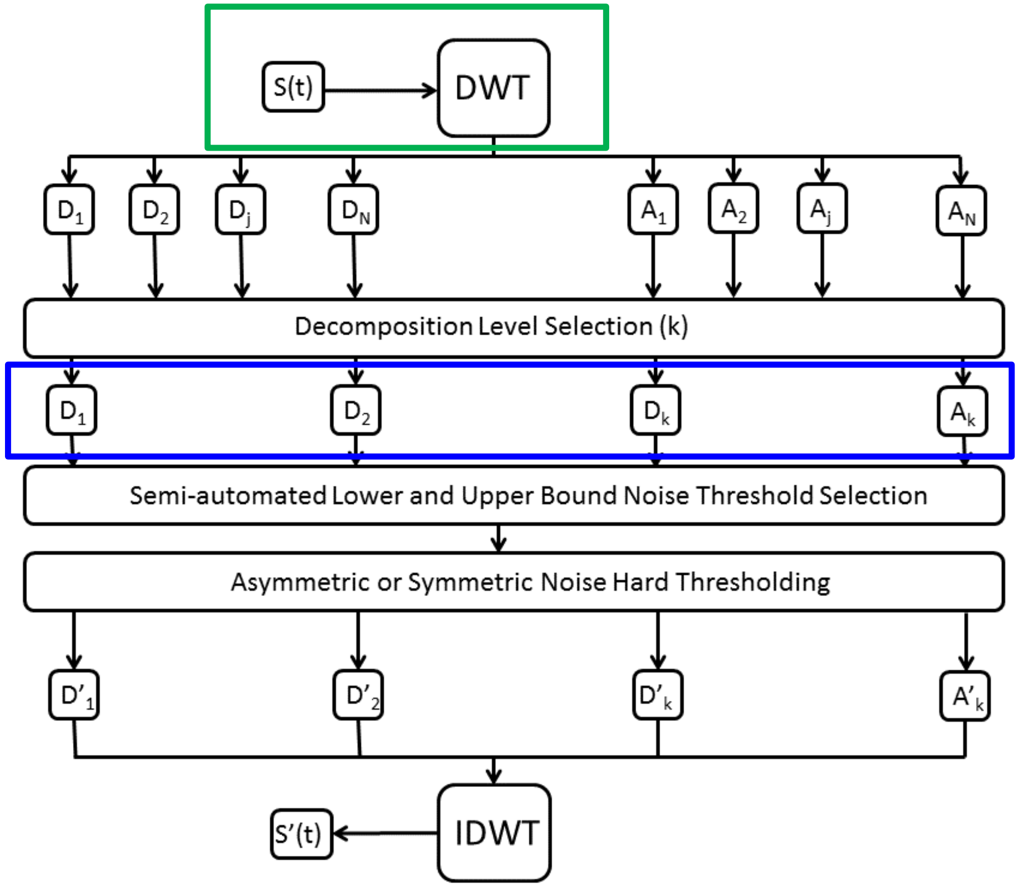


1. Flips the signal before applying DWT
2. Divides the signal into high and low SNR before noise thresholding

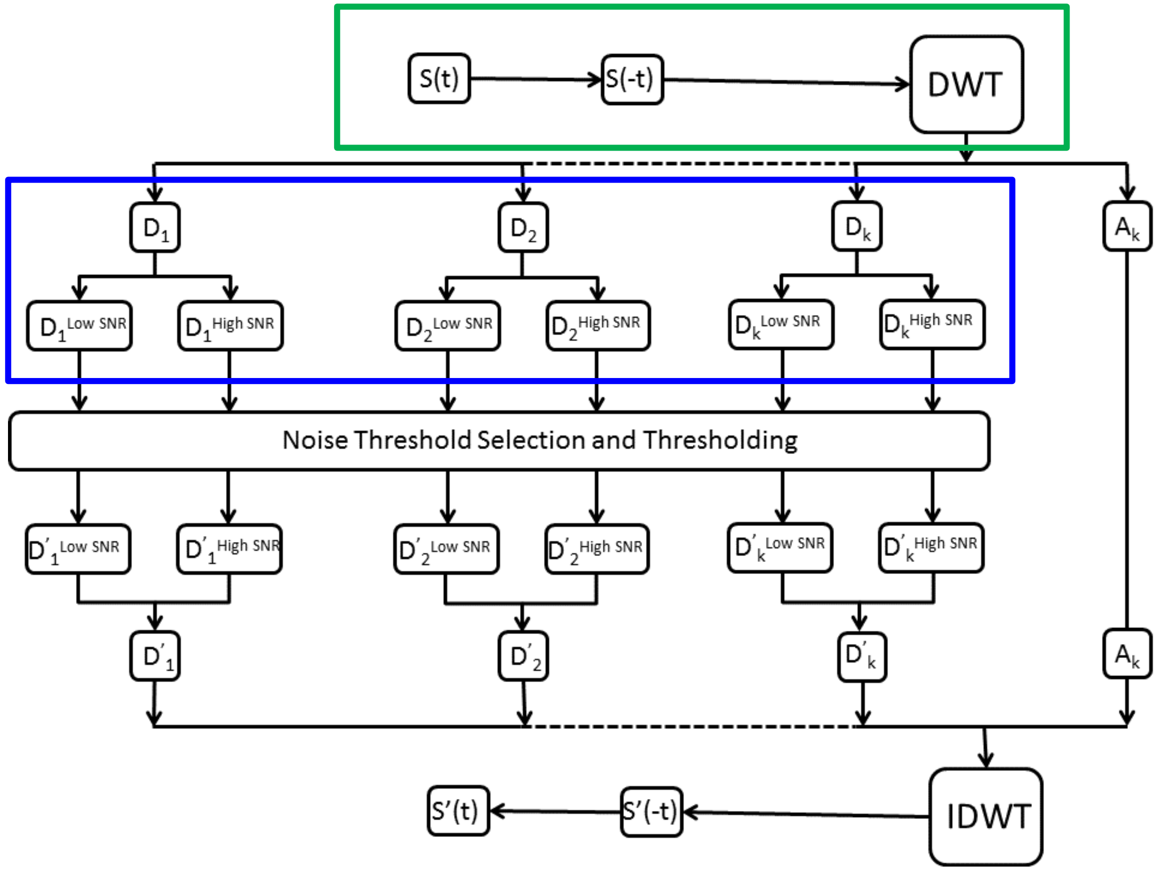
Srivastava, Georgieva, Freed (2017) *J. Phys. Chem. A*

WavPDS Method

New Method (IEEE Paper):



WavPDS

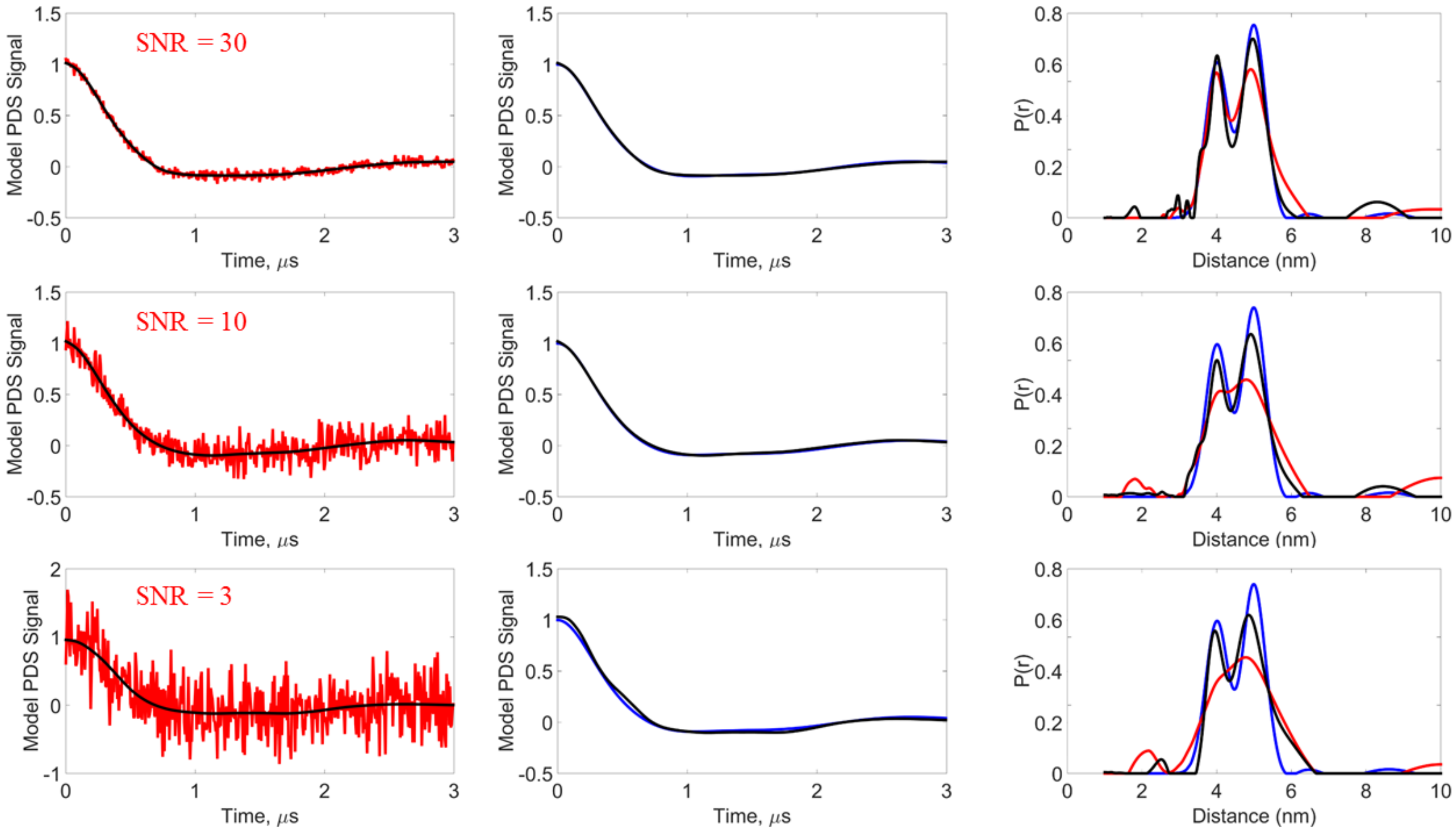


1. Flips the signal before applying DWT
2. Divides the signal into high and low SNR before noise thresholding

Srivastava, Georgieva, Freed (2017) *J. Phys. Chem. A*

WavPDS Results: Model Data Case 2

- Noisy
- Reference
- Denoised



		X^2	SNR	SSIM
Noisy		4.3283	3	0.0077
		1.3999	10	0.1068
		0.4347	30	0.5412
Denoised		0.0363	378	0.7532
		0.0073	1850	0.9530
		0.0042	3186	0.9971

Model Data Generation: Two-Gaussians distance distribution with peaks at 4 and 5 nm were created, which was then converted to time-domain pulse dipolar signals.

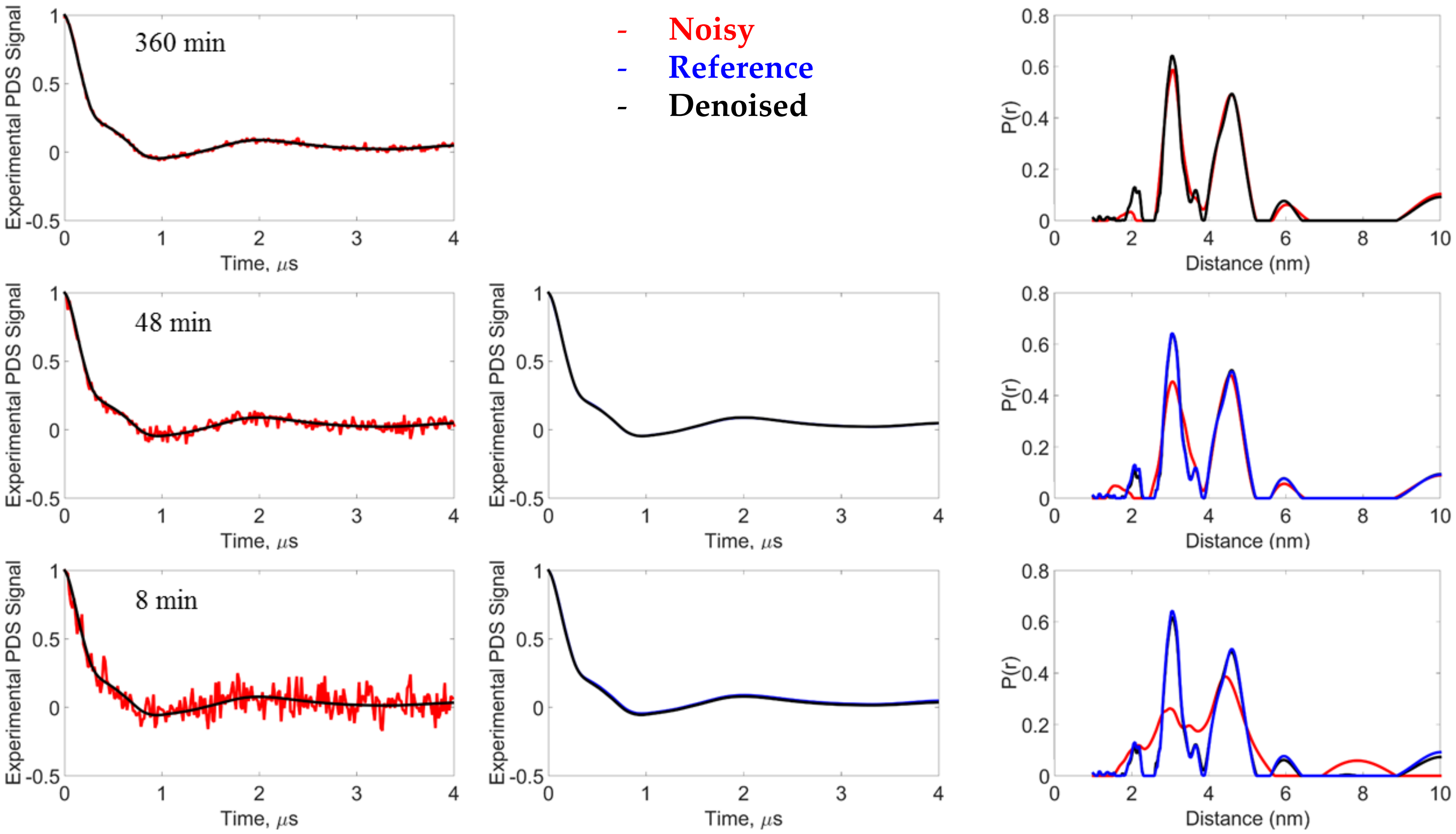
Noise: Gaussian noise was added to create the signal with different SNRs.

$$\chi^2 \equiv \sqrt{\frac{1}{p}\sum_{i=1}^{p}(f^{Ref}[i] - f[i])^2}$$

Wavelet: Daubechies 6

*Srivastava, Georgieva, Freed (2017) *J. Phys. Chem. A*

WavPDS Results: Experimental Data



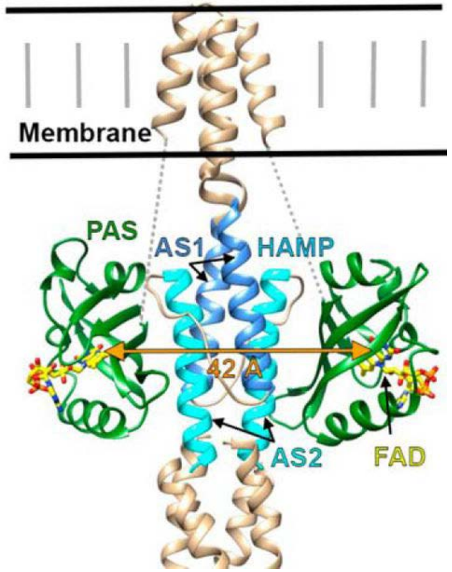
Wavelet: Daubechies 6

Sample:

- Mut1/Mut2 MIX = 44μM/47μM.
- Mutants are T4 Lysozyme spin-labeled at H2O buff, 10% Gly + 20% Gly-d8

*Srivastava, Georgieva, Freed (2017) *J. Phys. Chem. A*

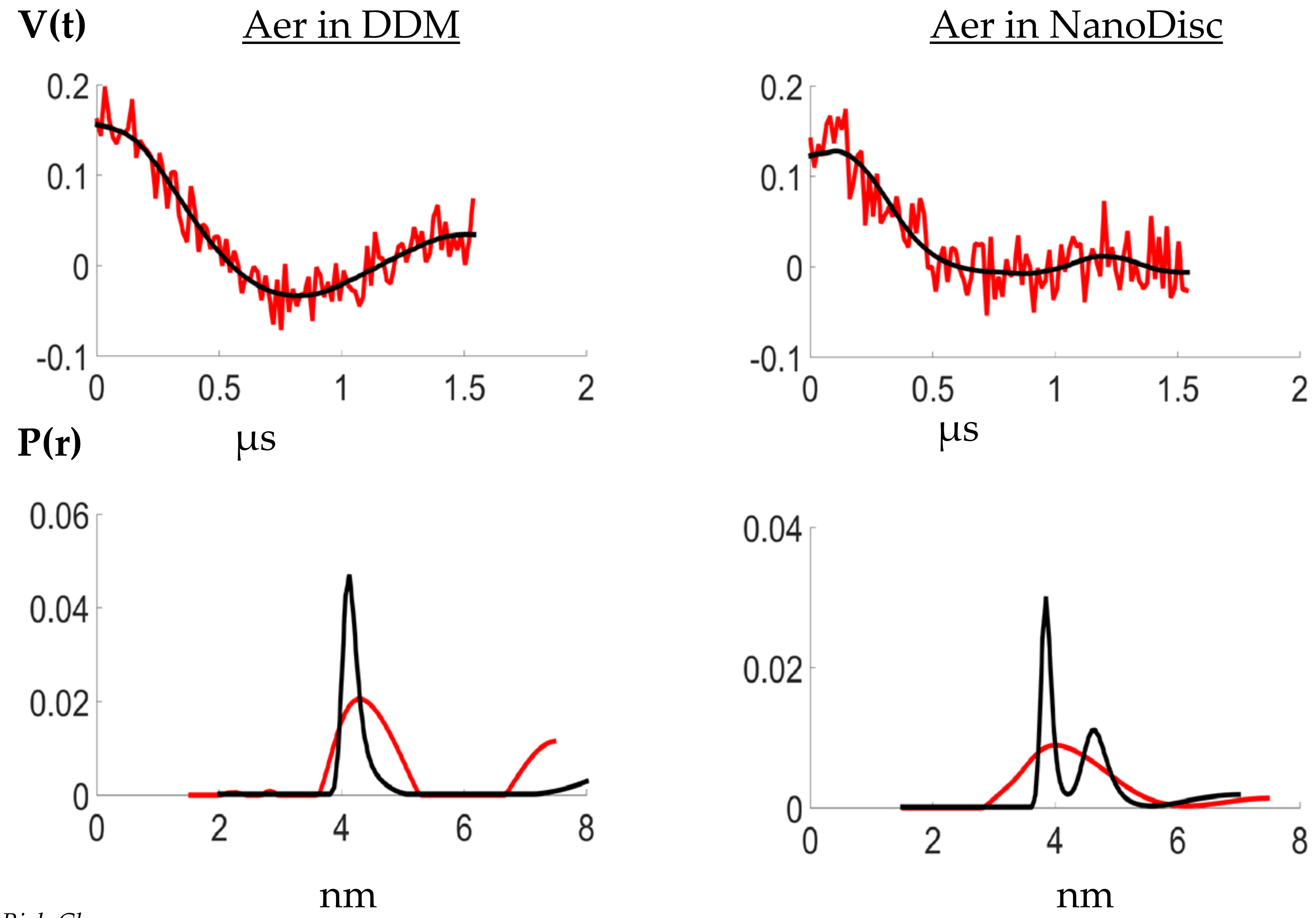
Revealing Multiple Conformations



Aer

Signal Acquisition Time: 40 hrs

- Denoised
- Noisy



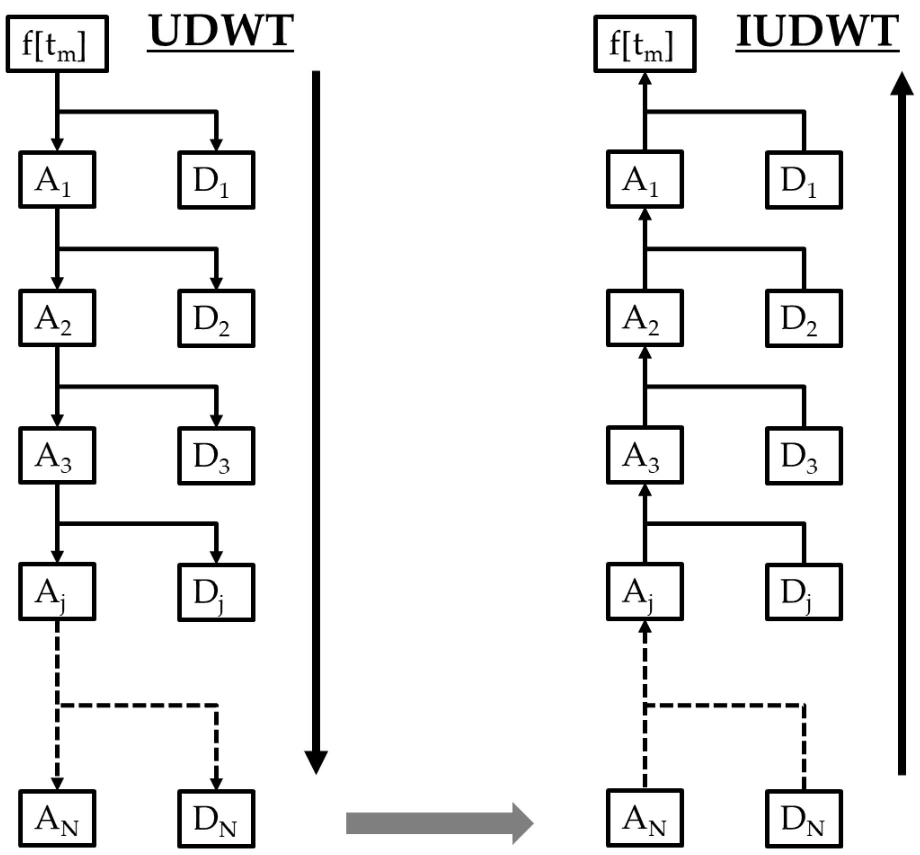
Sample:

- Flavin Adenine Dithionite spin-labeled Aer Solution = 60 μM.
- Solution contains H2O buff, 35% Gly

Samanta, ….Freed , Crane (2016) *J. Biol. Chem.*

Fast Wavelet Transform

Undecimated DWT and IDWT



$l[n]$ and $\tilde{l}[n]$ = low pass filters
$h[n]$ and $\tilde{h}[n]$ = high pass filters

Approximation component

$$A_{j+1}[k] = \sum_{n=0}^{L-1} l[n]\, A_j[2k+n]$$

Detail component

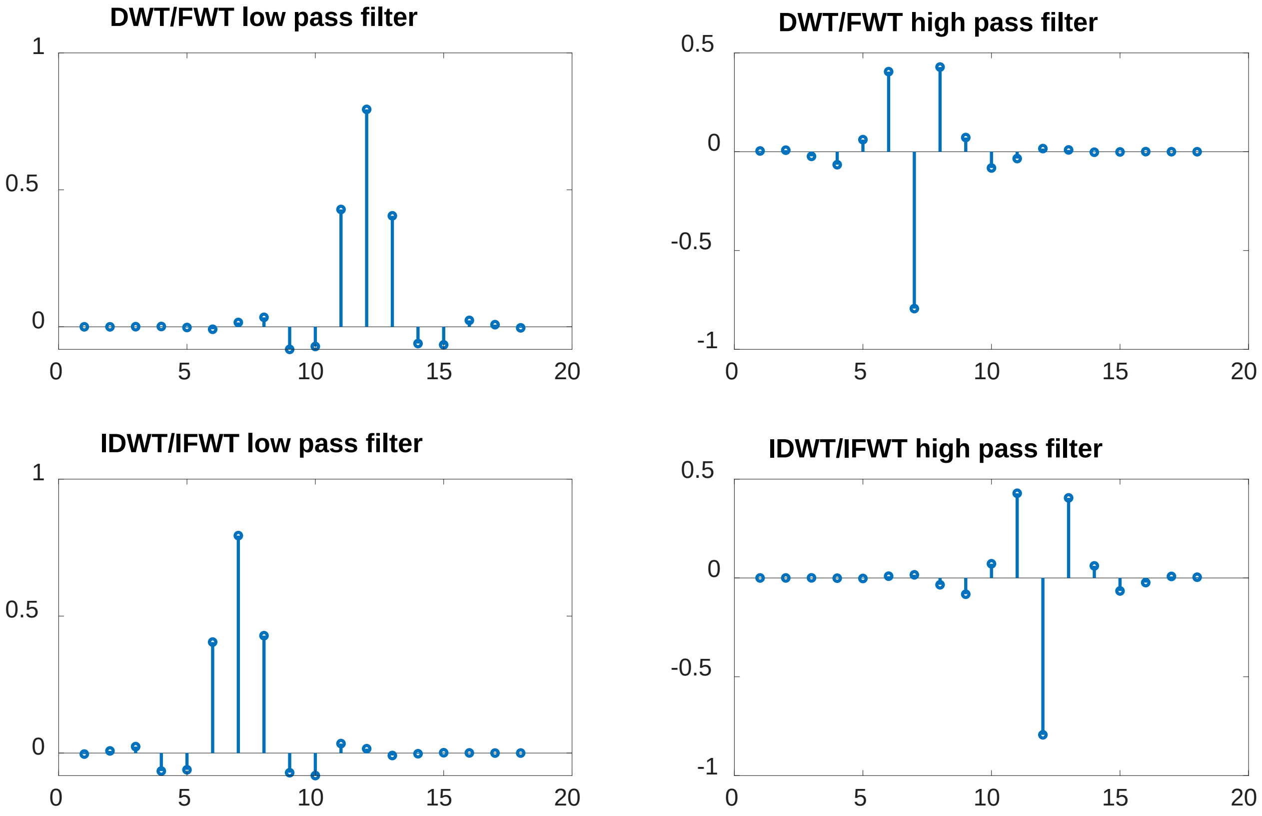
$$D_{j+1}[k] = \sum_{n=0}^{L-1} h[n]\, A_j[2k+n]$$

Inverse Fast Wavelet Transform

$$A_j[k] = \sum_{n=1}^{L-1} \tilde{l}[n]\, A_{j+1}[2k+n] + \sum_{n=1}^{L-1} \tilde{h}[n]\, D_{j+1}[2k+n]$$

Filters and their Relationship

Coiflet 3



FWT: Relation between low and high pass filters

$$h[n] = (-1)^n l[L-1-n]$$

IFWT: Relation between low and high pass filters

$$\tilde{h}[n] = (-1)^n \tilde{l}[L-1-n]$$

Relation between FWT and IFWT filters

$$\tilde{h}[n] = h[L-1-n]$$

$$\tilde{l}[n] = l[L-1-n]$$

Orthogonal and Non-orthogonal Frequency Sub-ban