

arPLS-vignette

Introduction

In the domain of (Raman) Spectroscopy it is a common problem and nuisance that the measured signal is a combination of “chemical information”, a (background) baseline and random noise (Zhang, Chen, and Liang (2010)). The so called baseline signal appears in the measurement as a smooth curve over the measured spectrum and it is important to estimate it and correct for it to allow e.g. for the correct integration of the part of the measured signal that truly belongs to chemical characteristics of the sample of interest.

A sample of a raw Raman spectrum (for the mineral Abelsonite) is shown in the below picture. The data was taken from Lafuente et al. (2016)

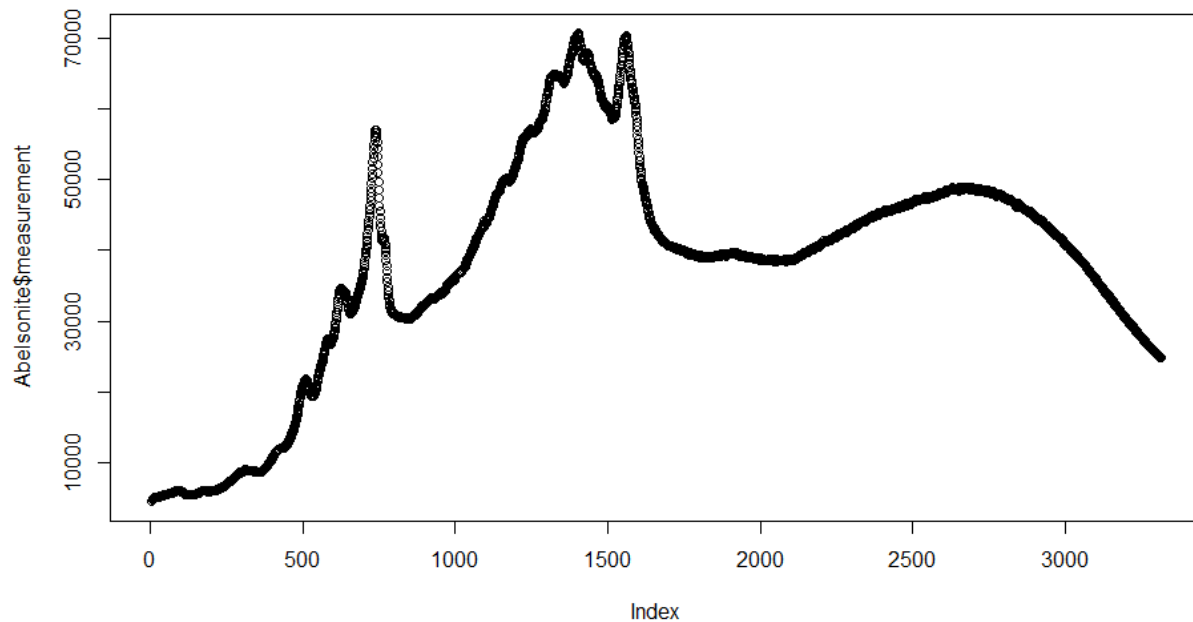


Figure 1: Raw raman spectrum of Abelsonite

The package at hand implements a semi-automatic baseline correction using asymmetrically reweighted penalized least squares smoothing as described in Baek et al. (2015). This algorithm estimates a baseline by trying to solve a multi criteria optimisation problem. It tries to find a line that satisfies (to various degrees the following criteria):

- closely follow the original measurements
- don't have much curvature (“wigglyness”)
- be located below the original measurements

To balance 1. and 2. a user provided smoothness parameter λ is taken into account. To satisfy 3., the algorithms uses a list of weights that put the estimation emphasis (error minimisation) of any given iteration

on areas where the baseline is over or close to the original signal. While areas with a large difference between baseline and original measurement are assumed to be due to a valid signal peak in that area. The algorithm will assign low weights for the optimisation efforts to those areas as it would be counter productive to try and force the baseline to mirror any actual signal peak, given that the whole point of a baseline estimation is to tell the background noise apart from the valid signal.

Usage

In terms of usage of the package, the end user will need to provide an input vector of a measured spectrum, a smoothness parameter λ to control the allowed curviness of the baseline estimate and a stopping criterion in terms of maximum number of iterations and/or percentage changes of the internal weight parameters from one iteration to the next.

Input Data

The main function of the package is `baseline_estimation()` and it requires as input data a vector of positive integers or floats representing the measurements across a range of wavelengths or so called wavenumbers¹. A sample of such data is e.g. the raw spectrum measured for Abelsonite² that can be obtained from the RRUFF database (Lafuente et al. (2016)). The first couple of rows of this spectrum are depicted in Figure below.

```
##NAME=Abelsonite
##RRUFFID=R070007
##IDEAL CHEMISTRY=Ni^2+^C_31_H_32_N_4
##LOCALITY=Green River Formation, Utah, USA
##OWNER=RRUFF
##SOURCE=Geophysical Laboratory, Carnegie Institution of Washington
##DESCRIPTION=Purple platy crystals embedded in drill core
##STATUS=The identification of this mineral is confirmed by single-crystal X-ray diffraction and chemical analysis.
##URL=rruff.info/R070007
##MEASURED CHEMISTRY=(Ni_0.92_Fe^2+^_0.05_Cr_0.02_)C_31_H_32_N_4_ ; C, H and N not measured but estimated by stoichiometry
175.0032, 4434.013
176.9317, 4464.471
178.8601, 4508.786
180.7886, 4587.709
182.7171, 4659.256
184.6455, 4705.039
186.5740, 4727.510
188.5025, 4759.603
190.4309, 4816.004
192.3594, 4880.960
194.2879, 4933.048
196.2163, 4971.668
198.1448, 5000.027
200.0733, 5016.268
202.0017, 5017.087
203.9302, 5027.395
```

It is left to the user to only feed the column with the measurements to the baseline estimation function. The algorithm performs reasonably fast on common consumer laptops for a couple of thousand rows, but slows down considerably for much larger spectra (of e.g. 10k rows). Further input data required from the user are the parameter values for λ (the smoothness parameter), ratio (one of the stopping criteria based on conversion of the results) and maximum number of iterations (a fall back stopping criterion in case the algorithm doesn't convert). For all of these parameters the estimation function will provide default values taken from p. 253 of Baek et al. (2015).

The function has a verbose mode that will render the current estimate of the baseline and print some diagnostic information to the console during the estimation process. This might be particularly useful for large spectra that can take a long time. The console output can serve as some kind of progress indication.

As part of the package the spectrum of Abelsonite from Lafuente et al. (2016) is provided and can be loaded as shown below.

¹Raman spectra are often recorded across so called wavenumbers with a unit of measurement that is the inverse wavelength expressed in cm, so 1/cm

²https://rruff.info/repository/sample_child_record_raman_full/by_minerals/Abelsonite__R070007__Broad_Scan__532__0__unoriented__Raman_Data_RAW__13756.txt

```
library(baselineARPLss)
data("Abelsonite")
head(Abelsonite,10)
```

```
##      wavenumber. measurement
## 1    175.0032,    4434.013
## 2    176.9317,    4464.471
## 3    178.8601,    4508.786
## 4    180.7886,    4587.709
## 5    182.7171,    4659.256
## 6    184.6455,    4705.039
## 7    186.5740,    4727.510
## 8    188.5025,    4759.603
## 9    190.4309,    4816.004
## 10   192.3594,    4880.960
```

Function call

With such input data at hand one of the most basic calls of the `baseline_estimation` function would be as shown below

```
result<-baseline_estimation(Abelsonite$measurement)
#due to default values that is the equivalent for the following function call
#result <- function(Abelsonite$measurement, lambda = 1e6,
#ratio = 1e-6, max_iter = 50,verbose=FALSE, algo="banded")
result
```

```
## $rawinput
##      [1] 4434.013 4464.471 4508.786 4587.709 4659.256 4705.039 4727.510
##      [8] 4759.603 4816.004 4880.960 4933.048 4971.668 5000.027 5016.268
##     [15] 5017.087 5027.395 5055.084 5088.089 5112.631 5127.084 5137.349
##     [22] 5145.543 5149.059 5151.471 5149.170 5148.275 5153.314 5171.389
##     [29] 5187.741 5195.132 5193.952 5203.059 5240.905 5283.491 5307.176
##     [36] 5282.429 5268.215 5282.618 5320.122 5351.076 5365.372 5375.111
##     [43] 5390.054 5412.359 5434.713 5456.928 5478.145 5493.906 5498.614
##     [50] 5502.327 5513.899 5537.156 5552.203 5547.243 5527.353 5521.505
##     [57] 5540.753 5563.373 5579.722 5588.578 5596.530 5605.131 5613.506
##     [64] 5619.818 5621.479 5625.213 5632.903 5644.857 5660.721 5684.257
##     [71] 5709.706 5730.428 5743.120 5757.442 5777.541 5802.995 5824.949
##     [78] 5836.334 5850.521 5875.493 5921.310 5955.105 5964.096 5958.642
##     [85] 5966.655 5999.088 6030.275 6049.996 6053.533 6056.141 6054.667
##     [92] 6054.175 6059.972 6082.969 6091.712 6072.210 6021.534 5982.431
##     [99] 5963.741 5952.756 5937.752 5916.513 5892.463 5867.996 5844.500
##    [106] 5819.936 5796.394 5765.918 5726.714 5677.990 5637.361 5600.021
##    [113] 5564.526 5541.889 5536.986 5529.850 5513.429 5492.642 5478.016
##    [120] 5472.826 5465.034 5453.674 5440.145 5428.526 5414.075 5396.881
##    [127] 5386.313 5383.123 5392.441 5419.549 5457.421 5474.378 5445.438
##    [134] 5421.760 5432.687 5474.437 5502.414 5502.190 5492.960 5487.059
##    [141] 5483.334 5482.375 5484.531 5488.904 5496.142 5510.638 5526.097
##    [148] 5540.436 5553.340 5566.002 5582.685 5598.371 5606.247 5591.140
##    [155] 5591.178 5614.569 5651.980 5688.412 5727.797 5763.566 5794.774
##    [162] 5821.729 5846.551 5859.116 5877.464 5909.189 5953.889 5987.816
##    [169] 6015.687 6036.451 6047.976 6049.025 6051.085 6049.648 6046.973
##    [176] 6052.317 6080.697 6097.574 6092.191 6066.354 6038.197 6008.386
##    [183] 5983.443 5966.357 5961.506 5951.908 5928.690 5898.720 5874.339
```

##	[190]	5865.138	5865.833	5862.533	5856.711	5868.446	5922.256	5963.221
##	[197]	5969.248	5952.615	5951.133	5963.109	5970.177	5964.303	5957.388
##	[204]	5972.498	6008.389	6036.394	6038.876	6021.745	6023.376	6050.453
##	[211]	6082.957	6093.686	6076.549	6065.839	6078.110	6111.169	6146.998
##	[218]	6178.401	6202.161	6216.827	6230.260	6241.757	6241.719	6246.110
##	[225]	6265.100	6301.975	6329.585	6344.717	6360.825	6388.738	6423.651
##	[232]	6454.785	6478.662	6501.673	6530.924	6573.989	6603.842	6600.468
##	[239]	6590.875	6609.677	6661.850	6712.573	6757.018	6804.416	6854.524
##	[246]	6896.643	6930.960	6950.897	6977.974	7018.989	7069.979	7109.859
##	[253]	7127.924	7141.930	7167.425	7206.092	7240.479	7266.760	7296.922
##	[260]	7327.642	7355.262	7382.283	7411.293	7447.004	7485.287	7524.323
##	[267]	7561.252	7601.939	7659.261	7712.415	7753.495	7793.132	7846.387
##	[274]	7916.847	7982.374	8039.621	8085.801	8123.915	8147.888	8177.402
##	[281]	8212.935	8255.580	8306.008	8368.980	8425.948	8474.009	8512.990
##	[288]	8543.920	8563.053	8576.647	8588.007	8593.940	8583.849	8539.366
##	[295]	8517.129	8543.193	8599.695	8635.720	8634.760	8642.202	8673.919
##	[302]	8721.242	8768.535	8819.488	8862.878	8895.790	8918.497	8935.271
##	[309]	8946.692	8956.033	8966.008	8972.187	8970.450	8958.689	8943.193
##	[316]	8920.744	8891.624	8873.381	8868.753	8872.214	8887.198	8909.519
##	[323]	8920.136	8904.312	8887.696	8888.562	8915.080	8920.988	8890.604
##	[330]	8859.575	8852.537	8863.888	8861.879	8831.938	8798.481	8769.311
##	[337]	8753.484	8755.396	8784.128	8804.990	8805.150	8792.858	8778.707
##	[344]	8762.698	8748.044	8735.782	8719.614	8699.432	8675.607	8657.552
##	[351]	8645.188	8624.256	8615.992	8636.562	8655.493	8635.609	8603.534
##	[358]	8604.225	8648.656	8676.353	8666.815	8657.337	8674.339	8725.101
##	[365]	8766.086	8760.529	8751.306	8778.162	8847.973	8911.132	8958.785
##	[372]	9000.411	9040.645	9082.109	9133.785	9205.602	9274.946	9330.979
##	[379]	9381.243	9434.186	9484.369	9528.820	9583.919	9647.590	9705.165
##	[386]	9748.639	9791.749	9846.817	9913.149	9983.590	10058.130	10125.340
##	[393]	10175.670	10230.440	10309.790	10413.450	10506.660	10561.320	10604.630
##	[400]	10671.890	10778.460	10903.160	11016.470	11095.290	11153.780	11205.790
##	[407]	11260.550	11313.250	11377.160	11455.220	11530.080	11585.530	11622.210
##	[414]	11675.060	11719.900	11746.910	11768.770	11801.550	11830.120	11846.780
##	[421]	11872.010	11901.990	11923.790	11940.920	11962.530	11964.330	11962.370
##	[428]	11977.190	12008.120	12028.580	12052.030	12091.860	12137.390	12171.880
##	[435]	12166.660	12129.990	12107.730	12117.650	12161.590	12215.220	12268.760
##	[442]	12327.580	12384.150	12430.090	12464.750	12493.910	12524.110	12573.340
##	[449]	12646.540	12729.910	12809.240	12901.210	13006.120	13096.340	13180.450
##	[456]	13272.040	13379.250	13480.990	13588.320	13711.480	13846.450	13968.550
##	[463]	14072.470	14178.530	14282.190	14377.980	14469.300	14554.340	14649.490
##	[470]	14764.400	14909.090	15060.640	15201.280	15333.630	15488.550	15695.380
##	[477]	15919.270	16151.360	16371.320	16577.290	16791.090	17028.080	17298.590
##	[484]	17566.410	17809.980	18055.480	18317.490	18594.540	18884.060	19210.100
##	[491]	19509.400	19739.020	19892.790	20048.460	20219.320	20389.450	20556.720
##	[498]	20701.070	20809.860	20883.190	20963.880	21039.810	21129.600	21253.920
##	[505]	21416.510	21571.130	21739.840	21845.970	21860.510	21797.790	21698.690
##	[512]	21565.870	21404.650	21192.320	20972.170	20757.710	20553.290	20372.550
##	[519]	20223.500	20087.670	19965.590	19855.880	19759.160	19676.490	19601.210
##	[526]	19528.670	19465.640	19422.960	19398.590	19376.500	19343.080	19334.800
##	[533]	19374.940	19444.070	19505.850	19540.070	19615.160	19758.760	19924.770
##	[540]	20076.880	20205.840	20363.620	20575.230	20788.660	20975.310	21159.740
##	[547]	21382.500	21646.840	21907.290	22166.450	22411.300	22626.480	22810.790
##	[554]	22999.640	23217.360	23408.680	23547.550	23651.790	23754.580	23867.190
##	[561]	23988.350	24117.760	24248.100	24364.480	24485.750	24665.520	24924.260

##	[568]	25167.380	25348.860	25529.160	25757.020	26016.510	26275.210	26556.360
##	[575]	26806.030	26995.290	27122.250	27234.370	27371.630	27452.820	27447.320
##	[582]	27403.590	27352.930	27295.870	27226.860	27137.390	27048.070	26944.210
##	[589]	26855.660	26824.080	26835.020	26880.450	26987.830	27124.020	27281.150
##	[596]	27430.720	27540.880	27620.470	27765.020	28019.950	28282.500	28488.940
##	[603]	28657.550	28902.080	29257.590	29585.480	29829.040	30071.580	30410.500
##	[610]	30871.300	31284.990	31629.080	31986.350	32399.000	32809.750	33147.460
##	[617]	33412.180	33664.470	33936.850	34176.770	34347.180	34460.450	34551.980
##	[624]	34639.340	34683.630	34635.630	34552.300	34486.610	34447.560	34382.400
##	[631]	34235.600	34132.270	34120.990	34140.440	34145.650	34139.820	34116.300
##	[638]	34084.020	33992.280	33849.190	33678.090	33482.810	33247.430	33017.640
##	[645]	32781.630	32537.550	32292.920	32055.810	31826.030	31600.930	31421.940
##	[652]	31288.270	31189.200	31151.580	31157.800	31162.220	31153.860	31171.760
##	[659]	31249.520	31326.760	31373.880	31419.380	31490.990	31578.270	31646.240
##	[666]	31708.080	31798.480	31872.710	31945.860	32090.180	32349.950	32568.640
##	[673]	32695.440	32822.640	32965.160	33118.040	33282.720	33472.480	33645.050
##	[680]	33778.710	33911.390	34076.990	34257.910	34409.650	34515.960	34637.000
##	[687]	34796.740	34956.570	35088.190	35208.750	35350.430	35517.910	35698.860
##	[694]	35874.400	36083.510	36371.730	36679.460	36934.190	37154.300	37445.710
##	[701]	37829.650	38232.970	38676.830	39107.480	39448.480	39727.000	40058.880
##	[708]	40454.370	40893.200	41397.720	41916.620	42428.530	42934.150	43413.750
##	[715]	43856.810	44298.950	44719.110	45186.910	45748.420	46368.630	46970.310
##	[722]	47546.040	48153.860	48807.360	49482.570	50170.050	50874.260	51623.230
##	[729]	52421.780	53138.310	53732.450	54307.790	54916.720	55486.250	55969.330
##	[736]	56367.450	56694.790	57014.950	57113.570	56962.230	56610.060	56067.500
##	[743]	55338.930	54412.250	53226.930	52058.890	50924.250	49780.880	48551.850
##	[750]	47360.860	46331.720	45459.630	44654.750	43907.080	43246.300	42664.050
##	[757]	42182.440	41808.390	41547.540	41423.160	41471.850	41538.060	41675.040
##	[764]	41756.550	41782.230	41715.720	41515.050	41183.710	40797.130	40361.810
##	[771]	39856.850	39289.040	38644.050	37866.340	37028.340	36235.690	35483.760
##	[778]	34823.340	34263.550	33775.290	33373.760	33023.070	32693.680	32393.500
##	[785]	32157.740	32015.960	31868.460	31684.360	31536.020	31473.710	31436.730
##	[792]	31350.420	31222.440	31148.510	31173.550	31177.940	31165.450	31124.690
##	[799]	31016.580	30896.660	30853.850	30894.540	30897.370	30825.470	30774.280
##	[806]	30775.380	30772.710	30722.160	30654.730	30630.810	30660.410	30669.010
##	[813]	30652.240	30620.920	30536.410	30481.080	30543.210	30655.370	30664.460
##	[820]	30549.410	30473.500	30447.270	30450.280	30518.850	30571.700	30545.330
##	[827]	30474.440	30431.810	30418.840	30418.450	30436.080	30451.800	30476.430
##	[834]	30479.480	30411.550	30323.600	30333.870	30439.180	30470.150	30381.290
##	[841]	30313.570	30319.750	30339.010	30335.060	30322.530	30322.410	30333.270
##	[848]	30340.460	30340.630	30346.550	30367.460	30386.080	30377.800	30373.110
##	[855]	30420.270	30506.730	30567.290	30596.410	30616.400	30605.820	30620.560
##	[862]	30709.900	30806.680	30834.630	30819.960	30862.770	30998.650	31057.060
##	[869]	30959.430	30900.150	30934.810	30995.490	31047.270	31093.230	31132.200
##	[876]	31161.950	31230.430	31369.770	31480.050	31538.290	31583.260	31611.670
##	[883]	31647.140	31729.580	31840.260	31885.630	31855.470	31864.510	31937.780
##	[890]	32018.350	32107.150	32176.050	32204.560	32205.060	32177.520	32132.590
##	[897]	32130.630	32177.780	32251.700	32383.690	32482.320	32490.510	32477.500
##	[904]	32485.010	32512.950	32569.030	32655.680	32719.090	32736.120	32771.100
##	[911]	32839.950	32909.570	32978.490	33034.660	33062.200	33070.180	33074.620
##	[918]	33072.130	33116.070	33234.040	33319.170	33342.810	33345.500	33344.110
##	[925]	33328.660	33270.390	33200.050	33195.500	33251.130	33256.330	33182.130
##	[932]	33138.740	33150.350	33193.520	33300.960	33395.840	33381.120	33323.110
##	[939]	33372.210	33530.680	33629.530	33636.490	33650.350	33674.420	33704.840

##	[946]	33752.680	33793.420	33781.800	33773.750	33885.830	34078.020	34146.270
##	[953]	34077.690	34007.500	33940.250	33908.580	33938.490	33982.680	34026.150
##	[960]	34065.940	34091.000	34112.290	34160.110	34236.360	34306.120	34351.510
##	[967]	34424.430	34549.060	34666.970	34754.190	34843.490	34973.290	35100.530
##	[974]	35167.700	35188.260	35196.350	35193.500	35234.660	35338.770	35429.180
##	[981]	35499.770	35537.200	35492.250	35461.750	35534.290	35646.150	35710.890
##	[988]	35735.800	35758.560	35783.000	35781.940	35732.500	35721.310	35787.390
##	[995]	35843.460	35819.940	35826.110	35968.510	36150.630	36266.890	36329.780
##	[1002]	36365.700	36373.870	36400.160	36452.640	36505.700	36537.610	36600.510
##	[1009]	36749.320	36876.260	36926.590	36933.540	36900.240	36858.640	36894.650
##	[1016]	36987.800	37011.190	36954.700	36936.180	36974.340	37034.320	37139.550
##	[1023]	37220.950	37218.630	37229.610	37344.110	37483.160	37536.810	37543.370
##	[1030]	37610.210	37734.530	37878.360	38047.420	38153.540	38152.010	38208.510
##	[1037]	38410.940	38599.720	38712.520	38793.890	38853.170	38912.870	39012.620
##	[1044]	39128.170	39189.780	39201.630	39251.680	39340.830	39464.070	39635.250
##	[1051]	39775.420	39858.130	39930.500	39987.690	40066.300	40218.900	40366.840
##	[1058]	40420.500	40437.050	40504.910	40615.070	40729.540	40848.560	40989.820
##	[1065]	41158.920	41298.560	41392.510	41488.590	41597.110	41711.700	41857.020
##	[1072]	41973.770	41995.000	42008.200	42102.110	42233.640	42345.520	42435.770
##	[1079]	42485.560	42501.380	42535.050	42588.080	42678.740	42824.280	42959.110
##	[1086]	43083.380	43178.130	43197.180	43243.510	43436.400	43582.330	43398.110
##	[1093]	43236.820	43649.600	44249.180	44283.890	43915.750	43797.320	43936.390
##	[1100]	43990.250	43889.450	43928.320	44192.390	44390.670	44476.000	44534.730
##	[1107]	44578.480	44618.350	44640.980	44683.760	44779.960	44896.790	45004.650
##	[1114]	45111.820	45218.560	45338.340	45544.660	45813.140	45915.930	45858.880
##	[1121]	45918.350	46127.710	46328.900	46502.090	46667.260	46819.630	46976.110
##	[1128]	47158.090	47318.670	47418.380	47521.020	47680.830	47832.960	47911.260
##	[1135]	47966.570	48071.930	48192.030	48249.100	48260.730	48306.210	48382.810
##	[1142]	48379.850	48295.300	48292.240	48384.360	48535.550	48773.500	48962.720
##	[1149]	49039.460	49132.770	49280.430	49423.980	49554.970	49666.250	49760.100
##	[1156]	49826.200	49825.150	49827.280	49916.250	50029.350	50085.210	50104.590
##	[1163]	50131.670	50157.560	50145.470	50101.890	50048.360	49990.780	50027.100
##	[1170]	50189.000	50220.480	50006.340	49902.790	49971.090	50000.190	49957.660
##	[1177]	49900.090	49812.120	49775.010	49807.620	49913.530	50198.640	50419.100
##	[1184]	50364.170	50284.610	50349.330	50483.130	50651.530	50821.010	50941.310
##	[1191]	51045.330	51198.110	51373.040	51500.050	51591.150	51689.720	51799.080
##	[1198]	51950.950	52140.300	52307.820	52453.630	52531.640	52490.060	52552.310
##	[1205]	52745.150	52954.440	53173.290	53408.200	53676.540	53910.240	54070.000
##	[1212]	54234.400	54427.950	54620.360	54812.750	54987.140	55140.450	55268.710
##	[1219]	55334.030	55419.910	55641.600	55827.960	55804.080	55729.010	55719.720
##	[1226]	55767.960	55907.960	56063.150	56155.680	56187.210	56112.950	56004.320
##	[1233]	56027.570	56143.510	56234.120	56314.870	56457.150	56640.820	56766.740
##	[1240]	56837.360	56879.310	56890.810	56955.990	57076.060	57130.520	57114.260
##	[1247]	57080.880	57028.800	57006.400	57043.600	57028.600	56936.320	56900.260
##	[1254]	56954.670	56927.510	56745.360	56648.540	56731.500	56816.710	56913.610
##	[1261]	56955.280	56913.550	56864.310	56802.500	56793.880	56905.730	56998.870
##	[1268]	56993.710	57030.460	57160.390	57314.960	57487.380	57649.300	57769.050
##	[1275]	57902.730	58113.940	58290.540	58363.290	58406.050	58445.380	58477.520
##	[1282]	58479.180	58501.040	58579.310	58683.350	58799.390	58926.320	59072.690
##	[1289]	59216.680	59316.150	59438.010	59654.690	59894.000	60061.230	60260.380
##	[1296]	60656.170	61036.350	61166.270	61257.090	61529.340	61840.340	62036.510
##	[1303]	62209.210	62441.400	62703.260	62982.860	63261.150	63517.340	63763.360
##	[1310]	64066.210	64312.850	64294.370	64246.200	64465.270	64723.880	64746.830
##	[1317]	64691.380	64722.100	64786.540	64861.690	64905.420	64836.480	64751.450

##	[1324]	64765.110	64810.040	64810.290	64806.210	64856.220	64899.480	64872.100
##	[1331]	64811.280	64718.650	64651.440	64698.130	64759.750	64745.070	64716.150
##	[1338]	64749.710	64767.710	64659.320	64558.990	64609.050	64655.900	64555.840
##	[1345]	64448.000	64433.300	64450.970	64529.840	64529.430	64295.560	64063.010
##	[1352]	63962.130	63920.980	63966.250	63959.280	63756.800	63634.320	63779.450
##	[1359]	63949.700	64035.360	64136.520	64291.750	64466.510	64678.600	64844.980
##	[1366]	64833.750	64946.170	65396.100	65725.050	65811.720	65922.480	66123.000
##	[1373]	66347.590	66591.610	66850.110	67149.980	67348.580	67404.210	67501.380
##	[1380]	67673.390	67879.300	68144.800	68292.940	68310.660	68390.500	68547.440
##	[1387]	68819.050	69220.900	69457.120	69542.190	69668.660	69830.340	69964.370
##	[1394]	70064.600	70061.310	70007.860	70156.800	70406.840	70512.690	70537.640
##	[1401]	70627.160	70710.420	70668.090	70539.770	70371.940	70157.450	69849.060
##	[1408]	69537.480	69331.640	69126.400	68853.680	68552.080	68206.570	67895.450
##	[1415]	67657.740	67467.770	67338.570	67205.410	66990.080	66866.800	66903.640
##	[1422]	66977.020	67080.410	67192.570	67319.470	67407.000	67412.650	67551.690
##	[1429]	67831.650	67952.050	67902.080	67895.930	67930.510	67935.680	67902.880
##	[1436]	67786.790	67603.490	67371.670	67122.950	66925.760	66745.010	66517.650
##	[1443]	66295.750	66126.310	65992.380	65927.520	65824.280	65602.410	65371.000
##	[1450]	65144.910	64986.950	64928.120	64940.710	65074.290	65064.350	64739.570
##	[1457]	64638.170	64859.040	64977.060	64977.260	64885.140	64706.820	64554.700
##	[1464]	64426.490	64320.240	64218.880	64075.820	63907.230	63742.250	63567.890
##	[1471]	63366.200	63146.400	62915.860	62671.910	62382.710	62132.200	61972.240
##	[1478]	61806.230	61571.160	61392.980	61316.730	61250.740	61192.290	61104.410
##	[1485]	60976.880	60911.330	60905.410	60765.270	60545.290	60473.500	60472.500
##	[1492]	60322.830	60168.460	60280.160	60438.930	60476.180	60438.490	60275.950
##	[1499]	60187.540	60314.910	60362.270	60191.480	59991.970	59757.270	59626.620
##	[1506]	59617.470	59576.980	59494.780	59371.330	59220.420	59149.260	59096.960
##	[1513]	58882.700	58649.100	58618.280	58661.360	58687.120	58710.320	58715.130
##	[1520]	58765.630	58907.720	59012.390	58993.110	59159.390	59629.290	59972.130
##	[1527]	60188.250	60336.200	60455.610	60746.950	61144.100	61485.800	61815.500
##	[1534]	62206.690	62587.520	62857.610	63156.410	63561.470	63975.800	64334.840
##	[1541]	64777.360	65354.500	65770.800	65996.160	66344.640	66814.050	67336.950
##	[1548]	67864.160	68267.530	68593.490	68876.130	69151.390	69459.620	69753.450
##	[1555]	70058.410	70245.500	70238.050	70259.730	70354.890	70312.050	70111.570
##	[1562]	69893.170	69650.310	69340.110	68988.600	68645.520	68282.020	67862.890
##	[1569]	67414.950	66941.210	66461.450	65962.970	65516.390	65142.930	64728.710
##	[1576]	64247.350	63997.970	63906.040	63561.120	63115.520	62865.230	62671.540
##	[1583]	62380.790	62093.060	61889.870	61658.070	61340.640	61087.790	60944.090
##	[1590]	60624.900	60118.730	59634.680	59165.850	58714.900	58237.080	57662.180
##	[1597]	57033.690	56344.310	55695.530	55197.740	54615.450	53888.930	53242.330
##	[1604]	52701.870	52225.630	51804.140	51401.700	51002.430	50547.960	50125.450
##	[1611]	49802.450	49577.380	49512.500	49390.090	49130.980	48886.330	48662.960
##	[1618]	48479.750	48325.170	48147.640	47965.850	47846.840	47687.340	47335.070
##	[1625]	47036.530	46901.710	46747.660	46529.910	46280.540	46005.740	45833.110
##	[1632]	45717.250	45539.190	45313.950	45002.700	44745.790	44694.940	44591.870
##	[1639]	44356.390	44137.220	43953.470	43771.610	43608.300	43624.550	43690.290
##	[1646]	43594.210	43450.660	43319.180	43240.070	43275.580	43227.040	43053.960
##	[1653]	42886.690	42747.910	42776.130	42866.680	42812.460	42682.810	42469.660
##	[1660]	42323.070	42331.630	42346.160	42348.950	42339.890	42313.830	42149.250
##	[1667]	41962.860	41993.280	42067.750	42064.830	41983.830	41769.960	41634.330
##	[1674]	41613.350	41579.390	41539.310	41577.930	41614.500	41452.850	41298.830
##	[1681]	41328.290	41335.260	41242.610	41223.500	41298.770	41274.800	41177.440
##	[1688]	41095.370	41034.070	41002.710	40994.100	41026.620	41007.630	40888.200
##	[1695]	40836.650	40845.320	40809.560	40744.570	40649.950	40586.110	40613.840

##	[1702]	40639.840	40626.160	40609.820	40592.930	40605.300	40627.590	40599.270
##	[1709]	40551.230	40506.830	40469.000	40436.170	40420.370	40424.120	40423.140
##	[1716]	40415.120	40385.910	40355.160	40346.800	40344.420	40325.240	40367.460
##	[1723]	40525.580	40510.160	40355.510	40263.810	40213.050	40177.440	40170.160
##	[1730]	40220.540	40221.990	40113.670	40139.980	40262.810	40294.300	40265.890
##	[1737]	40211.450	40139.690	40001.880	39987.800	40142.630	40071.290	39837.240
##	[1744]	39863.820	39976.170	39945.540	39912.520	39963.700	40004.960	40028.020
##	[1751]	39934.020	39780.930	39825.270	39901.610	39808.510	39765.370	39887.070
##	[1758]	39847.690	39594.430	39559.910	39658.470	39749.220	39754.890	39500.740
##	[1765]	39368.410	39481.170	39486.680	39384.570	39428.730	39535.270	39639.790
##	[1772]	39648.520	39475.060	39389.700	39473.990	39438.820	39343.310	39363.590
##	[1779]	39414.910	39420.430	39422.980	39446.640	39436.410	39391.400	39281.070
##	[1786]	39181.280	39259.810	39312.090	39208.930	39134.780	39111.600	39127.180
##	[1793]	39165.940	39189.360	39218.360	39296.610	39308.770	39205.630	39110.920
##	[1800]	39045.150	39089.140	39162.330	39173.550	39177.130	39191.230	39220.580
##	[1807]	39257.170	39221.560	39165.930	39197.240	39209.980	39121.210	39080.770
##	[1814]	39096.030	39073.020	39028.300	38967.070	38961.320	39136.160	39169.590
##	[1821]	39024.040	39012.850	39085.120	39095.060	39088.030	39098.060	39091.100
##	[1828]	39058.820	39090.240	39162.230	39244.610	39246.690	39002.400	38895.480
##	[1835]	39003.540	39120.680	39205.460	39122.710	39023.050	39013.100	39057.390
##	[1842]	39155.350	39210.120	39213.160	39094.630	39016.230	39154.040	39216.050
##	[1849]	39135.710	39138.600	39198.860	39240.350	39251.470	39193.210	39201.370
##	[1856]	39302.100	39354.390	39347.170	39194.130	39103.140	39258.670	39296.590
##	[1863]	39175.010	39133.320	39154.150	39243.180	39294.830	39234.730	39214.530
##	[1870]	39245.720	39322.700	39403.110	39436.630	39431.770	39364.850	39410.730
##	[1877]	39534.980	39484.910	39397.520	39396.590	39446.040	39559.170	39589.220
##	[1884]	39541.610	39407.250	39278.840	39195.610	39226.820	39391.320	39393.630
##	[1891]	39349.000	39468.370	39546.640	39487.800	39505.070	39592.700	39568.600
##	[1898]	39524.660	39556.200	39584.790	39594.870	39582.100	39567.750	39625.290
##	[1905]	39672.820	39642.610	39641.710	39675.110	39721.730	39737.600	39728.700
##	[1912]	39675.060	39552.300	39472.300	39457.250	39587.860	39683.320	39636.660
##	[1919]	39605.430	39601.680	39673.930	39723.490	39532.170	39401.190	39480.180
##	[1926]	39441.270	39331.290	39362.950	39426.010	39468.760	39439.050	39331.290
##	[1933]	39218.490	39171.990	39274.680	39357.200	39371.380	39370.770	39374.810
##	[1940]	39369.640	39348.890	39307.440	39240.370	39165.420	39191.350	39261.410
##	[1947]	39356.930	39308.540	39158.720	39162.110	39196.020	39129.130	39106.360
##	[1954]	39188.550	39102.510	38986.580	39118.090	39197.540	39114.020	39046.500
##	[1961]	39012.840	39014.890	39027.780	39046.180	39045.280	39031.890	39072.230
##	[1968]	39094.700	39025.620	38964.930	38929.980	39014.620	39092.210	38958.110
##	[1975]	38877.740	38936.250	38957.330	38956.840	38885.940	38840.480	38881.000
##	[1982]	38900.590	38882.690	38785.350	38756.620	38870.930	38847.050	38715.580
##	[1989]	38694.290	38727.880	38758.370	38780.270	38806.050	38819.850	38762.710
##	[1996]	38643.250	38675.620	38824.970	38900.210	38915.840	38824.850	38738.790
##	[2003]	38768.040	38795.620	38734.860	38682.350	38660.110	38638.360	38666.870
##	[2010]	38713.450	38683.500	38642.310	38631.310	38664.190	38646.040	38542.200
##	[2017]	38536.640	38614.450	38564.600	38550.110	38615.140	38655.150	38672.890
##	[2024]	38672.010	38661.140	38636.720	38686.550	38753.470	38729.220	38733.580
##	[2031]	38731.130	38660.660	38605.180	38655.390	38685.500	38643.390	38621.350
##	[2038]	38656.710	38657.530	38626.510	38601.050	38624.790	38702.680	38740.040
##	[2045]	38603.340	38430.890	38508.120	38607.680	38532.600	38470.660	38539.560
##	[2052]	38686.400	38723.640	38623.890	38523.880	38446.900	38519.430	38600.850
##	[2059]	38616.470	38636.190	38610.260	38547.700	38505.620	38497.300	38552.330
##	[2066]	38604.940	38574.950	38579.480	38657.670	38621.530	38521.800	38519.890
##	[2073]	38539.910	38556.550	38609.290	38660.010	38637.840	38622.410	38631.930

##	[2080]	38657.670	38685.580	38671.870	38647.390	38627.380	38538.490	38440.360
##	[2087]	38470.120	38542.920	38654.870	38633.110	38544.920	38556.330	38617.760
##	[2094]	38723.460	38711.650	38644.130	38583.270	38570.920	38634.590	38659.130
##	[2101]	38671.630	38712.640	38720.310	38688.620	38708.670	38742.920	38754.410
##	[2108]	38726.860	38667.250	38757.910	38856.370	38791.260	38795.740	38873.710
##	[2115]	38811.820	38735.640	38757.610	38755.030	38747.570	38861.970	38984.080
##	[2122]	39055.290	39087.510	39094.270	39105.010	39115.180	39116.020	39160.460
##	[2129]	39220.070	39259.880	39261.680	39216.730	39194.770	39204.120	39275.800
##	[2136]	39335.550	39371.110	39343.510	39322.370	39338.080	39508.490	39746.580
##	[2143]	39671.240	39567.180	39550.930	39579.700	39638.580	39729.010	39778.500
##	[2150]	39767.180	39793.030	39800.670	39700.390	39708.380	39821.390	39757.430
##	[2157]	39727.460	39863.950	39963.650	40016.520	40018.800	40050.460	40132.780
##	[2164]	40087.770	40018.740	40084.390	40082.400	40017.080	40140.320	40232.170
##	[2171]	40094.740	40138.210	40290.020	40338.240	40304.250	40171.920	40319.590
##	[2178]	40520.310	40482.990	40433.370	40403.410	40406.830	40417.710	40411.590
##	[2185]	40490.180	40601.100	40642.450	40646.520	40625.070	40677.420	40749.520
##	[2192]	40800.340	40877.400	40923.880	40625.360	40559.730	40916.390	40878.570
##	[2199]	40702.400	40685.110	40779.730	40947.130	41064.230	41107.410	41024.300
##	[2206]	41019.650	41092.670	41319.720	41362.250	41198.370	41135.640	41154.560
##	[2213]	41254.630	41335.150	41376.130	41318.970	41334.640	41433.070	41492.840
##	[2220]	41474.710	41293.180	41323.680	41457.380	41485.800	41478.950	41453.640
##	[2227]	41423.770	41456.610	41612.690	41665.850	41650.030	41645.820	41561.090
##	[2234]	41430.010	41563.800	41712.590	41723.860	41786.320	41855.350	41848.710
##	[2241]	41822.590	41796.830	41841.290	41918.150	42016.930	42046.140	42009.890
##	[2248]	41876.220	41852.710	41925.310	41965.120	42059.490	42245.350	42259.930
##	[2255]	42215.730	42184.500	42277.810	42394.230	42282.130	42159.180	42089.470
##	[2262]	42213.680	42346.530	42391.650	42383.070	42358.340	42352.900	42383.680
##	[2269]	42443.990	42530.090	42549.890	42483.070	42494.410	42563.800	42696.300
##	[2276]	42670.140	42583.300	42619.270	42666.670	42707.700	42740.910	42803.980
##	[2283]	42910.100	42856.900	42744.150	42625.600	42686.290	42835.650	42911.530
##	[2290]	42936.180	42928.480	42969.190	43005.560	43019.460	43041.250	43094.130
##	[2297]	43217.980	43170.760	43051.500	43017.700	43090.500	43213.620	43091.140
##	[2304]	43108.760	43343.530	43325.960	43225.090	43120.570	43337.800	43590.970
##	[2311]	43468.630	43389.090	43389.500	43511.270	43554.910	43515.100	43577.540
##	[2318]	43593.660	43483.640	43646.660	43778.730	43633.530	43597.890	43629.920
##	[2325]	43642.730	43703.700	43807.810	43984.800	43971.360	43774.950	43870.540
##	[2332]	44006.430	44088.330	44049.710	44027.730	44148.130	44142.360	44117.720
##	[2339]	44209.220	44299.480	44313.160	44014.450	44012.820	44269.810	44355.730
##	[2346]	44295.630	44125.660	44257.770	44377.960	44363.130	44329.940	44307.410
##	[2353]	44301.360	44395.200	44493.700	44477.770	44617.660	44779.920	44665.420
##	[2360]	44641.420	44700.430	44675.520	44646.840	44630.030	44603.010	44605.540
##	[2367]	44656.770	44891.380	44986.260	44783.540	44778.440	44856.980	44943.050
##	[2374]	44995.760	44993.760	44887.900	44880.940	44943.070	45052.840	45036.530
##	[2381]	44950.900	44901.450	44999.080	45176.810	45184.510	45225.020	45300.270
##	[2388]	45255.430	45164.240	45066.020	45148.090	45202.130	45175.520	45269.450
##	[2395]	45379.450	45456.260	45439.600	45382.320	45313.030	45310.710	45335.730
##	[2402]	45351.480	45406.560	45441.700	45390.320	45452.290	45561.070	45652.080
##	[2409]	45592.940	45472.650	45400.240	45473.220	45606.690	45675.630	45600.810
##	[2416]	45469.630	45471.210	45516.250	45566.550	45552.010	45607.860	45698.950
##	[2423]	45622.720	45616.400	45682.450	45683.840	45628.690	45565.330	45733.540
##	[2430]	45818.910	45782.710	45805.480	45840.170	45864.520	45802.150	45793.210
##	[2437]	45848.390	45733.500	45732.890	45879.760	45877.650	45860.830	45875.390
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##	[2451]	46094.540	45993.340	45848.810	45850.310	46023.850	46020.330	46086.240

##	[2458]	46252.590	46214.460	46211.180	46281.810	46152.740	46118.160	46230.510
##	[2465]	46320.290	46278.840	46169.020	46453.800	46479.390	46224.400	46365.940
##	[2472]	46420.770	46342.550	46307.830	46336.340	46418.700	46540.900	46640.980
##	[2479]	46661.370	46418.030	46354.090	46445.860	46547.050	46582.080	46576.850
##	[2486]	46588.470	46600.480	46618.850	46670.880	46664.800	46634.840	46626.430
##	[2493]	46598.190	46621.230	46785.870	46693.880	46583.510	46708.770	46663.090
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##	[2507]	46873.050	46898.410	47003.200	47164.420	47178.020	47143.330	47103.110
##	[2514]	47108.770	47137.300	47160.640	47122.670	47090.590	47076.200	47095.060
##	[2521]	47062.100	47069.060	47228.680	47235.750	47223.510	47318.190	47300.770
##	[2528]	47256.270	47234.830	47214.870	47204.690	47218.220	47337.550	47432.110
##	[2535]	47452.550	47292.530	47302.410	47432.050	47441.530	47492.290	47550.860
##	[2542]	47552.140	47463.290	47401.890	47469.720	47546.130	47578.980	47546.570
##	[2549]	47489.880	47399.800	47310.610	47557.840	47590.780	47434.460	47527.400
##	[2556]	47583.070	47590.430	47591.960	47620.620	47623.420	47545.390	47541.220
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##	[2570]	47776.030	47725.630	47765.200	47811.090	47725.680	47708.900	47708.510
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```

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## [3271,] 26742.805
## [3272,] 26693.911
## [3273,] 26645.077
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## [3308,] 24960.178
## [3309,] 24912.369
## [3310,] 24864.563
## [3311,] 24816.758
## [3312,] 24768.954
## [3313,] 24721.151
## [3314,] 24673.348
## [3315,] 24625.546
##
## $last_iter
## [1] 50
##
## $last_ratio
## [1] 0.0001536236

```

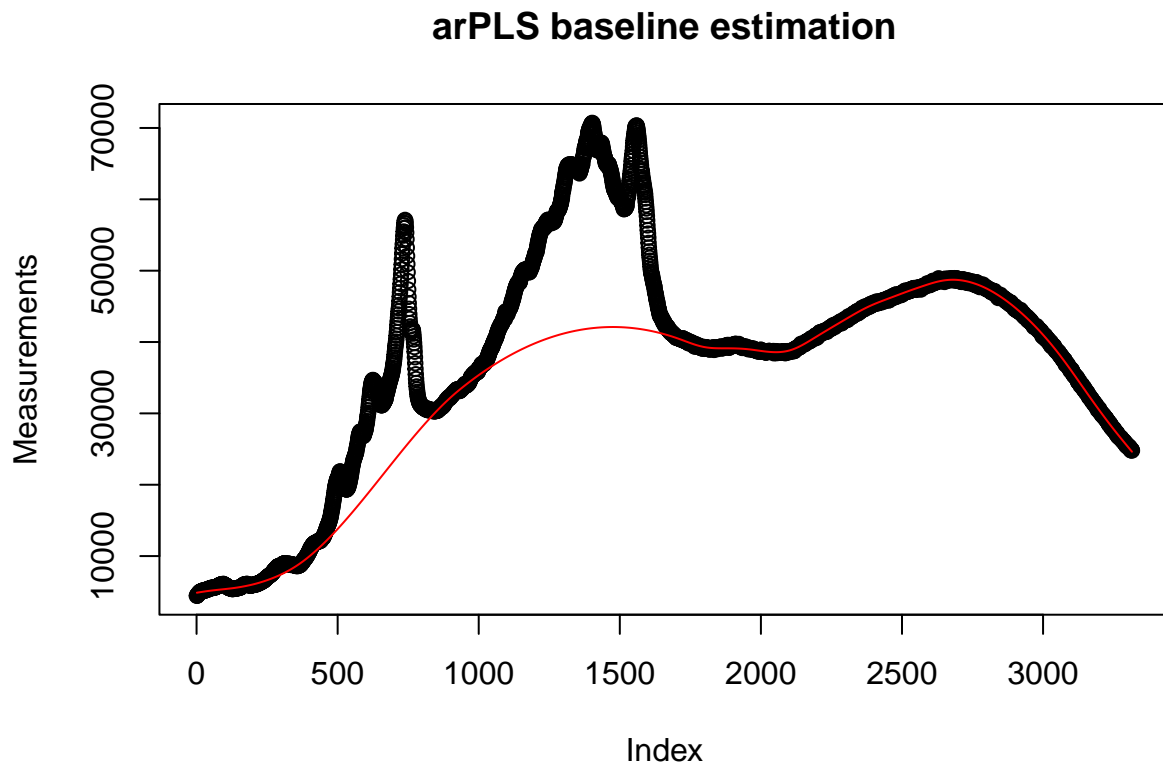
```
##
## attr("class")
## [1] "arPLSresult"
```

The package will use an S3 object of the class `arPLSresult` to store the results of the baseline estimation. The data structure behind this object is a named list with input data, result and parameter values. The rationale is that similarly to the result object of a `lm`-regression it would be important or at least useful to have contextual information beside the end result. This additional information includes the parameter values with which the algorithm was run:

- raw spectrum that was used as input data
- smoothness parameter λ that the user provided
- ratio parameter provided by the user as one stopping criterium
- maximum iteration parameter provided by the user as an additional stopping criterium
- estimated baseline after the algorithm stopped
- last iteration executed when the algorithm stopped
- last weight vector ration at the time when the algorithm stopped

The last two pieces of information allow to determine if the algorithm stopped because it converged or because it ran out of iteration. Given that the result is a custom data structure there is a summarize and plot function for this class included in the package. The custom plot function will plot the original raw spectrum with the estimated baseline overlaid. The usage is shown below.

```
plot(result)
```



The custom summary function will print the control parameter with which the algorithm was called as

well as the reason why it stopped (e.g. conversion vs. maximum iterations). The call of this function is demonstrated below.

```
summary(result)
```

```
## [1] "The lambda parameter value used was: 1e+06"
## [1] "The ratio parameter value used was: 1e-06"
## [1] "The max_iter parameter value used was: 50"
## [1] "The algorithm stopped after the following number of iterations: 50"
## [1] "The last weight ratio value was: 0.000153623596796175"
## [1] "It appears that the algorithm stopped because the maximum number of iterations was reached"
```

Bibliography

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