The LPML Method - Manual

Date: 6 July 2016

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This manual explains the code to the LPML method that was introduced in *Vandersteen et al.* [2015] and extensively applied on field data in *Anibas et al.* [2016].

The LPML (local polynomial (LP) method - maximum likelihood estimator (ML)) method can be used to quantify vertical components of the specific discharge vector (Darcy flux) across streambeds or lakebeds by solving the 1D heat transport equation as defined in *Stallman* [1965] and further discussed in *Vandersteen et al.* [2015], equations (1) - (4). It can also be used to estimate one thermal parameter of the streambed (thermal diffusivity, thermal conductivity, volumetric heat capacity).

To determine the parameters at one location the following input is needed:

(i) temperature-time series measured at the streambed top and at known distances in the vertical

(ii) Some reliable information regarding thermal parameters of the streambed that are not estimated

The 1D heat transport equation is solved in the frequency domain. In the first part, the spectrum of the measured temperature signal is determined with the Fast Fourier transform algorithm (FFT) for a set of equidistant discrete frequencies. Equation (1) in *Vandersteen et al.* [2015] then becomes Equation (5) and parameters alpha, beta and gamma are introduced. They are defined as shown in Equations (6) – (10). For a semi-infinite halfspace where in our case the upper boundary condition is a temperature-time series at the streambed top and the lower boundary condition approaches infinity in space, equation (5) can be solved analytically resulting in equation (14). The LPML method applies the concept of non-parametric transfer functions or frequency response functions (FRF) that can be computed between the temperature sensor used as upper boundary and each subsequent temperature sensor of known distance to the upper boundary. For the analytical solution, the FRF is defined as in equation (13). Each FRF contains a real and an imaginary part, which can be resolved into magnitude (amplitude in dB) and phase (in radians) information per frequency.

However, temperature data collected in field experiments usually contains periodic and transient signal parts as well as additional noise. Thus, a local polynomial method [*Pintelon and Schoukens*, 2012] is used to separate these parts of the temperature signal and to compute a new FRF (equation (15)) that can be compared to the FRF of the analytical solution (Figure 2b in *Vandersteen et al.* [2015]). For this new FRF a standard deviation can be computed, which serves as kind of a data quality indicator. If the standard deviation is above the value of the FRF the respective data will be excluded from subsequent parameter estimation (Figure 2a in*Vandersteen et al.* [2015]).

Afterwards, a maximum likelihood estimator is used (Equations (16) – (18)) to estimate alpha and gamma as well as their uncertainties (equations (20) – (24)). After optimizing alpha and gamma, the vertical components of the specific discharge and/or the estimated thermal parameter as well as their uncertainties can be quantified (equations (25) – (27)).

The LPML code as provided here is scripted in MATLAB (The MathWorks, Inc.) and contains the following files:

- ComputeTF (M-file) that computes the FRF for the analytical solution;
- LocalPolyAnal (M-file) that provides several options to determine the FRF using a local polynomial function;
- MLcost (M-file) that allows for a calculation of the cost function (equation (16) and following);
- MLEOptimization (M-file) that performs the parameter estimation using a Levenberg-Marquart/Gauss-Newton Algorithm);
- LPML_Aa (M-file), which was used to test the LPML method on simulated data as described in *Vandersteen et al.* [2015], section 3.1;
- LPML_ML1 (M-file), which was used to quantify the vertical specific discharge for location ML1 at the Slootbeek as described in *Vandersteen et al.* [2015], sections 3.2 and 3.3;
- Text files Aa.txt and ML1_90.txt, which contain the respective input temperature data with one data column per sensor.

To apply the LPML method, one has to provide their own input temperature data and adapt LPML_Aa or LPML_ML1.

LPML_Aa performs the following steps:

- Line 12: Load input temperature data.
- Line 13: Define sensor spacing in the vertical (here in m).
- Line 14: Define the length of the input data set (here in days).
- Line 15: Define the sampling frequency of input data and index all data (here 1 measurement every 1 hour).
- Line 16: Select input sensor.
- Line 17: Select response sensors.
- Line 23: True = only a frequency of 1/d is isolated from the entire signal as is often done by researchers using the methods of *Hatch et al.* [2006] or *Keery et al.* [2007]. In many cases the diel signal is the most pronounced one.
- Line 23: False = a frequency range is used.
- Line 27: Define the maximum frequency to be included in the analysis if line 23 = false.
- Lines 31 – 33: Determine input/output spectra and the frequency range used in the analysis.
- Lines 35 – 64: Use the local polynomial method to determine the FRFs and their uncertainties. Then draw them and isolate those frequencies for parameter estimation where the respective FRF was larger than its standard deviation.
- Line 74: Define the time unit.
- Lines 75 – 78: Define the starting values for parameter estimation.
- Lines 81 – 83: Determine the initial lumped parameters alpha (a), beta (b) and gamma(c).
- Line 88: Chose the free parameters, which will then be estimated.
- Lines 90 – 91: Use the maximum likelihood estimator for parameter estimation.
- Lines 92 – 101: Determine the FRFs applying the analytical solution and draw them in comparison to the FRFs determined using the local polynomial model.
- Lines 103 – 111: Determine estimated alpha and/or gamma and respectively estimated vertical specific discharge and in this case thermal conductivity. Also, standard deviations are calculated.
- Lines 113 – 120: Results for the estimated vertical specific discharge [mm/d], thermal conductivity [W/(m·K)], their standard deviations, actual model cost and expected model cost are printed.

Some additional comments on LPML_ML1:

- Line 13: For temperature measurements a probe as shown in Figure S1 [*Vandersteen et al.*, 2015] was used. It has 8 temperature sensors and the file ML1_90 contains 1 data column for each sensor. Data from sensor 1 was not used further. Sensor 2 represents the upper boundary. Sensors 3 to 8 show the system response.
- Lines 14 – 15: The length of the data set is 90 days with temperature measurements every 10 minutes.
- Line 17: 6 sensors show the system response.
- Line 27: The maximum frequency used was 1.5/d
- Lines 90: One can chose, whether only one parameter or two parameters by fixing the C parameter (set FixedC = 1 or 0);
- Lines 134 – 139: Results for the estimated vertical specific discharge [mm/d], thermal diffusivity [m^2/d], their standard deviations, actual model cost and expected model cost are printed.

References

Vandersteen, G., U. Schneidewind, C. Anibas, C. Schmidt, P. Seuntjens, and O. Batelaan (2015), Determining groundwater-surface water exchange from temperature-time series: Combining a local polynomial method with a maximum likelihood estimator, *Water Resour. Res.*, *51*(2), 922-939, doi: 10.1002/2014wr015994. → Please use this one for referencing the method!

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