Abstract: Lock in Feedback in Sequential Experiments

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Abstract

We often encounter situations in which an experimenter wants to find, by sequential experimentation, $x_{\text{max}} = \arg \max_x f(x)$, where $f(x)$ is a (possibly unknown) function of a well-controllable variable $x$. Taking inspiration from physics, we have designed a new method to address this problem.

1. Introduction

We often encounter situations in which an experimenter wants to find, by sequential experimentation, $x_{\text{max}} = \arg \max_x y = f(\vec{x})$, where $f(\vec{x})$ is a (possibly unknown) function of a well-controllable variable $\vec{x}$. To solve this problem in physics and engineering applications, scientists have routinely used methods that rely on the idea of systematically changing the value of the controllable variable in time and following, via so-called lock-in amplifier techniques, how those changes affect the dependent variable $y$ (see, e.g., [3]). Despite the fact that problem presents itself in many places, there is no single agreed upon method to approach it. It is thus worthwhile asking whether it is possible to adapt the lock-in amplifier approach used in physics as a generic tool to find $x_{\text{max}} = \arg \max_{\vec{x}} y = f(\vec{x})$ in sequential experiments. The goal of this abstract is to address this topic. We coin the novel method Lock-in Feedback (LiF) (for more details see [2]).

2. Finding the maximum of a curve with a lock-in algorithm: a short introduction

In this section we detail the principles behind LiF assuming continuous time. Let’s assume that $y$ is a continuous function $f$ of $x$: $y = f(x)$ and that $x$ oscillates with time according to $x(t) = x_0 + A \cos(\omega t)$ where $\omega$ is the angular frequency, $x_0$ its central value, and $A$ its amplitude. For relatively small values of $A$, Taylor expanding $f(x)$ around $x_0$ to the second order gives:

$$y(x(t)) = k - A \cos(\omega t) \left( \frac{\partial f}{\partial x} \bigg|_{x=x_0} \right) + \frac{1}{4} A^2 \cos(2\omega t) \left( \frac{\partial^2 f}{\partial x^2} \bigg|_{x=x_0} \right)$$

(1)

where $k = f(x_0) + 1/4 \left( \frac{\partial^2 f}{\partial x^2} \bigg|_{x=x_0} \right)$.

Suppose that $f$ only has one maximum and no minimum. Further suppose that our measurements of $y$ contain noise: $y(t) = f(x(t)) + \epsilon$. Following the scheme used in physical lock-in amplifiers (see, e.g., [3]), we can multiply the observed $y$ variable by $\cos(\omega t)$. Using eq. [1] we can obtain:

$$y_\omega = -\frac{A}{2} \left( \frac{\partial f}{\partial x} \bigg|_{x=x_0} \right) + k_\omega \cos(\omega t) + k_{2\omega} \cos(2\omega t) + k_{3\omega} \cos(3\omega t) + \epsilon \cos(\omega t)$$

(2)

where $y_\omega$ is the value of $y$ after it has been multiplied by $\cos(\omega t)$ and $k_\omega = k + A^2/8 \left( \frac{\partial^2 f}{\partial x^2} \bigg|_{x=x_0} \right)$, $k_{2\omega} = -A/2 \left( \frac{\partial^2 f}{\partial x^2} \bigg|_{x=x_0} \right)$, and $k_{3\omega} = A^2/8 \left( \frac{\partial^2 f}{\partial x^2} \bigg|_{x=x_0} \right)$.

Integrating $y_\omega$ over a time $T = \frac{2\pi N}{\omega}$, where $N$ is a positive integer and $T$ denotes the time needed to integrate $N$ full oscillations, we obtain:

$$y_\omega^* = -\frac{TA}{2} \left( \frac{\partial f}{\partial x} \bigg|_{x=x_0} \right) + \int_0^T \epsilon \cos(\omega t)$$

(3)

Depending on the noise level, one can tailor the integration time, $T$, to reduce the second addendum of the right hand of eq. [3] to negligible levels, effectively averaging out the noise. Under those circumstances, $y_\omega^*$ provides a direct measurement of the value of the first derivative of $f$ at $x = x_0$. This provides a logical update strategy of $x_0$: if $y_\omega^* < 0$, then $x_0$ is larger than the value of $x$ that maximizes $f$; likewise, if $y_\omega^* > 0$, $x_0$ is smaller than the value of $x$ that maximizes $f$. 


3. Algorithm for LiF in experiments

In discrete time we can use the same procedure as described above in which we start with \( x_0 \), and for each discrete sample oscillate around \( x_0 \) with a known frequency \( \omega \) and known amplitude \( A \):

\[
x_t = x_0 + A \cos \omega t
\]

which will result in measurements given by

\[
y_t = f(x_0 + A \cos \omega t) + \epsilon_t
\]

On the basis of the arguments given in the previous section, we can now implement a feedback loop that iteratively adjusts the value of \( x_0 \) until \( x \) reaches \( x_{\text{max}} \). Algorithm 1 presents a discrete time implementation of LiF. Note that in this presentation \( \gamma \) is the “learn-rate” of the procedure.

Algorithm 1 Implementation of LiF for single variable maximization in a data stream.

Require: \( x_0, A, T, \gamma, \tilde{y}_\omega = \{NA_1, \ldots, NA_T\} \)
\[
\omega = \frac{2\pi}{T}
\]

for \( t = 1, \ldots, T \) do

\[
x_t = x_0 + A \cos \omega t
\]

\[
y_t = f(x_0 + A \cos \omega t) + \epsilon_t
\]

\[
\tilde{y}_\omega = \text{push}(\tilde{y}_\omega, y_t \cos \omega t)
\]

if \( t > T \) then

\[
y_\omega^m = (\sum \tilde{y}_\omega) / T
\]

\[
x_0 = x_0 + \frac{\gamma}{T} y_\omega^m
\]

end if

end for

4. Simulation study: Performance of LiF in cases of concept drift

LiF, contrary to many other methods of finding \( x_{\text{max}} \), is feasible since the experimenter does not need to know the functional form of \( f() \). Additionally, LiF can also be used to find a maximum of a function in cases of concept drift: cases in which the location of the maximum changes over time. To illustrate this latter, we setup a simulation using the following data generating model:

\[
f(x, t) = -2((x - .0025t) - 5)^2 + \epsilon
\]

where the \((x - .0025t)\) ensures that during the data stream running from \( t = 0 \) to \( t = 10^4 = T \) the (expected) value of \( x_{\text{max}} \) moves from 5 to 30. We choose as starting values for the algorithm \( x_0 = -20, A = 1, T = 100, \gamma = .1 \) and \( \sigma^2 = 10 \). Subsequently, investigate the performance of LiF in this case of concept drift.

Figure 1 presents in the top panel \( y = f(x, t) \) for distinct values of \( t \in \{0, 1000, \ldots, 10000\} \). The concept drift is illustrated by the different locations of the parabola. Superimposed in blue is the value of \( x_0 \) as selected by LiF during the data stream. In the bottom panel the value of \( x_0 \) as a function of the length of the stream is presented. It is clear that LiF quickly finds \( x_{\text{max}} \) and follows the maximum as it moves during the stream.

Figure 1. Illustration of LiF in the case of concept drift. As the true maximum shifts (top panel) LiF is able to follow the maximum and keep \( x_0 \) close to \( x_{\text{max}} \).

5. Discussion and Future work

In this abstract we briefly presented Lock in Feedback as a method to find \( \arg \max_x f(x) \) through sequential experiments. The method is appealing since it a) does not require the functional form of \( f(x) \) to be known to find its maximum, b) performs well in situations in which measurements are obtained with large noise (not presented here), and c) allows following the maximum of a function even if that function changes over time. We have presented the basic mathematical arguments behind LiF, demonstrating how known (or imposed) oscillations in \( x \) can be used to determine the derivative(s) of \( f(x) \) which can subsequently be used to find \( \arg \max_x f(x) \). We then showed that a fully streaming implementation of LiF (Algorithm 1) is indeed robust in cases of concept drift.

References