1 Implicit Filtering

There are other methods for fitting without derivatives besides Brent's method and Parabolic Interpolation. One method that was investigated is known as the Implicit Filtering algorithm, which will only be briefly covered here[1]. The implicit filtering algorithm is designed for optimising problems where the objective function $f(\cdot)$ can only be evaluated up to an arbitary degree of accuracy, but the exact value is unavailable. The parameter h controls the degree of the desired accuarcy - the lower h, the lower the error.It is usually the case that getting a higher degree of accuaracy means a higher run time. For a Monte Carlo simulation for example, it would be reasonable to set $h = 1/\sqrt{N}$ where N is the number of samples used. If the objective function relies on numerically solving an ODE, h would be set to the step size.

Let $f(\mathbf{x}; h)$ denote the result of approximately evauluating $f(\cdot)$ at $\mathbf{x}$ with precision level h. To generate a search direction, Implicit Filtering uses a finite difference approximation to the gradient $\nabla f(\mathbf{x})$. The simplest such approximation is forward differencing, though other choices are available:

$$[\nabla_h f]_i = \frac{f(\mathbf{x} + h\mathbf{e}_i; h) - f(\mathbf{x}; h)}{h} \tag{1}$$

The approximate gradient is used to define a search direction. The algorithm proceeds to conduct a line search along this direction until a point that achieves a sufficient reduction is found [2].

If such a point cannot be found, or or the the approximate gradient is $\mathcal{O}(h)$ then the value of h is shrunk so that $h \leftarrow \delta h$ with $0 < \delta < 1$. The algorithm then proceeds again with a higher level of precision.

The algorithm terminates when the change in the value of the objective function produced by reducing the value of h and running again is within a chosen tolerance.

There are many disadvantages with Implicit Filtering compared to Brent's Method. First, it is much more complex to code, and is thus more difficult to maintain and debug[3]. Second, it's slow. Third, the results of the fitting are sensitive to the value of the shrink factor δ choosen. Fourth, it can be necessary to impose a penalty term to ensure convergence.

To test the implicit filtering method, the following quasi-linear fourth order ODE was fitted to the melanoma data[4].

$$y^{(4)} = \mu^2[1 - \sin(\pi y'')^2]y''' - \omega^2 y'' \tag{2}$$

The objective function used is a penalised sum of squared errors of the form:

$$PENSSE(f(t), \omega, \mu) = \rho \sum [y_i - f(t_i)]^2 + (1 - \rho) \int |f''(t)|^2 dt$$

The value of $PENSSE$ is influenced by ω and μ because $f(t)$ is required to be a solution of Equation 2 with given values of ω and μ. The Implicit Filtering algorithm will not converge correctly without the penalty term as illustrated in Figure 2.

To compute $PENSSE$, the package `deSolve` was used to numerically solve (2) with the appropriate values of ω and μ [25]. The precision factor h determines the stepsize used.

As can be seen in Table 1, the algorithm takes a long time to run. In addition, it can be seen in both the table and Figure 1 that changing the value of δ can introduce qualitative changes in behaviour.

[1] Interested readers are pointed towards [19, 11, 10].

[2] More precisely, the next point is required to satisfy a condition of the form $f(\mathbf{x}_{k+1}) \leq f(\mathbf{x}_k) - c\mathbf{d}_k^\top[\nabla_h f(\mathbf{x}_k)]$, where $\mathbf{d}_k = \mathbf{x}_{k+1} - \mathbf{x}_k$ and $0 < c < 1$. Note that there no requirement to decrease the norm of the approximate gradient $\nabla_h f(x)$.

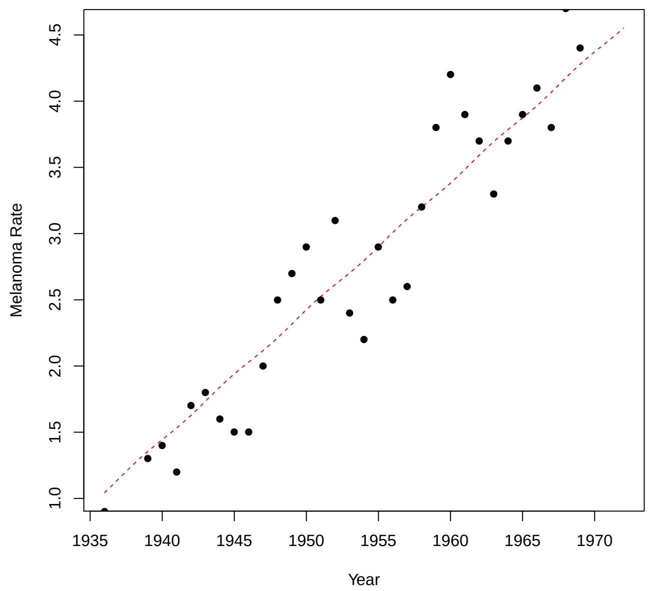
[3] The R code used to fit the ODE (2) came out at a little over 300 lines long. The code in the Data2LD package that performs optimisation is over 600 lines long. Code that uses Brent's Method tends to be much shorter.

[4] The version of Implicit Filtering used is actually a modified version of that described above. A Quasi-Newton algorithm was used instead of naive gradient descent to compute search directions, and central differences were used to estimate the gradient instead of forward differences as in (1).

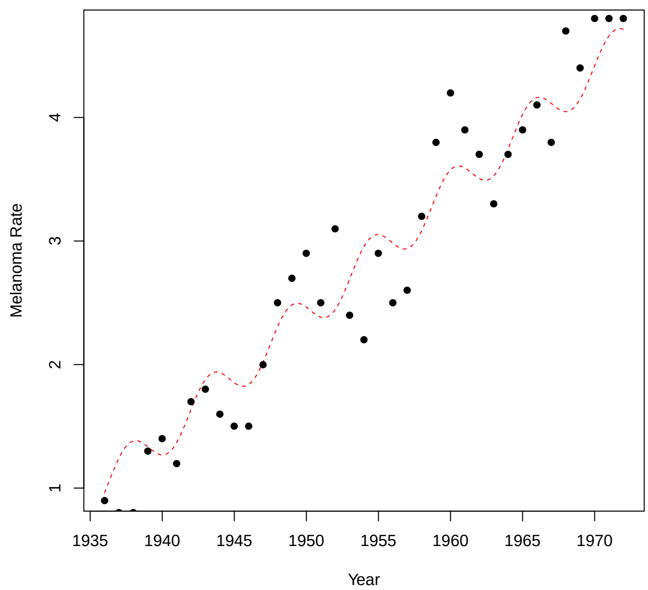
The algorithm is much quicker for $\delta = 0.9$, presumably because the algorithm is converging to a different fit than for the other cases.

δ	Running Time (Seconds)	Running Time (Minutes)
0.7	1717.807	28.63
0.8	1611.459	26.85
0.9	1013.165	16.88

Table 1: Time for Implicit Filtering to converge for various values of δ.



(a)



(b)

Figure 1: Fitting the ODE (2) to the Melanoma data. The exact value of the shrink value δ effects the fit the implicit filtering algorithm converges to. For $\delta = 0.7$, the fit in (a) resembles a straight line, but $\delta = 0.9$ results in a sinusodial plus linear trend as can be seen in (b).

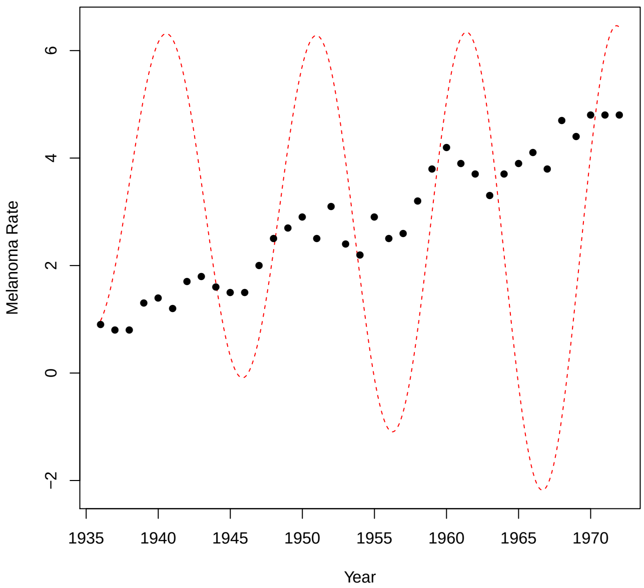


Figure 2: Without a penalty term, Implicit Filtering fails to fit the ODE (2) to the melanoma data.

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