Parameter Estimation

We have seen how mathematical models can be expressed in terms of differential equations. For example:

- Exponential growth

$$
\begin{aligned}
r'(t) &= ar(t) \quad \text{for } t > 0, && (347)\\
r(0) &= r_0. && (348)
\end{aligned}
$$

Parameter Estimation

- Logistic growth

$$
\begin{aligned}
r'(t) &= ar(t)\left(1-\frac{r(t)}{R}\right) \quad \text{for } t>0, && (349)\\
r(0) &= r_0. && (350)
\end{aligned}
$$

- Heat conduction

$$
\begin{aligned}
u_t = (ku_x)_x \quad \text{for } x\in(0,1),\, t>0, && (351)\\
u(0,t) = u(1,t) = 0 \quad \text{for } t>0, && (352)\\
u(x,0) = f(x) \quad \text{for } x\in(0,1). && (353)
\end{aligned}
$$

Parameter Estimation

In order to use such models we must somehow assign suitable values to the involved parameters;

- r_0 and a in the model for exponential growth,
- r_o, a and R in the model for logistic growth,
- and $f(x)$ and $k(x)$ in the model for heat conduction.

Exponential Growth

- We will consider the estimation of the growth rate a and the initial condition r_0 in the equations for exponential growth.
- We employ the notation

$$r(t;a,r_0) = r_0 e^{at} \tag{354}$$

Exponential Growth

- Total world population from 1950 to 1955:

$$
\begin{aligned}
1950: \; r(0;a,r_0) &= 2.555 \cdot 10^9 \\
1951: \; r(1;a,r_0) &= 2.593 \cdot 10^9 \\
1952: \; r(2;a,r_0) &= 2.635 \cdot 10^9 \\
1953: \; r(3;a,r_0) &= 2.680 \cdot 10^9 \\
1954: \; r(4;a,r_0) &= 2.728 \cdot 10^9 \\
1955: \; r(5;a,r_0) &= 2.780 \cdot 10^9
\end{aligned}
$$

Exponential Growth

$$
\begin{aligned}
r_0 &= 2.555 \cdot 10^9 && (355)\\
r_0 e^{a} &= 2.593 \cdot 10^9 && (356)\\
r_0 e^{2a} &= 2.635 \cdot 10^9 && (357)\\
r_0 e^{3a} &= 2.680 \cdot 10^9 && (358)\\
r_0 e^{4a} &= 2.728 \cdot 10^9 && (359)\\
r_0 e^{5a} &= 2.780 \cdot 10^9. && (360)
\end{aligned}
$$

- Six equations, but only two unknowns; a and r_0.

Cost-functional

Consider the function

$$\begin{aligned} J(a,r_0) &= \frac{1}{2}\sum_{t=0}^{t=5}(r(t;a,r_0)-d_t)^2 \\ &= \frac{1}{2}\sum_{t=0}^{t=5}(r_0e^{at}-d_t)^2, \end{aligned}$$

where

$$\begin{aligned} d_0 &= 2.555\cdot 10^9, \quad d_1 = 2.593\cdot 10^9, \\ d_2 &= 2.635\cdot 10^9, \quad d_3 = 2.680\cdot 10^9, \\ d_4 &= 2.728\cdot 10^9, \quad d_5 = 2.780\cdot 10^9. \end{aligned}$$

Cost-functional

- $J(a, r_0)$ is a sum of quadratic terms which measure the deviation between the output of the model and the observation data.
- If $J(a, r_0)$ is small, then equations (355)-(360) are approximately satisfied.
- We thus seek to minimize J;

$$\min_{a, r_0} J(a, r_0).$$

Cost-functional

- The first order necessary conditions for a minimum:

$$\begin{aligned} \frac{\partial J}{\partial a} &= 0 \\ \frac{\partial J}{\partial r_0} &= 0 \end{aligned}$$

Cost-functional

- A nonlinear 2×2 system of algebraic equations for a and r_0:

$$\sum_{t=0}^{t=5}(r_0e^{at} - d_t)r_0te^{at} = 0 \tag{361}$$

$$\sum_{t=0}^{t=5}(r_0e^{at} - d_t)e^{at} = 0 \tag{362}$$

Cost-functional

- Note that the standard output least squares form of the present problem is;

$$\min_{a,r_0}\left[\frac{1}{2}\sum_{t=0}^{t=5}(r(t;a,r_0)-d_t)^2\right]$$

subject to the constraints

$$r'(t) = ar(t) \quad \text{for } t > 0, \tag{363}$$

$$r(0) = r_0. \tag{364}$$

- Due to the formula (354) available for the solution of (363)-(364), it can be analyzed in the manner presented above.

A simpler problem

- Instead of seeking to compute both the growth rate a and the initial condition r_0 we might consider a somewhat simpler, but less sophisticated, approach.
- Choose

$$r_0 = 2.555 \cdot 10^9.$$

- Estimate a by defining an objective function only involving the observation data from 1951 to 1955;

$$G(a) = \frac{1}{2} \sum_{t=1}^{t=5} (2.555 \cdot 10^9 e^{at} - d_t)^2. \tag{365}$$

A simpler problem

- The necessary condition for a minimum is

$$G'(a) = 0.$$

- This leads to the equation

$$\sum_{t=1}^{t=5} (2.555 \cdot 10^9 e^{at} - d_t) 2.555 \cdot 10^9 t e^{at} = 0, \tag{366}$$

which must be solved to determine an optimal value for a.

A simpler problem

- In this case, the standard output least squares form is;

$$\min_a \left[\frac{1}{2} \sum_{t=1}^{t=5} (r(t;a) - d_t)^2 \right]$$

subject to the constraints

$$\begin{aligned} r'(t) &= ar(t) \quad \text{for } t > 0, \\ r(0) &= 2.555 \cdot 10^9. \end{aligned}$$

Backwards heat equation

- Assume that a substance in an industrial process must have a prescribed temperature distribution, say $g(x)$, at time T in the future.
- The substance must be introduced/implanted to the process at time $t = 0$. (This could typically be the case in various molding process or in steel casting).
- What should the temperature distribution $f(x)$ at time $t = 0$ be in order to assure that the temperature is $g(x)$ at time T?

Backwards heat equation

- Consider a medium with constant heat conductivity $k(x) = 1$ for all x, occupying the unit interval.
- Determine the initial condition $f = f(x)$ such that the solution $u = u(x,t;f)$ of

$$u_t = u_{xx} \quad \text{for } x \in (0,1),\, t > 0, \tag{367}$$

$$u(0,t) = u(1,t) = 0 \quad \text{for } t > 0, \tag{368}$$

$$u(x,0) = f(x) \quad \text{for } x \in (0,1), \tag{369}$$

is such that

$$u(x,T;f) = g(x) \quad \text{for all } x \in (0,1).$$

Backwards heat equation

- $g(x)$ is our observation data, and the output least squares formulation of the problem becomes;

$$\min_{f}\left[\int_0^1 (u(x,T;f)-g(x))^2\,dx\right] \tag{370}$$

subject to $u = u(x,t;f)$ satisfying (367)-(369).

Fourier Analysis

- The solution $u(x,t;f)$ of (367)-(369) can be written

$$u(x,t,f) = \sum_{k=1}^{\infty} c_k e^{-k^2\pi^2 t} \sin(k\pi x)$$

where

$$f(x) = \sum_{k=1}^{\infty} c_k \sin(k\pi x) \quad \text{for } x \in (0,1),$$

- Equation (370) can be expressed in terms of the Fourier coefficients;

$$\min_{c_1,c_2,\ldots} \left[\int_0^1 \left(\sum_{k=1}^{\infty} c_k e^{-k^2\pi^2 T} \sin(k\pi x) - g(x) \right)^2 dx \right]. \quad (371)$$

Fourier Analysis

- Next, we insert the Fourier sine expansion

$$g(x) = \sum_{k=1}^{\infty} d_k \sin(k\pi x) \quad \text{for } x \in (0,1)$$

of g into (371) and obtain the following form of our problem

$$\min_{c_1,c_2,\ldots} \left[\int_0^1 \left(\sum_{k=1}^{\infty} c_k e^{-k^2\pi^2 T} \sin(k\pi x) - \sum_{k=1}^{\infty} d_k \sin(k\pi x) \right)^2 dx \right]. \tag{372}$$

Fourier Analysis

$$\left[\int_0^1 \left(\sum_{k=1}^{\infty} c_k e^{-k^2\pi^2 T}\sin(k\pi x) - \sum_{k=1}^{\infty} d_k \sin(k\pi x)\right)^2 dx\right] \geq 0$$

for all choices of $c_1, c_2, \ldots$.
We can solve (372) by determining $c_1, c_2, \ldots$ such that

$$c_k e^{-k^2\pi^2 T}\sin(k\pi x) = d_k \sin(k\pi x) \quad \text{for } k = 1, 2, \ldots,$$

which is satisfied if

$$c_k = e^{k^2\pi^2 T} d_k \quad \text{for } k = 1, 2, \ldots.$$

Fourier Analysis

- The solution $f(x)$ of (370) is

$$f(x) = \sum_{k=1}^{\infty} e^{k^2\pi^2 T} d_k \sin(k\pi x) \quad \text{for } x \in (0,1),$$

where

$$g(x) = \sum_{k=1}^{\infty} d_k \sin(k\pi x) \quad \text{for } x \in (0,1).$$

Stability

- From a mathematical point of view, one might argue that the backwards heat equation is a simple problem since an analytical solution is obtainable.
- On the other hand, the problem itself has an undesirable property.
- The heat distribution $f(x)$ at time $t = 0$ is determined by multiplying the Fourier coefficients of $g(x)$ by factors on the form $e^{k^2\pi^2 T}$.

Stability

- These factors are very large, even for moderate k, e.g. with $T = 1$;

$$e^{\pi^2} \approx 1.93 \cdot 10^4,$$
$$e^{2^2\pi^2} \approx 1.40 \cdot 10^{17},$$
$$e^{3^2\pi^2} \approx 3.77 \cdot 10^{38}.$$

- If $T = 1$ and $g(x) = \sin(3\pi x)$, then the solution of the backwards heat equation is

$$f(x) = e^{3^2\pi^2} \sin(3\pi x) \approx 3.77 \cdot 10^{38} \sin(3\pi x).$$

Stability

- If a very small amount of noise is added to g, say

$$\widehat{g}(x) = g(x) + 10^{-20}\sin(3\pi x) = (1 + 10^{-20})\sin(3\pi x),$$

then the corresponding solution $\hat{f}$ of (370) changes dramatically, i.e.

$$\widehat{f}(x) = (1+10^{-20})e^{3^2\pi^2}\sin(3\pi x) \approx f(x) + 3.77\cdot 10^{18}\sin(3\pi x).$$

Stability

- The problem is extremely unstable; very small changes in the observation data g can cause huge changes in the solution f of the problem:

$$\widehat{g}(x) - g(x) = 10^{-20}\sin(3\pi x)$$

$$\widehat{f}(x) - f(x) = 3.77 \cdot 10^{18}\sin(3\pi x)$$

Stability

- One can argue that it is almost impossible to estimate the temperature distribution backwards in time, only using the present temperature and the heat equation.
- Further information is needed.
- This has lead mathematicians to develop various techniques for incorporating a priori data, for example that $f(x)$ should be almost constant.
- More precisely, a number of methods for approximating unstable problems with stable equations have been proposed, commonly referred to as *regularization techniques*.

Stability

- Do the mathematical considerations presented above agree with our practical experiences with heat conduction?
- Is it possible to track the temperature distribution backwards in time in the room you are sitting?
- What kind of information do you need to do so?

Estimating the heat conductivity

- The examples discussed above are rather simple since explicit formulas for the solutions of the involved differential equations are known.
- This is not always the case, and we will now briefly consider such a problem.
- Assume that one wants to use surface measurements of the temperature to compute a possibly non-constant heat conductivity $k = k(x)$ inside a medium.

Estimating the heat conductivity

- With our notation, the output least squares formulation of this task is;

$$\min_k \left[\int_0^T (u(0,t;k) - h_1(t))^2 \, dt + \int_0^T (u(1,t;k) - h_2(t))^2 \, dt \right]$$

subject to $u = u(x,t;k)$ satisfying

$$\begin{aligned}
u_t &= (ku_x)_x \quad \text{for } x \in (0,1),\ t > 0,\\
k(0)u_x(0,t) &= 0 \quad \text{for } t > 0,\\
k(1)u_x(1,t) &= 0 \quad \text{for } t > 0,\\
u(x,0) &= f(x) \quad \text{for } x \in (0,1).
\end{aligned}$$

Estimating the heat conductivity

- This is a very difficult problem.
- To solve it, a number of mathematical and computational techniques developed throughout the last decades must be employed.
- This exceeds the ambitions of the present text, but we encourage the reader to carefully evaluate their understanding of the output least squares method by formulating such an approach for a problem involving, e.g., a system of ordinary differential equations.