The Polynomial Option

(Thoughts on Homework 12)

1 Background

As presented in the problem formulation, groundwater mechanics dictates that the leakage, $\gamma(x)$, is a smooth, continuous function. The heads in both aquifers, at both ends, equal the heads in the rivers. The difference in heads between the aquifers, at both ends, equal zero. Therefore, the leakage, at both ends, equal zero.

$$\gamma(0) = 0 \tag{1}$$
$$\gamma(w) = 0 \tag{2}$$

The sought after function, $\Gamma(x)$, is defined by

$$\gamma(x) = \frac{d^2\Gamma}{dx^2} \tag{3}$$

for $0 \leqslant x \leqslant w$. Since the second derivative of $\Gamma(x)$ is a smooth, continuous function, $\Gamma(x)$ must be a smooth, continuous function. We also know that, by definition, $\Gamma(x)$ is equal to zero at both ends.

$$\Gamma(0) = 0 \tag{4}$$
$$\Gamma(w) = 0 \tag{5}$$

Our goal in this note is to find a general representation for $\Gamma(x)$, and $\gamma(x)$, that satisfies all five of these conditions: (1) through (5).

2 Change of variables

To diminish anticipated numerical problems we introduce a dimensionless location variable, denoted χ.

$$\chi = \frac{x}{w} \tag{6}$$

We repose Γ and γ as functions of χ, and rewrite the boundary conditions as

$$\gamma(0) = 0 \tag{7}$$
$$\gamma(1) = 0 \tag{8}$$
$$\Gamma(0) = 0 \tag{9}$$
$$\Gamma(1) = 0 \tag{10}$$

Applying the chain rule of differentiation to evaluate (3) yields

$$\frac{d\Gamma}{dx} = \frac{d\Gamma}{d\chi}\frac{d\chi}{dx} = \frac{1}{w}\frac{d\Gamma}{d\chi} \tag{11}$$

Differentiating (11), again using the chain rule, yields

$$\frac{d^2\Gamma}{d\chi^2} = \frac{1}{w}\frac{d^2\Gamma}{d\chi^2}\frac{d\chi}{dx} = \frac{1}{w^2}\frac{d^2\Gamma}{d\chi^2} \tag{12}$$

Substituting (12) into (3) yields

$$\gamma(\chi) = \frac{1}{w^2}\frac{d^2\Gamma}{d\chi^2} \tag{13}$$

3 Andrew's proposal

In class last week, Andrew made a modest proposal[1]. Andrew recommended that we represent $\Gamma(\chi)$ as a polynomial. A polynomial is continuous, infinitely differentiable (i.e. very smooth), easy to manipulate, and efficient to compute. Furthermore, the theory of *Taylor series expansions*[2] suggests that we can get arbitrarily close to the true answer by selecting a sufficiently high-degree polynomial.

4 Representing $\Gamma(\chi)$

4.1 Initial representation

We consider a general polynomial of the form[3]:

$$\Gamma(\chi) = \sum_{n=0}^{\infty} a_n \chi^n \tag{14}$$

The conditions imposed by (9) and (10) will restrict the coefficients.

4.2 Left-hand boundary

Evaluating $\Gamma(0)$ we find

$$\begin{aligned}
\Gamma(0) &= \left[\sum_{n=0}^{\infty} a_n \chi^n\right]_{\chi=0} && (15)\\
&= \left[\sum_{n=0}^{\infty} a_n (0)^n\right] && (16)\\
&= \left[a_0 + a_1(0)^1 + a_2(0)^2 + \ldots\right] && (17)\\
&= a_0 && (18)
\end{aligned}$$

Thus, condition (9) requires

$$a_0 = 0 \tag{19}$$

In light of (19) we rewrite (14) as

$$\Gamma(\chi) = \sum_{n=1}^{\infty} a_n \chi^n \tag{20}$$

[1] This is not to be confused with Jonathan Swift's famous 1729 satirical essay *A Modest Proposal*. See, for example, `http://en.wikipedia.org/wiki/A_Modest_Proposal`.

[2] See, for example, `http://en.wikipedia.org/wiki/Taylor_series`.

[3] The representation given in (14) has an infinite number of terms, which seems a bit excessive for our modest purposes. However, the use of an infinite upper bound on the summation allows us to put off the selection of the polynomial degree to a later time. Note, by setting $c_n = 0$ for all $n > N$, (14) is an appropriate representation even for a polynomial of finite degree.

4.3 Right-hand boundary

Evaluating $\Gamma(1)$ we find

$$\Gamma(1) = \left[\sum_{n=1}^{\infty} a_n \chi^n\right]_{\chi=1} \tag{21}$$

$$= \left[\sum_{n=1}^{\infty} a_n (1)^n\right] \tag{22}$$

$$= \left[a_1(1)^1 + a_2(1)^2 + a_3(1)^3 + \ldots\right] \tag{23}$$

$$= [a_1 + a_2 + a_3 + \ldots] \tag{24}$$

$$= \sum_{n=1}^{\infty} a_n \tag{25}$$

Thus, condition (10) requires

$$\sum_{n=1}^{\infty} a_n = 0 \tag{26}$$

An alternative representation for (26) is

$$a_1 = -\sum_{n=2}^{\infty} a_n \tag{27}$$

Substituting (27) into (20) yields

$$\Gamma(\chi) = \sum_{n=1}^{\infty} a_n \chi^n \tag{28}$$

$$= a_1\chi + \sum_{n=2}^{\infty} a_n \chi^n \tag{29}$$

$$= \left(-\sum_{n=2}^{\infty} a_n\right)\chi + \sum_{n=2}^{\infty} a_n \chi^n \tag{30}$$

$$= \sum_{n=2}^{\infty} a_n \chi^n - \sum_{n=2}^{\infty} a_n \chi \tag{31}$$

$$= \sum_{n=2}^{\infty} a_n \left(\chi^n - \chi\right) \tag{32}$$

4.4 New representation

This new representation of $\Gamma(\chi)$ is guaranteed to satisfy both (9) and (10) for any values of the coefficients.

$$\Gamma(\chi) = \sum_{n=2}^{\infty} a_n \left(\chi^n - \chi\right) \tag{33}$$

5 Representing $\gamma(\chi)$

5.1 Initial representation

Differentiating (33) with respect to χ yields[4]

$$\frac{d\Gamma}{d\chi} = \sum_{n=2}^{\infty} a_n \left(n\chi^{n-1} - 1\right) \tag{34}$$

Differentiating (34) with respect to χ yields

$$\frac{d^2\Gamma}{d\chi^2} = \sum_{n=2}^{\infty} a_n(n-1)(n)\chi^{n-2} \tag{35}$$

Reorganizing the summation, we rewrite (35) as

$$\frac{d^2\Gamma}{d\chi^2} = \sum_{n=0}^{\infty} a_{n+2}(n+1)(n+2)\chi^{n} \tag{36}$$

Substituting (36) into (13) yields

$$\gamma(\chi) = \frac{1}{w^2}\sum_{n=0}^{\infty} b_n\chi^n \tag{37}$$

where

$$b_n = (n+1)(n+2)a_{n+2} \tag{38}$$

The conditions imposed by (7) and (8) will further restrict the coefficients.

5.2 Left-hand boundary

Evaluating $\gamma(0)$ we find

$$\begin{aligned}
\gamma(0) &= \left[\sum_{n=0}^{\infty} b_n\chi^n\right]_{\chi=0} && (39)\\
&= \left[\sum_{n=0}^{\infty} b_n(0)^n\right] && (40)\\
&= \left[b_0 + b_1(0)^1 + b_2(0)^2 + \ldots\right] && (41)\\
&= b_0 && (42)
\end{aligned}$$

Thus, condition (7) requires

$$b_0 = 0 \tag{43}$$

In light of (43) we rewrite (37) as

$$\gamma(\chi) = \frac{1}{w^2}\sum_{n=1}^{\infty} b_n\chi^n \tag{44}$$

[4]See Appendix A for a tutorial on differentiating power series using summation notation.

5.3 Right-hand boundary

Evaluating $\gamma(1)$ we find

$$\gamma(1) = \left[\sum_{n=1}^{\infty} b_n \chi^n\right]_{\chi=1} \tag{45}$$

$$= \left[\sum_{n=1}^{\infty} b_n (1)^n\right] \tag{46}$$

$$= \left[b_1(1)^1 + b_2(1)^2 + b_3(1)^3 + \ldots\right] \tag{47}$$

$$= [b_1 + b_2 + b_3 + \ldots] \tag{48}$$

$$= \sum_{n=1}^{\infty} b_n \tag{49}$$

Thus, condition (10) requires

$$\sum_{n=1}^{\infty} b_n = 0 \tag{50}$$

An alternative representation for (50) is

$$b_1 = -\sum_{n=2}^{\infty} b_n \tag{51}$$

Substituting (51) into (44) yields

$$w^2\gamma(\chi) = \sum_{n=1}^{\infty} b_n \chi^n \tag{52}$$

$$= b_1\chi + \sum_{n=2}^{\infty} b_n \chi^n \tag{53}$$

$$= \left(-\sum_{n=2}^{\infty} b_n\right)\chi + \sum_{n=2}^{\infty} b_n \chi^n \tag{54}$$

$$= \sum_{n=2}^{\infty} b_n \chi^n - \sum_{n=2}^{\infty} b_n \chi \tag{55}$$

$$= \sum_{n=2}^{\infty} b_n \left(\chi^n - \chi\right) \tag{56}$$

5.4 New representation

This new representation of $\gamma(\chi)$ is guaranteed to satisfy both (7) and (8) for any values of the coefficients.

$$\gamma(\chi) = \frac{1}{w^2} \sum_{n=2}^{\infty} b_n \left(\chi^n - \chi\right) \tag{57}$$

6 Re-representing $\Gamma(\chi)$ and $\gamma(\chi)$

6.1 Further simplification

Substituting (38) into (43) yields

$$b_0 = (1)(2)a_2 = 0 \tag{58}$$

Or more simply,

$$a_2 = 0 \tag{59}$$

Incorporating (59) into (57) yields a newer representation:

$$\Gamma(\chi) = \sum_{n=3}^{\infty} a_n \left(\chi^n - \chi\right) \tag{60}$$

Using this representation, a_0, a_1, and a_2 are of no consequence. Only coefficients a_n for $n \geqslant 3$ matter.

6.2 A less obvious step

Substituting (38) into (50) yields

$$\sum_{n=1}^{\infty} (n+1)(n+2)a_{n+2} = 0 \tag{61}$$

or equivalently

$$\sum_{n=3}^{\infty} (n-1)(n)a_n = 0 \tag{62}$$

We pull the a_3 term out of the sum in (62) and write

$$(3-1)(3)a_3 + \sum_{n=4}^{\infty} (n-1)(n)a_n = 0 \tag{63}$$

Solving (63) for a_3 we find

$$a_3 = -\sum_{n=4}^{\infty} \frac{(n-1)(n)}{6} a_n \tag{64}$$

6.3 Final $\Gamma(\chi)$ representations

We substitute (64) into (60) and reorganize the resulting expression as follows.

$$\Gamma(\chi) = \sum_{n=3}^{\infty} a_n \left(\chi^n - \chi\right) \tag{65}$$

$$= a_3 \left(\chi^3 - \chi\right) + \sum_{n=4}^{\infty} a_n \left(\chi^n - \chi\right) \tag{66}$$

$$= \left(-\sum_{n=4}^{\infty} \frac{(n-1)(n)}{6} a_n\right) \left(\chi^3 - \chi\right) + \sum_{n=4}^{\infty} a_n \left(\chi^n - \chi\right) \tag{67}$$

$$= \sum_{n=4}^{\infty} a_n \left(\chi^n - \chi\right) - \sum_{n=4}^{\infty} a_n \frac{(n-1)(n)}{6} \left(\chi^3 - \chi\right) \tag{68}$$

$$= \sum_{n=4}^{\infty} a_n \left[\left(\chi^n - \chi\right) - \frac{(n-1)(n)}{6} \left(\chi^3 - \chi\right)\right] \tag{69}$$

Using this representation, a_0, a_1, a_2, and a_3 are of no consequence. Only coefficients a_n for $n \geqslant 4$ matter. Furthermore, since

$$\left(\chi^n - \chi\right) = \left(\chi^3 - \chi\right) = 0 \tag{70}$$

for $\chi = 0$ and $\chi = 1$, conditions (9) and (10) are satisfied by this representation for any set of coefficients $\{a_4, a_5, a_6, \ldots\}$.

6.4 And $\gamma(\chi)$ too

Differentiating (69) with respect to χ yields

$$\frac{d\Gamma}{d\chi} = \sum_{n=4}^{\infty} a_n \left[\left(n\chi^{n-1} - 1\right) - \frac{(n-1)(n)}{6} \left(3\chi^2 - 1\right)\right] \tag{71}$$

Differentiating (71) with respect to χ yields

$$\frac{d^2\Gamma}{d\chi^2} = \sum_{n=4}^{\infty} a_n \left[\left((n-1)(n)\chi^{n-2}\right) - \frac{(n-1)(n)}{6} (6\chi)\right] \tag{72}$$

$$= \sum_{n=4}^{\infty} a_n \left[(n-1)(n) \left(\chi^{n-2} - \chi\right)\right] \tag{73}$$

Substituting (73) into (13) yields

$$\gamma(\chi) = \frac{1}{w^2} \sum_{n=4}^{\infty} a_n \left[(n-1)(n) \left(\chi^{n-2} - \chi\right)\right] \tag{74}$$

By visual inspection, we see that the representation offered by (74) satisfies conditions (7) and (8) for any set of coefficients $\{a_4, a_5, a_6, \ldots\}$.

7 Summary

For any set of coefficients $\{a_4, a_5, a_6, \ldots\}$,

$$\boxed{\Gamma(\chi) = \sum_{n=4}^{\infty} a_n \left[(\chi^n - \chi) - \frac{(n-1)(n)}{6} \left(\chi^3 - \chi \right) \right]} \tag{75}$$

$$\boxed{\gamma(\chi) = \frac{1}{w^2} \sum_{n=4}^{\infty} a_n \left[(n-1)(n) \left(\chi^{n-2} - \chi \right) \right]} \tag{76}$$

satisfy the required conditions.

8 Computational considerations

8.1 Control points

We consider a specific set of M evenly-spaced locations along the aquitard, $\{x_1, x_2, \ldots, x_M\}$, where

$$x_m = \frac{mw}{M+1} \tag{77}$$

for $m = 1, 2, \ldots, M$. We will call these the *control points*.

The associated dimensionless control points are then given by the remarkably simple form

$$\chi_m = \frac{x_m}{w} = \frac{mw}{w(M+1)} = \frac{m}{M+1} \tag{78}$$

8.2 Evaluation at the control points

Create a $(M \times N)$ matrix $\mathbf{G}$ such that

$$G(m, j) = \left(\chi_m^{j+3} - \chi_m \right) - \frac{(j+2)(j+3)}{6} \left(\chi_m^3 - \chi_m \right) \tag{79}$$

for $m = 1, 2, \ldots, M$ and $j = 1, 2, \ldots, N$.

Similarly, create a $(M \times N)$ matrix $\mathbf{g}$ such that

$$g(m, j) = (j+2)(j+3) \left(\chi_m^{j+1} - \chi_m \right) \tag{80}$$

for $m = 1, 2, \ldots, M$ and $j = 1, 2, \ldots, N$.

Create a $(N \times 1)$ parameter matrix $\mathbf{a}$ where

$$\mathbf{a} = \begin{bmatrix} a_4 \\ a_5 \\ \vdots \\ a_{N+3} \end{bmatrix} \tag{81}$$

We are, essentially, setting a_n for $n \geqslant N+4$ equal to zero.

Compute the simple matrix product

$$\mathbf{H} = \mathbf{G}\mathbf{a} \tag{82}$$

The resulting $(M \times 1)$ matrix $\mathbf{H}$ will have terms

$$H(m) = \Gamma(\chi_m) = \sum_{n=4}^{N+3} a_n \left[(\chi_m^n - \chi_m) - \frac{(n-1)(n)}{6} \left(\chi_m^3 - \chi_m \right) \right] \tag{83}$$

Similarly, compute the simple matrix product

$$\mathbf{h} = \frac{1}{w^2}\,\mathbf{g}\mathbf{a} \tag{84}$$

The resulting $(M \times 1)$ matrix $\mathbf{h}$ will have terms

$$h(m) = \gamma(\chi_m) = \frac{1}{w^2} \sum_{n=4}^{N+3} a_n \left[(n-1)(n) \left(\chi_m^{n-2} - \chi_m \right) \right] \tag{85}$$

The **BIG** computational advantage of this matrix formulation is that matrix $\mathbf{G}$ and matrix $\mathbf{g}$ need only be computed once. Given the number of control points M and the number of non-zero coefficients N, $\mathbf{G}$ and $\mathbf{g}$ are fully defined – fixed. Thus, even as the coefficients change (e.g. from iteration to iteration), only two matrix multiplications are required to reevaluate Γ and γ at all of the control points.

A Differentiation of a power series

Differentiation of a power series represented using summation notation is a learned skill. The manipulation of the symbols is compact, but confusing to the neophyte.

Consider a general power series

$$f(x) = \sum_{n=0}^{\infty} a_n x^n \tag{86}$$

Expanding the right-hand-side of (86) using ellipsis notation instead of summation notation yields

$$f(x) = a_0 x^0 + a_1 x^1 + a_2 x^2 + a_3 x^3 + \ldots \tag{87}$$

In this form, the derivative of $f(x)$ with respect to x follows from our standard rules for differentiation learned in Calculus I.

$$\frac{df}{dx} = 0 + 1a_1 x^0 + 2a_2 x^1 + 3a_3 x^2 + \ldots \tag{88}$$

Note that the a_0 term disappears, since the derivative of a constant, $a_0 x^0$, is zero.

Translating (88) back into summation notation we have

$$\frac{df}{dx} = \sum_{n=1}^{\infty} n a_n x^{n-1} \tag{89}$$

The representation given by (89) is a recognizable form: the original power of x comes down as a multiplier, and then the power is decreased by one. The disappearance of the a_0 term is reflected in the change of the lower limit of the summation from $n = 0$ in (86) to $n = 1$ in (89).

An equally valid re-representation of (88) using summation notation is

$$\frac{df}{dx} = \sum_{n=0}^{\infty} (n+1) a_{n+1} x^{n} \tag{90}$$

This form has the advantage of looking like (86), just with new coefficients. That is,

$$\frac{df}{dx} = \sum_{n=0}^{\infty} b_n x^{n} \tag{91}$$

where

$$b_n = (n+1) a_{n+1} \tag{92}$$

for all $n = 0, 1, 2, \ldots$.

The representation given by (90) is not obvious to most engineering students on the first exposure. The comforting recognizable form in (89) is hidden in (90).

There are two ways to arrive at (90). First, stare at (88) until the pattern emerges, and then write it down. This is my favorite approach, but it is difficult to teach and is error prone. Sometimes the pattern is hard to see, and often the pattern is incorrectly identified. The second approach is more formal. We start with (89) and apply the change of variables $m = n - 1$, which is the same as $n = m + 1$.

$$\frac{df}{dx} = \sum_{n=1}^{\infty} n a_n x^{n-1} \tag{93}$$

Substituting $m + 1$ in for each occurance of n, we find

$$= \sum_{m+1=1}^{\infty} (m+1) a_{m+1} x^{m+1-1} \tag{94}$$

$$= \sum_{m=0}^{\infty} (m+1) a_{m+1} x^{m} \tag{95}$$

In (95) it does not matter what we call the summation variable, so we may as well use n instead of m and write

$$\frac{df}{dx} = \sum_{n=0}^{\infty} (n+1) a_{n+1} x^{n} \tag{96}$$

which is the same as (90)