Inferring Local Flow Directions using the Conic Discharge Potential Model

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1   INTRODUCTION

Determining the likely groundwater flow direction from water level data is a common practical problem. Since the advent of the personal computer, this problem domain has been well trodden (e.g. Kelly and Bogardi, 1989). "Two points determine a line," and "three points determine a plane" are common mantras in introductory geometry. Given a plane, we have a dip and dip direction: a lesson from structural geology. Pinder et al. (1981) furnishes the details of the *three-point problem* for computing the hydraulic head gradient based on these principles. Introductory hydrogeology classes commonly include a method to determine the hydraulic head gradient from three head measurements (e.g. Fetter, 1994, Section 4.12).

The purely geometric perspective embraced by most authors ignores the inherent uncertainty in all head measurements. Piezometric data are subject to many sources of perturbations, deviations, and outright errors; for example, uncertain collar locations, imprecise collar elevations, error-prone depth measurements, fluctuating pumping influences, unquantified seasonal effects, climatic variations, and changing usage of groundwater resources. This list is not exhaustive. We propose that head measurements must be understood as stochastic quantities. Furthermore, errors and fluctuations in the head measurements will have significant impacts on the inferred flow directions (e.g. Devlin and McElwee, 2007).

The approach outlined in this paper (project name: *Akeyaa*) uses the $O_n e_{ka}$-type conic discharge potential model[1] to infer local flow directions from noisy head measurements. The statistical inference provides a probability distribution for local flow directions. As will be shown, we can infer flow directions without knowing the base elevation, the aquifer thickness, or the hydraulic conductivity. All we need is lots of data.

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[1]See Appendix A.

2 OUR MODEL

2.1 Coordinates and Notation

We introduce a Cartesian coordinate system (x, y, z), where x [m] and y [m] are the horizontal coordinates and z [m] is the vertical coordinate. The origin of the coordinate system is arbitrary.

2.2 Aquifer Model

Our aquifer model embraces the following simplifications:

- a single layer,
- fully confined,
- homogeneous,
- horizontally isotropic,
- on a flat-lying base.

The base elevation, z_b [m], aquifer thickness, H [m], horizontal hydraulic conductivity, k [m/d], and vertical hydraulic conductivity, k_v [m/d], characterize such an aquifer for our purposes.

2.3 Discharge and Discharge Potential

We denote the piezometric head in the aquifer by $\phi(x, y, z)$ [m], and the two horizontal components of the specific discharge vector by $q_x(x, y, z)$ [m/d] and $q_y(x, y, z)$ [m/d].

We define the components of the discharge vector, $Q_x(x, y)$ [m²/d] and $Q_y(x, y)$ [m²/d], as the vertically integrated specific discharge.

$$Q_x(x, y) = \int_{z_b}^{z_b+H} q_x(x, y, z)\,dz \qquad\qquad Q_y(x, y) = \int_{z_b}^{z_b+H} q_y(x, y, z)\,dz \qquad (1)$$

Following Bear (1979, p. 77-78) and Strack et al. (2006), we integrate (1) using Leibnitz's rule, apply Darcy's law, and obtain the following expressions:

$$Q_x(x, y) = -\frac{\partial \Phi}{\partial x} \qquad\qquad Q_y(x, y) = -\frac{\partial \Phi}{\partial y} \qquad (2)$$

where the discharge potential, $\Phi(x, y)$ [m³/d], is given by

$$\Phi(x, y) = kH\bar{\phi}(x, y) \qquad (3)$$

with the vertically averaged piezometric head, $\bar{\phi}(x, y)$ [m], defined by

$$\bar{\phi}(x, y) = \frac{1}{H} \int_{z_b}^{z_b+H} \phi(x, y, z)\,dz \qquad (4)$$

We observe, following Youngs (1966), that (3) is a valid discharge potential even when the hydraulic conductivity is vertically anisotropic.

2.4 Regional Flow Model

The O_ne_ka-type regional flow model captures two features: regional uniform recharge, and regional uniform flow. The result form for the discharge potential is a second-order polynomial in x and y:

$$\Phi(x, y) = Ax^2 + By^2 + Cxy + Dx + Ey + F \tag{5}$$

where A, B, C, D, E, and F are model parameters[2]. All conic sections can be represented by the general form of (5), thus the name "conic discharge potential".

The components of the associated discharge vector, (Q_x, Q_y) $[m^2/d]$, are

$$-Q_x(x, y) = \frac{\partial \Phi}{\partial x} = 2Ax + Cy + D \tag{6}$$

$$-Q_y(x, y) = \frac{\partial \Phi}{\partial y} = 2By + Cx + E \tag{7}$$

The resulting flow direction[3], $\alpha(x, y)$ $[rad]$, is computed using the standard four quadrant arctangent[4] function as

$$\alpha(x, y) = \text{atan2}\left(-Q_y(x, y), -Q_x(x, y)\right)$$

$$= \text{atan2}\left((2By + Cx + E), (2Ax + Cy + D)\right) \tag{8}$$

3 MEASUREMENTS AND NOISE

We consider a set of N observed piezometric heads:

$$\left\{ (x_1, y_1, \hat{\phi}_1), (x_2, y_2, \hat{\phi}_N), \dots, (x_N, y_N, \hat{\phi}_N) \right\} \tag{9}$$

where $\hat{\phi}_n$ denotes the measured head at location (x_n, y_n), for $n = 1, 2, \dots, N$.

Head measurements contain errors and deviations. We model the relationship between the measured head at location (x_n, y_n) and the vertically averaged head at the same location using

$$\hat{\phi}_n = \bar{\phi}(x_n, y_n) + \epsilon_n \tag{10}$$

for $n = 1, 2, \dots, N$, where ϵ_n $[n]$ denotes the net error and deviation (noise) associated with the n'th head measurement.

The sources of the errors and deviations of head measurements are legion. Typically, these sources are well-modeled as statistically independent and additive. As such we will embrace the promise of the *Central Limit Theorem*[5] and model the ϵ_n as independent, Normal random variables, with 0 mean and standard deviation σ_n,

$$\epsilon_n \Rightarrow \text{Normal}(0, \sigma_n) \tag{11}$$

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[2]See Appendix A for more details.

[3]In this note we define the "flow direction" as the direction from which the flow originates. This is consistent with the usage of the term in atmospheric physics and meteorology; e.g. a "north wind" blows from the north toward the south. This definition is useful in well-head protection because it helps identify the source areas.

[4]See, for example, Wikipedia contributors (2020a).

[5]See, for example, Wikipedia contributors (2020b).

for $n = 1, 2, \ldots, N$.

The measurement standard deviations are known based upon physical characteristics of the wells and the measurements. Note, we are assuming that the measurements are unbiased, but we are not assuming that they are homoscedastic. For example, older measurements may have larger standard deviations than newer measurements.

4   FITTING THE MODEL

4.1   Matching the Measured Heads

The conic discharge potential model has six free parameters, A through F. Values for these parameters are inferred using an inverse modelling approach: we select the parameters to best fit the measured piezometric heads.

We can divide (3) by kH, solve for $\bar{\phi}(x, y)$, and substitute the result into (10). These steps yield

$$\hat{\phi}_n = \frac{\Phi(x_n, y_n)}{kH} + \epsilon_n \tag{12}$$

Substituting (5) into (12) we arrive at

$$\hat{\phi}_n = ax_n^2 + by_n^2 + cx_ny_n + dx_n + ey_n + f + \epsilon_n \tag{13}$$

for $n = 1, 2, \ldots, N$, where $a = \frac{A}{kH}$, $b = \frac{B}{kH}$, ..., and $f = \frac{F}{kH}$.

4.2   Matrix Representation

For notational convenience, we introduce the following matrices.

$$\mathbf{X} = \begin{bmatrix} x_1^2 & y_1^2 & x_1y_1 & x_1 & y_1 & 1 \\ x_2^2 & y_2^2 & x_2y_2 & x_2 & y_2 & 1 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ x_N^2 & y_N^2 & x_Ny_N & x_N & y_N & 1 \end{bmatrix} \quad \mathbf{p} = \begin{bmatrix} a \\ b \\ \vdots \\ f \end{bmatrix} \quad \mathbf{z} = \begin{bmatrix} \hat{\phi}_1 \\ \hat{\phi}_2 \\ \vdots \\ \hat{\phi}_N \end{bmatrix} \quad \mathbf{e} = \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \vdots \\ \epsilon_N \end{bmatrix} \tag{14}$$

Using this notation, we can write (13) in the following compact form.

$$\mathbf{z} = \mathbf{X}\mathbf{p} + \mathbf{e} \tag{15}$$

4.3   Mathematical Program

The *best, linear, unbiased estimator* for the parameters $\mathbf{p}$ is given by the solution of a weighted least squares optimization problem (e.g. Ryan, 1997, Chapter 3):

$$E(\mathbf{p}) = \left(\mathbf{X}^\mathsf{T}\mathbf{V}^{-1}\mathbf{X}\right)^{-1}\mathbf{X}^\mathsf{T}\mathbf{V}^{-1}\mathbf{z} \tag{16}$$

where

$$\mathbf{V} = \begin{bmatrix} \sigma_1^2 & 0 & 0 & \ldots & 0 \\ 0 & \sigma_2^2 & 0 & \ldots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \ldots & \sigma_N^2 \end{bmatrix} \tag{17}$$

Furthermore, the covariance matrix of the fitted parameters is

$$Var(\mathbf{p}) = \left(\mathbf{X}^\mathsf{T}\mathbf{V}^{-1}\mathbf{X}\right)^{-1} \tag{18}$$

Equations (16) and (17) assume that $\left(\mathbf{X}^\mathsf{T}\mathbf{V}^{-1}\mathbf{X}\right)^{-1}$ exists. This is true if $\sigma_n^2 > 0$ for $n = 1, 2, \ldots, N$, and $\mathbf{X}$ has full column rank. This last condition means that we must have at least six unique locations for our measured heads, and that these locations cannot all fall on an ellipse.

4.4   Scaling and Such

In real-world settings our observation locations can be separated by thousands, or even tens of thousands, of meters. As such, the columns of $\mathbf{X}$ span many orders of magnitudes. The condition number of $\mathbf{X}^\mathsf{T}\mathbf{V}^{-1}\mathbf{X}$ is typically on the order of 10^{26}. This can be numerically disconcerting. To counter this concern, we are going to employ a simple *column scaling* strategy[6].

We define the (6×6) diagonal scaling matrix $\mathbf{S}$ by

$$S_{jj} = \frac{1}{\max\limits_{\forall i} |X_{ij}|} \tag{19}$$

for $j = 1, 2, \ldots, 6$. Note that $\mathbf{S}$ is invertible.

We define the $(N \times N)$ diagonal weighting matrix $\mathbf{W}$ by

$$W_{ii} = \frac{1}{\sigma_i^2} \tag{20}$$

for $i = 1, 2, \ldots, N$. We note that $\mathbf{W} = \mathbf{V}^{-1}$, but we do not need to compute the inverse of $\mathbf{V}$ using an inversion algorithm. We simply do the needed computations term-by-term.

We define the $(N \times 6)$ matrix $\mathbf{Y}$ by

$$\mathbf{Y} = \mathbf{X}\mathbf{S} \tag{21}$$

We define the (6×6) matrix $\mathbf{A}$ by

$$\mathbf{A} = \mathbf{Y}^\mathsf{T}\mathbf{W}\mathbf{Y} \tag{22}$$

The condition number of $\mathbf{A}$ will be on the order of 10.

We substitute $\mathbf{X} = \mathbf{Y}\mathbf{S}^{-1}$, $\mathbf{A}$, and $\mathbf{W}$ into (16) and (18), we rearrange the results, and we arrive at the following scaled version of our equations.

$$\boxed{E(\mathbf{p}) = \mathbf{S}\mathbf{A}^{-1}\mathbf{Y}^\mathsf{T}\mathbf{W}\mathbf{z}} \tag{23}$$

$$\boxed{Var(\mathbf{p}) = \mathbf{S}\mathbf{A}^{-1}\mathbf{S}} \tag{24}$$

Furthermore, since $\mathbf{p}$ is a linear combination of normal random variables, $\mathbf{p}$ follows a multivariate normal distribution.

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[6]Row and column scaling do not always improve the quality of a solution. See for example, Golub and Loan (1996, Section 3.5.2) and Higham (1996, Section 9.7). Nonetheless, if we do not scale our linear algebra package yells nasty things at us, so we are going to scale.

5   FLOW DIRECTION

5.1   A Convenient Choice

Without lose of generality, we assume that our location of interest is at the origin, $(x, y) = (0, 0)$. Applying (8) the flow direction at our location of interest becomes

$$
\begin{aligned}
\alpha = \alpha(0, 0) &= \texttt{atan2}\left((2B \cdot 0 + C \cdot 0 + E), (2A \cdot 0 + C \cdot 0 + D)\right) \\
&= \texttt{atan2}\left(E, D\right) \\
&= \texttt{atan2}\left(e, d\right)
\end{aligned}
\tag{25}
$$

This last step is possible because the hydraulic conductivity, k [m], and the aquifer thickness, H [m] are strictly positive numbers.

   We may carry out our analysis in terms of heads and never need to consider the discharge potential. Using unknown parameters $\{a, b, c, d, e, f\}$, the aquifer properties k and H will never need to explicitly enter into our computations. In this simple confined model, we can infer flow directions without knowing z_b, H, k, or k_v. All we need is lots of data.

5.2   Flow Direction Probability Distribution

The flow direction is a function of d and e only, so we need to extract the associated bivariate marginal distribution from the multivariate distribution. For a multivariate normal distribution, this is a simple process of extracting the fourth and fifth row of the expected value matrix, (18), and the fourth and fifth rows and columns of the variance matrix, (18) (e.g., Roussas (1973, Section 18.2, Theorem 3)). We use the following notation to denote these extracted rows and columns.

$$
\mathbf{u} = \begin{bmatrix} \mu_d \\ \mu_e \end{bmatrix}
\qquad\qquad
\mathbf{S} = \begin{bmatrix} \sigma_d^2 & \sigma_{de} \\ \sigma_{de} & \sigma_e^2 \end{bmatrix}
\tag{26}
$$

The resulting distribution of the flow direction, α, follows Smith's distribution[7] (Justus (1978, Equation (4-11)) or Carta et al. (2008, Equation (6))):

$$
f(\alpha) = \frac{\sqrt{|\mathbf{S}^{-1}|}}{\mathbf{r}^\mathsf{T}\mathbf{S}^{-1}\mathbf{r}} \cdot \frac{1}{2\pi}\left[1 + \sqrt{2\pi}D \cdot \exp\left(\tfrac{1}{2}D^2\right) \cdot \mathcal{F}(D)\right] \exp\left(-\tfrac{1}{2}\mathbf{u}^\mathsf{T}\mathbf{S}^{-1}\mathbf{u}\right)
\tag{27}
$$

with

$$
D = \frac{\mathbf{r}^\mathsf{T}\mathbf{S}^{-1}\mathbf{u}}{\sqrt{\mathbf{r}^\mathsf{T}\mathbf{S}^{-1}\mathbf{r}}}
\qquad\qquad
\mathbf{r} = \begin{bmatrix} \cos\alpha \\ \sin\alpha \end{bmatrix}
\tag{28}
$$

and $\mathcal{F}$ denotes the standard normal cumulative distribution function.

   Smith's distribution model is relatively uncommon in the literature on directional data analysis. The most common model is the von Mises distribution (Mardia (1972) or Watson (1983)). Nonetheless, in our case, Smith's is appropriate because we are not analyzing directional measurements. We are inferring the distribution of the flow directions from a quadratic fit to head measurements.

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[7]Smith's distribution is also called the "General Projected Normal distribution". See, for example, Lark et al. (2014) and Hernandez-Stumpfhauser et al. (2017).

6 SUMMARY

In this simple confined model, we can infer the flow directions without knowing z_b, H, k, or k_v. All we need is lots of data.

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A   Conic Discharge Potential

A.1   Using real variables

A.1.1   Discharge potential

The *conic discharge potential* is given by

$$\boxed{\Phi(x,y) = Ax^2 + By^2 + Cxy + Dx + Ey + F} \tag{29}$$

where the coefficient, $\{A, B, C, D, E, F\}$, are real constants.

This form is called the *conic discharge potential* because the level-sets of $\Phi(x,y)$ are conic sections[8]. If $C^2 < 4AB$ the contours are ellipses[9], if $C^2 = 4AB$ the contours are parabolas, and if $C^2 > 4AB$ the contours are hyperbolas.

A.1.2   Discharge

The components of the associated discharge vector are

$$-Q_x(x,y) = \frac{\partial \Phi}{\partial x} = 2Ax + Cy + D \tag{30}$$

$$-Q_y(x,y) = \frac{\partial \Phi}{\partial y} = 2By + Cx + E \tag{31}$$

A.1.3   Divergence

The divergence of the discharge is

$$\nabla^2 \Phi = 2(A + B) \tag{32}$$

A.2   Using complex variables

A.2.1   Discharge potential

Let

$$z = x + iy \qquad \text{and} \qquad \bar{z} = x - iy \tag{33}$$

then

$$x = \frac{z + \bar{z}}{2} \qquad \text{and} \qquad y = \frac{z - \bar{z}}{2i} \tag{34}$$

Substituting (34) into (29) yields

$$\Phi(z, \bar{z}) =$$
$$A\left(\frac{z + \bar{z}}{2}\right)^2 + B\left(\frac{z - \bar{z}}{2i}\right)^2 + C\left(\frac{z + \bar{z}}{2}\right)\left(\frac{z - \bar{z}}{2i}\right) + D\left(\frac{z + \bar{z}}{2}\right) + E\left(\frac{z - \bar{z}}{2i}\right) + F \tag{35}$$

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[8]See, for example, Wikipedia contributors (2020c).
[9]This is the form of the discharge potential used in O_ne^ka.

Expanding out the products in (35) yields

$$\Phi(z, \bar{z}) = $$
$$A \left(\frac{z^2 + 2z\bar{z} + \bar{z}^2}{4} \right) + B \left(\frac{z^2 - 2z\bar{z} + \bar{z}^2}{-4} \right) + C \left(\frac{z^2 - \bar{z}^2}{4i} \right) + D \left(\frac{z + \bar{z}}{2} \right) + E \left(\frac{z - \bar{z}}{2i} \right) + F \tag{36}$$

Collecting like terms in (36) yields

$$\Phi(z, \bar{z}) = $$
$$\left(\frac{A - B - Ci}{4} \right) z^2 + \left(\frac{A - B + Ci}{4} \right) \bar{z}^2 + \left(\frac{A + B}{2} \right) z\bar{z} + \left(\frac{D - Ei}{2} \right) z + \left(\frac{D + Ei}{2} \right) \bar{z} + F \tag{37}$$

We define two complex constants $\{a, b\}$, and two real constants $\{c, d\}$, as

$$a = \frac{A - B - Ci}{4} \tag{38}$$

$$b = \frac{D - Ei}{2} \tag{39}$$

$$c = \frac{F}{2} \tag{40}$$

$$d = \frac{A + B}{2} \tag{41}$$

Substituting (38) through (41) into (37) yields

$$\boxed{\Phi(z, \bar{z}) = \left(az^2 + bz + c \right) + \overline{\left(az^2 + bz + c \right)} + dz\bar{z}} \tag{42}$$

The level sets for $\Phi(z, \bar{z})$ are conic sections. If $2|a| < |d|$ the contours are ellipses, if $2|a| = |d|$ the contours are parabolas, and if $2|a| > |d|$ the contours are hyperbolas.

A.2.2   Discharge

The complex discharge, denoted W, is given by

$$W(z, \bar{z}) = Q_x - iQ_y = -2\frac{\partial \Phi}{\partial z} = -2\left(2az + b + d\bar{z} \right) \tag{43}$$

A.2.3   Divergence

The divergence of the discharge is given by

$$\nabla^2 \Phi = 4\frac{\partial^2 \Phi}{\partial z \partial \bar{z}} = 4d \tag{44}$$