Two applications of interval analysis to parameter estimation in hydrology

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16th GAMM-IMACS International Symposium on Scientific Computing, Computer Arithmetic and Validated Numerics, 2014

Outline

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Hydrology

- Measure
- Describe
- Understand
- Model
- Predict

Prediction needs:

- Qualitative understanding (model)
- Quantative understanding (model parameters)

Numerics

- Limited data
- Numerical approximation of model needed
- Relatively large measurement uncertainty
- Automated parameter search
  - computer: no common sense
  - computer: no math insight

Outline

Koblenz 2013

Floods.

- Extreme and not so extreme events
- Need for probability estimates.
- Estimation of parameters of Probability Distribution.
    - for instance the Gamma distribution

Tracer experiments.

- Understanding catchments.
- Convolution integral as model of transport.
  - with Gamma distribution probability density function ...
- Estimation of parameters of the “transfer function”.

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Outline

The (incomplete) Gamma function

- Upper incomplete Gamma function

$$\Gamma(\alpha, x) = \int_{y=x}^{\infty} y^{\alpha-1} e^{-y} dy$$

- Lower incomplete Gamma function

$$\gamma(\alpha, x) = \int_{y=0}^{x} y^{\alpha-1} e^{-y} dy$$

- Gamma function

$$\Gamma(\alpha) = \int_{y=0}^{\infty} y^{\alpha-1} e^{-y} dy$$

The polygamma function

- Digamma

$$\psi(\alpha) = \frac{d}{d\alpha} \log \Gamma(\alpha)$$

- Trigamma

$$\psi^{(1)}(\alpha) = \frac{d^2}{d\alpha^2} \log \Gamma(\alpha)$$

- Polygamma

$$\psi^{(m)}(\alpha) = \frac{d^{m+1}}{d\alpha^{m+1}} \log \Gamma(\alpha)$$

The Gamma probability density function

- One parameter

$$f_\Gamma(x;\alpha) = \frac{1}{\Gamma(\alpha)} x^{\alpha-1} e^{-x}$$

- Two parameter

$$f_\Gamma(x;\alpha,\zeta) = \frac{1}{\zeta^\alpha \Gamma(\alpha)} x^{\alpha-1} e^{-x/\zeta}$$

- Three parameter or Pearson III

$$f_\Gamma(x;\alpha,\zeta) = \frac{1}{\zeta^\alpha \Gamma(\alpha)} (x-\lambda)^{\alpha-1} e^{-(x-\lambda)/\zeta}$$

The Gamma Cumulative Distribution Function

- One parameter

$$F_{\Gamma}(x;\alpha) = \frac{\gamma(\alpha,x)}{\Gamma(\alpha)} = \frac{1}{\Gamma(\alpha)} \int_{y=0}^{x} y^{\alpha-1} e^{-y} dy$$

- Two parameter

$$F_{\Gamma}(x;\alpha,\zeta) = \frac{\gamma(\alpha,x/\zeta)}{\Gamma(\alpha)}$$

- Three parameter or Pearson III

$$F_{\Gamma}(x;\alpha,\lambda,\zeta) = \frac{\gamma(\alpha,(x-\lambda)/\zeta)}{\Gamma(\alpha)}$$

Generalized Gamma Distribution

- pdf

$$f_{g\Gamma}(x;\alpha,\beta,\zeta) = \frac{\beta}{\zeta^{\alpha\beta}\Gamma(\alpha)} x^{\alpha\beta-1} e^{-(x/\zeta)^{\beta}}$$

- cdf

$$F_{g\Gamma}(x;\alpha,\beta,\zeta) = \frac{\gamma\left(\alpha,(x/\zeta)^{\beta}\right)}{\Gamma(\alpha)}$$

Reparametrized three parameter Gamma Distribution

$$f_\Gamma(x;\alpha,\lambda,\zeta) = \frac{1}{\zeta} f_\Gamma\left(\frac{x-\lambda}{\zeta};\alpha\right)$$

$$f(x;\gamma,\mu,\sigma) = \frac{1}{\sigma\gamma} f_\Gamma\left(\frac{1}{\gamma^2}\left(1+\gamma\frac{x-\mu}{\sigma}\right);\frac{1}{\gamma^2}\right)$$

Outline

Fitting a distribution to the data

- Maximum Likelihood
- Method of moments
- L-moments

Maximum likelihood

Given a sample $\{x_i\}_{i=1}^n$ find the maximum of

$$\mathscr{L}(x;\alpha,\zeta) = \prod_{i=1}^{n} f_\Gamma(x_i;\alpha,\zeta)$$

for $\alpha > 0$, $\zeta > 0$ or equivalently the maximum of

$$\ell(x;\alpha,\zeta) = \sum_{i=1}^{n} \log f_\Gamma(x_i;\alpha,\zeta)$$

Gradient and Hessian

$$\frac{\partial}{\partial \alpha}\ell(x;\alpha,\zeta) = -n\log\zeta - n\psi(\alpha) + \sum_{i=1}^{n}\log x_i$$

$$\frac{\partial}{\partial \zeta}\ell(x;\alpha,\zeta) = -n\alpha\frac{1}{\zeta} + \frac{1}{\zeta^2}\sum_{i=1}^{n}x_i$$

$$\frac{\partial^2}{\partial \alpha^2}\ell(x;\alpha,\zeta) = -n\psi^{(1)}(\alpha) < 0$$

$$\frac{\partial^2}{\partial \alpha\partial\zeta}\ell(x;\alpha,\zeta) = -\frac{n}{\zeta} < 0$$

$$\frac{\partial^2}{\partial \zeta^2}\ell(xx;\alpha,\zeta) = -\frac{n\alpha}{\zeta^2} - \frac{2}{\zeta^3}\sum_{i=1}^{n}x_i < 0$$

Needed ingredients

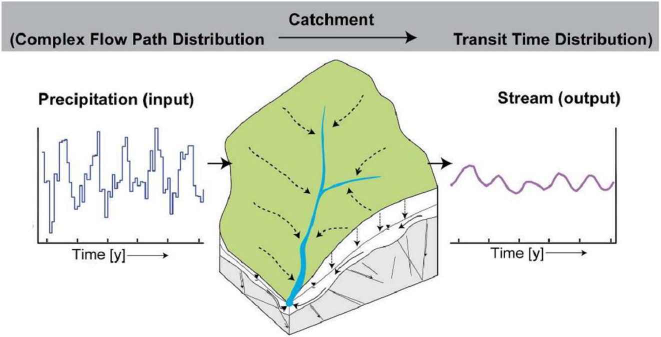
Need to solve

$$0 = -n \log \zeta - n \psi(\alpha) + \sum_{i=1}^{n} \log x_i$$

$$n\alpha = \frac{1}{\zeta} \sum_{i=1}^{n} x_i$$

Outline

Tracer experiments



Role of tracer

- Rain with a detectible chemical: the tracer
- Passes through catchment
- Ends up in stream or river
- Aim: establish catchment transit time distribution

What we know

- Measurement: rain per time interval (day, week) $\Longrightarrow$ average daily or weekly intensity
- Measurement: tracer in accumulated sample$\Longrightarrow$ average concentration
- Measurement: concentration in stream sample $\Longrightarrow$ concentration

The big unknowns

- Catchment history before start of experiment
- Details of catchment pathways
- Details of input

Catchment = low pass filter

- Convolution
- Numerator: convolution of mass signal with Gamma distribution
- Denominator: convolution of precipitation signal with Gamma distribution
  - Proxy for streamflow

Parameter estimate

Find best α, ζ to fit

$$\sum_{i=1}^{n} \left(c_{\mathrm{s}}(t_i) - z(t_i, \alpha, \zeta)\right)^2$$

with

$$z(t_i, \alpha, \zeta) = \frac{\int_{\tau=0}^{\infty} \frac{\tau^{\alpha-1}}{\Gamma(\alpha)} \exp\left(-\frac{\tau}{\zeta}\right) (p \cdot c_{\mathrm{p}})(t_i - \tau)\, d\tau}{\int_{\tau=0}^{\infty} \frac{\tau^{\alpha-1}}{\Gamma(\alpha)} \exp\left(-\frac{\tau}{\zeta}\right) p(t_i - \tau)\, d\tau}$$

where p is “the” precipitation, c_{p} is “the” tracer concentration in precipitation and c_{s} is “the” tracer concentration in stream.

Currently used

- Warmup period
- Numerical integration
- Parameter optimization (classical method)

Interval version

- Interval estimate of integral replaces warmup period
- Interval estimate of integral replaces numerical integration
- Interval analysis based optimization to find parameters

Interval approximation of convolution

- Decomposition (assume $t_0 = 0$ and $p \geq 0$ and bounded)

$$g(t_k) = \sum_{j=0}^{\infty} \int_{\tau=t_j}^{t_{j+1}} f_\Gamma(\tau)\, p(t_k - \tau)\, d\tau$$

Interval approximation of convolution

- Decomposition (assume $t_0 = 0$ and $p \geq 0$ and bounded)

$$g(t_k) = \sum_{j=0}^{\infty} \int_{\tau=t_j}^{t_{j+1}} f_\Gamma(\tau)\, p(t_k - \tau)\, d\tau$$

At zero

$$\int_{\tau=0}^{t_1} f_\Gamma(\tau)\, p(t_k - \tau)\, d\tau \in$$

$$p([0,\varepsilon]) \int_{\tau=0}^{\varepsilon} f_\Gamma(\tau)\, d\tau + f_\Gamma([\varepsilon, t_1]) \int_{\tau=\varepsilon}^{t_1} p(t_k - \tau)\, d\tau$$

Interval approximation of convolution

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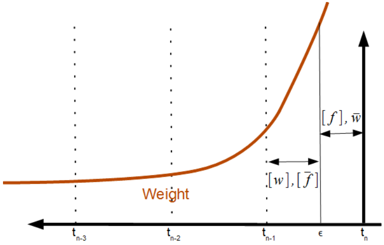

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Simple case

$$\int_{\tau=t_{k-1}}^{t_k} f_\Gamma(\tau)\, p(t_k - \tau)\, d\tau \in f_\Gamma([t_{k-1}, t_k]) \int_{\tau=t_{k-1}}^{t_k} p(t_k - \tau)\, d\tau$$

Interval approximation of convolution

- Decomposition (assume $t_0 = 0$ and $p \geq 0$ and bounded)

$$g(t_k) = \sum_{j=0}^{\infty} \int_{\tau=t_j}^{t_{j+1}} f_\Gamma(\tau)\, p(t_k - \tau)\, d\tau$$

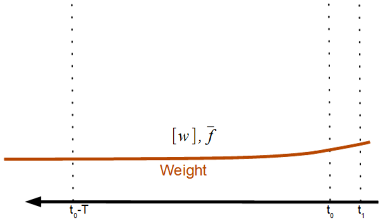
Tail

$$\int_{\tau=t_k}^{\infty} f_\Gamma(\tau)\, p(t_k - \tau)\, d\tau \in f_\Gamma((-\infty, 0]) \int_{\tau=t_k}^{\infty} p(t_k - \tau)\, d\tau$$

Interval approximation of convolution

- Decomposition (assume $t_0 = 0$ and $p \geq 0$ and bounded)

$$g(t_k) = \sum_{j=0}^{\infty} \int_{\tau=t_j}^{t_{j+1}} f_\Gamma(\tau)\, p(t_k - \tau)\, d\tau$$



Needed ingredient

Multi-dimensional interval inclusion of

$$f_\Gamma\,(x;\alpha,\zeta)$$

Outline

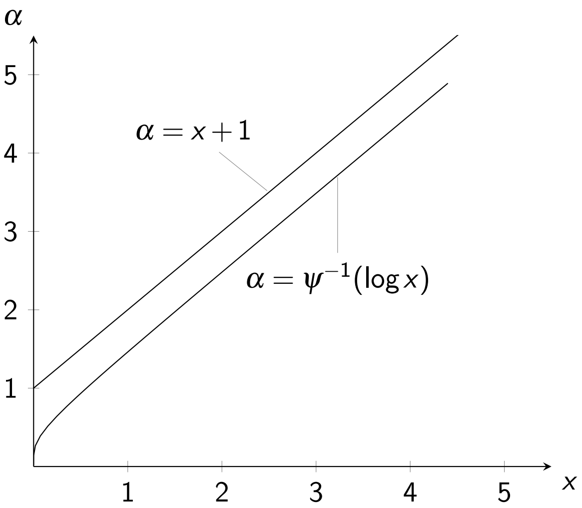
Starting point.

$$f_\Gamma(x;\alpha) = \frac{1}{\Gamma(\alpha)} x^{\alpha-1} e^{-x}$$

We look for g_Γ such that

$$\{f_\Gamma(x;\alpha) \mid \langle x,\alpha\rangle \in [x_1,x_2] \times [\alpha_1,\alpha_2]\} \subseteq g_\Gamma([x_1,x_2],[\alpha_1,\alpha_2])$$

Situation



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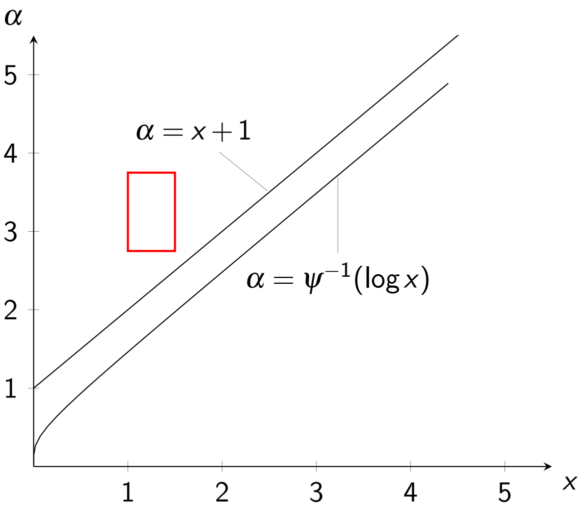

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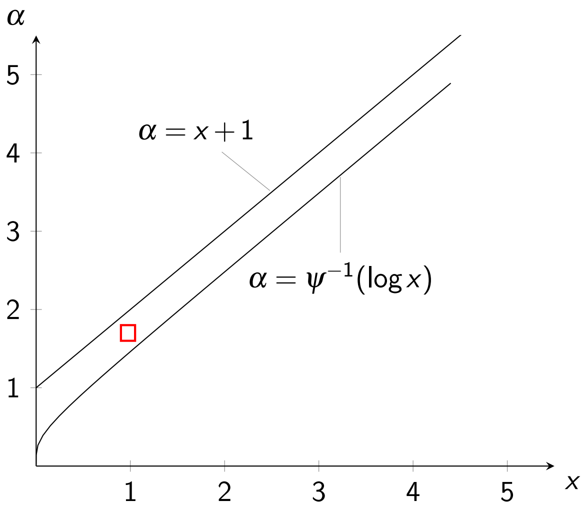
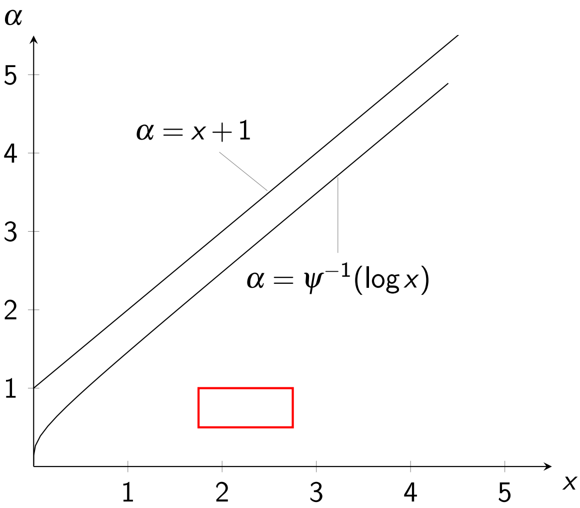


Situation



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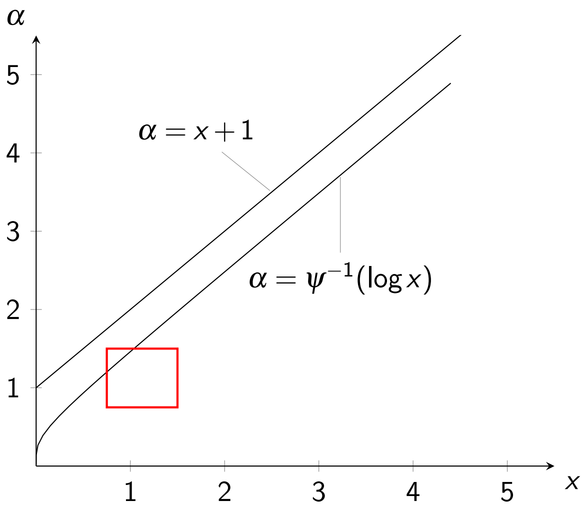

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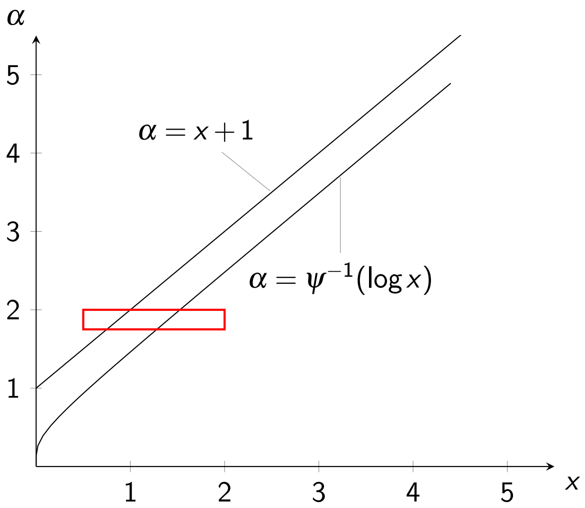

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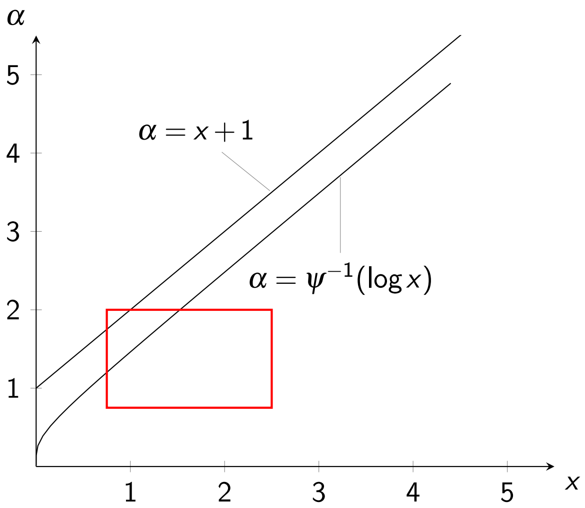

Result of basic analysis.

- Extremum in one of the following
  - corner of $[x_1, x_2] \times [\alpha_1, \alpha_2]$
  - intersection of edge of $[x_1, x_2] \times [\alpha_1, \alpha_2]$ with $\alpha = \psi^{-1}(\log x)$
  - intersection of edge of $[x_1, x_2] \times [\alpha_1, \alpha_2]$ with $\alpha = x + 1$

Outline

Plug and play?

- digamma and trigamma are rarely found in interval libraries
- would be nice to reuse
- Portable routine in interval arithmetic?
  - Basic interval arithmetic supported in C++, Fortran 90, Java (more or less), Python, Matlab (INTLAB)

Di/Tri-gamma preliminaries

Definitions

(From [Spouge 1994])

$$a \geq 2, c_0 = 1;\; c_{k,a,\theta} = \frac{1}{\sqrt{2\pi}} \frac{(-1)^{k-1}}{(k-1)!} (-k+a)^{k-\theta}\, e^{-k+a}$$

$$\tilde{F}_{a,\frac{1}{2}}(z) = c_0 + \sum_{k=1}^{\lceil a \rceil - 1} \frac{c_{k,a,\frac{1}{2}}}{z+k}$$

Digamma approximation

Theorem

([Spouge 1994, Theorem 1.4.1]) If for $\Re z \geq 0$ and $a \geq 3/2$ we define

$$\tilde{\psi}_a(z) \quad = \quad \ln(z+a) - \frac{a-\frac{1}{2}}{z+a} + \frac{1}{\tilde{F}_{a,\frac{1}{2}}} \frac{d}{dz}\left(\tilde{F}_{a,\frac{1}{2}}\right)$$

then

$$|\psi(z) - \tilde{\psi}_a(z)| \quad \leq \quad D(\ln 2a)\sqrt{a}\frac{1}{(2\pi)^{a+\frac{1}{2}}}\frac{1}{\Re(z+a)}$$

where

$$D = \left(1 - \sqrt{\frac{2}{3}\frac{1}{(2\pi)^2}}\right)^{-1}$$

Trigamma approximation

Theorem

([Spouge 1994]) If for $\Re z \geq 0$ and $a \geq 3/2$ we define

$$\tilde{\psi}_a^{(1)}(z) = \frac{1}{z+a} + \frac{a-\frac{1}{2}}{(z+a)^2} + \frac{1}{\tilde{F}_{a,\frac{1}{2}}(z)} \frac{d^2}{dz^2} \tilde{F}_{a,\frac{1}{2}}(z) - \left(\frac{1}{\tilde{F}_{a,\frac{1}{2}}(z)} \frac{d}{dz} \tilde{F}_{a,\frac{1}{2}}(z) \right)^2$$

then

$$\left| \psi^{(1)}(z) - \tilde{\psi}_a^{(1)}(z) \right| \leq D \left(3 \ln^2 2a - \ln 2a + 2 \right) \sqrt{a} \frac{1}{(2\pi)^{a+\frac{1}{2}}} \frac{1}{\Re(z+a)}$$

where

$$D = \left(1 - \sqrt{\frac{2}{3}} \frac{1}{(2\pi)^2} \right)^{-1}$$

Conclusions

- Computers are not specialists: interval based algorithms better at signalling problems.
- Limited interval support for special functions: portable reference would be nice.

For Further Reading I

John L. Spouge.
Computation of the gamma, digamma, and trigamma functions.
SIAM J. Numer. Anal. 31(3):931–944, 1994.