The Lambert W Function in Optimization

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CARMA, University of Newcastle

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https://www.carma.newcastle.edu.au/jon/WinOpt.pdf



Meetings with the Lambert W function and other special functions in optimisation and analysis

Dedicated to Prof: Michel Théra on his 70th birthday

Jonathan Borwein Laureate Professor and Director **CARMA**

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7th International Seminar on Optimization and Variational Analysis

Alicante, June 1-3, 2016

"I never run for trains." Nasim Nicholas

Revised 24-05-2016

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2016 Presentations

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2016 Presentations as Distinguished Scholar in Residence Western University, London Ontario



April 12-13 : Owens Lectures Wayne State University

1. Lambert W in Optimization

2. Walking on Numbers

"I never run for trains." Nasim Nicholas Taleb (The Black Swan)





Revised 4-02-2016

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Jon's website:

https://www.carma.newcastle.

edu.au/jon/WinOpt.pdf



Computer Assisted Research Mathematics and its Applications (CARMA) Priority Research Centre

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Scott's website:

https://carma.newcastle.edu.au/

findsem.php?n=395

Outline I



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Outline II

- Occurrences in Composition
- Occurrences in Infimal Convolution
- Occurrences in Homotopy
- 5 Homotopy and Entropy Solutions of Inverse Problems

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- An Optimization Problem
- A General Implementation
- Computed Examples
- 6 Conclusion
 - Further Merits of SCAT and CCAT
 - Bibliography

Definition Basic Properties The Power of Naming

Definition

 Lambert W is the inverse of x → x exp(x). The real inverse is two-valued, as shown in Figure 1.

Meeting with Lambert W

Meeting with Meijer-G Experimental Mathematics and *W* Convex Analysis Homotopy and Entropy Solutions of Inverse Problems Conclusion

Definition Basic Properties The Power of Naming

Definition

- Lambert W is the inverse of x → x exp(x). The real inverse is two-valued, as shown in Figure 1.
- We are interested in the principal branch with Taylor series

$$W(x) = \sum_{k=1}^{\infty} \frac{(-k)^{k-1}}{k!} x^k$$

with radius of convergence 1/e.

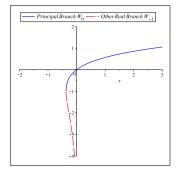


Figure: The real branches of the Lambert *W* function.

Definition Basic Properties The Power of Naming

Basic Properties

Implicit differentiation leads to

$$W'(x) = \frac{W(x)}{x (1 + W(x))}.$$

- **2** *W* is concave on $(-1/e, \infty)$ and positive on $(0, \infty)$.
- (log ∘ W)(z) = log(z) W(z) is concave; since W is log concave on (0,∞).
- $\exp(W(z)) = z/W(z)$ is concave.

Definition Basic Properties The Power of Naming

The Power of Naming

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The Power of Naming

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• *W* is an excellent counter-example to Stigler's Law of Eponymy (which asserts that an idea is always named after the *last* person to discover it).



Figure: Johann Heinrich Lambert (1728–1777)

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Trefethen's Problem Random Walks

Trefethen's Problem

In **2002** Nick Trefethen published ten numerical challenge problems in *SIAM Review* [3]. Several are in optimization.

Trefethen's Problem Random Walks

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Example (Trefethen's ninth problem [3])

The problem is posed as follows.

The integral

$$I(\alpha) = \int_0^2 [2 + \sin(10\alpha)] x^\alpha \, \sin\left(\frac{\alpha}{2 - x}\right) \, \mathrm{d}x$$

depends on the parameter α . What is the value $\alpha \in [0, 5]$ at which $I(\alpha)$ achieves its maximum?

Trefethen's Problem Random Walks

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The Computer Informs the Scientist

 What we know about a function often matters less than what our CAS (say Maple, Mathematica, or SAGE) does.

Trefethen's Problem Random Walks

The Computer Informs the Scientist

- What we know about a function often matters less than what our CAS (say Maple, Mathematica, or SAGE) does.
- At left: what Maple knows about Meijer-G.

```
MeijerG - Meijer G function
Calling Sequence
  MeijerG([as, bs], [cs, ds], z)
Parameters
          - list of the form [a1, ..., am]: first group of numerator [] parameters

    list of the form [b1, ..., bn]; first group of denominator [] parameters

             list of the form [c1, ..., cp]; second group of numerator [ parameters
              list of the form [d1, ..., do]: second group of denominator [] parameters
              expression
Description

    The Meijer G function is defined by the inverse Laplace transform

                MeijerG{[ar, bs], [cr, ds], z} = \frac{1}{2\pi 1} \oint \frac{\Gamma(1 - ar + y) \Gamma(cs - y)}{\Gamma(bs - y) \Gamma(1 - ds + y)} z^{y} dy
    where
                   as = [al, ..., am], \Gamma(1 - as + y) = \Gamma(1 - al + y) ... \Gamma(1 - am + y)
                           bs = [b1, ..., bn], \Gamma(bs - y) = \Gamma(b1 - y) ... \Gamma(bn - y)
                           cs = [cl, ..., cp], \Gamma(cs = y) = \Gamma(cl = y) ... \Gamma(cp = y)
                    ds = [dl, ..., dq], \Gamma(1 - ds + y) = \Gamma(1 - dl + y) ... \Gamma(1 - dq + y)
    and \,{\rm L} is one of three types of integration paths L_{\eta\,+\,\,\omega\,\,|},L_{\infty}, and L_{-\,\omega}
    Contour L_{-} starts at \infty + 1.07 and finishes at \infty + 1.02(07 < 02).
    Contour L _ starts at -\infty + 16/ and finishes at -\infty + 162(6/ < 62)
    Contour L_{\gamma + \infty 1} starts at \gamma - \infty and finishes at \gamma + \infty 1
```

Trefethen's Problem Random Walks

A Solution to Trefethen's Problem

- $I(\alpha)$ is expressible in terms of a *Meijer-G* function.
- Unlike most humans, Mathematica and Maple will figure this out.
 - Help files or a web search then inform the scientist.
 - This is a measure of the changing environment.
- Below: the exact form of $I(\alpha)$ as given by *Maple*.

$$I(\alpha) = 4\sqrt{\pi} \Gamma(\alpha) G_{2,4}^{3,0} \left(\frac{\alpha^2}{16} \middle| \begin{array}{c} \frac{\alpha+2}{2}, \frac{\alpha+3}{2} \\ \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, 1, 0 \end{array} \right) [\sin(10\alpha) + 2].$$

Trefethen's Problem Random Walks

Short Random Walks

- Assuming the Meier-G function is well implemented, one can now use any good numerical optimiser.
- The Meijer-G function has also been instrumental in producing new results on a hundred-year-old topic:

Trefethen's Problem Random Walks

Short Random Walks

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Example (Moments of random walks [10])

The moment function of an n-step random walk in the plane is:

$$M_n(s) = \int_{[0,1]^n} \left| \sum_{k=1}^n e^{2\pi x_k i} \right|^s d(x_1, \dots, x_{n-1}, x_n)$$

Trefethen's Problem Random Walks

A Moment Function

The first breakthrough in [10] makes use of Meijer-G:

Theorem (Meijer-G form for M_3)

For s not an odd integer,

$$M_3(s) = \frac{\Gamma(1+\frac{s}{2})}{\sqrt{\pi} \ \Gamma(-\frac{s}{2})} \ G_{33}^{21} \left(\begin{array}{c} 1,1,1\\ \frac{1}{2},-\frac{s}{2},-\frac{s}{2} \end{array} \middle| \frac{1}{4} \right). \tag{1}$$

Trefethen's Problem Random Walks

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- Equation (1) was first found by Crandall via CAS and proven in [10] using residue calculus methods.
- M₃(s) is among the first non-trivial higher order Meijer-G functions to be placed in closed form. (Also M₄(s).)

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Trefethen's Problem Random Walks

A New Result on an Old Topic

Theorem (Meijer-G form for M_4)

For $\Re s > -2$ and s not an odd integer

$$M_4(s) = \frac{2^s}{\pi} \frac{\Gamma(1+\frac{s}{2})}{\Gamma(-\frac{s}{2})} G_{44}^{22} \begin{pmatrix} 1, \frac{1-s}{2}, 1, 1\\ \frac{1}{2} - \frac{s}{2}, -\frac{s}{2}, -\frac{s}{2} \end{pmatrix} |1 \end{pmatrix}.$$

(2)

Trefethen's Problem Random Walks

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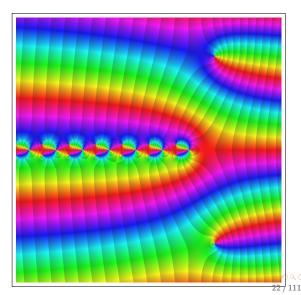
$$M_4(s) = \frac{2^s}{\pi} \frac{\Gamma(1+\frac{s}{2})}{\Gamma(-\frac{s}{2})} G_{44}^{22} \begin{pmatrix} 1, \frac{1-s}{2}, 1, 1\\ \frac{1}{2} - \frac{s}{2}, -\frac{s}{2}, -\frac{s}{2} \end{pmatrix} |1 \end{pmatrix}.$$

This, together with the first result, led to useful results, including:

Closed hypergeometric form for the radial density of a 3-step walk:

$$p_{3}(\alpha) = \frac{2\sqrt{3}\alpha}{\pi (3+\alpha^{2})} {}_{2}F_{1}\left(\frac{\frac{1}{3},\frac{2}{3}}{1} \left|\frac{\alpha^{2} (9-\alpha^{2})^{2}}{(3+\alpha^{2})^{3}}\right.\right)$$
(3)

Trefethen's Problem Random Walks



The moment function M_4 drawn from (2) in the Calendar Complex Beauties 2016.

Knuth's Series Problem An Open Question

Knuth's Series Problem

We continue with an account of the solution in [5], to a problem posed by Donald E. Knuth in the November 2000 issues of the *American Mathematical Monthly*.

Problem 10832

Evaluate

$$S = \sum_{k=1}^{\infty} \left(\frac{k^k}{k! e^k} - \frac{1}{\sqrt{2\pi k}} \right).$$

See [18] for the published solution.

Knuth's Series Problem An Open Question

A Numerical Solution

Problem 10832

$$S = \sum_{k=1}^{\infty} \left(\frac{k^k}{k! e^k} - \frac{1}{\sqrt{2\pi k}} \right).$$

Maple produced the approximation

 $S \approx -0.08406950872765599646.$

With "Smart Lookup" feature, the Inverse Symbolic Calculator* yielded:

$$S \approx -\frac{2}{3} - \frac{1}{\sqrt{2\pi}} \zeta\left(\frac{1}{2}\right).$$
 (4)

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Knuth's Series Problem An Open Question

- Calculations to higher precision (50 decimal digits) confirmed this approximation. Are we done?
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 - One clue was the speed with which *Maple* calculated the precise value of this slowly convergent sum. *Maple* clearly knew something we did not ...
 - We discovered *Maple* was using the Lambert W function.
- Another clue was the appearance of ζ(1/2) in the above experimental identity, together with an obvious allusion to Stirling's formula in the original problem.

Knuth's Series Problem An Open Question

A Conjectured Identity

We Conjectured the Identity

$$\sum_{k=1}^{\infty} \left(\frac{1}{\sqrt{2\pi k}} - \frac{P(1/2, k-1)}{(k-1)!\sqrt{2}} \right) = \frac{1}{\sqrt{2\pi}} \zeta\left(\frac{1}{2}\right)$$

- Here P(x, n) denotes the Pochhammer symbol $x(x+1)\cdots(x+n-1)$, and the binomial coefficients on the left hand side are the same as those of the function $1/\sqrt{2-2x}$.
- *Maple* successfully evaluated this summation as shown on the right hand side.

Knuth's Series Problem An Open Question

We now needed to establish that

$$\sum_{k=1}^{\infty} \left(\frac{k^k}{k! e^k} - \frac{P(1/2, k-1)}{(k-1)! \sqrt{2}} \right) = -\frac{2}{3}.$$

Guided by the presence of the Lambert W function,

$$W(z) = \sum_{k=1}^{\infty} \frac{(-k)^{k-1} z^k}{k!},$$

an appeal to Abel's limit theorem suggested

$$\lim_{z\to 1}\left(\frac{dW(-z/e)}{dz}+\frac{1}{\sqrt{2-2z}}\right)=\frac{2}{3}.$$

Maple was able to evaluate this limit and so establish the identity.

Knuth's Series Problem An Open Question

Proving the Identity

The identity relies on the following reversion [16]. Let $p = \sqrt{2(1 + ez)}$ with $z = We^W$, so that

$$\frac{p^2}{2} - 1 = W \exp(1 + W) = -1 + \sum_{k \ge 1} \left(\frac{1}{k!} - \frac{1}{(k-1)!}\right) (1 + W)^k$$

and revert to $1 + W = p - \frac{p^2}{3} + \frac{11}{72} p^3 + \dots$ for $|p| < \sqrt{2}$.

This combines with $W'(x) = \frac{W(x)}{x(1+W(x))}$ to prove the identity.

Knuth's Series Problem An Open Question

Remark on Generalisation

Proposition. $(\zeta(s) \text{ for } 0 < s < \infty, s \neq 1)$

For 0 < Re s < 1 in the complex plane,

$$\sum_{k=1}^{\infty} \left(\frac{1}{k^{s}} - \frac{\Gamma(k-s)}{\Gamma(k)} \right) = \zeta(s).$$
 (5)

Knuth's Series Problem An Open Question

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 (5)

Now Maple's summation tools can reduce this to

$$\sum_{k=1}^{N} \frac{1}{k^{s}} - \frac{\Gamma(N+1-s)}{(1-s)\Gamma(N)} \to \zeta(s).$$
(6)

For any given rational $s \in (0, \infty)$ Maple will evaluate the limit by the Euler-Maclaurin method.

Now Maple's summation tools can reduce this to

$$\sum_{k=1}^{N} \frac{1}{k^s} - \frac{\Gamma\left(N+1-s\right)}{\left(1-s\right)\Gamma\left(N\right)} \to \zeta(s).$$
(7)

For any given rational $s \in (0, \infty)$ Maple will evaluate the limit by the Euler-Maclaurin method. Consulting the DLMF* we discover

$$\zeta(s) = \sum_{k=1}^{N} \frac{1}{k^s} + \frac{N^{1-s}}{s-1} - s \int_{N}^{\infty} \frac{x - \lfloor x \rfloor}{x^{s+1}} \, \mathrm{d}x.$$

*Found at http://www.dlmf.gov.

Remark on Generalisation

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Since the integral tends to zero for s > 0 and

$$\lim_{N\to\infty}\frac{\Gamma\left(N+1-s\right)}{\left(1-s\right)\Gamma\left(N\right)}-\frac{N^{1-s}}{1-s}=0,$$

we can also produce an explicit human proof.

*Found at http://www.dlmf.gov

Knuth's Series Problem An Open Question

An Open Question

Can one find a solution for general $s \neq \frac{1}{2} \in (0,1)$?

Based on (5) and the Stirling approximation for $\Gamma(k+s) \approx \sqrt{2\pi} e^{-k} k^{k+s-1/2}$ we obtain

$$\sum_{k=1}^{\infty} \left(\frac{1}{\sqrt{2\pi}k^s} - \frac{k^{k+1/2-s}}{k! e^k} \right) - \frac{\zeta(s)}{\sqrt{2\pi}} = \kappa(s).$$
(8)

We have $\kappa(1/2) = 2/3$, but it remains to evaluate $\kappa(s) \in \mathbb{R}$ more generally. Our question is closely allied to that of asking if

$$W_{s}(x) = \sum_{k=1}^{\infty} \frac{k^{k+1/2-s}}{k!} x^{k}$$
(9)

for $s \neq 1/2$ can be analysed in terms of W.

Knuth's Series Problem An Open Question

A Plot of the Function in Question

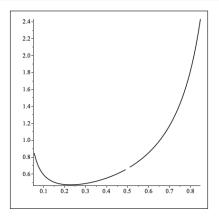


Figure: The function κ to the left and right of s = 1/2.

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Preliminaries on Convex Conjugates W in Conjugation of Log Convex Functions Occurrences in Composition Occurrences in Infimal Convolution Occurrences in Homotopy

Definition of Convex Conjugate

For a function $f: X \rightarrow [-\infty, \infty]$ the convex conjugate is

the function $f^*: X^* \to [-\infty, \infty]$ given by

$$f^*(y) = \sup_{x \in X} \langle y, x \rangle - f(x).$$
 (10)

Here X is a Euclidean, Hilbert, or Banach space.

Meeting with Lambert W Preliminaries on Convex Conjugates Meeting with Meijer-G Experimental Mathematics and W Convex Analysis Homotopy and Entropy Solutions of Inverse Problems Conclusion

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- The function f^* is always convex (if possibly always infinite).
- If f is lower semicontinuous, convex, proper, $(f^*)^* = f$.
- In particular if we show (by CAS) a function $g = f^*$ for some alert f, then g is necessarily convex.

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Homotopy and Entropy Solutions of Inverse Problems Conclusion Preliminaries on Convex Conjugates W in Conjugation of Log Convex Functions Occurrences in Composition Occurrences in Infimal Convolution Occurrences in Homotopy

Visualizing Convex Conjugates

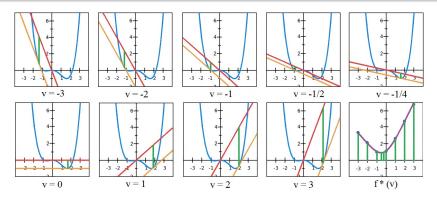


Figure: The construction of f^* is shown for a blue function f. The inputs of f^* may be thought of as slopes of the lines through the origin. For each input, we obtain the corresponding output by taking a parallel line and sliding it down as far away from the original line as as it can go while still touching the curve of the function f. The output is the vertical distance between the two lines [19]

Preliminaries on Convex Conjugates W in Conjugation of Log Convex Functions Occurrences in Composition Occurrences in Infimal Convolution Occurrences in Homotopy

Computing a Closed Form

Let
$$f : \mathbb{R} \to \mathbb{R}$$
 by $f(x) = x^2$.
Then

$$f^*(y) = \sup_{x \in \mathbb{R}} \{ \langle y, x \rangle - f(x) \}$$
$$= \sup_{x \in \mathbb{R}} \{ yx - x^2 \}.$$

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• Differentiating $yx - x^2$ and using y - 2x = 0, we find that $yx - x^2$ attains its supremum when $x = \frac{y}{2}$. Preliminaries on Convex Conjugates W in Conjugation of Log Convex Functions Occurrences in Composition Occurrences in Infimal Convolution Occurrences in Homotopy

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• Differentiating $yx - x^2$ and using y - 2x = 0, we find that $yx - x^2$ attains its supremum when $x = \frac{y}{2}$.

We substitute to obtain $f^*(y) = y(\frac{y}{2}) - (\frac{y}{2})^2 = \frac{y^2}{4}.$ Preliminaries on Convex Conjugates W in Conjugation of Log Convex Functions Occurrences in Composition Occurrences in Infimal Convolution Occurrences in Homotopy

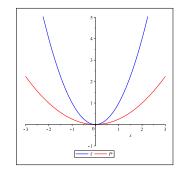


Figure: The function $f(x) = x^2$ and its conjugate $f^*(y) = \frac{y^2}{4}$ [19].

Preliminaries on Convex Conjugates W in Conjugation of Log Convex Functions Occurrences in Composition Occurrences in Infimal Convolution Occurrences in Homotopy

Some Important Examples

• For
$$1/p + 1/q = 1$$
 with $p, q > 1$,

 $\left(\frac{|\cdot|^p}{p}\right)^* = \frac{|\cdot|^q}{q}.$

- The energy function $\frac{|\cdot|^2}{2}$ is the only self-conjugate function.
- The log barrier f(x) = -log x for x > 0 has conjugate conjugate f*(y) = -1 log y for x < 0.
- The Boltzmann-Shannon entropy y log(y) y is the convex conjugate of exp(x) (and vice-versa since exp(x) is convex).

Our *Maple* packages SCAT & CCAT [7] automate all this and more subtle ideas such as iterated conjugation: see http: //carma.newcastle.edu.au/ConvexFunctions/SCAT.ZIP.

Preliminaries on Convex Conjugates W in Conjugation of Log Convex Functions Occurrences in Composition Occurrences in Infimal Convolution Occurrences in Homotopy

Addition and Convolution

The convex conjugate exchanges addition of functions with their infimal convolution

$$(f \Box g)(y) = \inf_{x \in X} f(y - x) + g(x).$$

Indeed $(f \Box g)^* = f^* + g^*$ always holds and under mild hypotheses

$$(f+g)^*=f^*\,\Box\,g^*.$$

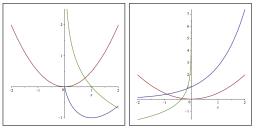


Figure: The energy, log barrier and negative entropy (L) and duals (R).

Variable Separability

Suppose f is variable separable. That is to say that

$$f(x_1, x_2, \ldots, x_n) = \sum_{j=1}^n f_j(x_j)$$

where each f_j is convex. Then f is convex and

$$f^*(y_1, y_2, \dots, y_n) = \sum_{j=1}^n f_j^*(y_j).$$

From such building blocks, and the *Fenchel duality* theorem – for $f + g \circ A - [8]$ or Theorem 5 below, many other convex conjugates engaging W are accessible.

Matrix Functions

Preliminaries on Convex Conjugates W in Conjugation of Log Convex Functions Occurrences in Composition Occurrences in Infimal Convolution Occurrences in Homotopy

It is also possible to induce functions of matrices as follows.

Matrix Functions

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• Let f be a symmetric proper and lower semicontinuous convex function of n variables, and let A be a symmetric matrix with real spectrum $\lambda(A)$.

Then

$$\widehat{f}(A) = f(\lambda(A))$$

induces a proper and lower semicontinuous convex matrix function.

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• So $f(x) = -\sum_{k=1}^{n} \log(x_k)$ induces $\widehat{f}(A) = -\log(\det(A))$.

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• So $f(x) = -\sum_{k=1}^{n} \log(x_k)$ induces $\hat{f}(A) = -\log(\det(A))$. Moreover,

$$\widehat{f^*}(A) = \left(\widehat{f}(A)\right)^*$$

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Meeting with Lambert W Preliminaries on Convex Conjugates Meeting with Meijer-G Experimental Mathematics and W **Convex Analysis** Homotopy and Entropy Solutions of Inverse Problems Conclusion

A Note on Closed Forms

- The notion of a closed form for a given function is an always-changing issue.
 - While $x \exp x$ is elementary W(x) is not, since arbitrary inversion is not permitted in the definition of *elementary*.

A Note on Closed Forms

- The notion of a closed form for a given function is an always-changing issue.
 - While $x \exp x$ is elementary W(x) is not, since arbitrary inversion is not permitted in the definition of *elementary*.
- We consider a closed form roughly to be a form which is finitary and computationally effective. See, for example, [6] available at https:

//www.carma.newcastle.edu.au/jon/closed-form.pdf.

• Once a computationally effective closed form is available, all of classical convex duality theory is accessible.

Preliminaries on Convex Conjugates W in Conjugation of Log Convex Functions Occurrences in Composition Occurrences in Infimal Convolution Occurrences in Homotopy

Log Convex Functions

Definition

A log convex function g is a positive function such that $f = \log g$ is convex. Thence

 $g(x)=e^{f(x)}.$

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- log convexity useful in statistics may be thought of as a strengthening of convexity and is implied by 1/g > 0 being concave.
- We are interested in the convex conjugates of such functions:

$$g^*(y) = \sup_{x \in X} \{yx - e^{f(x)}\}$$

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Meeting with Lambert W Meeting with Meijer-G Experimental Mathematics and W Convex Analysis Homotopy and Entropy Solutions of Inverse Problems Conclusion Convex Conjugates of Log Convex Functions

Given the function f, we may solve, as before, by taking the derivative and setting it equal to zero to obtain

 $y = f'(x)e^{f(x)}.$

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Given the function f, we may solve, as before, by taking the derivative and setting it equal to zero to obtain

 $y = f'(x)e^{f(x)}.$

If we can solve this equation for x = s(y), we can express the conjugate in closed form as

$$g^*(y) = y \cdot s(y) - g(s(y)).$$

We will explore a useful class of functions for which W shows up quite naturally in their closed forms.

Two Examples with W

Our *Maple* package *SCAT* provides two such examples which we can also easily verify by the methods above.

• For $g(x) = e^{e^x}$, we have

$$g^{*}(y) = \begin{cases} y \left(\log (y) - W (y) - \frac{1}{W(y)} \right) & \text{if } y > 0 \\ -1 & \text{if } y = 0 \\ \infty & \text{if } y < 0 \end{cases}$$

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• For $g(x) = e^{\frac{x^2}{2}}$, we have

$$g^*(y) = |y| \left(\sqrt{W(y^2)} - \frac{1}{\sqrt{W(y^2)}}\right)$$
 for all y .

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Seeking a General Closed Form

If we can first solve the equation

$$f'(x)^{\alpha+1} = \gamma f(x) \tag{11}$$

for some α and nonzero γ , we will be able to express g^* in closed form using W.

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for some α and nonzero γ , we will be able to express g^* in closed form using W. Indeed, since

 $y=f'(x)e^{f(x)},$

we raise both sides to the $\alpha + 1$ power to obtain

$$y^{\alpha+1} = f'(x)^{\alpha+1}e^{(\alpha+1)f(x)} = \gamma f(x)e^{(\alpha+1)f(x)}.$$

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$$y^{\alpha+1} = f'(x)^{\alpha+1}e^{(\alpha+1)f(x)} = \gamma f(x)e^{(\alpha+1)f(x)}$$

Finally, we multiply both sides by $\frac{\alpha+1}{\gamma}$ and can use W to write:

$$(\alpha+1)f(x) = W\left((\alpha+1)\frac{y^{\alpha+1}}{\gamma}\right).$$

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We obtain the following closed forms for $(\exp \circ f)^*(y)$: we write

$$f(x) = \frac{W\left((\alpha+1)\frac{y^{\alpha+1}}{\gamma}\right)}{\alpha+1}$$
$$x = b\left(\frac{W\left((\alpha+1)\frac{y^{\alpha+1}}{\gamma}\right)}{\alpha+1}, y\right)$$

Here $b(x, y) = f^{-1}(x)$ in the invertible case and b(x, y) is the pre-image choice in $f^{-1}(x)$ such that $x \cdot y$ is maximized otherwise.

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These yield the closed form for g^* :

$$g^*(y) = y \cdot b(d(y), y) - \exp(d(y)) \text{ where}$$
$$d(y) = \frac{W\left((\alpha + 1)\frac{y^{\alpha+1}}{\gamma}\right)}{\alpha + 1}.$$

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Comparing to our Previous Examples

We can see quite nicely how this relates to our previous examples.

• In the case of our example $g(x) = \exp(\exp(x))$, we have

 $b(x, y) = f^{-1}(x) = \log(x).$

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• In the case of our example $g(x) = \exp(\exp(x))$, we have

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• In the case of our example $g(x) = \exp\left(\frac{|x|^{\rho}}{\rho}\right)$, we have

$$b(x,y) = \begin{cases} (p \cdot x)^{\frac{1}{p}} & \text{if } y \ge 0\\ -(p \cdot x)^{\frac{1}{p}} & \text{if } y < 0 \end{cases}.$$
 (12)

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A Simplified General Form

Using the fact that $\exp(W(x)) = x/W(x)$, we can further simplify the expression of our general closed form to:

Closed form when (11) holds

$$g^{*}(y) = y \cdot b\left(\frac{W\left((\alpha+1)\frac{y^{\alpha+1}}{\gamma}\right)}{\alpha+1}, y\right) - \left(\frac{(\alpha+1)\frac{y^{\alpha+1}}{\gamma}}{W\left((\alpha+1)\frac{y^{\alpha+1}}{\gamma}\right)}\right)^{\frac{1}{\alpha+1}}.$$

While this isn't especially nice to look at, it simplifies greatly for certain choices of f (ergo, choices of γ, α). More importantly, it is very clean from a computational standpoint.

A Class of Functions

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With initial condition $f(0) = \beta$, *Maple*'s built-in ODE solver returns

$$f(\mathbf{x}) = \left(\frac{1}{\alpha+1}\left(\alpha\gamma^{\frac{1}{\alpha+1}}\mathbf{x} + (\alpha+1)\mathrm{e}^{\frac{\alpha\ln(\beta)}{\alpha+1}}\right)\right)^{\frac{\alpha+1}{\alpha}}$$

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- As $\alpha \to 0$, we retrieve the familiar $f(x) = \beta(\exp(\gamma x))$.
- Also, for $\alpha = 1, \gamma = 2$, when $\beta \to 0$, we recover $f(x) = \frac{x^2}{2}$.
- Thus, we obtain a large class of closed forms from which our previous examples emerge as limiting cases.

Preliminaries on Convex Conjugates W in Conjugation of Log Convex Functions Occurrences in Composition Occurrences in Infimal Convolution Occurrences in Homotopy

Simplified Closed Forms

• The closed form of the convex conjugates for functions of form $\beta \cdot \exp(x)$ simplifies to

$$g^{*}(y) = \begin{cases} y \left(\log (y) - W (y) - \frac{1}{W(y)} - \log(\beta) \right) & \text{if } y > 0 \\ -1 & \text{if } y = 0 \\ \infty & \text{if } y < 0 \end{cases}$$

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Where ¹/_q + ¹/_p = 1, the closed form of the convex conjugates for functions of form f(x) = ^{|x|^p}/_p, (p > 1) simplifies to

$$g^*(y) = |y| \left(\left(\frac{p}{q} W \left(\frac{q}{p} |y|^q \right) \right)^{\frac{1}{p}} - \left(\frac{p}{q} W \left(\frac{q}{p} |y|^q \right) \right)^{-\frac{1}{q}} \right)$$

• Compare the former to the case $\beta = 1$ and the latter to the case p = q = 2, both of which we have seen before.

Preliminaries on Convex Conjugates W in Conjugation of Log Convex Functions Occurrences in Composition Occurrences in Infimal Convolution Occurrences in Homotopy

Conjugates of Compositions

Theorem (Conjugates of Compositions)

Consider the convex composition $h \circ g$ of a nondecreasing convex function $h: (-\infty, \infty] \to (-\infty, \infty]$ with a convex function $f: X \to (-\infty, \infty]$. We interpret $f(+\infty) = +\infty$, and we assume there is a point \hat{x} in X satisfying $f(\hat{x}) \in \operatorname{int} \operatorname{dom}(h)$. For y in X^{*},

$$(h \circ f)^*(y) = \inf_{t \ge 0} \left\{ h^*(t) + tf^*\left(\frac{y}{t}\right) \right\}.$$

Here $0f^*\left(\frac{y}{0}\right) = \iota^*_{\text{dom}f}(y)$ in terms of the convex indicator function $\iota^*_{\text{dom}f}$ which is zero on domf and is $+\infty$ otherwise.

An Example with Composition

We may use Theorem 5 with

 $h(t) = \exp(t), h^*(t) = t \log t - t$ (the Shannon entropy)

to compute the conjugate for $g(x) = \exp \circ f(x)$ for various f.

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$$(h \circ f)^*(y) = \inf_{t \ge 0} \left\{ h^*(t) + tf^*\left(\frac{y}{t}\right) \right\} = \inf_{t \ge 0} \left\{ t \log t - t + t \left(\frac{|y|}{t}\right)^q / q \right\}.$$

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Differentiating, setting equal to zero, and solving for t, we arrive at

$$t = \exp\left(rac{W\left((q-1)|y|^q
ight)}{q}
ight)$$

which we substitute to obtain the same answer as before. $A \equiv A = A$

Preliminaries on Convex Conjugates W in Conjugation of Log Convex Functions Occurrences in Composition Occurrences in Infimal Convolution Occurrences in Homotopy

Infimal Convolution

Consider for $\mu > 0$ the convolutions

$$g_{\mu} = (x
ightarrow x \log(x) - x) \Box \mu \left(x
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This family – of everywhere continuous functions – is also called the Moreau envelope of $x \log(x) - x$.

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SCAT provides:

$$g_{\mu}(y) = \frac{\mu}{2}y^2 - \frac{1}{\mu}W(\mu e^{\mu y}) - \frac{1}{2\mu}W(\mu e^{\mu y})^2.$$

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$$g_{\mu}(y) = rac{\mu}{2}y^2 - rac{1}{\mu}W(\mu e^{\mu y}) - rac{1}{2\mu}W(\mu e^{\mu y})^2.$$

• g_{μ} is fully explicit in terms of W.

Preliminaries on Convex Conjugates W in Conjugation of Log Convex Functions Occurrences in Composition Occurrences in Infimal Convolution Occurrences in Homotopy

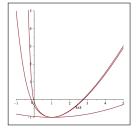


Figure: Convolution of entropy $x \log x - x$ and energy $\mu x^2/2$ for $\mu = 1/10, 10, 100.$

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Homotopy

Consider for $0 \le t \le 1$ the combination

$$f_t(x) = (1-t)(x\log x - x) + t\frac{x^2}{2}$$
(13)

2

so that f_0 is the Shannon entropy and f_1 the energy.

Homotopy

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The conjugate of (13) is

$$f_t^*(y) = \frac{(1-t)^2}{2t} \left(W\left(\frac{t}{1-t}e^{\frac{y}{1-t}}\right) + 2 \right) W\left(\frac{t}{1-t}e^{\frac{y}{1-t}}\right).$$

In the limit at t = 1 we recover the positive energy which is infinite for y < 0 and at t = 0 we reobtain $x \log(x) - x$.

An Optimization Problem A General Implementation Computed Examples

Minimization with Constraints

Consider the (negative) entropy functional $I_f : L^1([0,1],\lambda) \to \mathbb{R}$ defined as follows:

$$I_f(x) = \int_0^1 f(x(s)) \, \mathrm{d}s$$

where λ is Lebesgue measure and f is a proper, closed convex function.

Suppose we wish to minimize l_f subject to finitely many continuous linear constraints of the form

$$\langle a_k, x \rangle = \int_0^1 a_k(s) x(s) \, \mathrm{d}s = b_k$$

for $1 \le k \le n$. We may write this for $A : L^1([0,1]) \to \mathbb{R}^n$ with $Ax = \left(\int_0^1 a_1(s)x(s) \, \mathrm{d}s, \dots, \int_0^1 a_n(s)x(s) \, \mathrm{d}s\right) = b.$ BX = b. BX = b.

An Optimization Problem A General Implementation Computed Examples

Reformulation as Dual Problem

When f^* is smooth and everywhere finite on the real line, our problem

 $\inf_{x\in L^1} \left\{ I_f(x) | Ax = b \right\}$

reduces – via subtle Fenchel duality – to solving a finite nonlinear equation.

Solve for $\lambda_1, \lambda_2, \dots, \lambda_n$ $\int_0^1 (f^*)' \left(\sum_{j=1}^n \lambda_j a_j(s) \right) a_k(s) \, \mathrm{ds} = \mathrm{b}_k \qquad (1 \le \mathrm{k} \le \mathrm{n}). \quad (14)$

An Optimization Problem A General Implementation Computed Examples

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Solve for $\lambda_1, \lambda_2, \ldots, \lambda_n$

$$\int_{0}^{1} \underbrace{(f^{*})'\left(\sum_{j=1}^{n} \lambda_{j} a_{j}(s)\right)}_{a_{k}(s) \operatorname{ds} = \operatorname{b}_{k}} \quad (1 \leq k \leq n). \quad (14)$$

Details are reprised in the paper accompanying this talk. More information – including the matter of primal attainment and constraint qualification – can be found in [9].

An Optimization Problem A General Implementation Computed Examples

The Role of Lambert W

To illustrate the role of for W, we choose f in our optimization problem to be of the form

$$f_t(x) = (1-t)(x\log x - x) + t\frac{x^2}{2}.$$

An Optimization Problem A General Implementation Computed Examples

The Role of Lambert W

To illustrate the role of for W, we choose f in our optimization problem to be of the form

$$f_t(x) = (1-t)(x \log x - x) + t \frac{x^2}{2}.$$

Then we have the following:

- f₀ is the Shannon Entropy
- f_1 is the energy

•
$$(f_t^*)'(y) = \frac{(1-t)}{t} W\left(\frac{t}{1-t} \exp\left(\frac{y}{1-t}\right)\right)$$

- $\lim_{t\to 0} (f_t^*)'(y) = \exp(y)$
- $\lim_{t\to 1} (f_t^*)'(y) = \max\{y, 0\}.$

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An Optimization Problem A General Implementation Computed Examples

A Computational Example

We illustrate by implementing a program with m algebraic moments of the form

$$a_k(s) = s^{k-1}$$
 $(k = 1 \dots m).$

An Optimization Problem A General Implementation Computed Examples

A Computational Example

We illustrate by implementing a program with m algebraic moments of the form

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 $(k = 1 \dots m).$

Our subgradient (dual problem) is represented more explicitly by following the set of equations for $k = 1 \dots 10$:

$$\int_0^1 \frac{(1-t)}{t} W\left(\frac{t}{1-t} \exp\left(\frac{\sum_{j=1}^n \lambda_j s^{j-1}}{1-t}\right)\right) s^{k-1} \mathrm{d}s - b_k = 0.$$
(15)

We can solve for λ using any standard numerical solver or, say, by a Newton-type method.

An Optimization Problem A General Implementation Computed Examples

Cost-Effective Computing

Newton's method is cost-effective for this formulation. The Hessian is a Hankel matrix:

 $\begin{aligned} H(\lambda) &= (h_{i,k}) \\ h_{i,k} &= \int_0^1 \frac{(1-t)}{t} W\left(\frac{t}{1-t} \exp\left(\frac{\sum_{j=1}^n \lambda_j a_j(s)}{1-t}\right)\right) a_k(s) a_i(s) \mathrm{d}s \\ &= \int_0^1 \frac{(1-t)}{t} W\left(\frac{t}{1-t} \exp\left(\frac{\sum_{j=1}^n \lambda_j s^{j-1}}{1-t}\right)\right) s^{k+i-2} \mathrm{d}s. \end{aligned}$

An Optimization Problem A General Implementation Computed Examples

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- When *m* is the number of moments specified, for each iteration we need only to compute the 2m 1 cases $k + i = 2 \dots 2m$.
- The gradient G(λ) may be obtained by taking the first row (or column) of the Hessian and subtracting b_k from the kth entry. ³_{90/111}

An Optimization Problem A General Implementation Computed Examples

Saving Computation on the Quadrature

We adopt a Gaussian quadrature rule with weights $\{a_l\}_{l=1}^m$ and abcissas $\{x_l\}_{l=1}^m$. Then, where

$$F(x_l) = \frac{(1-t)}{t} W\left(\frac{t}{1-t} \exp\left(\frac{\sum_{j=1}^n \lambda_j x_l^{j-1}}{1-t}\right)\right),$$

for a single iteration we need only use numerical integration on the W function m times rather than order $m \cdot n$ times.

An Optimization Problem A General Implementation Computed Examples

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for a single iteration we need only use numerical integration on the W function m times rather than order $m \cdot n$ times.

• To see more clearly why this is the case, notice that we can reuse the values $a_l F(x_l)$, $l = 1 \dots m$ as follows:

$$h_{1,1} = \sum_{l=0}^{m} a_l F(x_l), h_{(i+k=\alpha)} = \sum_{l=0}^{m} a_l F(x_l) x_l^{\alpha-2}.$$

• Thus, we need only compute each once for each iteration. We can also reuse $x_l^{\alpha-2}$ for $l = 1 \dots m$, $\alpha = 2 \dots 20$.

An Optimization Problem A General Implementation Computed Examples

Complete Optimized Process

An Optimization Problem A General Implementation Computed Examples

Complete Optimized Process

Our full method for computing with minimal cost is as follows:

Precompute the weights {a_l}^m_{l=1}, and the abscissas raised to various powers x^α_l, l = 1...m, α = 0...18, storing the weights in a vector and the powers of the abscissas in a matrix.

An Optimization Problem A General Implementation Computed Examples

Complete Optimized Process

- Precompute the weights {a_l}^m_{l=1}, and the abscissas raised to various powers x^α_l, l = 1...m, α = 0...18, storing the weights in a vector and the powers of the abscissas in a matrix.
- 2 At each step compute the function values $a_l F(x_l)$, $l = 1 \dots m$, storing them in a vector.

An Optimization Problem A General Implementation Computed Examples

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- 2 At each step compute the function values $a_l F(x_l)$, $l = 1 \dots m$, storing them in a vector.
- Compute the necessary 19 Hessian values ∑_{l=0}^m a_lF(x_l)x_l^{α-2}, α = 2...20. If we properly create our matrix – of stored abscissa values raised to powers – we will be able to compute the Hessian values by simply multiplying our vector from Step 2 by this matrix.

An Optimization Problem A General Implementation Computed Examples

Complete Optimized Process

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- Compute the necessary 19 Hessian values ∑_{l=0}^m a_lF(x_l)x_l^{α-2}, α = 2...20. If we properly create our matrix – of stored abscissa values raised to powers – we will be able to compute the Hessian values by simply multiplying our vector from Step 2 by this matrix.
- Use the resultant 19 values to build the Hessian and gradient and then solve for the next iterate.

An Optimization Problem A General Implementation Computed Examples

For consistency, all examples in this subsection used:

- 24 digits of precision
- 20 abscissas
- A Newton step size of 1/2
- 8 moments unless otherwise specified
- A t value of $\frac{1}{2}$ unless otherwise specified
- The objective function of $s \rightarrow \frac{6}{10} + sin(3\pi s^2)$ unless otherwise specified.

An Optimization Problem A General Implementation Computed Examples

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- 20 abscissas
- A Newton step size of 1/2
- 8 moments unless otherwise specified
- A t value of $\frac{1}{2}$ unless otherwise specified
- The objective function of $s \rightarrow \frac{6}{10} + sin(3\pi s^2)$ unless otherwise specified.

This reduced step dramatically improved convergence for t near 1. While this precision is higher than would be used in production code, it allows us to see the optimal performance of the algorithm.

An Optimization Problem A General Implementation Computed Examples

Visualizing Accuracy

We ask *Maple* to compute until the error, as measured by the norm of the gradient, is less than 10^{-10} . At 46 iterations we obtain λ values:

> -0.7079161355, 10.64405426, -126.5979784, 656.6020449, -1458.868219, 1329.347874 -299.1180785, -112.3114246

where the error is about 6.84330e - 11.

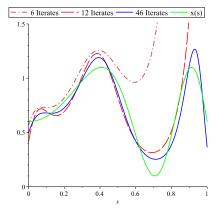


Figure: The primal solutions for iterates 6, 12, and 46. The primal $\frac{9000}{100}$

An Optimization Problem A General Implementation Computed Examples

Variation of t

- We consider five different possible values for *t*: 0, .25, .5, .75, 1.
- We run Newton's Method for each case until meeting the requirement that the norm of the gradient is less than or equal to 10⁻¹⁰.
- Notice that as t increases the visual fit increases substantially. One cannot determine this from looking at the numerical error alone.

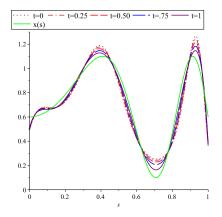


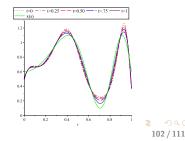
Figure: The associated primal solutions for various choices of $t_{101/111}^{\circ,\circ,\circ}$

An Optimization Problem A General Implementation Computed Examples

Solutions for Various Choices of t

| t | 0 | .25 | .5 | .75 | 1 |
|-------------|-------------|-------------|-------------|------------|-------------|
| λ_1 | 707916 | 404828 | 101065 | .204002 | .512307 |
| λ_2 | 10.6440 | 9.46383 | 8.23003 | 6.90162 | 5.36009 |
| λ_3 | -126.597 | -114.651 | -101.923 | -87.8556 | -70.8919 |
| λ_4 | 656.602 | 605.686 | 550.755 | 488.934 | 412.561 |
| λ_5 | -1458.86 | -1368.32 | -1269.02 | -1154.26 | -1007.13 |
| λ_6 | 1329.34 | 1282.68 | 1227.95 | 1157.70 | 1054.85 |
| λ_7 | -299.118 | -329.937 | -358.596 | -381.447 | -391.764 |
| λ_8 | -112.311 | -85.1887 | -57.6202 | -30.1516 | -3.12491 |
| Error | 6.84330e-11 | 9.81661e-11 | 8.26865e-11 | 9.6666e-11 | 7.05698e-11 |
| Iterates | 46 | 46 | 47 | 47 | 47 |

Dual solutions corresponding to various choices of t are shown in the Table while primal solutions are shown to the right.



An Optimization Problem A General Implementation Computed Examples

Varying the Number of Moments

- We consider the choice of 4, 8, 12, and 20 moments.
- We run Newton's Method for each case until meeting the requirement that the norm of the gradient is less than or equal to 10⁻¹⁰.
- While we used 26 digits of precision for all of these examples (for consistency), this was the only case wherein we used 20 moments and so exploited the employment of such high precision.

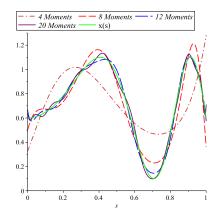


Figure: The primal solutions for various numbers of moments

Changing the Objective Function: A Pulse

- We compute with the pulse: $x(s) = \chi_{[0,\frac{1}{2}]}(s).$
- The pulse is a more computationally challenging example because of its jump discontinuity and constancy on an open interval.
- This slowed the convergence of the gradient to zero with more moments, especially for values of *t* nearer to 1.
- The desired properties can still be seen visually.

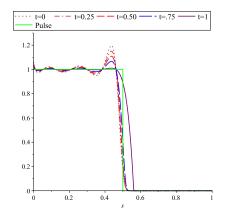


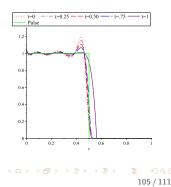
Figure: The primal solutions for various numbers of moments

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Meeting with Lambert W Meeting with Meijer-G Experimental Mathematics and W Convex Analysis Homotopy and Entropy Solutions of Inverse Problems Conclusion Changing the Objective Function: A Pulse

| t | 0 | .25 | .5 | .75 | 1 |
|----------|-------------|-------------|-------------|------------|-----------|
| Error | 6.87225e-11 | 7.45516e-11 | 9.69259e-11 | 1.9136e-11 | .21252e-5 |
| Iterates | 70 | 62 | 55 | 48 | 200 |

- We instruct *Maple* to stop computing once the norm of the gradient is less than 10⁻¹⁰ or after reaching 200 iterates.
- For t = 1, we reached 200 iterates before the norm of the gradient was less than 10^{-10} , but the primal solution we obtained is still a good proxy for the pulse. This can be seen in the Figure, where the Gibbs Phenomenon may also be clearly observed for the the other values of t.



Meeting with Lambert W Meeting with Meijer-G Experimental Mathematics and W Convex Analysis Homotopy and Entropy Solutions of Inverse Problems Conclusion When a Closed Form is not Forthcoming

Even when one is not able to produce a closed form, *SCAT* and its numerical partner *CCAT* may still help.

Example:
$$f := (0, \infty) \to \mathbb{R}$$
 by
$$f(x) = \left(\frac{x}{e}\right)^x$$

SCAT does not return a closed form but still produces the plot shown.

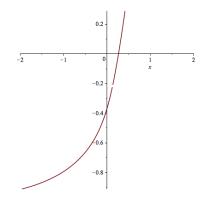


Figure: The Conjugate of f

Further Merits of SCAT and CCAT Bibliography

Another Example: log Γ

For the conjugate, SCAT returns:

$$RootOf(-\Psi(_Z) + x)x - \log(\Gamma(RootOf(-\Psi(_Z) + x))).$$

where Ψ is the Psi function.

Maple's root finder struggles, leaving the plot incomplete. This can be obviated by a Newton solver for x > 0 of $\Psi(x) = y$. Set

$$x_0 = \begin{cases} \exp(y) + 1/2 & \text{if } y \ge -2.2\\ -1/(y - \Psi(1)) & \text{otherwise} \end{cases}$$
$$x_{n+1} = x_n - \frac{\Psi(x_n) - y}{\Psi'(x_n)}.$$

– Ψ and Ψ' are also known as digamma and trigamma functions.

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Further Merits of SCAT and CCAT Bibliography

Another Example: log Г

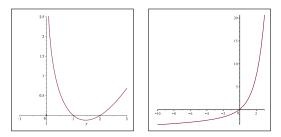


Figure: The function $\log \Gamma$ (L) and its conjugate (R).

- We hope that we have made a good advertisement for the value of W in optimisation and elsewhere.
- We also hope we have highlighted the usefulness of SCAT and its numerical partner CCAT.

Further Merits of SCAT and CCAT Bibliography

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