Maximum Entropy-type Methods and (Non-)Convex Programming

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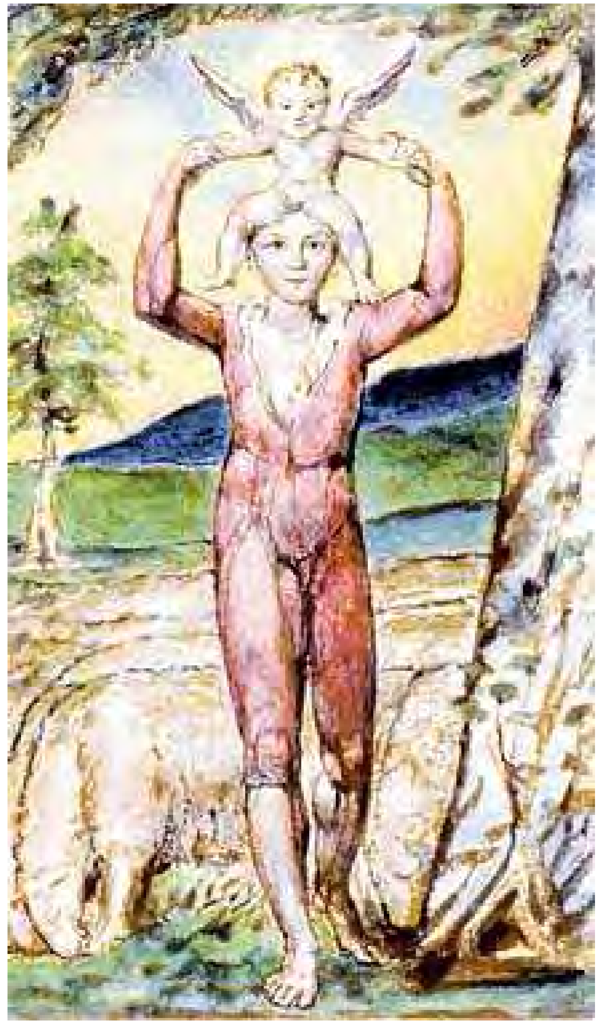
BRAGG and BLAKE

"I feel so strongly about the wrongness of reading a lecture that my language may seem immoderate. ··· The spoken word and the written word are quite different arts. ··· I feel that to collect an audience and then read one's material is like inviting a friend to go for a walk and asking him not to mind if you go alongside him in your car."

(**Sir Lawrence Bragg**)
Nobel Crystallographer



Songs of Innocence and Experience (1825)

SANTAYANA

"If my teachers had begun by telling me that mathematics was pure play with presuppositions, and wholly in the air, I might have become a good mathematician. But they were overworked drudges, and I was largely inattentive, and inclined lazily to attribute to incapacity in myself or to a literary temperament that dullness which perhaps was due simply to lack of initiation."

(**George Santayana**)
Persons and Places, 1945, 238–9.

TWO FINE REFERENCES

1. J.M. Borwein and Qiji Zhu, *Techniques of Variational Analysis*, CMS/Springer-Verlag, New York, 2005.

2. J.M. Borwein and A.S Lewis, *Convex Analysis and Nonlinear Optimization*, CMS/Springer-Verlag, 2nd expanded edition, New York, 2005.

OUTLINE

I shall discuss in "tutorial mode" the formalization of inverse problems such as signal recovery and option pricing as (convex and non-convex) optimization problems over the infinite dimensional space of signals. I shall touch on* the following:

1. The impact of the choice of "entropy" (e.g., Boltzmann-Shannon, Burg entropy, Fisher information) on the *well-posedness* of the problem and the form of the solution.

2. Convex programming duality: what it is and what it buys you.

3. Algorithmic consequences.

4. Non-convex extensions: life is hard.

♠ Related papers at `http://locutus.cs.dal.ca:8088/`

*More is an unrealistic task!

THE GENERAL PROBLEM

• Many applied problems reduce to "**best**" solving (under-determined) systems of linear (or non-linear) equations $\boxed{Ax = b}$, where $b \in \mathbb{R}^n$, and the unknown x lies in some appropriate function space.

Discretization reduces this to a finite-dimensional setting where A is now a $m \times n$ matrix.

◇ In many cases, I believe it is better to address the problem in its function space home, discretizing only as necessary for computation.

• Thus, the problem often is *how do we estimate x from a finite number of its 'moments'*? This is typically an under-determined linear inversion problem where the unknown is most naturally a function, not a vector in $\mathbb{R}^m$.

EXAMPLE 1. AUTOCORRELATION

• Consider, extrapolating an *autocorrelation function* $R(t)$ given sample measurements.

◇ The Fourier transform $S(z)$ of the autocorrelation function is the power spectrum of the data.

> Fourier moments of the power spectrum are the same as samples of the autocorrelation function, so by computing several values of $R(t)$ directly from the data, we are in essence computing moments of $S(z)$.

• If we compute a finite number of moments of S, we can then estimate S from these moments, and *we may compute more moments* from the estimate $\widehat{S}$ by direct numerical integration, thereby affording an *extrapolation* of R, without directly computing R from the potentially noisy data.

THE ENTROPY APPROACH

• Following (B-Zhu) I sketch a maximum entropy approach to under-determined systems where the unknown, x, is a function, typically living in a *Hilbert space*, or more general space of functions.

This technique picks a "best" representative from the infinite set of *feasible* functions (functions that possess the same n moments as the sampled function) by minimizing an integral functional, f, of the unknown.

http://projects.cs.dal.ca/ddrive

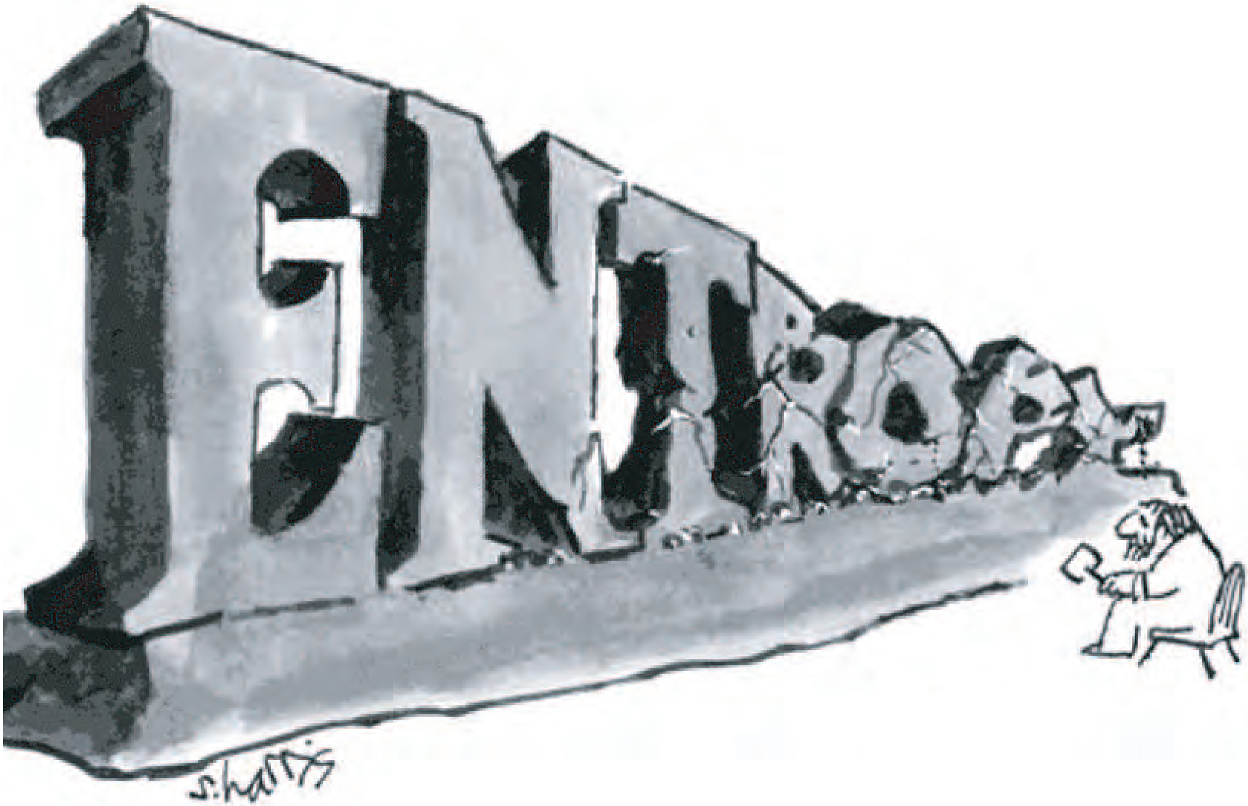
◇ The approach finds applications including:

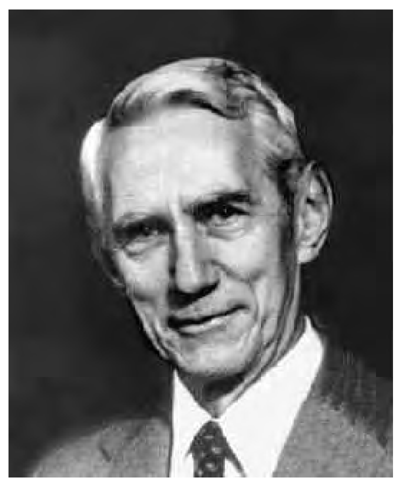
acoustics, constrained spline fitting, image reconstruction, inverse scattering, optics, option pricing, multidimensional NMR, tomography, statistical moment fitting, and time series analysis, etc (1,000's of papers).

• However, the derivations and mathematics are fraught with subtle errors.

I will discuss some of the difficulties inherent in infinite dimensional calculus, and provide a simple theoretical algorithm for correctly deriving maximum entropy-type solutions.

WHAT is





Boltzmann (1844-1906) **Shannon (1916-2001)**

WHAT is ENTROPY?

Despite the narrative force that the concept of entropy appears to evoke in everyday writing, in scientific writing entropy remains a thermodynamic quantity and a mathematical formula that numerically quantifies disorder. When the American scientist Claude Shannon found that the mathematical formula of Boltzmann defined a useful quantity in information theory, he hesitated to name this newly discovered quantity entropy because of its philosophical baggage. The mathematician John Von Neumann encouraged Shannon to go ahead with the name entropy, however, since "no one knows what entropy is, so in a debate you will always have the advantage."

- **19C**: **Boltzmann**—thermodynamic *disorder*
- **20C**: **Shannon**—information *uncertainty*
- **21C**: **JMB**—potentials with *superlinear growth*

CHARACTERIZATIONS of ENTROPY

- Information theoretic characterizations abound. A nice one is:

Theorem 1 $H(\overrightarrow{p}) = -\sum_{k=1}^{N} p_k \log p_k$ *is the unique continuous function (up to a positive scalar multiple) on finite probabilities such that*

I. Uncertainly grows:

$$H\left(\overbrace{\frac{1}{n}, \frac{1}{n}, \cdots, \frac{1}{n}}^{n}\right)$$

increases with n.

II. Subordinate choices are respected: for distributions $\overrightarrow{p_1}$ and $\overrightarrow{p_2}$ and $0 < p < 1$,

$$H\left(p\,\overrightarrow{p_1}, (1-p)\,\overrightarrow{p_2}\right) = p\,H(\overrightarrow{p_1}) + (1-p)\,H(\overrightarrow{p_2}).$$

ENTROPIES FOR US

• Let X be our *function space*, typically Hilbert space $L^2(\Omega)$, or the function space $L^1(\Omega)$ (or a Sobelov space).

◇ For $p \geq 1$,

$$L^p(\Omega) = \left\{ x \text{ measurable } : \int_\Omega |x(t)|^p dt < \infty \right\}.$$

It is well known that $L^2(\Omega)$ is a Hilbert space with *inner product*

$$\langle x, y \rangle = \int_\Omega x(t)y(t)dt.$$

• A *bounded linear map* $A : X \to \mathbb{R}^n$ is determined by

$$(Ax)_i = \int x(t)a_i(t)\, dt$$

for $i = 1, \ldots, n$ and $a_i \in X^*$ the 'dual' of X (L^2 in the Hilbert case, L^∞ in the L^1 case).

• To pick a solution from the infinitude of possibilities, we may freely define "**best**".

$\otimes$ The most common approach is to find the minimum norm solution*, by solving the *Gram system*

$$\boxed{AA^T\lambda = b}\ .$$

$\oplus$ The solution is then $\widehat{x} = A^T\lambda$. This recaptures all of *Fourier analysis*!

• This actually solved the following *variational problem*:

$$\inf\left\{\int_\Omega x(t)^2 dt : Ax = b \ \ x \in X\right\}.$$

*Even in the (realistic) infeasible case.

• We generalize the norm with a *strictly convex functional* f as in

$$\min\{f(x) : Ax = b,\ \ x \in X\}, \qquad (P)$$

where f is what we call, an *entropy functional*, $f : X \to (-\infty, +\infty]$. Here we suppose f is a strictly convex integral functional* of the form

$$f(x) = \int_\Omega \phi(x(t))dt.$$

The functional f can be used to include other constraints†. For example, the constrained L^2 norm functional ('**positive energy**'),

$$f(x) = \begin{cases} \int_0^1 x(t)^2 dt & \text{if } x \geq 0 \\ +\infty & \text{else} \end{cases}$$

is used in constrained *spline fitting*.

• Entropy constructions abound: *Bregman* and *Csizar distances* model statistical divergences.

*Essentially $\phi''(t) > 0$.

†Including nonnegativity, by appropriate use of $+\infty$.

• Two popular choices for f are the *Boltzmann-Shannon* entropy (in image processing)

$$f(x) = \int x \ln x,$$

and the *Burg entropy* (in time series analysis),

$$f(x) = -\int \ln x.$$

⋄ *Both implicitly impose nonnegativity* (positivity in Burg case) constraint.

• There has been much information-theoretic debate about which entropy is best.

This is more theology than science!

• More recently, the use of *Fisher Information*

$$f(x, x') = \int \frac{{x'}^2}{2x}$$

has become more usual as it *penalizes* large derivatives; and can be argued for physically.

WHAT 'WORKS' BUT CAN GO WRONG?

• Consider solving $Ax = b$, where, $b \in I\!R^n$ and $x \in L^2[0,1]$. Assume further that A is a continuous linear map, hence represented as above.

• As L^2 is infinite dimensional, and $I\!R^n$ is not, the null space of A is infinite dimensional: if there are any solutions to $Ax = b$, there is an infinite number.

We pick our solution to *minimize*

$$f(x) = \int \phi(x(t))\,dt$$

[$\phi(x(t), x'(t))$ in Fisher-like cases (BN1,BN2)].

• We introduce the *Lagrangian*

$$L(x,\lambda) := \int_0^1 \phi(x(t))dt + \sum_{i=1}^{n} \lambda_i \left(b_i - \langle x, a_i\rangle\right),$$

and the associated *dual problem*

$$\max_{\lambda \in I\!R^n} \min_{x \in X} \{L(x,\lambda)\}. \qquad (D)$$

• So we formally have a "dual pair" (BL1)

$$\min\{f(x) : Ax = b,\ \ x \in X\}, \qquad (P)$$

and

$$\max_{\lambda \in I\!R^n} \min_{x \in X} \{L(x, \lambda)\}. \qquad (D)$$

• Moreover, for the solutions $\widehat{x}$ to (P), $\widehat{\lambda}$ to (D), the derivative (w.r.t. x) of $L(x, \widehat{\lambda})$ should be zero, since $L(\widehat{x}, \widehat{\lambda}) \leq L(x, \widehat{\lambda}), \forall\, x$.

This implies

$$\begin{aligned} \widehat{x}(t) &= (\phi')^{-1} \left(\sum_{i=1}^{n} \widehat{\lambda}_i a_i(t) \right) \\ &= (\phi')^{-1} \left(A^T \widehat{\lambda} \right). \end{aligned}$$

- This allows us to reconstruct the primal solution (qualitatively and quantitatively) from a presumptively easier dual computation.

A DANTZIG ANECDOTE

George wrote in his paper "**Reminiscences about the origins of linear programming,**" 1, 2, *Oper. Res. Letters*, April 1982 (p. 47):

> *"The term Dual is not new. But surprisingly the term Primal, introduced around 1954, is. It came about this way. W. Orchard-Hays, who is responsible for the first commercial grade L.P. software, said to me at RAND one day around 1954: 'We need a word that stands for the original problem of which this is the dual.'*
> *I, in turn, asked my father, Tobias Dantzig, mathematician and author, well known for his books popularizing the history of mathematics. He knew his Greek and Latin. Whenever I tried to bring up the subject of linear programming, Toby (as he was affectionately known) became bored and yawned.*

But on this occasion he did give the matter some thought and several days later suggested Primal as the natural antonym since both primal and dual derive from the Latin. It was Toby's one and only contribution to linear programming: his sole contribution unless, of course, you want to count the training he gave me in classical mathematics or his part in my conception."

A lovely story. I heard George recount this a few times and, when he came to the "conception" part, he always had a twinkle in his eyes. (Saul Gass, Oct 2006)

- In a Sept 2006 *SIAM book review*, I asserted George assisted his father—for reasons I believe but cannot reconstruct.

  I also called Lord Chesterfield, Chesterton (*gulp*!).

PITFALLS ABOUND

There are 2 major problems to this approach.*

1. *The assumption that a solution $\hat{x}$ exists*. For example, consider the problem

$$\inf_{x \in L^1[0,1]} \left\{ \int_0^1 x(t)dt : \int_0^1 tx(t)dt = 1, x \geq 0 \right\}.$$

$\diamond$ The optimal value is not attained. Similarly, existence can fail for the Burg entropy with trig moments. Additional conditions on ϕ are needed to insure solutions exist.† (BL2)

2. *The assumption that the Lagrangian is differentiable*. In the above, f is $+\infty$ for every x negative on a set of positive measure.
$\diamond$ This implies the Lagrangian is $+\infty$ on a dense subset of L^1, the set of functions *not* nonnegative a.e.. The Lagrangian is *nowhere continuous*, much less differentiable.

*A third, the existence of $\hat{\lambda}$, is less difficult to surmount.

†The solution is actually the *absolutely continuous part of a measure* in $C(\Omega)^*$.

FIXING THE PROBLEM

• One approach to circumvent the differentiability problem, is to pose the problem in $L^\infty(\Omega)$, or in $C(\Omega)$, the space of essentially bounded, or continuous, functions. However, in these spaces, even with additional side qualifications, we are not necessarily assured solutions to (P) exist.

◇ In (BL2), there is an example of a problem on $\Omega \subset I\!R^3$, moments the first four Fourier coefficients, and the entropy is Burg's, yet no solutions exist for certain feasible data values.

• Another example, Minerbo poses the problem of tomographic reconstruction in $C(\Omega)$ with the Boltzmann-Shannon entropy. However, there the functions a_i are characteristic functions of strips across Ω, and the solution is piecewise constant, not continuous.

CONVEX ANALYSIS (AN ADVERT)

We prepare to state a theorem that guarantees that the form of solution found in the above faulty derivation $\boxed{\widehat{x} = (\phi')^{-1}(A^T\widehat{\lambda})}$ is, in fact, correct. A full derivation is given in (BL2).

• We introduce the *Fenchel (Legendre) conjugate* (see BL1) of a function $\phi : I\!R \to (-\infty, +\infty]$:

$$\phi^*(u) = \sup_{v \in I\!R}\{uv - \phi(v)\}.$$

• Often this can be (pre-)computed explicitly, using Newtonian calculus. Thus,

$$\phi(v) = v \log v - v, \; -\log v \text{ and } v^2/2$$

yield

$$\phi^*(u) = \exp(u), \; -1 - \log(-u) \text{ and } u^2/2$$

respectively. The red is the *log barrier* of interior point fame!

• The Fisher case is similarly explicit.

EXAMPLE 2. CONJUGATES & NMR

The *Hoch and Stern information measure*, or *neg-entropy*, is defined in complex $n-$space by

$$H(z) = \sum_{j=1}^{n} h(z_j/b),$$

where h is convex and given (for scaling b) by:

$$\boxed{h(z) \triangleq |z| \ln\left(|z| + \sqrt{1+|z|^2}\right) - \sqrt{1+|z|^2}}$$

for *quantum theoretic* (NMR) reasons.

• Recall the *Fenchel-Legendre conjugate*

$$f^*(y) := \sup_x \langle y, x\rangle - f(x).$$

• Our *symbolic convex analysis* package (stored at `www.cecm.sfu.ca/projects/CCA/`, also in Chris Hamilton's package at Dal) produced:

$$h^*(z) = \cosh(|z|)$$

◇ Compare the *Shannon entropy*:

$$(z \ln z - z)^* = \exp(z).$$

COERCIVITY AND DUALITY

• We say ϕ possess *regular growth* if either $d = \infty$, or $d < \infty$ and $k > 0$, where $d = \lim_{u\to\infty} \phi(u)/u$ and $k = \lim_{v\uparrow d}(d-v)(\phi^*)'(v)$.*

• The *domain* of a convex function is $\mathrm{dom}(\phi) = \{u : \phi(u) < +\infty\}$; ϕ is *proper* if $\mathrm{dom}(\phi) \neq \emptyset$. Let $\imath = \inf \mathrm{dom}(\phi)$ and $\sigma = \sup \mathrm{dom}(\phi)$.

• Our *constraint qualification*,† (CQ), reads

$$\exists\, \overline{x} \in L^1(\Omega), \text{ such that } A\overline{x} = b, \\ f(\overline{x}) \in \mathbb{R}, \ \ \imath < \overline{x} < \sigma \ \ a.e.$$

◇ *In many cases, (CQ) reduces to feasibility*, and trivially holds.

• In this language, the *dual problem* for (P) is

$$\sup \left\{ \langle b, \lambda \rangle - \int_\Omega \phi^*(A^T \lambda(t))dt \right\}. \qquad (D)$$

*-log does nor possess regular growth; $v \to v \ln v$ does.

†The standard Slater's condition fails; this is what guarantees dual solutions exist.

Theorem 1 *(BL2) Suppose Ω is a finite interval, μ is Lebesgue measure, each a_k continuously differentiable (or just locally Lipschitz) and ϕ is proper, strictly convex with regular growth.*

Suppose (CQ) holds and also
(1)

$$\exists\, \tau \in I\!R^n \text{ such that } \sum_{i=1}^{n} \tau_i a_i(t) < d \quad \forall t \in [a,b],$$

then the unique solution to (P) is given by

$$\hat{x}(t) = (\phi^*)'(\sum_{i=1}^{n} \hat{\lambda}_i a_i(t)) \tag{2}$$

where $\hat{\lambda}$ is any solution to dual problem (D).

• This theorem generalizes to cover $\Omega \subset I\!R^n$, and more elaborately in Fisher-like cases. These results can be found in (BL2, BN1).

• What this means is that the form of the maximum entropy solution can be legitimated simply by validating the *easily* checked conditions of Theorem 1.

♠ Also, any solution to $Ax = b$ of the form in (2) is automatically a solution to (P).

Thus, solving (P) is equivalent to solving for $\lambda \in \mathbb{R}^n$

$$(3) \qquad \langle (\phi^*)'(A^T\lambda), a_i \rangle = b_i, \quad i = 1, \ldots, n,$$

a *finite dimensional* set of non-linear equations.

> One can then apply a standard 'industrial strength' nonlinear equation solver, like Newton's method, to this system, to find the optimal λ.

• Often, $\boxed{(\phi')^{-1} = (\phi^*)'}$ and so the 'dubious' solution agrees with the 'honest' solution.

Importantly, we may tailor $(\phi')^{-1}$ to our needs.

• Note that discretization is only needed to compute the terms in (3). Indeed, *these integrals can sometimes be computed exactly* (in some tomography and option estimation problems, [BCM]). This is what we gain by *not discretizing* too early.

> By waiting to see what form the dual problem takes, one can customize one's integration scheme to the problem at hand.

◇ Even when this is not the case one can often use the shape of the dual solution to fashion very *efficient heuristic reconstructions* that avoid any iterative steps (see BN2).

$\mathcal{M}$om$\mathcal{E}$nt+

• The $\mathcal{M}$om$\mathcal{E}$nt+ project at CECM, provides teaching code (`www.cecm.sfu.ca/interfaces/`, soon being moved to Dalhousie) implementing the entropic reconstructions described above.

◇ Moments, entropies and problem dimension are easily varied. It also allows adding noise and allowing relaxations of the constraints, and several methods of solving the dual, including

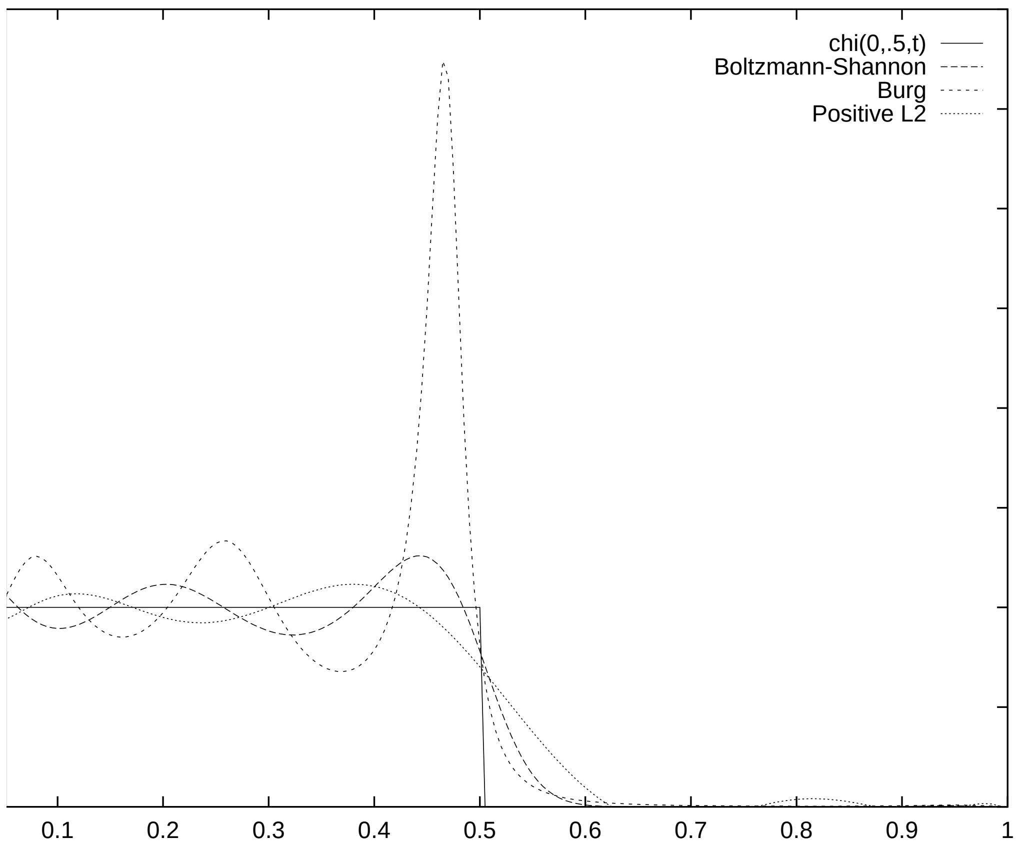
Newton and quasi-Newton methods (BFGS, DFP), conjugate gradients, Barzilai-Borwein line-search free method.

• For iterative methods I recommend:

H.H. Bauschke and J.M. Borwein, "On projection algorithms for solving convex feasibility problems," *SIAM Review*, **38** (1996), 367–426, (cited over 133 times!) and a forthcoming CMS book by *Bauschke and Combettes*.

COMPARISON OF ENTROPIES

• The positive L^2, Boltzmann-Shannon and Burg entropy reconstruction of the **characteristic function** of $[0, 1/2]$ using *10 algebraic moments* ($b_i = \int_0^{1/2} t^{i-1} dt$) on $\Omega = [0, 1]$.



• **Solution**: $\widehat{x}(t) = (\phi^*)'(\sum_{i=1}^{n} \widehat{\lambda}_i t^{i-1})$.
Burg over-oscillates since $(\phi^*)'(t) = 1/t$.

THE NON-CONVEX CASE

• In general non-convex optimization is a much less satisfactory field. We can usually hope only to find critical points ($f'(x) = 0$) or local minima. Thus, problem-specific heuristics dominate.

• **Crystallography**: We of course wish to estimate x in $L^2(\mathbb{R}^n)$* Then the modulus $c = |\widehat{x}|$ is known ($\widehat{x}$ is the Fourier transform of x).†

Now $\{y\colon |\widehat{y}| = c\}$, is not convex. So the issue is to find x given c and other convex information. An appropriate optimization problem extending the previous one is

$$\min \{f(x) : Ax = b, \|Mx\| = c, \ \ x \in X\}, \quad (NP)$$

where M models the modular constraint, and f is as in Theorem 1.

*Here $n = 2$ for images, 3 for holographic imaging, etc.

†Observation of the modulus of the **diffracted image in crystallography**. Similarly, for **optical aberration** correction.

A CRYSTALLOGRAPHIC CAUTION

• My Parisian collaborator Patrick Combettes is expert on various optimization perspectives on cognates to (NP) and related feasibility problems.

◇ Most methods rely on a two-stage (easy convex, hard non-convex) decoupling schema—the following from Decarreau et al. (D). They suggest solving

$$\min\left\{f(x) : Ax = y, \|B_k y\| = b_k,\ \ x \in X\right\}, \tag{NP^*}$$

where $\|B_k y\| = b_k,\ k \in K$ encodes the hard modular constraints.

• They solve formal *first-order Kuhn-Tucker conditions* for a relaxed form of (NP^*). The easy constraints are treated by Thm 1.

I am obscure, largely because the results were largely negative:

• They applied these ideas to **a prostaglandin molecule (25 atoms)**, with <u>known</u> structure, using quasi-Newton (which could fail to find a local min), truncated Newton (better) and trust-region (best) numerical schemes.

◇ They observe that the "*reconstructions were often mediocre*" and highly dependent on the amount of prior information – a small proportion of unknown phases to be satisfactory.

> "**Conclusion**: It is fair to say that the entropy approach has limited efficiency, in the sense that it requires a good deal of information, especially concerning the phases. Other methods are wanted when this information is not available."

• Thus, I offer this part of my presentation largely to illustrate the difficulties.

AND SOME HOPE FROM HUBBLE

• The (human-ground) lens was mounted upside-down. It had a micro-metric asymmetry. The back-up (computer-ground) lens is perfect, back here on earth!

◇ NASA challenged ten teams to devise algorithmic fixes.

• **Optical aberration correction**, using the *Misell algorithm*, a *method of alternating projections*, works much better than it should—given that it is being applied to find a member of a version of

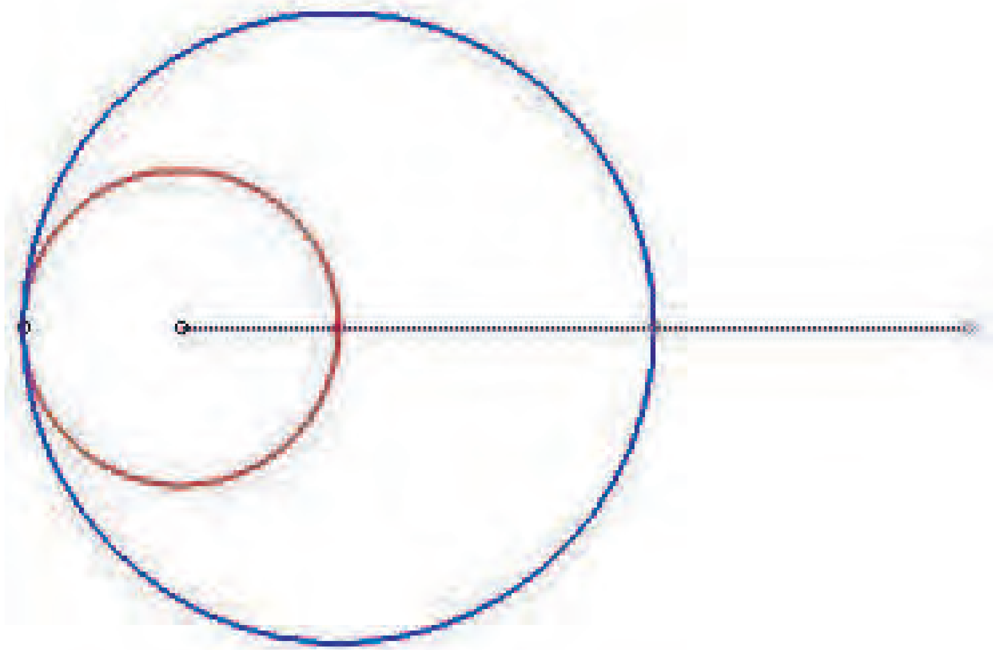
$$\Psi := \bigcap_{k \in K} \{x : Ax = b, \|M_k x\| = c_k, \ \ x \in X\}, \tag{NCFP}$$

which is a **non-convex feasibility problem**.

Hidden Convexity?

NON-CONVEX PROJECTION CAN FAIL

• Consider the **alternating projection method** to find the point on the **line-segment A** (convex) and the blue **circle B** (non-convex)



• If we start on the line-segment outside the *red circle*, we converge to the intersection. If we start inside the red circle we find a period two 'least-distance' solution.

EXAMPLE 3. HUBBLE TELESCOPE

- **Electromagnetic field:** $u : \mathbb{R}^2 \to \mathbb{C} \in L^2$

- **Data:** Field intensities for $m = 1, 2, \ldots, M$:

$$\psi_m : \mathbb{R}^2 \to \mathbb{R}_+ \in L^1 \cap L^2 \cap L^\infty$$

- **Model:** For $\mathcal{F}_m : L^2 \to L^2$, a *modified Fourier Transform*,

$$|\mathcal{F}_m(u)| = \psi_m \quad \forall m = 1, 2, \ldots, M$$

♣ **Inverse problem:** Given transforms $\mathcal{F}_m$ and field intensities ψ_m (for $m = 1, \ldots, M$), **find** u.

TWO APPROACHES

I. Non-convex (in)feasibility problem: Given $\psi_m \neq 0$, define $\mathbb{Q}_0 \subset L^2$ convex, and

$$\mathbb{Q}_m := \left\{u \in L^2 \mid |\mathcal{F}_m(u)| = \psi_m \; a.e.\right\} \quad \text{(nonconvex)}$$

we wish to find

$$u \in \bigcap_{m=0}^{M} \mathbb{Q}_m = \emptyset.$$

⊙ via an *alternating projection method*: e.g., for two sets A and B, **compute**

$$x \to P_A(x) =: y \to P_B(y) =: x$$

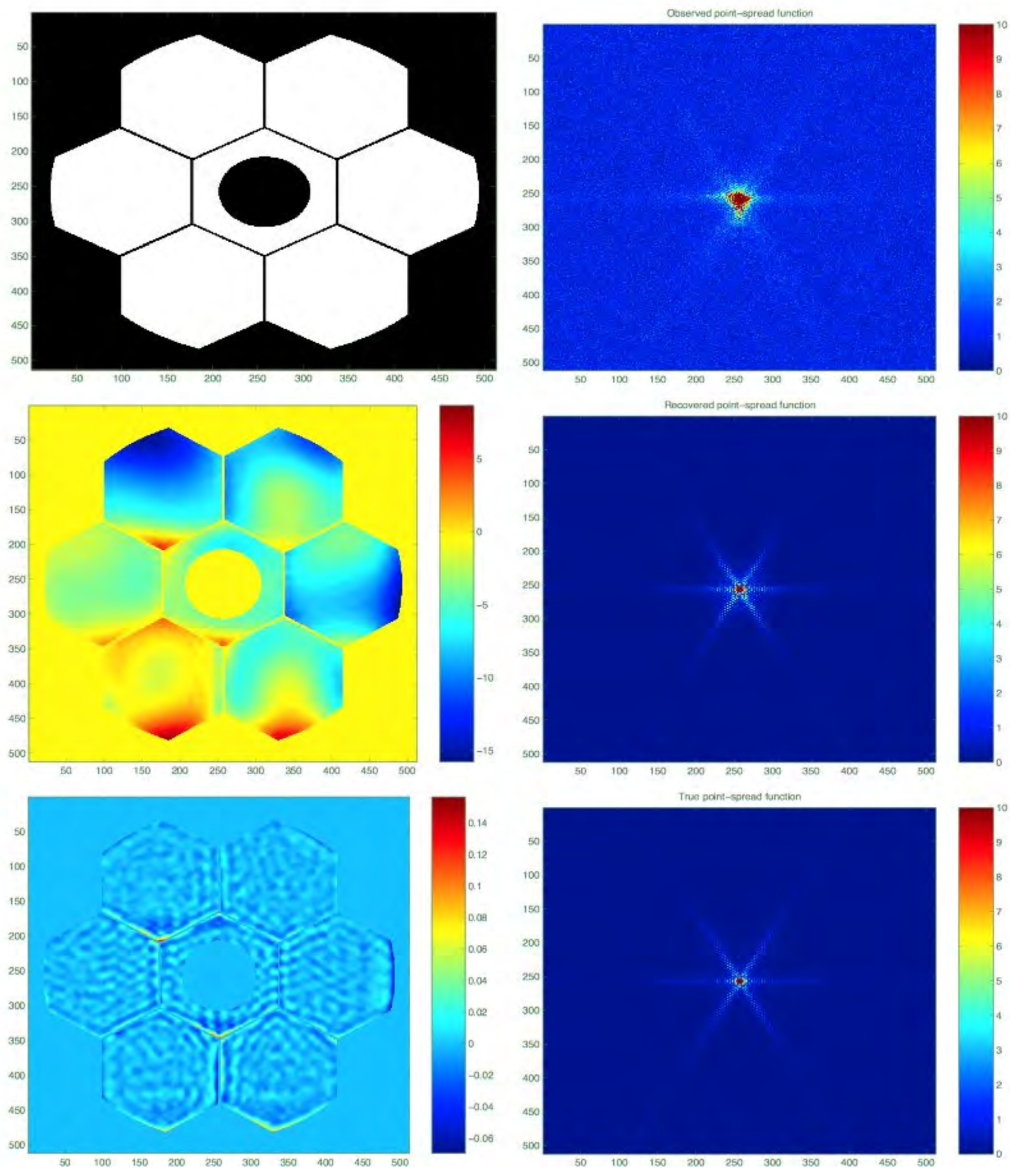
and **repeat** (this parallelizes neatly).

II. Error reduction of a nonsmooth objective: for fixed $\beta_m > 0$, we attempt to solve

$$\text{minimize} \quad E(u) := \sum_{m=0}^{M} \frac{\beta_m}{2} \text{dist}^2(u, \mathbb{Q}_m)$$

$$\text{over} \quad u \in L^2.$$

A SAMPLE RECONSTRUCTION (via II)



Top row: data

Middle: reconstruction

Bottom: truth and error

NOTE FROM RUSSELL LUKE

- **The optics community** calls the projection algorithms *Iterative Transform Algorithms*.

  They used an algorithm which they call the *Misell Algorithm* on Hubble, but it's really just averaged projections. The best projection algorithm I found was *cyclic projections* (with no relaxation).

- **The crystallography problem** is similar, but not the same. For this, the best known algorithm is what the optics community calls the *Hybrid Input-Output algorithm*.

  Heinz, Patrick and I showed thi is the *Lyons-Mercier*,also called the *Douglas-Rachford algorithm*, depending on who you talk to.

EXAMPLE 4. INVERSE SCATTERING

• **Central problem:** determine the location and shape of buried objects from measurements of the *scattered field* after illuminating a region with a known *incident field.*

• **Recent techniques:** determine if a point z is inside or outside of the scatterer by determining *solvability* of the linear integral equation

$$\mathcal{F} g_z \stackrel{?}{=} \varphi_z$$

where $\mathcal{F} \to X$ is a compact linear operator constructed from the observed data, and $\varphi_z \in X$ is a known function parameterized by z.

• $\mathcal{F}$ has *dense range*, but if z is on the exterior of the scatterer, then $\varphi_z \notin$Range($\mathcal{F}$).

• Since $\mathcal{F}$ is compact, any numerical implementation to solve the above integral equation will need some *regularization scheme*.

• If *Tikhonov regularization* is used—in a restricted physical setting—the solution to the regularized integral equation, $g_{z,\alpha}$, has the behaviour

$$||g_{z,\alpha}|| \to \infty \quad \text{as} \quad \alpha \to 0$$

if and only if z is a point outside the scatterer.

• **An important open problem** is to determine the behavior of regularized solutions $g_{z,\alpha}$ under different regularization strategies.

In other words, when can these techniques fail? (On going joint work with Russell Luke: also in *Experimental Math in Action*, AKP, 2006)

OTHER REFERENCES

BCM J.M. Borwein, R. Choksi and P. Maréchal, "Probability distributions of assets inferred from option prices via the Principle of Maximum Entropy," *SIAM J. Optimization*, **4** (2003), 464–478.

BL1 J.M. Borwein and A.S. Lewis, *Convex Analysis and Nonlinear Optimization. Theory and Examples*, CMS Books, Springer-Verlag, New York, 2000.

BL2 J. M. Borwein and A. S. Lewis, "Duality relationships for entropy–like minimization problems," *SIAM J. Control and Optim.*, **29** (1991), 325–338.

BLi J.M. Borwein and M.A. Limber, "Under-determined moment problems: a case for convex analysis," *SIAMOPT*, Fall 1994.

BN1 J.M. Borwein, A.S. Lewis, M.N. Limber and D. Noll, "Maximum entropy spectral analysis using first order information. Part 2," *Numerische Mathematik*, **69** (1995), 243–256.

BN2 J. Borwein, M. Limber and D. Noll, "Fast heuristic methods for function reconstruction using derivative information," *App. Anal.*, **58** (1995), 241–261.

D A. Decarreau, D. Hilhorst, C. LeMaréchal and J. Navaza, "Dual methods in entropy maximization. Application to some problems in crystallography," *SIAM J. Optim.* **2** (1992), 173–197.