What Sparsity and ℓ_1 Optimization Can Do For You

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(Joint with many people)

Begin with related notions

(1) Compressive Sensing
D. Donoho, E. Candes, T. Tao (2006)
Sparse Recover via L1 Minimization

(2) Fast Optimization Algorithms for L1 Related Problems
(Including Total Variation)
S.O., W. Yin, M. Burger, D. Goldfarb (2006)

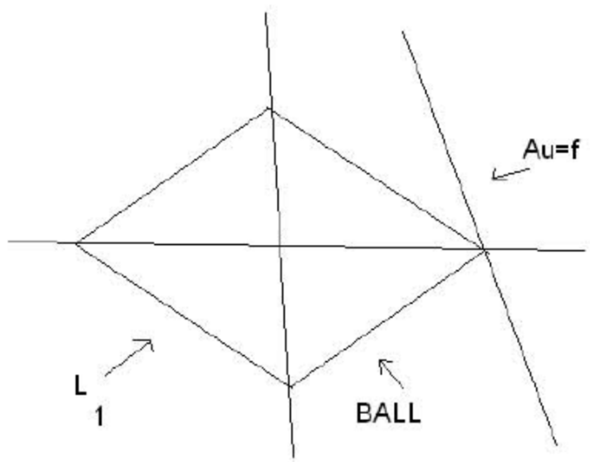
(3) PDE and Variational Methods for Image Processing
L.I. Rudin, S.O., E. Fatemi (1989)

(4) Level Set Methods
S.O., J.A. Sethian (1987)

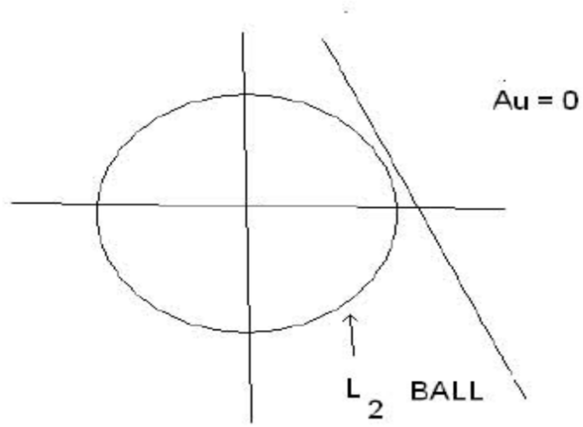
L_1 minimization $\Rightarrow L_0$ minimization

Old idea (Galileo?!!)

$$u = \arg\min_{u \, \varepsilon \, R^N} |u|_1 \quad \text{such that} \quad Au = f$$



Intersection on an axis with probability = 1 sparse!



Intersects off axes with probability = 1 nonsparse!

Example:

$$A_{1XN} = [a_1 \ldots a_N], \;\; u \,\varepsilon\, R^N, \;\; f \,\varepsilon\, R^1$$

$$\sum_{i=1}^{N} a_i u_i = f$$

$$L_1 \text{ minimum: Suppose } |a_k| > a_j, \;\; j \neq k$$

$$L_1 \text{ minimum}: U_{\text{opt}} = \left[0 \ldots, \frac{f}{a_k}, 0 \ldots 0 \right]^T \text{ sparse}$$

$$L_2 \text{ minimum}: U_{\text{opt}} = \left(\sum_{i=1}^{N} (a_i)^2 \right)^{-1} \left[a, \ldots a_N \right]^T f, \text{ nonsparse}$$

Compressed Sensing (CS)

- Compressed sensing techniques constructs high resolution images from a small number of measurements
- If done properly, then the image constructed from the small data set is exactly equivalent to the original image constructed from the large data set.
  - T. Tao, E. Candes, and D.L. Donoho
  - For this to work, the data must be acquired in a different “basis” than the underlying image

CS MRI

- In MRI, we do not directly acquire images, we acquire “K-Space” data

  -- The actual image is reconstructed by taking the Fourier transform of the K-Space data

- With CS, we can reconstruct a high-quality/high-resolution image from a fraction of the K-space data

  -- This allows image acquisition to be done 3-5 times faster

Work being done at UCLA

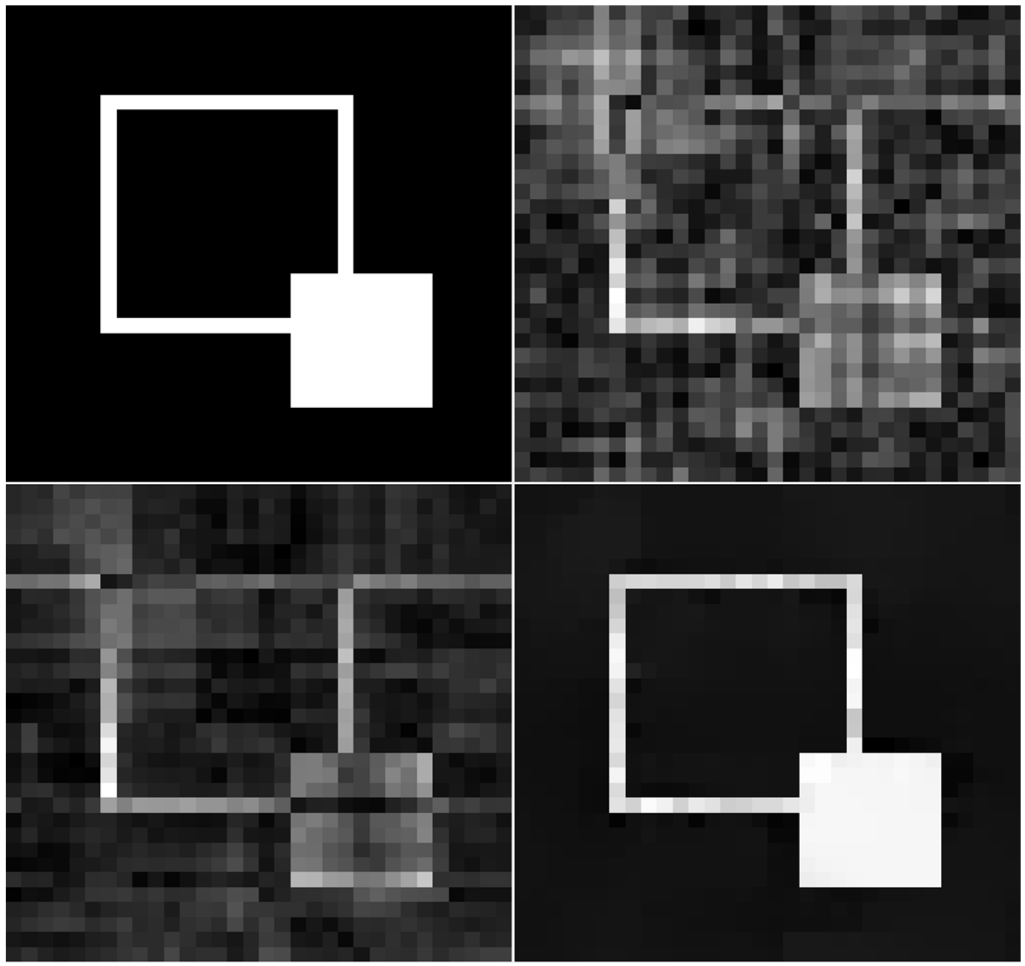
- CS allows high resolution images to be acquired much faster than conventional techniques
- Drawback: It is very difficult to compute the image reconstructions
- At UCLA, we develop new algorithms, such as the “Split Bregman Method” that allow these images to be reconstructed quickly (less than 1 second per image)
- Our techniques also allow CS to be done using “TV regularization” – an idea pioneered in Los Angeles that yields results superior to other CS methods

A simulated Example (artificial data)

Original Image

(Full K-Space)

Conventional Reconstruction using 25% of K-space data



CS reconstruction using Wavelet Basis

CS - Split Bregman method using only 25% of K-Space data

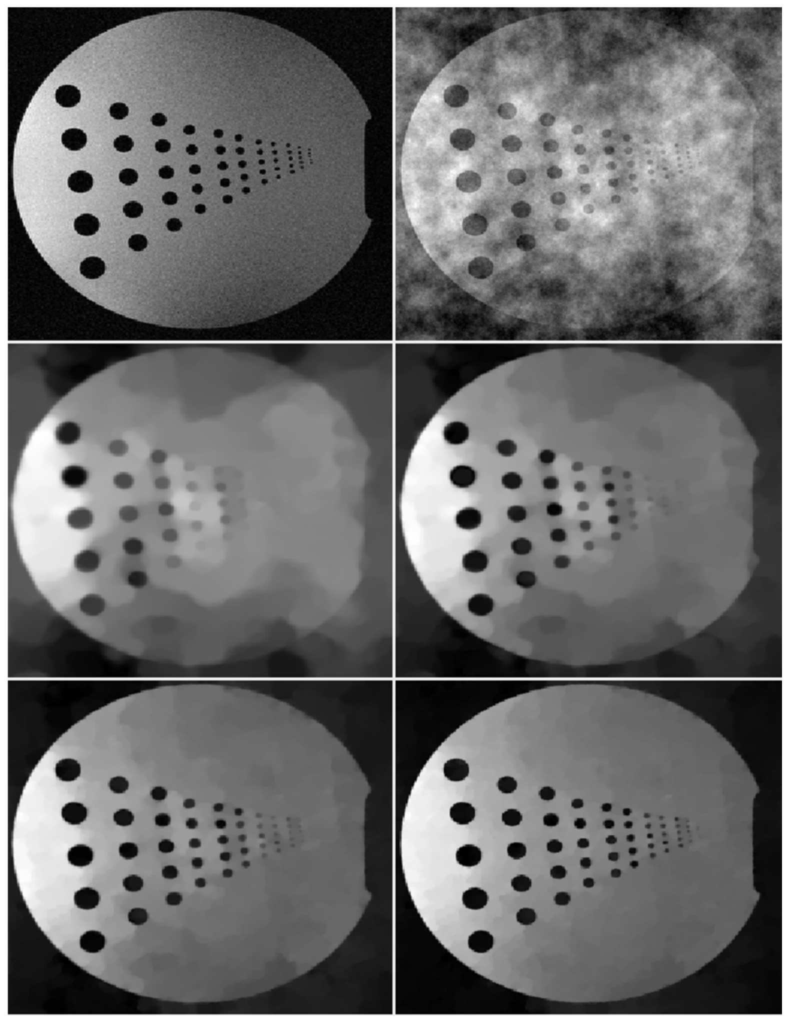
An Example using a real MR image (a phantom)

Original Image

(Full K-Space)

Conventional Fast Acquisition Method

(30% OF k-Space data)



10 iterations of Split Bregman Method

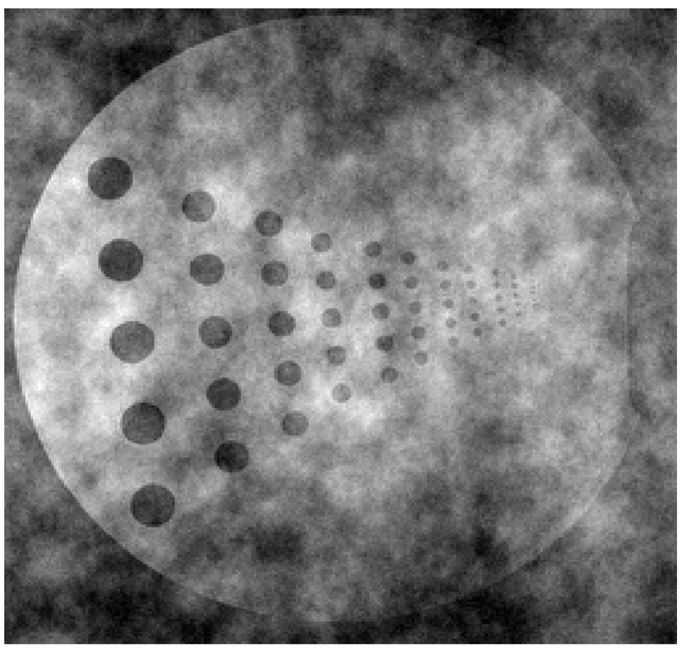
20 iterations of Split Bregman Method

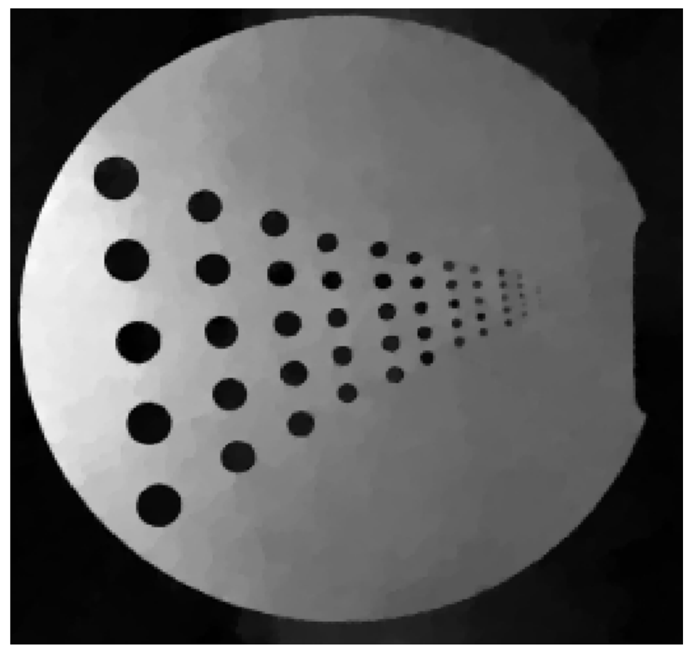
30 iterations of Split Bregman Method

Final reconstruction using only 30% of K-Space data

Comparison of CS to conventional techniques

- Both images below were acquired using only 35% of K-Space data
- Image on the left was reconstructed using a conventional technique (fill all unknown K-Space data with zeros)
- Image on right was reconstructed using Compressed Sensing





Conclusion

- CS is a technique that allows MR images to be reconstructed from small amounts of K-Space data without sacrificing resolution or quality
- Using this technique, MRI acquisition can be sped up to 3-5 times the speed of conventional techniques that use full K-Space acquisitions

The Bregman Methods: Reviews and New Error Cancellation Results

With Wotao Yin

Bregman iteration has been unreasonably successful in

1. Better regularization quality over ℓ_1, total variation, ...
2. Fast, accurate iterations for *constrained* ℓ_1-like minimization.

Points 1 and 2 are different!

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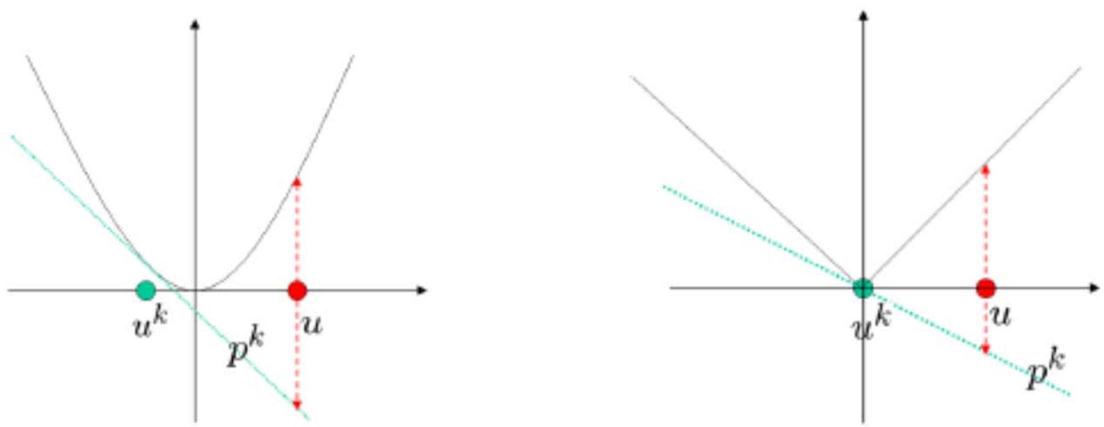
Bregman Distance

- Original model: $\min J(u) + f(u)$. Regularizer $J(\cdot)$
- Given u^k, $p^k \in \partial J(u^k)$
- Bregman distance:

$$D(u, u^k) := J(u) - \left(J(u^k) + \langle p^k, u - u^k \rangle\right)$$



- New model: $u^{k+1} \leftarrow \min \alpha D(u, u^k) + f(u)$. E.g.: $\alpha = 5$. p^k is obtainable from previous iteration.

Bregman = Add Back Residuals

- Original model:

$$u \leftarrow \min \ \mu J(u) + \frac{1}{2}\|Au - b\|_2^2.$$

- Bregman original form:

$$\begin{aligned} u^{k+1} &\leftarrow \min \ \mu\left[J(u) - (J(u^k) + \langle p^k, u - u^k\rangle)\right] + \frac{1}{2}\|Au - b\|_2^2 \\ p^{k+1} &\leftarrow p^k + A^\top(b - Au^{k+1}). \end{aligned}$$

- Add-Back form:

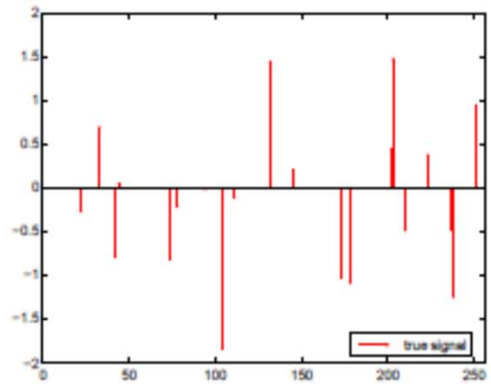
$$\begin{aligned} u^{k+1} &\leftarrow \min \ \mu J(u) + \frac{1}{2}\|Au - b^k\|_2^2 \\ b^{k+1} &\leftarrow b + (b^k - Au^{k+1}). \end{aligned}$$

Each subproblem has the same form of the original problem.

Bregman Regularization: Better Solution Quality

Example: Compressive Sensing Reconstruction from Noise Input

Original signal u, sparse



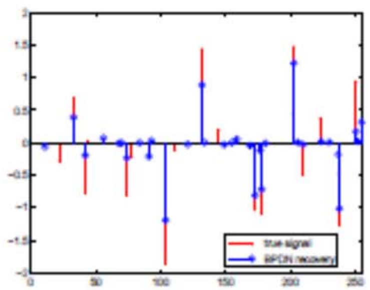
Noisy Gaussian measurements: $b = Au + \omega$, where A: 100×250.

Compare:

1. Basis pursuit: $u \leftarrow \min \mu \|u\|_1 + \frac{1}{2}\|Au - b\|_2^2$
2. Bregman: $u^{k+1} \leftarrow \min \bar{\mu}\|u\|_1 + \frac{1}{2}\|Au - b^k\|_2^2$, $b^{k+1} \leftarrow$ add back

Basis Pursuit (Non-Bregman) vs Bregman

1. Recover u by: $\min \ \mu\|u\|_1 + \frac{1}{2}\|Au - b\|_2^2$



$\mu = 48.5$

Not sparse

μ too small

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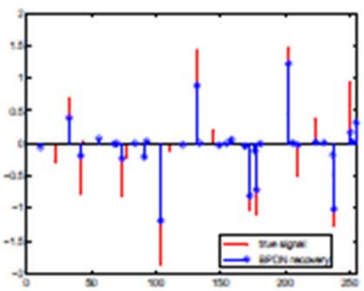

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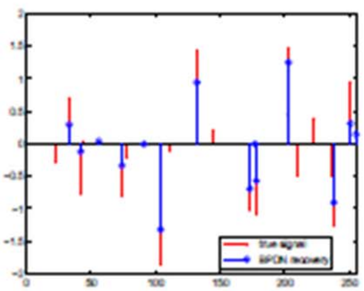

$\mu = 49$
Sparse but poor fitting

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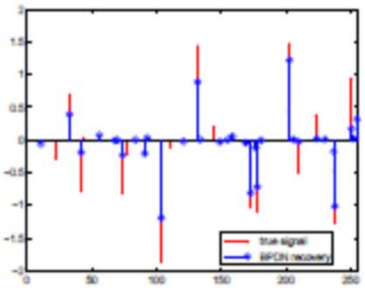

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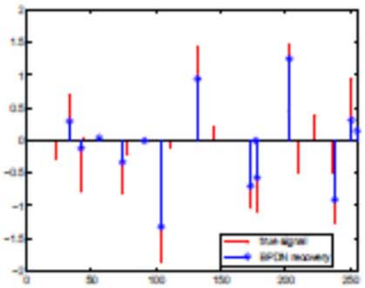
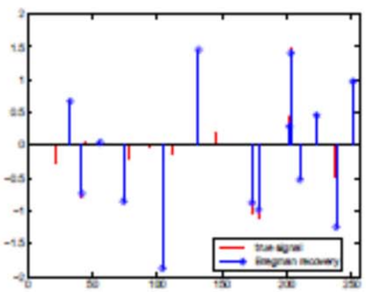


$\mu = 49$
Sparse but poor fitting

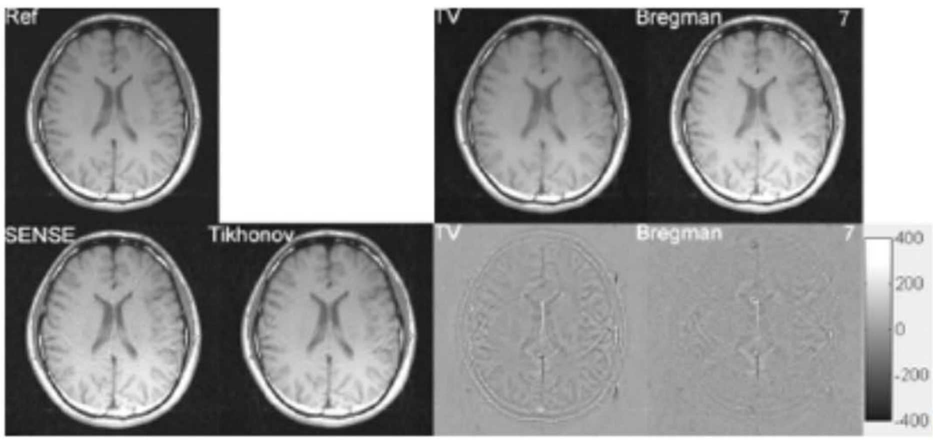
2. Recover u by Bregman: set $\bar{\mu} = 150$, after 5 iterations



Sparse, better fitting

Example: image deblurring and/or denoising

- $J(u) = \mu TV(u)$
- $f(u) = \frac{1}{2}\|Au - b\|_2^2$
- Stop when $\|Au^k - b\|_2^2 \approx \text{est.}\|Au^{true} - b\|_2^2$



(UWM-CMRI Lab)

Less signal in the residual.

- For ℓ_1, Bregman gives *sparser, better fitted* signals
- For TV, Bregman gives *less staircasing, higher contrast*

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- Reasons: *iterative boosting*
  1. For small k, u^k is over-regularized yet correctly captures larger nonzeros/edges.
  2. Minimizing $D(u, u^k)$ does not penalize the nonzeros/edges in u^k.

1. Better regularization quality over ℓ_1, total variation, ...
   - Work for noisy data
   - Start with over-regularization
   - $f(u^k)\downarrow$, stop $f(u^k) \approx f(\textit{real } u)$ est.
2. Fast, accurate methods for constrained ℓ_1 and TV minimization.
   - Work for *noiseless* data
   - $f(u^k)\downarrow$, stop $f(u^k) = 0$.

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Applied to Constrained Minimization

Y.-Osher-Goldfarb-Burger 07

- Purpose: $u_{real} \leftarrow \min\{J(u) : Au = b\}$, constrained
- Bregman: $u^{k+1} \leftarrow \min D_J(u, u^k) + \frac{1}{2}\|Au - b\|_2^2$, unconstrained
- Properties:
  - $u^k \to u_{real}$
  - Fast, finite convergence for ℓ_1–like $J(u)$
  - Even if subproblems are solved inexactly, under some conditions, solution is accurate and error converges to machine precision.

Convergence results

Assumption: J is convex, f is convex & differentiable, subproblem solutions exist; p^k starts from 0 (equivalent, b^k starts from b).

Theorem (General convergence)

Under the Assumption, $\{u^k\}$ of (1) satisfies

1. *Monotonic decrease:* $f(u^{k+1}) \leq D(u^{k+1}) + f(u^{k+1}) \leq f(u^k)$.
2. *Convergence: if u^* minimizes f and $J(u) < \infty$, then* $f(u^k) \leq f(u^*) + J(u^*)/k$ *and, thus,* $f(u^k) \to f(u^*)$.
3. *Denoise b, noise reduction: let* $f(\cdot) = f(\cdot; b)$ *(e.g.,* $f(\cdot) = \frac{1}{2}\|A \cdot - b\|_2^2$*) and suppose* $f(\bar{u}, \bar{b}) = 0$ *($\bar{b}$ and $\bar{u}$ are noiseless input and signal, resp); then* $D(\bar{u}, u^{k+1}) < D(\bar{u}, u^k)$ *as long as* $f(u^{k+1}; b) > f(\bar{u}; b)$.

Convergence results

Lemma

If $f(\cdot) = \frac{1}{2}\|A\cdot - b\|_2^2$ *and an* u^k *satisfies* $f(u^k) = 0$*, then* u^k *is a solution of* $\min\{J(u) : f(x) = 0\}$*. This holds even if subproblems are inexactly solved.*

Theorem (Finite convergence for ℓ_1)

Let $J(\cdot) = \mu\|\cdot\|_1$ *and* $f(\cdot) = \frac{1}{2}\|A\cdot - b\|_2^2$*. If* $Ax = b$ *is consistent, then there exists* K *such that any* u^k*,* $k > K$*, is a solution of* $\min\{J(u) : f(x) = 0\}$*.*

The theorem extends to any piece-wise linear J.

Error Cancellation

- Error cancellation is a happy result due to *adding back*!

$$b^k \leftarrow b + (b^{k-1} - Au^k) \tag{2}$$

$$u^{k+1} \leftarrow \min J(u) + \frac{1}{2}\|Au - b^k\|_2^2. \tag{3}$$

- Suppose we computed $u^k_{inexact} = u^k + w^k$. w^k is error.
- (2) becomes $b^k_{inexact} \leftarrow b + (b^{k-1} - Au^k_{inexact}) = b^k - Aw^k$.
- (3) becomes

$$u^{k+1} \leftarrow \min J(u) + \frac{1}{2}\|A(u + w^k) - b^k\|_2^2$$

which includes the *model error* w^k.

Let w be a model error, and consider

$$\min J(u) + f(u + w). \tag{4}$$

Define

- u_{exact}: exact solution of (4)
- $u_{inexact} = u_{exact} + \epsilon$: computed inexact sol of (4)
- u_{real}: exact solution of $\min J(u) + f(u)$.

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Theorem (General case)

If u_{exact} and $u_{exact} - w$ are on the same face of $\mathrm{graph}(J)$, then

$$u_{inexact} - u_{real} = \epsilon - w.$$

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Corollary (J is ℓ_1)

If u_{exact}^{k+1} and $u_{exact}^{k+1} - w^k$ have no opposite signs, then

$$u_{inexact}^{k+1} - u_{real}^{k+1} = \epsilon^{k+1} - w^k.$$

Error Cancellation Example

- u_{real}: 500 entries, 25 nonzero, sparse
- $b = Au_{real}$: 250 linear projections, A has Gaussian random entries
- Recover u_{real} by solving $\min\{\|u\|_1 : Au = b\}$
- Run Bregman, each subproblem inexactly solved with the same tol $\equiv$ 1e-6

  by: FPC, FPC-BB, GPSR, GPSR–BB, or SpaRSA

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Itr k	1	2	3	4	5
$\frac{\|u_{real} - u^k_{inexact}\|}{\|u_{real}\|}$	6.5e-2	2.3e-7	6.2e-14	7.9e-16	5.6e-16.

Relative error converged to the machine precision!

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  Relative error converged to the machine precision!

- Classical results require *diminishing tolerances* for convergence, but they are *not* needed for ℓ_1 and above solvers. Why?

Short Answer:

In $u^{k+1}_{inexact} - u^{k+1}_{real} = \epsilon^{k+1} - w^k$, ϵ^{k+1} almost cancels w^k for all k large.

A Slightly Long Answer:

1. **Finiteness.** With enough accuracy, Bregman u^k reaches the optimal face in finitely many iterations (denoted by K) and stays.
   - The Theorem applies for $k \geq K$.
2. **Error forgetting.** For any $k > K$, two *exact* Bregman iterations yields the global solution. In other words, errors before K can be forgotten.
   - For any $k \geq K$, $u_{real}^{k+1} = u_{real}$, the global solution.
   - $w^k = \epsilon^k$ and, thus, $u_{inexact}^{k+1} - u_{real} = \epsilon^{k+1} - \epsilon^k$.
3. **Convergence.** Use a first-order solver with a fixed tol. Given $\epsilon^{k+1} - \epsilon^k$ is small enough, $\|\epsilon^{k+1} - \epsilon^k\| \to 0$ geometrically in k.
   - $u_{inexact}^k$ converges to u_{real}, the global solution, geometrically in k.

Generalizations

- Inverse scale space (Burger, Gilboa, Osher, Xu, etc.)
- Linearized Bregman (Yin, Osher, Mao, etc.)
- Logistic Regression (Shi, et al. Rice CAAM 08-08)
- Split Bregman (Goldstein, Osher, UCLA CAM08-29)
- A unified primal-dual framework, BOS (X.Zhang, et al. UCLA CAM09-99)
- More ... People use the words “Bregmanize”

Linearized Bregman

Idea: Linearize the fidelity term at u^k

Work: Y.-Osher-Goldfarb-Darbon 07, Osher-Mao-Dong-Y. 08, Cai-Osher-Shen 08, Y. 09

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- Example: data fitting $= \frac{1}{2}\|Au - b\|_2^2$

$$u^{k+1} \leftarrow \min_u D(u, u^k) + \langle A^\top (Au^k - b), u\rangle + \frac{1}{2\delta}\left\|u - u^k\right\|_2^2$$

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- For $D(u, u^k)$ induced by $J(u) = \mu\|u\|_1$, iterations become

$$\begin{aligned} u^{k+1} &\leftarrow \delta\ \mathrm{shrink}(v^k, \mu) \\ v^{k+1} &\leftarrow v^k + A^\top(b - Au^{k+1}). \end{aligned}$$

Note: Second equation above is NOT $v^{k+1} = u^{k+1} + A^T(b - Au^{k+1})$

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- Application: non-negative least–squares, matrix completion

Linearized Bregman, Cont'd

Properties:

- gradient-ascend the dual of $\min\{\mu\|u\|_1 + \frac{1}{2\delta}\|u\|^2 : Au = b\}$
- Exact regularization: $\exists\bar{\delta}$: if $\delta > \bar{\delta}$, then solves $\min\{\|u\|_1 : Au = b\}$
- Empirically, # nonzeros of u^k grows monotonically in k

Yin, W. Analysis and Generalizations of the Linearized Bregman Method, Rice CAAM Report TR09-02. [link]

Operator Splitting ADM

Operator splitting + ADM gives Split Bregman (Goldstein–Osher 08)

- Operator splitting by (Wang–Yang–Y.–Zhang 07,08): Split $TV(u)$ to Du and $\sum_i \|(\cdot)_i\|$. Great payoff for many imaging problems.
- Apply the alternating direction of multipliers (ADM) method to above splitting.

Operator Splitting ADM

Alternating direction method: (Douglas–Rachford 60s, Glowinski–Marocco, Gabay–Mercier, 70s)

1. fix u, minimize w.r.t. v
2. fix v, minimize w.r.t. u
3. update λ

Example (Wang–Yang–Y.–Zhang 07,08) Compressed MRI, image deblr

$$\min_u \mu TV(u) + \frac{1}{2}\|Au - b\|_2^2 \Leftrightarrow \min_u \{\mu\|w\|_1 + \frac{1}{2}\|Au - b\|_2^2 : w = Du\}$$

where A is partial Fourier or convolution. ADM extends to color images, duals, rank-minimization

Summary

1. Bregman improves ℓ_1-like regularization quality for noisy data
2. Bregman applied to constrained ($Au = b$) minimization is not new but is fast and accurate due *adding back*
3. Various extensions take advantages of model structures

L1 Based Bregman Iteration Forgives & Forgets Errors

Stan Osher & Wotao Yin

We are solving

$$\min_u \left\{ D_J(u, u_v) + \frac{1}{2}\|Au - f\|^2 \right\}$$

$$v = 1, 2, \ldots$$

$$J = \mu |u|_1$$

$$\|\;\| \text{ means L2 norm}$$

We are sloppy, making numerous errors.

But at the k^{th} step:

we arrive at u_k such that

(1) The subgradient $p(u_k) = A^T g \quad \text{for some } g.$

(2) There is a vector u^* having the property that

$$Au^* = f$$
$$D(u^*, u_k) = 0$$

Then u_{k+1} solves $u_{k+1} = \arg\min |u|_1 \quad \text{such that } Au = f$

We have finished the iterative procedure!

Note $D_J\left(u^*, u_k\right)=0$ for this J means, for every component $u(i)$

$$\left|u^*(i)\right| - u^*(i)\left(\operatorname{sign} u_k(i)\right) = 0$$

If $u^*(i) \neq 0$, then $u_k(i)$ has the same sign as $u^*(i)$

That's all that's needed!!

Similar results for BV.

However, for strictly convex $J(u)$

$$D\left(u^*, u\right) = 0 \Leftrightarrow u^* = u_k$$

Not interesting!

Proof

$$u_{k+1} = \arg\min \left\langle D(u, u_k) + \frac{1}{2}\|Au - f\| \right\rangle$$

we know $D(u,u_k) \geq 0,\ \|Au - f\|^2 \geq 0$ and they are both zero for $u = u^*$

Therefore, the u_{k+1} from Bregman satisfies $Au_{k+1} = f$

Also, let u satisfy $Au = f$. Then:

$$\begin{aligned}
J(u_{k+1}) &\leq |u| - \langle u - u_{k+1}, P(u_{k+1}) \rangle \\
&= J(u) - \langle u - u_{k+1}, A^T g \rangle \\
&= J(u) - \langle Au - Au_{k+1}, g \rangle \\
&= J(u) - \langle f - f, g \rangle \\
&= J(u)
\end{aligned}$$

Minimizing for $u \varepsilon R^n$, $|u|_1$ such that $Au = f$

$A_{m \times n}$ m < n

get sparse solutions.
Also, penalized problem, for $\mu > 0$

$$\min \frac{1}{\mu} |u|_1 + \frac{1}{2} \|Au - f\|_2^2$$

get sparser than just least squares.

Sparsity increases as $\mu \downarrow 0$.

Now: Suppose we think about calculus of variations type problems in physics?

Think continuously

e.g. Let $u, f: R^1 \to R, \quad u\, \varepsilon\, H^1$

$f\, \varepsilon\, L^2$

Toy problem

$$\min_u \left\{ \frac{1}{2}\int |u_x|^2 - \int fu + \frac{1}{\mu}\int |u| \right\}$$

$$\mu > 0$$

Leads to

$$u_{xx} = -f + \frac{1}{\mu}\, p(u)$$

$p(u)$ is a subgradient of u, i.e. for any u

$$|v|_1 - |u|_1 - \langle v - u, p(u) \rangle \geq 0$$

Or $|v|_1 \geq \langle v, p(u) \rangle$

The addition of the L^1 term shrinks the support of u, support decreases with μ ↓

Similarly for the "heat equation"

$$u_t - u_{xx} = f - \frac{1}{\mu} p(u)$$

which is gradient descent on the toy problem.

This was noticed (in some generality) by H. Brezis [1974] and H. Brezis and A. Friedman [1976].

Generalized a bit recently by R. Caflisch, S.O., H. Schaeffer and G. Tran.

An easy intuitive explanation of the shrinking support for the elliptic equation:

Suppose u(x) > 0 in an interval $x_i \leq x \leq x_{i+1}$ with

u(x_i) = u(x_{i+1}) = 0. Then $p(u) = 1$ in this interval.

We have

$$x_2 - x_1 = \mu(u_x(x_2) - u_x(x_1)) + \mu \int_{x_1}^{x_2} f(s)us$$

$$x_2 - x_1 \leq \mu \int_{x_1}^{x_2} f(s)ds$$

which diminishes with μ.

Similarly for intervals in which $u(x) < 0$.

This concept is very useful in obtaining spatially localized solutions to a class of problems in mathematical physics, such as finding compactly supported approximations to eigenfunctions of the Schrodinger equation.

Joint work: V. Ozolins, R. Lai, R. Caflisch, S.O., F. Barekat and K. Yin.

Motivated by localized Wannier functions developed in solid state physics and quantum chemistry.

Consider the Hamiltonian

$$\hat{H} = -\frac{1}{2}\Delta + V(x), \text{ e. values } \lambda_1 < \lambda_2 \ldots$$

Ground state energy for a finite system with N electrons

$$E_0 = \sum_{j=1}^{N} \lambda_j$$

This is obtained by solving the variational problem

$$E_0 = \sum_{j=1}^{N} \langle \varphi_j, \widehat{H} \varphi_j \rangle \text{ such that } \langle \varphi_j, \varphi_k \rangle = \delta_{jk}$$

Get densely supported φ_j

We want short-ranged interaction.

Wannier functions (1937) involve a subspace rotation of the φ_j (unitary transformation). Usually cut off by hand to get compact support.

We just replace the variational problem by adding an L^1 regularization:

$$E = \min_{\psi_1,\psi_2,\dots,\psi_N} \sum_{j=1}^{N} \left(\frac{1}{\mu} \left|\psi_j\right|_1 + \left\langle \psi_j, \hat{H}\psi_j \right\rangle \right)$$

$$\text{such that } \left\langle \psi_j, \psi_k \right\rangle = \delta_{jk}$$

This can be solved by split Bregman with an extra step of projecting onto the constraint set (R. Lai & S.O., (2012)). Nonconvex, but works (Faster with “more L^1” added). Get localized modes.

Proven

(1) These “compressed modes” have compact support in R^d. There exists μ_0 depending on N, d and $\|V\|_\infty$

$$|\sup \psi_i| \leq C\mu^{2d/4+d} \text{ for } i = 1,\dots,N.$$

for $0 < \mu < \mu_0$

(2) As $\mu \uparrow \infty$, i.e. the L^1 term diminishes to 0 the compressed modes converge in L^2 to a unitary transformation of eigenfunctions of the original Hamiltonian.

(3) The sub-eigenspace spanned by the first M eigenfunctions can be approximated by the first N compressed modes as N increases (with improvable accuracy) for any fixed μ.

Shift Invariance:

Wannier Function Based Variational Formalism for Electronic Structure Calculations
V. Ozolins, F. Barekat, R. Lai, K. Yin, S.O. & R. Caflisch

Wannier functions

Unitary transformations of eigenstates of the Hamiltonian

Subject to constraint of orthogonality to all their translations by lattice vectors, shift orthogonality. Usually they are localized after first going through the construction by first calculating the eigenstates. The localization is problematic.

We will use L_1 regularization in a very fast algorithm to obtain localized approximations directly.

3D Lattice

$$R_\alpha (\alpha = 1,2,3)$$

any point on the lattice

$$R = \sum_{\alpha}^{3} n_\alpha R_\alpha$$

Reciprocal lattice

$$Q_\alpha R_B = 2T\delta_{\alpha B}$$

Supercell

$$L_\alpha R_\alpha, L_\alpha \text{ positive integers}$$

Periodic B.C. on supercell

$\psi(x) = \psi(x + R_{sc})$, wave functions ψ

$$R_{sc} = \sum_{\alpha} n_\alpha L_\alpha R_\alpha, \forall n_\alpha \ \varepsilon \ Z$$

Eigenfunctions ψ are in general not lattice periodic.

Reciprocal lattice vector

$$G = \Sigma m_\alpha Q_\alpha, m_\alpha \ \varepsilon \ Z$$

$$e^{iGR} = 1 \quad \forall R$$

Fourier expansion of ψ contains only plane waves with wave vectors k + G.

k belongs to the first Brillouin zone.

i.e. first Voronoi cell in the reciprocal lattice, also called Wigner-Seitz cell, WS, the volume is |WS|

$$\Gamma = \{R | R\,\varepsilon\, WS\}$$

$$\psi(x) = \sum_{G}\sum_{k} \hat{\psi}(k+G)e^{i(k+G)x}$$

$$\hat{\psi}(k+G) = \frac{1}{|WS|}\int_{WS} \psi(x)e^{-i(k+G)x}dx$$

Function is shift-orthogonal iff

$$\langle \psi(x-R'), \psi(x-R)\rangle = \delta(R, R')$$

for $R, R'\,\varepsilon\,\Gamma$

Well known result

Supercell-Periodic function

$\psi(x)$ is shift orthogonal

iff

$$\Sigma\left|\hat{\psi}(k+G)\right|^2 = \frac{1}{|WS|(\Gamma)} \quad \forall k \; \varepsilon \; BZ$$

$|\Gamma|$ is the cardinality of set Γ. Also, if $\psi(x), \varphi(x)$ supercell periodic.

$$\langle\psi(\text{x-R}), \varphi(\text{x-R}')\rangle = 0 \quad \forall R, R' \varepsilon \; \Gamma$$

iff

$$\Sigma\hat{\psi}(k+G)\hat{\varphi}(k+G) = 0, \forall \; k \; \varepsilon \; BZ$$

Simple to project.

Given f, supercell periodic $f(x+R_{sc}) = f(x)$

Find

$$\Pi f = \underset{\psi}{\operatorname{argmin}} \|f - \psi\|_2$$

such that ψ is shift orthogonal.

Easy. (Not unique)

in 1D

Compute $$C_k = \sum_{m=-N}^{N} \left|\hat{f}\big(\Sigma(k+mQ)\big)\right|^2$$

If $C_k \neq 0$ then

$$\widehat{\Pi}f\big((k+mQ)\big) = \frac{\hat{f}(k+mQ)}{|\Gamma||WS|C_k}$$

else (non unique)

$$\widehat{\Pi f}(k+mQ) = \text{any unit vector.}$$

Now we use the split Bregman for orthogonal constrained problems SOC method, algorithm, very fast.

Algorithm for level-k Wannier function

Input

$$\widehat{H}: \psi_j\{; j = 1, \ldots, k-1\}, \lambda, \gamma, \mu$$

Output ψ_k.

(1) Initialize: $u(x), v(x)$ norm, random

$$b(x) = c(x) = 0$$

(2) While not converged do:

$$(3)\ \psi = \underset{\psi}{\operatorname{argmin}}\{\langle\psi, \widehat{H}\psi\rangle + \frac{\lambda}{2}\|\psi - u + b\|^2{}_2$$

$$+ \frac{\gamma}{2}\|\psi - v + c\|^2{}_2\}$$

(4) $u = \Pi_{\psi_1,\psi_2,\ldots,\psi_{k-1}}(\psi + \mathrm{b}) \longleftarrow$ This is now fast!!

(5) $v = \arg\min\left\{\frac{1}{u}\|v\|_1 + \frac{\gamma}{2}\|\varphi - v + c\|^2{}_2\right\}$

(6) $b = \psi - u + b$

(7) $c = \psi - v + c$

(8) Return $\psi_k(x)$

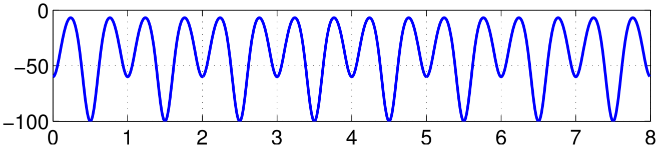

Figure : Model potential $V(x) = -\sum_{j=-\infty}^{\infty} \sum_{m=1}^{2} V_m \exp\left[-\frac{(x - x_m - ja)^2}{2\sigma^2}\right]$, where $a = 1$, $\sigma = 0.1a$, $V_1 = 60$, $V_2 = 100$, $x_1 = 0$, and $x_2 = a/2$.

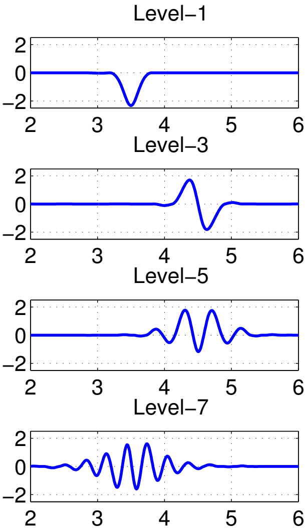

Figure : Compressed Wannier Functions at levels 1-8. $\lambda = \gamma = 10^3$, parameter for L^1 term $\mu = 10/\sqrt{L}$ ($L = 8$ is the length of the supercell).

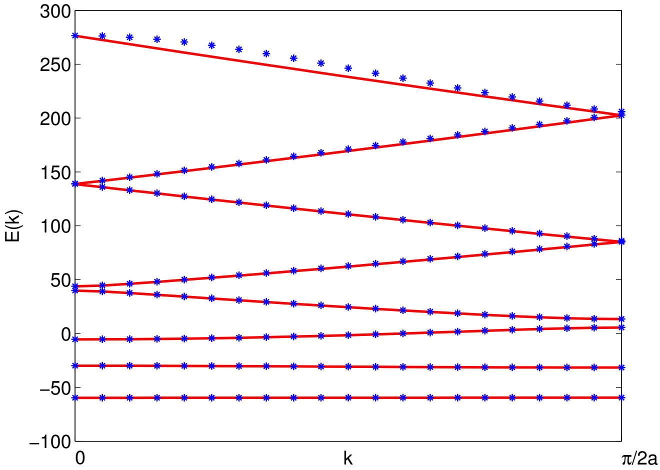

Figure : "Spaghetti plot": Eigenvalue dispersion for bands 1-8 calculated by exact diagonalization (continuous line) and by using the lowest 8 Wannier modes (filled circles).