Compressed Modes for Material Interface Problems

Russel Caflisch
IPAM
Mathematics Department, UCLA

math changes everything.

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Collaborators

- Edward Chou (UCLA)
- Stan Osher (UCLA)
- Vidvuds Ozolins (UCLA Materials Sci)
- Omer Tekin (UCLA→Google)

Outline

- Compressed Sensing
- Phase Transitions
- Deposition

Compressed Sensing

- Problem statement
  - Donoho 2006, Candes, Romber & Tao 2006
  - Find x that is m-sparse and solves Ax = f
  - Assuming that an m-sparse solution exists
- Standard methods

  min $\|x\|_0$ subject to constraint Ax = f

  - note $\|x\|_0 = \#\{i : x_i \neq 0\}$
- Compressed sensing

  min $\|x\|_1$ subject to constraint Ax = f

  - note $\|x\|_1 = \sum_{i=1}^{N} |x_i|$

How many measurements are required?

- For m << N, find m-sparse solution $x \in R^N$ of

$$Ax = f \in R^n \quad A \text{ is } n \times N$$

- Standard methods require: n = N
  - #(equations)=#(unknowns), NP hard = intractable
- Compressed sensing: n = m (log N)
  - n << N. Many fewer equations than unknowns!
  - Solution is exact with high probability!
    - Reduced isometry property (RIP)
  - convex programming, tractable and fast

Why Does L^1 Promote Sparsity?

- Compressed sensing

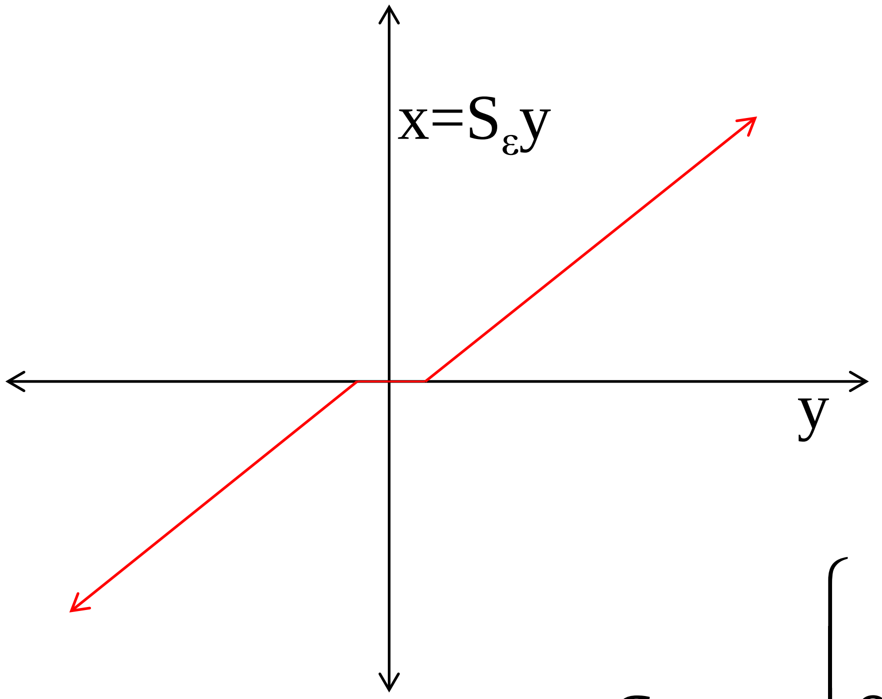
  $\min \|x\|_1$ subject to constraint Ax = f

- Simplified problems: Find x solving
  - $\min \ (x-y)^2 + \varepsilon |x|$ for given y in R
  - Solution

$$x = S_\varepsilon y = \begin{cases} y-\varepsilon & \text{if } y > \varepsilon \\ 0 & \text{if } |y| < \varepsilon \\ y+\varepsilon & \text{if } y < -\varepsilon \end{cases}$$

  - Operator S_ε is "soft-thresholding"

Soft Thresholding



$$S_\varepsilon y = \begin{cases} y - \varepsilon & if\ \ y > \varepsilon \\ 0 & if\ \ |y| < \varepsilon \\ y + \varepsilon & if\ \ y < -\varepsilon \end{cases}$$

Subgradient

- Euler-Lagrange eqtn for $\min\,(x-y)^2+\varepsilon|x|$

$$2(x-y)+\varepsilon\,p(x)=0$$

- Subgradient

$$p(x)=\partial_x|x|=\begin{cases}1 & \text{if } x>0\\ [-1,1] & \text{if } x=0\\ -1 & \text{if } x<0\end{cases}$$

- Write sgn(x)=p(x)

COMPRESSION FOR PHASE TRANSITIONS

Phase Transitions

- Cahn-Hilliard equations

$$\partial_t c = -\partial_x^2(\partial_c J[c])$$
$$J_0[c] = \int \frac{1}{2}\gamma c_x^2 + \frac{1}{4}(c^2-1)^2\,dx$$

  - Pure phase regions c=-1 and c=1
  - Steady eqtn $\partial_c J[c]=0$ has solution

$$c(x) = \tanh(x/\sqrt{2\gamma})$$

- Goals of compression
  - c=-1 and c=1 reached at finite distance
  - Similar to classification problem in machine learning

Compression for Cahn-Hilliard

- Variational quantity for Cahn-Hilliard

$$J_0[c] = \int \frac{1}{2}\gamma c_x^2 + \frac{1}{4}(c^2-1)^2\, dx$$

- Variational quantity with compression

$$J[c] = \int \frac{1}{2}\gamma c_x^2 + \frac{1}{4}(c^2-1)^2 + \varepsilon\left|c^2-1\right| dx$$

  – Euler-Lagrange for steady minimizer

$$-\gamma c_{xx} + c(c^2-1) + 2\varepsilon c\,\mathrm{sgn}(c^2-1) = 0$$

  – Look for solution that is odd in x and reaches ±1 at x= ±L

$$\begin{aligned} c(x) &= -1 \quad && x \le -L \\ \left|c(x)\right| &< 1 && \left|x\right| < L \\ c(x) &= 1 && x \ge L \end{aligned}$$

  – ODE and BCs

$$-\gamma c_{xx} + c(c^2-1) - 2\varepsilon c = 0 \quad \left|x\right| < L$$

$$c(\pm L) = \pm 1, \quad c_x(\pm L) = 0$$

Numerical Method for Compressed Cahn-Hilliard

- Numerical Method: Split Bregman

$$\phi(c) = \varepsilon(c^2 - 1)$$

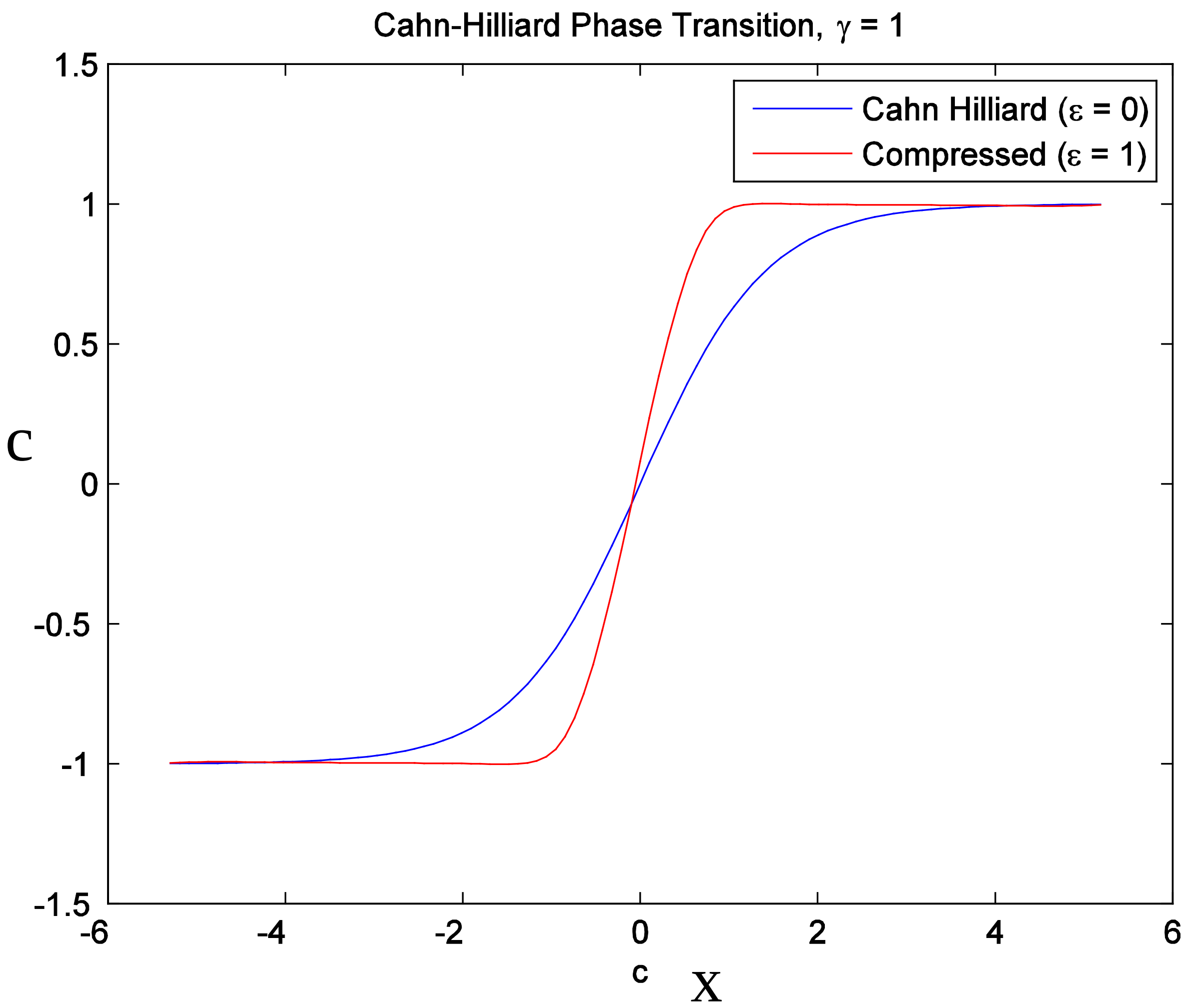
$$c^{(k+1)} = \min_u J_0[c] + \frac{\lambda}{2}\int d^{(k)} - \phi(c) - b^{(k)} dx$$

$$d^{(k+1)} = \min_d \|d\|_1 + \frac{\lambda}{2}\int d^{(k)} - \phi(c^{(k+1)}) - b^{(k)} dx$$

$$b^{(k+1)} = b^{(k)} + \phi(c^{(k+1)}) - d^{(k+1)}$$

  - Use gradient descent to update c, soft-thresholding to update d
  - λ is a fixed parameter, influences convergence but not solution

Numerical Solution for Compressed Cahn-Hilliard



COMPRESSION FOR DEPOSITION

Simplified Deposition Model

- Deposition model
  - u(x) = height of deposited material
  - Diffusion with source s(x) and removal rate λ

$$\partial_t u = \partial_x^2 u - \lambda u + s \quad -\pi < x < \pi$$

- Steady state problem

$$u = Gs \qquad G = (-\partial_x^2 + \lambda)^{-1}$$

  - Desired height profile f(x)=cos(x)
  - Choose s(x) so that $\int_{-\pi}^{\pi} (u - f(x))^2 dx \le \sigma^2$
- Goals of compression
  - Choose s which is smooth and has small support

Compression for Deposition

- Variational quantity
  - $J[s]=\int_{-\pi}^{\pi}\frac{1}{2}(u-f(x))^2+\varepsilon|s|+\frac{1}{2}\gamma^2 s_x^2\,dx$ with $u=Gs$

    $=\int_{-\pi}^{\pi}\frac{1}{2}(Gs-f(x))^2+\varepsilon|s|+\frac{1}{2}\gamma^2 s_x^2\,dx$
  - Euler-Lagrange eqtn

    $$G^2 s-Gf+\varepsilon\,\mathrm{sgn}(s)-\gamma^2 s_{xx}=0$$
  - Solution s doesn't have compact support (?)
- Modified variational quantity

  $$J[s]=\int_{-\pi}^{\pi}\frac{1}{2}(Gs-f(x))^2+\varepsilon G^2|s|+\frac{1}{2}\gamma^2(Gs_x)^2\,dx$$
  - Euler-Lagrange eqtn

    $$G^2 s-Gf+\varepsilon G^2\,\mathrm{sgn}(s)-\gamma^2 G^2 s_{xx}=0$$

    $$\Longrightarrow\quad s-G^{-1}f+\varepsilon\,\mathrm{sgn}(s)-\gamma^2 s_{xx}=0$$

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Modified Variational Quantity

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- Variational quantity
  - Original $J[s]=\int_{-\pi}^{\pi}\frac{1}{2}(Gs-f(x))^2+\varepsilon|s|+\frac{1}{2}\gamma^2 s_x^2 dx$
  - Modified $J_m[s]=\int_{-\pi}^{\pi}\frac{1}{2}(Gs-f(x))^2+\varepsilon G^2|s|+\frac{1}{2}\gamma^2 (Gs_x)^2 dx$

    $\min J_m[s] \Rightarrow s-g+\varepsilon\,\mathrm{sgn}(s)-\gamma^2 s_{xx}=0 \qquad g=G^{-1}f$
  - Equivalent $J_{\varepsilon,\gamma}[s]=\int_{-\pi}^{\pi}\frac{1}{2}(s-g)^2+\varepsilon|s|+\frac{1}{2}\gamma^2 s_x^2 dx$
- Thresholding
  - For γ=0, $\min J_{\varepsilon,0}[s] \Rightarrow s=S_\varepsilon g$ soft-thresholding
  - For γ>0, $\min J_{\varepsilon,\gamma}[s] \Rightarrow s=S_{\varepsilon,\gamma} g$ "smooth-thresholding"

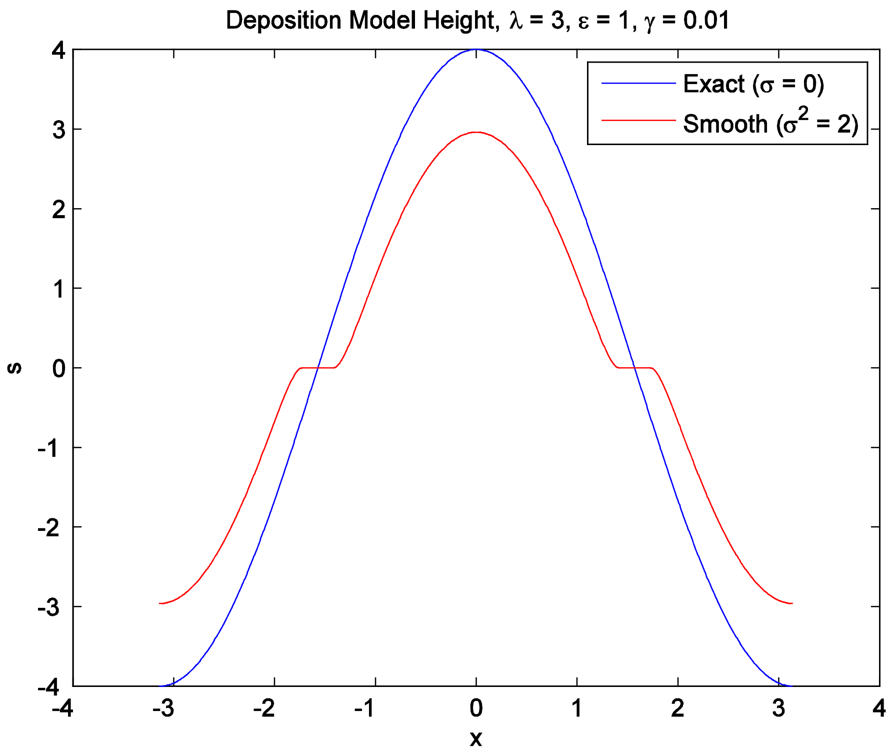
Solution of Modified Compressed Deposition Equations

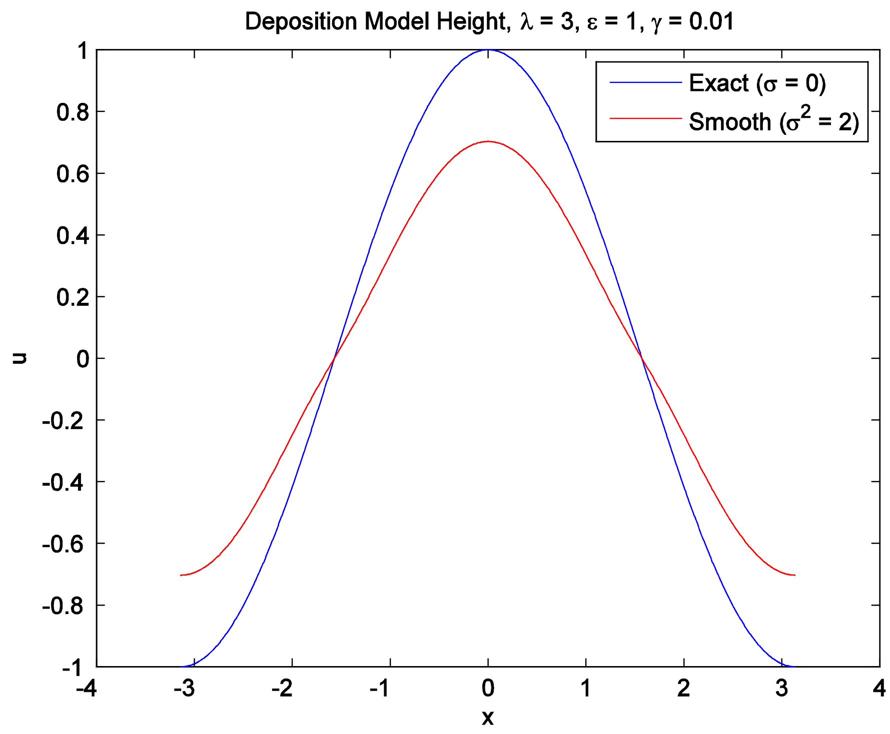
- Equation for s
  - $s - G^{-1} f + \varepsilon\,\mathrm{sgn}(s) - \gamma^2 s_{xx} = 0$ periodic on |x|<π, f=cos(x)
  - Look for solution s to be nonnegative and even for |x|<π/2 with
    $$s(x) > 0 \quad |x| < L$$
    $$s(x) = 0 \quad L < |x| < \pi/2$$
  - Antisymmetric around π/2
- Equation for s on |x|<L (using s>0)
  $$s - G^{-1} f + \varepsilon - \gamma^2 s_{xx} = 0 \qquad s(L) = s_x(L) = 0$$
  - Solution $s(x) = a + b\cos(x) + c\cos(x/\gamma)$
  - $a = -\varepsilon$, $b = \dfrac{1+\lambda}{1+\gamma^2}$ and $\begin{aligned} a + b\cos(L) - c\gamma^2\cos(L/\gamma) &= 0 \\ -b\sin(L) + c\gamma\sin(L/\gamma) &= 0 \end{aligned}$ 2 eqtns for c, L

Numerical Solution for Compressed Deposition

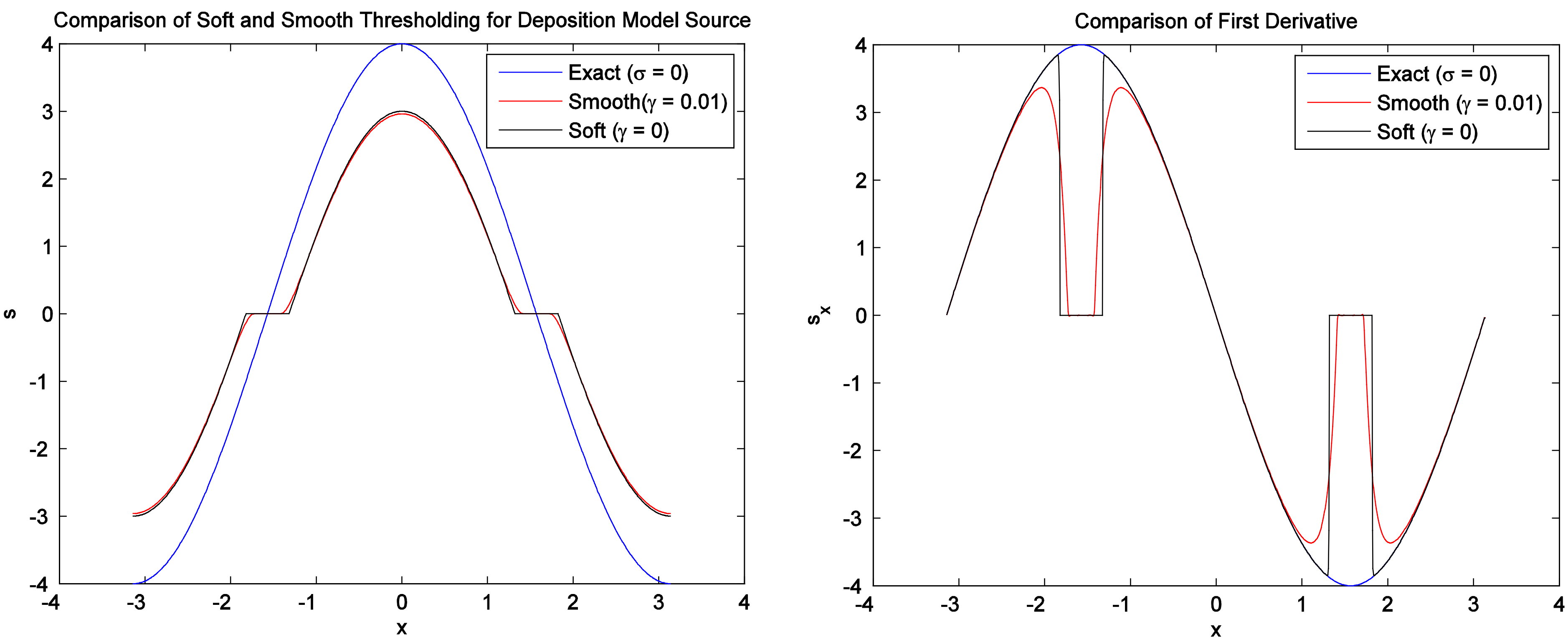
- The analytic solution, for σ large enough, takes the form

$$s(x) = c_1 + c_2 \cos(x) + c_3 \cosh(kx)$$





Comparison of Soft and Smooth Thresholding



Ongoing and Future Work

- Compression of Schrodinger equation
  - Wannier modes
  - Application to DFT, including symmetries
- Signal fragmentation
  - Decompose a desired signal into a sum of fragments
  - Fragments have compact support
- Multiscale method
  - Use compression to mediate interaction between micro and macro scales