Hamilton-Jacobi theory for Inverse PDE

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for some optimal controlled PDE

- regularization
- discretization
- error estimates

based on Hamiltonians and Hamilton-Jacobi theory

Optimal Control

$$\frac{dX_t}{dt} = f(X_t, \alpha_t),$$

$$\inf_{\alpha \in \mathcal{A}} \Big(g(X_T) + \int_0^T h(X_s, \alpha_s) ds \Big),$$

given $X_0, f, g, h, \quad \mathcal{A} = \{\alpha : [0,T] \to B\}$.

Ex: Calibration in math finance. Find $\sigma : [0,T] \times \mathbb{R}_+ \to \mathbb{R}_+$

$$\partial_t C(t,x) = \frac{\sigma^2(t,x)x^2}{2} \partial_{xx} C(t,x), \quad C(0,x) = \max(S - x, 0)$$

$$\min_\sigma \sum_{i,j} |C(t_j, x_i) - \hat{C}(t_j, x_i)|^2$$

Two Computational Alternatives

1. Dynamic programming and Hamilton-Jacobi PDE

$$u(x,t) := \inf_{\alpha} \Big(g(X_T + \int_t^T h(X_s, \alpha_s) ds\,;\ X_t = x \Big),$$

$$\partial_t u(x,t) + \underbrace{\min_{\alpha \in B} \big(f(x,\alpha) \cdot \partial_x u(x,t) + h \big)}_{H(\partial_x u(x,t),x)} = 0, \quad t < T$$

$$u(\cdot, T) = g$$

2. Minimization with ODE-constraint: Hamiltonian system

$$\dot{X}_t = H_\lambda(\lambda_t, X_t) \qquad X_0 \text{ given}$$

$$\dot{\lambda}_t = -H_x(\lambda_t, X_t) \qquad \lambda_T = g'(X_T)$$

Compare HJB-PDE and Hamiltonian system

Hamilton-Jacobi by FEM or FD:

$+$ Global minimum

$+$ Theory also for non smooth

$+$ Stochastics

$-$ Not $d \gg 1$

Minimization with ODE-constraint:

$-$ Local minimum

$-$ Need smooth

$-$ No stochastics

$+$ $d \gg 1$!

Idea here:

use HJ theory to find regularizations & estimates for H-systems

Approximation of Optimal Controls

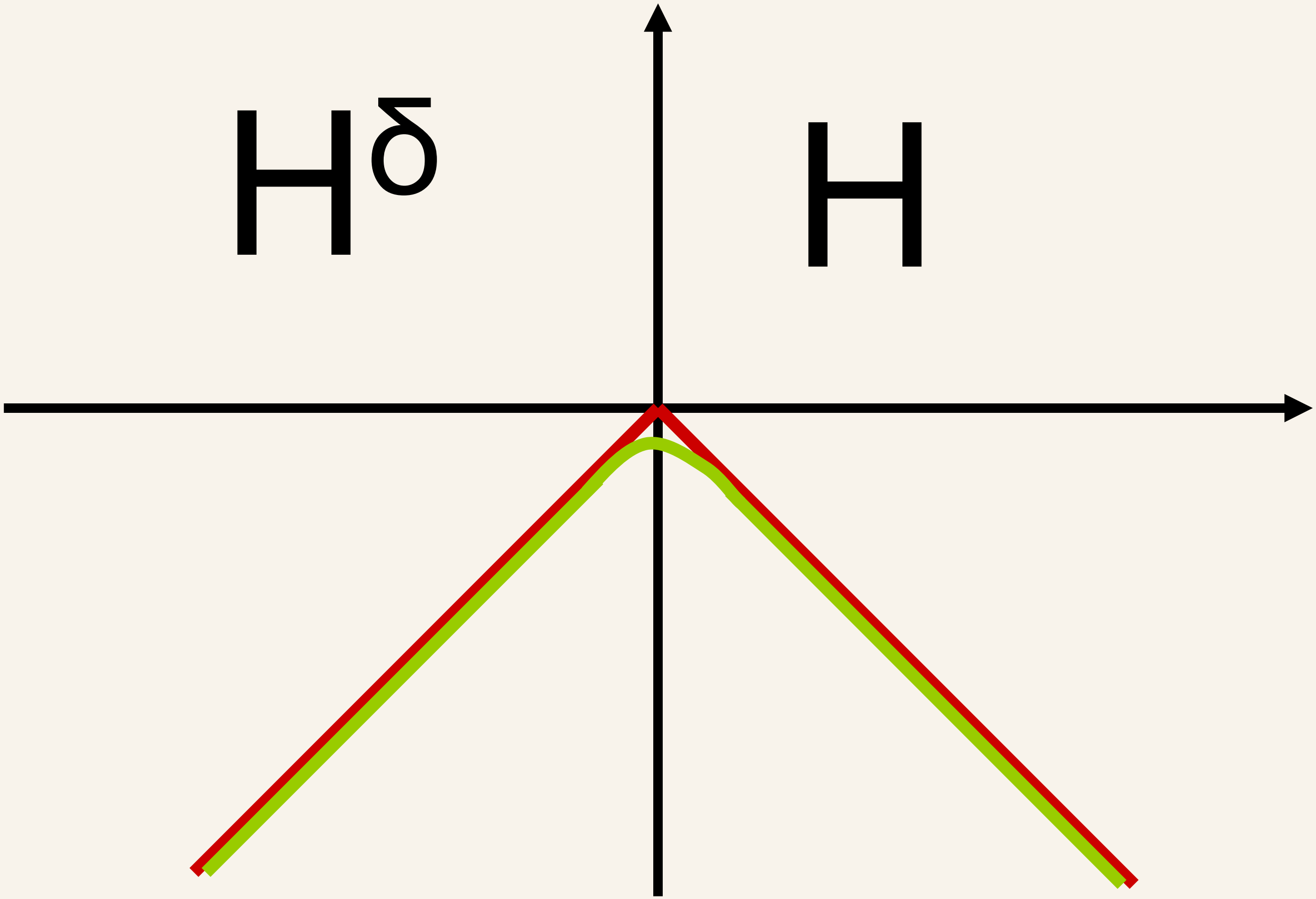
- Convergence for *symplectic* ODE method with
- non smooth control (two reasons)
- regularization by consistency with Hamilton-Jacobi PDE and Pontryagin principle.

Non smooth control:

- H only Lipschitz
- Colliding backward paths X, i.e. shocks!

Regularized H^δ:

Ex: $f = \alpha \implies H(\lambda) = \min_{\alpha \in [-1,1]} (\lambda\, \alpha) = -|\lambda|$.



H^{δ}
H

Pontryagin Principle and the Symplectic Euler

$$\bar X_{n+1} = \bar X_n + \Delta t\ H^\delta_\lambda(\bar\lambda_{n+1}, \bar X_n), \quad \bar X_0 = X(0),$$

$$\bar\lambda_n = \bar\lambda_{n+1} + \Delta t\ H^\delta_x(\bar\lambda_{n+1}, \bar X_n), \quad \bar\lambda_N = g'(\bar X_N).$$

Motivation

The Hamilton equations are the characteristics for the Hamilton-Jacobi PDE and

$$\begin{aligned} &f\big(X_s, \alpha^*(X_s, \lambda_s)\big) = H_\lambda(\lambda_s, X_s) \\ &h = H - \lambda H_\lambda \\ &\alpha^*_t = \mathsf{argmin}_a\big(\lambda_t \cdot f(X_t, a) + h(x, a)\big) \end{aligned}$$

Implied volatility

Find $\tilde{\sigma} : [0,T] \longrightarrow [\sigma_-, \sigma_+]^M$

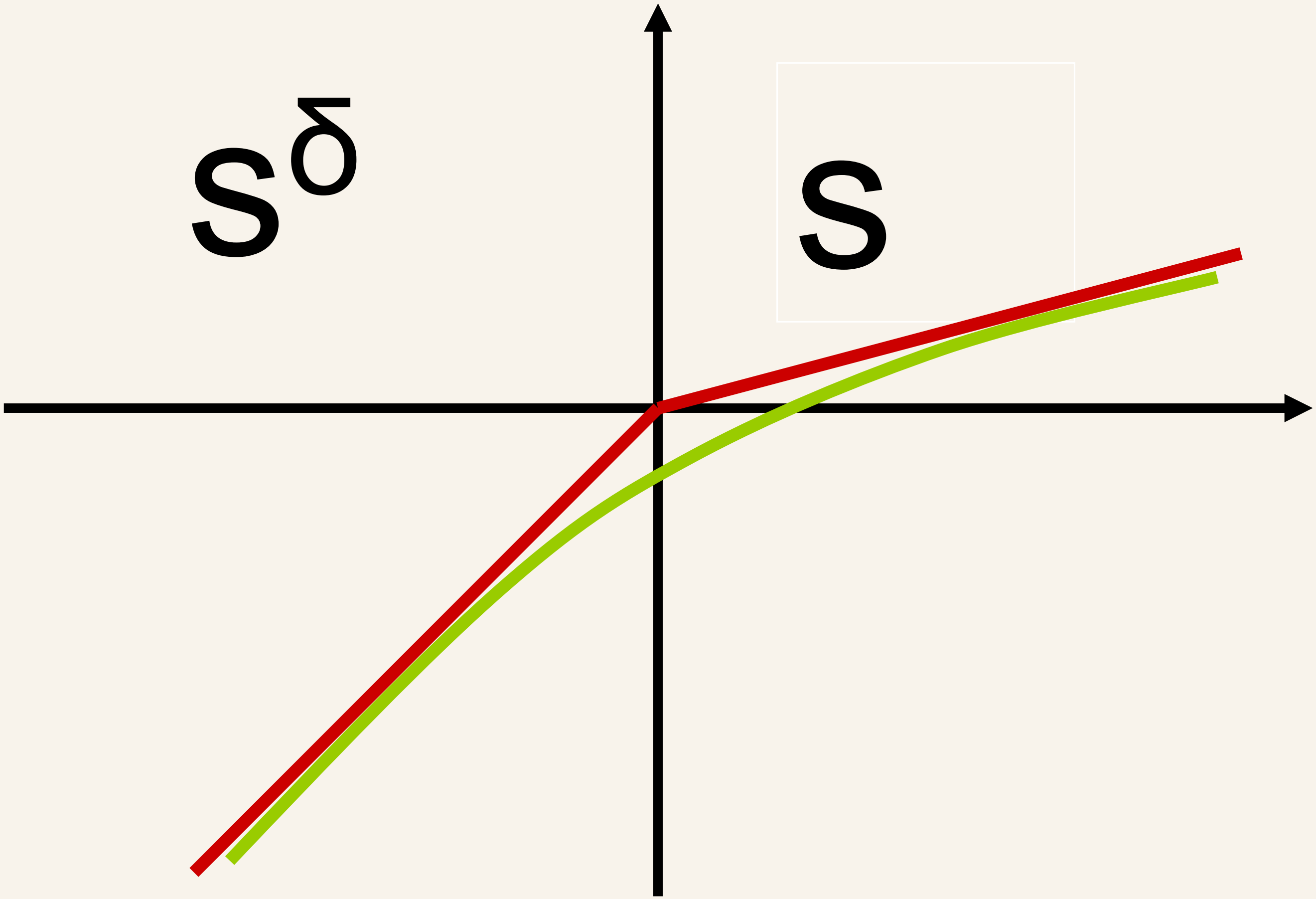
$$\min_{\tilde{\sigma}} \sum_{i,j} \left(C(t_j, x_i) - \hat{C}(t_j, x_i) \right)^2$$

subject to $\partial_t C_i(t) = \tilde{\sigma}_i(t) D_i^2 C(t)$ (Dupire's eq.)

$$\begin{aligned} H(\lambda, C) &= \min_{\tilde{\sigma}} \sum_{i=1}^{M-1} \left(\tilde{\sigma}_i \underbrace{D_i^2 C \lambda_i}_{v_i} + (C - \hat{C})_i^2 \right) \\ &= \sum_{i=1}^{M-1} \left(\underbrace{\min_{\tilde{\sigma}} (\tilde{\sigma}_i v_i)}_{s(v_i)} + (C - \hat{C})_i^2 \right) \end{aligned}$$

Regularized:

$$H^\delta(\lambda, C) := \sum_{i=1}^{M-1} \left(s_\delta(D_i^2 C \lambda_i) + (C - \hat{C})_i^2 \right)$$



S δ
S

The corresponding Hamiltonian system

$$\partial_t C_i = s'_\delta(D_i^2 C \lambda_i) D_i^2 C, \quad C_0 = S, C_M = 0$$
$$-\partial_t \lambda_i = D_i^2\big(s'_\delta\big(D_\cdot^2 C \lambda_\cdot\big)\lambda_\cdot\big) + 2(C - \hat{C})_i, \quad \lambda_0 = \lambda_M = 0$$

and Hamilton-Jacobi equation for the value function

$$u(c,t) = \min_{\tilde{\sigma}} \Big[\sum_{i,t_j>t} |C_i(t_j) - \hat{C}_i(t_j)|^2 \; ; \; C(t) = c \Big]$$

is

$$\partial_t u(C,t) + H^\delta(\partial_C u(C,t), C) = 0 \quad t < T,$$
$$u(\cdot, T) = 0.$$

ODE Convergence for $d \gg 1$

Theorem. Assume f, g, h Lipschitz,

$$\|\partial_{\bar{X}(t_n)} \bar{\lambda}_{n+1}\|_{L^\infty(\Omega_- \cup \Omega_+)} \leq K,$$

then

$$|u - \bar{u}| = \mathcal{O}(\delta + \Delta t + \Delta t^2/\delta).$$

Proof.

1. $\bar{u}(x, t_n) := \min_{\bar{X}_n = x} \Big(g(\bar{X}_N) + \sum_{m \geq n} h(\bar{X}_m, \bar{\lambda}_{m+1}) \Delta t \Big)$
2. $\partial_{\bar{X}_n} \bar{u} = \bar{\lambda}_n$
3. $\partial_t \bar{u}(\bar{X}_t, t) + H(\partial_x \bar{u}, \bar{X}_t) = \mathcal{O}(\delta + \Delta t + \frac{(\Delta t)^2}{\delta}),$
4. 2 & 3 and stability of viscosity solutions
5. H concave, subdifferential empty at shocks.

HJ-Stability

L^2 projection $P : V \to \bar{V}$ gives $\bar{H}(\bar{\lambda}, \bar{X}) = H^\delta(P\bar{\lambda}, \bar{X})$ and

$$\begin{aligned}
&\int_0^T (\bar{H} - H)\big(\partial u(\bar{X}_t, t), \bar{X}_t\big)dt \leq \bar{u}(X_0, 0) - u(X_0, 0) \\
&\leq \int_0^T (\bar{H} - H)\big(\partial \bar{u}(PX_t, t), PX_t\big)dt \\
&\quad + \int_0^T H\big(\partial \bar{u}(PX_t, t), PX_t\big) - H\big(\partial \bar{u}(PX_t, t), X_t\big)dt \\
&\quad + g(PX_T) - g(X_T)
\end{aligned}$$

Allen-Cahn Ex. (Sandberg)

$$u(X_0, 0) - \bar{u}(X_0, 0) = \mathcal{O}(\Delta t + (\Delta x)^2)$$

$$\partial_t X_t = \delta \partial_{xx} X_t - \delta^{-1} V'(X_t) + \alpha_t \quad x \in (0,1) \quad t < T$$

Stability for case $\bar{X}^0 = X^0$ and $\bar{g} = g$:

$$\underbrace{\int_0^T \bar{h}(\bar{X}^t, \bar{\alpha}^t)\,\mathrm{d}t + \bar{g}(\bar{X}^T)}_{\bar{u}(\bar{X}^0,0)} - \underbrace{\int_0^T h(X^t, \alpha^t)\,\mathrm{d}t + g(X^T)}_{u(X^0,0)}$$

$$= \int_0^T \bar{h}(\bar{X}^t, \bar{\alpha}^t)\,\mathrm{d}t + u(\bar{X}^T, T) - \underbrace{u(X^0, 0)}_{u(\bar{X}^0,0)}$$

$$= \int_0^T \bar{h}(\bar{X}^t, \bar{\alpha}^t)\,\mathrm{d}t + \int_0^T \mathrm{d}u(\bar{X}^t, t)$$

$$= \int_0^T \underbrace{\partial_t u(\bar{X}^t, t)}_{=-H\left(\partial_x u(\bar{X}^t,t),\bar{X}^t\right)} + \underbrace{\partial_x u(\bar{X}^t, t) \cdot \bar{f}(\bar{X}^t, \bar{\alpha}^t) + \bar{h}(\bar{X}^t, \bar{\alpha}^t)}_{\geq \bar{H}\left(\partial_x u(\bar{X}^t,t),\bar{X}^t\right)}\,\mathrm{d}t$$

$$\geq \int_0^T (\bar{H} - H)\big(\partial_x u(\bar{X}^t, t), \bar{X}^t\big)\,\mathrm{d}t.$$

Implied volatility: from Heston plus jumps 20 strikes in price and 5 in time

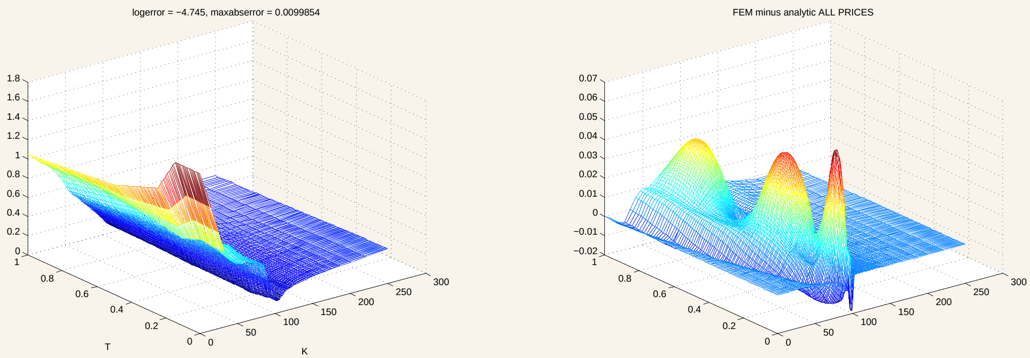


Figure 1: Volatility surface and error in option prices with piecewise linears

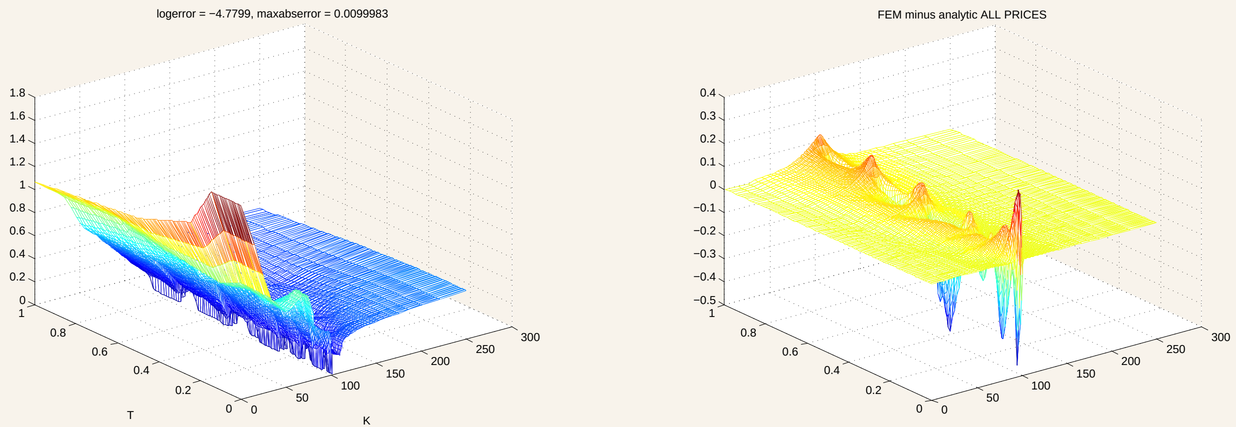


Figure 2: Volatility surface and error in option prices; volatility on fine mesh

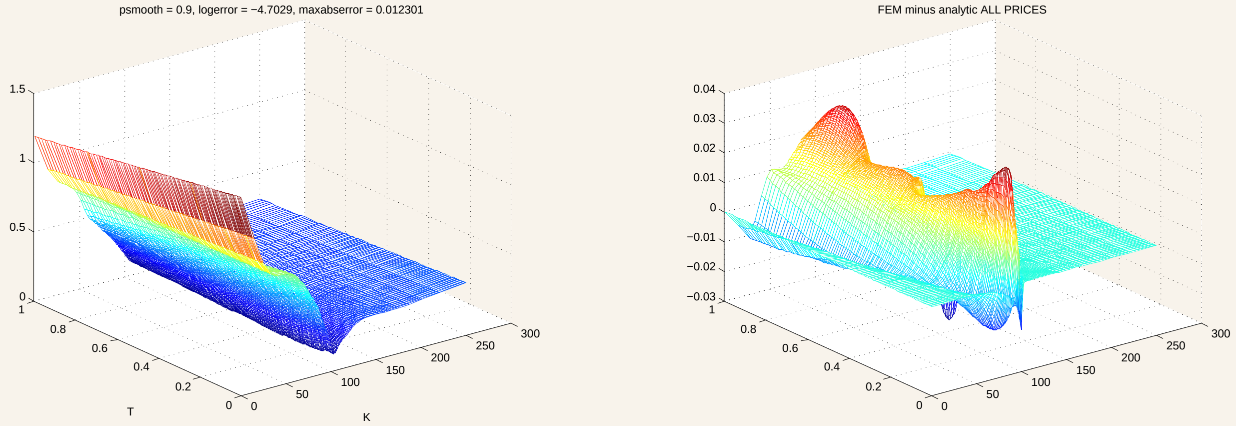


Figure 3: Volatility surface and error in option prices with splines

Relation to Tikhonov

Want

$$\min_{\alpha \in B} \big(\lambda \cdot f(X,\alpha) + \hat{T}(X,\alpha)\big) = H^\delta(\lambda, X)?$$

instead $$\min_{\phi \in \hat{f}(X,B)} \big(\lambda \cdot \phi + T(X,\phi)\big) = H^\delta(\lambda, X)$$

Legendre solution

$$T(X,\phi) = \sup_{\lambda \in \mathbb{R}^d} \big(-\lambda \cdot \phi + H^\delta(\lambda, X)\big)$$

Our inverse approach

- choose controls
- determine Hamiltonian (if possible)
- regularize Hamiltonian (by convolution)
- solve Hamiltonian system (by Newton)

More Examples

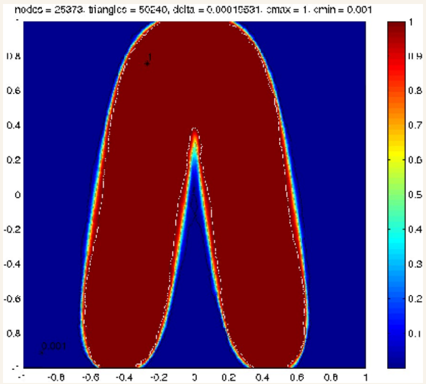
- optimal design
- reconstruction
- use MD to find Allen-Cahn SPDE for phase changes
- accuracy of MD compared to Schrödinger
- calibration of jump-diffusion (Kiessling)
- optimal design and reconstruction for heat equation and wave equation (Carlsson)

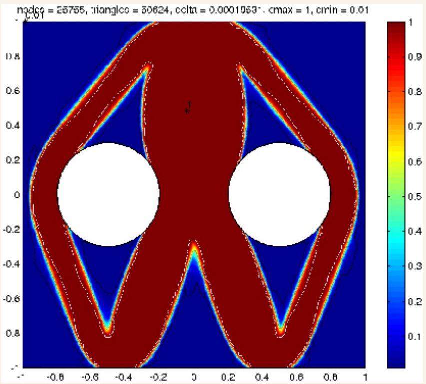
A Convex Minimization Problem

Ex: Computation of optimal designs. Find $\sigma : \Omega \longrightarrow \{\sigma_-, \sigma_+\}$

$$\operatorname{div}(\sigma \partial_x \varphi(x)) = 0 \quad x \in \Omega, \qquad \sigma \frac{\partial \varphi}{\partial n}\Big|_{\partial\Omega} = I$$

$$\min_{\sigma}\left(\int_{\partial\Omega} I \varphi ds + \eta \int_{\Omega} \sigma dx \right).$$





- Convex problem
- $\delta \longrightarrow 0$ possible

Non Convex/Concave Problem

Change to $\max_\sigma$

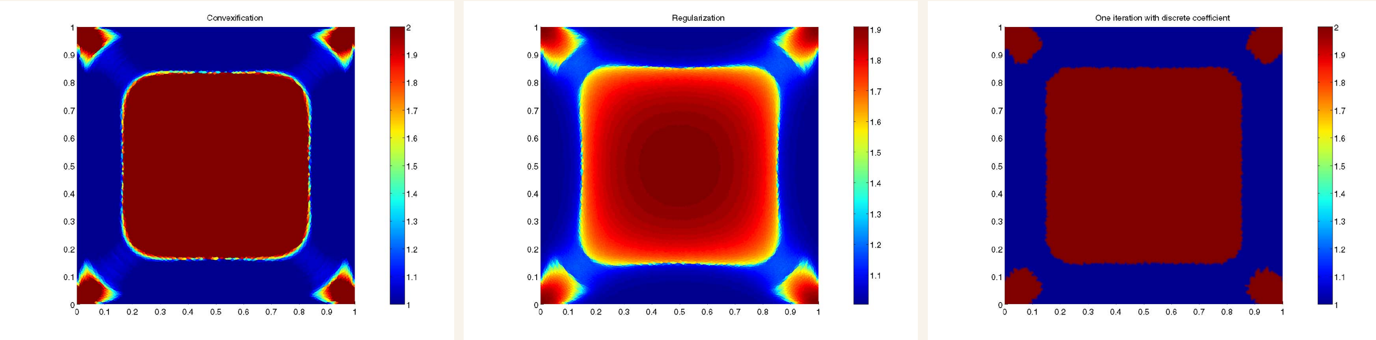


Figure 4: Convexified reference, H^δ, iterations in $\{\sigma_-, \sigma_+\}$

- $\delta \sim 1$
- Convexified functional optimal, or do η/σ

Parameter estimation from measurements

Change to $\min_\sigma \int_{\partial\Omega} (\varphi - \bar{\varphi})^2$

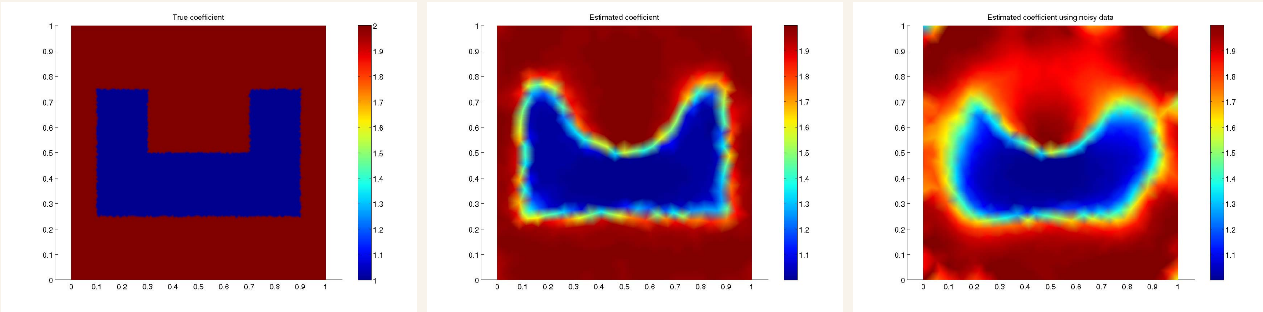


Figure 5: Conductivity: true, estimated no noise, 5% noise

- Seems to behave as convex/non-convex problem depending on σ_+/σ_-
- Optimal choice of input currents?

Elasticity

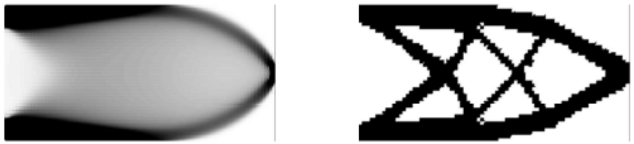


FIGURE 3. Plot of $\mathfrak{h}'_\delta$ as an approximation of the relative material density when minimizing compliance of an elastic plate with a fixed right side and an external load $f_s(2, y) = -10$, $y \in [0.45, 55]$. A uniform mesh with 80×40 nine-node quadrilateral finite elements and a multiplier $\eta = 0.005$ was used. In the left figure, (4) was solved with the Newton method and by successively reducing the regularization δ until $\delta \approx 3.5 \cdot 10^{-4}$. The right figure shows the density after 100 iterations using (25) with $\delta = 0$ and with the solution from the left part taken as initial guess.

FIGURE 4. Plot of $\mathfrak{h}'_\delta$ calculated with data as in Figure 3 but using a 240×120 mesh. Note that the unregularized design on the right is mesh dependent. The discrete designs are also sensitive to the initial data and the fraction of elements allowed to change in each iteration. Although the discrete design here differs a lot from the one in Figure 3, the compliance only differs by less than 0.1 percent.