Graz, Austria

Semi-Smooth Newton Methods in Function Spaces and Applications to Variational Problems in Optimal Control and Imaging

K. Kunisch

Department of Mathematics and Computational Sciences
University of Graz, Austria

Mathematical Optimization and Applications in the Biomedical Sciences

JOHANN·RADON·INSTITUTE FOR COMPUTATIONAL AND APPLIED MATHEMATICS

Collaborators

- K. Ito, North Carolina State University

- M. Hintermüller, Humbold University, Berlin
- M. Bergounioux, Univ. Orleans

- C. Clason, Univ. Graz
- J.C. De Los Reyes, Univ. Quito
- R. Griesse, Univ. Chemnitz
- T. Karkkainnen, Univ. Yvaaskyla
- V. Kovtunenko, Univ. Novosibirsk
- F. Rendl, Univ. Klagenfurt
- A. Rösch, Univ. Dortmund
- G. Stadler, Univ. Texas at Austin
- B. Vexler, Techn. Univ. Munich

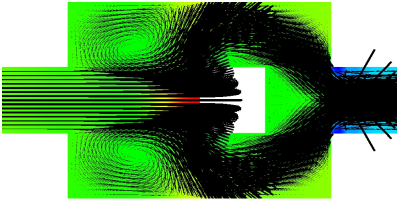

Figure: uncontrolled flow, $t = 2.4$

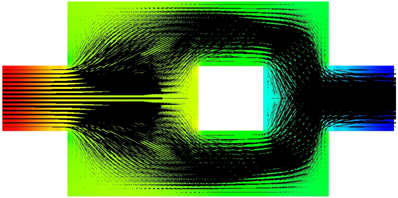

Figure: Stokes solution, $t = 2.4$

$$
(P) \qquad \begin{cases} \min J(y,u) = J_1(y) + J_2(u) \\ \\ y_t = F(y,\pi) \quad \text{on} \ \ (0,T] \\ y(0) = y_0, \qquad\qquad \text{for } t = 0 \\ \text{boundary conditions} \end{cases}
$$

inflow condition:

$$
y = u(t)\,\hat{y}_{in}(x) \quad \text{on } \Gamma_{in}, \quad \hat{y}_{in} \text{ fixed, parabolic}
$$

$$
\int_0^T u(t)\,dt = C_0
$$

total inflow in $(0,T)$ is independent of control.

Cost-functionals for vortex reduction

- Tracking functional: $$J_1(y) = \int_0^T \int_\Omega |y(t,x) - y_{des}(t,x)|^2$$
- curl functional: $$J_2(y) = \int_0^T \int_\Omega |\mathrm{curl}\, y(t,x)|^2$$
- Galilean functional: $$J_3(y) = \int_0^T \int_\Omega |(\det \nabla y(x))^+|$$
  $$\sim \mathrm{spectrum}(\nabla y(x)) \not\subseteq \mathcal{I}m$$
- Objective functional: $$J_4(y,\pi) = \int_0^T \int_\Omega (|r(y,\pi)| - 1)^+$$
  $$x \to \mathcal{Q}(t)x + d(t)$$

$$r(y,\pi) = \frac{\omega}{\sigma} - \frac{\sigma_s(\pi_{x_1x_1} - \pi_{x_2x_2}) - 2\sigma_n \pi_{x_1x_2}}{\sigma^{\frac{3}{2}}},$$

$$\omega = (y_2)_{x_1} - (y_1)_{x_2},\ \sigma_s = (y_2)_{x_1} + (y_1)_{x_2},\ \sigma_n = (y_1)_{x_1} - (y_2)_{x_2}.$$

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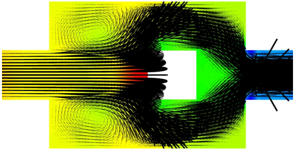
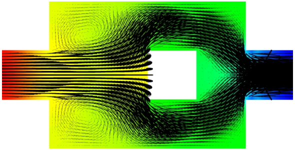
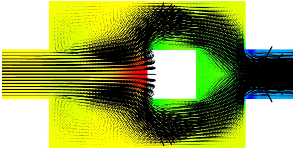
Optimal Vortex Reduction for Non-Stationary Flows



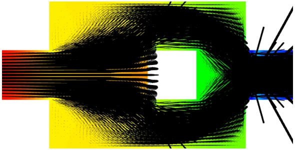
tracking functional



curl functional



Galilean functional



Objective functional

Inverse Elastohydrodynamic Problem

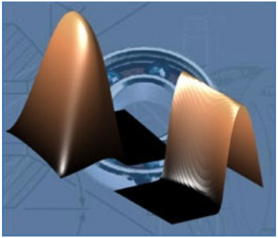
$$
(P) \qquad \begin{cases} \min \frac{1}{2} \int_{\tilde{\Omega}} |y - y_{data}|^2 \, dx + \frac{\alpha}{2} |u|^2 \\ u \in U \\ y = y(u) = argmin \, \{ J^u(y) \, : \, y \in K \} \end{cases}
$$

$$
J^u(y) = \int_\Omega u^3 \, |\nabla y|^2 \, dx - \int_\Omega \frac{\partial u}{\partial x_2} \, y \, dx
$$

$$
K = \{ y \in H_0^1(\Omega) : y \geq 0 \}
$$

Reynolds lubrication problem

Inverse Elastohydrodynamic Problem



$$
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Reynolds lubrication problem

Control Constrained Optimal Control

$$(P) \qquad \begin{cases} \min \frac{1}{2}\,|y-z|^2_{L^2} + \frac{\alpha}{2}|u|^2_{L^2} \\ -\Delta y = u \ \text{ in } \ \Omega\,, \qquad y = 0 \ \text{ on } \ \partial\Omega\,, \qquad u \le \psi \ \text{ in } \ \Omega \end{cases}$$

$$G := u - \psi \le 0; \qquad G : L^2(\Omega) \to L^2(\Omega)$$

G' surjective

$$\mathcal{L}(y,u,p,\lambda) = \frac{1}{2}\,|y-z|^2_{L^2} + \frac{\alpha}{2}|u|^2_{L^2} + (p, -\Delta y - u)_{L^2} + (\lambda, u-\psi)_{L^2}$$

$$(OS) \qquad \begin{cases} -\Delta y = u \\ -\Delta p = -(y-z) \\ \alpha\, u + \lambda = p\,, \quad u \le \psi\,, \quad \lambda \ge 0\,, \quad (\lambda, u-\psi)_{L^2} = 0 \end{cases}$$

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Primal-Dual Active Set Algorithm for Control Constraints

$$(OS) \qquad \begin{cases} -\Delta y = u \\ -\Delta p = -(y - z) \\ \alpha\, u + \lambda = p\,, \quad u \le \psi\,, \quad \lambda \ge 0\,, \quad (\lambda, u - \psi)_{L^2} = 0 \end{cases}$$

$\lambda^* = \max(0, \lambda^* + c(u^* - \psi))$ for any $c > 0$

Moreau - Yosida approximation

PDA-Algorithm

(i) choose $c > 0,\ (u_0, \lambda_0); \quad k = 0$

(ii) $\mathcal{A}_{k+1} = \{x \in \Omega :\ \lambda_k(x) + c(u_k(x) - \psi(x)) > 0\}$

(iii) $y_{k+1} = \text{argmin}\,\{(P) : u = \psi \text{ on } \mathcal{A}_{k+1}\}$

(iv) λ_{k+1} associated L.M., with $\lambda_{k+1} = 0 \quad \text{on} \quad \mathcal{I}_{k+1}$.

Remarks:

1. solve (iii) only on $\mathcal{I}_{n+1}$
2. termination $\mathcal{A}_{n+1} = \mathcal{A}_n$, globalization
3. $\mathcal{A}_{n+1}$ may be very different from $\mathcal{A}_n$
4. typically the iterates are primarily feasible
5. bilateral constraints:

$$\lambda^* = \max(0, \lambda^* + c(y^* - \psi)) + \min(0, \lambda^* + c(y - \phi))$$

6. polygonial constraints

Theorem

If $\|\Delta^{-1}\|^2_{\mathcal{L}(L^2(\Omega))} < \alpha$, then global convergence, also in bilateral case.

$$M(u, \lambda) = \alpha^2 \int_\Omega |(u - \psi)^+|^2 + \int_{\mathcal{A}} |\lambda^-|^2,$$

Semi-smoothness Newton Method

Definition

$F : D \subset X \to Z$ is called Newton differentiable in $U \subset D$, if there exist $G : U \to \mathcal{L}(X, Z)$:

$$(A)\ lim_{h\to 0} \frac{1}{\mid h \mid} \mid F(x+h) - F(x) - G(x+h)h \mid = 0, \text{ for all } x \in U.$$

Example

$F : L^p(\Omega) \to L^q(\Omega),\ F(\varphi) = \max(0, \varphi)$ is Newton differentiable if $q < p$, and

$$G_{\max}(\varphi)(x) = \begin{cases} 1 & \text{if } \varphi(x) > 0 \\ 0 & \text{if } \varphi(x) < 0 \\ \delta & \text{if } \varphi(x) = 0,\ \delta \in \mathbb{R} \text{ arbitrary.} \end{cases}$$

Example

$\psi : \mathbb{R} \to \mathbb{R}$ semi-smooth, glob. Lip.-cont., $1 \le p < q < \infty$.

$\Psi(y)(x) = \psi(y(x)), \quad \Psi : L^q(\Omega) \to L^p(\Omega)$

Theorem

Let $F(x^*) = 0$, F Newton differentiable in $U(x^*)$, and $\{||G(x)^{-1}||_{\mathcal{L}(X,Z)} : x \in U(x^*)\}$ bounded.

Then the Newton iteration converges locally superlinearly.

PDA and Newton applied to (OC) coincide

$$(OS) \qquad \begin{cases} -\Delta y = u, \\ -\Delta p = -(y - z) \\ \alpha\, u + \lambda = p \\ \lambda = \max(0, \lambda + c(u - \psi)) \end{cases}$$

$$c = \alpha : \qquad F(u) = \alpha u - p(u) + \max(0, p(u) - \alpha\psi) = 0$$

Rate of convergence, chain rules

Ref.: Hintermüller-Ito-K, Chen-Nashed, Kummer, M. Ulbrich.

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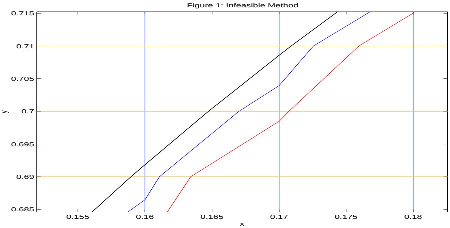
Numerical tests, control constraints

k	1	2	3	4	5	6	7
q_u^k	1.0288	0.8354	0.6837	0.4772	0.2451	0.0795	0.0043
q_λ^k	0.6130	0.5997	0.4611	0.3015	0.1363	0.0399	0.0026

$$q_u^k = \frac{|u_h^k - u_h^*|}{|u_h^{k-1} - u_h^*|}, \quad q_\lambda^k = \frac{|\lambda_h^k - \lambda_h^*|}{|\lambda_h^{k-1} - \lambda_h^*|},$$



Active-inactive interface

State Constrained Optimal Control

$$(P) \quad \begin{cases} \min \frac{1}{2}\,|y-z|^2_{L^2} + \frac{\alpha}{2}|u|^2_{L^2} \\ \\ -\Delta y = u \ \text{ in } \ \Omega, \qquad y = 0 \ \text{ on } \ \partial\Omega\,, \qquad y \le \psi \ \text{ in } \ \Omega \end{cases}$$

$$G : H^2(\Omega) \cap H^1_0(\Omega), \qquad G \text{ not surjective to } L^2(\Omega).$$

$$(OS) \quad \begin{cases} -\Delta y = u \\ -\Delta p + \lambda = -(y-z)\,, \quad \lambda \in H^{-2}(\Omega) \cap C^*(\Omega). \\ \alpha\, u = p\,, \quad y \le \psi\,, \quad \lambda \ge 0\,, \quad \langle \lambda, y-\psi \rangle_{H^{-2},H^2} = 0 \end{cases}$$

Mesh size h	1/16	1/32	1/64	1/128	1/256
PDAS	14	27	54	113	226

Speed of propagation, state constraints.

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State Constraints - Low Multiplier Regularity

$$(P_\gamma) \quad \begin{cases} \min \frac{1}{2}\,|y-z|^2 + \frac{\alpha}{2}\,|u|^2 + \frac{1}{2\gamma}\int_\Omega |(\bar{\lambda}+\gamma(y_\gamma-\psi))^+|^2 dx \\ -\Delta y = u, \ \text{ in } \ \Omega, \quad y=0 \ \text{ on } \partial\Omega. \end{cases}$$

$$\gamma \to \infty$$

$$(OS_\gamma) \quad \begin{cases} -\Delta y = u \ \text{ in } \Omega, & y = 0 \ \text{ on } \ \partial\Omega \\ -\Delta p + \lambda_\gamma = -(y-z) \ \text{ in } \Omega, & p = 0 \ \text{ on } \ \partial\Omega \\ \alpha u = p & \\ \lambda_\gamma = \bar{\lambda} + \gamma(y-\psi) & \end{cases}$$

compare to $\lambda = \max(0, \lambda + c(y-\psi))\,, \quad c > 0$ fixed.

Theorem

- $(y_\gamma, p_\gamma, \lambda_\gamma) \underset{\gamma\to\infty}{\longrightarrow} (y^*, p^*, \lambda^*)$ *in* $H^2(\Omega) \times L^2(\Omega) \times H^2(\Omega)^*_{weak}$
- *If* $\frac{\gamma}{\alpha}||\Delta^{-1}||_{\mathcal{L}(L^2(\Omega))} < 1$ *, then global convergence.*
- $(y_k, p_k, \lambda_k) \underset{k\to\infty}{\longrightarrow} (y_\gamma, p_\gamma, \lambda_\gamma)$ *locally superlinearly.*

regularized reduced iteration function

$$\lambda = \max\left(0, \bar{\lambda} + \gamma((I + \alpha A^2)^{-1}(z - \lambda) - \psi)\right)$$

reduced iteration function (unregularized)

$$\lambda = \max\left(0, \lambda + y - \psi\right) = \max(0, \lambda + (I + \alpha\Delta^2)^{-1}(z - \lambda) - \psi)$$

γ	10^3	10^4	10^5	10^6	10^8	10^9	10^{10}
iter	10	17	27	30	30	31	31
active	791	667	606	587	577	575	575

γ	10^3	10^6	10^9	
iter	10	6	3	$\Sigma = 19$

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Path Following for State Constrained Problems

$\bar{\lambda} = 0$.

$$\mathcal{P} = \{(y_\gamma, u_\gamma, p_\gamma, \lambda_\gamma) \in H^2 \times L^2 \times H^2 \times L^2 : \gamma > 0\}$$

$(P_{\gamma=0})$ unconstrained, $\quad$ $(P_{\gamma=\infty})$ constrained.

Theorem

$\mathcal{P}$ *is locally Lipschitz continuous.*

$$(H) \quad S_\gamma^0 := \{x \in \Omega : \; y_\gamma - \psi = 0\}, \quad meas\, S_\gamma^0 = 0$$

Theorem

$\gamma \to (y_\gamma, u_\gamma, p_\gamma) \in H^2 \times L^2 \times L^2_{weak}$ *is differentiable and*

$$-\Delta \dot{y} = \dot{u}, \quad -\Delta \dot{p} + (y_\gamma - \psi + \gamma \dot{y})\mathcal{X}_{S_\gamma} = 0, \quad \alpha \dot{u} = \dot{p}$$

$S_\gamma = \{x : y_\gamma - \psi > 0\}.$

$$V(\gamma) = \min J(y_\gamma, u_\gamma) + \frac{\gamma}{2} \int_\Omega |(y_\gamma - \psi)^+|^2$$

Theorem

$$\dot{V}(\gamma) = \frac{1}{2} \int_\Omega |(y_\gamma - \psi)^+|^2 \,, \qquad \ddot{V}(\gamma) = \int_\Omega (y_\gamma - \psi)^+ \dot{y}$$

Corollary

$$\dot{V}(\gamma) > 0\,, \quad \ddot{V}(\gamma) < 0\,, \quad V(0) \triangleq (P_{unconstr.})\,, \quad V(\infty) \triangleq (P)$$

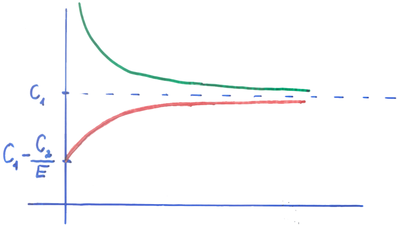
Model Function for Path

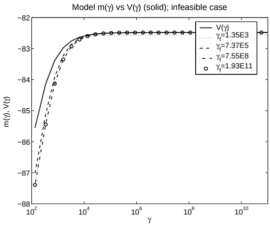
$$m(\gamma) = C_1 - \frac{C_2}{E+\gamma} \qquad\qquad m(\gamma) = C_1 - \frac{C_2}{E+\gamma} + \frac{B}{\gamma}$$

$$\bar{\lambda} = 0. \qquad\qquad \bar{\lambda} = \max\left(0, f + \Delta\psi\right).$$

approximate ODE

$$(E+\gamma)\ddot{m}(\gamma) + 2\,\dot{m}\,(\gamma) = 0$$





Exact Path-Following

$$|V^* - V(\gamma_{k+1})| \leq \tau_k \, |V^* - V(\gamma_k)|$$

$$m(\gamma) = C_1 - \frac{C_2}{(E+\gamma)}.$$

$$|C_{1,k} - V(\gamma_{k+1})| \leq \tau_k \, |C_{1,k} - V(\gamma_k)| =: \alpha_k$$

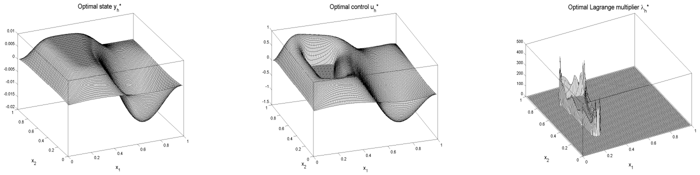
$$\gamma_{k+1} = (\frac{C_{2,k}}{\alpha_k})^{1/r} - E_k.$$

Theorem

(exact path following)

$$\lim_{k\to\infty} (y_{\gamma_k}, u_{\gamma_k}, \lambda_{\gamma_k}) \to (y^*, u^*, \lambda^*).$$

Inexact Path-following : $\gamma_{k+1} = \mathcal{F}$(primal/dual feasibilies), compare interior point methods



Optimal state (left), optimal control (middle), and optimal multiplier (right) for problem 1 with $h = 1/128$.

Mesh size h	1/16	1/32	1/64	1/128	1/256
PDAS	14	27	54	113	226
PDIP	12	14	15	19	19
IPF	11	15	14	13	15

Comparison of iteration numbers for different mesh sizes and methods.

Mesh size h	1/4	1/8	1/16	1/32	1/64	1/128	1/256	total
PDAS	3	4	4	5	6	6	6	34
PDIP	3	2	4	4	5	6	7	31
IPF	4	3	3	4	5	5	5	29

Comparison of iteration numbers for different mesh sizes and methods based on nested iteration.

Important further Issues and Applications

- Discretization, adaptivity
- Gradient and (approximate) Hessian
- Discretize before or after optimize
- Saddle point solvers, preconditioning
- Globalization

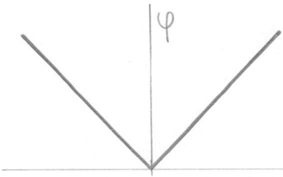
- Optimal control of variational inequalities, calibration of American options
- Time optimal control
- Crack modelling with non-penetration condition
- Contact and friction problems
- L^1- tracking functionals: robust statistics
- Sparsity

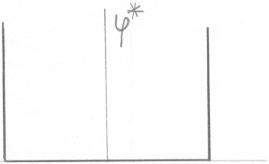
Dualisation of BV

$$\begin{cases} \min & \frac{1}{2}\int_\Omega |Ku - f|^2 dx + \frac{\alpha}{2}\int_\Omega |u|^2 dx + \beta \int_\Omega |Du| \\ \text{over} & u \in BV, \end{cases}$$

$$\alpha \geq 0, \beta > 0$$

$$\int_\Omega |Du| = \sup \left\{ \int_\Omega u \, div \, \vec{v} : \vec{v} \in (C_0^\infty(\Omega))^2, \, |\vec{v}(x)| \leq 1 \right\}$$





Dualisation of BV

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Theorem

$$\begin{cases} \inf \ \frac{1}{2}|div\, \vec{p} + K^* f|_B^2 \\ s.t. \ -\beta\vec{1} \le \vec{p}(x) \le \beta\vec{1} \ for\ a.e.\ x \in \Omega, \end{cases}$$

$$|v|_B^2 = (v, B^{-1}v), \quad B = \alpha\,\mathrm{I} + K^*K$$

$$div\vec{p} = Bu - K^*f, \quad \vec{p} = \beta\left(\frac{u_{x_i}}{|u_{x_i}|}\right)_{i=1}^n \text{ on } \{x : u_{x_i}(x) \neq 0 \text{ for all } i\}.$$

Dualisation of BV

$$\begin{cases} \min & \frac{1}{2}\int_\Omega |Ku-f|^2 dx + \frac{\alpha}{2}\int_\Omega |u|^2 dx + \beta\int_\Omega |Du| \\ \text{over} & u \in BV, \end{cases}$$

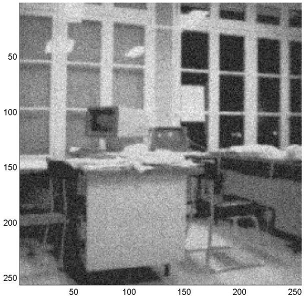
Theorem

$$\begin{cases} \inf\ \frac{1}{2}|div\,\vec{p} + K^* f|_B^2 \\ s.t.\ -\beta\vec{1} \le \vec{p}(x) \le \beta\vec{1}\ \textit{for a.e. } x \in \Omega, \end{cases}$$

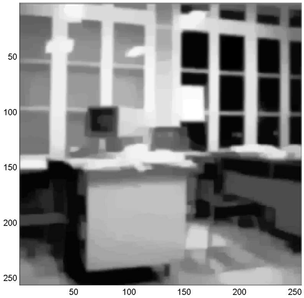
$$|v|_B^2 = (v, B^{-1}v), \quad B = \alpha\,\mathrm{I} + K^*K$$

$$div\vec{p} = Bu - K^*f, \quad \vec{p} = \beta\left(\frac{u_{x_i}}{|u_{x_i}|}\right)_{i=1}^n \text{ on } \{x : u_{x_i}(x) \ne 0 \text{ for all } i\}.$$

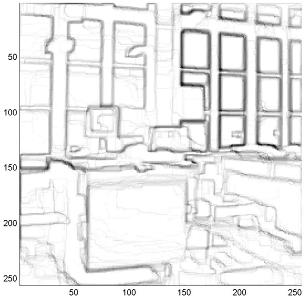
Data



Reconstruction



Edge detector, i.e. l_1-norm of λ.



Portfolio Optimization

$$dX_0(t) = rX_0(t)\,dt - (1+\gamma)dL(t) + (1-\gamma)dM(t)$$

$$dX_1(t) = \mu X_1(t)\,dt + \sigma X_1(t)dW(t) + dL(t) - dM(t)$$

X_0, X_1 wealth processes for bank account /stock

r, μ, σ, γ interest rate, trend, volatility, trading costs

L, M cumulative processes describing purchases/sales of stock

jointly with J. Sass

Portfolio Optimization

$$J(t, x_0, x_1)$$
$$= \sup_{L,M} E[\tfrac{1}{\alpha}(X_0(T) + (1-\gamma)X_1(T))^\alpha \mid X_0(t) = x_0, X_1(t) = x_1]$$

Theorem

J is concave, continuous, and a viscosity solution of

$$\max \{ J_t + \mathcal{A}J \ , \quad -(1+\gamma)J_{x_0} + J_{x_1} \ , \quad (1-\gamma)J_{x_0} - J_{x_1} \} = 0$$

on $[0, T) \times \mathcal{D}$ *with* $J(T, x_0, x_1) = \frac{1}{\alpha}(x_0 + (1-\gamma)x_1)^\alpha$

$$\mathcal{A}\, h(x_0, x_1) = r x_0 h_{x_0}(x_0, x_1) + \mu h_{x_1}(x_0, x_1) + \tfrac{1}{2}\sigma^2 x_1^2\, h_{x_1, x_1}(x_0, x_1)$$

NO TRADING – BUY – SELL

c.f. Shreve and Soner, 1994.

Portfolio Optimization

$$J(t, x_0, x_1)$$

$$= \sup_{L,M} E[\tfrac{1}{\alpha}(X_0(T) + (1-\gamma)X_1(T))^\alpha \,|\, X_0(t) = x_0, X_1(t) = x_1]$$

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on $[0, T) \times \mathcal{D}$ with $J(T, x_0, x_1) = \frac{1}{\alpha}(x_0 + (1-\gamma)x_1)^\alpha$

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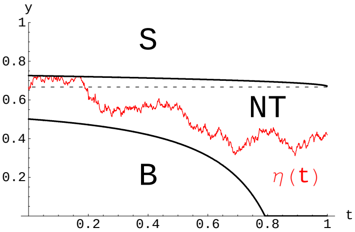
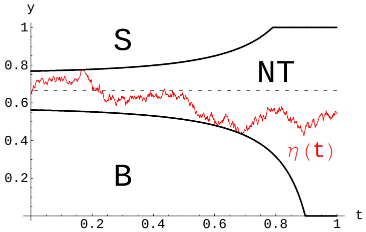




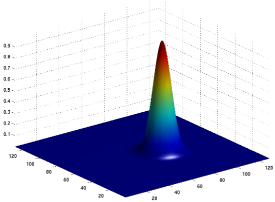
without liquidation costs

optimally controlled risky fraction

Which control norm to choose ?

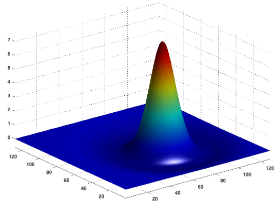
$$\min_{u \in U} \int_\Omega |y - z|^2 + |u|_U$$

$$-\Delta y = u$$

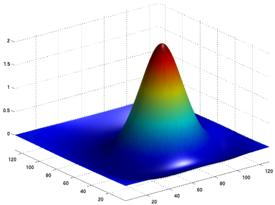


Target

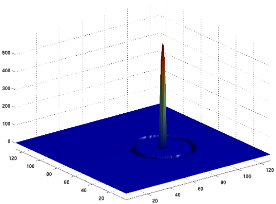
Which control norm to choose ?



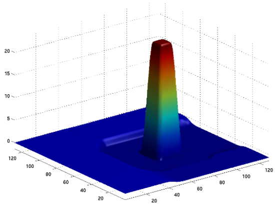
L^2 control



H^1 control



$\mathcal{M}$ control



BV control

On the Lagrange Multiplier Approach to Variational Problems and Applications, with K.Ito, SIAM, 2008.

karl.kunisch@uni-graz.at

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