Semismooth Hybrid Systems

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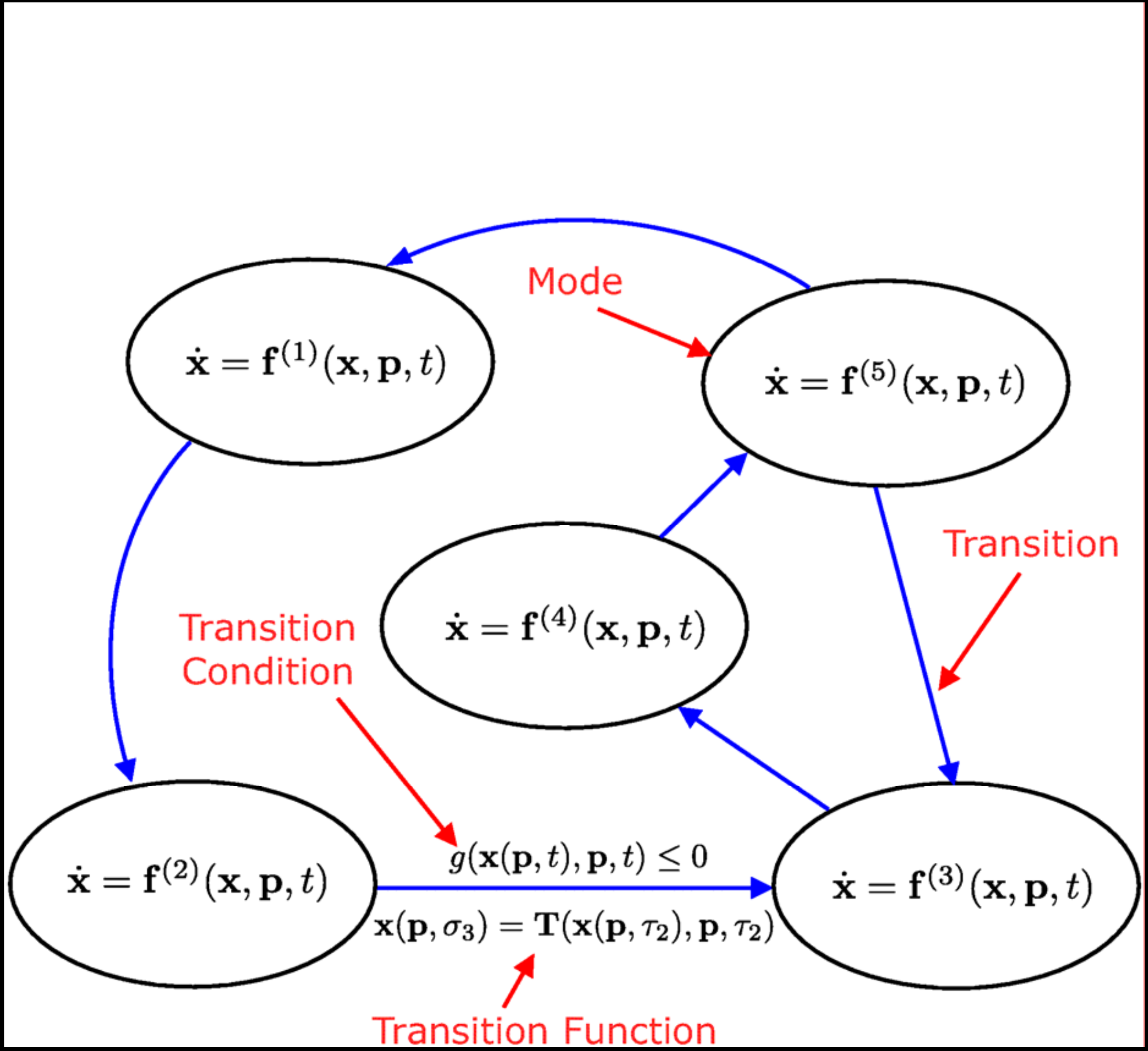
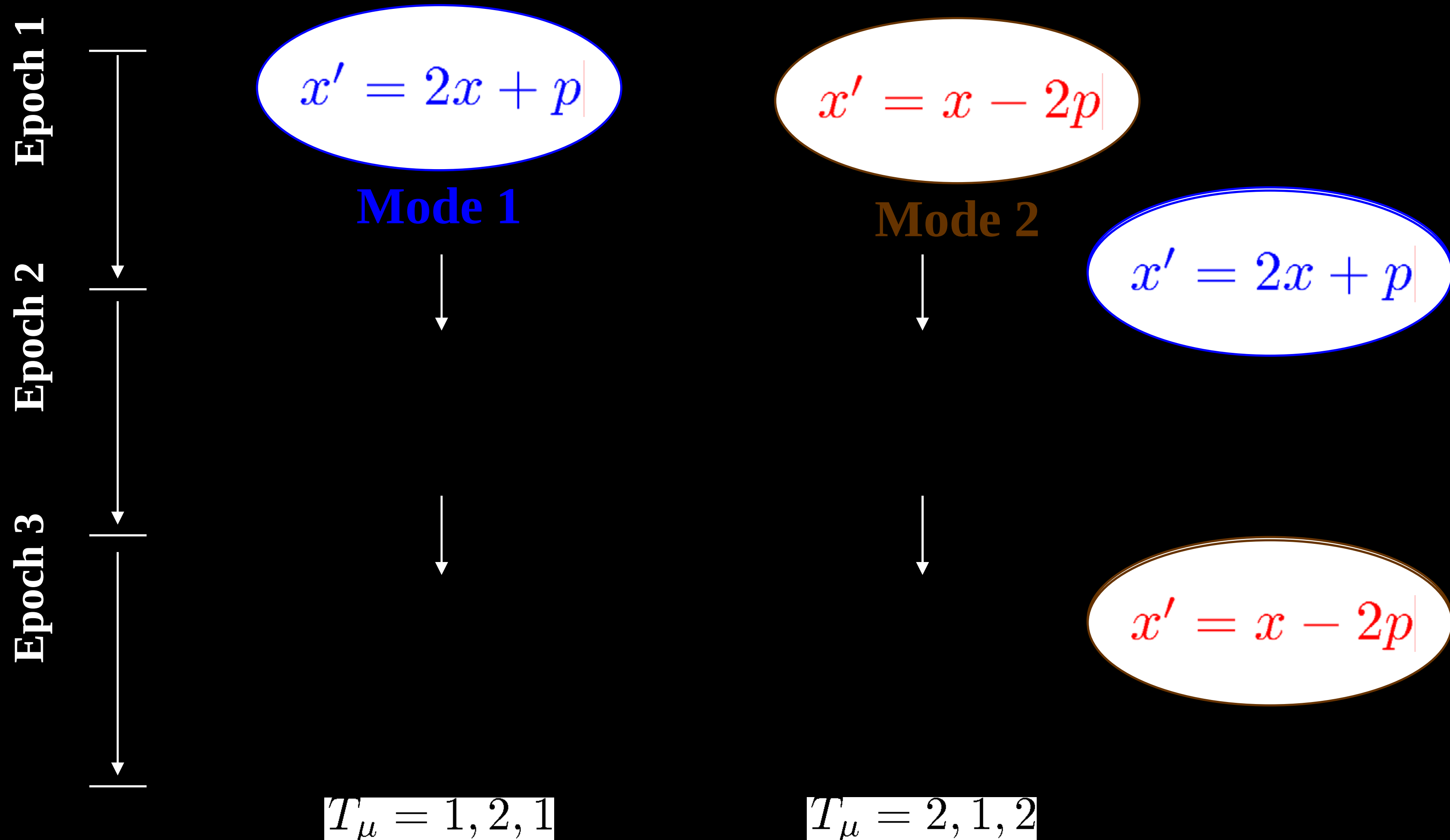
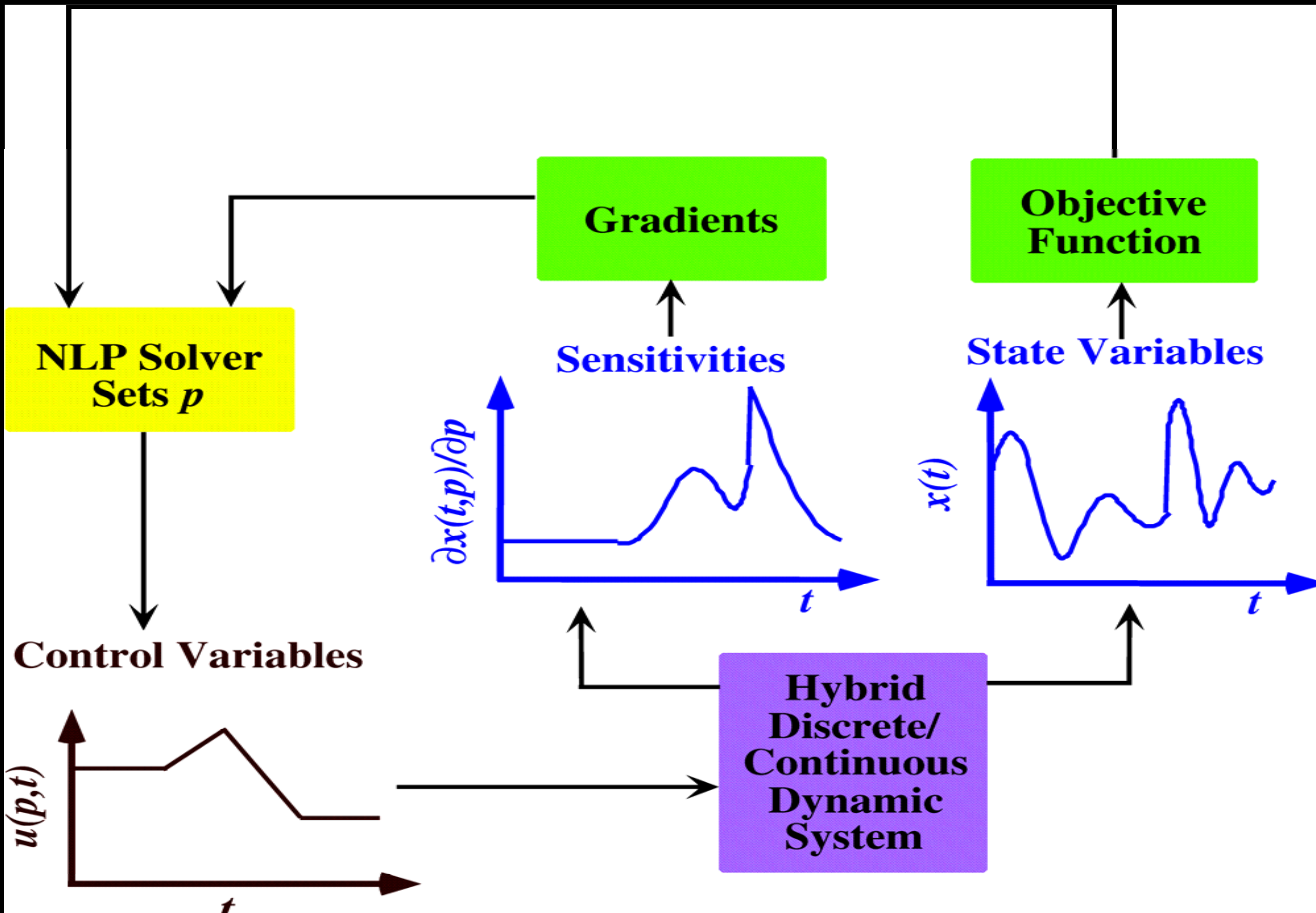
Continuous Time Hybrid Automaton (deterministic)



Hybrid Automaton
Epoch and Mode Sequences



Control Parameterization



Jacobian®

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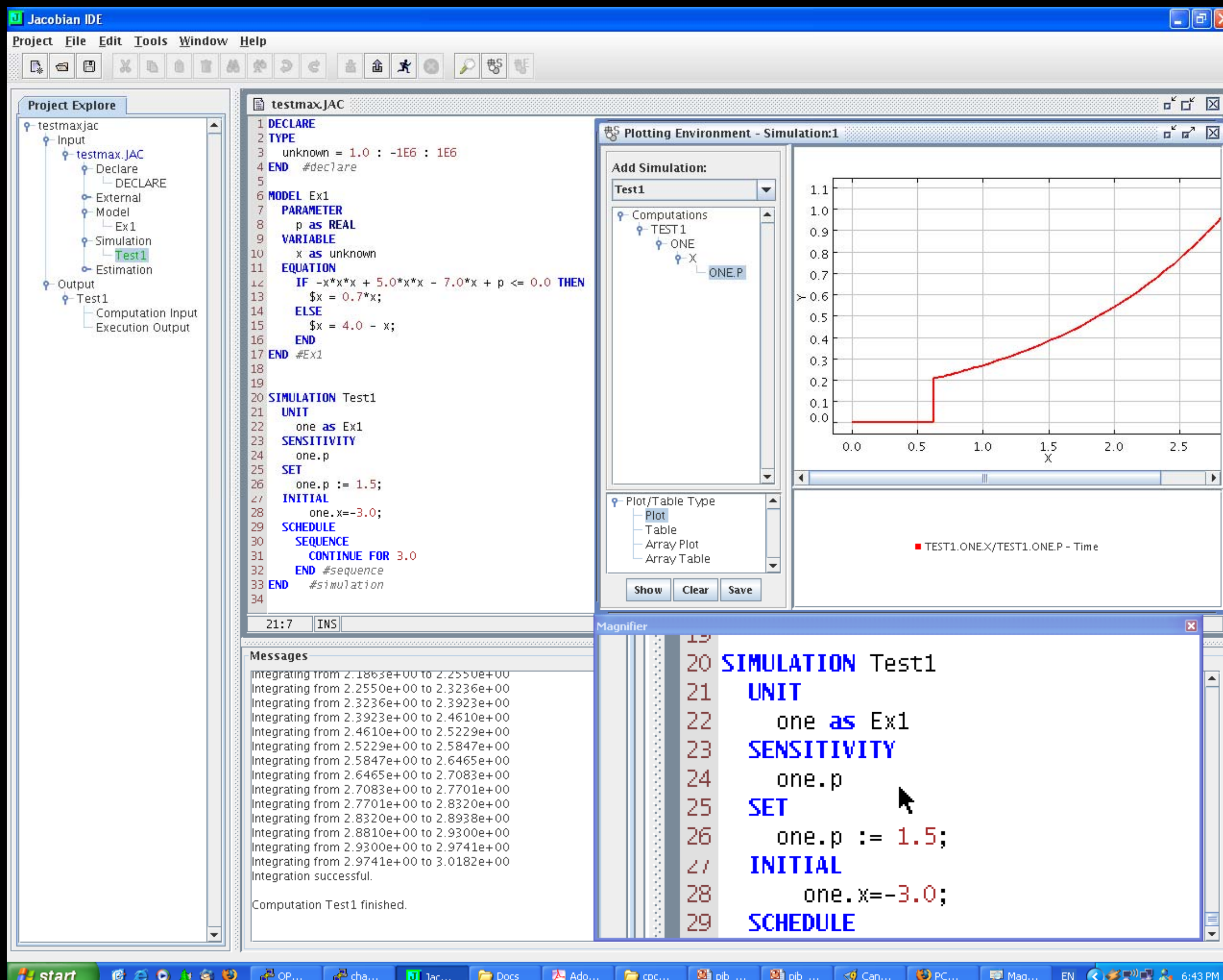


Nonsmoothness Example

$$\min_{p \in [0,7.5]} f(p) = -x(p,3)$$

subject to:

$$\text{Mode 1: } \dot{x} = 4 - x,$$

$$\text{switch to Mode 2 if } g(x,p) \leq 0$$

$$\text{Mode 2: } \dot{x} = 0.7x,$$

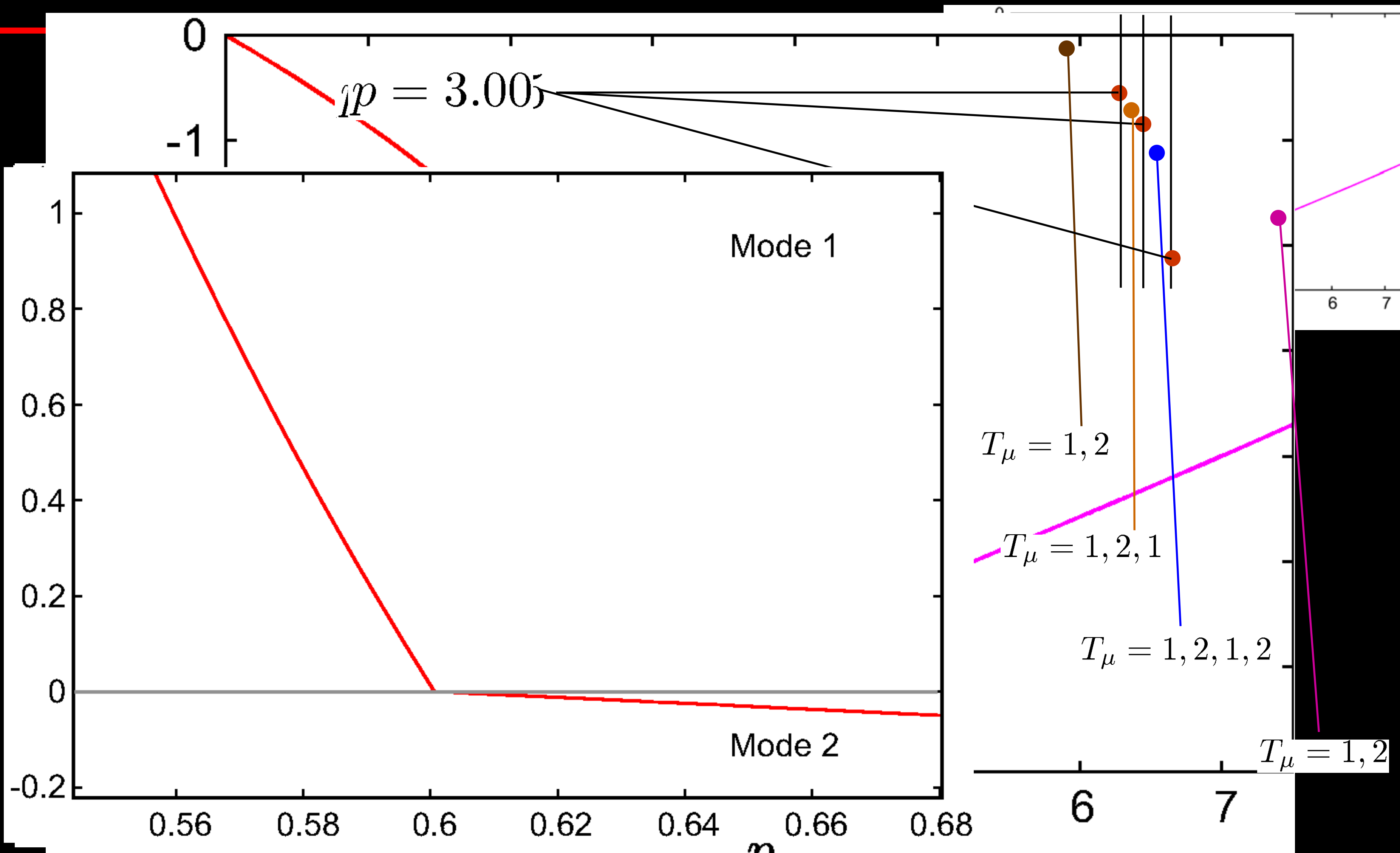
$$\text{switch to Mode 1 if } g(x,p) \geq 0$$

where $g(x,p) = -x^3 + 5x^2 - 7x + p,$

$$x(p,0) = -3,$$

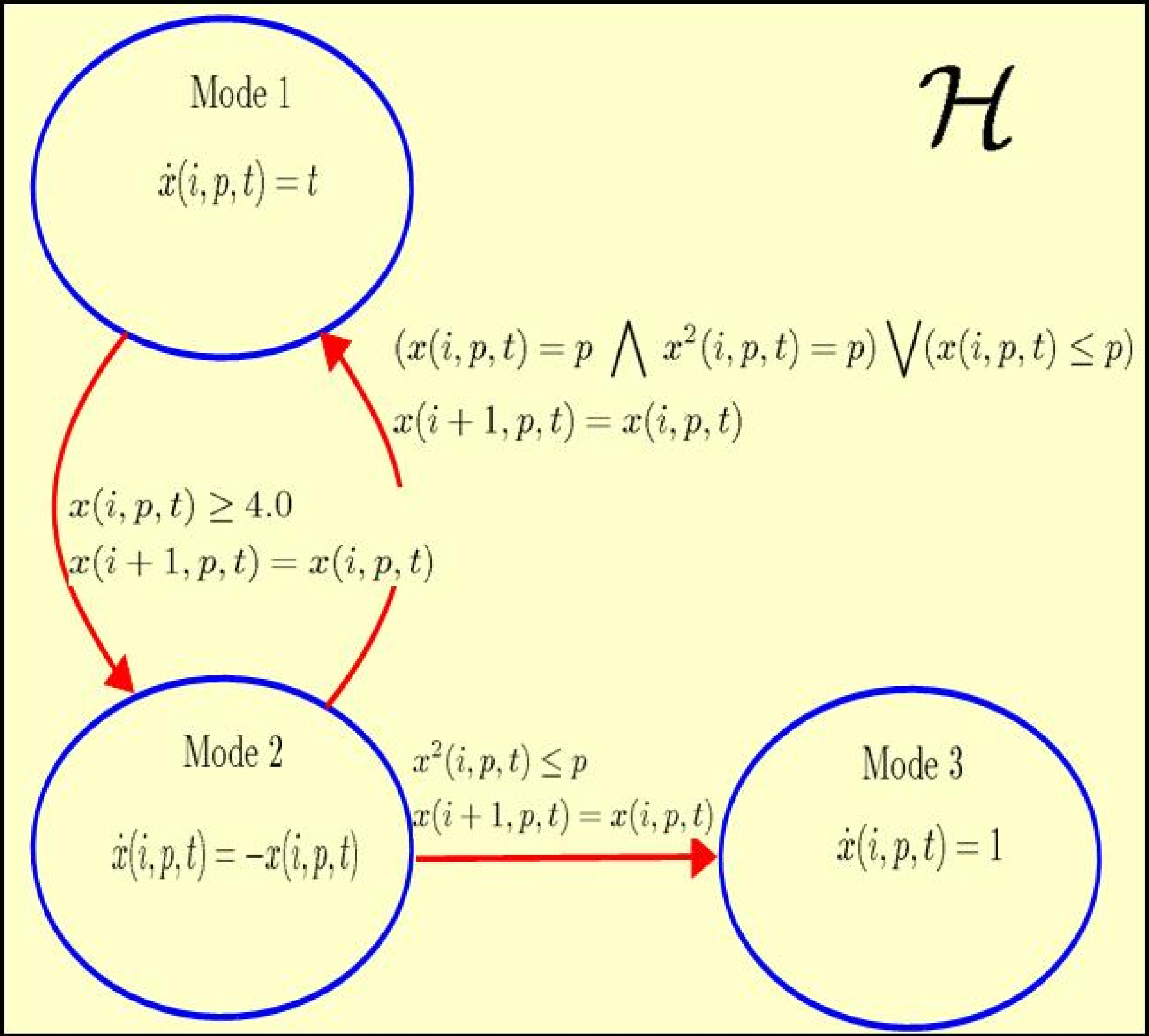
and state continuity is preserved at all transitions.

Nonsmoothness Example

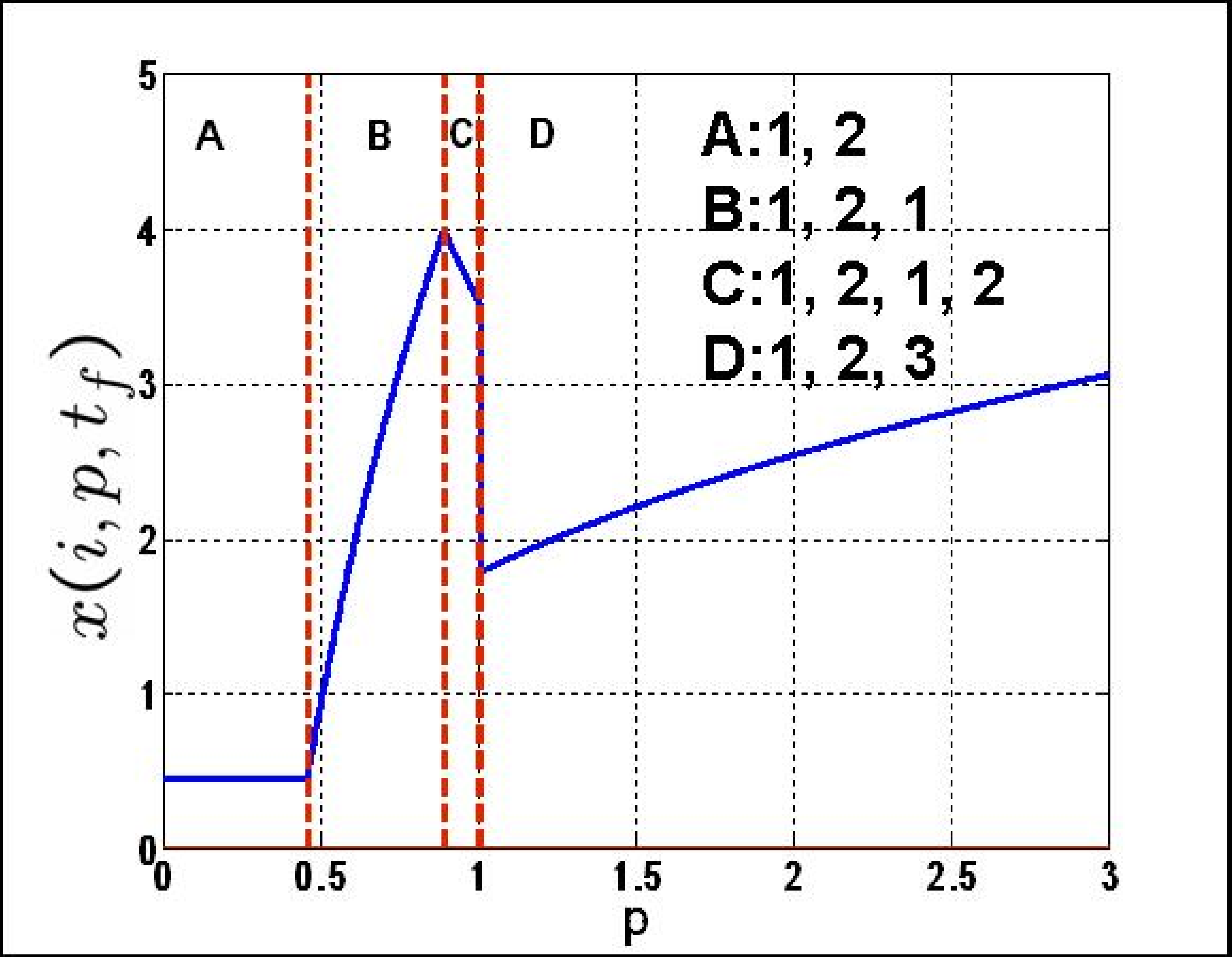


Discontinuity function $-x^3 + 5x^2 - 7x + p$

Discontinuous Example



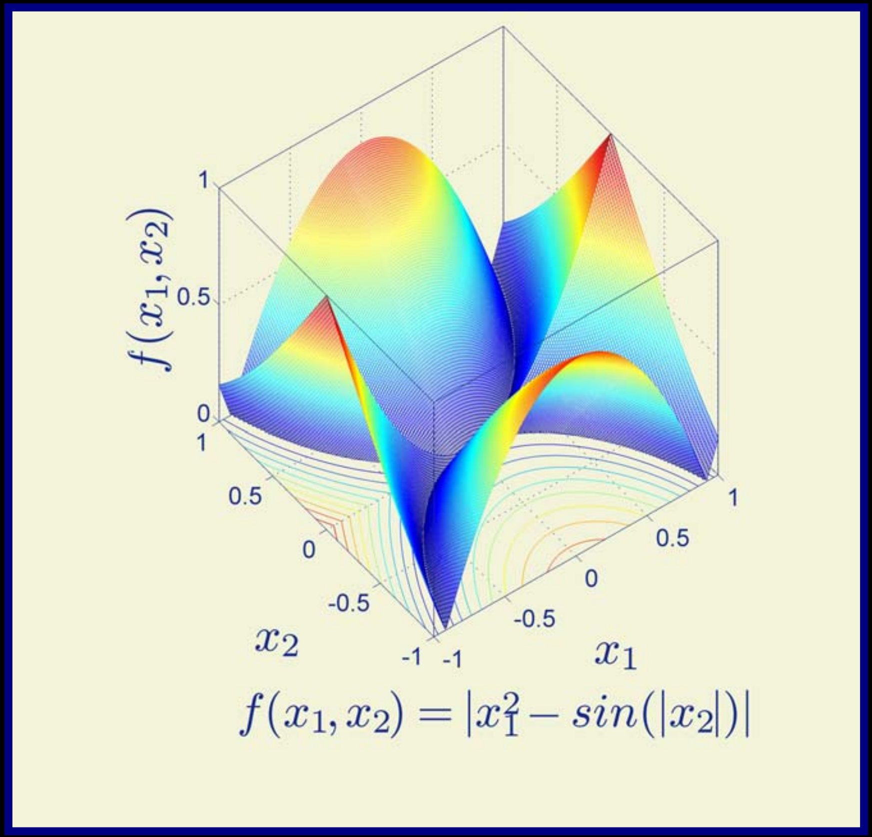
Discontinuous Example



Classification of Optimization Problems with Hybrid Systems Embedded

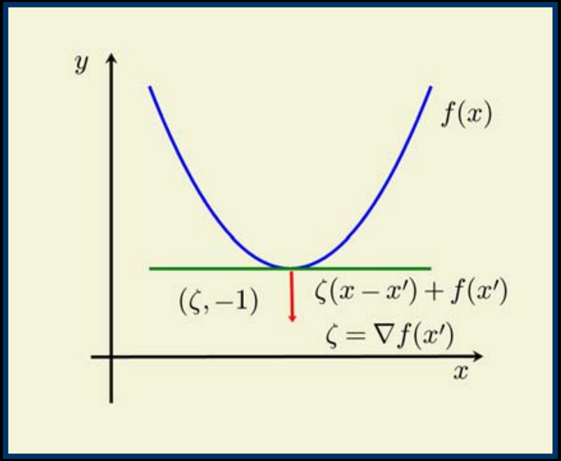
- Mode sequence does not vary - usually smooth
  - multi-stage dynamic optimization
- Semismooth hybrid systems
  - nonsmooth, mode sequence can vary
- Continuous but not semismooth hybrid systems
- Discontinuous hybrid systems

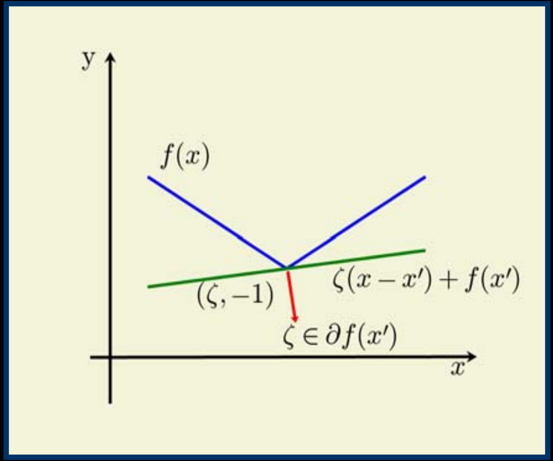
Nonsmooth Analysis
Locally Lipschitz Continuous Functions

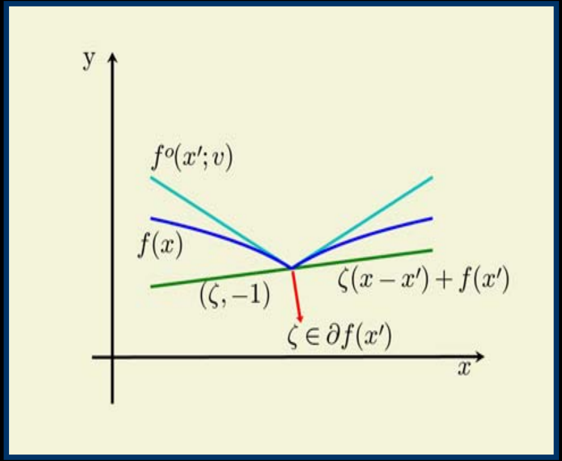


f locally Lipschitz continuous on an open neighborhood if
$\exists K \in \mathbb{R}_+ : \; |f(\mathbf{z}) - f(\mathbf{y})| \leq K\|\mathbf{z} - \mathbf{y}\|, \; \forall \mathbf{z}, \forall \mathbf{y} \in N_\varepsilon(\mathbf{x}), \; \forall \mathbf{x} \in X.$

Nonsmooth Analysis: Generalized Gradient



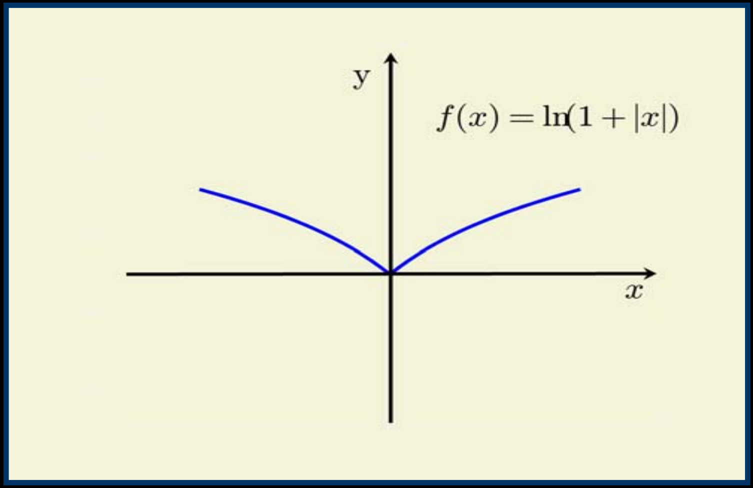


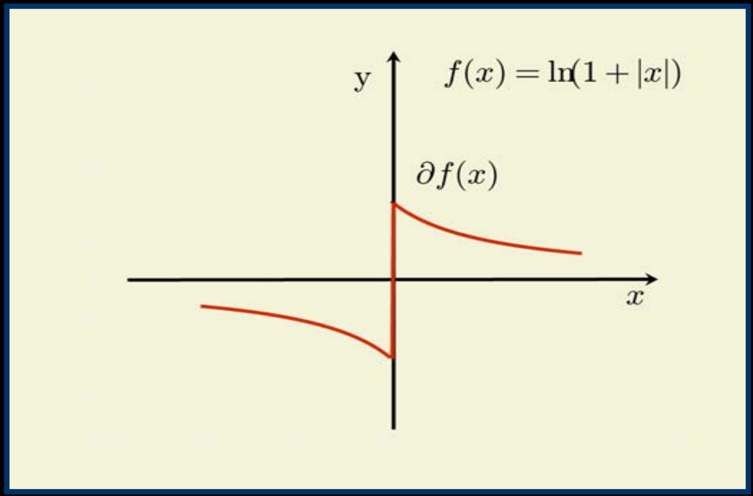


- Differentiable functions → gradients
- Convex functions → subdifferentials
- Locally Lipschitz continuous functions → generalized gradient*

***F. H. Clarke, Optimization and Nonsmooth Analysis, Classics in Applied Mathematics 5, SIAM, 1990**

Nonsmooth Analysis: Calculation of the Generalized Gradient





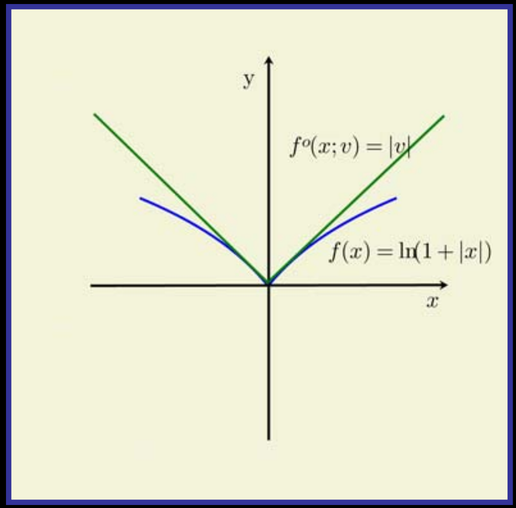
A locally Lipschitz continuous function, f:

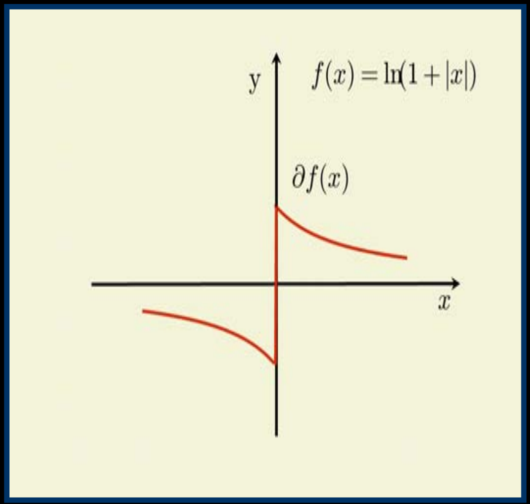
- is differentiable almost everywhere and
- its *generalized gradient* at $\mathbf{x}$ is:

$$\partial f(\mathbf{x}) = \mathrm{co}\{\lim \nabla f(\mathbf{x}_i) : \mathbf{x}_i \to \mathbf{x},\ \mathbf{x}_i \notin S\}$$

where S is a set of measure zero of points where the derivative does not exist

Nonsmooth Analysis: Optimization using Generalized Gradients

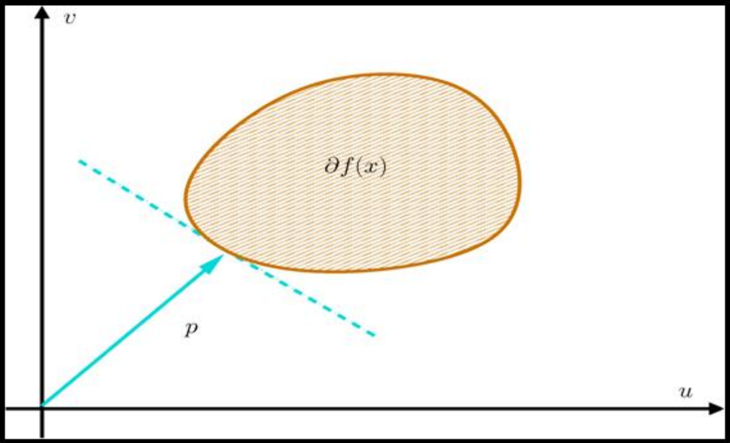




- $f : \mathbb{R}^n \to \mathbb{R}$ be locally Lipschitz continuous on $\mathbb{R}^n$ and $\mathbf{x}^*$ be a local minimum , then $\mathbf{0} \in \partial f(\mathbf{x}^*)$.
- Necessary conditions similar to KKT conditions for continuously differentiable optimization exist.

Nonsmooth Analysis: Descent Direction

Let $f : \mathbb{R}^n \to \mathbb{R}$ be locally Lipschitz continuous, then $\mathbf{p}$ s.t. $-\mathbf{p} \in \operatorname{argmin}\{\|\mathbf{g}\|,\ \text{s.t} : \mathbf{g} \in \partial f(\mathbf{x})\}$ is a descent direction.



- Main issue: the whole generalized gradient usually cannot be calculated.

Nonsmooth Optimization: Bundle Methods [1,2]

- Question:
  - How do we obtain a direction of descent given only an element of the generalized gradient and the objective value at x?
- Answer:
  - Keep a set of auxiliary points “close” to x called the bundle.
  - Create a piecewise linear approximation of the generalized directional derivative at x using the bundle and improve the approximation if necessary.
  - Calculate an approximation to the generalized gradient using the piecewise linear approximation.
  - Calculate a direction of descent for the piecewise linear approximation
  - Update the bundle as necessary.
- Bundle methods require the existence of the directional derivative with certain continuity properties w.r.t. to the direction (semismoothness) for convergence [3].

1. Nonsmooth Optimization, Analysis and Algorithms and Applications to Optimal Control, Marko Makela and Pekka Neittaanmaki, World Scientific, Singapore, 1992.
2. Krzysztof C. Kiwiel, Methods of Descent for Nondifferentiable Optimization, Lecture Notes in Mathematics, no. 1133, Springer-Verlag, Berlin, 1985.
3. R. Mifflin, “Semismooth and Semiconvex Functions in Constrained Optimization”, SIAM Journal of Control and Optimization, vol. 15, no. 6, pp. 959-972, November 1977.

Semismooth Hybrid Systems

- Under which assumptions are the states of the hybrid system semismooth mappings of the parameters and time?
- Two distinct classes:
  - Class A: Continuous Vector Field Across Transitions
  - Class B: Discontinuous Vector Field Across Transitions

Semismooth Hybrid Systems: Class A

- Class A Semismooth Hybrid Systems:
  - Reset functions are identities
  - All functions are continuously differentiable w.r.t. parameters and states
  - A single continuous vector field can be constructed on the product space of states and parameters irrespective of modes
  - The dynamics do not explicitly depend on time
  - Transitions have a reversible nature. Transitions depend on parameters and states
- As a consequence, the states are locally Lipschitz continuous and semismooth functions with respect to the parameters

Class A Semismooth Hybrid Systems

Tumor Chemotherapy Example [1]

$$\dot{P} = (a - m - n)P + bQ \quad \text{if } V_A - V_{THA} \leq 0$$

$$\dot{P} = (a - m - n)P + bQ - k_A(V_A - V_{THA})P \quad \text{if } V_A - V_{THA} \geq 0$$

$$\dot{Q} = mP - bQ \quad \text{if } V_B - V_{THB} \leq 0$$

$$\dot{Q} = mP - bQ - k_B(V_B - V_{THB})Q \quad \text{if } V_B - V_{THB} \geq 0$$

$$\dot{Y} = \sigma Y(1 - \frac{Y}{K}) - k_{yA}V_A Y - k_{yB}V_B Y$$

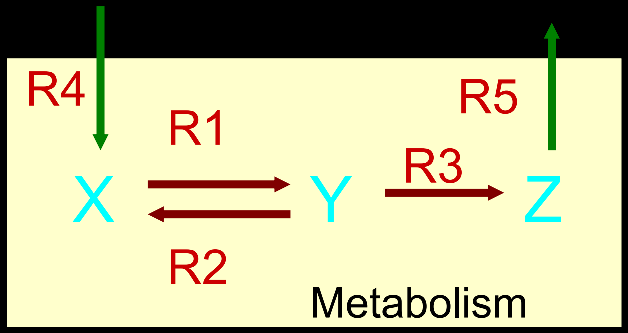
$$\dot{V}_A = u_A - \gamma_A V_A$$

$$\dot{V}_B = u_B - \gamma_B V_B$$

This hybrid system satisfies the conditions to be a class A semismooth hybrid system

1. Model modified from J. C. Panetta & J. Adam, “A mathematical model of cycle-specific chemotherapy.” Mathematical and Computer Modeling, 22, 67-82, 1995

Class A Semismooth Hybrid Systems
Flux Balance Analysis Models I



Chemical Reactions

	Internal		External
R1	X → Y	R4	X
R2	Y → X	R5	-Z
R3	Y → Z		

	R1	R2	R3	R4	R5
X	-1	1	0	1	0
Y	1	-1	-1	0	0
Z	0	0	1	0	-1

Stoichiometry Matrix, A

$$\dot{C} = Av$$

- C: Concentrations of X,Y,Z
- v: Reaction fluxes

Class A Semismooth Hybrid Systems

Flux Balance Analysis Models II

- Reactions inside the organism occur at a very fast time scale: quasi steady-state approximation
- Steady-state does not determine all fluxes uniquely
- The metabolism can be formulated as a linear program where the metabolism is assumed to optimize an objective (e.g., growth of biomass)
- The linear program is solved to determine the fluxes

$$\min_{\mathbf{v},\mathbf{b}} \mathbf{w}^{\mathrm{T}}\mathbf{v}$$

$$\text{s.t: } A\mathbf{v} = \mathbf{b}$$

$$\mathbf{v}^L \leq \mathbf{v} \leq \mathbf{v}^U$$

$$\mathbf{b}^L \leq \mathbf{b} \leq \mathbf{b}^U$$

- $\mathbf{w}$: objective vector
- A: stoichiometry matrix
- $\mathbf{b}$: exchange and accumulation rates
- $\mathbf{v}$: reaction fluxes

Class A Semismooth Hybrid Systems
Flux Balance Analysis Models III

- The dynamics of the mass of external chemical species and reaction volume are:

$$\mathbf{x} = [\mathbf{M}, V]$$

$$\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}, \mathbf{v}^*, \mathbf{p}, t)$$

$$\mathbf{v}^* \in arg \min_{\mathbf{v},\mathbf{b}} \mathbf{w}^{\mathsf{T}} \mathbf{v}$$

$$\text{s.t: } A\mathbf{v} = \mathbf{b}$$

$$\mathbf{v}^L(\mathbf{x}, \mathbf{p}, t) \leq \mathbf{v} \leq \mathbf{v}^U(\mathbf{x}, \mathbf{p}, t)$$

$$\mathbf{b}^L(\mathbf{x}, \mathbf{p}, t) \leq \mathbf{b} \leq \mathbf{b}^U(\mathbf{x}, \mathbf{p}, t)$$

- **M**: Mass of chemical species
- V: Volume
- **w**:objective vector
- A: stoichiometry matrix
- **b**: exchange and accumulation rates
- **v**: reaction fluxes

Class A Semismooth Hybrid Systems
Flux Balance Analysis Models IV

- Flux Balance Models can be analyzed as hybrid systems
- The discrete state is determined by the embedded linear program
  - Substitute with equivalent KKT conditions to yield a complementarity system
- The solution of the linear program is determined by a selection of columns of the stoichiometry matrix
- Each selection represents a potential discrete state
- There are exponentially many discrete states, hence mixed-integer reformulations are not practical

Semismooth Hybrid Systems: Class A
Flux Balance Analysis Models V

- v and b are locally Lipschitz continuous functions of their bounds.
- States are locally Lipschitz continuous and semismooth functions of the parameters and time.
- Assumptions
  - The linear program has always a unique solution for the elements of v and b of interest,
  - f, v_L, v_U, b_L, b_U are continuously differentiable functions of their arguments.

Class A Semismooth Hybrid Systems
Flux Balance Analysis Models VI: S. Cerevisiae

$$\dot{V} = F$$

$$\dot{X} = \mu X$$

$$\dot{G} = FG_f/V - v_g X$$

$$\dot{E} = v_e X$$

$$v_e, v_g \in \mathbf{v}^*$$

$$\mathbf{v}^* \in arg \max_{\mathbf{v},\mathbf{b}} \mu = \mathbf{w}^\top \mathbf{v}$$

$$\text{s.t: } A\mathbf{v} = \mathbf{b}$$

$$\mathbf{v}^L \leq \mathbf{v} \leq \mathbf{v}^U$$

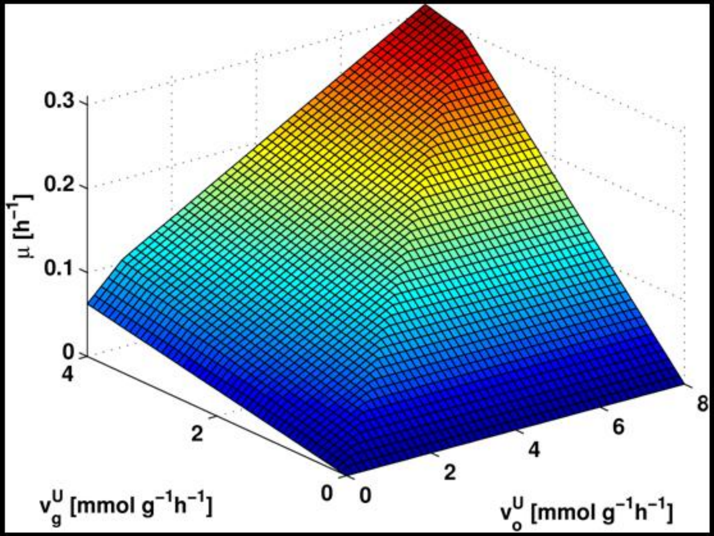
$$v_g^L \leq v_g \leq v_g^U(G,E)$$

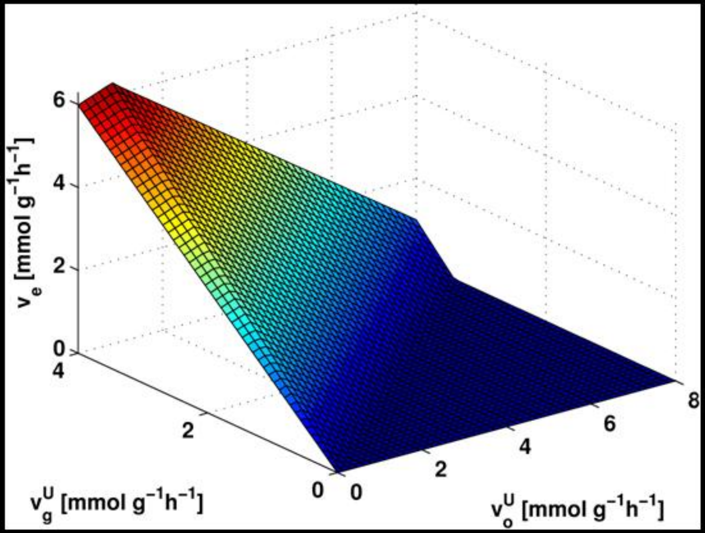
$$v_o^L \leq v_o \leq v_o^U(O)$$

$$\mathbf{b}^L \leq \mathbf{b} \leq \mathbf{b}^U$$

- F: Glucose feed rate
- O: Oxygen concentration
- G_f: Glucose concentration in feed
- V: Volume
- X: Biomass concentration
- E: Ethanol concentration
- G: Glucose concentration
- v_g: Glucose membrane exchange flux
- v_e: Ethanol membrane exchange flux
- v_o: Oxygen membrane exchange flux
- μ: Cellular Growth rate

Class A Semismooth Hybrid Systems
Flux Balance Analysis Models VII: S. Cerevisiae*



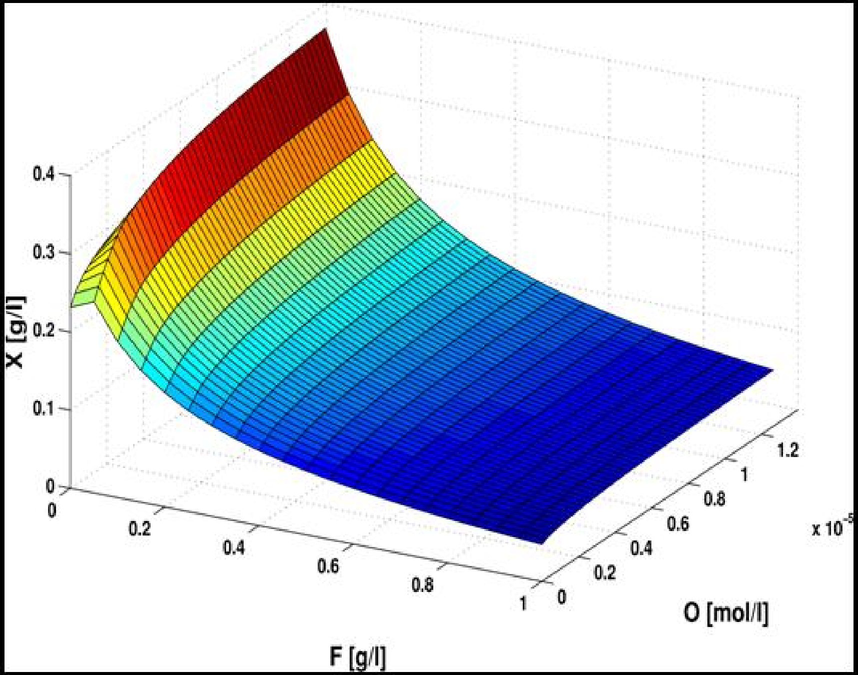


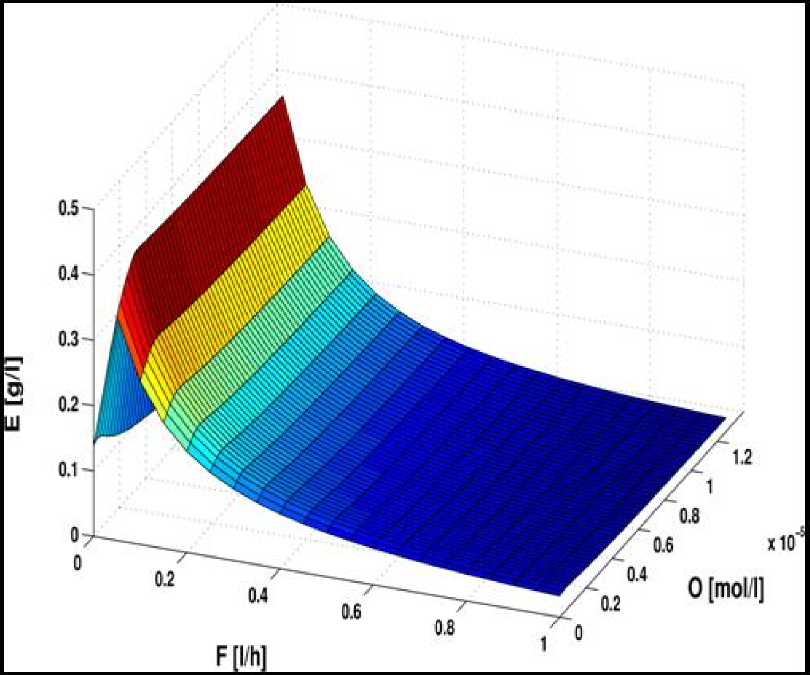
- Ethanol membrane exchange rate and biomass production rate as functions of the glucose and oxygen membrane exchange bounds

* FBA model courtesy of Jared Hjersted and Professor Michael A. Henson, University of Massachusetts, Amherst

Class A Semismooth Hybrid Systems

Flux Balance Analysis Models VIII: S. Cerevisiae





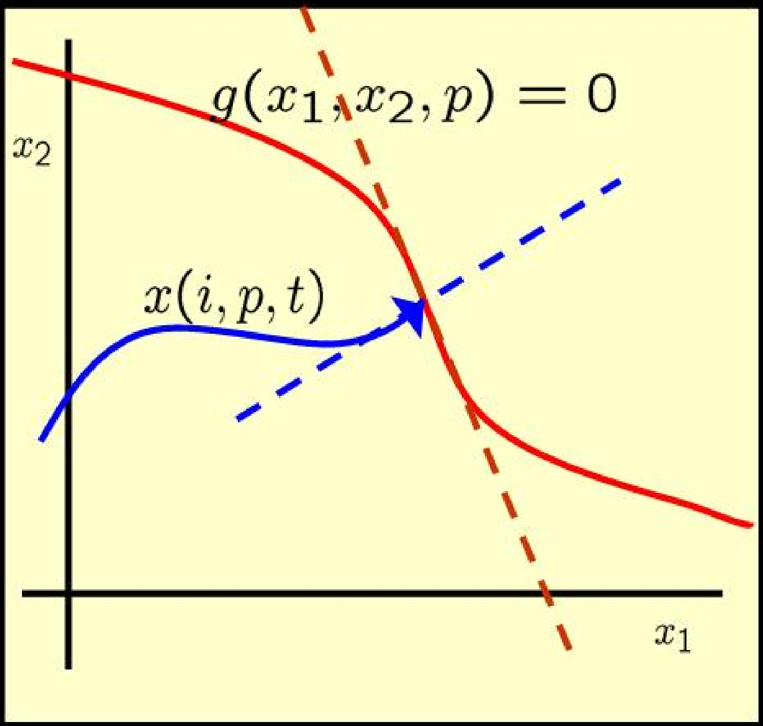
- The biomass and ethanol concentrations after 1 hour for different feed rates and oxygen concentrations.

Class B Semismooth Hybrid Systems

- Restrictions on the structure of the hybrid system
  - A subset of the states which have identity resets across all transitions is considered in objective function and constraints
  - All functions are continuously differentiable w.r.t. parameters and states
  - The vector fields may be discontinuous across transitions
  - The initial discrete state is not a function of the parameters and initial continuous state cannot trigger an event at the initial time
  - Events occur when the evolution of the continuous state reaches non-intersecting smooth surfaces in the state space
  - Intersection of these surfaces is only allowed if all intersecting surfaces correspond to transitions to the same mode

Class B Semismooth Hybrid Systems

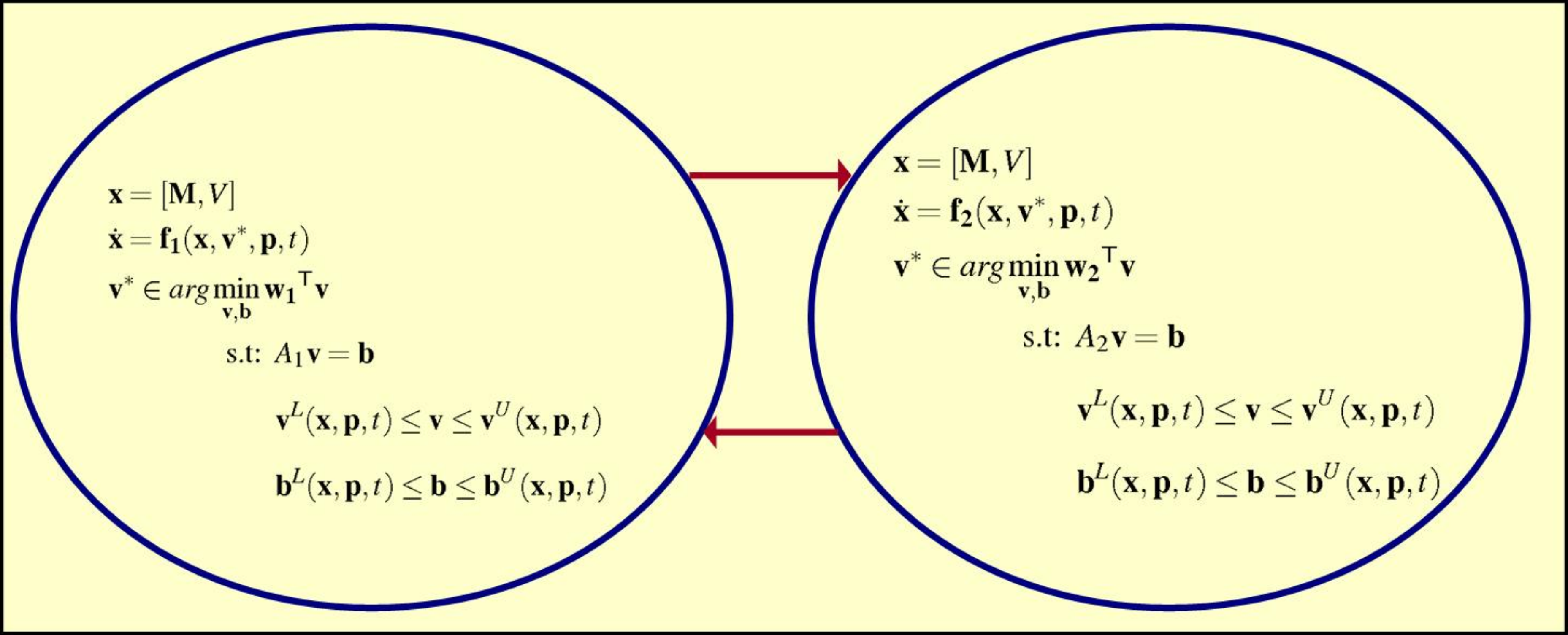
- Restrictions on the execution of the hybrid system
  - No Zeno or deadlock phenomena
  - Transversality condition: when the continuous evolution reaches an event triggering surface, it does so non-tangentially to the surface



Class B Semismooth Hybrid Systems

Flux Balance Analysis Models IX

- A change in the stoichiometry matrix or the objective for a FBA model can also be analyzed in the framework of hybrid systems
- Local Lipschitz continuity and semismoothness can be recovered if the transitions and events satisfy conditions for class B systems



$$
\begin{aligned}
&\mathbf{x} = [\mathbf{M}, V] \\
&\dot{\mathbf{x}} = \mathbf{f_1}(\mathbf{x}, \mathbf{v}^*, \mathbf{p}, t) \\
&\mathbf{v}^* \in arg \min_{\mathbf{v},\mathbf{b}} \mathbf{w_1}^{\mathsf{T}} \mathbf{v} \\
&\quad \text{s.t: } A_1 \mathbf{v} = \mathbf{b} \\
&\quad \mathbf{v}^L(\mathbf{x}, \mathbf{p}, t) \le \mathbf{v} \le \mathbf{v}^U(\mathbf{x}, \mathbf{p}, t) \\
&\quad \mathbf{b}^L(\mathbf{x}, \mathbf{p}, t) \le \mathbf{b} \le \mathbf{b}^U(\mathbf{x}, \mathbf{p}, t)
\end{aligned}
$$

$$
\begin{aligned}
&\mathbf{x} = [\mathbf{M}, V] \\
&\dot{\mathbf{x}} = \mathbf{f_2}(\mathbf{x}, \mathbf{v}^*, \mathbf{p}, t) \\
&\mathbf{v}^* \in arg \min_{\mathbf{v},\mathbf{b}} \mathbf{w_2}^{\mathsf{T}} \mathbf{v} \\
&\quad \text{s.t: } A_2 \mathbf{v} = \mathbf{b} \\
&\quad \mathbf{v}^L(\mathbf{x}, \mathbf{p}, t) \le \mathbf{v} \le \mathbf{v}^U(\mathbf{x}, \mathbf{p}, t) \\
&\quad \mathbf{b}^L(\mathbf{x}, \mathbf{p}, t) \le \mathbf{b} \le \mathbf{b}^U(\mathbf{x}, \mathbf{p}, t)
\end{aligned}
$$

Class B Semismooth Hybrid Systems

Diver Example I

Semismooth Hybrid Systems: Class B:
Diver Example II

$$\mathcal{M} = \{Descent = 1, Deco = 1, Nondeco = 3, Terminal = 4\},$$

$$\mathrm{p} = \{u\} \in \mathbb{R},\ s(i,\mathrm{p}) \in \mathcal{M},\ \mathrm{x}(i,\mathrm{p},t) = [P_{\mathrm{N}}, P, P_t, t_{Deco}],$$

$$\mathcal{F}(\cdot) = \begin{cases} \dot{P}_{\mathrm{N}} = \frac{\ln(2)}{5}(0.79P - P_{\mathrm{N}}), \\ \dot{P}_t = -\frac{q}{V_t}P, \\ \dot{P} \begin{cases} 0 & \text{if } s(i,\mathrm{p}) = Terminal \bigvee s(i,\mathrm{p}) = Deco, \\ v_d & \text{if } s(i,\mathrm{p}) = Descent \\ u & \text{if } s(i,\mathrm{p}) = Nondeco \end{cases} \\ \dot{t}_{Deco} \begin{cases} 1 & \text{if } s(i,\mathrm{p}) = Deco, \\ 0 & \text{otherwise} \end{cases} \end{cases}$$

$$\mathcal{E}(\cdot) = \begin{cases} 1 & \text{if } L_1 : P \geq P_t = \text{true}, \\ 1 & \text{if } L_2 : s(i,\mathrm{p}) = Deco \bigwedge t_{Deco} = 4.0 = \text{true}, \\ 1 & \text{if } L_3 : s(i,\mathrm{p}) = Nondeco \bigwedge P_{\mathrm{N}}/0.79P \geq 2 = \text{true}, \\ 1 & \text{if } L_4 : s(i,\mathrm{p}) = Descent \bigwedge P_t = h_d = \text{true}, \\ 0 & \text{otherwise}, \end{cases}$$

$$\mathcal{S}(\cdot) = \begin{cases} Terminal & \text{if } L_1 = \text{true} \\ Nondeco & \text{if } L_2 = \text{true} \\ Deco & \text{if } L_3 = \text{true} \\ Nondeco & \text{if } L_4 = \text{true} \end{cases}$$

$$\mathcal{R}(\cdot) = \begin{cases} P_t(i+1,u,t) = P_t(i,u,t); \\ P(i+1,u,t) = P(i,u,t); \\ P_{\mathrm{N}}(i+1,u,t) = P_{\mathrm{N}}(i,u,t); \\ t_{Deco}(i+1,u,t) = 0; \end{cases}$$

$$s_0(\mathrm{p}) = Descent,\ \mathrm{x}_0(\mathrm{p}) = [0.79, 1.0, 200, 0.0];$$

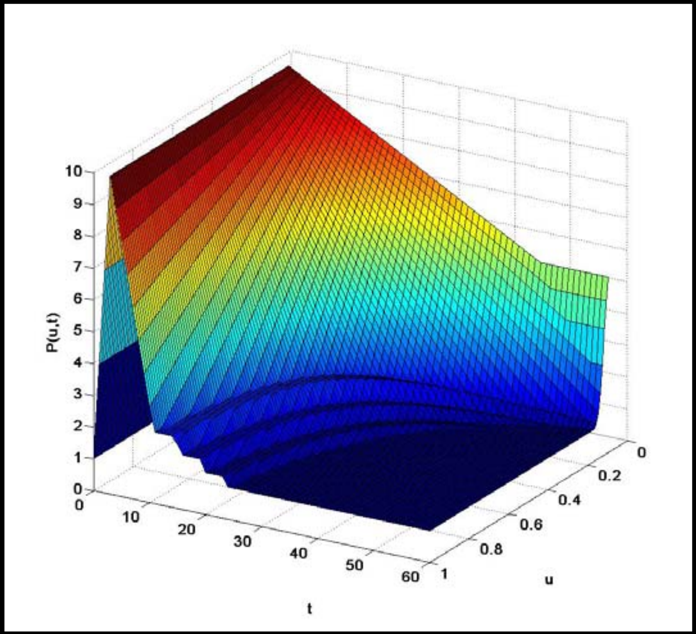
Semismooth Hybrid Systems: Class B:
Diver Example III

$$\min_{u,\, t_f} t_f$$

$$\text{s.t.} \quad P(i, u, t_f) = 1.0$$

$$u \in [0, 1]$$

$$P \in \mathcal{H}$$



- The constraint is nonsmooth.
- The hybrid system has discontinuous vector fields.
- There are resetting states.
- The transitions are not reversible

Semismooth Hybrid System: Calculation of an Element of the Generalized Gradient

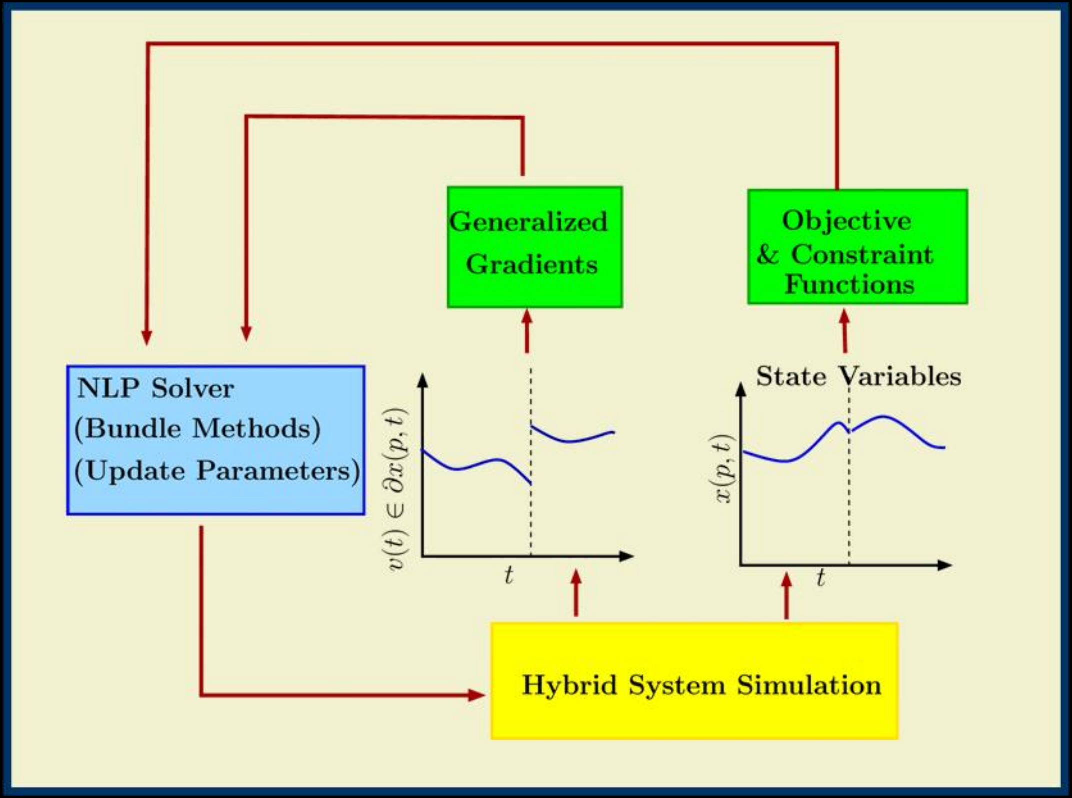
- Under the assumptions for semismooth hybrid systems, the following formula is used to calculate an element of the generalized gradient:

$$\partial f(\mathbf{x}) = \mathrm{co}\{\lim \nabla f(\mathbf{x}_i) : \ \mathbf{x}_i \to \mathbf{x}, \ \mathbf{x}_i \notin S\}$$

- One of the limits can exactly be calculated with the algorithms used to calculate parametric sensitivities in case the discrete state trajectory is constant [I].

I. S. Galán, W. F. Feehery, P. I. Barton, "Parametric Sensitivity Functions for Hybrid Discrete/Continuous Systems", Applied Numerical Mathematics, 31(1):17-48, (1999)

Semismooth Hybrid Systems: Optimization



- Once an element of the generalized gradient is obtained, a direct method can be used for optimization

Optimization

Tumor Chemotherapy Example II

$$\dot{P} = (a - m - n)P + bQ \qquad \text{if } v_A - v_{THA} \leq 0$$

$$\dot{P} = (a - m - n)P + bQ - k_A(v_A - v_{THA})P \qquad \text{if } v_A - v_{THA} \geq 0$$

$$\dot{Q} = mP - bQ \qquad \text{if } v_B - v_{THB} \leq 0$$

$$\dot{Q} = mP - bQ - k_B(v_B - v_{THB})Q \qquad \text{if } v_B - v_{THB} \geq 0$$

$$\dot{Y} = \sigma Y(1 - \frac{Y}{K}) - k_{yA}v_AY - k_{yB}v_BY$$

$$\dot{V}_A = u_A - \gamma_A v_A$$

$$\dot{V}_B = u_B - \gamma_B v_B$$

- The hybrid system satisfies the conditions to be a class A semismooth hybrid system

Optimization

Tumor Chemotherapy Example III

- The optimal drug profile for a thirty day treatment is determined using control vector parameterization.
- The aim is to minimize the number of tumor cells (Q + P) subject to the constraint that the healthy cell population is above a certain number at the end of thirty days.

$$\min_{\boldsymbol{p}} P(i, \boldsymbol{p}, t_f) + Q(i, \boldsymbol{p}, t_f)$$

$$s.t: \qquad Y(i, \boldsymbol{p}, t_f) \geq 1 \times 10^6$$

$$t_f = 30$$

$$\boldsymbol{p} = \{u_A^j, u_B^j : 1, 2, \ldots, 30\}$$

$$0 \leq u_A^j \leq 20.0$$

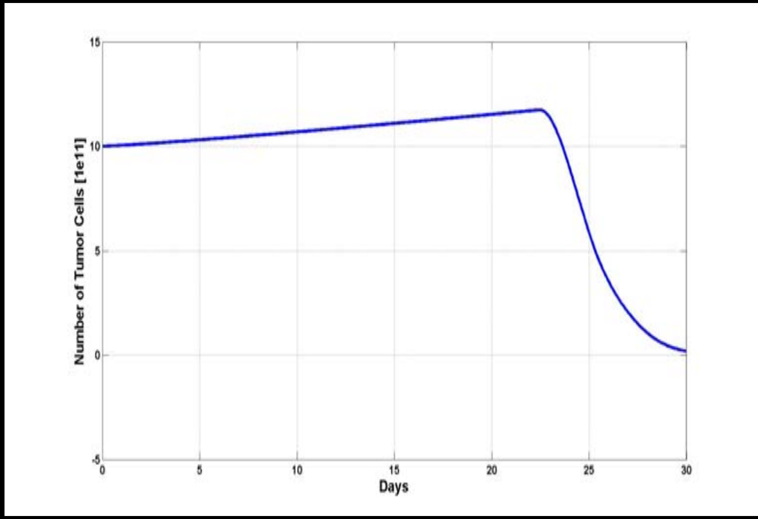
$$0 \leq u_B^j \leq 20.0$$

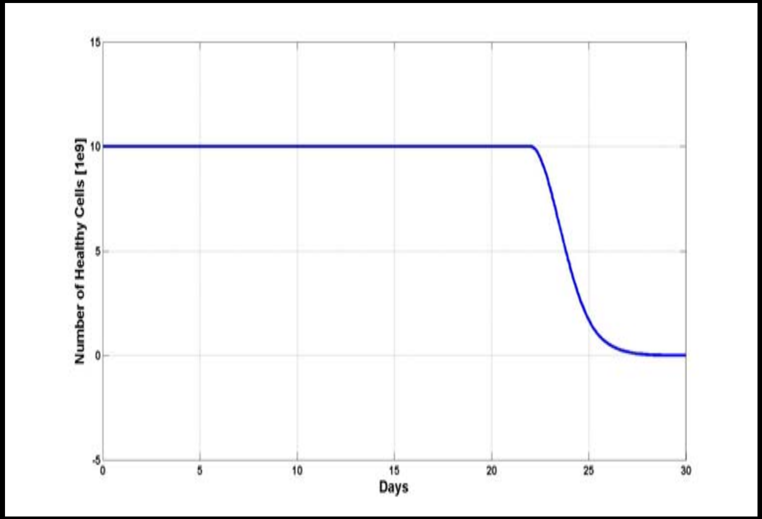
Optimization
Tumor Chemotherapy Example IV

- Exact penalty is used with a freely available bundle solver [I].
- Multi-start is needed due to nonconvexity of the optimization problem.

I. Ladislav Lukšan, Jan Vlček, "Algorithm 811: NDA: algorithms for nondifferentiable optimization", ACM Transactions on Mathematical Software , 27(2) :193 - 213, (2001)

Optimization
Tumor Chemotherapy Example IV

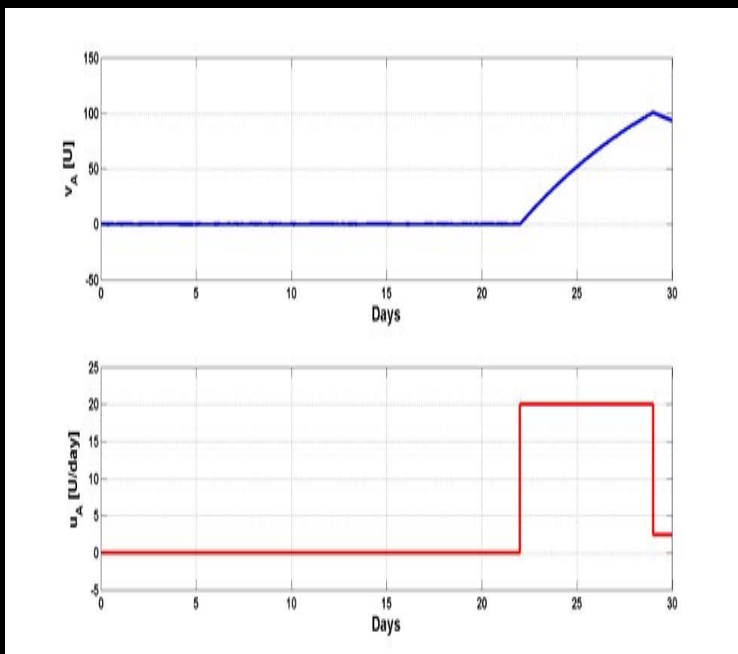


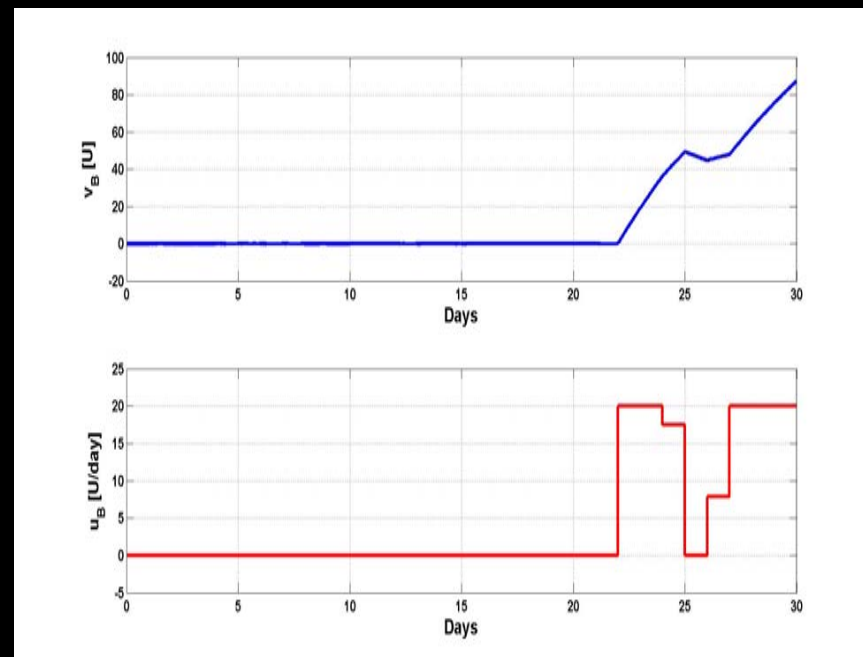


- Tumor Cell Population and Healthy Cell Population Evolution

	P +Q	Y
Initial	1.0e12	1.0e9
Final	1.8e10	1.0e6

Optimization
Tumor Chemotherapy Example VI





- Drug A concentration and doses
- Drug B concentration and doses

Optimization

- Drug doses were obtained in case drug resistance is ignored.
- Smooth problem solved with SNOPT using multi-start.
- Doses applied to the original model.

	P +Q	Y
Initial	1.0e12	1.0e9
Final (Original) Final (Smooth)	1.8e10 3.9e10	1.0e6 1.0e6

Conclusions

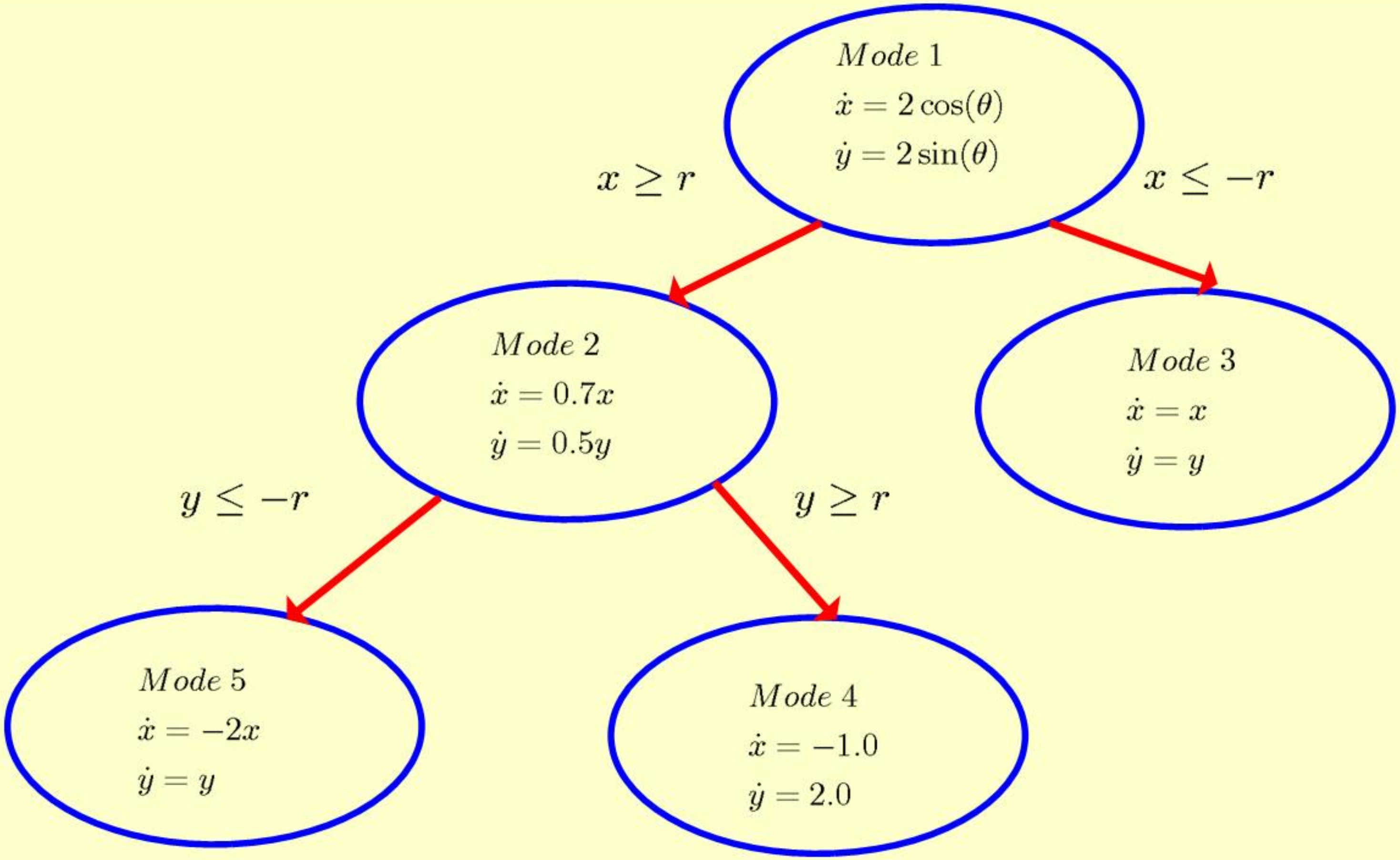
- Finding the optimal mode sequence is a fundamental challenge in the optimization of hybrid systems
- Broad class of semismooth hybrid systems for which nonsmooth optimization can find optimal mode sequences
- Mixed-integer formulations also possible
  - Global mixed-integer dynamic optimization

Future Work

- Exploit structure of semismooth hybrid automata in nonsmooth optimization methods
- Methods for nonsemismooth and discontinuous hybrid automata?

THE END

Another Simple Example



State continuity across transitions is enforced.

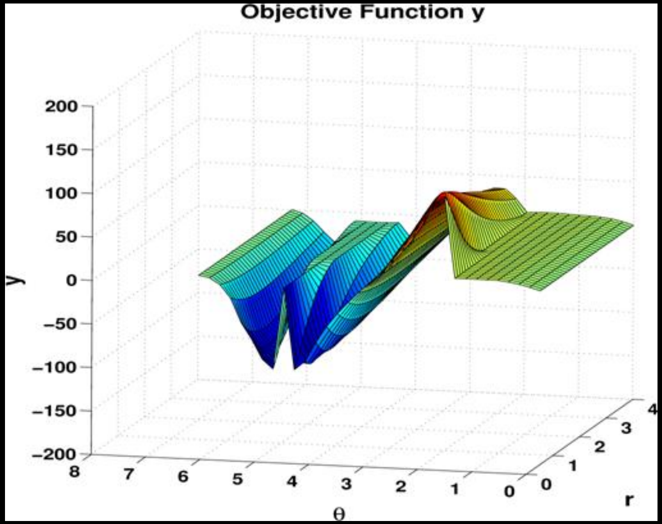
Another Simple Example II

$$\min_{r,\,\theta} y(r, \theta, t_f)$$

subject to:

$$r \in [0.5, 4],\ \theta \in [0, 2\pi]$$

$$t_f = 5.0,\ x_o = 0.0,\ y_o = 0.0$$



Mode Sequence	Conditions on $r \in [0.5, 4]$, $\theta \in [0, 2\pi]$ and $t_f = 5.0$
1	$\lvert r/2t_f \rvert > \cos(\theta)$
1,3	$-r/2t_f \geq \cos(\theta)$
1,2,4	$r/2t_f \leq \cos(\theta) \vee \sqrt{e^{r/2\cos(\theta) - t_f}} \leq \tan(\theta)$
1,2,5	$r/2t_f \leq \cos(\theta) \vee -\sqrt{e^{r/2\cos(\theta) - t_f}} \geq \tan(\theta)$
1,2	$r/2t_f \leq \cos(\theta) \vee -\sqrt{e^{r/2\cos(\theta) - t_f}} < \tan(\theta) < \sqrt{e^{r/2\cos(\theta) - t_f}}$

- Analysis of the nonsmoothness requires some mathematics: “Nonsmooth Analysis”.

Semismooth Hybrid Systems: Class A:
Valves

- Q is the flow across the valve, pressures P_{in} and P_{out} are the states of the system, valve opening, u, is the parameter.
- Slight reformulation is necessary to make the equations continuously differentiable at zero pressure difference due to the square root.

$$Q = uK_v\sqrt{P_{in} - P_{out}} \qquad \text{if } \; P_{in} \geq P_{out}$$

$$Q = 0 \qquad \text{if } \; P_{in} \leq P_{out}$$

Semismooth Hybrid Systems: Class A:
Models with Friction

- Certain models with friction are of class A.
- The friction force is a continuously differentiable function of the states and parameters.

$$\dot{v}_x = \frac{F_x - F_f(v_x, \mathbf{p})}{m} \qquad \text{if } |F_x| \geq |F_f(v_x, \mathbf{p})|$$

$$\dot{v}_x = 0 \qquad \text{if } |F_x| \leq |F_f(v_x, \mathbf{p})|$$