

Optimal Control and Applications in Biomath

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UNIVERSITÄT
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DSABNS-Workshop

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...joint work of...



Contents

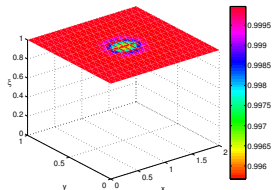
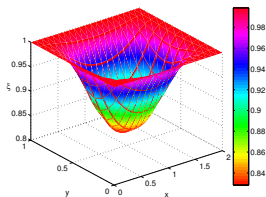
- 1 Optimal Control
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Task: Optimal Control

Real world process in nature or technology can be modeled with (partial) **differential equations**. However, one is often not just interested in the solution (=simulation) of the DE for a given set of parameters, but in **identifying** the parameters from measurements or **optimizing** the solution w.r.t. those parameters.

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Mathematical Problem

Minimize the cost functional J on a set of **admissible control parameters** $u \in \mathcal{U}$ **subject to** the constraint that some differential equation is satisfied.

Model Problem

$$x' = f(t, x, u), \quad x(0) = x_0$$

- Solution $x \in \mathcal{X} = H^1([0, 1]) \subset C([0, 1])$ (Sobolev–Lemma).

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- Minimization in ∞ –dimensional spaces \mathcal{X} , \mathcal{U}

“Brute Force” Approach

First Discretize – Then Optimize

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$$x_{k+1} = x_k + h\varphi(t, x_k, u_k, u_{k+1}) \quad \text{or} \quad F(t, x, u) = 0$$

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- ▶ **Solution depends on discretization** ⚡

Constrained Minimization

Theorem (Lagrange–Multiplier)

A local solution x^* of the problem

$$\min J(x) \text{ s.t. } F(x) = 0$$

is a stationary point of the *Lagrangian*

$$\mathcal{L}(x, \lambda) := J(x) + \langle \lambda, F(x) \rangle$$

i.e.

$$\nabla \mathcal{L}(x^*, \lambda^*) = 0$$

We call λ^* the *adjoint variable* of x^* (Lagrange–multiplier).

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- Lagrangian

$$\begin{aligned} \mathcal{L}(x, u, z) &= \frac{1}{2} \|x - x_d\|^2 + \frac{\alpha}{2} \|u\|^2 + \langle F, z \rangle \\ &= xz \Big|_0^1 + \int_0^1 \frac{(x - x_d)^2 + \alpha u^2}{2} - xz' - f(t, x, u) \cdot z dt \end{aligned}$$

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- $\partial_u \mathcal{L} \stackrel{!}{=} 0$ $\alpha u - \partial_u f \cdot z = 0$

Pontryagin Maximum (Minimum) Principle

$$x' = f(x, u) \quad x(0) = x_0, \quad u \in \mathcal{U}$$

- Solution x^* , u^* , z^* of Control Problem

$$J = \int_0^T g(x(t), u(t)) dt \longrightarrow \min$$

leads to extremal value of *Hamiltonian* $H(z, x, u) = z \cdot f + g$.

- Costate / Adjoint z solves

$$-z' = z f_x + g_x, \quad z(T) = 0$$

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- Need subdifferentials $\lambda \in \partial \|x\|_{L^1}$ instead of derivatives $\nabla \|x\|_{L^2}$

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- Leads to Bang-Bang-Control

Optimal Control Problem; Solution

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Optimal Control Problem

$$\begin{aligned} \min J(x, u) &= \int_0^T j(x, u) = \frac{1}{2} \left(\|x - x_d\|_2^2 + \alpha \|u\|_2^2 \right) \\ \text{s.t. } x' &= f(t, x, u), \quad x(0) = x_0 \end{aligned}$$

is equivalent to solving the KKT-system

$$\begin{aligned} x' &= f(t, x, u) & x(0) &= x_0 \\ z' &= j_x - \partial_x f \cdot z & z(T) &= 0 \\ 0 &= j_u - \partial_u f \cdot z \end{aligned}$$

How to Solve the KKT–System ?

Iterative Gradient algorithm

① Solve $x' = f(t, x^{(k)}, u^{(k)})$, $x(0) = x_0$ for $x^{(k+1)}$

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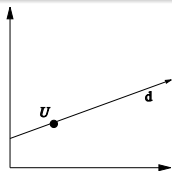
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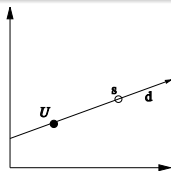
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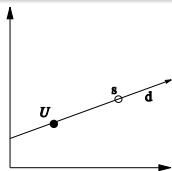
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- 5 Iterate, until $\|\nabla J\| < \varepsilon$



Approaches for Step Size Selection

$$\hat{J}(u) := J(x(u), u)$$

- **Optimal:** 1d-search: $s_{opt} = \operatorname{argmin}_{\delta > 0} \hat{J}(u^{(k)} - \delta d^{(k+1)})$

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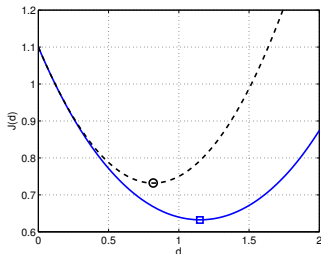
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- ▶ Given $u^{(k)}$, $\hat{J}(u^{(k)})$
- ▶ Compute $\hat{J}(u^{(k)} - s_1 d^{(k+1)})$
- ▶ Polynomial approximation

$$\tilde{J}(t) = \hat{J}(u^{(k)} + t d^{(k+1)})$$



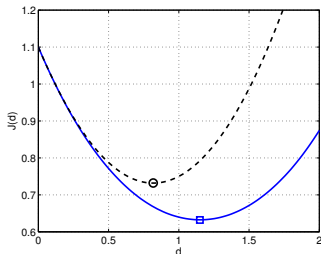
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- Adjoint System

$$-\partial_t z = \Delta z + \partial_y f \cdot z + (y - y_d)$$

with $z(T) = 0$ and boundary conditions

Single-Objective vs. Multi-Objective Control

- So far: Objective = weighted sum of goal and cost

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 - ▶ Optimize both criteria at the same time!

$$\min (J_1(x, u), J_2(x, u))$$

Single-Objective vs. Multi-Objective Control

- So far: Objective = weighted sum of goal and cost

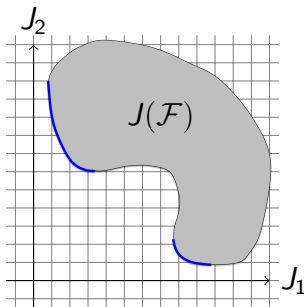
$$J(x, u) := \frac{1}{2} \left(\|x - x_d\|_2^2 + \alpha \|u\|_2^2 \right)$$

weighting / regularization parameter $\alpha > 0$

- How to choose α ?
 - ▶ Choice of α influences result
 - ▶ Optimize both criteria at the same time!

$$\min (J_1(x, u), J_2(x, u))$$

- ▶ Find points/solutions such that for fixed J_1 , there is no better J_2 and vice versa.



Multi-Objective Control

Typical Situation: *More than one optimization task*

- Dynamical system $x' = f(t, x, u)$, $x(0) = x_0$

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Multi-Objective Control

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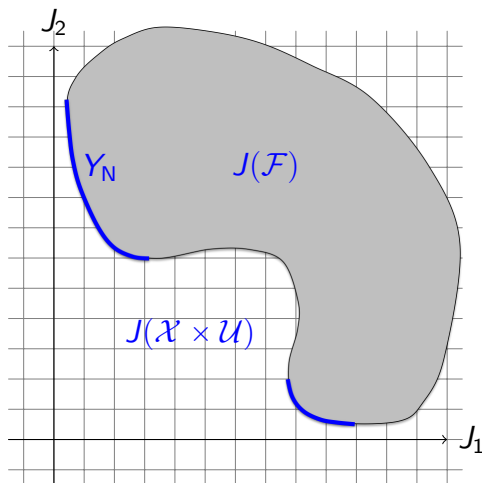
- Dynamical system $x' = f(t, x, u)$, $x(0) = x_0$
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- Task

$$\min J(x, u) = \min (J_1(x, u), J_2(x, u))$$

- Ordering in \mathbb{R}^2 , \mathbb{R}^n ? \rightsquigarrow Product order

$$(x_1, x_2) < (y_1, y_2) \text{ if } x_1 < y_1 \text{ and } x_2 < y_2$$

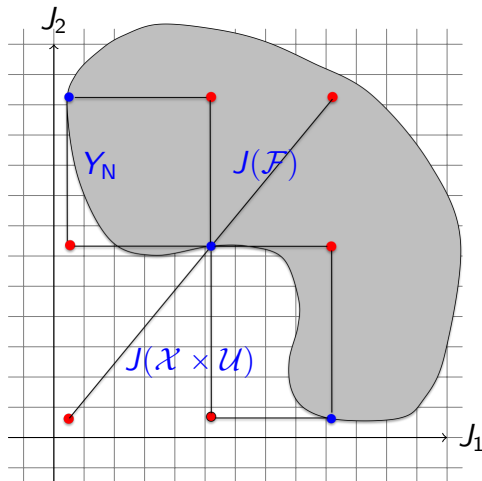
Non-dominated Points



- $J(\mathcal{F})$: set of feasible outcomes
- Y_N : set of non-dominated points
- Any point $y \in Y_N$ is an “optimal” solution of the problem

$$\min J = \min (J_1, J_2)$$

Computing the Set of Non-dominated Points



Rectangular framing

Divide-and-Conquer Method

- Generate anchor points
- Subdivide using mid-point
- ▶ Solve SO-problem
- Get two new rectangles
- Iterate

Idea: K.Putra

Fishing Model



[adapted from toonpool.com]

Model

Objective:

$$\min_{(x,u) \in \mathcal{X} \times \mathcal{U}} \left(\int_0^T x^2 dt, \int_0^T u^2 dt \right)$$

Constraints:

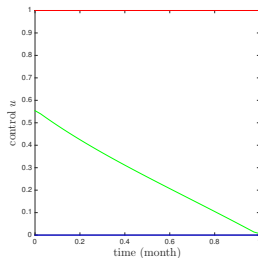
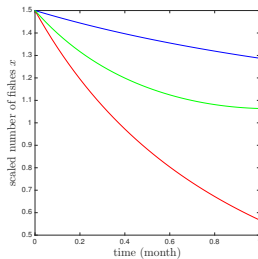
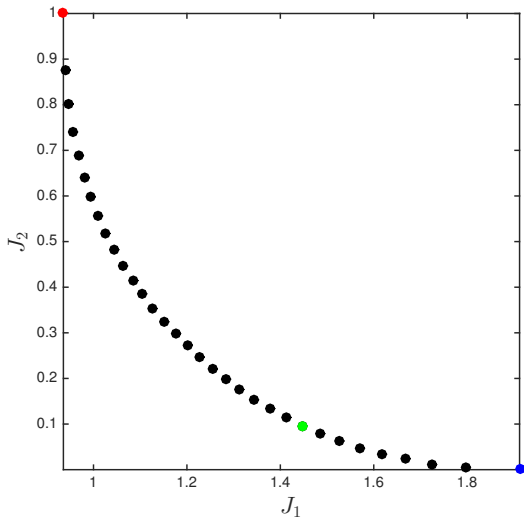
$$x' = r x (1 - x) - u(t)x$$

$$x(0) = x_0$$

$$u(t) \in [0, 1]$$

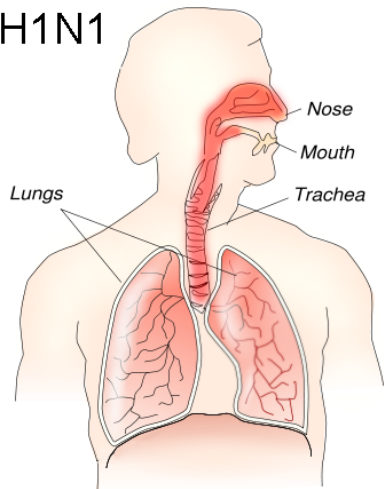
$$t \in [0, T]$$

Fishing Model – Pareto Front



Influenza Model

H1N1



© Wikipedia 2009

Model

Objective:

$$\min_{(x,u) \in \mathcal{X} \times \mathcal{U}} \left(\int_0^T I^2 dt, \int_0^T u^2 dt \right)$$

Constraints:

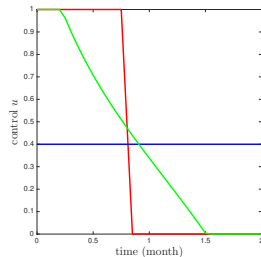
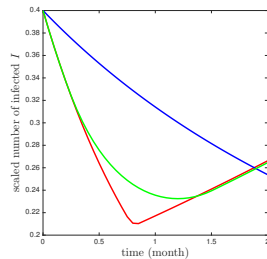
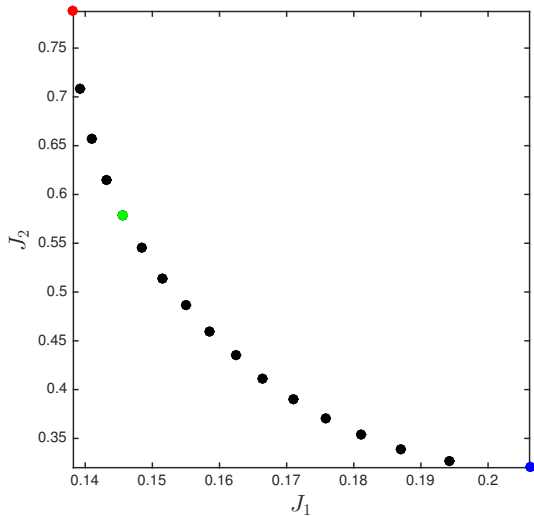
$$S' = -bSI + cI + uI \quad S(0) = S_0$$

$$I' = bSI - cI - uI \quad I(0) = I_0$$

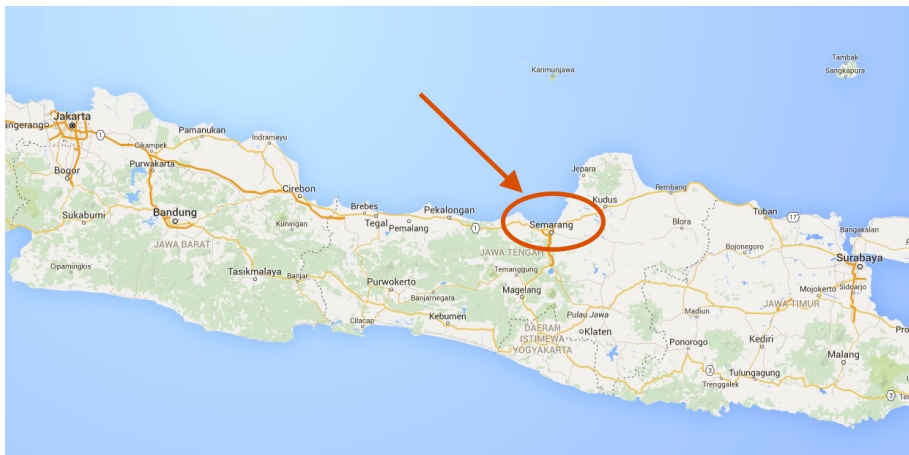
$$u(t) \in [0, 1]$$

$$A = \int_0^T u(t) dt$$

Influenza Model – Pareto Front

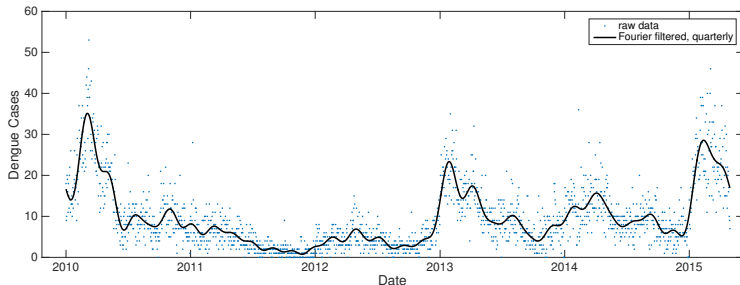


Dengue in Semarang, Java, Indonesia



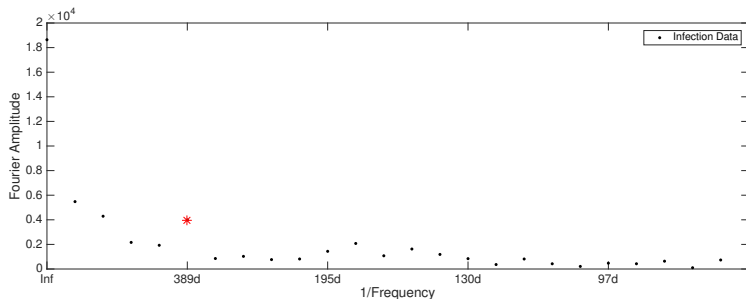
- Population: approx. 1.5 Mio.
- Tropical climate, wet season in Dec–Mar, dry season Jun–Aug

Dengue Data from Semarang



- Hospitalized cases of Dengue
 - ▶ DF: Dengue Fever
 - ▶ DHF: Dengue Haemorrhagic Fever
 - ▶ DSS: Dengue Shock syndrome
- January 2010 – April 2015
- Age structured data also available (?)

Data Analysis



- $n = 1946$ data
- Low-pass filter
- Fourier-transform shows peak at period $\tau = 389d$

SIR UV-Model

$$S' = \mu(N - S) - \frac{\beta(t)}{M} S \cdot V$$

$$I' = \frac{\beta(t)}{M} S \cdot V - (\gamma + \mu)I$$

$$R' = \gamma I - \mu R$$

$$(U', V') = \dots$$

Idea from time-scale separation (Rocha, Aguiar, e.a.)

$$V \simeq \frac{I}{I + \nu N} M, \quad \nu = \frac{1}{2}$$

Time-dependent *biting-rate* $\beta(t)$

IR-Model

$$I' = \beta(t)(N - I - R) \frac{I}{I + \nu N} - (\gamma + \mu)I$$

$$R' = \gamma I - \mu R$$

Parameters

$$\mu = 1/65a \quad \gamma = 1/30d \quad N = 1.5 \cdot 10^6 \quad I(0) = \text{given}$$

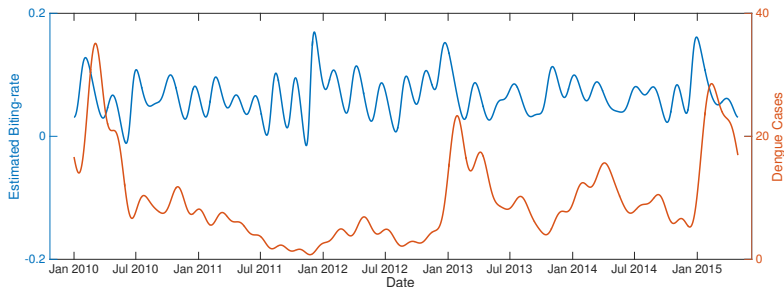
$$R_0 \stackrel{?}{=} R^* = \rho N \text{ from equilibrium, } \rho = \frac{3\delta^2 - \delta}{4\delta^2 + 6\delta + 2}, \quad \delta = \frac{\mu}{\gamma} \gg 1$$

- Biting-rate $\beta(t)$ as *Control-function*

A-priori Estimate for β

$$\beta_{est} = \frac{\nu}{1 - \rho} \frac{I' + (\gamma + \mu)I}{I}$$

with average $\bar{\beta}_{est} = \frac{\nu}{1 - \rho} \left[\frac{1}{T} \ln \frac{I_0}{I_n} + \gamma + \mu \right] \rightarrow 2\gamma$



Estimating β using Optimal Control

Find $\beta(t)$ such, that $\|I - I_{obs}\|_2 \rightarrow \min$, where I solves IR-system

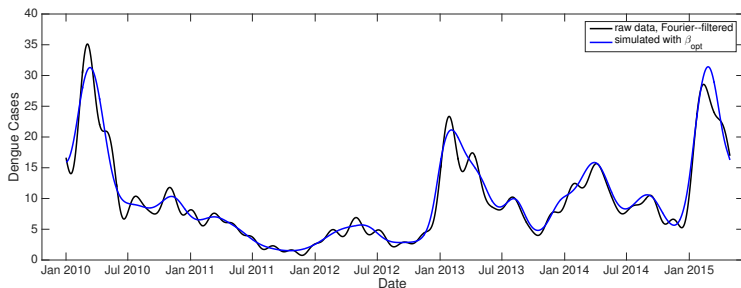
$$I' = \beta(t)(N - I - R) \cdot \frac{I}{I + N/2} - (\gamma + \mu)I$$

$$R' = \gamma I - \mu R$$

Parameter

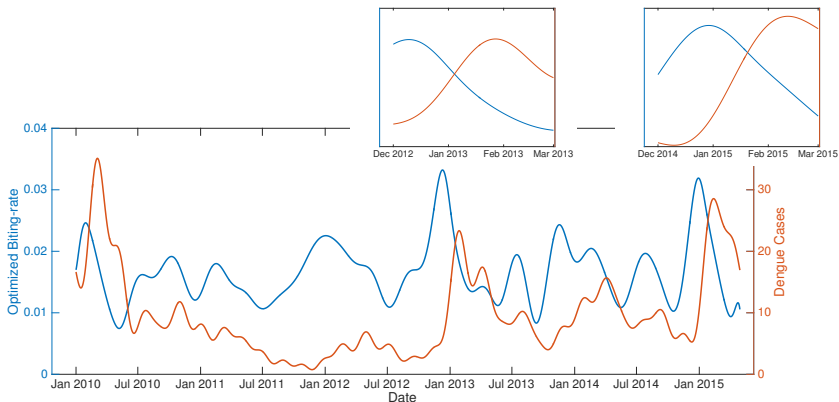
- $\gamma = 1/(30 \text{ d})$
- $\mu = 1/(365 \cdot 65 \text{ d})$
- $N = 1.5 \cdot 10^6$
- $I_0 = 16$
- $R_0 = \sum_{k=1}^{30} I_{obs,k} (?)$

Optimal Control Solution vs. Data



- Observed data (Fourier-filtered)
- Simulation result with β_{opt}
- Good agreement — as to be expected

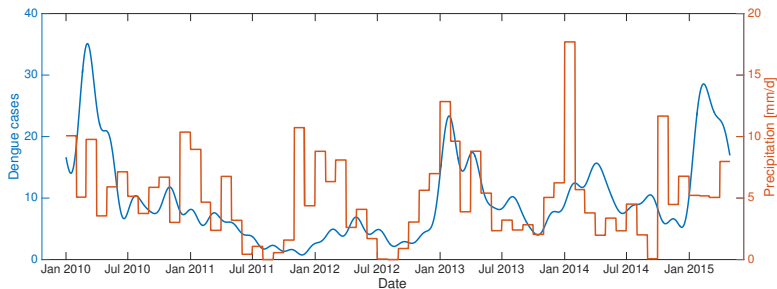
Optimal Control Solution vs. Data



- Biting rate β_{opt} from Optimal Control vs. **Dengue Data**
- Peaks in Dengue lag behind peaks in β_{opt}
- Delay $t \simeq 40d$ (Jan 2013 and Jan 2015)

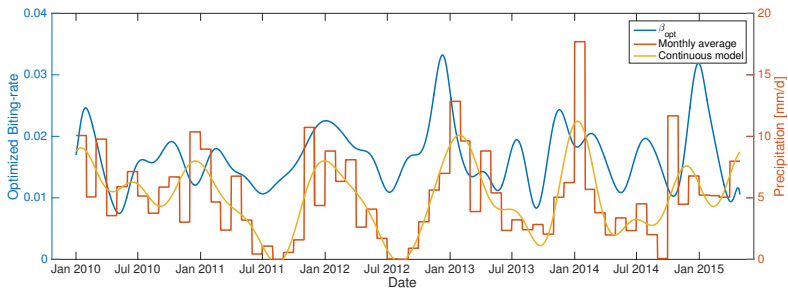
Influence of Precipitation

- *Aedes aegyptii* breed in stagnant water
- Eggs viable in dry state, can re-emerge later on
- Pronounced wet season in Semarang
- Historic precipitation data (monthly) $p(t)$

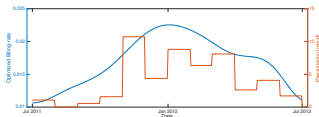


- Good agreement in 2013

Influence of Precipitation



- Biting-rate $\beta(t)$ depends on precipitation data $p(t)$
- July 2011 – July 2012



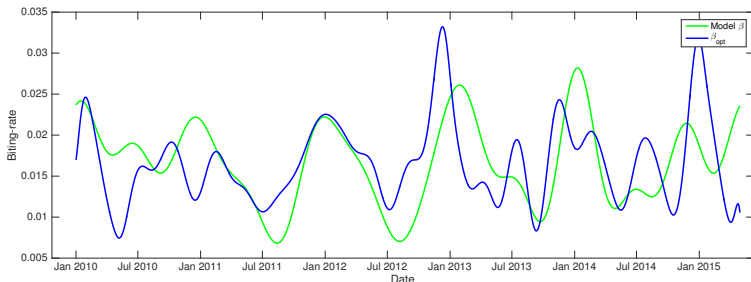
Modeling the Influence of Precipitation

- Normalize precipitation data

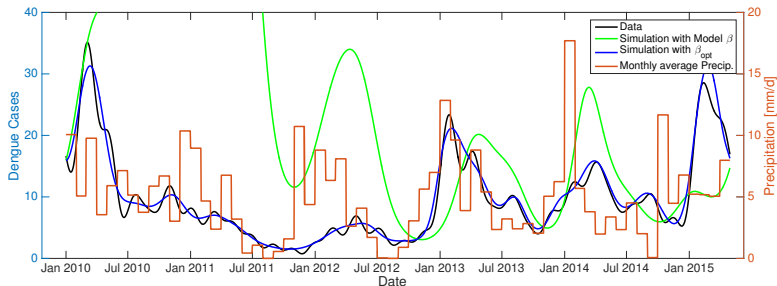
$$p_0 := \frac{p(t) - \bar{p}}{\sigma(p)}$$

with average $\bar{p} = \frac{1}{T} \int_0^T p(t) dt$ and standard deviation $\sigma(p)$

- Model *biting-rate* $\beta(t) := \bar{\beta}_{opt} + \sigma(\beta_{opt}) p_0$



Modeling the Influence of Precipitation II



- Observed Dengue Cases
- Simulation using precipitation data and $\beta = \bar{\beta}_{opt} + \sigma(\beta_{opt}) p_0$
- Simulation using β_{opt} from Optimal Control
- Precipitation Data

Conclusion & Outlook

- Optimal Control & Pontryagin

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- Solution using Adjoint Equations

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- ▶ Improve this model !

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Thanks.