TRAJECTORY FOLLOWING AND REGULATION OF CHEMICAL BATCH REACTORS VIA GENEALOGICAL DECISION TREES

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Contents:
- Application of particle filtering to solving an optimal control problem

Outline:
- Background
- GDT algorithm and some properties
- Numerical illustrations
- Regulation using GDT
- Discussion

BACKGROUND

- *Optimal filtering*
  - Bayesian approach: Estimate the evolving posterior distribution recursively in time (prediction + updating)
  - Kalman filter (linear Gaussian)
  - **Particle filtering** aka **Sequential Monte Carlo** (non-linear non-Gaussian)

- *Importance Sampling & Resampling*

Step 0. Initialization

(Set initial particle positions)

Step 1. Importance Sampling

- **Predict** (using model)
- **Evaluate** importance weights (using observation)

Step 2. **Resampling**

(Sample from weighted distribution)

- *Duality* between optimal filtering and regulation

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PROBLEM FORMULATION

Model:

$$\mathbf{X}_n = F_n(\mathbf{X}_{n-1}, \mathbf{U}_n);\ \mathbf{X}_0$$

$$\mathbf{Y}_n = h_n(\mathbf{X}_n)$$

Control objective:

$$J_T(\mathbf{U}_1, \mathbf{U}_2, \ldots, \mathbf{U}_T) = \sum_{n=1}^{T} \left\| \mathbf{U}_n \right\|_{\mathbf{A}_n}^2 + \sum_{n=1}^{T} \left\| \mathbf{Y}_n - \mathbf{Y}_n^{ref} \right\|_{\mathbf{B}_n}^2$$

T length of trajectory (horizon)

$\mathbf{A}_n, \mathbf{B}_n$ control and error costs (covariances)

Find the sequence of control actions that will minimize the control objective for open-loop control.

OPTIMIZATION OF THE CONTROL SEQUENCE

Idea: Associate Gaussian distributions to the norms of the control actions and tracking errors, and translate the cost function as the likelihood of a conditional probability

Algorithm:

Initialize recursions: $\hat{\mathbf{X}}_0^i = \mathbf{X}_0,\ i = \overline{1,N}\ , n = 1.$

Generate iid controls: $\mathbf{U}_n^i \sim \mathrm{N}(\mathbf{0}, \mathbf{A}_n).$

Evaluate model: $\mathbf{X}_n^i = F_n\left(\hat{\mathbf{X}}_{n-1}^i, \mathbf{U}_n^i\right);\ \mathbf{Y}_n^i = h_n\left(\mathbf{X}_n^i\right).$

Weight according to $p_n^i = \dfrac{\exp\left(-\frac{\beta}{2}\left\|\mathbf{Y}_n^i - \mathbf{Y}_n^{\mathrm{ref}}\right\|_{\mathbf{B}_n}^2\right)}{\sum_{j=1}^{N} \exp\left(-\frac{\beta}{2}\left\|\mathbf{Y}_n^j - \mathbf{Y}_n^{\mathrm{ref}}\right\|_{\mathbf{B}_n}^2\right)}.$

Resample controls from $p_n(\mathbf{u}) = \sum_{i=1}^{N} p_n^i \delta_{\mathbf{U}_n^i}$ for each $j = \overline{1,N}$

which leads to:

$$\hat{\mathbf{X}}_n^j = F_n\left(\hat{\mathbf{X}}_{n-1}^i, \mathbf{U}_n^i\right); \qquad \mathbf{Y}_n^j = h_n\left(\hat{\mathbf{X}}_n^j\right) \qquad \begin{matrix} \text{for each } j \\ i \in \left\{\overline{1,N}\right\} \end{matrix}.$$

Repeat for $n = \overline{2,T}$.

GENEALOGICAL DECISION TREE

Interpretation as a genetic particle evolution model

Interpret state $\hat{\mathbf{X}}_{n-1}^{j}$ as the parent of individual $\hat{\mathbf{X}}_{n}^{i}$:

- denote $\hat{\mathbf{X}}_{n-1,n}^{i} = \hat{\mathbf{X}}_{n-1}^{j}$, etc.

Ancestral lines:

$$\hat{\mathbf{X}}_{0,n}^{i} \leftarrow \dots \leftarrow \hat{\mathbf{X}}_{n-2,n}^{i} = \hat{\mathbf{X}}_{n-2}^{k} \leftarrow \hat{\mathbf{X}}_{n-1,n}^{i} = \hat{\mathbf{X}}_{n-1}^{j} \leftarrow \hat{\mathbf{X}}_{n,n}^{i} = \hat{\mathbf{X}}_{n}^{i}$$

$$\hat{\mathbf{U}}_{1,n}^{i} \leftarrow \dots \leftarrow \hat{\mathbf{U}}_{n-2,n}^{i} = \hat{\mathbf{U}}_{n-2}^{k} \leftarrow \hat{\mathbf{U}}_{n-1,n}^{i} = \hat{\mathbf{U}}_{n-1}^{j} \leftarrow \hat{\mathbf{U}}_{n,n}^{i} = \hat{\mathbf{U}}_{n}^{i}$$

Solution at $n = T$:

$$I = \arg \inf_{i=1,N} J_n\left(\hat{\mathbf{U}}_{1,n}^{i}, \hat{\mathbf{U}}_{2,n}^{i}, \dots, \hat{\mathbf{U}}_{n,n}^{i}\right)$$

CONVERGENCE

Idea:
- Associate Gaussian distributions to the norms in the cost function
- Translate the cost function as the likelihood of a conditional probability
- Duality between control and filtering problems

Corresponding **filtering problem:**

$$\mathbf{X}_n = F_n(\mathbf{X}_{n-1}, \mathbf{W}_n);\ \mathbf{Y}_n = h_n(\mathbf{X}_n) + \mathbf{V}_n$$

where **W** and **V** are Gaussian random vectors with covariances $\mathbf{A}_n$ and $\mathbf{B}_n$.

We can show the following (see works with P. Del Moral):

1. To find control actions which minimize the control objective, it is equivalent to look for most likely W.
2. The conditional probability mass of W is concentrated around the optimal control sequence:

$$\Pr\{(\mathbf{W}_1,\ldots,\mathbf{W}_n) \in d(\mathbf{w}_1,\ldots,\mathbf{w}_n) \,|\, \mathbf{Y}_1 = \mathbf{Y}_1^{\mathrm{ref}},\ldots,\mathbf{Y}_n = \mathbf{Y}_n^{\mathrm{ref}}\}$$

$$= \frac{1}{Z_n}\exp\left(\frac{-\beta}{2}\left(\sum_{k=1}^{n}\|\mathbf{w}_k\|_{\mathbf{A}_k}^2 + \sum_{k=1}^{n}\left\|\mathbf{Y}_k^{\mathrm{ref}} - h_k(\mathbf{X}_k)\right\|_{\mathbf{B}_k}^2\right)\right)d\mathbf{w}_1\ldots d\mathbf{w}_n$$

$$= \frac{1}{Z_n}\exp\left(\frac{-\beta}{2}J_n(\mathbf{w}_1,\ldots,\mathbf{w}_n)\right)d\mathbf{w}_1\ldots d\mathbf{w}_n$$

3. **Convergence of actions to optimal actions** (as $N \to \infty$).

NUMERICAl EXAMPLES (1) 'ABC'-batch plant

Plant

nonlinear equations:

$$\frac{dc_A}{dt} = -k_1(T)c_A^2$$

$$\frac{dc_B}{dt} = k_1(T)c_A^2 - k_2(T)c_B$$

$$\frac{dT}{dt} = \gamma_1 k_1(T)c_A^2 + \gamma_2 k_2(T)c_B + (a_1 + a_2 T) + (b_1 + b_2 T)u$$

temperature target trajectory:

$$T^{ref} = 20\exp(-0.02t)$$

GDT

optimize sequence of Δu's

$A = 2^2$ ('tolerated dev. on input')

$B = 0.2^2$ (tolerated dev. on output')

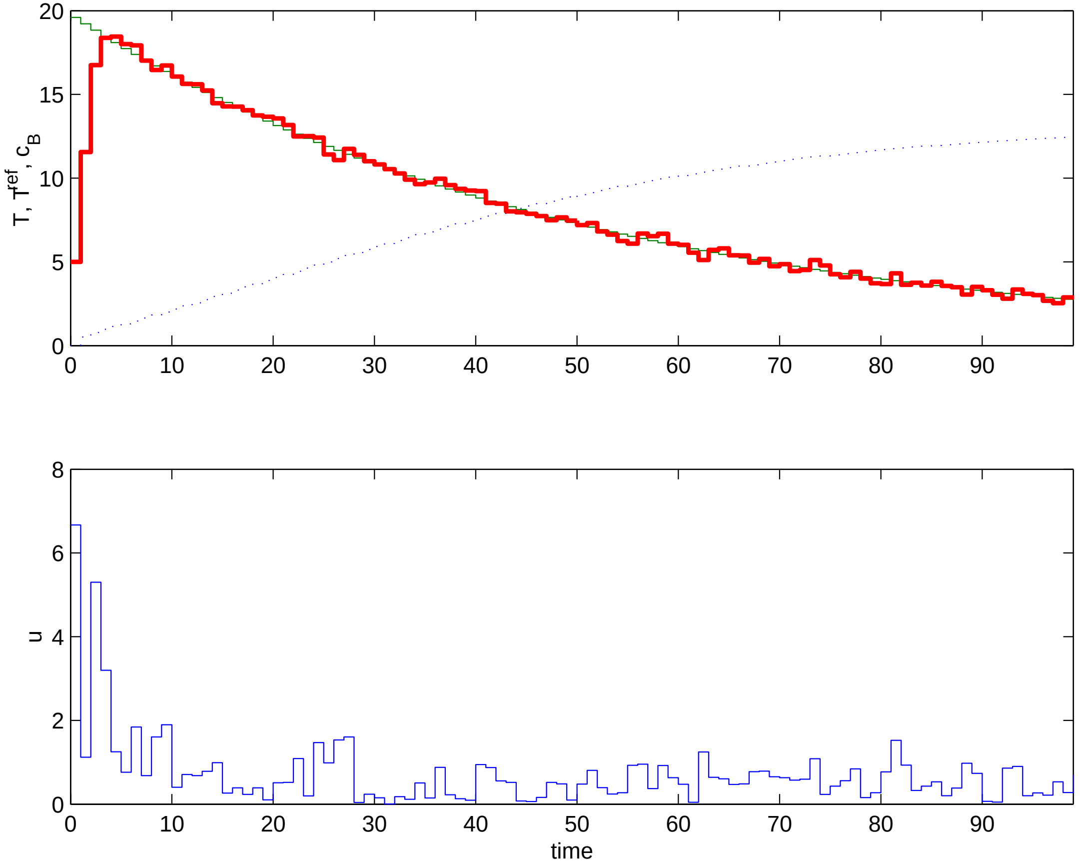
$\beta = 1$,

$N = 2500$ (# particles)

Results

design specs fulfilled

randomness apparent



temperature (output)

temperature reference (target)

dimensionless scaling (input)

NUMERICAL EXAMPLES (2) RTP-repetitive plant

Plant

nonlinear equations:

$$\frac{dT_F}{dt} = b_u u - c_1\left(T_F^4 - T_P^4\right) - c_2\left(T_F - T_A\right)$$

$$\frac{dT_P}{dt} = c_3\left(T_F^4 - T_P^4\right)$$

temperature target trajectory consisting of ramp and constant phases

GDT

optimize sequence of u's

$A = 1$ ('tolerated dev. on input')

$B = 1$ (tolerated dev. on output')

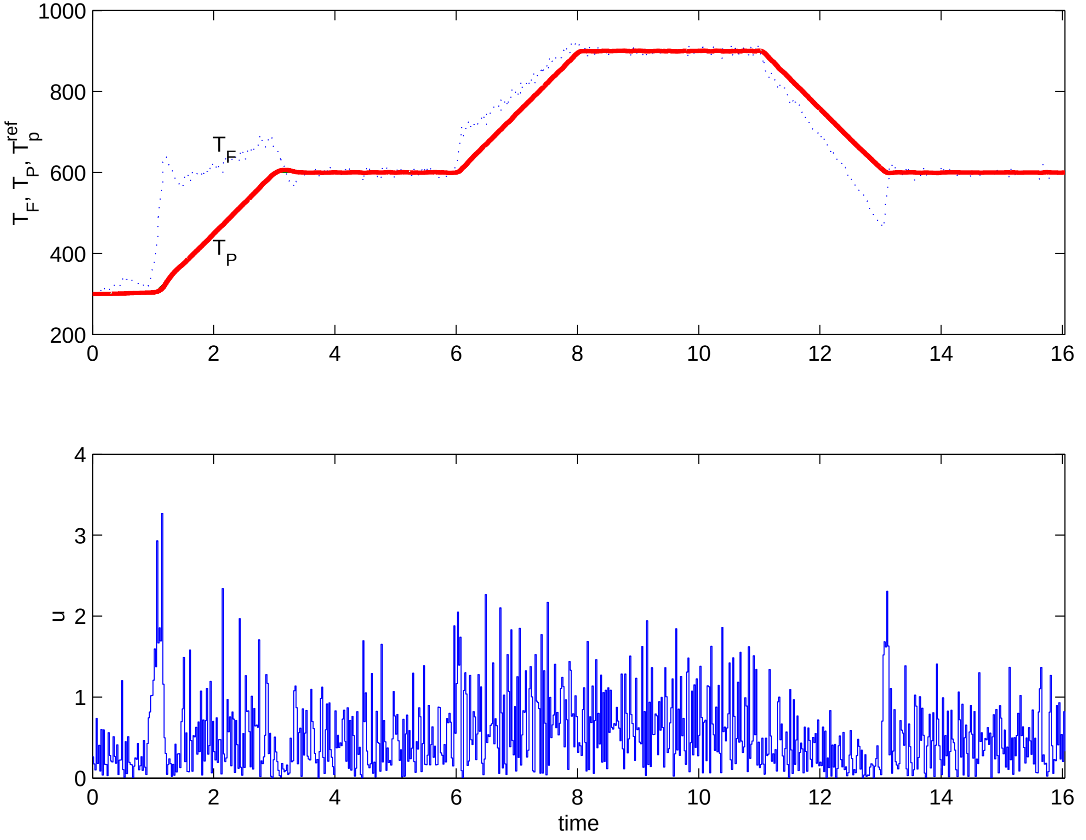
$\beta = 1$,

$N = 500$ (# particles)

Results

design specs fulfilled

randomness apparent



part temperature

heating intensity

More examples available:
3x3 power plant, 2-joint robot arm,

GDT-BASED REGULATION

Feedback:

1. Add (**SISO linear**) feedback based on output deviation (PI, for example)
   - suitable, e.g., for partially measured output/state trajectories
2. Receding-horizon **MPC**
   - solve optimization problem from current (disturbed) state
   - computationally heavy => discretized approximation with precomputed solutions

'Assumptions':

- **Accuracy** can be increased by making the discretization more dense (for non-chaotic plants)
- Given a minimal finite horizon $T_{min}<T$, each sequence contains a number of optimal **sub-sequences**
- **Regulation** problems (=setpoint trajectory) + time-invariant plants make the approach feasible

Algorithm

off-line:

1. **Solve** optimal trajectories of length T from K initial states $\mathbf{x}_0$
2. **Store** all sequences.

on-line:

3. a) *if measurement of* $\mathbf{x}$ *is available*:
   Compare state $\mathbf{x}$ with $K*(T-T_{min}+1)$ states in memory and find the closest match $\mathbf{x}*$.
   Set next and future controls equal to controls in the selected solution from point $\mathbf{x}*$ forward.
   b) *if no new measurements*:
   Select **next** control from the sequence.
4. **Apply** control to plant.
5. Return to Step 3.

NUMERICAL EXAMPLE (3): van der Vusse-regulation

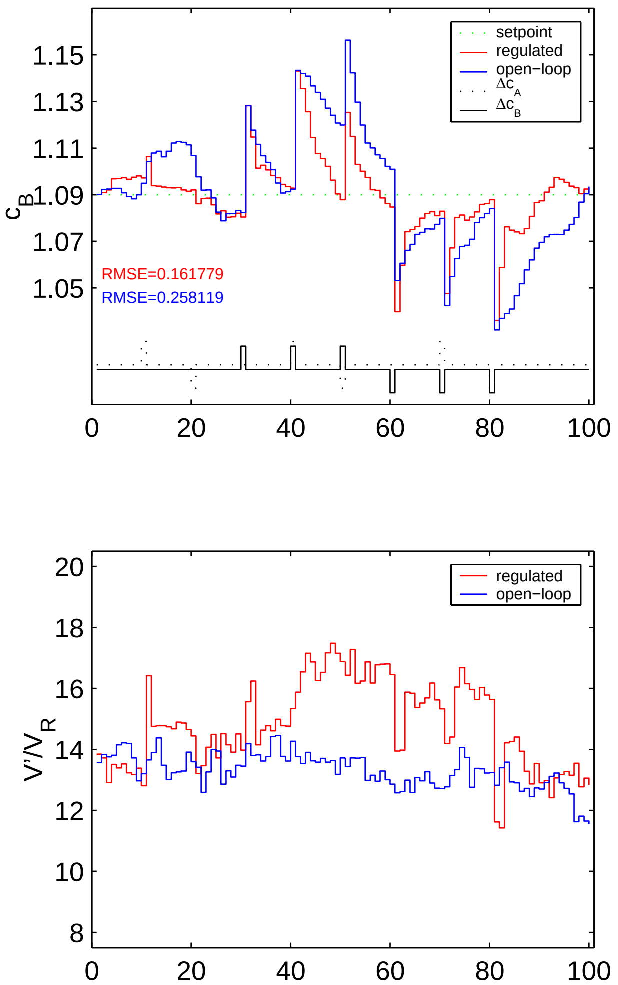
van der Vusse CSTR:
A→B→C
non-monotone ss-gain
non-minimum phase dyn.

Simulations (dbase):
isothermal simulations
$T = 100$ (traj. length)
controlled: c_B
manipulated: V'/V_R

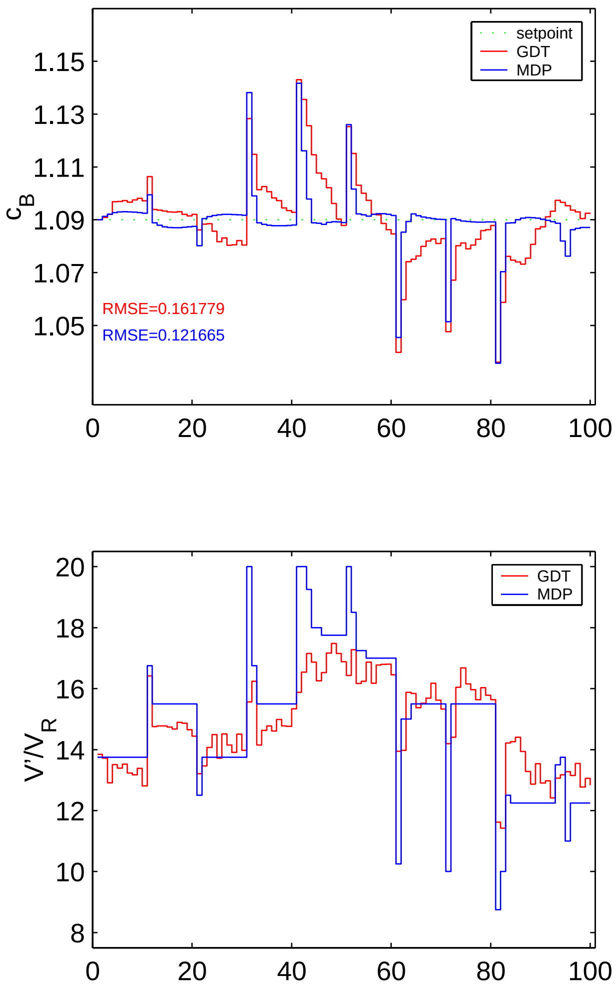
GDT parameters:
$A = 0.5^2$, $B = 0.01^2$
$\beta = 1$, $N = 2000$
Δu optimized

GDT-regulation:
$K = 300$ random init. states:
$c_A(0)=2.126 \pm 10\%$
$c_B(0)=1.09 \pm 10\%$
$J_T < 700$, $T_{min} = 60$
⇨ finite state dbase of 5760 state entries

Simulations (regulation):
impulse disturb. in states



Open-loop GDT vs. state disturbances
GDT regulation vs state disturbances



MDP-based optimal control
GDT-based regulation
with input constraints

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DISCUSSION

Why (..do we need the approach)?

- an optimization technique suitable for solving (potentially) difficult problems
  - nonlinear, discontinuous, sequential open loop trajectory problems
- main drawback: a noiseless state-space model is required/assumed

(How to use GDT in..) feedback control ?

- Linear feedback for disturbances
  - e.g., GDT + PI
- Receding-horizon model predictive control
  - approximate on-line solutions to open loop problems
  - requires state measurements and/or state estimators

(Selection of) GDT-algorithm parameters ?

- not always simple (trial and error)
- future directions: non-gaussian non-diagonal distributions in **A** and **B**

(Large) number of particles *N* needed ?

- Computations are realizable on office PC (at least for small dimensional problems)

(Theoretical..) properties ?

duality btw. optimal control and optimal filtering => ...

(How to assess potential..) usefulness of GDT ?

- What to compare with?
- MDP (finite state MC + Bellman equation)
  - what else would be fair / interesting?
- Real industrial applications ?

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Thank you

For more info, see:

http://cc.oulu.fi/~iko/MGDT.htm

- MATLAB-code
- a users' guide with examples