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
PROBLEM FORMULATION

Model:
\[
X_n = F_n(X_{n-1}, U_n); \quad X_0
\]
\[
Y_n = h_n(X_n)
\]

Control objective:
\[
J_T(U_1, U_2, ..., U_T) = \sum_{n=1}^{T} \|U_n\|_A^n + \sum_{n=1}^{T} \|Y_n - Y_n^{ref}\|_B^n
\]

- \(T\): length of trajectory (horizon)
- \(A_n, B_n\): 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: \( \hat{X}_0^i = X_0, \quad i = 1, \overline{N}, \quad n = 1 \).

Generate iid controls: \( U_n^i \sim N(0, A_n) \).

Evaluate model: \( X_n^i = F_n(\hat{X}_{n-1}^i, U_n^i); \quad Y_n^i = h_n(X_n^i) \).

\[
\exp\left( -\frac{\beta}{2} \| Y_n^i - Y_n^{\text{ref}} \|_{B_n}^2 \right)
\]

Weight according to \( p_n^i = \frac{N}{\sum_{j=1}^{N} \exp\left( -\frac{\beta}{2} \| Y_n^j - Y_n^{\text{ref}} \|_{B_n}^2 \right)} \).

Resample controls from \( p_n(u) = \sum_{i=1}^{N} p_n^i \delta_{U_n^i} \) for each \( j = 1, \overline{N} \) which leads to:

\[
\hat{X}_n^j = F_n(\hat{X}_{n-1}^i, U_n^i); \quad Y_n^j = h_n(\hat{X}_n^j) \quad \text{for each } j \in \{1, N\}.
\]

Repeat for \( n = 2, T \).
GENEALOGICAL DECISION TREE

Interpretation as a genetic particle evolution model

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

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

Ancestral lines:

$\hat{X}_{0,n}^i \leftarrow \ldots \leftarrow \hat{X}_{n-2}^i = \hat{X}_{n-2}^k$  \quad  $\hat{U}_{1,n}^i \leftarrow \ldots \leftarrow \hat{U}_{n-2,n}^i = \hat{U}_{n-2}^k$

$\hat{X}_{n-1,n}^i = \hat{X}_{n-1}^j$  \quad  $\hat{U}_{n-1,n}^i = \hat{U}_{n-1}^j$

$\hat{X}_{n,n}^i = \hat{X}_n^i$  \quad  $\hat{U}_{n,n}^i = \hat{U}_n^i$

Solution at $n = T$:

$I = \arg \inf_{i=1}^{N} J_n(\hat{U}_1^i, \hat{U}_2^i, \ldots, \hat{U}_n^i)$
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:
\[ X_n = F_n(X_{n-1}, W_n); \ Y_n = h_n(X_n) + V_n \]
where \( W \) and \( V \) are Gaussian random vectors with covariances \( A_n \) and \( B_n \).

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:
\[
\Pr\left\{ (W_1, \ldots, W_n) \in d(w_1, \ldots, w_n) \mid Y_1 = Y_{1 \text{ref}}, \ldots, Y_n = Y_{n \text{ref}} \right\} \\
= \frac{1}{Z_n} \exp\left( -\frac{\beta}{2} \left( \sum_{k=1}^{n} \|w_k\|_{A_k}^2 + \sum_{k=1}^{n} \|Y_k^{\text{ref}} - h_k(X_k)\|_{B_k}^2 \right) \right) \, dw_1 \ldots dw_n \\
= \frac{1}{Z_n} \exp\left( -\frac{\beta}{2} J_n(w_1, \ldots, w_n) \right) \, dw_1 \ldots dw_n
\]
3. Convergence of actions to optimal actions (as \( N \to \infty \)).
NUMERICAL EXAMPLES (1) ‘ABC’-batch plant

**Plant**
nonlinear equations:
\[
dc_A = -k_1(T)c_A^2 \\
dc_B = k_1(T)c_A^2 - k_2(T)c_B \\
dT = \gamma_1(T)c_A^2 + \gamma_2(T)c_B + (a_1 + a_2 T) + (h_1 + h_2 T)u
\]
temperature target trajectory:
\[T_{\text{ref}} = 20 \exp(-0.02t)\]

**GDT**
optimize sequence of \( \Delta u \)'s
\[A = 2^2 \text{ (tolerated dev. on input)}\]
\[B = 0.2^2 \text{ (tolerated dev. on output)}\]
\[\beta = 1, \quad N = 2500 \text{ (# particles)}\]

**Results**
design specs fulfilled
randomness apparent

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**Graphs**
- Temperature (output)
- Temperature reference (target)
- Dimensionless scaling (input)
NUMERICAL EXAMPLES (2) RTP-repetitive plant

**Plant**
nonlinear equations:
\[
\frac{dT_F}{dt} = b_x u - c_1 (T_F^1 - T_p^1) - c_2 (T_F - T_d)
\]
\[
\frac{dT_p}{dt} = c_3 (T_F^1 - T_p^1)
\]

temperature target trajectory consisting of ramp and constant phases

**GDT**
optimize sequence of u’s
\[ A = 1 \text{ (‘tolerated dev. on input’)} \]
\[ B = 1 \text{ (tolerated dev. on output’)} \]
\[ \beta = 1, \]
\[ N = 500 \text{ (# particles)} \]

**Results**
design specs fulfilled randomness apparent

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 $T_{\text{min}} < T$, 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 $x_0$
2. Store all sequences.

**on-line:**
3. a) if measurement of $x$ is available:
   - Compare state $x$ with $K^* (T-T_{\text{min}}+1)$ states in memory and find the closest match $x^*$.
   - Set next and future controls equal to controls in the selected solution from point $x^*$ 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:
\( A = 0.5^2, B = 0.01^2 \)
\( \beta = 1, N = 2000 \)
\( \Delta u \) optimized

GDT-regulation:
\( K = 300 \) random init. states:
\( c_A(0) = 2.126 \pm 10\% \)
\( c_B(0) = 1.09 \pm 10\% \)
\( J_T < 700, T_{\text{min}} = 60 \)
\( \Rightarrow \) 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
## 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