A Dynamic Programming Approach to Sequential and Nonlinear Bayesian Experimental Design

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Motivation

Goal:
To determine the sequence of experiments that together produce the most informative data

(Source: www.weather.com)
Bayesian Inference

\[
p(\theta|w, u) = \frac{\text{likelihood prior}}{p(w|\theta, u) p(\theta)}
\]

\(\theta\) — parameters of interest
\(w\) — noisy measurements
\(u\) — design variables or controls
Experimental Design of Multiple Experiments

- Open-loop vs. closed-loop
- Open-loop design chooses experiments all-at-once
- Numerical tools validated in open-loop design [Huan & Marzouk (2011)]: information-theoretic based objective, polynomial chaos surrogates, stochastic optimization

Contribution from this study: the first step to develop numerical tools for solving the closed-loop design problem
Finite-horizon, discrete-time, perfect state information

**State:** posterior PDFs $x_k = p(\theta|w_0, \ldots, w_{k-1}, u_0, \ldots, u_{k-1})$

**Control:** design variable $u_k = \mu_k(x_k) \in U \subseteq \mathbb{R}^{nu}$; $\pi = \{\mu_0, \mu_1, \ldots, \mu_{N-1}\}$ is a policy

**Disturbance:** measurements $w_k \in \mathbb{R}^{nw}$ from the experiment conducted under design $u_k$; assumed to be distributed according to a given likelihood function $p(w_k|\theta, u_k)$

**System:** Bayes’ Theorem, for $k = 0, \ldots, N - 1$

$$x_{k+1} = f(x_k, u_k, w_k) = \frac{p(w_k|\theta, u_k)x_k}{p(w_k|w_0, \ldots, w_{k-1}, u_0, \ldots, u_k)}$$
**Setup**

**System:** Bayes’ Theorem, for $k = 0, \ldots, N - 1$

$$x_{k+1} = f(x_k, u_k, w_k) = \frac{p(w_k | \theta, u_k) x_k}{p(w_k | w_0, \ldots, w_{k-1}, u_0, \ldots, u_k)}$$
Optimal Policy

**Cost and DP Algorithm:** information-theoretic approach [Lindley (1956)] using Kullback-Leibler divergence

\[
J_N(x_N) = \int_{\Theta} x_N \ln \left[ \frac{x_N}{x_0} \right] d\theta
\]

\[
J_k(x_k) = \max_{u_k \in U} \mathbb{E}_{w_k} [g_k(x_k, u_k, w_k) + J_{k+1}(f(x_k, u_k, w_k))]
\]

for \(k = 0, \ldots, N - 1\)
Optimal Policy

**Cost and DP Algorithm:** information-theoretic approach [Lindley (1956)] using Kullback-Leibler divergence

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\[
J_k(x_k) = \max_{u_k \in U} E_{w_k} \left[ g_k(x_k, u_k, w_k) + J_{k+1}(f(x_k, u_k, w_k)) \right]
\]

for \( k = 0, \ldots, N - 1 \)

How does the optimal policy \( \pi^* = \{\mu_0^*, \mu_1^*, \ldots, \mu_{N-1}^*\} \) come in?

Evaluating \( J_k \) at a particular \( x_k \) and finding the corresponding arg-max \( u_k^* \) is exactly evaluating \( u_k^* = \mu_k^*(x_k) \)
Exponential Growth

\[ J_k(x_k) = \max_{u_k \in U} \mathbb{E}_{w_k} \left[ g_k(x_k, u_k, w_k) + J_{k+1}(f(x_k, u_k, w_k)) \right] \]

Number of \( J_N(x_N) \) evaluations exponential in \( N \)
Successive Cost-To-Go Approximation

\[ J_k(x_k) \approx \max_{u_k \in U} \mathbb{E}_{w_k} \left[ g_k(x_k, u_k, w_k) + \tilde{J}_{k+1}(f(x_k, u_k, w_k)) \right] \]

Number of \( J_N(x_N) \) evaluations independent of \( N \)
Number of \( \tilde{J}_k(x_k) \) evaluations linear in \( N \)
Polynomial Spectral Expansion

Construct \( \tilde{J}_k(x_k) \) with expansions

\[
J_k(\xi) = \sum_{|i|_1=0}^{\infty} a_i \psi_i(\xi_1, \xi_2, \ldots) \approx \tilde{J}_k(\xi) = \sum_{|i|_1=0}^{p} a_i \psi_i(\xi_1, \xi_2, \ldots, \xi_n)
\]

\[
\psi_i(\xi_1, \xi_2, \ldots, \xi_n) = \prod_{j=1}^{n} \psi_{ij}(\xi_j)
\]

- \( a_i \in \mathbb{R} \) expansion coefficients, \( \xi_i \) base variables
- \( \psi_{ij} \) is the \( ij \)th order univariate orthogonal polynomial with respect to some weight function
- Non-intrusive approach to compute expansion coefficients

\[
a_i = \frac{\langle J_k \psi_i \rangle}{\langle \psi_i^2 \rangle} = \frac{\int J_k(x(\xi)) \psi_i(\xi) p(\xi) \, d\xi}{\int \psi_i^2(\xi) p(\xi) \, d\xi}
\]
Recall

\[ J_k(x_k) \approx \max_{u_k \in \mathcal{U}} \mathbb{E}_{w_k} \left[ g_k(x_k, u_k, w_k) + \tilde{J}_{k+1} (f(x_k, u_k, w_k)) \right] \]

Robbins-Monro (RM)

\[ u^{m+1} = u^m - \gamma(m) \hat{\nabla}(u^m) \]

\( m \) is the RM sub-iteration number, \( \gamma(m) \) is the gain sequence, and \( \hat{\nabla}(u^m) \) is an unbiased gradient estimator

- convergence requires \( \sum_{i=1}^{\infty} \gamma(i) = \infty \) and \( \sum_{i=1}^{\infty} \gamma^2(i) < \infty \) (e.g., \( \gamma(m) = \frac{\alpha}{m} \), \( \alpha \) some constant)
- \( \hat{\nabla}(u^m) \) from differentiating the Monte Carlo approximation to \( \mathbb{E} [\cdot] \)
Optimal Designs

After constructing all surrogate functions $\tilde{J}_0, \ldots, \tilde{J}_N$, once the current state $x_k$ becomes known, we can recover optimal controls by evaluating

$$u_k^* = \mu_k^*(x_k) \approx \arg \max_{u_k \in U} \mathbb{E}_{w_k} \left[ g_k(x_k, u_k, w_k) + \tilde{J}_{k+1}(f(x_k, u_k, w_k)) \right]$$
Linear-Gaussian Problem

\[ F_k = m_k a + \epsilon_k \]
\[ (or \ w_k = u_k \theta + \epsilon_k) \]

- Prior: \( \theta \sim \mathcal{N}(\mu_0, \sigma_0^2) \)
- Noise: \( \epsilon_k \sim \mathcal{N}(0, \sigma_\epsilon^2) \)
- Linear Gaussian problem: conjugate family, posteriors (i.e., all states) will be Gaussian:

\[
\mathbf{x}_{k+1} = \left( \mu_{k+1}, \sigma_{k+1}^2 \right) = \left( \frac{w_k / u_k}{\sigma_\epsilon^2 / u_k^2 + \sigma_k^2} + \frac{\mu_k}{\sigma_k^2}, \frac{1}{\sigma_\epsilon^2 / u_k^2 + \sigma_k^2} \right)
\]

We would like to sequentially choose \( N \) test-masses \( m_0, \ldots, m_{N-1} \in [1, M] \) such that we can best infer the value of \( a \).
Results

Approximate cost-to-go functions at different stages
A simulated experimental design scenario

<table>
<thead>
<tr>
<th>$k$</th>
<th>$x_k$</th>
<th>$u^*_k$</th>
<th>$w_k$</th>
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<td>98.5</td>
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<td>(9.73, 0.07$^2$)</td>
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<td>98.2</td>
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<tr>
<td>3</td>
<td>(9.76, 0.06$^2$)</td>
<td>–</td>
<td>–</td>
</tr>
</tbody>
</table>
Conclusions:

- Provided a general dynamic programming framework for solving *optimal Bayesian sequential experimental design* problems
- Achieved computational-feasibility through *successive approximation of the cost-to-go functions*
- Recommended numerical algorithms (polynomial surrogates, Robbins-Monro, etc)
- Presented numerical results on a simple proof-of-concept linear-Gaussian problem

Future work:

- State representation (general PDFs)
- Surrogate building from noisy function
- Weight function selection in the context of polynomial spectral expansion
KAUST Global Research Partnership

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