A note on optimal experiment design for nonlinear systems using dynamic programming

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March 26, 2015

1 Main result

We consider a discrete-time dynamical system with noisy observations

\[ x_{t+1} = f(x_t, u_t, \theta) \]
\[ Y_t \sim p_{x_t}(y_t) \]  

where \( x_t \in \mathbb{R}^n \) denotes the system’s state, \( u_t \in \mathbb{R}^m \) is a sequence of inputs to be designed and \( \theta \in \mathbb{R}^p \) is a vector of unknown parameters that we wish to estimate. Observations are drawn independently from a known distribution that is parametrized by the system state \( x_t \). We assume that for all \( x_t \in \mathbb{R}^n \) the probability distribution is absolutely continuous with respect to some measure \( \mu \) and we denote its density with respect to \( \mu \) by \( p_{x_t}(y_t) \). We further assume that this density is differentiable with respect to the parameter \( x_t \) and define the Fisher information matrix as

\[ I_Y(\theta) = \mathbb{E}_{\theta} \left[ \left( \nabla_{x_t} \log p_{x_t}(Y_t) \right) \left( \nabla_{x_t} \log p_{x_t}(Y_t) \right)^T \right]. \]

We consider this system over a finite horizon \( 0 \leq t \leq N \). Our goal is to design a sequence \( u \) that provides a maximal amount of information about the unknown parameter vector \( \theta \) for \( \theta \) in a neighbourhood of some nominal value of the parameters \( \theta_0 \). Mathematically, we wish to choose \( u \) to maximize a function \( \phi(I_Y(\theta_0)) \) of the Fisher information that the joint output \( Y = (Y_0, \ldots, Y_N) \) carries about the parameter \( \theta \). The function \( \phi \) is chosen to be a measure of the “largeness” of the positive semidefinite matrix \( I \). Multiple choices for the function \( \phi \) have been proposed [1]; here we use \( \phi(I) = \text{tr}(I) \) (often called “T-optimal design”). In general this problem is nonconvex as a function of \( u \), but due to the fact that the trace is linear our objective function is additive so a global solution can be found using dynamic programming.

The following result allows us to compute the information contained in the observed data. A proof of this proposition is given in Section 3.

**Proposition 1.** Suppose that for all \( x_t \in \mathbb{R}^n \) the density \( p_{x_t}(y_t) \) is differentiable with respect to \( x_t \) and that there exists a \( \mu \)-integrable function \( q \) with \( \left| \frac{\partial p_{x_t}(y_t)}{\partial x_t} \right| \leq q(y_t) \) for all \( y_t \in \mathbb{R} \). If \( f \) is \( C^1 \) in \( x_t \) and \( \theta \), then the Fisher information with respect to the parameter \( \theta \) can be computed as

\[ I_Y(\theta) = \sum_{t=0}^{N} (\nabla_{\theta} x_t)^T I_{Y_t}(x_t)(\nabla_{\theta} x_t) \]  

where \( \nabla_{\theta} x_t \) denotes the Jacobian of \( x_t \) with respect to \( \theta \).

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1 arXiv:1503.07232v1 [cs.SY] 24 Mar 2015
Applying the chain rule to (1), we get a dynamical system
\[ \nabla_{\theta} x_{t+1} = \nabla_{\theta} f(x_t, u_t, \theta) + \nabla_{x} f(x_t, u_t, \theta) \nabla_{\theta} x_t \]

(4)
describing the time evolution of the sensitivities \( \nabla_{\theta} x_t \). The dynamics (1) and (4) together with the cost function (3) define a discrete-time finite-horizon optimal control problem that can be solved via dynamic programming [2]. In particular, we define the sequence of value functions \( J_k \)

\[ J_N(x_N, \nabla_{\theta} x_N) = \text{tr} \left( (\nabla_{\theta} x_N)^T I_N(x_N) (\nabla_{\theta} x_N) \right) \]

\[ J_k(x_k, \nabla_{\theta} x_k) = \max_{u_k} \left\{ \text{tr} \left( (\nabla_{\theta} x_k)^T I_N(x_k) (\nabla_{\theta} x_k) \right) + J_{k+1} \left( f(x_k, u_k, \theta), \nabla_{\theta} f(x_k, u_k, \theta) + \nabla_{x} f(x_k, u_k, \theta) \nabla_{\theta} x_k \right) \right\} \]

If the control policy \( u^*_k(x_k, \nabla_{\theta} x_k) \) maximizes the right hand side of (4) then \( u^* \) is globally optimal.

Related approaches to the optimal experiment design problem appear in [3] and [4] for continuous-time dynamical systems with Gaussian noise. However, a different objective function \( \phi \) is used and these approaches requires appending a nonlinear matrix differential equation for the dispersion (the inverse of the Fisher information) to the system state in addition to equation (4). By choosing the \( T \)-optimal design criterion \( \phi(I) = \text{tr}(I) \), we are able to avoid adding an equation for the dispersion to the system state, allowing us to efficiently solve problems of larger dimension.

2 Example problem

We consider a population of fruit flies, whose dynamics are modelled using the discrete logistic equation

\[ x_{t+1} = x_t + rx_t(K - x_t) \]

We want to estimate the reproduction rate \( r \) along with the carrying capacity \( K \). To generate data from which to estimate the model parameters, we place a sequence of traps into the fly cage, each capturing a fraction \( u_t \) of the current fly population. By measuring the number of fruit flies caught in the trap, we wish to infer the model parameters. The optimization problem thus consists of choosing the size of the traps (and hence the proportion of flies trapped) at each sampling interval.

This leads to a model for the population dynamics together with the number of fruit flies trapped \( Y_t \)

\[ x_0 = K \]
\[ x_{t+1} = x_t(1 - u_t) + rx_t(1 - u_t)(K - x_t(1 - u_t)) \]
\[ Y_t \sim \text{Poisson}(x_t u_t) \]

(5)

For this problem, we approximate the functions \( J_k \) by evaluation on a grid of size \( 100 \times 100 \times 100 \). We optimize about the nominal parameter values \( r_0 = 5 \times 10^{-4} \) and \( K_0 = 1000 \). This is implemented in MATLAB using the dynamic programming routine introduced in [5]. The optimal inputs are computed in 33.01 seconds and are shown in Figure 1a. The corresponding state trajectory is shown in Figure 1b.

We see that the optimal observation scheme is to first capture a large fraction \( u_1 = 0.9795 \) of the flies allowing us to get a reliable estimate for the carrying capacity \( K \). After this, we capture a fraction \( u_t \approx 0.32 \) of the flies, just enough to keep the population constant. This provides maximal sensitivity to the growth rate \( r \) in a neighbourhood of \( r_0 \). Indeed, if \( r > r_0 \) we will see the the population of flies grow over time, whereas if \( r < r_0 \) the population will shrink toward zero.
3 Proof of Proposition 1

Proof. First, note that the hypotheses of this proposition provide sufficient regularity to exchange the order of differentiation with respect to $\theta_i$ and integration with respect to $y_t$. Therefore for all $i = 1, \ldots, p$ and $t = 0, \ldots, N$

$$
\mathbb{E}_\theta \left[ \frac{\partial \log p_\theta(Y_t)}{\partial \theta_i} \right] = \int \frac{\partial \log p_\theta(y_t)}{\partial \theta_i} p_\theta(y_t) d\mu(y_t) = \int \frac{\partial p_\theta(y_t)}{\partial \theta_i} d\mu(y_t)
$$

$$
= \frac{\partial}{\partial \theta_i} \int p_\theta(y_t) d\mu(y_t) = \frac{\partial}{\partial \theta_i} 1 = 0.
$$

Now for all $i, j = 1, \ldots, p$ we can compute the $(i, j)$-th entry of $\mathcal{I}_\theta(Y)$ as

$$
\mathcal{I}_{Y}(\theta)_{i,j} = \mathbb{E}_\theta \left[ \frac{\partial \log p_\theta(Y)}{\partial \theta_i} \frac{\partial \log p_\theta(Y)}{\partial \theta_j} \right]
$$

$$
= \mathbb{E}_\theta \left[ \frac{\partial }{\partial \theta_i} \left( \sum_{t=0}^{N} \frac{\partial \log p_\theta(Y_t)}{\partial \theta_i} \right) \left( \sum_{s=0}^{N} \frac{\partial \log p_\theta(Y_s)}{\partial \theta_j} \right) \right]
$$

$$
= \sum_{t=0}^{N} \mathbb{E}_\theta \left[ \frac{\partial \log p_\theta(Y_t)}{\partial \theta_i} \frac{\partial \log p_\theta(Y_t)}{\partial \theta_j} \right] + \sum_{t=0}^{N} \sum_{s=0, s \neq t}^{N} \mathbb{E}_\theta \left[ \frac{\partial \log p_\theta(Y_t)}{\partial \theta_i} \right] \mathbb{E}_\theta \left[ \frac{\partial \log p_\theta(Y_s)}{\partial \theta_j} \right]
$$

$$
= \sum_{t=0}^{N} \mathbb{E}_\theta \left[ \frac{\partial \log p_{x_t(\theta)}(Y_t)}{\partial \theta_i} \frac{\partial \log p_{x_t(\theta)}(Y_t)}{\partial \theta_j} \right]
$$

$$
= \sum_{t=0}^{N} \mathbb{E}_\theta \left[ \nabla x_t \log p_{x_t}(Y_t) \frac{\partial }{\partial \theta_i} \left( \nabla x_t \log p_{x_t}(Y_t) \right) \nabla x_t \log p_{x_t}(Y_t) \frac{\partial }{\partial \theta_j} \right]
$$

$$
= \sum_{t=0}^{N} \frac{\partial x_t}{\partial \theta_i} \mathbb{I}_{Y_t}(x_t) \frac{\partial x_t}{\partial \theta_j}.
$$

Figure 1: Numerically-computed solution to the optimal experiment design problem
So

\[ I_Y(\theta) = \sum_{t=0}^{N} (\nabla_\theta x_t)^T I_Y(x_t)(\nabla_\theta x_t). \]

References

[1] F. Pukelsheim, *Optimal Design of Experiments*. Society for Industrial and Applied Mathematics, 2006.

[2] D. P. Bertsekas, *Dynamic Programming and Optimal Control, Volume 1*. Athena Scientific, 1995.

[3] R. T. N. Chen, “Input design for aircraft parameter identification: Using time-optimal control formulation,” in *Methods for Aircraft State and Parameter Identification, Advisory Group for Aerospace Research and Development (AGARD), Conference Proceedings no. 172*, 1975.

[4] E. A. Morelli and V. Klein, “Optimal input design for aircraft parameter estimation using dynamic programming principles,” in *AIAA Atmospheric Flight Mechanics Conference paper 90-2801*, 1990.

[5] O. Sundström and L. Guzzella, “A generic dynamic programming Matlab function,” in *IEEE International Symposium on Control Applications and Intelligent Control (CCA & ISIC)*, 2009, pp. 1625–1630.