Optimal Design for estimation in stochastic LIF models - Mutual Information + Maximum Principle / Dynamic Programing Approach

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Abstract

Given a stochastic differential equation with unknown parameters and a control in the drift term - we discuss optimal design-type questions on what is the best external perturbation in order to facilitate the estimation of the unknown parameters

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1 Problem Formulation

The basic goal of 'Optimal Design' is to perturb a dynamical system in an 'optimal' way such as to 'best' estimate its structural parameters.

Consider the generic parametrized and controlled SDE system

$$dX = U(x, \alpha(x,t); \theta)\,\mathrm{d}t + \sqrt{2D}dW \tag{1}$$

and for illustration case also consider the simplest non-trivial example of eq. (1), the OU system:

$$dX = \underbrace{(\alpha + \beta(\mu - X)}_{U(x,\alpha;\theta)}\,\mathrm{d}t + \underbrace{\sigma}_{\sqrt{2D}} dW \tag{2}$$

Whose parameter set is:

$$\theta = \{\mu, \beta, \sigma\}$$

Sometimes, to make things simpler, we will assume that we know the diffusion coefficient, σ, in which case the parameter set to-be-estimated for the OU system becomes:

$$\theta = \{\mu, \beta\}$$

Out ultimate goal is to choose the control policy $\alpha(\cdot)$, such as to facilitate the estimation of the parameter set θ given a single observed trajectory $\{X_t\}_0^T$. At first we will idealize that we have cts. observations (i.e. very-high-frequency observations). Later we can try addressing the problem of low-frequency observations.

A fundamental concept in the sequel is the probabilty transition density associated with X_t, we will call this f

$$f(x, t|x_0; \theta, \alpha(\cdot))dx = \mathbb{P}[X_t \in x + dx|x_0, \alpha, \theta] \tag{3}$$

It is well-known that for a fixed, $\theta, \alpha(\cdot)$, f is the solution to a Fokker-Planck equation:

$$\partial_t f = \mathcal{L}_{\theta,\alpha(\cdot)}[f] \tag{4}$$

where the differential operator $\mathcal{L}$ is given by:

$$\mathcal{L}_{\theta,\alpha(\cdot)}[f] = D \cdot \partial_x^2[f] - \partial_x[U(x, \alpha(x,t); \theta) \cdot f]$$

We will call $\mathcal{L}$ the forward operator and its adjoint $\mathcal{L}^*$, the backward operator.

2 Optimal Design using Mutual Information

Our main point-of-departure in obtaining $\alpha(\cdot)$ is the concept of Mutual Information (here are two books on information theory - [1, 4], see appendix A for definitions).

In particular, two references suggest that one should use the Mutual Information [5, 2] as the criterion for designing the experiment. (Designing the experiment is synonymous to choosing the control policy $\alpha(\cdot)$.

In order to apply the concept of mutual information, we need to have a prior on the parameter set, θ. We will call this prior:

$$\rho(\theta).$$

Naturally a optimally-designed experiment is one which reveals most the actual value of θ. That is we want to choose $\alpha(\cdot)$ such as to maximize the Information in the random variable θ, given observations of the random variable X_t.

First we need to consider the posterior of θ, $p(\theta|X_t)$ given an observation X_t for t fixed

$$p(\theta|X_t;\alpha) = \frac{f(X_t,t|\theta;\alpha)\cdot\rho(\theta)}{\int_\Theta f(X_t,t|\theta;\alpha)\cdot\rho(\theta)\,\mathrm{d}\theta} \tag{5a}$$

That is the transition density is the likelihood of the parameters.

$$L(X_t|\theta) = f(X_t,t|x_0,0;\theta,\alpha(\cdot)) \tag{5b}$$

However, if we have many observations $\{X_{t_n}\}$, the likelihood is, of course, more complicated. Then

$$L(\{X_n\}|\theta) = \prod_n (f(X_{t_{n+1}},t_{n+1}|X_{t_n},t_n;\theta) \tag{6a}$$

and the parameter posterior is then

$$p(\theta|\{X_{t_n}\};\alpha) = \frac{L(\{X_{t_n}\},t|\theta;\alpha)\cdot\rho(\theta)}{\int_\Theta L(\{X_{t_n}\},t|\theta;\alpha)\cdot\rho(\theta)\,\mathrm{d}\theta} \tag{6b}$$

Once we have the concepts of the prior, posterior and likelihood, ρ, p, L, then the mutual information, I, between the two random variables, θ, X_t is:

$$I(\alpha) = \int_\Theta\int_X \log\left[\frac{p(\theta|x;\alpha)}{\rho(\theta)}\right]\cdot L(x|\theta;\alpha)\cdot\rho(\theta)\,\mathrm{d}\theta\,\mathrm{d}x \tag{7}$$

This is straight from equations 6,8,9 of [5] (That paper is on the OptEstimate Mendeley group). Also see appendix A.

Replacing the posterior in eq. (7), with the bayesian formula from eq. (5a) or 6b, we get:

$$I(\alpha) = \int_\Theta\int_X \log\left[\frac{L(x|\theta;\alpha)}{\int_\Theta L(x|\theta;\alpha)\cdot\rho(\theta)\,\mathrm{d}\theta}\right]\cdot L(x|\theta;\alpha)\cdot\rho(\theta)\,\mathrm{d}\theta\,\mathrm{d}x \tag{8}$$

It is a small step then to seek the policy $\alpha(\cdot)$ that maximizes I.

However eq. (8) can appear deceptively simple. The integral over X, $\int_X \mathrm{d}x$, is really a multi-dimensional integral over all observations. Thus just the evaluation of I is only possible through Monte Carlo methods (unless there are very few, say $N < 5$ observations). However if you have only one observation, as with the posterior given eq. (5a), then we have a very simple single integral over x, which can be easily evaluated approximately using any quadrature rule.

A crucial assumption in the sequel is that we will NOT be updating the prior on the fly, that is we will always have the same $\rho(\theta)$ in eq. (8), even though new observations can obviously be used to update the prior, ρ, through Bayes' formula.

3 Finding the optimal design $\alpha(\cdot)$ - Dynamic Programing

In principle now, we have a criterion, the mutual information in eq. (8), using which to select the most informative perturbation $\alpha(\cdot)$.

However, in its most generality, $\alpha(\cdot)$ is a stochastic process measurable wrt. the filtration of X_t. I.e. we will choose different control values $\alpha(t)$ depending on the up-to t realization of $X_s; s \leq t$.

This is clearly a problem from optimal stochastic control. However, the objective in eq. (8) is not in the form needed to apply dynamic programing (or the maximum principle for that matter). The multi-dimensional integral in X makes things 'too' complicated.

On the other hand, what we propose to do is to take the mutual information criterion in eq. (8) using the single observation likelihood in eq. (5b) and just integrate it over time.

$$J(\alpha) = \int_\theta \int_0^T \int_X \log \left(\frac{f(x,t|\theta;\alpha(\cdot))}{\int_\theta f(x,t|\theta;\alpha(\cdot))\rho(\theta)\,\mathrm{d}\theta} \right) f(x,t|\theta;\alpha(\cdot))\cdot\rho(\theta)\,\mathrm{d}x\,\mathrm{d}t\,\mathrm{d}\theta \tag{9}$$

where the dx integral has the same dimension as the dimension of the SDE not the dimension of the number of observations. I should repeat that J is NOT the mutual information between a realization of the process, $\{X_t\}_0^T$ and the parameter set, θ. It is the time-integral of the individual mutual informations between each X_t at time t and the parameter set θ. The reason we do this is that now J can be written as

$$J(\alpha) = \mathbb{E}_\theta \left[\mathbb{E}_{X_t|\theta;\alpha(\cdot)} \left[\int_0^T \log \left(\frac{f(X_t,t|\theta;\alpha(\cdot))}{\int_\theta f(X_t,t|\theta;\alpha(\cdot))\rho(\theta)\,\mathrm{d}\theta} \right) \mathrm{d}t \right] \right] \tag{10}$$

which almost has the classical form of a stochastic optimal control problem, except for two non-standard features:

1. We have an extra outer expectation, the one wrt. to the parameter prior.
2. There is a forward-backward coupling in the determinations of the optimal control, meaning we can't just back out, the optimal control with a backwards solution to an HJB equation

Of these two features, we discuss pt. 1 first.

3.1 Stochastic Optimal Control with a Prior

We would like to apply Dynamic Programing to the problem of maximizing eq. (10). However section 3.1.1 shows why this is impossible (or at least why the first thing one thinks of does not work).

Instead, in order to find the optimal $\alpha(\cdot)$ we turn to the maximum principle in section 3.1.2.

3.1.1 Dynamic Programing with a Prior

WARNING: THIS SECTION ULTIMATLY EXPLAINS WHY YOU CANNOT! USE eq. (16). I.E. WHY DYNAMIC PROGRAMING CANNOT! BE USED TO FIND THE CONTROL.

In order to apply Dynamic Programing, i.e. in order to set up an HJB PDE, let us write our objective as:

$$J(x_0, 0; \alpha) = \mathbb{E}_\theta \left[\mathbb{E}_{X_0^T|\theta,\alpha} \left[\int_0^T r(X_t|\theta) \, \mathrm{d}t \right] \right] \tag{11}$$

where, in our case, the reward r is the mutual information between X_t and θ

$$r(x|\theta) = \log \left(\frac{f(x, t|\theta; \alpha(\cdot))}{\int_\theta f(x, t|\theta; \alpha(\cdot)) \rho(\theta)} \right) \tag{12}$$

But we can consider $r(\cdot)$ as a generic function of X_t.

Now we try to follow the standard dynamic programing approach to obtain an HJB-type equation.

Call w the value function, i.e. the optimal reward-to-go.

$$w(x_t, t) = \sup_{\alpha(\cdot)} \mathbb{E}_\theta \left[\mathbb{E}_{X_t^T|\theta,\alpha} \left[\int_t^T r(X_t|\theta) \, \mathrm{d}t \right] \right] \tag{13}$$

Or in particular, starting from x_0 at $t = 0$

$$w(x_0, 0) = \sup_{\alpha(\cdot)} \mathbb{E}_\theta \left[\mathbb{E}_{X_0^T|\theta,\alpha} \left[\int_0^T r(X_t|\theta) \, \mathrm{d}t \right] \right] \tag{14}$$

$$\mathbb{E}_{X_0^T|\theta,\alpha}[\cdot]$$

means the expectation over the full trajectory of X from 0 to T^*, X_0 held fixed, while evolving under the parameter set θ and the control policy α.

$$\mathbb{E}_{\Delta X|\theta,\alpha}[\cdot]$$

Is the expectation over the single point realization of $\Delta X = X(\Delta t) = X_{\Delta t}$, again under a given parameter set and policy, θ, α.

The Markovian nature of $X_t|\theta$ implies that for x_0 fixed.

$$\mathbb{E}_{X_0^T|\theta,\alpha}[\cdot] = \mathbb{E}_{\Delta X|\theta} \left[\mathbb{E}_{X_{\Delta t}^T|\theta,\alpha}[\cdot|\Delta X] \right]$$

With that we can start deriving an equation for w, starting from

$$\begin{aligned} w(x_0, 0) &= \sup_{\alpha(\cdot)} \mathbb{E}_\theta \left[\mathbb{E}_{X_0^T|\theta,\alpha} \left[\int_0^T r(X_t|\theta) \, \mathrm{d}t \right] \right] \\ &= \sup_{\alpha(\cdot)} \mathbb{E}_\theta \left[r(x_0)\Delta t \right] + \mathbb{E}_\theta \left[\mathbb{E}_{X_0^T|\theta,\alpha} \left[\int_{\Delta t}^T r(X_t|\theta) \, \mathrm{d}t \right] \right] \end{aligned}$$

All we've done so far is split the time integral into an incremental initial part which is approximately equal to $r(x_0)\Delta t$ and the rest $\int_{\Delta t}^T$. Now let's focus on the second term, $\mathbb{E}_\theta\left[\mathbb{E}_{X_0^T|\theta,\alpha}\left[\int_{\Delta t}^T r(X_t|\theta)\,\mathrm{d}t\right]\right]$ and condition on $x_0+\Delta X$:

$$\mathbb{E}_\theta\left[\mathbb{E}_{X_0^T|\theta,\alpha}\left[\int_{\Delta t}^T r(X_t|\theta)\,\mathrm{d}t\right]\right] = \mathbb{E}_\theta\left[\mathbb{E}_{\Delta X|\theta,\alpha}\left[\mathbb{E}_{X_{\Delta t}^T|\theta,\alpha}\int_{\Delta t}^T r(X_t|\theta)\,\mathrm{d}t|X_{\Delta t}\right]\right]$$

Now here is the main problem! We WOULD LIKE to say that

$$\mathbb{E}_\theta\left[\mathbb{E}_{\Delta X|\theta,\alpha}\left[\mathbb{E}_{X_{\Delta t}^T|\theta,\alpha}\int_{\Delta t}^T r(X_t|\theta)\,\mathrm{d}t|X_{\Delta t}\right]\right] =$$
$$\mathbb{E}_\theta\left[\mathbb{E}_{\Delta X|\theta,\alpha}\left[\underbrace{\mathbb{E}_{\boldsymbol{\theta}}}_{\uparrow\texttt{add this?}\uparrow}\left[\mathbb{E}_{X_{\Delta t}^T|\theta,\alpha}\int_{\Delta t}^T r(X_t|\theta)\,\mathrm{d}t|X_{\Delta t}\right]\right]\right] \tag{15}$$

Because then we could plug in $w(x_0+\Delta X,\Delta t)$ in:

$$\mathbb{E}_\theta\left[\mathbb{E}_{X_{\Delta t}^T|\theta,\alpha}\int_{\Delta t}^T r(X_t|\theta)\,\mathrm{d}t|X_{\Delta t}\right] = w(x_0+\Delta X,\Delta t)$$

And then the rest rolls off easily to get the PDE:

$$\partial_t w(x,t) + \sup_{\alpha(x,t)}\left\{\mathbb{E}_\theta\left[\mathcal{L}^*{}_\theta[w] + r(x|\theta)\right]\right\} = 0 \tag{16}$$

Where $\mathcal{L}^*{}_\theta$ is the generator (backward Kolmogorov operator) corresponding to the SDE eq. (1) for fixed parameters, θ,

$$\mathcal{L}^*{}_\theta[\cdot] = U(x,\alpha;\theta)\partial_x[\cdot] + D\partial_x^2[\cdot]$$

HOWEVER! Can we just put the extra $\mathbb{E}_\theta$ in eq. (15)?

It comes down to what exactly is the meaning of the prior on SDE parameters. Is it that:

1. You choose θ at each time-step (infinitesimally going to 0) let X evolve accordingly for an increment dt and then choose θ again.
   or
2. You choose θ at time 0 and then let X evolve accordingly to this once-and-for-all fixed θ

If it is the former, then we can indeed add the extra expectation wrt. θ in eq. (15) and then use eq. (16) to compute w. If it is the latter, then we cannot.

HOWEVER! Assuming pt.1, i.e. that we re-choose θ at each incremenent, fundamentally violates the basic point of the parameter estimation.

Let me explain.

We suppose that the underlying process X is governed by a single value of θ, we just don't know which. We would like to observe the trajectory of X so as to determine which is the underlying value of θ, but if we rechoose θ at each time-increment of X's evolution, then there is NO single θ and indeed the whole estimation problem is moot.

So adding the inner expectation wrt. θ in eq. (15) is wrong! And solving eq. (16) will not at all help in finding the maximally informative stimulus $\alpha(\cdot)$.

Thus we must try something else!

3.1.2 Maximum Principle with a Prior

Let us go back to the original objective, eq. (9) or equivalently eq. (10)

$$J(\alpha) = \int_\theta \int_0^T \int_X \log\left(\frac{f(x,t|\theta;\alpha(\cdot))}{\int_\theta f(x,t|\theta;\alpha(\cdot))\rho(\theta)\,\mathrm{d}\theta}\right) f(x,t|\theta;\alpha(\cdot))\cdot\rho(\theta)\,\mathrm{d}x\,\mathrm{d}t\,\mathrm{d}\theta$$

J then is a functional of a family of distributions $f(|\theta)$ parametrized by θ.

We will write this as:

$$J(\alpha) = \mathbb{E}_\theta\left[\int_0^T \int_{\Omega_X} r(f(x,t|\theta;\alpha(\cdot)))\cdot f(x,t|\theta;\alpha(\cdot))\,\mathrm{d}x\,\mathrm{d}t\right]$$

Then optimizing J looks a lot like the a generic problem in optimizing over PDEs with the added complexity of the outer expectation (the one wrt. θ).

We now attempt to set up a Pontryagin-Type equation for the optimal value of α: We start by augmenting the objective with the dynamics:

$$J = \mathbb{E}_\theta\left[\int_0^T \int_{\Omega_X} r(f)\cdot f - p\cdot(\partial_t f - \mathcal{L}_{\theta;\alpha}[f])\,\mathrm{d}x\,\mathrm{d}t\right] \tag{17}$$

where $p = p(x,t|\theta;\alpha(\cdot))$ is the adjoint co-state and $\partial_t f - \mathcal{L}_{\theta;\alpha}[f]$ is the Fokker-Planck equation, eq. (4).

What we are going to do is calculate the differential of J wrt. $\alpha(\cdot)$ and then use this in a gradient ascent procedure. First what we would like to do is transfer all the differentials from f to p. That is we will integrate $p\cdot(\partial_t f - \mathcal{L}[f])$ by parts so that only f appears in the expression without any of its derivatives. This is a standard exercise, we show it in detail:

$$\begin{aligned}
&-\int_0^T \int_{\Omega_X} p\cdot(\partial_t f - \mathcal{L}[f])\,\mathrm{d}x\,\mathrm{d}s = \\
&= -\int_0^T \int_{\Omega_X} p\cdot(\partial_t f_0 - D\cdot\partial_x^2 f + \partial_x[U\cdot f]\,\mathrm{d}x\,\mathrm{d}t \quad \text{// what is } \mathcal{L} \\
&= \int_0^T \int_{\Omega_X} \partial_t p f\,\mathrm{d}x\,\mathrm{d}t + \int_{\Omega_X} pf\,\mathrm{d}x\Big|_{t=0}^{T} \quad \text{// the time-derivative pieces} \\
&\quad + \int_0^T \int_{\Omega_X} (D\partial_x^2 p + U\partial_x p)\cdot f\,\mathrm{d}t\,\mathrm{d}x \text{// the space-derivative pieces} \\
&\quad + \int_0^T \Big(pUf - pD\partial_x f + \partial_x pDf\Big|_{x=x_-}^{x_+}\,\mathrm{d}t \text{// the BC terms in 1-d}
\end{aligned}$$

Thus the terminal and boundary conditions of p are chosen given those of f and the objective J. Since there are no boundary or terminal terms contributing to our J, only the boundary conditions for f impact the choice of boundary conditions for p. In particular the following has to be true:

$$\begin{aligned}
pf\Big|_{t=T} &= 0 && \text{Null TCs} \\
pUf - pD\partial_x f + \partial_x pDf\Big|_{x=x_-,x_+} &= 0 && \text{Null BCs}
\end{aligned}$$

This usually implies that $p(T) \equiv 0$, since there are usually no a priori restrictions on f at the terminal time. For the boundary terms, if the forward density has reflecting boundaries such that:

$$Uf - D\partial_x f\Big|_{x=x_-,x_+} = 0$$

then the BC terms for the adjoint are just the simple Neumann BCs:

$$\partial_x p\Big|_{x=x_-,x_+} = 0$$

Once this integration-by-parts is done and the appropriate BCs applied, we can return to the augmented objective, eq. (17) which now looks like:

$$J = \mathbb{E}_\theta\left[\int_0^T \int_{\Omega_X} \log\left(\frac{f_\theta}{\int_\theta f_\theta \cdot \rho(\theta)\,\mathrm{d}\theta}\right) \cdot f_\theta + (\partial_t p_\theta + \mathcal{L}^*{}_{\theta;\alpha}[p_\theta]) \cdot f_\theta \,\mathrm{d}x\,\mathrm{d}t\right] \tag{18}$$

with $\mathcal{L}^*$ the adjoint operator to $\mathcal{L}$.

The next step is to take the differential of J wrt. the control $\alpha(x,t)$

In order to make things simpler, we will write the integral wrt. θ as a sum, i.e.:

$$\int_\Theta f(\theta)\rho(\theta)\,\mathrm{d}\theta = \mathbb{E}_\theta[f(\theta)] = \sum_\theta w_\theta(f(\theta))$$

where the weights w_θ approximate the density $\rho(\theta)$. If one assumes a discrete prior this is just a different way of writing the integral, if the prior is assumed continuous, then this is an approximation. Then J reads like:

$$J = \mathbb{E}_\theta\left[\int_0^T \int_{\Omega_X} \log(f_\theta) \cdot f_\theta - \log(\sum_\theta w_\theta f_\theta) \cdot f_\theta + (\partial_t p_\theta + \mathcal{L}^*{}_{\theta;\alpha}[p_\theta]) \cdot f_\theta \,\mathrm{d}x\,\mathrm{d}t\right]$$

and its differential wrt. α for given x, t is:

$$\begin{aligned}
\delta J|_{x,t} = &\sum_\theta \Big[\frac{\delta f_\theta}{f_\theta} \cdot f_\theta - \frac{w_\theta \delta f_\theta}{\sum_\theta w_\theta f_\theta} \cdot f_\theta + \log\left(\frac{f_\theta}{\sum_\theta w_\theta f_\theta}\right) \cdot \delta f_\theta \\
&+ (\partial_t p_\theta + \mathcal{L}^*{}_{\theta;\alpha} p_\theta) \cdot \delta f_\theta + \delta\alpha \cdot (\partial_x p_\theta \cdot f_\theta)\Big] \\
= &\sum_\theta \left[\left(1 - \frac{w_\theta f_\theta}{\sum_\theta w_\theta f_\theta} + \log\left(\frac{f_\theta}{\sum_\theta w_\theta f_\theta}\right) + (\partial_t p_\theta + \mathcal{L}^*{}_{\theta;\alpha} p_\theta)\right) \cdot \delta f_\theta \right. \\
&\left. + \delta\alpha \cdot (\partial_x p_\theta \cdot f_\theta)\right]
\end{aligned}$$

Now we need to knock out the δf_θ terms so that we are left with only $\delta\alpha$ terms. Thus we set the coeffiecent of δf_θ to zero, which completes the evolution equation for a given p_θ

$$-\partial_t p_\theta = \mathcal{L}^*{}_{\theta;\alpha}[p_\theta] + 1 - \frac{w_\theta f_\theta}{\sum_\theta w_\theta f_\theta} + \log\left(\frac{f_\theta}{\sum_\theta w_\theta f_\theta}\right) \tag{19}$$

And once p_θ, f_θ are solved for, the differential wrt. α comes out to:

$$\frac{\delta J}{\delta \alpha}\Big|_{x,t} = \sum_\theta (\partial_x p_\theta \cdot f_\theta) \tag{20}$$

Equation (20) forms the key ingredient in our gradient search for the most informative perturbation $\alpha^*(x,t) = \arg\max J(\alpha)$.

3.1.3 Stationary Maximum Principle with a Prior

Let us now consider another approach, when we just maximize the Mutual Information between the stationary distribution and the prior.

This ammounts to changing the objective in eq. (9) to

$$J(\alpha) = \int_\theta \int_X \log\left(\frac{f(x|\theta;\alpha(\cdot))}{\int_\theta f(x|\theta;\alpha(\cdot))\rho(\theta)\,\mathrm{d}\theta}\right) f(x|\theta;\alpha(\cdot)) \cdot \rho(\theta)\,\mathrm{d}x\,\mathrm{d}\theta$$

In effect this is a simplified version of section 3.1.2, where we ignore the time evolution of f and focus on its long-term equilibrium.

The calculations are very similar with the exception of $\partial_t f = 0$. We start by augmenting the objective with the dynamics:

$$J = \mathbb{E}_\theta\left[\int_{\Omega_X} r(f)\cdot f + p\cdot \mathcal{L}_{\theta;\alpha}[f]\,\mathrm{d}x\right] \tag{21}$$

where $p = p(x|\theta;\alpha(\cdot))$ is the statinoary adjoint co-state and $\mathcal{L}_{\theta;\alpha}[f]$ is the right hand of the Fokker-Planck equation, eq. (4).

What we are going to do is calculate the differential of J wrt. $\alpha(\cdot)$ and then use this in a gradient ascent procedure. First what we would like to do is transfer all the differentials from f to p. That is we will integrate $p\cdot(\mathcal{L}[f])$ by parts so that only f appears in the expression without any of its derivatives. This is done exactly as before:

$$\begin{aligned}
&\int_{\Omega_X} p\cdot(\mathcal{L}[f])\,\mathrm{d}x = \\
= &\int_{\Omega_X} (\mathcal{L}^*[p])\cdot f\,\mathrm{d}x // \text{ the space-derivative pieces} \\
+ &\int_0^T \Big(pUf - pD\partial_x f + \partial_x pDf\Big|_{x=x_-}^{x_+} // \text{ the BC terms in 1-d}
\end{aligned}$$

Thus we keep the BCs as in the time-dependent section section 3.1.2, and ditch the TCs:

$$pUf - pD\partial_x f + \partial_x pDf\Big|_{x=x_-,x_+} = 0 \qquad \text{Null BCs}$$

Once this integration-by-parts is done and the appropriate BCs applied, we can return to the augmented objective, eq. (17) which now looks like:

$$J = \mathbb{E}_\theta\left[\int_{\Omega_X} \log\left(\frac{f_\theta}{\int_\theta f_\theta\cdot\rho(\theta)\,\mathrm{d}\theta}\right)\cdot f_\theta + (\mathcal{L}^*{}_{\theta;\alpha}[p_\theta])\cdot f_\theta\,\mathrm{d}x\right] \tag{22}$$

Taking the differential of J wrt. the control $\alpha(x,t)$ gives

$$\delta J|_x = \sum_\theta \left[\left(1 - \frac{w_\theta f_\theta}{\sum_\theta w_\theta f_\theta} + \log\left(\frac{f_\theta}{\sum_\theta w_\theta f_\theta}\right) + \mathcal{L}^*{}_{\theta;\alpha} p_\theta\right) \cdot \delta f_\theta \right.$$
$$\left. + \delta\alpha \cdot (\partial_x p_\theta \cdot f_\theta)\right]$$

This gives us the differential equation for the adjoint p

$$0 = \mathcal{L}^*{}_{\theta;\alpha}[p_\theta] + 1 - \frac{w_\theta f_\theta}{\sum_\theta w_\theta f_\theta} + \log\left(\frac{f_\theta}{\sum_\theta w_\theta f_\theta}\right) \tag{23}$$

And once p_θ, f_θ are solved for, the differential wrt. α comes out to:

$$\frac{\delta J}{\delta \alpha}\Big|_x = \sum_\theta (\partial_x p_\theta \cdot f_\theta) \tag{24}$$

Equation (24) forms the key ingredient in our gradient search for the most informative *stationary* perturbation $\alpha^*(x) = \arg\max J(\alpha)$.

4 Illustrative Example - Double Well Potential

4.1 Maximum Principle Approach - Time-Dependent Case

We now follow up the theoretical developments from section 3.1.2 with a concrete example.

Our first test problem will be the problem on estimating the double-well potential barrier height as in Sec. 4 of the latest draft of [3] on arXiv. (From June 7th, 2013). We shall use exactly the same parameter values etc. as in sec. 4 in [3].

We would now like to compute the forward density and the adjoint functions $\{f_\theta, p_\theta\}$ for the double-well problem.

Let's explicitly state the evolution equations for f_θ, p_θ

$$\partial_t f_\theta(x,t;\theta,\alpha(\cdot)) = -\partial_x[U(x;A,\alpha)\cdot f_\theta(x,t)] + D\partial_x^2 f_\theta(x,t)$$
$$\begin{cases} f_\theta(x,0) & = & \delta(x-x_0) & \text{delta function at some } x_0 \\ Uf_\theta - D\partial_x f_\theta\big|_{x=x_-,x_+} & \equiv & 0 & \text{reflecting BCs at some } x_-, x_+ \end{cases} \tag{25}$$

$$-\partial_t p_\theta(x,t) = D\partial_x^2 p_\theta(x,t) + U(x;A,\alpha(x,t))\cdot\partial_x p_\theta(x,t)$$
$$+1 - \frac{w_\theta f_\theta}{\sum_\theta p_{\theta\theta} f_\theta} + \log\left(\frac{f_\theta}{\sum_\theta w_\theta f_\theta}\right) \tag{26}$$
$$\begin{cases} \partial_x p_\theta(x,t)|_{x=x_-,x_+} & = & 0 & \text{BCs} \\ p_\theta(x,T^*) & = & 0 & \text{TCs} \end{cases}$$

where,

$$\begin{aligned}
U(x;A,\alpha) &= -\left(4x^3 - 4x - A\tfrac{x}{c}e^{-(x/c)^2/2}\right) + \alpha(x,t) \\
&= -\nabla_x\left(x^4 - 2x^2 + Ae^{-(x/c)^2/2}\right) + \alpha(x,t) \\
&= -\nabla_x\left(\mathcal{V}(x) + \mathcal{A}(x)\right)
\end{aligned}$$

Having computed f_θ, p_θ, we compute the gradient $\delta J/\delta\alpha$ as

$$\frac{\delta J}{\delta\alpha}|_{x,t} = \sum_\theta w_\theta(\partial_x p_\theta \cdot f_\theta)$$

This just restates eq. (20).

Following [3] (with some deviation in the exact values) we set the parameters as $\sigma = 1. \implies D = 0.5$, (actually it is a little smaller in [3], but this eases the numerics) and $c = 0.3$.

We will use $A = 4$ as the value of A under which the actual process evolves, but that is not important in the computation of the optimal control, α^*. For the prior on A we use a uniform over $[2, 5]$, which we represent with only $N_\theta = 2$ uniform points - $[2.0, 5.0]$. In general it is not clear how to start the forward density (what its ICs should be). For now, let's use a delta mass at $x_0 = 0$, i.e. we assume the process starts at the crest of the barrier. The control is constrained to lie in the set $[-10, 10]$, i.e. $\alpha_{\max} = 10$. The space is constrained to $x \in [-2., 2.]$, i.e. $x_-, x_+ = -2., 2.$, using It is further discretized using $\Delta x = .1$, i.e. with 101 uniform points, $[-5, -4.9 \ldots 5.]$.

Let's first see what happens when we run the solver until $T = 5.$.

The experiment proceeds as follows: For our initial guess we take

$$\alpha_0(x,t) \equiv 0$$

Then we would like to see that

$$\operatorname{sgn}\left(\frac{\delta J}{\delta\alpha}\right)\Big|_{x,t} = -\operatorname{sgn}(x)$$

That is that for negative x we want to drive to the right, $\alpha > 0$ and for positive x we want to drive to the right $\alpha < 0$. Let's see.

The results are visualized in fig. 6. Let's discuss fig. 6. The most important plots are on the right, δJ which indicate how we are supposed to be changing α. It is clear that except for the very beginning $t \approx 0$, and the end $t \approx T$, δJ is essentially constant in time.

Let's focus then on what happens in the bulk of time in the middle. Indeed we have that

$$\operatorname{sgn}\left(\frac{\delta J}{\delta\alpha}\right)\Big|_{x,t} = -\operatorname{sgn}(x)$$

which implies that we should push the particle to the right (resp. left) depending on whether we are to the left (resp. right) of the barrier at $x = 0$. Everything looks good, except for two points.

1. The magnitude of δJ is very small. If we were to take steps of size $s = 1.$, it would take us thousands of iteratons to get to what we expect to be the right solution, i.e. bang-bang at $\alpha_{\max} = 10$.
2. The behaviour of δJ is 'wrong' or 'surprising near the end, $t \approx T$, which appear around $t > 4.75$ and there is also some discrepancies near the beginning, the negative wiggles for $t \approx 0$, which vanish by the time $t > 0.5$

Both issues are minor, but we shall keep them in mind when we go through a full iteration of the gradient descent.

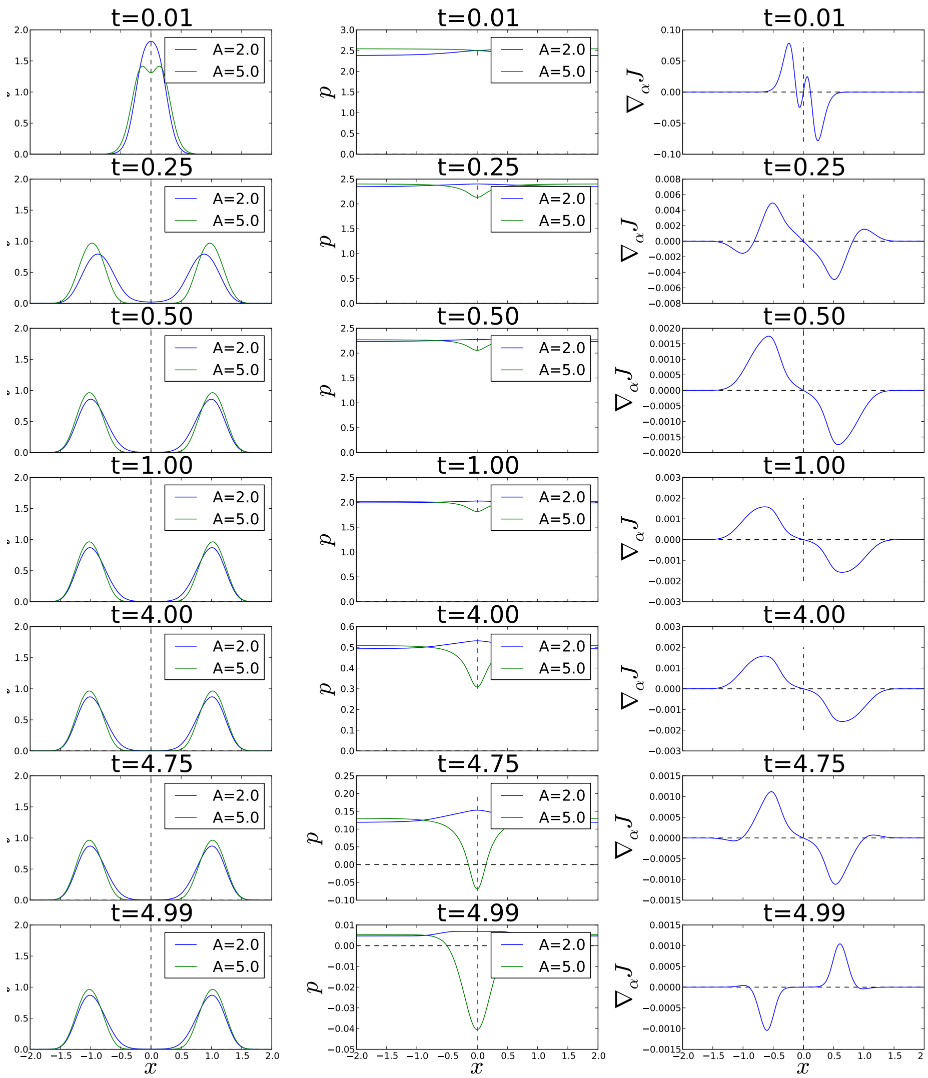

Figure 1: Solution to the test Double Well potential problem using $\alpha \equiv 0$. On the left, the density f, in the middle the adjoint p, on the right the gradient $\delta J/\delta\alpha$, sampled at different times $t = .0, .01, 1.0, \ldots 5.0$

4.1.1 Going through a full gradient descent iteration

We start with the simplest possible approach which is just to push the alpha in the gradient direction K number of times. We see that for $K > 15$, J doesn't change much and so we stop there.

The α_k iterates and the evolution of J are shown in resp.

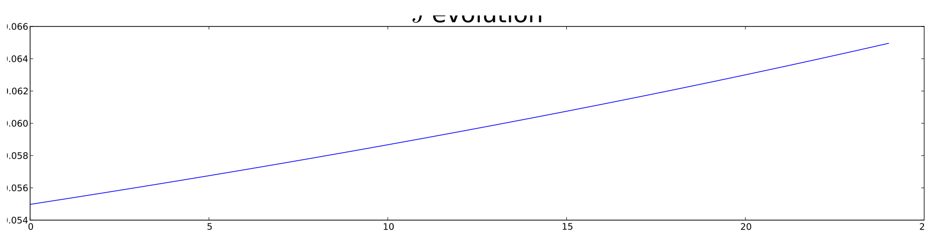

Figure 2: Evolution of J_k during a gradient ascent procedure

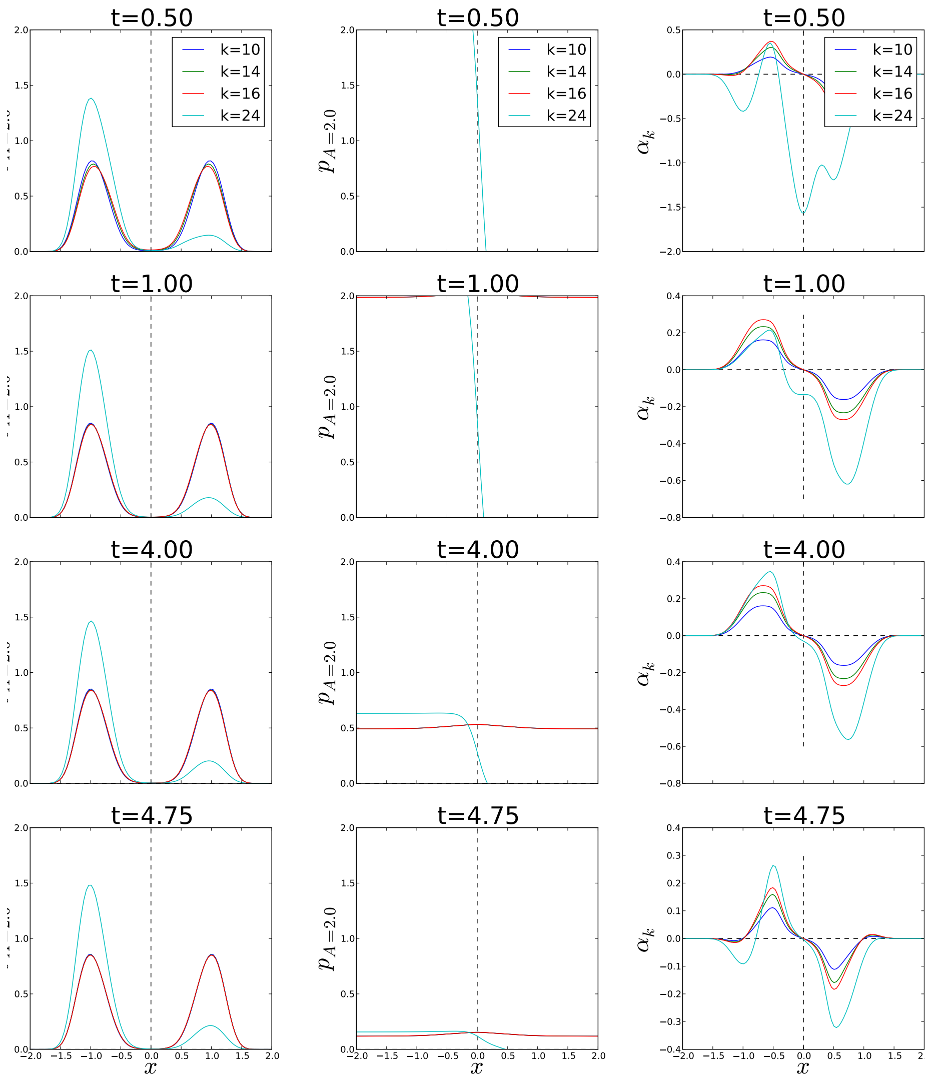

Figure 3: Evolution of α_k during a gradient ascent procedure. On the left we show one of the transition densities f_A and on the right we show the control field for different iterates k in the ascent procedure

4.2 MP Approach - Stationary

Unfortunately, we saw that the gradient ascent procedure used in section 5 had the tendency to converge to something 'wrong' (see fig. 8.

We now try to see whether restricting ourselves to the statinoary case will make things better...

Let's explicitly restate the stationarity equations for f_θ, p_θ

$$\begin{aligned} 0 &= -\partial_x[U(x;A,\alpha)\cdot f(x)] + D\partial_x^2 f(x) \\ \Big\{ \; Uf - D\partial_x f\big|_{x=x_-,x_+} &\equiv 0 \quad \text{reflecting BCs at some } x_-, x_+ \end{aligned} \tag{27}$$

$$\begin{aligned} D\partial_x^2 p_\theta(x) + U(x;A,\alpha(x))\cdot\partial_x p(x) &= -1 + \frac{w_\theta f_\theta}{\sum_\theta w_\theta f_\theta} - \log\left(\frac{f_\theta}{\sum_\theta w_\theta f_\theta}\right) \\ \Big\{ \; \partial_x p_\theta(x,t)|_{x=x_-,x_+} &= 0 \qquad \text{BCs} \end{aligned} \tag{28}$$

Having computed f_θ, p_θ, we compute the gradient $\delta J/\delta\alpha$ as

$$\frac{\delta J}{\delta \alpha}|_x = \sum_\theta w_\theta(\partial_x p_\theta \cdot f_\theta)$$

This just restates eq. (24).

4.2.1 Gradient Ascent for the Stationary-MP

We start by setting our initial guess

$$\alpha_0(x) \equiv 0$$

Again, we would like to see that

$$\operatorname{sgn}\left(\frac{\delta J}{\delta\alpha}\right)\Big|_x = -\operatorname{sgn}(x)$$

That is that for negative x we want to drive to the right, $\alpha > 0$ and for positive x we want to drive to the right $\alpha < 0$. Let's check.

The results are visualized in fig. 4. Let's discuss fig. 4. In general we have the right tendency, but something is obviously wrong.... All these wiggles and stuff. In general we cannot get to the bang-bang solution. At least not using the simple-minded gradient ascent procedure we have implemented so far. Although we do have improvement in the objective, fig. 5 with the ascent procedure, we just can't reach the bang-bang solution.... On the other hand if we were to try the bang-bang solution, we will find that it is much better than the gradient ascent optimal. In fact:

$$J_{\text{bang-bang}} = 0.31 \gg 0.09 = J_{\text{opt}}$$

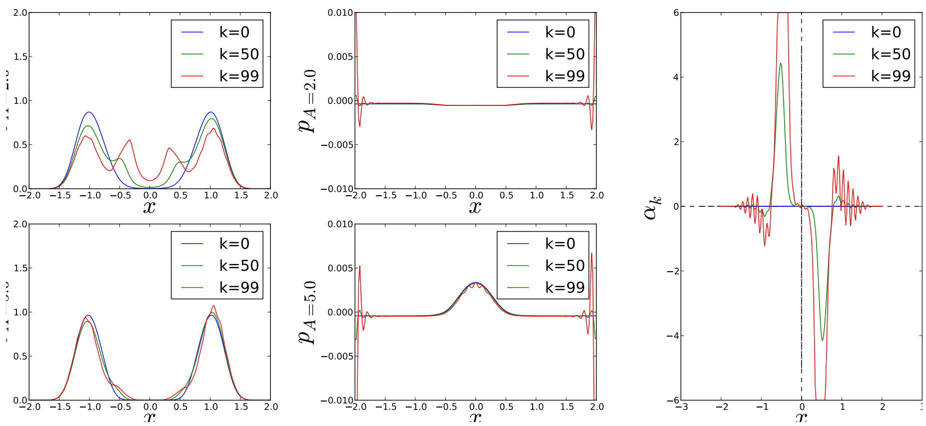

Figure 4: Gradient Ascent for the stationary Double-Well potential problem starting from $\alpha \equiv 0$. On the left, the density $f_\theta(x)$, in the middle the adjoint p_θ, on the right the gradient $\delta J/\delta\alpha$

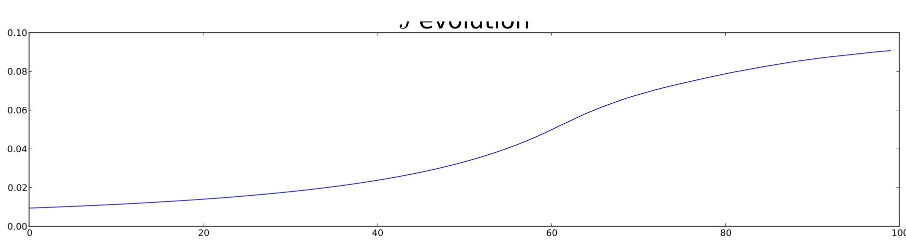

Figure 5: Objective Evolution for the Gradient Ascent for the stationary Double Well potential problem starting from $\alpha \equiv 0$.

4.3 DP appraoch

I DON"T THINK THIS IS FEASBILE - AT LEAST I HAVEN"T FIGURED OUT HOW TO DO IT YET, SEE section 3 for DISCUSSION OF PROBLEMS.

5 Second Illustrative Example - the time-constant for the OU model

We now follow up the theoretical developments from section 3.1.2 with a concrete example.

Our first test problem will be the problem on estimating the double-well potential barrier height as in Sec. 4 of the latest draft of [3] on arXiv. (From June 7th, 2013). We shall use exactly the same parameter values etc. as in sec. 4 in [3].

We would now like to compute the forward density and the adjoint functions $\{f_\theta, p_\theta\}$ for the double-well problem.

Let's explicitly state the evolution equations for f_θ, p_θ

$$\partial_t f_\theta(x,t;\theta,\alpha(\cdot)) = -\partial_x[U(x;A,\alpha)\cdot f_\theta(x,t)] + D\partial_x^2 f_\theta(x,t)$$

$$\left\{\begin{array}{lcll} f_\theta(x,0) & = & \delta(x-x_0) & \text{delta function at some } x_0 \\ Uf_\theta - D\partial_x f_\theta\big|_{x=x_-,x_+} & \equiv & 0 & \text{reflecting BCs at some } x_-, x_+ \end{array}\right. \tag{29}$$

$$\begin{aligned} -\partial_t p_\theta(x,t) &= D\partial_x^2 p_\theta(x,t) + U(x;A,\alpha(x,t))\cdot\partial_x p_\theta(x,t) \\ &\quad +1 - \frac{w_\theta f_\theta}{\sum_\theta p_{\theta\theta} f_\theta} + \log\left(\frac{f_\theta}{\sum_\theta w_\theta f_\theta}\right) \\ &\quad \left\{\begin{array}{lcll} \partial_x p_\theta(x,t)|_{x=x_-,x_+} & = & 0 & \text{BCs} \\ p_\theta(x,T^*) & = & 0 & \text{TCs} \end{array}\right. \end{aligned} \tag{30}$$

where,

$$\begin{aligned} U(x;A,\alpha) &= -\tfrac{1}{\tau_c}(\mu - x) + \alpha(x,t) \\ &= -\nabla_x(\mathcal{V}(x) + \mathcal{A}(x)) \end{aligned}$$

Having computed f_θ, p_θ, we compute the gradient $\delta J/\delta\alpha$ as

$$\frac{\delta J}{\delta \alpha}|_{x,t} = \sum_\theta w_\theta(\partial_x p_\theta \cdot f_\theta)$$

This just restates eq. (20).

For the fixed params we assume $\sigma = 1. \implies D = 0.5$, $\mu = 0$.

For the prior on τ_c we use a uniform over $[10, 40]$, which we represent with only $N_\theta = 2$ uniform points - $[10, 40]$. In general, it is not clear how to start the forward density, i.e., what its ICs should be.

For now, let's use a delta mass at $x_0 = 0$, i.e. we assume the process starts at the crest of the barrier. The control is constrained to lie in the set $[-10, 10]$, i.e. $\alpha_{\max} = 10$. The space is constrained to $x \in [-2., 2.]$, i.e. $x_-, x_+ = -2., 2.$, using It is further discretized using $\Delta x = .1$, i.e. with 101 uniform points, $[-5, -4.9 \ldots 5.]$.

Let's first see what happens when we run the solver until $T = 5.$.

The experiment proceeds as follows: For our initial guess we take

$$\alpha_0(x,t) \equiv 0$$

Then we would like to see that

$$\operatorname{sgn}\left(\frac{\delta J}{\delta \alpha}\right)\Big|_{x,t} = -\operatorname{sgn}(x)$$

That is that for negative x we want to drive to the right, $\alpha > 0$ and for positive x we want to drive to the right $\alpha < 0$. Let's see.

The results are visualized in fig. 6. Let's discuss fig. 6. The most important plots are on the right, δJ which indicate how we are supposed to be changing α. It is clear that except for the very beginning $t \approx 0$, and the end $t \approx T$, δJ is essentially constant in time.

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$$\operatorname{sgn}\left(\frac{\delta J}{\delta \alpha}\right)\Big|_{x,t} = -\operatorname{sgn}(x)$$

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1. The magnitude of δJ is very small. If we were to take steps of size $s = 1.$, it would take us thousands of iteratons to get to what we expect to be the right solution, i.e. bang-bang at $\alpha_{\max} = 10$.
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Both issues are minor, but we shall keep them in mind when we go through a full iteration of the gradient descent.

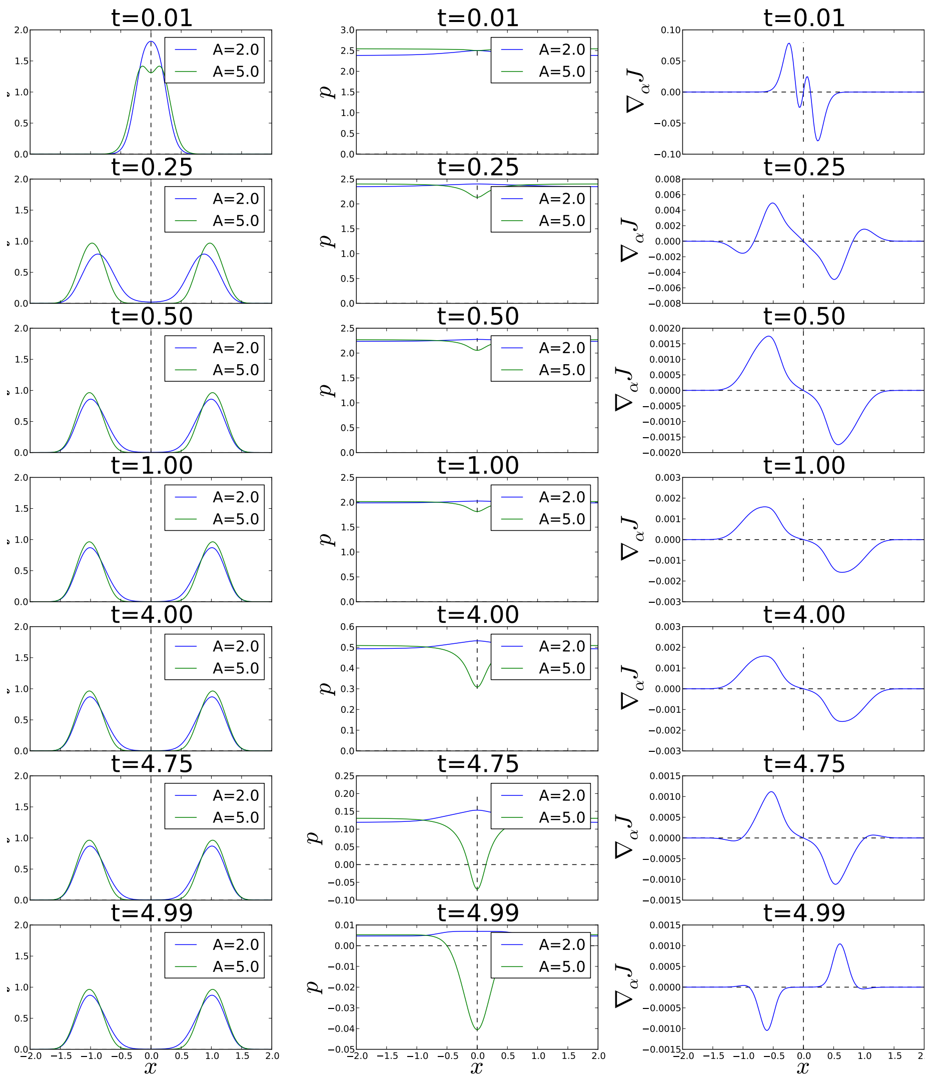

Figure 6: Solution to the test Double Well potential problem using $\alpha \equiv 0$. On the left, the density f, in the middle the adjoint p, on the right the gradient $\delta J/\delta\alpha$, sampled at different times $t = .0, .01, 1.0, \ldots 5.0$

5.0.1 Going through a full gradient descent iteration

We start with the simplest possible approach which is just to push the alpha in the gradient direction K number of times. We see that for $K > 15$, J doesn't change much and so we stop there.

The α_k iterates and the evolution of J are shown in resp.

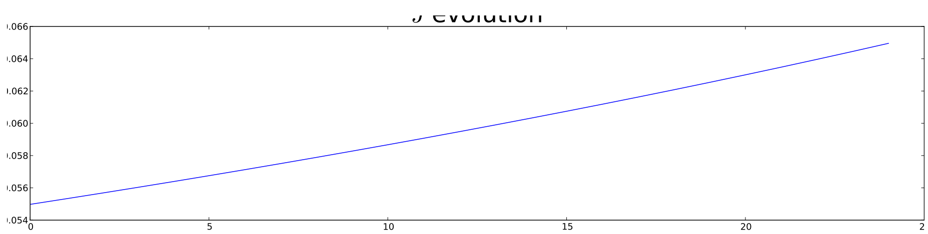

Figure 7: Evolution of J_k during a gradient ascent procedure

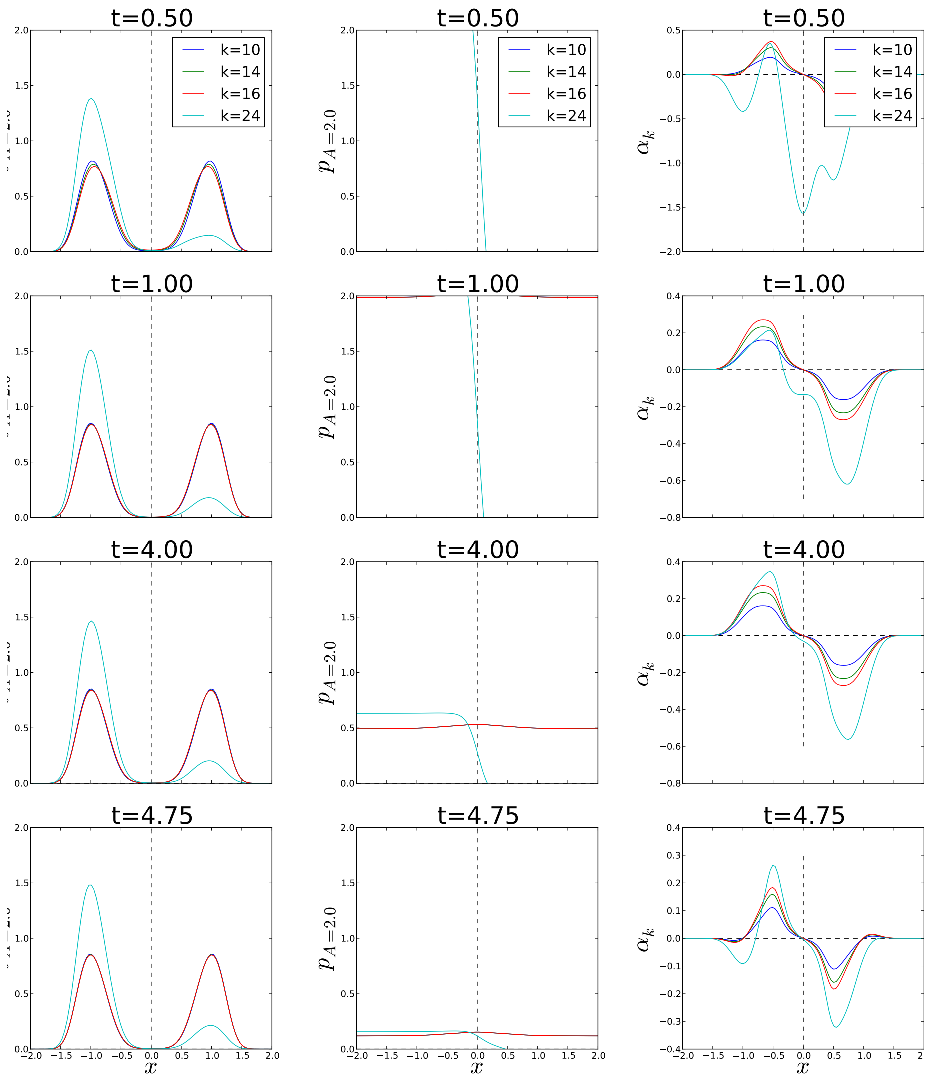

Figure 8: Evolution of α_k during a gradient ascent procedure. On the left we show one of the transition densities f_A and on the right we show the control field for different iterates k in the ascent procedure

A Mutual Info calculation

Here we show why eq. (7) for the Mutual Information agrees with the usual definition of the Mutual Information, which for the two random variables, X, θ is

$$I(X,\theta) = \int_\Theta \int_X p(x,\theta) \cdot \log\left(\frac{p(x,\theta)}{p(x)p(\theta)}\right) \mathrm{d}x\,\mathrm{d}\theta \tag{31}$$

First of all, $p(\theta)$ is just the prior of θ,

$$p(\theta) = \rho(\theta)$$

. The joint distribution is

$$p(x,y) = L(x|\theta)\rho(\theta)$$

, while the x marginal is

$$p(x) = \int_\Theta L(x|\theta)\rho(\theta)\,\mathrm{d}\theta$$

. Plugging the three expressions into the definition in eq. (31) gives:

$$I = \int_\Theta \int_X L(x|\theta)\rho(\theta) \cdot \log\left(\frac{L(x|\theta)\rho(\theta)}{\int_\Theta L(x|\theta)\rho(\theta)\,\mathrm{d}\theta \cdot \rho(\theta)}\right) \mathrm{d}x\,\mathrm{d}\theta. \tag{32}$$

And after canceling $\rho(\theta)$ inside the log, we get eq. (8) which is equivalent to eq. (7).

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[1] Thomas Cover and Joy Thomas. Elements of Information Theory. Wiley-Interscience; 2 edition, 2006 edition, 2006.

[2] Jeremy Lewi, Robert Butera, and Liam Paninski. Sequential optimal design of neurophysiology experiments. Neural computation, 21(3):619–87, March 2009.

[3] Kevin K Lin, Giles Hooker, and Bruce Rogers. Control Theory and Experimental Design in Diffusion Processes. pages 1–23.

[4] David J. C. MacKay. Information Theory, Inference and Learning Algorithms. Cambridge University Press, 2003.

[5] Jay I Myung, Daniel R Cavagnaro, and Mark a Pitt. A Tutorial on Adaptive Design Optimization. Journal of mathematical psychology, 57(3-4):53–67, January 2013.