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Sensitivity analysis in HMMs with application to likelihood maximization

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Abstract
This paper considers a sensitivity analysis in Hidden Markov Models with continuous state and observation spaces. We propose an Infinitesimal Perturbation Analysis (IPA) on the filtering distribution with respect to some parameters of the model. We describe a methodology for using any algorithm that estimates the filtering density, such as Sequential Monte Carlo methods, to design an algorithm that estimates its gradient. The resulting IPA estimator is proven to be asymptotically unbiased, consistent and has computational complexity linear in the number of particles.

We consider an application of this analysis to the problem of identifying unknown parameters of the model given a sequence of observations. We derive an IPA estimator for the gradient of the log-likelihood, which may be used in a gradient method for the purpose of likelihood maximization. We illustrate the method with several numerical experiments.

1 Introduction
We consider a parameterized hidden Markov model (HMM) defined on continuous state and observation spaces. The HMM is defined by a state process \((X_t)_{t \geq 0} \in X\) and an observation process \((Y_t)_{t \geq 1} \in Y\) that are parameterized by a continuous parameter \(\theta = (\theta_1, \ldots, \theta_d) \in \Theta\), where \(\Theta\) is a compact subset of \(\mathbb{R}^d\).

The state process is a Markov chain taking its values in a (measurable) state space \(X\), with initial probability measure \(\mu \in \mathcal{M}(X)\) (i.e. \(X_0 \sim \mu\)) and Markov transition kernel \(K(\theta, x_t, dx_{t+1})\). We assume that we can sample this Markov chain using a transition function \(F\) and independent random numbers, i.e. for all \(t \geq 0\),

\[ X_{t+1} = F(\theta, X_t, U_t), \text{ with } U_t \overset{i.i.d.}{\sim} \nu, \]  

where \(F : \Theta \times X \times U \rightarrow X\) and \((U, \sigma(U), \nu)\) is a probability space. In many practical situations \(U = [0, 1]^p\), \(\nu\) is uniform, thus \(U_t\) is a \(p\)-uple of uniform random numbers. For simplicity, we adopt the notations \(F(\theta, x_{-1}, u) \triangleq F_\mu(\theta, u)\), where \(F_\mu\) is the first transition function (i.e. \(X_0 = F_\mu(\theta, U_{-1})\) with \(U_{-1} \sim \nu\)).

The observation process \((Y_t)_{t \geq 1}\) lies in a (measurable) space \(Y\) and is linked with the state process by the conditional probability measure \(\mathbb{P}(Y_t \in dy_t | X_t = x_t) = g(\theta, x_t, y_t) dy_t\), where \(g : \Theta \times \mathbb{R}^d \rightarrow \mathbb{R}\) is a continuous function.
we are interested in the continuous state case since numerous applications in signal processing, financial, robotics, or telecommunications naturally fit in this framework. In the general setting there exists no closed-form expression of the filtering distribution (unlike in finite spaces where the Viterbi algorithm may apply or in linear-Gaussian models where the Kalman filter can be used). Thus, in this paper, we will make use of the so-called Sequential Monte Carlo methods (SMC) also known as Particle Filters which are numerical tools that can be applied to a large class of models, see e.g. [DFG01]. For illustration, a challenging example in finance is the problem of parameter estimation in the stochastic volatility model, which is a non-linear non-Gaussian continuous space HMM parameterized by three continuous parameters (see e.g. [ME07]) which will be described in the experimental section.

A usual approach for parameter estimation consists in performing a maximum likelihood estimation (MLE), i.e. search for the most likely value of the parameter, given the observed data. For finite state space problems, the Expectation Maximization (EM) algorithm is a popular method for solving the MLE problem. However, in continuous space problems, see [CM05], the EM algorithm is difficult to use mainly because the Expectation part relies on the estimation of the posterior path measure which is intractable in many situations. The Maximization part may also be very complicated and time-consuming when the model does not belong to a linear or exponential family. An alternative method consists in using brute force optimization methods based on the evaluation of the likelihood such as grid-based or simulated annealing methods. These approaches, which can be seen as black-box optimization are not very efficient in high dimensional parameter spaces.
Another approach is to treat the parameter as part of the state variable and then compute the optimal filter (see [DFG01] and [Sto02]). In this case, the Bayesian posterior distribution of the parameter is a marginal of the optimal filter. It is well known that those methods are stable only under certain conditions, see [Pap07], and do not perform well in practice for a large number of time steps.

A last solution consists in using an optimization procedure based on the evaluation of the gradient of the log-likelihood function with respect to the parameter. These approaches have been studied in the field of continuous space HMMs e.g. in [DT03, FLM03, PDS05, Poy06]. The idea was to use a likelihood ratio approach (also called score method) to evaluate the gradient of the likelihood. This approach suffers from high variance of the estimator, in particular for problems with small noise in the dynamic. To tackle this issue, [PDS05] proposed to use a marginal particle filter instead of a simple path-based particle filter as Monte Carlo approximation method. This approach is efficient in terms of variance reduction but its computational complexity becomes quadratic in the number of particles instead of being linear, like in path-based particle methods.

The IPA approach proposed in this paper is an alternative gradient-based maximum likelihood approach. Compared with works on gradient approaches previously cited, the IPA provides usually a lower variance estimators than the likelihood ratio methods, and its numerical complexity is linear in the number of particles.

A work related to ours is the Finite-Difference (FD) approach described in a different setting (i.e. policy gradient in Partially Observable Markov Decision Processes) in [CDM08]. A similar FD estimator could be designed in our setting too but the resulting FD estimator would be biased (like usual FD schemes) whereas the IPA estimator is not.

3 Sequential Monte Carlo methods (SMC)

Given a measurable test function $f : X \rightarrow \mathbb{R}$, we have:

$$
\pi_n(f) \triangleq \mathbb{E}[f(X_n)|Y_{1:n} = y_{1:n}] = \frac{\int f(x_n) \prod_{t=0}^{n} K(x_{t-1}, dx_t) G_t(x_t)}{\int \prod_{t=0}^{n} K(x_{t-1}, dx_t) G_t(x_t)} = \frac{\mathbb{E}[f(X_n) \prod_{t=0}^{n} G_t(X_t)]}{\mathbb{E}[\prod_{t=0}^{n} G_t(X_t)]}.
$$

where we used the simplified notation: $G_t(x_t) \triangleq g(x_t, y_t)$ and $G_0(x_0) \triangleq 1$.

In general, it is impossible to write $\pi_n(f)$ analytically except for specific cases (such as linear/Gaussian with Kalman filtering). In this paper, we consider a numerical approximation of $\pi_n(f)$ based on a SMC method. But it should be mentioned that other methods (such as Extended Kalman filter, quantization methods, Markov Chain Monte Carlo methods) may be used as well to build the IPA estimator that we propose in the next section.

The basic SMC method, called Bootstrap Filter, see [DFG01] for details, approximates $\pi_n(f)$ by an empirical distribution $\pi_n^N(f) \triangleq \frac{1}{N} \sum_{i=1}^{N} f(x^i_n)$ made of $N$ particles $x^i_{1:N}$.

**Algorithm 1** Generic Sequential Monte Carlo

```
for $t = 1$ to $n$
    **Sampling:** Sample $u^i_{t-1} \sim \nu$ and set $\bar{x}^i_t = F(x^i_{t-1}, u^i_{t-1}) \forall i = 1, ..., N$. Then define the importance sampling weights $w^i_t = \frac{G_t(\bar{x}^i_t)}{\sum_{j=1}^{N} G_t(\bar{x}^j_t)} \forall i$.
    **Resampling:** Set $x^i_t = \bar{x}^{k^i_t}_t \forall i$, where $k^i_{1:N}$ are indices selected from the weights $w^i_{1:N}$.
end for
RETURN: $\pi^N_n(f) = \frac{1}{N} \sum_{i=1}^{N} f(x^i_n)$
```

The sampling (or transition) step generates a successor particle population $\bar{x}^i_{1:N}$ according to the state dynamics from the previous population $x^i_{1:N}$. The importance sampling weights $w^i_{1:N}$ are evaluated, and the resampling (or selection) step resamples (with replacement) $N$ particles $x^i_{1:N}$ from the set $\bar{x}^i_{1:N}$ according to the weights $w^i_{1:N}$. Resampling is used to avoid the problem of degeneracy of the algorithm, i.e. that most of the weights decreases to zero. It consists in selecting new particle positions such as to preserve a consistency property (i.e. $\sum_{i=1}^{N} w^i_{1:N} \phi(\bar{x}^i_t) = \mathbb{E}[\frac{1}{N} \sum_{i=1}^{N} \phi(x^i_t)]$).

The simplest version introduced in [GSS93] chooses the selection indices $k^i_{1:N}$ by an independent
sampling from the set $1 : N$ according to a multinomial distribution with parameters $u_{i}^{1:N}$, i.e. $$\mathbb{P}(k_{i}^{t} = j) = u_{i}^{j},$$ for all $1 \leq i \leq N$. The idea is to replicate the particles in proportion to their weights. Many variants have been proposed in the literature, among which the stratified resampling method [Kit96] which is optimal in terms of variance minimization.

Convergence issues of $\pi_{n}^{N}(f)$ to $\pi_{n}(f)$ (e.g. Law of Large Numbers or Central Limit Theorems) are discussed in [Del04] or [DM08]. For our purpose we note that under mild conditions on $f$, $\pi_{n}^{n}(f)$ is an asymptotically unbiased (see [DMDP07] for the asymptotic expression of the bias) and consistent estimator of $\pi_{n}(f)$.

4 Infinitesimal Perturbation Analysis in HMMs

4.1 Sensitivity analysis of the filtering distribution

The following decomposition of the gradient of the filtering distribution $\pi_{n}$ applied to a function $f$:

$$\nabla[\pi_{n}(f)] = \nabla \left[ \frac{\mathbb{E}[f(X_{n}) \prod_{t=0}^{n} G_{t}(X_{t})]}{\mathbb{E}[\prod_{t=0}^{n} G_{t}(X_{t})]} \right] = \frac{\nabla \mathbb{E}[f(X_{n}) \prod_{t=0}^{n} G_{t}(X_{t})]}{\mathbb{E}[\prod_{t=0}^{n} G_{t}(X_{t})]} - \pi_{n}(f) \frac{\nabla \mathbb{E}[\prod_{t=0}^{n} G_{t}(X_{t})]}{\mathbb{E}[\prod_{t=0}^{n} G_{t}(X_{t})]}$$

(3)

shows that the problem of finding an estimator of $\nabla \pi_{n}(f)$ is reduced to the problem of finding an estimator of $\nabla \mathbb{E}[f(X_{n}) \prod_{t=0}^{n} G_{t}(X_{t})]$. There are two dominant infinitesimal methods for estimating the gradient of an expectation in a Markov chain: the Infinitesimal Perturbation Analysis (IPA) method and the Score Function (SF) method (also called likelihood ratio method), see for instance [Gla91] and [Pfl96] for a detailed presentation of both methods. SF has been used in [DT03, FLM03] to estimate $\nabla \pi_{n}$. Although IPA is known for having a lower variance than SF in general, as far as we know, it has never been used in this context. This is therefore the object of this Section.

Under appropriate smoothness assumptions (see Proposition 1 below), the gradient of an expectation over a random variable $X$ is equal to an expectation involving the pair of random variables $(X, \nabla X)$.

$$\nabla \mathbb{E}[f(X)] = \mathbb{E}[\nabla f(X)] = \mathbb{E}[f'(X) \nabla X],$$

(where $'$ refers to the derivative with respect to the state variable). Applying this property to estimate $\nabla \mathbb{E}[f(X_{n}) \prod_{t=0}^{n} G_{t}(X_{t})]$, we deduce

$$\nabla \mathbb{E} \left[ f(X_{n}) \prod_{t=0}^{n} G_{t}(X_{t}) \right] = \mathbb{E} \left[ \nabla f(X_{n}) \prod_{t=0}^{n} G_{t}(X_{t}) \right]$$

$$= \mathbb{E} \left[ \nabla f(X_{n}) + f(X_{n}) \sum_{t=0}^{n} \frac{\nabla G_{t}(X_{t})}{G_{t}(X_{t})} \prod_{t=0}^{n} G_{t}(X_{t}) \right]$$

$$= \mathbb{E} \left[ f'(X_{n}) \nabla X_{n} + f(X_{n}) \sum_{t=0}^{n} \frac{G'_{t}(X_{t}) \nabla X_{t} + \nabla G_{t}(X_{t})}{G_{t}(X_{t})} \prod_{t=0}^{n} G_{t}(X_{t}) \right].$$

(4)

Now we define an augmented Markov chain $(X_{t}, Z_{t}, R_{t})_{t \geq 0}$ by the following recursive relations (where $Z_{t} \triangleq \nabla X_{t}$)

$$\left\{ \begin{array}{ll}
X_{0} &= F_{0}(U_{-1}), \quad U_{-1} \sim \nu \\
Z_{0} &= \nabla F_{0}(U_{-1}), \\
R_{0} &= 0,
\end{array} \right. \quad \forall t \geq 0, \quad \left\{ \begin{array}{ll}
X_{t+1} &= F(X_{t}, U_{t}), \quad \text{where } U_{t} \sim \nu \\
Z_{t+1} &= \nabla F(X_{t}, U_{t}) + f'(X_{t}) U_{t} Z_{t}, \\
R_{t+1} &= R_{t} + G'_{t+1}(X_{t+1}) Z_{t+1} + \nabla G_{t+1}(X_{t+1}),
\end{array} \right.$$

By introducing this augmented Markov Chain in Equation (4) and using Equation (3) we can rewrite $\nabla \pi_{n}(f)$ as:

$$\nabla \pi_{n}(f) = \frac{\mathbb{E}[f'(X_{n}) Z_{n} + f(X_{n}) R_{n} \prod_{t=0}^{n} G_{t}(X_{t})]}{\mathbb{E}[\prod_{t=0}^{n} G_{t}(X_{t})]} - \pi_{n}(f) \frac{\mathbb{E}[R_{n} \prod_{t=0}^{n} G_{t}(X_{t})]}{\mathbb{E}[\prod_{t=0}^{n} G_{t}(X_{t})]}$$

$$= \frac{\mathbb{E}[f'(X_{n}) Z_{n} + R_{n}(f(X_{n}) - \pi_{n}(f)) \prod_{t=0}^{n} G_{t}(X_{t})]}{\mathbb{E}[\prod_{t=0}^{n} G_{t}(X_{t})]}.$$  

(5)

We now state some sufficient conditions under which the previous derivations are sound.
Proposition 1. Equation (5) is valid on $\Theta$ whenever the following conditions are satisfied:

- for all $\theta \in \Theta$, the path $\theta \mapsto (X_0, X_1, \cdots, X_n)(\theta)$ is almost surely (a.s.) differentiable,
- for all $\theta \in \Theta$, $f$ is a.s. continuously differentiable at $X_0(\theta)$, and for all $1 \leq t \leq n$, $G_t$ is a.s. continuously differentiable at $(\theta, X_t(\theta))$.
- $\theta \mapsto f(X_t(\theta))$ and for all $1 \leq t \leq n$, $\theta \mapsto G_t(\theta, X_t(\theta))$ are a.s. continuous and piecewise differentiable throughout $\Theta$.
- Let $D$ be the random subset of $\Theta$ at which $f(X_n(\theta))$ or $G_t(\theta, X_t(\theta))$ fails to be differentiable. We require that $\exists \theta \in D$.
- Equations (5) is valid on $\Theta$.

The proof of this Proposition is a direct application of Theorem 1.2 from [Gla91]. We notice that Proposition 2.

Algorithm 2 IPA estimator of $\nabla \pi_n(f)$ by using a SMC algorithm:

\begin{equation}
I_n^N \triangleq \frac{1}{N} \sum_{i=1}^{N} \left[ f'(x_n^i)z_n^i + f(x_n^i)\left(r_n^i - \frac{1}{N} \sum_{j=1}^{N} r_n^j\right) \right],
\end{equation}

where $(x_n^i, z_n^i, r_n^i)$ are particles derived by using a SMC algorithm on the augmented Markov chain $(X_t, Z_t, R_t)$ described in Algorithm 2.

Proposition 2. Under the assumptions of Proposition 1, the estimator $I_n^N$ defined by (6) is asymptotically unbiased, more precisely the bias $\mathbb{E}[I_n^N] - \nabla \pi_n(f)$ is in $O\left(\frac{1}{N}\right)$, and consistent with $\nabla \pi_n(f)$, i.e. $\lim_{N \to \infty} I_n^N = \nabla \pi_n(f)$ almost surely. In addition, its (asymptotic) variance is $O(N^{-1})$.

Proof. We use the general SMC convergence properties for Feynman-Kac (FK) models (see [Del04] or [DM08]) which, applied to a FK flow with Markov chain $X_{0:n}$, (random) potential functions $G(X_{0:n})$, and test function $H(X_{0:n})$, states that the SMC estimate: $\frac{1}{N} \sum_{i=1}^{N} H(x_{0:n}^i)$ is consistent with $\mathbb{E}[H(X_{0:n}) \prod_{i=0}^{n-1} G(X_t^i)]$. Moreover, an asymptotic expression of the bias, given in [DMDP07], shows that it is of order $O\left(\frac{1}{N}\right)$. Applying those results to the test function $H \triangleq f'(X_n)Z_n + R_n(f(X_n) - \pi_n(f))$, using the representation (5) of the gradient, we deduce that the SMC estimator (6) is asymptotically unbiased and consistent with $\nabla \pi_n(f)$. Now the asymptotic variance is $O(N^{-1})$ since the Central Limit Theorem (see e.g. [Del04, DM08]) applies to the IPA estimator (6) of (5).

Remark 1. Notice that the computation of the gradient estimator requires $O(nNmd)$ (where $m$ is the dimension of $X$) basic operations, which is linear in $N$, and has memory requirement $O(Nmd)$.
4.2 Gradient of the log-likelihood

In the Maximum Likelihood approach for the problem of parameter identification, one may follow a stochastic gradient method for maximizing the log-likelihood $l_n(\theta)$ where the gradient

$$\nabla l_n(\theta) = \sum_{i=1}^{n} \nabla \pi_{t+1|i}(G_{t+1})$$

is obtained by estimating each term $\nabla \pi_{t+1|i}(G_{t+1})$ of the sum using a similar decomposition as in (5) and (4) for the predictive distribution applied to $G_{t+1}$:

$$\nabla \pi_{t+1|i}(G_{t+1}) = \nabla \left[ \frac{E[G_{t+1}(X_{t+1}) \prod_{k=0}^{t} G_k(X_k)]}{E[\prod_{k=0}^{t} G_k(X_k)]} \right]$$

$$= \frac{\nabla E[G_{t+1}(X_{t+1}) \prod_{k=0}^{t} G_k(X_k)]}{E[\prod_{k=0}^{t} G_k(X_k)]} - \pi_{t+1|i}(G_{t+1}) \frac{\nabla E[\prod_{k=0}^{t} G_k(X_k)]}{E[\prod_{k=0}^{t} G_k(X_k)]}$$

with

$$\nabla E[G_{t+1}(X_{t+1}) \prod_{k=0}^{t} G_k(X_k)] = E \left[ (\nabla G_{t+1}(X_{t+1}) + G'_{t+1}(X_{t+1}) \nabla X_{t+1} \right]$$

$$+ G_{t+1}(X_{t+1}) \sum_{k=0}^{t} \frac{G'_k(X_k) \nabla X_k + \nabla G_k(X_k)}{G_k(X_k)} \prod_{k=0}^{t} G_k(X_k) \right].$$

We deduce the IPA estimator of $\nabla l_n(\theta)$

$$J^N_n \triangleq \sum_{i=1}^{n} \sum_{i=1}^{N} \left( \nabla G_{\tilde{x}_i^t} + G'_{\tilde{x}_i^t} \tilde{z}_i^t + G_{\tilde{x}_i^t}(r_{t-1}^i - \frac{1}{N} \sum_j r_{t-1}^j) \right),$$

where $(x^i_n, z^i_n, r^i_n)$ and $(\tilde{x}_i^t, \tilde{z}_i^t, \tilde{r}_i^t)$ are particles derived by using a SMC algorithm on the augmented Markov chain $(X_t, Z_t, R_t)$ described in the previous subsection. Using similar arguments as those detailed in proofs of Propositions 1 and 2, we have that this estimator is asymptotically unbiased and consistent with $\nabla l_n(\theta)$.

The resulting gradient algorithm is described in Algorithm 3. The steps $\gamma_k$ are chosen appropriately so that local convergence occurs (e.g. such that $\sum_{k \geq 1} \gamma_k = \infty$ and $\sum_{k \geq 1} \gamma_k^2 < \infty$), see e.g. [KY97] for a detailed analysis of Stochastic Approximation algorithms.

**Algorithm 3** Likelihood Maximization by gradient ascent using the IPA estimator of $\nabla l_n(\theta)$

```plaintext
for $k = 1, 2, \ldots$, Number of gradient steps do
  Initialize $J^N_0 = 0$
  for $t = 1$ to $n$ do
    Sample $u_{t-1}^{1:N} \overset{IID}{\sim} \nu$ and set $\tilde{x}_i^t = F(x_{t-1}^i, u_{t-1}^i) \forall i = 1, \ldots, N$,
    Set $\tilde{z}_i^t = \nabla F(x_{t-1}^i, u_{t-1}^i) + F'(x_{t-1}^i, u_{t-1}^i) \tilde{z}_{i-1}^t \forall i$,
    Set $J^N_{t} = J^N_{t-1} + \sum_{i=1}^{N} (\nabla G_{\tilde{x}_i^t} + G'_{\tilde{x}_i^t} \tilde{z}_i^t + G_{\tilde{x}_i^t}(r_{t-1}^i - \frac{1}{N} \sum_j r_{t-1}^j))$,
    Set $r_i^t = r_{t-1}^i + \frac{G_{\tilde{x}_i^t} \tilde{z}_i^t + \nabla G_{\tilde{x}_i^t} \tilde{z}_i^t}{G_{\tilde{x}_i^t}}$ and compute the weights $w_i^t = \frac{G_{\tilde{x}_i^t}}{\sum_j G_{\tilde{x}_j^t}} \forall i$,
    Set $(x^t_i, z^t_i, r^t_i) = (\tilde{x}_i^t, \tilde{z}_i^t, \tilde{r}_i^t) \forall i$, where $k_{1:N}$ are indices selected from $u_{t-1}^{1:N}$.
  end for
  Perform a gradient ascent step: $\theta_{k} = \theta_{k-1} + \gamma_k J^N_n(\theta_{k-1})$
end for
```

5 Numerical experiments

We consider two typical problems and report our results focussing on the variance of the estimator:
focused our study on $\sigma$, $\phi$, $\beta$. Figure 1: Box-and-whiskers plots of the three parameters ($\phi$, $\sigma$, $\beta$).

Figure 3 shows the variance of the IP A and Score estimators of the partial derivative

\[ \n \]

exact value (using Kalman).

We observe that in terms of estimation accuracy, IP A is very competitive to the other methods, $\theta = (0, 1, 1)$.

\[ \n \]

estimates of the corresponding estimators of the gradient $\nabla l_0$. $\theta = (0, 1, 1)$.

\[ \n \]

5.2 Variance study for Score and IP A algorithms

IPA and Score methods provide gradient estimators for general models. We compare the variance of the corresponding estimators of the gradient $\nabla l_0$ for the $AR_1$ since for this model we know its exact value (using Kalman).

Figure 3 shows the variance of the IPA and Score estimators of the partial derivative $\partial_\theta l_0$ (we focused our study on $\sigma$ since the problem of volatility estimation is challenging, and also because
the value of $\sigma$ influences the respective performances of the two algorithms, which is not the case for the other parameters $\phi, \beta).$ We used $n = N = 10^3.$ The IPA estimator performs better than the Score estimator for small values of $\sigma.$ On the other hand, in case of huge variance in the state model, it is better to use the Score estimator.

Let us mention that the variance of the IPA (as well as Score) estimator increases when the number of observations $n$ increases. However, under weak conditions on the HMM [LM00], the filtering distribution and its gradient forget exponentially fast the initial distribution. This property has already been used for EM estimators in [CM05] to show that fixed-lag smoothing drastically reduces the variance without significantly raising the bias. Similar smoothing (either fixed-lag or discounted) would provide efficient variance reduction techniques for the IPA estimator as well.

6 Conclusions

We proposed a sensitivity analysis in HMMs based on an Infinitesimal Perturbation Analysis and provided a computationally efficient gradient estimator that provides an interesting alternative to the usual Score method. We showed how this analysis may be used for estimating the gradient of the log-likelihood in a gradient-based likelihood maximization approach for the purpose of parameter identification. Finally let us mention that estimators of higher-order derivatives (e.g. Hessian) could be derived as well along this IPA approach, which would enable to use more sophisticated optimization techniques (e.g. Newton method).
References


