BAYESIAN STATISTICS PROJECT

FRANK-WOLFE BAYESIAN QUADRATURE: PROBABILISTIC INTEGRATION WITH THEORETICAL GUARANTEES

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Notations

We start with some notations we will use along this report.

- For any function, $g(\cdot)$ denotes the function $g : x \mapsto g(x)$.
- In integrals, $\mathrm{d}x$ denote $\mathrm{d}\lambda(x)$, *i.e.* with respect to the Lebesgue measure.

Introduction

The goal of the article [3] is to compute efficiently the integrals of the form $\int_{\mathcal{X}} f(x)p(x)\mathrm{d}x$ where $\mathcal{X} \subseteq \mathbb{R}^d$ is a measurable space, $d \geq 1$ integer representing the dimension of the problem, p a probability density with respect to the Lebesgue measure on $\mathcal{X}$ and $f : \mathcal{X} \to \mathbb{R}$ is a *test*-function.
We will use the common approximation

$$\int_{\mathcal{X}} f(x)p(x)\,\mathrm{d}x \approx \sum_{i=1}^{n} w_i f(x_i) \qquad (1)$$

but of course the real challenge lies in the choice of sequences $\{x_i\}$ and $\{w_i\}$:

• **Monte Carlo** : $w_i = \frac{1}{n}$ and x_i realization of multivariate random variable $X_i \overset{iid}{\sim} X$ where X has $p(\cdot)$ as probability distribution.

• **Quasi-Monte Carlo** :$w_i = \frac{1}{n}$ and x_i are chosen according to a low-discrepancy sequence. The Quasi-Monte Carlo method converges with rate $\mathrm{O}\left(\frac{1}{n}\right)$ whereas the classical Monte Carlo method converges with rate $\mathrm{O}\left(\frac{1}{\sqrt{n}}\right)$.

• **Kernel herding** : the sequences (w_i) and (x_i) are updated according to the following equations : $x_{t+1} = \arg\max_{x\in\chi} \langle w_t, \Phi(x)\rangle$ and $w_{t+1} = w_t + \mathbb{E}_{x\sim p}[\Phi(x)] - \Phi(x_{t+1})$ where $\Phi(\cdot)$ denotes the feature map function from $\mathcal{X}$ to an Hilbert space that we will later introduce. This method has the same rate of convergence than the Quasi-Monte Carlo method.

• **Frank-Wolfe Bayesian Quadrature** :

- $\{w_i\}$ appear naturally in the Bayesian Quadrature by taking the expectation of a posterior distribution (described in section 2),
- $\{x_i\}$ are selected by the Frank-Wolfe algorithm in order to minimize a posterior variance (described in section 3).

The main interest of the method developed in [3] is the super fast *exponential* convergence to the true value of the integral compared to the other methods mentioned above.

Through this report, we will detail every results from [3] with the goal to clarify and explain details that could have been omitted intentionally or not and which, in our view, make the Briol's and al. approach more natural, intuitive and easier to understand.

Lastly, we were able to successfully reproduce all the simulations from [3] with an additional application in pricing of financial derivatives with real worlds dataset. The full code can be found here :

https://github.com/ncloarec/FWBQ_project

1 Background

Let $\mathcal{X} \subseteq \mathbb{R}^d$ be a measurable space, μ a measure on $\mathcal{X}$ such that $p = \frac{\mathrm{d}\mu}{\mathrm{d}\lambda}$ where λ denotes the Lebesgue measure on $\mathcal{X}$, $\mathcal{H} \subset L^2(\mathcal{X}, \mathbb{R}; \mu)$ be an RKHS with a reproducing kernel $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$, Φ its canonical feature map associated. We denote respectively by $\langle \cdot, \cdot \rangle_{\mathcal{H}}$ and $\|\cdot\|_{\mathcal{H}}$ the bigps product and norm induced on $\mathcal{H}$.

Recall that the following relations hold:

$$\forall x \in \mathcal{X}, \quad k(\cdot, x) \in \mathcal{H} \tag{2}$$
$$\forall x \in \mathcal{X}, \forall f \in \mathcal{H}, \quad \langle f, k(\cdot, x)\rangle_{\mathcal{H}} = f(x) \tag{3}$$
$$\forall (x, y) \in \mathcal{X}^2 \quad k(x, y) = \langle \Phi(x), \Phi(y)\rangle_{\mathcal{H}} \tag{4}$$

Let's denote as [3]:

$$p[f] := \int_{\mathcal{X}} f(x) \mathrm{d}\mu(x) = \int_{\mathcal{X}} f(x) p(x) \mathrm{d}x$$
$$\hat{p}[f] := \sum_{i=1}^{n} w_i f(x_i).$$

We will use the *maximum mean discrepancy* (MMD) as our main metric to measure the accuracy of the approximation $p[f] \approx \hat{p}[f]$ in the worst case scenario and which is defined as

$$\mathrm{MMD}\left(\{x_i, w_i\}_{i=1}^n\right) := \sup_{f \in \mathcal{H} : \|f\|_{\mathcal{H}} = 1} |p[f] - \hat{p}[f]|.$$

Let's show (formula 3. in [3]) that MMD can be rewrite as

$$\mathrm{MMD}\left(\{x_i, w_i\}_{i=1}^n\right) = \left\|\mu_p - \mu_{\hat{p}}\right\|_{\mathcal{H}} \tag{5}$$

where $\mu_p(\cdot) = p[\Phi(\cdot)]$ and $\mu_{\hat{p}}(\cdot) = \hat{p}[\Phi(\cdot)]$.

- **For all f in $\mathcal{H}$, we have $p[f] = \langle f, \mu_p\rangle_{\mathcal{H}}$.** By using the dirac delta function, the continuity of the inner product and viewing integral as a limit of a sum, we get

$$\begin{aligned} p[f] &= \int_{\mathcal{X}} f(x) \mathrm{d}\mu(x) \\ &= \int_{\mathcal{X}} \delta_x[f] \mathrm{d}\mu(x) \\ &= \int_{\mathcal{X}} \langle f, \Phi(x)\rangle_{\mathcal{H}} \mathrm{d}\mu(x) \\ &= \left\langle f, \int_{\mathcal{X}} \Phi(x) \mathrm{d}\mu(x)\right\rangle_{\mathcal{H}} \\ &= \langle f, \mu_p\rangle_{\mathcal{H}} \end{aligned}$$

- **For all f in $\mathcal{H}$, we have $\hat{p}[f] = \langle f, \mu_{\hat{p}}\rangle_{\mathcal{H}}$.**

$$\begin{aligned} \hat{p}[f] &= \sum_{i=1}^{n} w_i f(x_i) \\ &= \sum_{i=1}^{n} w_i \delta_{x_i}[f] \\ &= \sum_{i=1}^{n} w_i \langle f, \Phi(x_i)\rangle_{\mathcal{H}} \\ &= \left\langle f, \sum_{i=1}^{n} w_i \Phi(x_i)\right\rangle_{\mathcal{H}} \\ &= \langle f, \mu_{\hat{p}}\rangle_{\mathcal{H}} \end{aligned}$$

- By using previous results and the Cauchy-schwartz inequality, we get :

$$\begin{aligned} \mathrm{MMD}\left(\{x_i, w_i\}_{i=1}^n\right) &= \sup_{f \in \mathcal{H} : \|f\|_{\mathcal{H}} = 1} \left|\langle f, \mu_p - \mu_{\hat{p}}\rangle_{\mathcal{H}}\right| \\ &\leq \sup_{f \in \mathcal{H} : \|f\|_{\mathcal{H}} = 1} \|f\|_{\mathcal{H}} \left\|\mu_p - \mu_{\hat{p}}\right\|_{\mathcal{H}} \\ &= \left\|\mu_p - \mu_{\hat{p}}\right\|_{\mathcal{H}} \end{aligned}$$

with equality if and only if f and $\mu_p - \mu_{\hat{p}}$ are linearly dependent. We deduce the desired result by taking $f = \dfrac{1}{\left\|\mu_p - \mu_{\hat{p}}\right\|_{\mathcal{H}}} \left(\mu_p - \mu_{\hat{p}}\right)$.

2 Bayesian Quadrature

Let's place a functional prior on the integrand f and denote by $(\Omega, \mathcal{F}, \mathbb{P})$ its probability space associated. We will assume that f to be a *centered* **gaussian process** with the kernel k as its covariance function, *i.e.*

$$\forall x \in \mathcal{H}, \quad \mathbb{E} f(x) = 0$$
$$\forall x, y \in \mathcal{H}, \quad \mathrm{Cov}\left[f(x), f(y)\right] = k(x, y)$$

A useful property is that $p[f]$ is a gaussian variable and then completely defined by its second-order statistics:

$$\mathbb{E}\, p[f] = 0 \tag{6}$$
$$\mathbb{V}\, p[f] = \int_{\mathcal{X}^2} k(x, y) \mathrm{d}\mu(x) \mathrm{d}\mu(y) \tag{7}$$

By switching integrals using Fubini's theorem, we get

$$\begin{aligned}\mathbb{E}\,p[f] &= \int_\Omega p[f](w)\,\mathrm{d}\mathbb{P}(w)\\ &= \int_\Omega \int_{\mathcal{X}} f(x,w)\,\mathrm{d}\mu(x)\,\mathrm{d}\mathbb{P}(w)\\ &= \int_{\mathcal{X}} \underbrace{\int_\Omega f(x,w)\,\mathrm{d}\mathbb{P}(w)}_{\mathbb{E}f(x)=0}\,\mathrm{d}\mu(x) = 0\end{aligned}$$

$$\begin{aligned}\mathbb{V}\,p[f] = \mathbb{E}\,p[f]^2 &= \int_\Omega p[f](w)^2\,\mathrm{d}\mathbb{P}(w)\\ &= \int_\Omega \left(\int_{\mathcal{X}} f(x,w)\,\mathrm{d}\mu(x)\right)^2 \mathrm{d}\mathbb{P}(w)\\ &= \int_\Omega \int_{\mathcal{X}^2} f(x,w)f(y,w)\,\mathrm{d}\mu(x)\,\mathrm{d}\mu(y)\,\mathrm{d}\mathbb{P}(w)\\ &= \int_{\mathcal{X}^2} \underbrace{\int_\Omega f(x,w)f(y,w)\,\mathrm{d}\mathbb{P}(w)}_{=\mathrm{Cov}[f(x),f(y)]=k(x,y)}\,\mathrm{d}\mu(x)\,\mathrm{d}\mu(y)\\ &= \int_{\mathcal{X}^2} k(x,y)\,\mathrm{d}\mu(x)\,\mathrm{d}\mu(y)\end{aligned}$$

Assume that samples $\{x_i\}$ and $\{f_i\} := \{f(x_i)\}$ are given for $i = 1$ to n and denote by $K := \big(k(x_i,x_j)\big)_{1\le i,j\le n}$. A natural question arises: how to update the weights $\{w_i\}_{i=1}^n$?

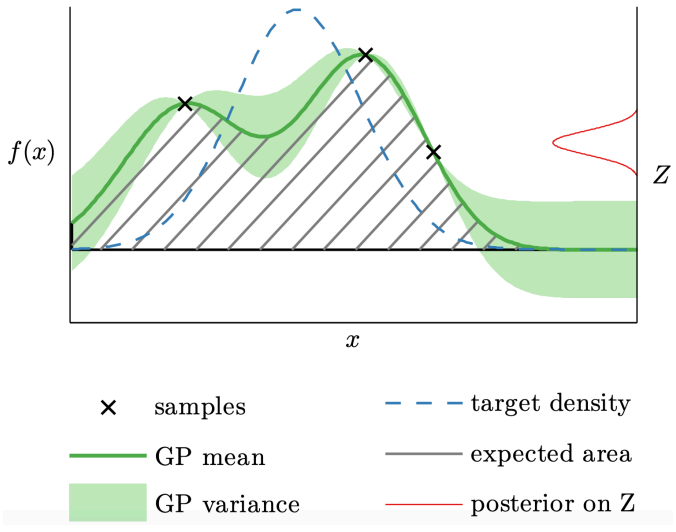


Figure 1: **An illustration of Bayesian Quadrature.** *Source:* [6]

First of all, let's determine the conditional distribution $p[f]|\,\mathbf{f}$ where $\mathbf{f} = (f_1,\dots,f_n)^T$. Since both $p[f]$ and $\mathbf{f}$ are gaussian, we can use the conditional gaussian rule:

[1] formula 4 in [3]

By denoting, $y_1 := p[f]$, $y_2 = \mathbf{f}$, $y = \begin{pmatrix} y_1 \\ y_2 \end{pmatrix}$, $\Sigma = \begin{pmatrix} \Sigma_{1,1}, \Sigma_{1,2} \\ \Sigma_{2,1}, \Sigma_{2,2} \end{pmatrix}$ its covariance matrix by blocks, we have :

$$p[f]|\,\mathbf{f} \sim \mathcal{N}(\mu, \widetilde{\Sigma})$$

where

$$\begin{cases} \mu &= \Sigma_{12}\,\Sigma_{22}^{-1}\,\mathbf{f} \\ \widetilde{\Sigma} &= \Sigma_{11} - \Sigma_{12}\,\Sigma_{22}^{-1}\,\Sigma_{21}. \end{cases}$$

Let's determine what μ and $\widetilde{\Sigma}$ look like in our context.

$$\begin{aligned}\Sigma_{22} &= \big(\mathrm{Cov}\,[f_i,f_j]\big)_{1\le i,j\le n}\\ &= \big(\mathrm{Cov}\,[f(x_i),f(x_j)]\big)_{1\le i,j\le n}\\ &= \big(k(x_i,x_j)\big)_{1\le i,j\le n}\\ &= K\\ \mu &= \begin{pmatrix} \mathrm{Cov}\,[p[f],f_1] \\ \dots \\ \mathrm{Cov}\,[p[f],f_n] \end{pmatrix} K^{-1}\mathbf{f}\end{aligned}$$

Let's rewrite the vector from the left:

$$\begin{aligned}\mathrm{Cov}\,[p[f],f_i] &= \int_\Omega p[f](w)f(x_i,w)\,\mathrm{d}\mathbb{P}(w)\\ &= \int_\Omega \int_{\mathcal{X}} f(x,w)\,\mathrm{d}\mu(x)f(x_i,w)\,\mathrm{d}\mathbb{P}(w)\\ &= \int_{\mathcal{X}} \underbrace{\int_\Omega f(x,w)f(x_i,w)\,\mathrm{d}\mathbb{P}(w)}_{=\mathrm{Cov}[f(x),f(x_i)]=k(x,x_i)}\,\mathrm{d}\mu(x)\\ &= \int_{\mathcal{X}} k(x,x_i)\,\mathrm{d}\mu(x)\\ &= \int_{\mathcal{X}} \Phi(x_i)(x)\,\mathrm{d}\mu(x)\\ &= p[\Phi(x_i)]\\ &= \mu_p(x_i)\end{aligned}$$

By denoting $z := (z_i)_{i=1}^n = \big(\mu_p(x_i)\big)_{i=1}^n \in \mathbb{R}^n$, we get the desired formula[1] for the expectation:

$$\mu = z^T K^{-1}\mathbf{f} \tag{8}$$

The variance is then straightforward :

$$\begin{aligned}\widetilde{\Sigma} &= \mathbb{V}\,p[f] - z^T K^{-1} z \\ &= \int_{\mathcal{X}^2} k(x,y)\,\mathrm{d}\mu(x)\,\mathrm{d}\mu(y) - z^T K^{-1} z\end{aligned}$$

We need to simplify the integral to obtain the desired formula for the variance:

$$\begin{aligned}\int_{\mathcal{X}^2} k(x,y)\,\mathrm{d}\mu(x)\,\mathrm{d}\mu(y) &= \int_{\mathcal{X}}\int_{\mathcal{X}} \Phi(x)(y)\,\mathrm{d}\mu(y)\,\mathrm{d}\mu(x) \\ &= \int_{\mathcal{X}} p[\Phi(x)]\,\mathrm{d}\mu(x) \\ &= \int_{\mathcal{X}} \mu_p(x)\,\mathrm{d}\mu(x) \\ &= p[\mu_p]\end{aligned}$$

which leads us to the desired result:

$$\widetilde{\Sigma} = p[\mu_p] - z^T K^{-1} z$$

Both the conditional expectation and variance are essentials in the FWBQ[2] algorithm:

- $\mu = z^T K^{-1}\mathbf{f}$ which can be written as $\mu = \sum_{i=1}^{n} w_i^{BQ} f_i$ where $w^{BQ} := \left(K^{-1}\right)^T z$. μ appears to be the **most natural estimation of our integral** $p[f]$. It also gives us the **new weights to update**.
- $\widetilde{\Sigma} = p[\mu_p] - z^T K^{-1} z$ which is also equal to $\mathrm{MMD}\left(\{x_i, w_i\}_{i=1}^n\right)^2$ according to [6] and can be interpreted as our **uncertainty**. Therefore we need to **choose** $\{x_i\}$ **which minimize this quantity**. This will be achieved by using the Frank Wolfe algorithm described in the next section.

3 Frank-Wolfe algorithm

Let's J be a convex differentiable real-valued function on a domain $\mathcal{G} \subset \mathcal{H}$ which is supposed to be a compact and convex.
The Frank-Wolfe algorithm [7] proposes a method to solve the following optimization problem :

$$\begin{aligned}&\text{Minimize } \{J(\mathbf{x})\} \\ &\text{subject to } \mathbf{x} \in \mathcal{G}\end{aligned} \tag{9}$$

Let's describe here both the Frank-Wolfe algorithm and its variant with the Line Search :

- **Initialization** $g_1 = \overline{g}_1 \in \mathcal{G}$ and step-size sequence $\{\rho_i\}_{i=1}^n$ (not required in the FWLS algorithm).
- **Iterations** For $i = 2$ to n :
- **Search direction** we replace in (9) J by its first-order Taylor expansion around g_k to solve the following subproblem :

$$\begin{aligned}&\text{minimize } \left\{J(g_{i-1}) + \nabla J(g_{i-1})^{\mathrm{T}}(g - g_{i-1})\right\} \\ &\text{subject to } g \in \mathcal{G}\end{aligned} \tag{10}$$

Let's denote as [3]

$$\overline{g}_i := \arg\min_{g\in\mathcal{G}} \left\langle g, \nabla J(g_{i-1})\right\rangle_{\mathcal{H}} \tag{11}$$

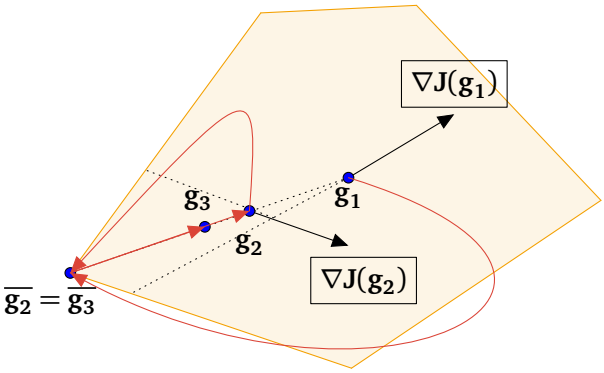
where we have removed in (10) terms independent of the optimization variable.

- **New iteration point** : we choose g_i as a *convex*-combination of g_{i-1} and $\overline{g}_i$.

$$g_i = (1-\rho_i)\,g_{i-1} + \rho_i \overline{g}_i \tag{12}$$

- **FW** ρ_i is determined by the sequence given at the initialization
- **FWLS**

$$\rho_i := \mathrm{argmin}_{\rho\in[0,1]} J\left((1-\rho)g_{i-1} + \rho\overline{g}_i\right)$$



An illustration of the Frank Wolfe algorithm.

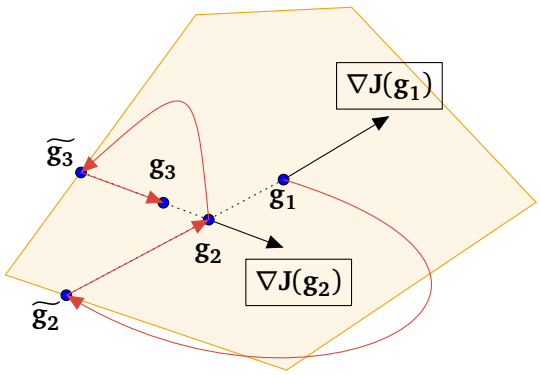
In equation (11), we don't have necessarily $\overline{g}_i \in \mathrm{span}\{\nabla J(g_{i-1})\}$. In fact, we can clearly see in the illustration above that the point

$$\begin{aligned}\widetilde{g}_i &:= \arg\min_{g\in\mathcal{G}\cap\mathrm{span}\{\nabla J(g_{i-1})\}} \left\langle g, \nabla J(g_{i-1})\right\rangle_{\mathcal{H}} \\ &= \arg\min_{\alpha\geq 0} \{-\alpha\nabla J(g_{i-1}) \mid \alpha\nabla J(g_{i-1}) \in \mathcal{G}\}\end{aligned}$$

would not be optimal as

$$\langle \overline{g}_i, \nabla J(g_{i-1})\rangle_{\mathcal{H}} < \langle \widetilde{g}_i, \nabla J(g_{i-1})\rangle_{\mathcal{H}}.$$

[2] Frank-Wolfe Bayesian Quadrature



Comparison with a descent algorithm.

Another important fact of the Frank Wolfe algorithm is that the output g_n can easily be expressed as a linear combination of atoms $\overline{g_i}$.
In fact we have the following formula, which corresponds to the equation (7) in [3]:

For all $n \geq 2$:

$$g_n = \sum_{k=1}^{n} \underbrace{\rho_k \left\{ \prod_{k<i\leq n} (1-\rho_i) \right\}}_{:=w_k^{FW}} \cdot \overline{g_k} = \sum_{k=1}^{n} w_k^{FW} \cdot \overline{g_k} \tag{13}$$

with $\rho_1 = 1$.

The formula in [3] is slightly different :

$$g_n = \sum_{i=1}^{n} \rho_{i-1} \left\{ \prod_{j=i+1}^{n} (1-\rho_{j-1}) \right\} \cdot \overline{g}_i$$

with $\rho_0 = 1$ but clearly doesn't work. In fact according to the algorithm, by taking $n = 2$ we should have :

$$g_2 = (1-\rho_2) \cdot \overline{g_1} + \rho_2 \cdot \overline{g_2}$$

while their formula gives

$$\begin{aligned} g_2 &= \sum_{i=1}^{2} \rho_{i-1} \left\{ \prod_{j=i+1}^{2} (1-\rho_{j-1}) \right\} \overline{g}_i \\ &= (1-\rho_1) \cdot \overline{g_1} + \rho_1 \cdot \overline{g_2}. \end{aligned}$$

Let's prove (13) by induction.

- **Base case** : $n = 2$. Our formula gives :

$$\begin{aligned} g_2 &= \sum_{k=1}^{2} \rho_k \left\{ \prod_{k<i\leq 2} (1-\rho_i) \right\} \cdot \overline{g_k} \\ &= (1-\rho_2) \cdot \overline{g_1} + \rho_2 \cdot \overline{g_2} \end{aligned}$$

as we have set $\rho_1 = 1$, as expected.

- **Step case** : Assume the formula holds for $n-1$ and let's prove it for n. Using the recurrence relation of (12) and our assumption, we have :

$$\begin{aligned} g_n &= (1-\rho_n) \cdot g_{n-1} + \rho_n \cdot \overline{g}_n \\ &= (1-\rho_n) \cdot \sum_{k=1}^{n} \rho_k \left\{ \prod_{k<i\leq n-1} (1-\rho_i) \right\} \cdot \overline{g_k} + \rho_n \cdot \overline{g}_n \\ &= \sum_{k=1}^{n} \rho_k \left\{ \prod_{k<i\leq n} (1-\rho_i) \right\} \cdot \overline{g_k} + \rho_n \cdot \overline{g}_n \\ &= \sum_{k=1}^{n} \rho_k \left\{ \prod_{k<i\leq n} (1-\rho_i) \right\} \cdot \overline{g_k} \end{aligned}$$

which ends the proof.

It is common to take harmonic coefficients in the standard FW algorithm[3] as a choice for $\{\rho_i\} := \left\{\frac{1}{i}\right\}_{i=1}^{n}$, which gives us uniform weights as showed bellow :

$$w_k^{FW} = \frac{1}{k} \left\{ \prod_{k<i\leq n} \left(1 - \frac{1}{i}\right) \right\} = \frac{1}{k} \cdot \frac{k}{n} = \frac{1}{n}.$$

Let's set here the framework of our optimization problem.

We want to approximate the mean element μ_p with a linear combination of elements of the form :

$$\Phi(x) = k(\cdot\,,\, x)\,.$$

In fact, let's say we have:

$$\mu_p \approx \hat{\mu_p} := \sum_{k=1}^{n} w_k \Phi(x_k).$$

Using the reproducing property, we will then have :

$$\hat{p}[f] = \langle f, \mu_p \rangle_{\mathscr{H}} = \sum_{k=1}^{n} w_k f(x_k),$$

which is a quadrature rule.
In order to do this, let's assume that we optimize the following convex function :

$$J(g) := \frac{1}{2} \left\| g - \mu_p \right\|_{\mathscr{H}}^2 \tag{14}$$

on the domain $\mathscr{G} \subseteq \mathscr{H}$ where $\mathscr{G}$ refers to the closure of the convex hull of $\Phi(\mathscr{X})$, which is assumed to be uniformly bounded, *i.e.*

$$\exists R > 0 : \forall x \in \mathscr{X}, \|\Phi(x)\|_{\mathscr{H}} \leq R$$

But a question rises : Why atoms g_i should be of the form $\Phi(x_i)$?
In fact, let's g be a point in the domain. Because of its definition, g can simply be expressed as a convex combination of elements in the feature space $\Phi(\mathscr{X})$, *i.e.* $g = \sum_k \alpha_k \Phi(x_k)$ with $\sum_k \alpha_k = 1$ and thus we have :

[3] Let's remember that in the FWLS algorithm, $\{\rho_i\}$ and thus $\left\{w_k^{FWLS}\right\}$ are determined by the line search step.

$$\begin{aligned}\left\langle g, \nabla J(g_{i-1})\right\rangle_{\mathscr{H}} &= \sum_k \alpha_k \cdot \left\langle \Phi(x_k), \nabla J(g_{i-1})\right\rangle_{\mathscr{H}} \\ &\geq \left(\sum_k \alpha_k\right) \cdot \min_k \left\langle \Phi(x_k), \nabla J(g_{i-1})\right\rangle_{\mathscr{H}} \\ &= \left\langle \Phi(x_{k_0}), \nabla J(g_{i-1})\right\rangle_{\mathscr{H}}\end{aligned}$$

for k_0 such that $k_0 \in \arg\min \left\langle \Phi(x_k), \nabla J(g_{i-1})\right\rangle_{\mathscr{H}}$.

We now understand how can the Frank Wolfe algorithm be useful here : because the minimization of (11) can be restricted at extreme points of the domain, selecting atoms of the form $\Phi(x_k)$ allow us to select interesting points $\{x_k\}$ which are needed for the bayesian quadrature which are solution of the following optimization problem :

$$x_k \in \arg\min_{x\in\mathscr{X}} \left\langle \Phi(x), g_{k-1} - \mu_p\right\rangle_{\mathscr{H}} \tag{15}$$

where $g \in \mathscr{G}$ in the left term of the inner product has been replaced by $\Phi(x) \in \mathscr{G}$ with $x \in \mathscr{X}$.
Therefore, if we denote by $\{w_l\}_{l=1}^{i-1}$ the coefficients in front of $\{\Phi(x_l)\}_{l=1}^{i-1}$ in g_{i-1} and using the reproducing kernel property, we have :

$$\begin{aligned}\left\langle \Phi(x), g_{i-1} - \mu_p\right\rangle_{\mathscr{H}} &= \left\langle \Phi(x), \sum_{l=1}^{i-1} w_l^{(i-1)} \Phi(x_l) - \mu_p \right\rangle_{\mathscr{H}} \\ &= \sum_{l=1}^{i-1} w_l^{(i-1)} k(x, x_l) - \mu_p(x)\end{aligned}$$

which gives an explicit formula for the optimization problem[4] with known quantities. In fact, in the simulations that we have been able to reproduce successfully, the choice of a gaussian kernel k allow us to compute $\mu_p(\cdot)$ easily. See [3] *Appendix C* for more details.

4 The Frank-Wolfe Bayesian Quadrature algorithm

We describe here the final algorithm which is a combination of the two previous ones. At each iteration `i`:

- **Selecting a new x_i** through the Frank Wolfe algorithm with g_{i-1} depending on the BQ weights of the iteration `i-1` and FW design points of all previous iteration `j` with $1 \leq j < i$.

- **Selecting new weights $\left\{w_k^{BQ}\right\}_{k=1}^{i}$** with the bayesian quadrature.

It's important to note that weights at each iteration `i` are used only for the next iteration `i+1` while the design points x_i are used for all iteration `j` with $i < j \leq n$.

5 Consistency

We will establish here the main result of the article [3] and referred as Theorem 1:

The posterior mean $\hat{p}_{\text{FWBQ}}[f]$ converges to the true integral $p[f]$ at the following rates:

$$\begin{aligned}\left|p[f] - \hat{p}_{\text{FWBQ}}[f]\right| &\leq MMD\left(\{x_i, w_i\}_{i=1}^n\right) \\ &\leq \begin{cases} \frac{2D^2}{R} n^{-1} & \text{for FWBQ} \\ \sqrt{2} D \exp\left(-\frac{R^2}{2D^2} n\right) & \text{for FWLSBQ} \end{cases}\end{aligned} \tag{16}$$

where the FWBQ uses step-size $\rho_i = 1/(i+1)$, $D \in (0, \infty)$ is the diameter of the marginal polytope $\mathscr{G}$ and $R \in (0, \infty)$ gives the radius of the **largest**[a] ball of center μ_p included in $\mathscr{G}$.
We will suppose n iterations in the FW algorithm (from $i = 2$ to $n+1$) instead of $n-1$ (from $i = 2$ to n) otherwise one should replace n in the rates above by $n-1$[b].

[a] There was a typo here in [3] as the authors mentioned the radius of the smallest ball which is clearly zero. In fact, greater is the radius and better is the inequality, so of course we are more interested in large radius rather than smaller ones.

[b] It was not necessarily a good idea to initialize the algorithm at $i = 1$ for the authors of [3] while all authors of [1], [2] and [4] have decided to initialize at $i = 0$. Despite that we have decided to keep their notations in order to be consistent with the results in [3].

It was a bit disappointing to see that the authors of [3] did not prove the most interesting part of the theorem, which is the introduction of the diameter of the marginal polytope (D) and the radius of the largest ball of center μ_p (R). Instead, it came out of nowhere quoting [1], which is of course deeply unsatisfactory from a scientific standpoint as it gives no clear understanding about the intuition behind this result.

We were able to find more details about this result in [2] and [4]. We will focus here on the proof of the FWLSBQ's consistency as it is the most difficult one involving few other results and propositions that we will also explore. The proof of the FWBQ's consistency in the case of uniform weights $\left(\rho_i = \frac{1}{i+1}\right)$ can be adapted from [4] proposition 1 when they show with same arguments that we will expose here that $w_n := n \cdot \left(\mu_p - g_n\right)$ is bounded.

[4] We remark that if the optimization problem on $g \in \mathscr{G}$ was a classic convex problem, this is not the case anymore when we perform the optimization on $x \in \mathscr{X}$.

Frank Wolfe Bayesian Quadrature with line search

Let's start assuming as [1] that μ_p is in the relative interior of $\mathscr{G}$:

$$\exists r > 0 \text{ such that } B(\mu_p, r) \subset \mathscr{G}. \tag{17}$$

• **Step 1** We start with a proposition[5] :

> We denote by R the radius of the largest ball of center μ_p. Using the same notations as previously and the assumption above, we have at iteration i:
>
> $$\left\langle \mu_p - g_{i-1}, \mu_p - \overline{g_i} \right\rangle_{\mathscr{H}} + R \left\| \mu_p - g_{i-1} \right\|_{\mathscr{H}} \leq 0 \tag{18}$$

By denoting $d = \mu_p - g_{i-1}$ and using the definition of R we have :

$$g = \mu_p + R \cdot \frac{d}{\|d\|_{\mathscr{H}}} \in \mathscr{G}.$$

Moreover by using the definition of $\overline{g_i}$ we get:

$$\begin{aligned}
\left\langle \mu_p - g_{i-1}, \mu_p - \overline{g_i} \right\rangle_{\mathscr{H}} &= \left\langle -\nabla J(g_{i-1}), \mu_p - \overline{g_i} \right\rangle_{\mathscr{H}} \\
&\leq \left\langle -\nabla J(g_{i-1}), \mu_p - g \right\rangle_{\mathscr{H}} \\
&\leq -R \cdot \left\langle \mu_p - g_{i-1}, \frac{d}{\|d\|_{\mathscr{H}}} \right\rangle_{\mathscr{H}} \\
&\leq -R \|d\|_{\mathscr{H}}
\end{aligned}$$

which is the desired result.

• **Step 2** There is an explicit formula for ρ_i at the i^{th} iteration.

> If we denote by $\rho^\star$ the optimum in the line search at the i^{th} iteration, the following formula holds :
>
> $$\rho^\star = \frac{\left\langle g_{i-1} - \mu_p, g_{i-1} - \overline{g_i} \right\rangle_{\mathscr{H}}}{\|g_{i-1} - \overline{g_i}\|^2_{\mathscr{H}}} \tag{19}$$

We will show here the proof from [2] instead of the one in [3] as it requires less computation and more intuition[6]. Let

$$f : \left| \begin{array}{ccc} [0;1] & \longrightarrow & \mathbb{R} \\ \rho & \longmapsto & J((1-\rho)\, g_{i-1} + \rho \overline{g_i}) \end{array} \right.$$

Because J is quadratic so is f and we can replace f by its quadratic approximation :

$$\begin{aligned}
f(\rho) = J(g_{i-1}) &+ \rho \langle \overline{g_i} - g_{i-1}, \nabla J(g_{i-1}) \rangle \\
&+ \frac{1}{2} \rho^2 \|g_{i-1} - \overline{g_i}\|^2
\end{aligned}$$

Taking the derivative of this expression, gives :

$$\rho^\star = \frac{\left\langle g_{i-1} - \mu_p, g_{i-1} - \overline{g_i} \right\rangle_{\mathscr{H}}}{\|g_{i-1} - \overline{g_i}\|^2_{\mathscr{H}}}.$$

which is the desired result but we need to ensure that $\rho^\star$ is between 0 and 1.
By definition of $\overline{g_i}$:

$$\begin{aligned}
\overline{g}_i = &\arg\min_{g \in \mathscr{G}} \langle g, \nabla J(g_{i-1}) \rangle_{\mathscr{H}} \\
&\arg\min_{g \in \mathscr{G}} \langle g - g_{i-1}, \nabla J(g_{i-1}) \rangle_{\mathscr{H}}
\end{aligned}$$

Because $g_{i-1} \in \mathscr{G}$[7], we have

$$\begin{aligned}
\left\langle \underbrace{g_{i-1} - \mu_p}_{=\nabla J(g_{i-1})}, g_{i-1} - \overline{g_i} \right\rangle_{\mathscr{H}} &\geq \langle \nabla J(g_{i-1}), g_{i-1} - g_{i-1} \rangle_{\mathscr{H}} \\
&\geq 0
\end{aligned}$$

so $\rho^\star \geq 0$. Using (18), we have

$$\left\langle \mu_p - g_{i-1}, \mu_p - \overline{g_i} \right\rangle_{\mathscr{H}} \leq 0. \tag{20}$$

Thus

$$\begin{aligned}
&\left\langle g_{i-1} - \mu_p, g_{i-1} - \overline{g_i} \right\rangle_{\mathscr{H}} \\
&= \left\langle \mu_p - g_{i-1}, (\mu_p - g_{i-1}) - (\mu_p - \overline{g_i}) \right\rangle_{\mathscr{H}} \\
&= \left\| \mu_p - g_{i-1} \right\|^2_{\mathscr{H}} - \left\langle \mu_p - g_{i-1}, \mu_p - \overline{g_i} \right\rangle_{\mathscr{H}} \\
&\leq \left\| \mu_p - g_{i-1} \right\|^2_{\mathscr{H}} - \left\langle \mu_p - g_{i-1}, \mu_p - \overline{g_i} \right\rangle_{\mathscr{H}} \\
&\quad + \left(\left\| \mu_p - \overline{g_i} \right\|^2_{\mathscr{H}} - \underbrace{\left\langle \mu_p - g_{i-1}, \mu_p - \overline{g_i} \right\rangle_{\mathscr{H}}}_{\leq 0} \right) \\
&= \left\| (\mu_p - g_{i-1}) - (\mu_p - \overline{g_i}) \right\|^2_{\mathscr{H}} \\
&= \|g_{i-1} - \overline{g_i}\|^2_{\mathscr{H}}
\end{aligned}$$

which gives us $\rho^\star \leq 1$.

• **Step 3** We show here the linear convergence rate of the algorithm :

> $$\left\| \mu_p - g_i \right\|^2_{\mathscr{H}} \leq \left(1 - q^2\right) \cdot \left\| \mu_p - g_{i-1} \right\|^2_{\mathscr{H}} \tag{21}$$
>
> where $q = \frac{R}{D} > 0$.

Using (12) and the fact that J is equal to its quadratic approximation, we have :

$$\begin{aligned}
\left\| \mu_p - g_i \right\|^2_{\mathscr{H}} = &(\rho^\star)^2 \|\overline{g_i} - g_{i-1}\|^2_{\mathscr{H}} \\
&+ 2\rho^\star \left\langle \mu_p - g_{i-1}, g_{i-1} - \overline{g_i} \right\rangle_{\mathscr{H}} \\
&+ \left\| \mu_p - g_{i-1} \right\|^2_{\mathscr{H}}
\end{aligned}$$

[5] Proposition 3.1 in [2].
[6] the authors of [3] do not give a full proof of this result the most important (showing that $\rho^\star \in [0;1]$).
[7] Remember that g_{i-1} is a convex combination of elements of $\Phi(\mathscr{X})$.

Substituting the value of $\rho^\star$ from step 2 yields to :

$$\begin{aligned}&\left\|\mu_p - g_i\right\|^2_{\mathscr{H}}\\ &= \frac{\left\|\mu_p - g_{i-1}\right\|^2_{\mathscr{H}}\left\|\mu_p - \overline{g_i}\right\|^2_{\mathscr{H}} - \left\langle \mu_p - g_i, \mu_p - \overline{g_i}\right\rangle^2_{\mathscr{H}}}{\left\|\overline{g_i} - g_{i-1}\right\|^2_{\mathscr{H}}}\end{aligned}$$

We will need the two following inequalities in this third step:

$$\left\|\mu_p - \overline{g_i}\right\|^2_{\mathscr{H}} \leq \left\|\overline{g_i} - g_{i-1}\right\|^2_{\mathscr{H}} \tag{22}$$

$$R^2\left\|\mu_p - g_{i-1}\right\|^2_{\mathscr{H}} \leq \left\langle \mu_p - g_{i-1}, \mu_p - \overline{g_i}\right\rangle^2_{\mathscr{H}} \tag{23}$$

The first one can be showed introducing μ_p in the right term and using (20), while the second one comes from (18) and the fact that the square function is decreasing on $\mathbb{R}_-$.
We are now able to prove the result :

$$\begin{aligned}&\left\|\mu_p - g_i\right\|^2_{\mathscr{H}}\\ &= \frac{\left\|\mu_p - g_{i-1}\right\|^2_{\mathscr{H}}\left\|\mu_p - \overline{g_i}\right\|^2_{\mathscr{H}} - \left\langle \mu_p - g_i, \mu_p - \overline{g_i}\right\rangle^2_{\mathscr{H}}}{\left\|\overline{g_i} - g_{i-1}\right\|^2_{\mathscr{H}}}\\ &\leq \frac{\left\|\mu_p - g_{i-1}\right\|^2_{\mathscr{H}}\left\|\mu_p - \overline{g_i}\right\|^2_{\mathscr{H}} - R^2\left\|\mu_p - g_{i-1}\right\|^2_{\mathscr{H}}}{\left\|\overline{g_i} - g_{i-1}\right\|^2_{\mathscr{H}}}\\ &\leq \frac{\left\|\mu_p - g_{i-1}\right\|^2_{\mathscr{H}}\left\|\mu_p - \overline{g_i}\right\|^2_{\mathscr{H}} - R^2\left\|\mu_p - g_{i-1}\right\|^2_{\mathscr{H}}}{\left\|\mu_p - \overline{g_i}\right\|^2_{\mathscr{H}}}\\ &\leq \left(1 - \frac{R^2}{\left\|\mu_p - \overline{g_i}\right\|^2_{\mathscr{H}}}\right)\cdot\left\|\mu_p - g_{i-1}\right\|^2_{\mathscr{H}}\\ &\leq \left(1 - \frac{R^2}{D^2}\right)\cdot\left\|\mu_p - g_{i-1}\right\|^2_{\mathscr{H}}\end{aligned}$$

where the last inequality comes from

$$\left\|\mu_p - \overline{g_i}\right\|_{\mathscr{H}} \leq \sup_{g_1, g_2 \in \mathscr{G}} \|g_1 - g_2\|_{\mathscr{H}} := D$$

• **Step 4** Using the results from step 3 , we will show the following inequality

$$\left\|\mu_p - \mu_{\hat{p}}\right\|^2_{\mathscr{H}} \leq D^2 \cdot \mathrm{e}^{-\frac{R^2 n}{D^2}} \tag{24}$$

Remember that we perfom n iterations, so $\mu_{\hat{p}} = g_{n+1}$. By direct induction and using (21), we have :

$$\begin{aligned}\left\|\mu_p - \mu_{\hat{p}}\right\|^2_{\mathscr{H}} &= \left\|\mu_p - g_{n+1}\right\|^2_{\mathscr{H}}\\ &\leq \left(1 - \frac{R^2}{D^2}\right)^n \cdot \left\|\mu_p - g_1\right\|^2_{\mathscr{H}}\\ &\leq \mathrm{e}^{n\cdot\log\left(1-\frac{R^2}{D^2}\right)}\cdot D^2\\ &\leq D^2 \cdot \mathrm{e}^{-\frac{R^2 n}{D^2}}\end{aligned}$$

where we have used the classic inequality $\log(1+x) \leq x$ for $x > -1$.
• **Step 5** For this last step we show the convergence rate for the FWLSBQ :

$$\left|p[f] - \hat{p}_{\mathrm{FWLSBQ}}[f]\right| \leq \sqrt{2} D \exp\left(-\frac{R^2}{2D^2} n\right) \tag{25}$$

By using the optimality of the weights in bayesian quadrature for $\{x_i\}$ given, we have :

$$\begin{aligned}\mathrm{MMD}\left(\left\{x_i^{\mathrm{FW}}, w_i^{\mathrm{BQ}}\right\}_{i=1}^n\right) &= \inf_{w \in \mathbb{R}^n} \mathrm{MMD}\left(\left\{x_i^{\mathrm{FW}}, w_i\right\}_{i=1}^n\right)\\ &\leq \mathrm{MMD}\left(\left\{x_i^{\mathrm{FW}}, w_i^{\mathrm{FW}}\right\}_{i=1}^n\right).\end{aligned}$$

Using (5) and the previous step, we have :

$$\begin{aligned}\mathrm{MMD}^2\left(\left\{x_i^{\mathrm{FW}}, w_i^{\mathrm{FW}}\right\}_{i=1}^n\right) &= 2 \cdot J(g_{n+1})\\ &\leq 2 \cdot D^2 \cdot e^{-\frac{R^2 n}{D^2}}\end{aligned}$$

Moreover, Cauchy schwartz inequality[8] yields to

$$\left|p[f] - \hat{p}_{\mathrm{FWBQ}}[f]\right| \leq \mathrm{MMD}\left(\left\{x_i^{\mathrm{FW}}, w_i^{\mathrm{BQ}}\right\}_{i=1}^n\right) \underbrace{\|f\|_{\mathscr{H}}}_{\leq 1}$$

which allow us to conclude.

6 Contraction

We expose here the second theorem of [3] which appears to us to be more like a corollary of the previous theorem rather than a whole new result. In fact, its proof requires very little effort compare to the precedent result.

Let $S \subseteq \mathbb{R}$ be an open neighbourhood of the true integral $p[f]$ and let $\gamma = \inf_{r \in S^c} |r - p[f]| > 0$. Then the posterior probability mass on $S^c = \mathbb{R}\backslash S$ vanishes at a rate:

$$\mathrm{prob}\left(S^c\right) \leq \begin{cases} \frac{2\sqrt{2}D^2}{\sqrt{\pi}R\gamma} n^{-1} \exp\left(-\frac{\gamma^2 R^2}{8D^4} n^2\right) \\ \frac{2D}{\sqrt{\pi\gamma}} \exp\left(-\frac{R^2}{2D^2} n - \frac{\gamma^2}{2D^2} \exp\left(\frac{R^2}{2D^2} n\right)\right) \end{cases} \tag{26}$$

for FWBQ and FWLSBQ respectively with the same notations used in theorem 1.

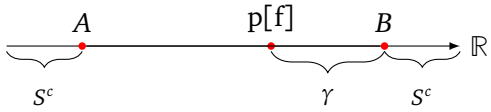


Figure 2: $A := \arg\max_{s \in S^c}\{s \leq p[f]\}$ and $B := \arg\min_{s \in S^c}\{s \geq p[f]\}$ with extremums reached since S^c is closed.

[8] referred as the Koksma Hlawka Inequality in this context. *See Lemma 5 in [4].*

Let's show the following proposition :

Let $\{m_n\} \subset \mathbb{R}$ and $\{\sigma_n\} \subset \mathbb{R}_+^*$ such that :

$$\begin{cases} m_n \to m^\star \\ \sigma_n \to 0 \\ \frac{|m_n - m^\star|}{\sigma_n} = O_{n\to\infty}(1) \end{cases}$$

with $m^\star$ a real number. Let $S \subseteq \mathbb{R}$ be an open neighbourhood of $m^\star$, $\gamma = \inf_{r\in S^c} |r - m^\star| > 0$ and denote by

$$M_n = \int_{S^c} \phi(x|m_n, \sigma_n)\,dx$$

the mass probability of a gaussian random variable on S^c with mean m_n and variance σ_n^2. The following inequality holds :

$$M_n \lesssim \left(\sqrt{2}\sigma_n/\sqrt{\pi}\gamma\right)\exp\left(-\gamma^2/2\sigma_n^2\right) \qquad (27)$$

where $\lesssim$ denotes an inequality which is true asymptotically.

Since

$$S^c \subseteq]-\infty\,; m^\star - \gamma] \cup [m^\star + \gamma\,; +\infty[$$

we have by monotony of integral:

$$\begin{aligned} M_n &\leq \int_{-\infty}^{m^\star-\gamma} \phi(x|m_n,\sigma_n)\,dx + \int_{m^\star+\gamma}^{+\infty} \phi(x|m_n,\sigma_n)\,dx \\ &\leq \underbrace{\Phi\left(\frac{m^\star - m_n}{\sigma_n} - \frac{\gamma}{\sigma_n}\right) + 1 - \Phi\left(\frac{m^\star - m_n}{\sigma_n} + \frac{\gamma}{\sigma_n}\right)}_{:=A_n} \end{aligned}$$

where $\Phi(\cdot)$ denotes the cumulative distribution function of a standard normal distribution. Since $\frac{p[f]-m_n}{\sigma_n}$ is bounded when n goes to infinity and because Φ is continuous over $\mathbb{R}$ we have :

$$\begin{aligned} A_n &\approx \Phi\left(\frac{-\gamma}{\sigma_n}\right) + 1 - \Phi\left(\frac{\gamma}{\sigma_n}\right) \\ &= 2\cdot\Phi\left(\frac{\gamma}{\sigma_n}\right). \end{aligned}$$

Now we need to find an equivalent of $\Phi(x)$ when x goes to infinity. Lets show the following inequality :

For $x > 0$:

$$\frac{1}{x}\left(1 - \frac{1}{x^2}\right)e^{-\frac{x^2}{2}} \leq \int_x^{+\infty} e^{-\frac{t^2}{2}}\,dt \leq \frac{1}{x}e^{-\frac{x^2}{2}} \qquad (28)$$

By integration by parts, we have :

$$\begin{aligned} \int_x^{+\infty} e^{-\frac{t^2}{2}}\,dt &= \int_x^{+\infty} \frac{1}{t}\cdot\left(t\cdot e^{-\frac{t^2}{2}}\right)dt \\ &= \left[-\frac{e^{-\frac{t^2}{2}}}{t}\right]_x^{+\infty} - \int_x^{+\infty} \frac{1}{t^2}\cdot\left(e^{-\frac{t^2}{2}}\right)dt \\ &= \frac{1}{x}\cdot e^{-\frac{x^2}{2}} - \int_x^{+\infty} \frac{1}{t^3}\cdot\left(t\cdot e^{-\frac{t^2}{2}}\right)dt \quad (29) \\ &= \frac{1}{x}\cdot e^{-\frac{x^2}{2}} - \frac{1}{x^3}\cdot e^{-\frac{x^2}{2}} + 3\int_x^{+\infty} \frac{1}{t^4}\cdot e^{-\frac{t^2}{2}}\,dt \\ &= \frac{1}{x}\left(1 - \frac{1}{x^2}\right)\cdot e^{-\frac{x^2}{2}} + 3\int_x^{+\infty} \frac{1}{t^4}\cdot e^{-\frac{t^2}{2}}\,dt. \quad (30) \end{aligned}$$

(29) proves the right inequality while (30) proves the left one. (28) is sufficient to shows that $\int_x^{+\infty} e^{-\frac{t^2}{2}}\,dt \sim \frac{1}{x}e^{-\frac{x^2}{2}}$, *i.e.*

$$A_n \sim 2\frac{1}{\sqrt{2\pi}}\cdot\frac{\sigma_n}{\gamma}e^{-\frac{\gamma^2}{\sigma_n^2}} = \sqrt{\frac{2}{\pi}}\cdot\frac{\sigma_n}{\gamma}e^{-\frac{\gamma^2}{\sigma_n^2}}$$

which concludes the proof of the intermediary proposition.

Substituting $m^\star$ by $p[f]$, m_n by the posterior mean $\hat{p}_{\text{FWBQ}}[f]$ and σ_n by the posterior standard deviation $MMD\left(\{x_i, w_i\}_{i=1}^n\right)$ and using the results from Theorem 1 show the second theorem.

7 Experimental Results

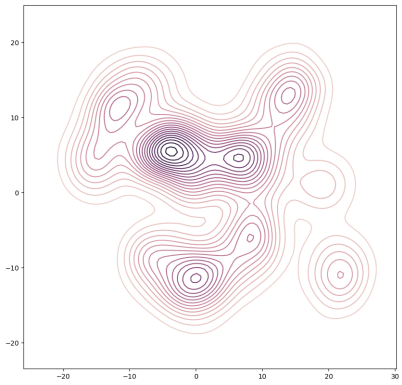
7.1 Overview of the code

We have implemented the following algorithms : – FW and FWBQ (when Line-Search mode is disabled) – FWLS and FWLSBQ (when Line-Search mode is enabled). Two notebooks are available. The first notebook applies the different algorithms to a simulation study. The second notebook is an example of how the algorithms can be used to solve a problem in a specific area.

7.2 Simulation Study

We also used an exponentiated-quadratic (EQ) kernel $k(x,x') := \lambda^2 exp(-\frac{1}{2}\sigma^2\|x - x'\|_2^2)$. EQ kernel is a relevant choice when p is a mixture of gaussians. Moreover, the mean element μ_p has a closed-form expression. In order to replicate the simulation study of the paper, we took p as a mixture of 20 two-dimensional gaussians. Using two dimensions for each gaussians allow us to plot selected points, the function f, the approximation of the mean element g_n and the mean element μ_p so that we can come up with a visual representation of the algorithms.

The following graph is a plot of the bivariate kernel density estimate of the 20 two-dimensional gaussians.



We start with a smooth function f that is the sum of 3 two-dimensional gaussians. Let us notice that the function f intervenes at the end of our algorithm. In other words, we can change f in order to obtain some other values of the integral without having to relaunch everything.

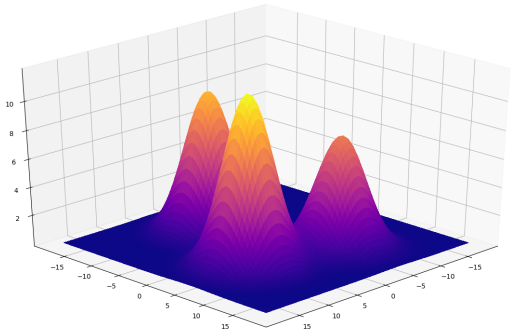


Figure 3: **KDE plot of the mixture of gaussians p.**

The next figures shows the 100 selected points in the FWBQ (FW algorithm) and the FWLSQB (FWLS algorithm) algorithms.

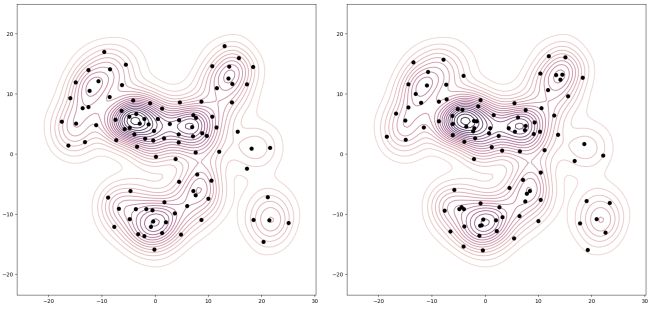


Figure 4: **Points selected by the FW (left) and FWLS (right) algorithm**

It is interesting to visualize what is happening when the point are selected by the FW and the FWLS algorithms throughout the iterations. What is important is how fast the mean element is reconstructed by carefully choosing the points and their weights.

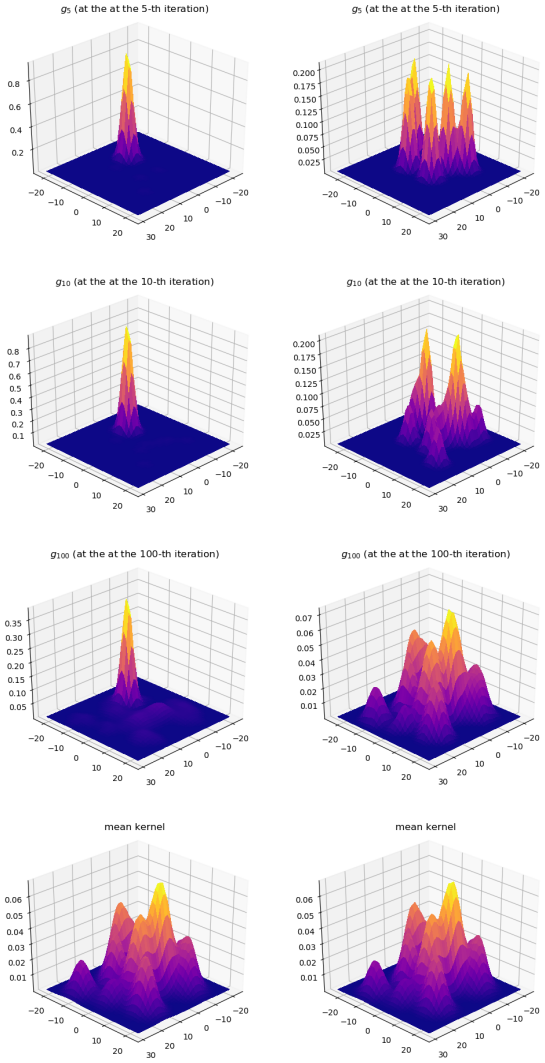


Figure 5: **Convergence towards the mean element of FW algorithm (left) and the FWLS algorithm (right).**

Adding the line-search allows for a much faster convergence towards the mean element. In no more than 50 points, the approximation of the mean element seems to perfectly match the analytically calcultated mean element. We conclude by saying the line-search (which choose the ρ_i) plays a crucial role in the algorithm. We can then compute the value of the integral with a 95% confidence interval.

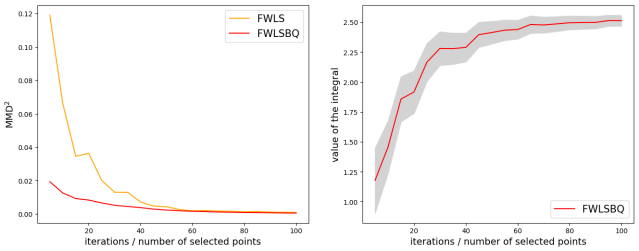


Figure 6: **MMD^2 and the value of the integral for the FWLSBQ algorithm.**

7.3 An example of application

In this section we have implemented from real data the two algorithms FWBQ and FWLSBQ. In order to have a basis of comparison, we have also implemented on our data the Monte Carlo integration. The data used represents the closing price of the shares of Apple, Facebook, Google and Microsoft of 2018. We compute the return of each stock. The return represents the design points of our theory.

We want to calculate the payoff of a basket option :

$$\mathbb{E}_P\Big(f(S(T))\Big) = \int f(s)p(s)ds$$

where for example $f(x) = \max\Big\{\sum_{i=1}^{d} \alpha_{(i)}x_{(i)} - K, 0\Big\}$ with $K = \sum_{i=1}^{d} \alpha_{(i)}S_{(i)}(0)$. The idea is to approximate this expectancy by the one given by FWLSBQ :

$$\mathbb{E}_P\Big(f(S(T))\Big) \simeq \sum_{i=1}^{N} w_{(i)}^{BQ} f(S_{(i)}^{FW}(T)))$$

where the $w_{(i)}^{BQ}$ are the BQ weights and the $S_{(i)}^{FW}(T)$ are the points selected by the FWLS algorithm.
We need a model for the stock prices. The evolution is modelled by the following stochastic differential equation :

$$dS(t) = \mu dS_t + \sigma S_t dB(t)$$

where S is the asset price, μ is the drift, σ is the volatility and B is a Brownian motion[9]. Let r be the risk-free rate. After using Ito's Lemma to get an expression of $d\log S_t$, the solution is given by :

$$S(t) = S(0) \cdot \exp\left\{\left(r - \frac{1}{2}\sigma^2\right) \cdot t + \sigma\sqrt{t} \cdot \mathcal{N}(0,1)\right\}.$$

In the case where we are studying a basket of d assets, $S_{(i)}(t) = S_{(i)}(0) \cdot \exp\left\{(r - \frac{1}{2}\sigma_{(i)}^2)t + \sigma\sqrt{t}W_{(i)}\right\}$ for $i \in \{0, ..., d-1\}$ where the vector $W = (W_{(0)}, ..., W_{(d-1)})$ follows a multivariate normal distribution with mean $MU = (0, ..., 0)$ and with a covariance matrix COR which is in fact the correlation matrix between assets.
The d assets will be d stocks. We first start by estimating the covariance matrix between the $d = 4$ assets (Apple, Facebook, Google and Microsoft) using the close on a 1-year history (year 2018).

We took some arbitrary values for r (5%) and T (10). We launched the FWLSBQ algorithm. We obtained the following results.

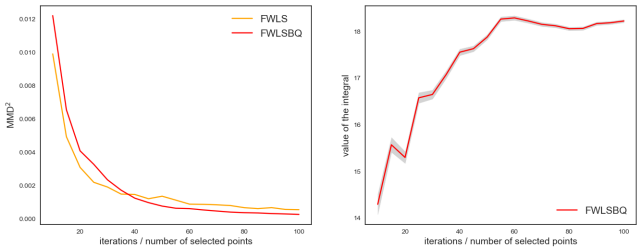


Figure 7: **MMD^2 and the value of the integral for the FWLSBQ algorithm.**

This graph is an exemple of how a real dataset can be used to model a distribution which will be then used to price any payoff given some known parameters such as r and T.

In finance, both giving a fast result and quantifying a result are useful. We used normal distributions to model the returns while we know that financial returns are leptokurtic. Modelling these returns with student distributions for example may be more realistic. However, we will need to use a kernel such that the mean element is analytically tractable.

7.4 Discussion about our implementation

Our implementation is a bit slow. A way to speed the implementation would be to use parallel computing for finding the point (15) at each iteration. For exemple, if we are calculating the value of M points of the space, we can compute X threads each responsible for M/X estimations in order to accelerate the process. Moreover, we believe that the way we keep track of the successive approximations of the mean element g_i can also be improved. We used a dictionnary of functions created by a function returning the convex-combination (with weights $1-\rho_i$ and ρ_i) of the previous function g_{i-1} and the atom $\overline{g_i}$. So, each time, we call a function, successive calculations are made to return a value. The higher the iteration, the longer it takes to return a value.

[9] which can be thought as $dB(t) \sim \mathcal{N}(0, dt)$.

Resources

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