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Monte Carlo Methods

1.1 Monte Carlo methods

Let $\lambda \geq 0$ be a probability density function on $G \subset \mathbb{R}^d$ such that

(1.1)
$$\int_{G} \lambda(\omega)d\omega = 1.$$

For example:

(1.2)
$$\lambda(\omega) = \frac{1}{|G|},$$

if G is bounded. The expectation is defined:

(1.3)
$$\mathbb{E}g := \int_{G} g(\omega) \lambda(\omega) d\omega$$

and for any $h = h(\omega_1, \omega_2, \dots, \omega_n) : G \times G \cdots G \mapsto \mathbb{R}$

$$(1.4) \quad \mathbb{E}_n h := \int_{G \times G \times ... \times G} h(\omega_1, \omega_2, \dots, \omega_n) \lambda(\omega_1) \lambda(\omega_2) \dots \lambda(\omega_n) d\omega_1 d\omega_2 \dots d\omega_n.$$

1.1.1 A basic result

Lemma 1. For any $g \in L^{\infty}(G)$, we have

$$(1.5) \qquad \mathbb{E}_{n}\left(\mathbb{E}g - \frac{1}{n}\sum_{i=1}^{n}g(\omega_{i})\right)^{2} = \begin{cases} \frac{1}{n}\mathbb{E}\left(\left(\mathbb{E}g - g\right)^{2}\right) \leq \frac{1}{n}\sup_{\omega,\omega\in G}|g(\omega) - g(\omega')|^{2} \\ \frac{1}{n}\left(\mathbb{E}(g^{2}) - \left(\mathbb{E}(g)\right)^{2}\right) \leq \frac{1}{n}\mathbb{E}(g^{2}) \leq \frac{1}{n}||g||_{L^{\infty}}^{2}, \end{cases}$$

Proof. First note that

(1.6)
$$\left(\mathbb{E}g - \frac{1}{n} \sum_{i=1}^{n} g(\omega_{i})\right)^{2} = \frac{1}{n^{2}} \left(n\mathbb{E}g - \sum_{i=1}^{n} g(\omega_{i})\right)^{2} = \frac{1}{n^{2}} \left(\sum_{i=1}^{n} (\mathbb{E}g - g(\omega_{i}))\right)^{2}$$
$$= \frac{1}{n^{2}} \sum_{i,j=1}^{n} (\mathbb{E}g - g(\omega_{i}))(\mathbb{E}g - g(\omega_{j}))$$
$$= \frac{I_{1}}{n^{2}} + \frac{I_{2}}{n^{2}}.$$

with

$$(1.7) \ I_1 = \sum_{i=1}^n (\mathbb{E}g - g(\omega_i))^2, \quad I_2 = \sum_{i\neq j}^n ((\mathbb{E}g)^2 - \mathbb{E}(g)(g(\omega_i) + g(\omega_j)) + g(\omega_i)g(\omega_j))).$$

Consider I_1 , for any i,

$$\mathbb{E}_n(\mathbb{E}g - g(\omega_i))^2 = \mathbb{E}_n(\mathbb{E}g - g)^2.$$

Thus,

$$\mathbb{E}_n I_1 = n \mathbb{E}((\mathbb{E}g - g)^2).$$

For I_2 , note that

$$\mathbb{E}_n g(\omega_i) = \mathbb{E}_n g(\omega_i) = \mathbb{E}(g)$$

and, for $i \neq j$,

$$\mathbb{E}_{n}(g(\omega_{i})g(\omega_{j})) = \int_{G\times G\times...\times G} g(\omega_{j})g(\omega_{j})\lambda(\omega_{1})\lambda(\omega_{2})\dots\lambda(\omega_{n})d\omega_{1}d\omega_{2}\dots d\omega_{n}$$

$$= \int_{G\times G} g(\omega_{j})g(\omega_{j})\lambda(\omega_{1})\lambda(\omega_{1})\lambda(\omega_{2})d\omega_{1}d\omega_{2}$$

$$= \mathbb{E}_{n}(g(\omega_{i}))\mathbb{E}_{n}(g(\omega_{j})) = [\mathbb{E}(g)]^{2}.$$

Thus

$$(1.9) \quad \mathbb{E}_n(I_2) = \mathbb{E}_n\left(\sum_{i\neq j}^n ((\mathbb{E}g)^2 - \mathbb{E}(g)(\mathbb{E}(g(\omega_i)) + \mathbb{E}(g(\omega_j))) + \mathbb{E}(g(\omega_i)g(\omega_j)))\right) = 0.$$

Consequently, there exist the following two formulas for $\mathbb{E}_n \left(\mathbb{E}g - \frac{1}{n} \sum_{i=1}^n g(\omega_i) \right)^2$:

(1.10)
$$\mathbb{E}_{n}\left(\mathbb{E}g - \frac{1}{n}\sum_{i=1}^{n}g(\omega_{i})\right)^{2} = \frac{1}{n^{2}}\mathbb{E}_{n}I_{1} = \begin{cases} \frac{1}{n}\mathbb{E}((\mathbb{E}g - g)^{2})\\ \frac{1}{n}(\mathbb{E}(g^{2}) - (\mathbb{E}g)^{2}). \end{cases}$$

Based on the first formula above, since

$$|g(\omega) - \mathbb{E}g| = |\int_G (g(\omega) - g(\tilde{\omega}))\lambda(\tilde{\omega})d\tilde{\omega}| \le \sup_{\omega,\omega \in G} |g(\omega) - g(\omega')|,$$

it holds that

(1.11)
$$\mathbb{E}_n \left(\mathbb{E} g - \frac{1}{n} \sum_{i=1}^n g(\omega_i) \right)^2 \le \frac{1}{n} \sup_{\omega, \omega \in G} |g(\omega) - g(\omega')|^2.$$

Due to the second formula above,

(1.12)
$$\mathbb{E}_{n} \left(\mathbb{E}g - \frac{1}{n} \sum_{i=1}^{n} g(\omega_{i}) \right)^{2} \leq \frac{1}{n} \mathbb{E}(g^{2}) \leq \frac{1}{n} ||g||_{L^{\infty}}^{2}$$

which completes the proof. \Box

Of course, we can use this to prove a high probability result.

Corollary 1. Under the assumptions of the preceding lemma, we have

(1.13)
$$\bar{\mathbb{P}}[(\mathbb{E}g - \frac{1}{n} \sum_{i=1}^{n} g(\omega_i))^2 > \frac{k}{n} ||g||_{L^{\infty}}^2] < \frac{1}{k}$$

Proof.

$$(1.14) \qquad \bar{\mathbb{P}}[(\mathbb{E}g - \frac{1}{n}\sum_{i=1}^n g(\omega_i))^2 > \epsilon] \le \epsilon^{-1}\bar{\mathbb{E}}(\mathbb{E}g - \frac{1}{n}\sum_{i=1}^n g(\omega_i))^2 \le \frac{1}{n\epsilon}\|g\|_{L^\infty}^2.$$

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This corollary implies that the set of ω_i where the estimate $n^{-1} \sum_{i=1}^n g(\omega_i)$ is far from the desired value $\mathbb{E}g$ is small.

The practical usefulness of this algorithm depends upon the existence of a *repeatable* process (for instance some physical process) which *generates* ω *according* to a desired distribution μ .

The precise meaning of this last statement is essentially that the strong law of large numbers holds. Specifically, if $\omega_1, ..., \omega_n, ...$ is a infinite sequence generated by the process, and $A \subset \Omega$ is any a measurable set, then

(1.15)
$$\lim_{n\to\infty} \frac{1}{n} \sum_{i=1}^{n} \chi_A(\omega_i) = \mu(A).$$

Generating n independent samples means generating $\omega_1, ..., \omega_n$ from μ^n according to the above notion. The existence of a realizable process generating samples from a probability distribution, and the practical use of such processes is an interesting topic in the intersection of statistics, physics, and computer science. In addition, statistics/probability theory studies how to take samples from one probability distribution and transform them to samples from another distribution.

1.1.2 Application

Lemma 2. Let

(1.16)
$$f(x) = \int_{G} g(x, \theta) \lambda(\theta) d\theta = \mathbb{E}(g)$$

with $\lambda(\theta) \geq 0$ and $\|\lambda(\theta)\|_{L^1(G)} = 1$. For any $n \geq 1$, there exist $\theta_i^* \in G$ such that

$$||f - f_n||_{L^2(\Omega)}^2 \le \frac{1}{n} \int_G ||g(\cdot, \theta)||_{L^2(\Omega)}^2 \lambda(\theta) d\theta = \frac{1}{n} \mathbb{E}(||g(\cdot, \theta)||_{L^2(\Omega)}^2)$$

where $\|g(\cdot,\theta)\|_{L^2(\Omega)}^2 = \int_{\Omega} [g(x,\theta)]^2 d\mu(x)$, and

$$f_n(x) = \frac{1}{n} \sum_{i=1}^n g(x, \theta_i^*).$$

Proof. Introducing a probability distribution $\lambda(\theta)$,

$$(1.17) f(x) = \mathbb{E}(g).$$

By Lemma 1,

$$\mathbb{E}_n\left(\left(\mathbb{E}(g(x,\cdot)) - \frac{1}{n}\sum_{i=1}^n g(x,\theta_i)\right)^2\right) \le \frac{1}{n}\mathbb{E}(g^2)$$

and

$$\mathbb{E}_n\left(h(\theta_1,\theta_2,\cdots,\theta_n)\right) \leq \frac{1}{n}\mathbb{E}\Big(\int_{\Omega} g^2 d\mu(x)\Big),$$

by taking integral where

$$h(\theta_1, \theta_2, \cdots, \theta_n) = \int_{\Omega} \left(\mathbb{E}(g(x, \cdot)) - \frac{1}{n} \sum_{i=1}^n g(x, \theta_i) \right)^2 d\mu(x).$$

Sine $\mathbb{E}_n(1) = 1$ and $\mathbb{E}_n(h) \leq \frac{1}{n} \mathbb{E} \Big(\int_{\Omega} g^2 d\mu(x) \Big)$, there exists $(\theta_1^*, \theta_2^*, \dots, \theta_n^*) \in G \times G \times \dots \times G$ such that

$$h(\theta_1^*, \theta_2^*, \cdots, \theta_n^*) \leq \frac{1}{n} \int_{\Omega} \mathbb{E}(g^2) d\mu(x).$$

Otherwise, $\mathbb{E}_n(h) > \frac{1}{n} \mathbb{E} \Big(\int_{\Omega} g^2 d\mu(x) \Big)$ if $h(\theta_1, \theta_2, \dots, \theta_n) > \frac{1}{n} \int_{\Omega} \mathbb{E}(g^2) d\mu(x)$. This implies that

$$||f - f_n||_{L^2(\Omega)}^2 \le \frac{1}{n} \int_G ||g(\cdot, \theta)||_{L^2(\Omega)}^2 \lambda(\theta) d\theta,$$

which completes the proof. \Box

We also have a more general version of the above lemma.

Lemma 3. Let

(1.18)
$$f(x) = \int_{G} g(x, \theta) \lambda(\theta) d\theta = \mathbb{E}(g)$$

with $\|\lambda(\theta)\|_{L^1(\Theta)} = 1$. For any $n \ge 1$, there exist $\theta_i^* \in G$ such that

$$||f - f_n||_{H^m(\Omega)}^2 \le \int_G ||g(\cdot, \theta)||_{H^m(\Omega)}^2 \lambda(\theta) d\theta = \frac{1}{n} \mathbb{E}(||g(\cdot, \theta)||_{H^m(\Omega)}^2)$$

where

$$f_n(x) = \frac{1}{n} \sum_{i=1}^n g(x, \theta_i^*)$$

In particular, if

$$(1.19) |D^{\alpha}g(x,\theta)| \le C, \quad \forall x, \theta, |\alpha| \le m$$

Then

$$||f - f_n||_{H^m(\Omega)} \le {m + d \choose m}^{1/2} |\Omega|^{1/2} n^{-1/2}.$$

For any $f(x) = \int_G g(x, \theta) \rho(\theta) d\theta$ with $\|\rho\|_{L^1(\Theta)} \neq 1$. Let $\lambda(\theta) = \frac{\rho(\theta)}{\|\rho\|_{L^1(\Theta)}}$. Thus,

(1.20)
$$f(x) = \|\rho\|_{L^1(\Theta)} \int_G g(x, \theta) \lambda(\theta) d\theta$$

with $\|\lambda(\theta)\|_{L^1(\Theta)} = 1$. We can apply the above two lemmas to the given function f(x).

1.2 Integral representations of functions

1.2.1 Fourier representation

Consider the Fourier transform:

(1.21)
$$\hat{f}(\omega) = \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} e^{-i\omega \cdot x} f(x) dx \quad \forall \omega \in \mathbb{R}^d.$$

We write $\hat{f}(\omega) = e^{i\theta(\omega)}|\hat{f}(\omega)|$. By Fourier inversion formula,

(1.22)
$$f(x) = \int_{\mathbb{R}^d} e^{i\omega \cdot x} \hat{f}(\omega) d\omega = \int_{\mathbb{R}^d} e^{i(\omega \cdot x + \beta(\omega))} |\hat{f}(\omega)| d\omega.$$

Since f(x) is real-valued, it implies that, for x

(1.23)
$$f(x) = \operatorname{Re} \int_{\mathbb{R}^d} e^{i\omega \cdot x} \hat{f}(\omega) d\omega$$
$$= \operatorname{Re} \int_{\mathbb{R}^d} e^{i\omega \cdot x} e^{i\beta(\omega)} |\hat{f}(\omega)| d\omega$$
$$= \int_{\mathbb{R}^d} \cos(\omega \cdot x + \beta(\omega)) |\hat{f}(\omega)| d\omega.$$

Then we have

(1.24)
$$f(x) = \int_{\mathbb{R}^d} k(x, \omega) d\omega,$$

with

(1.25)
$$k(x,\omega) = \cos(\omega \cdot x + \beta(\omega))|\hat{f}(\omega)|$$

and

$$(1.26) |k(x,\omega)| \le |\hat{f}(\omega)| = \rho(\omega).$$

Theorem 1. There exist $\omega_i \in \mathbb{R}^d$, s.t., $G = \mathbb{R}$ and

(1.27)
$$\int_{\Omega} (f(x) - f_n(x))^2 \le \frac{1}{n} \int_{\mathbb{R}^d} |\hat{f}(\omega)| d\omega,$$

where

(1.28)
$$f_n(x) = \frac{\|\hat{f}\|_{L^1}}{n} \sum_{i=1}^n \frac{\cos(\omega_i^* \cdot x + \beta_i^*)}{\rho(\omega_i^*)}.$$

Note that

(1.29)
$$f_n = \sum_{i=1}^n \frac{\cos(\omega_i^* \cdot x + \beta_i^*)}{\rho(\omega_i^*)} \in {}_n\mathbf{N}(\sigma, n),$$

with

(1.30)
$$\sigma(t) = \cos(t).$$

1.2.2 Double Fourier representation

Assume that σ is a locally Riemann integrable function and $\sigma \in L^1(\mathbb{R})$ and thus the Fourier transform of σ is well-defined and continuous. Since σ is non-zero and

(1.31)
$$\hat{\sigma}(\omega) = \frac{1}{2\pi} \int_{\mathbb{R}} \sigma(t) e^{-i\omega t} dt,$$

this implies that $\hat{\sigma}(a) \neq 0$ for some $a \neq 0$. Via a change of variables $t = w \cdot x + b$ and dt = db, this means that for all x and ω , we have

(1.32)
$$0 \neq \hat{\sigma}(a) = \frac{1}{2\pi} \int_{\mathbb{R}} \sigma(\omega \cdot x + b) e^{-ia(\omega \cdot x + b)} db$$
$$= e^{-ia\omega \cdot x} \frac{1}{2\pi} \int_{\mathbb{R}} \sigma(\omega \cdot x + b) e^{-ia + b} db,$$

and so

(1.33)
$$e^{ia\omega \cdot x} = \frac{1}{2\pi\hat{\sigma}(a)} \int_{\mathbb{D}} \sigma(\omega \cdot x + b)e^{-iab}db.$$

Likewise, since the growth condition also implies that $\sigma^{(k)} \in L^1$, we can differentiate the above expression under the integral with respect to x.

This allows us to write the Fourier mode $e^{ia\omega \cdot x}$ as an integral of neuron output functions. We substitute this into the Fourier representation of f (note that the assumption we make implies that $\hat{f} \in L^1$ so this is rigorously justified for a.e. x) to get

(1.34)
$$f(x) = \int_{\mathbb{R}^d} e^{i\omega \cdot x} \hat{f}(\omega) d\omega = \int_{\mathbb{R}^d} \int_{\mathbb{R}} \frac{1}{2\pi \hat{\sigma}(a)} \sigma\left(a^{-1}\omega \cdot x + b\right) \hat{f}(\omega) e^{-iab} db d\omega = \int_{\mathbb{R}^d \times \mathbb{R}} k(x, \theta) d\theta$$

where $\theta = (\omega, b)$ and

$$k(x,\theta) = \frac{1}{2\pi\hat{\sigma}(a)}\sigma(a^{-1}\omega \cdot x + b)\hat{f}(\omega)e^{-iab}.$$

Thus we have

(1.35)
$$|k(x,\theta)| \le \frac{1}{2\pi |\hat{\sigma}(a)|} \max_{x \in \Omega} |\sigma\left(a^{-1}\omega \cdot x + b\right)||\hat{f}(\omega)|,$$
$$\le h(\omega,b)|\hat{f}(\omega)| = \rho(\theta)$$

where

(1.36)
$$h(\omega, b) = \max_{x \in Q} |\sigma(a^{-1}\omega \cdot x + b)|.$$

if we ignore the coefficient. Thus, following the discussion in last section, the next step is to analyze $h(\omega, b)$ which we will discuss in the next section. Before that, let us introduce a special case of the above representation once the activation function is periodic.

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