Stochastic and deterministic algorithms for continuous black-box optimization

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APPENDIX A

Gaussian Distribution

Assume the probability space $(\Omega, \mathscr{F}, \mathbb{P})$ and a measurable space $(\mathbb{R}, \mathscr{B})$, where $\mathscr{B}$ is the Borel algebra on $\mathbb{R}$. A random variable $X : \Omega \to \mathbb{R}$ is said to be normally distributed if and only if its probability distribution $\mathbb{P}_X : \mathscr{B} \to [0, 1]$, defined as a push-forward measure, $\forall B \in \mathscr{B},\ \mathbb{P}_X(B) \coloneqq \mathbb{P}(X^{-1}[B])$, admits the following form:

$$\mathbb{P}_X(B) = \int_B \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(x-m)^2}{2\sigma^2}\right) \mathrm{d}\lambda, \tag{A.1}$$

where λ is the Lebesgue measure on $\mathbb{R}$ and m, σ^2 are the mean and variance of X, respectively. We typically use the notation $X \sim \mathcal{N}(m, \sigma^2)$. This distribution $\mathbb{P}_X$ is called *Gaussian measure* and the notation $\mathcal{G}_{m,\sigma^2}$ is assigned to it. The *cumulative distribution function* (c.d.f.) of X is

$$\Phi_{m,\sigma^2}(x) = \mathcal{G}_{m,\sigma^2}\left(\{X \in \mathbb{R} \ : \ X \leq x\}\right).$$

In addition, the *probability density function* (p.d.f.) of X is the Radon-Nikodym derivative of $\mathcal{G}_{m,\sigma^2}$ w.r.t. λ:

$$\phi_{m,\sigma^2}(x) = \frac{\mathrm{d}\mathcal{G}_{m,\sigma^2}}{\mathrm{d}\lambda} = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(x-m)^2}{2\sigma^2}\right), \tag{A.2}$$

that is, by definition, the integrand in Eq. (A.1). In the multivariate case, consider the measurable space $(\mathbb{R}^n, \mathscr{B}^n)$ where $\mathscr{B}^n$ is the Borel algebra on $\mathbb{R}^n$. A random vector $\mathbf{x} = (X_1, X_2, \ldots, X_n)^\top : \Omega \to \mathbb{R}^n$ is said to follow the multivariate Gaussian distribution, if and only if any linear combination $\mathbf{c}^\top\mathbf{x},\ \mathbf{c} \in \mathbb{R}^n$ admits the distribution as in Eq. (A.1). In addition, the distribution of $\mathbf{x}$ is

$$\forall B \in \mathscr{B}^n,\ \mathcal{G}^n_{\mathbf{m},\mathbf{K}}(B) = \int_B (2\pi)^{-\frac{n}{2}} \det(\mathbf{K})^{\frac{1}{2}} \exp\left(-\frac{1}{2}(\mathbf{y}-\mathbf{m})^\top \mathbf{K}^{-1}(\mathbf{y}-\mathbf{m})\right) \mathrm{d}\lambda^n,$$

where λ^n is the n-dimensional Lebesgue measure on $(\mathbb{R}^n, \mathscr{B}^n)$ and $\mathbf{m}, \mathbf{K}$ are the mean and covariance matrix of $\mathbf{x}$. As with the univariate case, we shall take the notation $\mathbf{x} \sim \boldsymbol{\mathcal{N}}(\mathbf{m}, \mathbf{K})$ and its cumulative distribution function is,

$$\Phi^n_{\mathbf{m},\mathbf{K}}(\boldsymbol{\zeta}) = \mathscr{G}^n_{\mathbf{m},\mathbf{K}}\left(\{\mathbf{x} \in \mathbb{R}^n \ : \ \mathbf{x} \leq \boldsymbol{\zeta}\}\right).$$

Given an arbitrary partition on $\mathbf{x} = (\mathbf{x}_1^\top, \mathbf{x}_2^\top)^\top$, in which $\mathbf{x}_1$, $\mathbf{x}_2$ have n_1 and n_2 components, respectively. The distribution of $\mathbf{x}$ can be re-written as

$$\begin{bmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \end{bmatrix} \sim \boldsymbol{\mathcal{N}}\left(\begin{bmatrix} \mathbf{m}_1 \\ \mathbf{m}_2 \end{bmatrix}, \begin{bmatrix} \mathbf{K}_{11} & \mathbf{K}_{12} \\ \mathbf{K}_{21} & \mathbf{K}_{22} \end{bmatrix} \right),$$

where all sub-mean vectors and sub-covariance matrices are obtained by applying the same partition on $\mathbf{m}$ and $\mathbf{K}$. The *marginal distribution* of $\mathbf{x}_1$ is Gaussian:

$$\mathbf{x}_1 \sim \boldsymbol{\mathcal{N}}\left(\mathbf{m}_1, \mathbf{K}_{11}\right). \tag{A.3}$$

The result holds for $\mathbf{x}_2$ in the same manner. In addition, the *conditional distribution* of $\mathbf{x}_1$ on $\mathbf{x}_2 = \mathbf{v}$ is Gaussian (Tong, 2012):

$$\mathbf{x}_1 \mid \mathbf{x}_2 = \mathbf{v} \sim \boldsymbol{\mathcal{N}}\left(\mathbf{m}_1 + \mathbf{K}_{12}\mathbf{K}_{22}^{-1}(\mathbf{v} - \mathbf{m}_2),\ \mathbf{K}_{11} - \mathbf{K}_{12}\mathbf{K}_{22}^{-1}\mathbf{K}_{21}\right). \tag{A.4}$$

Often, the value of Gaussian random variables is restricted:

$$X \sim \mathcal{N}(m, \sigma^2), \quad X_R = \max\{0, X\}.$$

The random variable X_R is known as the *Rectified Gaussian* and its distribution shall be denoted as $\mathcal{N}_R(m, \sigma^2)$. Note that the rectification "concentrates" all the probability measure in $(-\infty, 0)$ to the rectification point 0, leading to an infinite impulse at this point. Thus, the p.d.f. of X_R is:

$$p_{X_R}(x) = \Phi_{m,\sigma^2}(0)\delta(x) + \phi_{m,\sigma^2}(x)H(x), \tag{A.5}$$

where δ is the Dirac delta (distribution)[1] and H is the step function:

$$\delta(x) = \begin{cases} \infty & x = 0, \\ 0 & x \neq 0. \end{cases}, \quad H(x) = \begin{cases} 0 & x \leq 0, \\ 1 & x > 0. \end{cases}$$

The rectification is sometimes confused with the so-called *truncated Gaussian*, which is the distribution of a Gaussian variable $X \sim \mathcal{N}(m, \sigma^2)$ conditioning on an interval $(a, b) \subset \mathbb{R}$:

$$p(x \mid a < X < b) = \frac{\phi_{m,\sigma^2}(x)}{\Phi_{m,\sigma^2}(b) - \Phi_{m,\sigma^2}(a)}.$$

[1] Formally, the Dirac delta should be defined either as a distribution or measure. We use the heuristic characterization here for the sake of simplicity.

APPENDIX B

Proof

B.1 Theorem 5.3

Proof. Let us define $\mathbf{a} \coloneqq -\nabla f_1^{(2)}$ and $\mathbf{b} \coloneqq \nabla f_2^{(1)}$, such that $\tilde{\mathbf{A}}_1 = \mathbf{b}\mathbf{a}^\top$ and

$$\nabla^2 \mathcal{H}_{\mathbf{F}}(\mathbf{X}) = \begin{pmatrix} \mathbf{D}_1 & \mathbf{b}\mathbf{a}^\top \\ \mathbf{a}\mathbf{b}^\top & \mathbf{D}_2 \end{pmatrix}.$$

For two block matrices, their column vectors are denoted as: $\mathbf{D}_1 = (\mathbf{d}_1, \ldots, \mathbf{d}_n)$ and $\mathbf{D}_2 = (\mathbf{d}'_1, \ldots, \mathbf{d}'_n)$. The hypervolume Hessian is of size $2n \times 2n$ and its determinant can be simplified using the Laplace expansion along **the first n rows** of the $\nabla^2 \mathcal{H}_{\mathbf{F}}(\mathbf{X})$. To achieve this, n distinct columns need to be selected out of $2n$ rows. Let S be the set of the n-element subsets of $\{1, 2, \ldots, 2n\}$:

$$S = \{\{1, 2, \ldots, n\}, \{1, 2, \ldots, n-1, n+1\}, \ldots\}$$

For every $L \in S$, we define its complement $L' \coloneqq \{1, 2, \ldots, 2n\} \setminus L$. Note that a permutation is defined on $\{1, 2, \ldots, 2n\}$, by appending L' to L: $\{L, L'\}$ and we shall use $N(L)$ to denote the number of inversions in $\{L, L'\}$. According to the Laplace expansion, such a determinant can be expressed as:

$$\det\left(\nabla^2 \mathcal{H}_{\mathbf{F}}(\mathbf{X})\right) = \sum_{L \in S} (-1)^{N(L)}\, b_L c_{L'},$$

where b_L is the cofactor of the hypervolume Hessian, which is the determinant of the minor matrix obtained by keeping the first n rows and n columns given in L. Similarly, $c_{L'}$ is the *complementary* cofactor of b_L, obtained by removing the first n rows and n columns given in L. For example, if $L = \{1, 2, \ldots, n\}$, then $b_L = \det(\mathbf{D}_1)$ and $c_{L'} = \det(\mathbf{D}_2)$. In particular, when L contains two or more elements from $\{2n+1, 2n+2, \ldots, 2n\}$, meaning that at least two columns from

$\mathbf{ba}^\top$ are chosen to compute b_L, it is obvious that the cofactor b_L is zeros because all the columns from $\mathbf{ba}^\top$ are linear dependent. Using this observation, the expansion can be simplified:

$$\begin{aligned}\det\left(\nabla^2\mathcal{H}_{\mathbf{F}}(\mathbf{X})\right) &= \underbrace{\det\left(\mathbf{D}_1\right)\det\left(\mathbf{D}_2\right)}_{L=\{1,2,\ldots,n\}} \\ &+ \underbrace{(-1)^1\det\left((\mathbf{d}_1,\ldots,\mathbf{d}_{n-1},a_1\mathbf{b})\right)\det\left((b_n\mathbf{a},\mathbf{d}'_2\ldots,\mathbf{d}'_n)\right)}_{L=\{1,2,\ldots,n-1,n+1\}} \\ &+ \underbrace{(-1)^2\det\left((\mathbf{d}_1,\ldots,\mathbf{d}_{n-1},a_2\mathbf{b})\right)\det\left((b_n\mathbf{a},\mathbf{d}'_1,\mathbf{d}'_3,\ldots,\mathbf{d}'_n)\right)}_{L=\{1,2,\ldots,n-1,n+2\}}+\cdots \\ &+ \underbrace{(-1)^n\det\left((\mathbf{d}_1,\ldots,\mathbf{d}_{n-1},a_2\mathbf{b})\right)\det\left((b_n\mathbf{a},\mathbf{d}'_1,\mathbf{d}'_2,\ldots,\mathbf{d}'_{n-1})\right)}_{L=\{1,2,\ldots,n-1,2n\}}+\cdots\end{aligned}$$

There are n terms shown in the equation above, resulting from choosing the first $n-1$ columns and one column from $\{2n+1, 2n+2, \ldots, 2n\}$. Those terms can also be simplified:

$$\begin{aligned}&(-1)^1 a_1 b_n\det\left((\mathbf{d}_1,\ldots,\mathbf{d}_{n-1},\mathbf{b})\right)\det\left((\mathbf{a},\mathbf{d}'_2\ldots,\mathbf{d}'_n)\right) \\ &+(-1)^3 a_2 b_n\det\left((\mathbf{d}_1,\ldots,\mathbf{d}_{n-1},\mathbf{b})\right)\det\left((\mathbf{d}'_1,\mathbf{a},\mathbf{d}'_3\ldots,\mathbf{d}'_n)\right)+\cdots \\ &+(-1)^{2i-1} a_i b_n\det\left((\mathbf{d}_1,\ldots,\mathbf{d}_{n-1},\mathbf{b})\right)\underbrace{\det\left((\mathbf{d}'_1,\ldots,\mathbf{d}'_{i-1},\mathbf{a},\mathbf{d}'_{i+1},\ldots,\mathbf{d}'_n)\right)}_{\text{move } \mathbf{a} \text{ to the } i\text{-th column}} \\ &= -b_n\det\left((\mathbf{d}_1,\ldots,\mathbf{d}_{n-1},\mathbf{b})\right)\det\left(\mathbf{D}_2\right)\sum_{i=1}^{n} a_i\frac{\det\left((\mathbf{d}'_1,\ldots,\mathbf{d}'_{i-1},\mathbf{a},\mathbf{d}'_{i+1},\ldots,\mathbf{d}'_n)\right)}{\det\left((\mathbf{d}'_1,\mathbf{d}'_2,\ldots,\mathbf{d}'_n)\right)} \\ &= -b_n\det\left((\mathbf{d}_1,\ldots,\mathbf{d}_{n-1},\mathbf{b})\right)\det\left(\mathbf{D}_2\right)\mathbf{a}^\top\mathbf{D}_2^{-1}\mathbf{a}\end{aligned} \tag{B.1}$$

Note that the last step above is according to Cramer's rule for the equation $\mathbf{D}_2\mathbf{x}=\mathbf{a}$ ($\mathbf{D}_1$ and $\mathbf{D}_2$ are assumed to be nonsingular):

$$x_i = \frac{\det\left((\mathbf{d}'_1,\ldots,\mathbf{d}'_{i-1},\mathbf{a},\mathbf{d}'_{i+1},\ldots,\mathbf{d}'_n)\right)}{\det\left((\mathbf{d}'_1,\mathbf{d}'_2,\ldots,\mathbf{d}'_n)\right)}$$

In principle, the same simplification here can be applied to other terms in the hypervolume Hessian determinant:

$$
\begin{aligned}
&\det\left(\nabla^2 \mathcal{H}_{\mathbf{F}}(\mathbf{X})\right) = \det\left(\mathbf{D}_1\right)\det\left(\mathbf{D}_2\right) \\
&- \underbrace{b_n \det\left(\left(\mathbf{d}_1, \ldots, \mathbf{d}_{n-1}, \mathbf{b}\right)\right)\det\left(\mathbf{D}_2\right)\mathbf{a}^\top \mathbf{D}_2^{-1}\mathbf{a}}_{\text{drop column } n \text{ from } \mathbf{D}_1} \\
&- \underbrace{b_{n-1} \det\left(\left(\mathbf{d}_1, \ldots, \mathbf{d}_{n-2}, \mathbf{b}, \mathbf{d}_n\right)\right)\det\left(\mathbf{D}_2\right)\mathbf{a}^\top \mathbf{D}_2^{-1}\mathbf{a}}_{\text{drop column } n-1 \text{ from } \mathbf{D}_1} - \cdots \\
&- \underbrace{b_1 \det\left(\left(\mathbf{b}, \mathbf{d}_2, \ldots, \mathbf{d}_n\right)\right)\det\left(\mathbf{D}_2\right)\mathbf{a}^\top \mathbf{D}_2^{-1}\mathbf{a}}_{\text{drop column } 1 \text{ from } \mathbf{D}_1} \\
&= \det\left(\mathbf{D}_1\right)\det\left(\mathbf{D}_2\right)\left[1 - \mathbf{a}^\top \mathbf{D}_2^{-1}\mathbf{a}\sum_{i=1}^{n} b_i \frac{\det\left(\left(\mathbf{d}_1, \ldots, \mathbf{d}_{i-1}, \mathbf{b}, \mathbf{d}_{i+1}, \ldots, \mathbf{d}_n\right)\right)}{\det\left(\left(\mathbf{d}_1, \mathbf{d}_2, \ldots, \mathbf{d}_n\right)\right)}\right] \\
&= \left(1 - \left(\mathbf{a}^\top \mathbf{D}_2^{-1}\mathbf{a}\right)\left(\mathbf{b}^\top \mathbf{D}_1^{-1}\mathbf{b}\right)\right)\det\left(\mathbf{D}_1\right)\det\left(\mathbf{D}_2\right)
\end{aligned}
$$

Again, in the last step above the same argument as in Eq. (B.1) is applied. Because matrices $\mathbf{D}_1$ and $\mathbf{D}_2$ are nonsingular, the hypervolume Hessian matrix is nonsingular as long as $1 - \left(\mathbf{a}^\top \mathbf{D}_2^{-1}\mathbf{a}\right)\left(\mathbf{b}^\top \mathbf{D}_1^{-1}\mathbf{b}\right)$ is not zero. □

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Acronyms

BLP Best Linear Estimator. 50

BLUE Best Linear Unbiased Estimator. 48

BLUP Best Linear Unbiased Predictor. 48

ECDF Empirical Cumulative Distribution Function. 36, 101

EGO Efficient Global Optimization. 37, 90, 113, 114

EI Expected Improvement. 78, 90–93, 96, 103, 108, 114, 154

GEI Generalized Expected Improvement. 91, 92, 98, 100

GLS Generalized Least Squares. 48

GPR Gaussian Process Regression. 39, 43, 44, 56, 59, 63, 69, 87, 88, 95, 100, 152

KKT Karush-Kuhn-Tucker conditions. 57, 95, 125

LHS Latin Hypercube Sampling. 57, 101

LUP Linear Unbiased Predictor. 47

MAP Maximum a Posterior. 59

MGF Moment-Generating Function. 96

MGFI Moment-Generating Function of Improvement. 98, 100, 101, 103, 107, 154, 155

MSE Mean Squared Error. 37, 39, 49, 50, 69, 71, 73, 80, 82, 94, 108

Acronyms

RBF Radial Basis Functions. 46

RKHS Reproducing Kernel Hilbert Space. 54, 56, 57, 155

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