Stochastic and deterministic algorithms for continuous black-box optimization
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Gaussian Distribution

Assume the probability space \((\Omega, \mathcal{F}, \mathbb{P})\) and a measurable space \((\mathbb{R}, \mathcal{B})\), where \(\mathcal{B}\) 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 \(\mathbb{P}_X : \mathcal{B} \to [0,1]\), defined as a push-forward measure, \(\forall B \in \mathcal{B}, \mathbb{P}_X(B) := \mathbb{P}(X^{-1}(B))\), admits the following form:

\[
\mathbb{P}_X(B) = \int_B \frac{1}{\sqrt{2\pi\sigma^2}} \exp \left( -\frac{(x-m)^2}{2\sigma^2} \right) \, d\lambda,
\]

where \(\lambda\) is the Lebesgue measure on \(\mathbb{R}\) and \(m, \sigma^2\) 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. \(\lambda\):

\[
\phi_{m,\sigma^2}(x) = \frac{d\mathcal{G}_{m,\sigma^2}}{d\lambda} = \frac{1}{\sqrt{2\pi\sigma^2}} \exp \left( -\frac{(x-m)^2}{2\sigma^2} \right),
\]

that is, by definition, the integrand in Eq. (A.1). In the multivariate case, consider the measurable space \((\mathbb{R}^n, \mathcal{B}^n)\) where \(\mathcal{B}^n\) 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 \(c^\top \mathbf{x}\), \(c \in \mathbb{R}^n\) admits the distribution as in Eq. (A.1). In addition, the distribution of \(\mathbf{x}\) is

\[
\forall B \in \mathcal{B}^n, \mathcal{G}_{m,K}^n(B) = \int_B (2\pi)^{-n/2} \det(K)^{1/2} \exp \left( -\frac{1}{2} (\mathbf{y} - \mathbf{m})^\top K^{-1} (\mathbf{y} - \mathbf{m}) \right) \, d\lambda^n,
\]
A. GAUSSIAN DISTRIBUTION

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

\[
\Phi_{\mathbf{m}, \mathbf{K}}(\zeta) = \mathcal{G}_{\mathbf{m}, \mathbf{K}} \left( \{ \mathbf{x} \in \mathbb{R}^n : \mathbf{x} \leq \zeta \} \right).
\]

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

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

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:

\[
\mathbf{x}_1 \sim \mathcal{N}(\mathbf{m}_1, \mathbf{K}_{11}). \tag{A.3}
\]

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):

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

Often, the value of Gaussian random variables is restricted:

\[
X \sim \mathcal{N}(\mu, \sigma^2), \quad X_R = \max\{0, X\}.
\]

The random variable \( X_R \) is known as the Rectified Gaussian and its distribution shall be denoted as \( \mathcal{N}_R(\mu, \sigma^2) \). 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:

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

where \( \delta \) 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 \( X \sim \mathcal{N}(\mu, \sigma^2) \) conditioning on an interval \((a, b) \subset \mathbb{R} \):

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

\(^1\)Formally, the Dirac delta should be defined either as a distribution or measure. We use the heuristic characterization here for the sake of simplicity.
Proof

B.1 Theorem 5.3

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

$$\nabla^2 H_F(X) = \begin{pmatrix} D_1 & ba^\top \\ ab^\top & D_2 \end{pmatrix}.$$ 

For two block matrices, their column vectors are denoted as: $D_1 = (d_1, \ldots, d_n)$ and $D_2 = (d'_1, \ldots, d'_n)$. 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 $\nabla^2 H_F(X)$. 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 $L' := \{1, 2, \ldots, 2n\} \setminus L$. 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:

$$\det \left( \nabla^2 H_F(X) \right) = \sum_{L \in S} (-1)^{N(L)} b_{L} c_{L'},$$

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 $b_L = \det(D_1)$ and $c_{L'} = \det(D_2)$. In particular, when $L$ contains two or more elements from $\{2n+1, 2n+2, \ldots, 2n\}$, meaning that at least two columns from
\[ \text{b} \text{a}^T \text{ are chosen to compute } b_L, \text{ it is obvious that the cofactor } b_L \text{ is zeros because all the columns from } \text{b} \text{a}^T \text{ are linear dependent. Using this observation, the expansion can be simplified:} \]

\[
\det (\nabla^2 \mathcal{H}_F(X)) = \det (D_1) \det (D_2)
\]

\[
+ (-1)^1 \text{ det } ((d_1, \ldots, d_{n-1}, a_1 b)) \text{ det } ((b_n a, d'_2, \ldots, d'_n))
\]

\[
+ (-1)^2 \text{ det } ((d_1, \ldots, d_{n-1}, a_2 b)) \text{ det } ((b_n a, d'_1, d'_3, \ldots, d'_n)) + \cdots
\]

\[
+ (-1)^n \text{ det } ((d_1, \ldots, d_{n-1}, a_2 b)) \text{ det } ((b_n a, d'_1, d'_2, \ldots, d'_{n-1})) + \cdots
\]

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:

\[
(-1)^1 a_1 b_n \text{ det } ((d_1, \ldots, d_{n-1}, b)) \text{ det } ((a, d'_2, \ldots, d'_n))
\]

\[
+ (-1)^3 a_2 b_n \text{ det } ((d_1, \ldots, d_{n-1}, b)) \text{ det } ((d'_1, a, d'_3, \ldots, d'_n)) + \cdots
\]

\[
+ (-1)^{2i-1} a_i b_n \text{ det } ((d_1, \ldots, d_{n-1}, b)) \text{ det } ((d'_1, \ldots, d'_{i-1}, a, d'_{i+1}, \ldots, d'_n))
\]

\[
= -b_n \text{ det } ((d_1, \ldots, d_{n-1}, b)) \text{ det } (D_2) \sum_{i=1}^{n} a_i \frac{\det ((d'_1, \ldots, d'_{i-1}, a, d'_{i+1}, \ldots, d'_n))}{\det ((d'_1, d'_2, \ldots, d'_n))}
\]

\[
= -b_n \text{ det } ((d_1, \ldots, d_{n-1}, b)) \text{ det } (D_2) a^T D_2^{-1} a
\]

Note that the last step above is according to Cramer’s rule for the equation \( D_2 x = a \) (\( D_1 \) and \( D_2 \) are assumed to be nonsingular):

\[
x_i = \frac{\det ((d'_1, \ldots, d'_{i-1}, a, d'_{i+1}, \ldots, d'_n))}{\det ((d'_1, d'_2, \ldots, d'_n))}
\]
In principle, the same simplification here can be applied to other terms in the hypervolume Hessian determinant:

$$\det(\nabla^2 H_F(X)) = \det(D_1) \det(D_2)$$

$$= -b_n \det((d_1, \ldots, d_{n-1}, b)) \det(D_2) a^\top D_2^{-1} a$$

\text{drop column n from } D_1

$$- b_{n-1} \det((d_1, \ldots, d_{n-2}, b, d_{n})) \det(D_2) a^\top D_2^{-1} a - \ldots$$

\text{drop column n - 1 from } D_1

$$- b_1 \det((b, d_2, \ldots, d_n)) \det(D_2) a^\top D_2^{-1} a$$

\text{drop column 1 from } D_1

$$= \det(D_1) \det(D_2) \left[ 1 - a^\top D_2^{-1} a \sum_{i=1}^{n} b_i \frac{\det((d_1, \ldots, d_{i-1}, b, d_{i+1}, \ldots, d_n))}{\det((d_1, d_2, \ldots, d_n))} \right]$$

$$= (1 - (a^\top D_2^{-1} a) (b^\top D_1^{-1} b)) \det(D_1) \det(D_2)$$

Again, in the last step above the same argument as in Eq. (B.1) is applied. Because matrices $D_1$ and $D_2$ are nonsingular, the hypervolume Hessian matrix is nonsingular as long as $1 - (a^\top D_2^{-1} a) (b^\top D_1^{-1} b)$ is not zero. \qed
Bibliography


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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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