**Tutorial on Bayesian optimization**

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**Abstract**

**1. Introduction**

As a convention, lowercase and un-bold letters like *a*, *b*, *c*, *x*, *y*, and *z* denote scalar whereas lowercase and bold letters like ***a***, ***b***, ***c***, ***x***, ***y***, and ***z*** denote vector. In some cases, uppercase and un-bold letters like *A*, *B*, *C*, *X*, *Y*, and *Z* can denote vector. Uppercase and bold / un-bold letters like *A*, *B*, *C*,***A***,***B***,***C***, *X*, *Y*, *Z*,***X***,***Y***, and ***Z*** denote matrix. Variables can be denoted as *x*, *y*, *z*, ***x***, ***y***, ***z***, *X*, *Y*, *Z*, ***X***, ***Y***, and ***Z*** whereas constants can be denoted as *a*, *b*, *c*, ***a***, ***b***, ***c***, *A*, *B*, *C*, ***A***, ***B***, and ***C***. Uppercase and bold / un-bold letters like *X*, *Y*, *Z*,***X***, ***Y***, and ***Z*** can denote random variables. However, scalar, vector, matrix, variables, and random variables are stated explicitly in concrete cases.

**2. Bayesian optimization**

**3. Gaussian process regression**

Nonparametric BO is based on Gaussian process regression which, in turn, is based on Gaussian process. Therefore, we start the description of Gaussian process regression with a concept of Gaussian process. Given a random process ***X*** = (*X*1, *X*2,…, *Xn*) over *n* timepoints in which each *Xt* where *t* belongs to {1, 2,…, *n*} is random variable, if and only if for any finite index set {*t*1, *t*2,…, *tk*} of {1, 2,…, *n*} where *tj* belongs to {1, 2,…, *n*}, the subset considered as *tk*-dimension random vector follows multinormal distribution known as multivariate Gaussian distribution then ***X*** is called *Gaussian random process* or Gaussian process in brief. Note, each represents one dimension of the *k*-dimension random vector variable . Moreover, please pay attention that any combination of follows normal distribution too. Without loss of generality, we denote the random process as random variable ***X*** = (*X*1, *X*2,…, *Xn*)*T* where {*t*1, *t*2,…, *tk*} = {1, 2,…, *n*} obeying multinormal distribution (multivariate normal distribution or multivariate Gaussian distribution) as follows:

Where *μ*(***X***) and Σ(***X***) are mean vector and covariance matrix of ***X***, respectively. Note, the superscript “*T*” denotes transposition operator of vector and matrix whereas the tilde sign “~” indicates probabilistic distribution of a random variable. Gaussian process is known as infinite multinormal distribution which is the generalized form of *n*-dimension multinormal distribution because *n* can approach positive infinity *n* = +∞. Let *f*(***X*** | *μ*(***X***), Σ(***X***) be probability density function (PDF) of ***X*** when ***X*** is continuous, we have:

Indeed, mean *μ*(***X***) and covariance Σ(***X***) are functions of ***X***, respectively. In theoretical literature, *μ*(***X***) is assumed to be zero for convenience but it can be defined as the random process ***X*** itself.

Besides, *μ*(***X***) can be customized according to concrete applications, for example it can be constant as *μ*(***X***) = ***μ***. Covariance function Σ(***X***) measures the correlation between random variables when the random process “moves” them, in which the closer the given two random variables are, the larger their covariance. It is invertible, positive definite, and symmetric. The two most important properties based on covariance function Σ(***X***) of random process are stationarity and isotropy among four basic properties: stationarity, isotropy, smoothness, and periodicity. Stationarity implies that the PDF *f*(***X*** | *μ*(***X***) of random process ***X*** will not be changed when the process is shifted in time, for example, if new random variable *Xn*+1 raises to be added then means and covariances of old (previous) variables *Xi* where 1 ≤ *i* ≤ *n* in ***X*** will not be changed. It is proved that if Gaussian process ***X*** satisfies stationarity, Σ(***X***) will depend only on the deviation *Xi*–*Xj* but the inversed statement is not asserted. However, if Σ(***X***) depends only on the Euclidean distance |*Xi*–*Xj*| then, Gaussian process ***X*** will satisfy isotropy. If ***X*** satisfies both stationarity and isotropy, ***X*** is called homogeneous process. In cases where each element of matrix function Σ(***X***) depends only on *Xi* and *Xj* like stationarity case and isotropy, it will be formulated as following matrix.

In these cases, covariance function Σ(***X***) is identified with its element function Σ(*Xi*, *Xj*) if the formulation of Σ(*Xi*, *Xj*) is not changed formally and hence, Σ(*Xi*, *Xj*) is called *kernel function*. The following are some kernel functions.

Where *l* is the characteristic length-scale of the process which reinforces similarity of *Xi* and *Xj*. As a convention, let *Xi*:*j* where *i*≤*j* denote a sequential subset of ***X*** such that *Xi*:*j* = {*Xi*, *Xi*+1,…, *Xj*}. Of course, we have *Xi*:*i* = *Xi*. In general case, *Xi*:*j* is arbitrary subset of distinguish variables. Let Σ(*Xi*, *Xj*:*k*) denote a row covariance vector of *Xi* and *Xj*:*k* as follows:

Let Σ(*Xj*:*k*, *Xi*) denote a column covariance vector of *Xj*:*k* and *Xi* as follows:

As a convention, let Σ(*Xi*:*j*, *Xk*:*l*) denote a pseudo covariance matrix of *Xi*:*j* and *Xk*:*l* as follows:

Note, Σ(*Xi*:*j*, *Xk*:*l*) is not an actual covariance matrix because it may not be squared. Obviously, Σ(*Xi*:*j*, *Xk*:*l*) is a partition of Σ(***X***) and we have Σ(***X***) = Σ(*Xi*:*n*, *Xi*:*n*). If denoting ***X***1 =(*Xi*, *Xi*+1,…, *Xj*)*T* and ***X***2 = (*Xk*, *Xk*+1,…, *Xl*)*T*, we denote:

Gaussian process repression is based on Gaussian process when there is a target function which attaches to each *X* where *X* represents any *Xi* in ***X*** such that *Y* = *f*(*X*). Please distinguish the target function *f* from formal PDF notations *f*(.|.). Of course, *Y* or *Yi* is also random variable and we also have *Yi* = *f*(*Xi*). Gaussian process regression model tries to represent or draw a regressive PDF of ***Y*** from its previous ones (which will be explained later) and ***X***. Suppose we had a Gaussian process ***X*** = (*X*1, *X*2,…, *Xn*)*T* and target function ***Y*** = *f*(***X***), assuming that the prior PDF of ***Y*** = (*Y*1, *Y*2,…, *Yn*)*T* given ***X*** is also derived from the multinormal PDF of ***X***.

Therefore, we have:

Where *μ*(.) and Σ(.) denote mean function and covariance function (kernel function) in formality, respectively, and Σ(***X***, ***X***) = Σ(***X***). The equation above implies that the prior PDF of Gaussian process ***Y*** is initialized with the PDF of Gaussian process ***X***. Mean vector and covariance matrix of ***Y*** are *μ*(***Y***) and Σ(***X***, ***X***) *\**) within the PDF *f*(***Y*** | ***X***, *μ*(.), Σ(.)), respectively. The mean function *μ*(***Y***) is redefined here with variable ***Y*** but it should be the same to the mean function *μ*(***X***) in formulation if *μ*(***X***) can be extended with the lower/higher dimensional space. For instance, if *μ*(***X***) is defined as itself *μ*(***X***) = ***X*** then, *μ*(***Y***) will be defined as itself *μ*(***Y***) = ***Y*** = (*Y*1, *Y*2,…, *Yn*)*T*. Now suppose we randomize a new set of variables ***X***\* = (*Xn*+1, *Xn*+2,…, *Xn*+*k*)*T* and obtain their evaluated values ***Y***\* = *f*(***X***\*) = (*Yn*+1, *Yn*+2,…, *Yn*+*k*)*T*. Similarly, mean vector and covariance matrix of ***Y****\** are *μ*(***Y****\**) and Σ(***X****\**, ***X****\**) within the PDF *f*(***Y***\* | ***X***\*, *μ*(.), Σ(.)), respectively. Consequently, the joint PDF of ***Y*** and ***Y***\* which is of course multinormal distribution is denoted as follows:

Where mean vector and covariance matrix of the joint PDF of ***Y*** and ***Y***\* are and , respectively. As a result, the regressive Gaussian process (RGP) model of dependent variable *Y* is conditional PDF of ***Y***\* given ***Y***, ***X***, and ***X***\* such as *f*(***Y***\* | ***Y***, ***X***, ***X***\*, *μ*(.), Σ(.)) which is also predictive PDF of ***Y***\* because it can be used to predict next occurrence of *Y*. From interesting properties of multinormal distribution, it is easy to drawn RGP from the joint PDF *f*(***Y***, ***Y***\* | ***Y***, ***X***, ***X***\*, *μ*(.), Σ(.)) as follows:

Where,

Obviously, the RGP of ***Y***\* distributes normally with mean vector *μ*(***Y***\* | ***Y***, ***X***, ***X***\*) and covariance matrix Σ(***Y***\* | ***X***, ***X***\*). Indeed, the RGP *f*(***Y***\* | ***Y***, ***X***, ***X***\*, *μ*(.), Σ(.)) is posterior PDF of ***Y*** whose prior PDF is *f*(***Y*** | ***X***, *μ*(.), Σ(.)). Initializing such prior PDF by the PDF of ***X*** as *f*(***Y*** | ***X***, *μ*(.), Σ(.)) = *f*(***X*** | *μ*(.), Σ(.)) is not totally correct but implicit biases will be decreased after the posterior PDF *f*(***Y***\* | ***Y***, ***X***, ***X***\*, *μ*(.), Σ(.)) is updated. We have following summary:

Although the RGP of ***Y***\* depends on ***Y***, ***X***, and ***X***\*, the semantic meaning of regression model here is mentioned mainly that ***Y***\* is determined based on its previous one ***Y*** when both of them are assumed to be based on *X* via the PDF of ***Y*** as *f*(***Y*** | ***X***, *μ*(.), Σ(.)) and the PDF of ***Y***\* as *f*(***Y***\* | ***X***\*, *μ*(.), Σ(.)). This implies that *X* is the intermediate point for the dependence of ***Y***\* on ***Y***.

If ***X***\* and ***Y***\* are 1-element vectors such that ***X***\* = *Xn*+1 and ***Y***\* = *Yn*+1 and let ***x***1:*n* = ***X***, ***x*** = ***X***\*, *y*1:*n* = ***Y***, and *y* = ***Y***\*, the RGP becomes:

Where,

The equation above with single variables ***x*** and *y* (single posterior processes) is popular in BO, especially ***x*** is vector and *y* is scalar although ***x*** and *y* can be arbitrary such as scalar, vector, and matrix with note that high dimensional spaces require tensor products for example.

**4. Acquisition functions**

**5. Numerical simulation**

**6. Conclusions**

**Appendices**

**References**