Gaussian Process Regression and Classification under Mathematical Constraints with Learning Guarantees

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SUMMARY

We introduce constrained Gaussian process (CGP), a Gaussian process model for random functions that allows easy placement of mathematical constrains (e.g., non-negativity, monotonicity, etc) on its sample functions. CGP comes with closed-form probability density function (PDF), and has the attractive feature that its posterior distributions for regression and classification are again CGPs with closed-form expressions. Furthermore, we show that CGP inherents the optimal theoretical properties of the Gaussian process, e.g. rates of posterior contraction, due to the fact that CGP is an Gaussian process with a more efficient model space.

Some key words: Gaussian Process. Regression. Classification. Uncertainty Quantification. Posterior Convergence.
1. The Idea

Conceptually, the goal of a constrained Gaussian process (CGP) is to place mathematical constraints \( \mathcal{C} \) on the sample paths \( g \) of a Gaussian process, such that \( g \in \mathcal{C} \). Operationally, \( \mathcal{C} \) is defined through a system of \( k \) linear constraints characterized by matrices \( A_{k \times 1} \) and \( b_{k \times 1} \), e.g.:

\[
\text{sample } \quad g \sim GP(0,k) \\
\text{subject to } \quad g \in \mathcal{C} \quad \text{where } \quad \mathcal{C} = \{ g | Ag + b \geq 0 \}.
\]

For example, an inequality constraint \( \mathcal{C} = \{ g | g \geq 0 \} \) can be written as \( A = 1, b = 0 \), and a boundedness constraint \( \mathcal{C} = \{ g | 1 \geq g \geq 0 \} = \{ g | g \geq 0, 1 - g \geq 0 \} \) can be written as \( A = [1, -1] \top, b = [0, 1] \top \). Notice that since \( g \) is a random variable, the constraint \( \mathcal{C} \) is a random event with distribution \( f(\mathcal{C}|g) \). Consequently, CGP imposes constraints \( \mathcal{C} \) on a Gaussian process by augmenting the original distribution of a Gaussian process (GP) \( f(g) \) with the additional likelihood term \( P(\mathcal{C}|g) \).

As a result, given constraints \( \mathcal{C} \) and a standard GP with mean function \( \mu \) and kernel function \( k \), the likelihood function of CGP is defined to be:

\[
f(g|\mathcal{C}) \propto f(\mathcal{C}|g)f(g),
\]

where \( f(g) = GP(g|\mu,k) \) is the likelihood for the standard GP. \( f(\mathcal{C}|g) \) is designed such that it assigns near zero probability to \( g \)'s that violates \( \mathcal{C} \), and assign high probability otherwise. In this work, we use the Probit function (i.e. the cumulative density function (CDF) of a standard Gaussian distribution) to represent the likelihood functions for each individual constraint in \( \mathcal{C} \), and assume the \( k \) constraints are independent conditional on \( G \). As a result, \( P(\mathcal{C}|G) \) is the CDF of a standard multivariate Gaussian distribution:

\[
f(\mathcal{C}|g) \propto \Phi(Ag + b|\mu = 0, \Sigma = I)
\]

where we denote \( \Phi(.,|\mu, \Sigma) \) and \( \phi(.,|\mu, \Sigma) \) to be the CDF and PDF of a Gaussian distribution with mean \( \mu \) and covariance \( \Sigma \). To keep the notations uncluttered, we will drop the terms \( \mu \) and \( \Sigma \) unless they are different from the default values \( \mu = 0 \) and \( \Sigma = I \). Consequently, conditional on the function input \( z \), the likelihood function of CGP is:

\[
f(g|\mathcal{C}) \propto f(\mathcal{C}|g) * f(g),
\]

\[
\quad \propto \Phi(Ag + b) * \phi(g|\mu,k), \tag{2}
\]

where \( u \) and \( K \) are the mean vector and the kernel matrix of the standard GP \( f(g) = GP(g|\mu,k) \) evaluated at \( z \).

1.1. PDF, moment generating function (MGF) and Moments

Given constraints \( \mathcal{C} = \{ g | Ag + b \geq 0 \} \) and a standard Gaussian process \( GP(\mu,k) \), denote the Constrained Gaussian Process (CGP) as \( CGP(\mu,k,\mathcal{C}) \). For \( g \sim CGP(\mathcal{C},k,\mathcal{C}) \), given input \( z \), the PDF of \( g = g(z) \) is:

\[
f(g|u,K,\mathcal{C}) = \frac{\phi(g|u,K) * \Phi(Ag + b)}{C} \quad \text{where} \quad C = \Phi(Au + b|\Sigma = I + AK \top)
\]

and the MGF of \( CGP(\mathcal{C},k,\mathcal{C}) \) is:

\[
M_g(t) = exp(u \top t + \frac{1}{2}t \top Kt) * \frac{\Phi(Au + b + AK|\Sigma = I + AK \top)}{\Phi(Au + b|\Sigma = I + AK \top)} \tag{4}
\]

where recall \( \Phi(.,|\mu, \Sigma) \) and \( \phi(.,|\mu, \Sigma) \) are the CDF and PDF of a Gaussian distribution with mean \( \mu \) and covariance \( \Sigma \).

As a result, we can derive the moments of \( CGP(\mathcal{C},k,\mathcal{C}) \) by taking derivatives with respect to (4). In particular, the expression for the mean of CGP is

\[
E(g|u,K,\mathcal{C}) = u + KA \top (I + AK \top)^{-1}E(b|b' \geq -b, \Sigma = I + AK \top) \tag{5}
\]
In particular, the second term in (5) corrects the original mean vector $\mu$ with respect to the constraints such that $AE(\mathbf{g}|\mathbf{u}, \mathbf{K}, \mathcal{C}) + \mathbf{b} \geq 0$.

**Proof.** See Section A.1 □

2. **Regression and Classification**

An important feature of CGP is that the posterior distributions of $\mathbf{g}$ in regression and classification have closed forms. Specifically, assuming $g \sim \text{CGP}(\mu, k, \mathcal{C})$, for a regression model $\mathbf{y}_i \overset{\text{indep}}{\sim} \text{Normal}(g(\mathbf{z}_i), \sigma^2)$, the posterior distribution of $\mathbf{g}$ is again a constrained Gaussian process $\text{CGP}(\mu^*, k^*, \mathcal{C}^*)$ with parameters:

$$\mu^* = \mathbf{u} + \mathbf{K}(\mathbf{K} + \sigma^2 \mathbf{1})^{-1} (\mathbf{y} - \mathbf{u}), \quad \mathbf{K}^* = \mathbf{K} - \mathbf{K}(\mathbf{K} + \sigma^2 \mathbf{1})^{-1} \mathbf{K}, \quad \mathcal{C}^* = \mathcal{C},$$

and the predictive distribution for a new observation $\mathbf{z}^*$ also follows a constrained Gaussian process $\text{CGP}(\mu^*, k^*, \mathcal{C}^*)$ with parameters:

$$\mu^* = u(\mathbf{z}^*) + k(\mathbf{z}^*, \mathbf{z})(\mathbf{K} + \sigma^2 \mathbf{1})^{-1} (\mathbf{y} - \mathbf{u}),$$

$$\mathbf{K}^* = k(\mathbf{z}^*, \mathbf{z}^*) - k(\mathbf{z}^*, \mathbf{z})(\mathbf{K} + \sigma^2 \mathbf{1})^{-1} k(\mathbf{z}, \mathbf{z}^*),$$

$$\mathcal{C}^* = \mathcal{C}.$$

For a classification model under the Probit link function $\mathbf{y}_i \overset{\text{indep}}{\sim} \text{Bernoulli}(p_i)$ where $p_i = \Phi(g(\mathbf{z}_i))$, the posterior distribution of $\mathbf{g}$ is also a constrained Gaussian process $\text{CGP}(\mu^*, k^*, \mathcal{C}^*)$ with modified constraint $\mathcal{C}^*$:

$$\mu^* = \mathbf{u}, \quad \mathbf{K}^* = \mathbf{K}, \quad \mathcal{C}^* = \left\{ \mathbf{g} \mid \begin{bmatrix} \mathbf{A} \\ \mathbf{D} \end{bmatrix} \mathbf{g} + \begin{bmatrix} \mathbf{b} \\ \mathbf{0} \end{bmatrix} \geq \mathbf{0} \right\},$$

where $\mathbf{D} = \text{diag}(2 \ast \mathbf{y} - 1)$ is a diagonal matrix of $\pm 1$’s corresponding to the observations. Notice that the $\mathbf{Dg}$ term in $\Phi$ can be interpreted as imposing addition data-based constraints to $g(\mathbf{z}_i)$, i.e. $g(\mathbf{z}_i) \geq 0$ when $y_i = 1$ and $g(\mathbf{z}_i) \leq 0$ otherwise, such that during estimation, $g(\mathbf{z}_i)$ is pushed toward positive/negative values depending on the value of the observation $y_i$. The predictive distribution for $g$ at new location $\mathbf{z}^*$ is also a constrained GP $\text{CGP}(\mu^*, k^*, \mathcal{C}^*)$, with parameters:

$$\mu^* = u(\mathbf{z}^*) + k(\mathbf{z}^*, \mathbf{z}) \mathbf{K}^{-1} (\mathbf{y} - \mathbf{u}),$$

$$\mathbf{K}^* = k(\mathbf{z}^*, \mathbf{z}^*) - k(\mathbf{z}^*, \mathbf{z}) \mathbf{K}^{-1} k(\mathbf{z}, \mathbf{z}^*),$$

$$\mathcal{C}^* = \left\{ \mathbf{g} \mid \begin{bmatrix} \mathbf{A} \\ \mathbf{D} \end{bmatrix} \mathbf{g} + \begin{bmatrix} \mathbf{b} \\ \mathbf{0} \end{bmatrix} \geq \mathbf{0} \right\}.$$

**Proof.** See Section A.2 □

3. **Posterior Concentration**

3.1. **Feasibility Condition**

For a target function $g^* \in \mathcal{K}$ that is feasible with respect to constraint $\mathcal{C}$ (i.e. $g^* \in \mathcal{C}$), the interest of CGP is to better estimate $g^*$ by shifting its probability mass toward the region where $f(\mathcal{C}|g)$ is high. Consequently, to measure the convergence of CGP’s posterior toward $g^*$, we need a notion about the “degree” of feasibility of $g^*$ with respect to the probabilistic constraint $f(\mathcal{C}|g)$ specified by CGP, so that we can decide if our configuration of the CGP is “compatible enough” with $g^*$ to guarantee fast speed of posterior convergence. In this work, we establish such notion by considering how robust $f(\mathcal{C}|g^*)$ is under a small amount of random perturbation $s$ on $g^*$:
**Definition 1 (ε-feasibility).** Denote truncGP(0, k, S) the truncated Gaussian process with mean zero, covariance kernel k and its support truncated to be within the set S. For a small positive constant \( \varepsilon > 0 \), denote \( S_\varepsilon = \{ x | ||x|| \leq \varepsilon \} \) a set of perturbation noises with maximum magnitude \( \varepsilon \).

For a function \( g^* \in \mathcal{H}_k \), we say \( g^* \) is \( \varepsilon \)-feasible with respect to the probabilistic constraint \( f(\mathcal{C}|g) \) if for the "\( \varepsilon \)-perturbed" function \( g^*_\varepsilon \) truncGP(0, k, \( g^* + S_\varepsilon \)) and the random noise \( s_\varepsilon \sim \text{truncGP}(0, k, S_\varepsilon) \), we have

\[
E \left( f(\mathcal{C}|g^*_\varepsilon) \right) \geq E \left( f(\mathcal{C}|s_\varepsilon) \right)
\]

i.e. the \( \varepsilon \)-perturbed function \( g^*_\varepsilon \) is on average more feasible than the random noise \( s_\varepsilon \).

The notion of \( \varepsilon \)-feasibility requires \( g^* \) to be more feasible than the random noises under random perturbations of magnitude \( \varepsilon \). Notice that when \( \varepsilon \) is very small (as is the case for Theorem 1), the \( \varepsilon \)-feasibility condition is essentially requiring \( f(\mathcal{C}|g^*) \geq f(\mathcal{C}|0) \), i.e. the target function \( g^* \) should be no less feasible than the zero function \( \theta(x) = 0 \), which is the default mean function of a CGP prior.

### 3.2. Posterior Concentration for General CGP Prior

For a target function \( g^* \) that is \( \varepsilon \)-feasible, we can show that the CGP prior assigns sufficient probability mass around its neighborhood, which is important for guaranteeing reasonable speed of posterior convergence toward \( g^* \) (see Lemma 1 in Appendix). Furthermore, we can show that CGP enjoys an theoretical guarantee in the posterior convergence toward a target functions that are \( \varepsilon \)-feasible:

**Theorem 1 (Conditions for Posterior Consistency in CGP).** Let \( g \) be a Borel measurable, zero-mean constrained Gaussian random element in a separable Banach space \((\mathcal{B}, |||\cdot|||)\) with reproducing kernel Hilbert space (RKHS) \((\mathcal{H}_k, |||\cdot|||_{\mathcal{H}_k})\). Define the concentration function \( \psi^*(\varepsilon) = \inf_{\delta \in \mathcal{H}_k, ||g - g^*|| \leq \varepsilon} \left( \frac{1}{2} \log P(|||g||| \leq \varepsilon) - \log P(|||g - g^*||| \leq \varepsilon) \right) \).

For any number \( \varepsilon_n > 0 \) satisfying \( \psi^*(\varepsilon_n) \leq n\varepsilon_n^2 \), and any constant \( C \geq 1 \) with \( e^{-Cn\varepsilon_n^2} < \frac{1}{2} \), \( e^{-Cn\varepsilon_n^2} \leq \log P(g \notin B_n) \leq 2Cn\varepsilon_n^2 \)

In above theorem, \( B_n \) can be understood as the "large probability region" of a CGP model, i.e., region where the posterior distribution will put sufficiently large amount of probability mass in. Ideally, as the sample size \( n \) grow, we hope this region to move quickly from the initial location to concentrate around the target function \( g^* \). To this regard, the three conditions in Theorem 1 describes how the CGP prior behave with respect to the data-generating function \( g^* \) and a "model" \( B_n \). Specifically, condition (I) requires the CGP prior to put sufficient mass around \( g^* \), condition (II) requires the prior to be not too big compared to the model \( B_n \), and condition (III) puts a restriction on the size of the model \( B_n \) in the sense that the size of \( B_n \) when measured by the entropy number (i.e. the minimum number of balls of radius \( 3\varepsilon_n \) needed to cover \( B_n \)) is upper bounded.

Similar to Theorem 2.1 of van der Vaart & van Zanten (2007) which outlines the general convergence conditions of Gaussian processes, the three conditions in Theorem 1 can be matched one-to-one to the conditions for posterior convergence in Ghosal et al. (2000) (Theorem 2.1), with the exception that the distance measures in Theorem 1 are defined to be \( |||\cdot||| \) (i.e. the norm for the Banach space \( \mathcal{B} \) with which the constrained Gaussian process is defined) rather than the typical statistical distances (e.g. the Hellinger distance) that were used to measure convergence. Consequently, for a statistical problem under consideration (e.g. regression or classification), we can show convergence by showing that the statistical metric for measuring convergence is bounded by the Banach space norm \( |||\cdot||| \) and then invoke Theorem 1.
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A. Derivation

A.1. Derivation for CGP’s PDF, MGF and Mean

To derive the expression of PDF in (3), only need to derive the constant term \( C \) by integrating over CGP’s unnormalized likelihood function in (2):

**Proof.**

\[
C = \int_{g \in \mathbb{R}^n} \Phi(Ag + b) \cdot \phi(g|u, K)dg \\
= P(Z \leq Ag + b) \quad \text{where} \quad Z \sim \phi(0, I) \\
= P(Z \leq A(\Gamma Z' + u) + b) \quad \text{where} \quad Z' \sim \phi(0, I), Z' \parallel Z, A = \Gamma \Gamma^\top \\
= P(Z - A\Gamma Z' \leq \text{Au} + b) \quad \text{notice} \quad Z - A\Gamma Z' \sim \phi(0, \Sigma = I + \text{AKA}^\top) \\
= \Phi(\text{Au} + b|\Sigma = I + \text{AKA}^\top) \tag{1}
\]

Now derive the expression for MGF:

**Proof.**

\[
M_q(t) = E(exp(t^\top g)|\mathcal{C}, u, K) \\
= \int_{g \in \mathbb{R}^n} exp(t^\top g) \cdot \phi(g|u, K) \cdot \Phi(Ag + b)dg/C \\
\approx \int_{g \in \mathbb{R}^n} exp(-\frac{1}{2}gK^{-1}g + (K^{-1}u + t)^\top g) \cdot \Phi(Ag + b)dg/C \quad \text{complete square in exp term} \\
= \int_{g \in \mathbb{R}^n} exp(u^\top t + \frac{1}{2}t^\top Kt) \cdot \phi(g|\mu = u + Kt, \Sigma = K) \cdot \Phi(Ag + b)dg/C \\
= exp(u^\top t + \frac{1}{2}t^\top Kt) \cdot \Phi(A(u + Kt) + b|\Sigma = I + \text{AKA}^\top)/C \quad \text{compute integration as in (1)} \\
= exp(u^\top t + \frac{1}{2}t^\top Kt) \cdot \frac{\Phi(\text{Au} + b + \text{AK}(\Sigma = I + \text{AKA}^\top))}{\Phi(\text{Au} + b|\Sigma = I + \text{AKA}^\top)}
\]

Derive expression for CGP’s mean in (5):

**Proof.**

\[
E(g|u, K, \mathcal{C}) = \nabla_t M_q(t)\bigg|_{t=0} = u - KA^\top \frac{\nabla \Phi(\text{Au} + b|\Sigma = I + \text{AKA}^\top)}{\Phi(\text{Au} + b|\Sigma = I + \text{AKA}^\top)} \\
= u - K \frac{\nabla_u \Phi(\text{Au} + b|\Sigma = I + \text{AKA}^\top)}{\Phi(\text{Au} + b|\Sigma = I + \text{AKA}^\top)}
\]

where \( \nabla_u \Phi \) denotes the gradient of \( \Phi \) with respect to \( u \).

Furthermore, it can be shown that:

\[
\nabla_u \Phi(\text{Au} + b|\Sigma) = \int_{x \leq 0} \nabla_u \phi(x|\mu = \text{Au} + b, \Sigma)dx \\
= A^\top \Sigma^{-1} \int_{x \leq 0} (x - \text{Au})\phi(x|\mu = \text{Au} + b, \Sigma)dx \\
= A^\top \Sigma^{-1} \int_{x' \leq b} x'\phi(x'|\Sigma)dx,
\]
where recall 
\[
\mu = \Phi(A' \Sigma^{-1} E(b' | b' \geq -b, \Sigma)).
\]

This concludes the proof.

A.2. Derivation for CGP’s posterior PDF

First derive the posterior distribution for regression model:
\[
y_i \overset{\text{indep}}{\sim} \text{Normal}(g(z_i), \sigma^2)
\]
\[
g \sim \text{CGP}(\mu, k, \mathcal{G})
\]

Proof. To derive the posterior PDF, first write out its unnormalized form:
\[
f(g|\mathcal{G}, \mu, K, y) \propto f(y|g)f(g|\mathcal{G}, \mu, K)
\]
\[
\propto \exp\left(-\frac{1}{2\sigma^2}(y - g)^\top(y - g)\right) \times \phi(g|\mu, K) \times \Phi(A' g + b)
\]
\[
\propto \exp\left(-\frac{1}{2\sigma^2}(K' + \sigma^2 I)g + (y - K' u)\right) \times \Phi(A' g + b)
\]
\[
\propto \phi(g|\mu', \Sigma') \Phi(A' g + b)
\]
where \(\mu' = (K^{-1} + \sigma^{-2} I)^{-1}(\frac{1}{\sigma^2} y - K^{-1} u)\) and \(\Sigma' = (K^{-1} + \sigma^{-2} I)^{-1}\). Using spectral decomposition of \(K\), it can be shown easily that \(\mu' = u + K(K + \sigma^2 I)^{-1}(y - u)\) and \(\Sigma' = K - K(K + \sigma^2 I)^{-1} K\) as is done in the standard GP model (Rasmussen & Williams, 2006). Consequently, the expression for the posterior PDF is:
\[
f(g|\mathcal{G}, \mu, K, y) = \frac{\phi(g|\mu', \Sigma') \Phi(A' g + b)}{C}
\]
\[
C = \int_{g \in \mathbb{R}^n} \phi(g|\mu', \Sigma') \Phi(A' g + b) dg
\]
\[
= \Phi(A' \mu' + b) \Sigma = I + A \Sigma' A'\]
Using result from (1)

where recall \(\mu' = u + K(K + \sigma^2 I)^{-1}(y - u)\) and \(\Sigma' = K - K(K + \sigma^2 I)^{-1} K\).

Now derive the posterior distribution for classification model:
\[
y_i \overset{\text{indep}}{\sim} \text{Bernoulli}(p_i), p_i = \Phi(g(z_i))
\]
\[
g \sim \text{CGP}(\mu, k, \mathcal{G})
\]
Proof. To derive the posterior PDF, first write the expression for the likelihood $f(y|g)$. Denote $0 \leq i^+ \leq n^+$ and $0 \leq i^- \leq n^-$ the index set corresponding to positive and negative observations, then:

\[
    f(y|g) \propto \prod_{i^+} \Phi(g(z_i)) \cdot \prod_{i^-} (1 - \Phi(g(z_i)))
\]

\[
    = \prod_{i^=} \Phi(g(z_i)) \cdot \prod_{i^-} (\Phi(-g(z_i)))
\]

\[
    = \prod_i \Phi((2y_i - 1) g(z_i))
\]

\[
    = \Phi(Dg)
\]

where $D = \text{diag}(2 \cdot y - 1)$. Consequently, the posterior likelihood is:

\[
    f(g|h, u, K, y) \propto f(y|g) f(g|h, u, K)
\]

\[
    \propto f(g|h, u, K) \Phi(Dg)
\]

\[
    \propto \phi(g|\mu', \Sigma') \Phi(\mathbf{Ag} + \mathbf{b}) \Phi(Dg)
\]

\[
    \propto \phi(g|\mu', \Sigma') \Phi\left( \begin{bmatrix} A & | \mathbf{D} \mathbf{g} + \mathbf{b} \end{bmatrix} \right)
\]

B. ADDITIONAL DEFINITIONS

B.1. Full definition for $\varepsilon$-feasibility

We state the full definition of $\varepsilon$-feasibility:

DEFINITION 2 ($\varepsilon$-FEASIBILITY, FULL DEFINITION). Denote $\text{truncGP}(0,k,S)$ the truncated Gaussian process with mean zero, covariance kernel $k$ and its support truncated to be within the set $S$. For a small positive constant $\varepsilon > 0$, denote $S_\varepsilon = \{s | ||s|| \leq \varepsilon \}$ a “perturbation set” whose elements are random noise with maximum magnitude $\varepsilon$. Also denote $\alpha_\varepsilon = E\left(f(h|s_\varepsilon)\right)$ the “average feasibility” of random noise for $s_\varepsilon \sim \text{truncGP}(0,k,S_\varepsilon)$.

For a function $g^* \in \mathcal{H}$, we say $g^*$ is $\varepsilon$-feasible with respect to the probabilistic constraint $f(h|g)$ if the “$\varepsilon$-perturbed” function $g^* + s \sim \text{truncGP}(g^*,k,g^* + S_\varepsilon)$ satisfies any of the below conditions:

- ($\varepsilon$-feasibility, almost surely):

\[
    P\left(f(h|g^* + s) \geq \alpha_\varepsilon \right) = 1
\]

i.e. the $\varepsilon$-perturbed function $g^* + s$ is almost always more feasible than the random noise $s_\varepsilon$.

- ($\varepsilon$-feasibility, in probability):

\[
    P\left(f(h|g^* + s) < \alpha_\varepsilon \right) \leq \beta_\varepsilon
\]

i.e. the probability that the $\varepsilon$-perturbed function $g^* + s$ is less feasible than random noise is upper bounded by a constant $\beta_\varepsilon$.

In this work, we set $\beta_\varepsilon = P\left(f(h|g^* + s') < \alpha_\varepsilon \big| s' \in S_\varepsilon \right)$ for $g^* + s' \sim \text{CGP}(g^*,k,h)$.

- ($\varepsilon$-feasibility, in expectation):

\[
    E\left(f(h|g^* + s)\right) \geq \alpha_\varepsilon
\]

i.e. the $\varepsilon$-perturbed function $g^* + s$ is on average more feasible than the random noise $s_\varepsilon$. 
The definition of $\varepsilon$-feasibility requires $g^*$ to be “feasible enough” for $\mathcal{C}$ such that it is more feasible than the random noises even under random perturbation. The definition of "in probability" feasibility relaxes the almost-sure feasibility by only requiring the probability of violating the strong feasibility is small, i.e., upper bounded by a value $\beta_n$. Notice that in the above definition, $\beta_n$ measures the probability of the feasibility condition being violated by a "specially perturbed" function $g^* + s' \sim \text{CGP}(g^*, k, \varepsilon)$. Specifically, this function is similar to $g^* + s$ in that it perturbs $g^*$ using random noises with maximum magnitude $\varepsilon$, but it is "special" in the sense that the noise distribution is specially designed such that $g^* + s'$ still respects the probabilistic constraints $\mathcal{C}$ even after perturbation. Consequently, the weak feasibility condition essentially states that the perturbed $g^*$ should always be more feasible than the random noise regardless of how it is perturbed (i.e. if the perturbation noise respects $\mathcal{C}$ or not). Also notice that when $\varepsilon$ is very small (as is the case for Theorem 1), the $\varepsilon$-feasibility condition is essentially requiring $f(\mathcal{C}^* | g^*) \geq f(\mathcal{C}^* | 0)$, i.e. the target function $g^*$ needs to be as or more feasible than the prior mean function $0(x) = 0$.

C. Proof

C.1. Proof for CGP's posterior consistency

For a target function $g^*$ that is $\varepsilon$-feasible (in any sense as defined in Definition 2), we can show that the CGP prior assigns sufficient probability mass around its neighborhood, which is important for guaranteeing reasonable speed of posterior convergence toward $g^*$:

**Lemma 1 ($\varepsilon$-feasible function receives sufficient mass from CGP).** Let $g$ be distributed as a zero-mean CGP with covariance kernel $k$ and constraint $\mathcal{C}$. Consider a small ball $S_\varepsilon = \{g ||g|| \leq \varepsilon \}$, then for a $\varepsilon$-feasible function $g^* \in \mathcal{H}_k$, we have:

$$P(g : ||g - g^*|| \leq \varepsilon) \geq \exp\left( -||g||^2_{\mathcal{H}_k} \right) \* P(g : ||g|| \leq \varepsilon)$$

Intuitively, above result implies that for a function $g^*$ that is $\varepsilon$-feasible, the neighborhood surrounding $g^*$ with radius $\varepsilon$ is always receive ”sufficient” amount of probability mass from the CGP prior, in the sense that the amount of mass received is bounded away from zero by a function of $P(S_\varepsilon)$.

This result is analogous to the shifted-ball inequality for the standard Gaussian measures by Kuelbs et al. (1994) (Theorem 2), which played a key role in establishing the posterior convergence conditions for Gaussian processes (van der Vaart & van Zanten, 2008). We will use this result to establish the posterior convergence conditions for CGP. The proof is deferred to Section C.2.

Using Lemma 1, we are ready to establish the posterior convergence conditions for CGP:

**Proof.** Show Theorem 1 by showing conditions (I)-(III) are satisfied for suitable choices of $\varepsilon_n$ and $B_n$.

- Condition (I) is a direct consequence of Lemma 1 and the assumption on concentration function. Recall that the definition for concentration function is $\psi_{g^*}(\varepsilon) = \inf_{\hat{\theta} \in \mathcal{H}_k, ||\hat{\theta} - g^*|| \leq \varepsilon} ||\hat{\theta}||^2_{\mathcal{H}_k} - \log P(||g||_\infty \leq \varepsilon)$. Specifically, select $\hat{g}^*$ such that $||\hat{g}^* - g^*|| < \varepsilon_n$ and $||\hat{g}^*||^2_{\mathcal{H}_k} = \inf_{\hat{\theta} \in \mathcal{H}_k, ||\hat{\theta} - g^*|| \leq \varepsilon} ||\hat{\theta}||^2_{\mathcal{H}_k}$, then $||g - g^*||_\infty \leq \varepsilon_n + ||g - \hat{g}^*||_\infty$ and hence

$$P(||g - g^*||_\infty \leq 2\varepsilon_n) \geq P(||g - \hat{g}^*||_\infty \leq \varepsilon_n) \geq \exp\left(-\frac{1}{2}||\hat{g}^*||^2_{\mathcal{H}_k}\right) \* P(||g||_\infty \leq \varepsilon_n)$$

$$= \exp(-\psi_{g^*}(\varepsilon_n))$$

$$\geq \exp(-n\varepsilon_n^2)$$

where the second inequality follows by Lemma 1, and the third inequality follows by assumption on concentration function $\psi(\varepsilon_n) \leq n\varepsilon_n^2$. 
• Conditions (II) and (III) can be shown by construction, i.e., by showing that there exists a set \( B_n \) which satisfies (II) and (III).

Denote \( \mathbb{H}_1 \) a unit ball in the RKHS \( \mathcal{H} \), denote \( C_n \) the set of \( \epsilon_n \)-feasible functions such that \( f(\epsilon|g) > \alpha_n \), where \( \alpha_n \) is a small positive constant, and denote \( M_n \) a large positive constant.

We construct \( B_n \) as:

\[
B_n = M_n \mathbb{H}_1 \cap C_n,
\]

that is, \( B_n \) is a subset of the RKHS that contains highly feasible functions. We show that \( B_n \) satisfies (II) and (III) for suitable choices of \( \alpha_n \) and \( M_n \).

First show (II). Notice that by De Morgan’s law, \( (M_n \mathbb{H}_1 \cap C_n)^c = (M_n \mathbb{H}_1)^c \cup C_n^c \), which implies that \( P(g \not\in B_n) \leq P(g \not\in M_n \mathbb{H}_1) + P(g \not\in C_n) \), therefore only need to show \( P(g \not\in M_n \mathbb{H}_1) + P(g \not\in C_n) \leq e^{-n\epsilon_n^2} \) for suitable choice of \( M_n \) and \( \alpha_n \).

First consider \( P(g \not\in M_n \mathbb{H}_1) \):

\[
P(g \not\in M_n \mathbb{H}_1) = \int_{||g||_{\mathcal{H}} > M_n} \frac{\phi_k(g)f(\epsilon|g)}{E(f(\epsilon|g))} dg \\
\leq \int_{||g||_{\mathcal{H}} > M_n} \frac{\phi_k(g)}{E(f(\epsilon|g))} dg \\
= D \int_{||g||_{\mathcal{H}} > M_n} \phi_k(g) dg = D \cdot P(||g||_{\mathcal{H}} > M_n) \\
\leq D \cdot E\left(\exp(||g||_{\mathcal{H}}^2)\right) \cdot \exp(-M_n^2) \\
\leq D \cdot G \cdot \exp(-M_n^2)
\]

where we have denoted \( D, G \) two positive constants such that \( D = \frac{1}{E(f(\epsilon|g))} \) and \( G = E\left(\exp(||g||_{\mathcal{H}}^2)\right) \). In the above equation, the first inequality follows since \( f(\epsilon|g) \leq 1 \), and second inequality follows by first square and exponentiate both sides in \( P(||g||_{\mathcal{H}} > M_n) \), and then apply the Markov’s inequality.

Now consider \( P(g \not\in C_n) \):

\[
P(g \not\in C_n) = \int_{f(\epsilon|g) < \alpha_n} \frac{\phi_k(g)f(\epsilon|g)}{E(f(\epsilon|g))} dg \\
\leq \frac{\alpha_n}{E(f(\epsilon|g))} \int_{f(\epsilon|g) < \alpha_n} \phi_k(g) dg \\
= \frac{\alpha_n}{E(f(\epsilon|g))} \\
= D \cdot \alpha_n
\]

where the first inequality follows by the definition of \( C_n \), the second inequality follows since \( \int_{f(\epsilon|g) < \alpha_n} \phi_k(g) dg \leq 1 \), i.e. integrating a Gaussian measure \( \phi_k(g) \) over a subset of its full support yields a value less than 1.

Now for any \( C > 1 \) such that \( \exp(-Cn\epsilon_n^2) \leq \frac{1}{2} + \frac{1}{2} \cdot \frac{\alpha_n}{C^2} = \frac{1}{2} \cdot \frac{E(f(\epsilon|g))}{\exp(||g||_{\mathcal{H}}^2)} + \frac{1}{2} \), set

\[
M_n^2 = 2Cn\epsilon_n^2, \quad \alpha_n = e^{-2Cn\epsilon_n^2}, \quad (1)
\]
we then have

\[
P(g \not\in B_n) \leq P(g \not\in M_n H_1) + P(g \not\in C_n)
\leq D * G * \exp(-M_n^2) + D * \alpha_n
\leq \frac{1}{2} e^{-Cn^2} + \frac{1}{2} e^{-Cn^2} = e^{-Cn^2}.
\]

Therefore condition (II) is satisfied.

Now show $B_n$ satisfies the entropy number condition (III).

Recall that for the set $B_n$, its entropy number $N(\varepsilon_n, B_n, |||\cdot|||)$ is defined as the minimum number of balls of radius $\varepsilon_n$ needed to cover $B_n$ in a metric space with norm $|||\cdot|||$. Define $h_1, \ldots, h_N$ elements of $M_n H_1 \cap C_n$ that are $2\varepsilon_n$-separated with respect to the uniform norm $|||\cdot|||$, then $|||\cdot|||$-balls with radius $\varepsilon_n$ and centers at $h_j$ are mutually disjoint. Therefore, denote $E_n = \{ g |||g||| < \varepsilon_n \}$, for $g \in B_n$, we have:

\[
1 \geq \sum_{j=1}^{N} P(g \in (h_j + E_n) \cap C_n)
\geq \sum_{j=1}^{N} \exp \left( -\frac{1}{2} ||h_j||_{H_k}^2 \right) P(g \in E_n)
\geq N * \exp \left( -\frac{1}{2} M_n^2 \right) P(g \in E_n)
\]

where the second inequality follows by Lemma 1, the third inequality follows since $h_j \in M_n H_1$, which implies $||h_j||_{H_k}^2 \leq M_n$. It then follows that:

\[
\log N \leq \frac{1}{2} M_n^2 - \log P(g \in E_n)
\leq Cn\varepsilon_n^2 - \log P(g \in E_n)
\leq Cn\varepsilon_n^2 + n\varepsilon_n^2
\leq 2Cn\varepsilon_n^2,
\]

where the first inequality follows by the definition of $M_n$ in (1), second inequality follows by the assumption that the concentration function satisfy $\psi(\varepsilon_n) \leq n\varepsilon_n^2$, the last inequality follows since $C > 1$.

Finally, let $h_1, \ldots, h_N$ be maximal in the set $M_n H_1$ and recall that $h_j$'s are $2\varepsilon_n$ separated, then by the definition of entropy number, we have:

\[
\log N(2\varepsilon_n, B_n, |||\cdot|||) \leq \log N \leq 3Cn\varepsilon_n^2.
\]

Therefore condition (III) is satisfied. □

C.2. Proof for Lemma 1

Proof. Notice that the statement in the lemma is equivalent to:

\[
P(S_{\varepsilon} + g^*) \geq \exp \left( -\frac{1}{2} ||g^*||_{H_k}^2 \right) * P(S_{\varepsilon})
\]

therefore only need to show above statement is true.

- First show (2) holds for $g^*$ that is $\varepsilon$-feasible almost surely.
Recall that almost surely $\epsilon$ feasibility is defined as $f(\mathcal{E}|g^* + s) \geq E(f(\mathcal{E}|s)) \forall s \in S_{\epsilon}$. Start from the left hand side of (2), by the definition of zero-mean CGP:

$$P(S_{\epsilon} + g^*) = \int_{g' \in S_{\epsilon} + g^*} P(g') dg' = \int_{g \in S_{\epsilon}} P(g + g^*) dg$$

$$= \int_{g \in S_{\epsilon}} \frac{\phi_k(g + g^*) f(\mathcal{E}|g + g^*)}{E(f(\mathcal{E}|g))} dg$$

$$\geq \frac{E(f(\mathcal{E}|s))}{E(f(\mathcal{E}|g))} \int_{g \in S_{\epsilon}} \phi_k(g + g^*) * dg$$

$$= \frac{1}{\phi_k(S_{\epsilon})} \int_{z \in S_{\epsilon}} \frac{\phi_k(z) f(\mathcal{E}|z)}{E(f(\mathcal{E}|g))} * \int_{g \in S_{\epsilon}} \phi_k(g + g^*) * dg$$

$$= \frac{P(S_{\epsilon})}{\phi_k(S_{\epsilon})} \int_{g \in S_{\epsilon}} \phi_k(g + g^*) * dg$$

$$\geq P(S_{\epsilon}) \exp \left( -\frac{1}{2} ||g^*||^2_{H_{\epsilon}} \right)$$

where the first equality follows from change of variables, the second equality follows from the definition of CGP. The first inequality follows from the fact that $g^*$ is strongly $\epsilon$-feasible, the second inequality follows since $E(f(\mathcal{E}|g)) \leq 1$, the last inequality follows by the shift-ball inequality for Gaussian measures (Theorem 2 of Kuelbs et al. (1994)).

• Now show (2) also holds for $g^*$ that is $\epsilon$-feasible in probability.

Denote the event that a function $g$ violates the strong $\epsilon$ feasibility as $R_g = \{ g | f(\mathcal{E}|g) \leq \alpha_{\epsilon} \}$, and the event that a noise $s$ makes $g^*$ violating the strong $\epsilon$ feasibility as $R_s = \{ \epsilon | f(\mathcal{E}|g^* + \epsilon) \leq \alpha_{\epsilon} \}$.

Also denote $g^* + s \sim \text{truncGP}(g^*, k, g^* + S_{\epsilon})$ and $g^* + s' \sim \text{CGP}(g^*, k, \mathcal{E})$ two perturbed functions by random noises distributed as truncated and constrained GPs, respectively. Recall that weak $\epsilon$ feasibility upper bounds the probability of $g^* + s$ violating feasibility by requiring below to be true:

$$P(g^* + s \in R_g) \leq P(g^* + s' \in R_g | s' \in S_{\epsilon})$$

First derive a useful fact using the definition of weak $\epsilon$ feasibility. Notice that:

$$P(g^* + s \in R_g) = \int_{g^* + s \in R_g} \frac{\phi(g^* + s)}{\phi(g^* + S_{\epsilon})} d(g^* + s)$$

$$= \int_{s \in R_g} \frac{\phi(g^* + s)}{\phi(g^* + S_{\epsilon})} ds$$

$$P(g^* + s' \in R_g | s' \in S_{\epsilon}) = \frac{P(g^* + s' \in R_g, g^* + s' \in S_{\epsilon})}{P(s' \in S_{\epsilon})}$$

$$= \frac{1}{P(s' \in S_{\epsilon})} \int_{g^* + s' \in R_g | g^* + s' \in S_{\epsilon}} \frac{\phi(g^* + s') f(\mathcal{E}|g^* + s')}{E(f(\mathcal{E}|g))} d(g^* + s')$$

$$= \frac{1}{P(s' \in S_{\epsilon})} \int_{g^* + s' \in R_g | g^* + s' \in S_{\epsilon}} \frac{\phi(g^* + s') f(\mathcal{E}|g^* + s')}{E(f(\mathcal{E}|g))} ds'$$

we can then derive below:

$$\int_{s' \in S_{\epsilon}} \frac{\phi(g^* + s') f(\mathcal{E}|g^* + s')}{E(f(\mathcal{E}|g))} ds' \geq P(s' \in S_{\epsilon}) \int_{s \in R_g} \frac{\phi(g^* + s)}{\phi(g^* + S_{\epsilon})} ds.$$  (3)
Finally show (2) holds for $t\text{runcGP}_\varepsilon$ for Gaussian measures (Theorem 2 of Kuelbs et al. (1994)).

Using above fact, we are now ready to show (2). Starting from the left-hand side:

$$P(S_\varepsilon + g^*) = \int_{g^* \in S_\varepsilon + g^*} P(g') dg' = \int_{g^* \in S_\varepsilon} P(g + g^*) dg$$

$$= \int_{g^* \in S_\varepsilon \cap \mathcal{R}_\varepsilon} P(g + g^*) dg + \int_{g^* \in S_\varepsilon \cap \mathcal{R}_\varepsilon^c} P(g + g^*)$$

$$= \int_{g^* \in S_\varepsilon \cap \mathcal{R}_\varepsilon} \frac{\phi_k(g + g^*) f(\mathcal{C}^s | g + g^*)}{E(f(\mathcal{C}^s | g))} dg + \int_{g^* \in S_\varepsilon \cap \mathcal{R}_\varepsilon^c} \frac{\phi_k(g + g^*) f(\mathcal{C}^s | g + g^*)}{E(f(\mathcal{C}^s | g))} dg$$

$$\geq \int_{g^* \in S_\varepsilon \cap \mathcal{R}_\varepsilon} \frac{\phi_k(g + g^*) f(\mathcal{C}^s | g + g^*)}{E(f(\mathcal{C}^s | g))} dg + \frac{P(S_\varepsilon)}{\phi_k(S_\varepsilon)} \int_{g^* \in S_\varepsilon \cap \mathcal{R}_\varepsilon^c} \phi_k(g + g^*) dg$$

$$\geq \frac{P(S_\varepsilon)}{\phi_k(S_\varepsilon)} \int_{g^* \in S_\varepsilon \cap \mathcal{R}_\varepsilon} \phi_k(g + g^*) dg + \frac{P(S_\varepsilon)}{\phi_k(S_\varepsilon)} \int_{g^* \in S_\varepsilon \cap \mathcal{R}_\varepsilon^c} \phi_k(g + g^*) dg$$

$$= \frac{P(S_\varepsilon)}{\phi_k(S_\varepsilon)} \int_{g^* \in S_\varepsilon} \phi_k(g + g^*) dg$$

$$\geq P(S_\varepsilon) \exp \left( - \frac{1}{2} \| g^* \|^2_{\mathcal{R}_\varepsilon^c} \right),$$

where the last inequality follows by noticing $S_\varepsilon \cap \mathcal{R}_\varepsilon^c$ is the region where the strong $\varepsilon$-feasibility $f(\mathcal{C}^s | g + g^*) \geq E(f(\mathcal{C}^s | s))$ is satisfied, therefore the inequality in the second integral follows by the definition of strong $\varepsilon$-feasibility (see the proof for strong $\varepsilon$-feasibility for detail). We now handle the first integral by applying the fact (3):

$$= \frac{P(S_\varepsilon)}{\phi_k(S_\varepsilon)} \int_{g^* \in S_\varepsilon} \phi_k(g + g^*)$$

where the first inequality follows by the fact (3), the second inequality follows by the Anderson’s theorem (Anderson, 1955; Gardner, 2002), and the last inequality follows by the shift-ball inequality for Gaussian measures (Theorem 2 of Kuelbs et al. (1994)).

Finally show (2) holds for $g^*$ that is $\varepsilon$-feasible in expectation.

Recall that the in-expectation $\varepsilon$ feasibility is defined as $E(f(\mathcal{C}^s | g^* + s)) \geq E(f(\mathcal{C}^s | s'))$ for $g^* + s \sim \text{truncGP}(g^*, k, g^* + S_\varepsilon)$ and $s' \sim \text{truncGP}(0, k, S_\varepsilon)$. Also notice that:

$$E(f(\mathcal{C}^s | g^* + s)) = \int_{s \in S_\varepsilon} f(\mathcal{C}^s | g^* + s) \frac{\phi(g^* + s)}{\phi(g^* + S_\varepsilon)} ds$$

$$E(f(\mathcal{C}^s | s)) = \int_{s \in S_\varepsilon} f(\mathcal{C}^s | s) \frac{\phi(s)}{\phi(S_\varepsilon)} ds,$$

therefore the in-expectation $\varepsilon$ feasibility implies that

$$\int_{s \in S_\varepsilon} f(\mathcal{C}^s | g^* + s) \phi(g^* + s) ds \geq \frac{\phi(g^* + S_\varepsilon)}{\phi(S_\varepsilon)} \int_{s \in S_\varepsilon} f(\mathcal{C}^s | s) \phi(s) ds \tag{5}$$
We are now ready to show (2), start from the left hand side:

\[
P(S_\epsilon + g^*) = \int_{g' \in S_\epsilon + g^*} P(g')dg' = \int_{g \in S_\epsilon} P(g + g^*)dg
\]

\[
= \int_{g \in S_\epsilon} \frac{\phi_\delta(g + g^*)f(C|g + g^*)}{E(f(C|g))}dg
\]

\[
\geq \frac{\phi(g^* + S_\epsilon)}{\phi(S_\epsilon)} \ast \int_{s \in S_\epsilon} \frac{f(C|s)\phi(s)}{E(f(C|g))}ds
\]

\[
= \frac{\phi(g^* + S_\epsilon)}{\phi(S_\epsilon)} \ast P(S_\epsilon)
\]

\[
\geq \exp\left(-\frac{1}{2}\|g^*\|_{\mathcal{H}}^2\right) \ast P(S_\epsilon)
\]

where the first inequality follows from the fact (5) implied by the in-expectation \(\epsilon\)-feasibility, the second inequality follows by the shift-ball inequality for Gaussian measures (Theorem 2 of Kuelbs et al. (1994)).