Expected loss derviation from Osborne 2009 GPGO article

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1 Problem statement

In 2009, Osborne el al. introduced a novel Bayesian approach to global optimization using Gaussian processes [1]. In Section 3.1, they derive an analytical expression for a new loss function to determine where best to evaluate a function being optimized using Bayesian optimization. They call this new loss the Bayesian expected loss criterion.

The article sets up the problem as such:

Suppose $(\boldsymbol{x}_0, \boldsymbol{y}_0)$ are the function evaluations gathered thus far and define $\eta := \min \boldsymbol{y}_0$. Given this, we can define the loss of evaluating the function one last time at x and its returning y

$$\lambda(y) := \begin{cases} y; & y < \eta \\ n; & y \geq \eta \end{cases}$$

The loss at the new observed minimum is $\min(y, \eta)$. The analytic form is then dervied

$$\Lambda_1(x \,|\, I_0) := \int \lambda(y) \cdot p(y \,|\, x, I_0) \, dy = \sum_{i \in S} \rho_i V_i(x \,|\, I_0)$$

$V_i(x \,|\, I_0)$ is then shown to be

$$\begin{aligned} V_i(x \,|\, I_0) &:= \eta \int_{\eta}^{\infty} \mathcal{N}(y; m_i, C_i) \, dy + \int_{-\infty}^{\eta} y \, \mathcal{N}(y; m_i, C_i) \, dy \\ &= \eta + (m_i - \eta)\Phi(\eta; m_i, C_i) - C_i \mathcal{N}(\eta; m_i, Ci) \end{aligned}$$

Where m_i is $m_i(y|I_0)$—the mean function—and C_i is $C_i(y|I_0)$—the covariance function, with notation sometimes seen as $k(y_0, y \,|\, I_0)$.

2 Derivation

We focus on this derivation of $V_i(x \mid I_0)$. Our integral must be split at the critical value η. When $y < \eta$, $\lambda(y) = y$ and when $y \geq \eta$, $\lambda(y) = \eta$. Calling $\Lambda_1(x \mid I_0) = \mathbb{E}[\lambda(y)]$ and making explicit that we are integrating over y,

$$\mathbb{E}[\lambda(y)] := \int_{y=-\infty}^{y=\eta} y \cdot p(y \mid x, I_0)\, dy + \int_{y=\eta}^{y=\infty} \eta \cdot p(y \mid x, I_0)\, dy$$

Note that $p(y \mid x, I_0)$ is driven by the Gaussian process!

$$p(y \mid x, I_0) = \mathcal{N}\big(y; m(y \mid I_0), C_i(y|I_0)\big)$$

Plugging this into the integrals, we get

$$\mathbb{E}[\lambda(y)] = \int_{-\infty}^{\eta} y \cdot \mathcal{N}\big(y; m(y \mid I_0), C_i(y|I_0)\big)\, dy \\ + \int_{\eta}^{\infty} \eta \cdot \mathcal{N}\big(y; m_i(y \mid I_0), C_i(y|I_0)\big)\, dy$$

Let us work on each integral at a time. We can call the first integral A and the second integral B.

2.1 Integral B

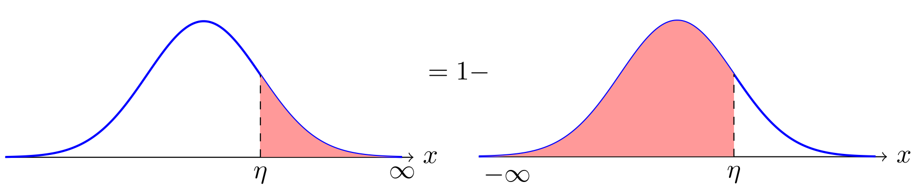
Starting with B,

$$B = \int_{\eta}^{\infty} \eta \cdot \mathcal{N}\big(y; m_i(y \mid I_0), C_i(y|I_0)\big)\, dy$$

Pulling out the η as the integral is with respect to y and replacing $m_i(y \mid I_0)$ and $C_i(y|I_0)$ with μ and σ^2, respectively, for notational simplicity.

$$B = \eta \int_{\eta}^{\infty} \mathcal{N}(y; \mu, \sigma^2)\, dy$$

Notice here that we are integrating the pdf of the normal distribution, which can be calculated using its cdf, $\Phi(\cdot)$. All that is needed to replace the intergral with $\Phi(\cdot)$ is to notice that the integral from a value x to infinity is equal to the integral of 1 minus the integral of negative infinity to that value.



Therefore,

$$
\begin{aligned}
B &= \eta \left(1 - \int_{-\infty}^{\eta} \mathcal{N}(y;\mu,\sigma^2)\,dy\right) \\
&= \eta(1 - \Phi(\eta;\mu,\sigma^2))
\end{aligned}
$$

2.2 Integral A

Now, we move to integral A:

$$
A = \int_{-\infty}^{\eta} y \cdot \mathcal{N}\big(y; m(y \mid I_0), C_i(y|I_0)\big)\,dy
$$

Substituting the pdf of the normal distribution

$$
A = \int_{-\infty}^{\eta} y \cdot \frac{1}{\sqrt{2\pi\sigma^2}} \cdot \exp\left\{-\frac{1}{2}\left(\frac{y-\mu}{\sigma}\right)^2\right\}\,dy
$$

Making the substitution $z = \frac{y-\mu}{\sigma}$,

$$
\begin{aligned}
dz &= d\left(\frac{y-\mu}{\sigma}\right) \\
&= d\left(\frac{y}{\sigma} - \frac{\mu}{\sigma}\right) \\
&= \frac{1}{\sigma}dy \\
\sigma \cdot dz &= dy
\end{aligned}
$$

We also have to substitute y, which is $\sigma z + \mu$ by simple rearrangement.

Plugging in z for y,

$$
A = \int_{-\infty}^{\eta} (\sigma z + \mu) \cdot \frac{1}{\sqrt{2\pi\sigma^2}} \cdot \exp\left\{-\frac{1}{2}z^2\right\}\,\sigma \cdot dz
$$

The limits of integration also need to be changed. When $y = \infty$,

$$
\begin{aligned}
z &= \frac{y-\mu}{\sigma} \\
&= \frac{-\infty-\mu}{\sigma} \\
&= -\infty
\end{aligned}
$$

And when $y = \eta$,

$$
z = \frac{\eta-\mu}{\sigma}
$$

Thus,

$$A = \int_{-\infty}^{\frac{\eta-\mu}{\sigma}} (\sigma z + \mu) \cdot \frac{1}{\sqrt{2\pi\sigma^2}} \cdot \exp\left\{-\frac{1}{2}z^2\right\} \sigma \cdot dz$$

Pulling out the constant and rearranging the sigma,

$$A = \frac{1}{\sqrt{2\pi\sigma^2}} \int_{-\infty}^{\frac{\eta-\mu}{\sigma}} \sigma(\sigma z + \mu) \cdot \exp\left\{-\frac{1}{2}z^2\right\} dz$$

Mutliplying out,

$$\begin{aligned} A &= \frac{1}{\sqrt{2\pi\sigma^2}} \int_{-\infty}^{\frac{\eta-\mu}{\sigma}} \sigma(\sigma z + \mu) \cdot \exp\left\{-\frac{1}{2}z^2\right\} dz \\ &= \frac{1}{\sqrt{2\pi\sigma^2}} \int_{-\infty}^{\frac{\eta-\mu}{\sigma}} (\sigma^2 z + \sigma\mu) \cdot \exp\left\{-\frac{1}{2}z^2\right\} dz \\ &= \frac{1}{\sqrt{2\pi\sigma^2}} \left[\int_{-\infty}^{\frac{\eta-\mu}{\sigma}} \sigma^2 z \exp\left\{-\frac{1}{2}z^2\right\} + \sigma\mu \exp\left\{-\frac{1}{2}z^2\right\} dz\right] \end{aligned}$$

Distributing the constant $\frac{1}{\sqrt{2\pi\sigma^2}}$ and the integral,

$$A = \frac{1}{\sqrt{2\pi\sigma^2}} \int_{-\infty}^{\frac{\eta-\mu}{\sigma}} \sigma^2 z \exp\left\{-\frac{1}{2}z^2\right\} dz + \frac{1}{\sqrt{2\pi\sigma^2}} \int_{-\infty}^{\frac{\eta-\mu}{\sigma}} \sigma\mu \exp\left\{-\frac{1}{2}z^2\right\} dz$$

We can split this integrals again,

$$A_1 = \frac{1}{\sqrt{2\pi\sigma^2}} \int_{-\infty}^{\frac{\eta-\mu}{\sigma}} \sigma^2 z \exp\left\{-\frac{1}{2}z^2\right\} dz \quad A_2 = \frac{1}{\sqrt{2\pi\sigma^2}} \int_{-\infty}^{\frac{\eta-\mu}{\sigma}} \sigma\mu \exp\left\{-\frac{1}{2}z^2\right\} dz$$

Taking the first integral A_1,

$$\begin{aligned} A_1 &= \frac{1}{\sqrt{2\pi\sigma^2}} \int_{-\infty}^{\frac{\eta-\mu}{\sigma}} \sigma^2 z \exp\left\{-\frac{1}{2}z^2\right\} dz \\ &= \frac{\sigma^2}{\sqrt{2\pi\sigma^2}} \int_{-\infty}^{\frac{\eta-\mu}{\sigma}} z \exp\left\{-\frac{1}{2}z^2\right\} dz \end{aligned}$$

This integral can be solved using u-substitution with $u = -\frac{1}{2}z^2$.

$$A_1 = \frac{\sigma^2}{\sqrt{2\pi\sigma^2}} \left[-\exp\left\{-\frac{1}{2}z^2\right\} \Bigg|_{-\infty}^{\frac{\eta-\mu}{\sigma}} \right]$$

At minus infinity, the above evaluates to 0. Thus, we have

$$\begin{aligned}
A_1 &= \frac{\sigma^2}{\sqrt{2\pi\sigma^2}} - \exp\left\{-\frac{1}{2}\left(\frac{\eta-\mu}{\sigma}\right)^2\right\} \\
&= -\sigma^2 \underbrace{\frac{1}{\sqrt{2\pi\sigma^2}} \exp\left\{-\frac{1}{2}\left(\frac{\eta-\mu}{\sigma}\right)^2\right\}}_{\text{pdf of normal}} \\
&= -\sigma^2 \mathcal{N}(\eta; \mu, \sigma^2)
\end{aligned}$$

Now for integral A_2,

$$\begin{aligned}
A_2 &= \frac{1}{\sqrt{2\pi\sigma^2}} \int_{-\infty}^{\frac{\eta-\mu}{\sigma}} \sigma\mu \exp\left\{-\frac{1}{2}z^2\right\} dz \\
&= \sigma\mu \frac{1}{\sqrt{2\pi\sigma^2}} \underbrace{\int_{-\infty}^{\frac{\eta-\mu}{\sigma}} \exp\left\{-\frac{1}{2}z^2\right\}}_{\text{the error function}} dz
\end{aligned}$$

The general form for the integral of the error function is

$$\int \exp\{-ax^2\}\, dx = \frac{1}{2}\sqrt{\frac{\pi}{a}} \cdot \text{erf}(\sqrt{a}x)$$

Using this, we complete the above integral as,

$$A_2 = \sigma\mu \frac{1}{\sqrt{2\pi\sigma^2}} \left(\frac{1}{2} \cdot \sqrt{\frac{\pi}{1/2}} \cdot \text{erf}\left(\sqrt{\frac{1}{2}} \cdot z\right) \Bigg|_{-\infty}^{\frac{\eta-\mu}{\sigma}} \right)$$

The limit as $z \to -\infty$ of the error function is -1. Thus, we have

$$\begin{aligned}
A_2 &= \sigma\mu \frac{1}{\sqrt{2\pi\sigma^2}} \left(\frac{1}{2} \cdot \sqrt{\frac{\pi}{1/2}} \cdot \text{erf}\left(\sqrt{\frac{1}{2}} \cdot \frac{\eta-\mu}{\sigma}\right) - -\frac{1}{2} \cdot \sqrt{\frac{\pi}{1/2}} \right) \\
&= \sigma\mu \frac{1}{\sqrt{2\pi\sigma^2}} \left(\frac{1}{2} \cdot \sqrt{2\pi} \cdot \text{erf}\left(\frac{1}{\sqrt{2}} \cdot \frac{\eta-\mu}{\sigma}\right) + \frac{1}{2} \cdot \sqrt{2\pi} \right)
\end{aligned}$$

Pull the $\sqrt{2\pi}$ all the way out,

$$A_2 = \sigma\mu \frac{1}{\sqrt{2\pi\sigma^2}} \cdot \sqrt{2\pi} \left(\frac{1}{2}\text{erf}\left(\frac{1}{\sqrt{2}} \cdot \frac{\eta-\mu}{\sigma}\right) + \frac{1}{2} \right)$$

Pull the $\frac{1}{2}$, but keep it within the paretheses. Also note that $\sqrt{2\pi}$ cancels and σ cancels with $1/\sigma^2$ leaving μ alone out front,

$$A_2 = \mu \left(\frac{1}{2} \left(1 + \text{erf}\left(\frac{1}{\sqrt{2}} \cdot \frac{\eta-\mu}{\sigma} \right) \right) \right)$$

Finally, we can use the definition of the cdf of the normal distribution,

$$\Phi\left(x;\mu,\sigma^2\right) = \frac{1}{2}\left(1 + \operatorname{erf}\left(\frac{x-\mu}{\sqrt{2}\sigma}\right)\right)$$

So,

$$A_2 = \mu\Phi\left(\eta;\mu,\sigma^2\right)$$

Combining the two, we get

$$A = -\sigma^2\mathcal{N}(\eta;\mu,\sigma^2) + \mu\Phi\left(\eta;\mu,\sigma^2\right)$$

Adding this to B,

$$\begin{aligned}
\mathbb{E}[\lambda(y)] &= \eta(1-\Phi(\eta;\mu,\sigma^2)) - \sigma^2\mathcal{N}(\eta;\mu,\sigma^2) + \mu\Phi\left(\eta;\mu,\sigma^2\right) \\
&= \eta + \mu\Phi\left(\eta;\mu,\sigma^2\right) - \eta\Phi(\eta;\mu,\sigma^2) - \sigma^2\mathcal{N}(\eta;\mu,\sigma^2) \\
&= \eta + (\mu-\eta)\Phi(\eta;\mu,\sigma^2) - \sigma^2\mathcal{N}(\eta;\mu,\sigma^2)
\end{aligned}$$

Substituting back in m_i for μ and C_i for σ^2, we can finally right,

$$\mathbb{E}[\lambda(y)] = \eta + (m_i-\eta)\Phi(\eta;m_i,C_i) - C_i\mathcal{N}(\eta;m_i,C_i). \quad \square$$

References

[1] Michael A. Osborne, Roman Garnett, and Stephen J. Roberts. "Gaussian Processes for Global Optimization". In: *Proceedings of the 3rd International Conference on Learning and Intelligent Optimization (LION3)*. 2009.