Supplementary Information

FOCAPO-CPC 27

Acquisition Functions for Gaussian Process Model Predictive Control

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DERIVATION OF EXPECTED IMPROVEMENT ACQUISITION FUNCTION FOR SCALED NON-CENTRAL CHI-SQUARE DISTRIBUTION

We define the Expected Improvement function for the objective value, which is a scaled non-central chi-square distribution with a constant offset, $J \sim \lambda\chi^2_{k=1}(\delta) + c$. The probability density function (PDF) of J and $\chi^2_k(\delta)$ is denoted ϕ_J and $\phi_{\chi^2_k(\delta)}$, respectively. The parameter k is the degree of freedom and δ is the non-centrality parameter. The variables j and z are samples from J and $\chi^2_k(\delta)$, respectively, and $j = \lambda z + c$.

$$
\begin{aligned}
EI(f_{min}, \lambda, \delta, c) &= \mathrm{E}_J[\max(f_{min} - J, 0)] \\
&= \int_0^\infty \max(f_{min} - j, 0)\phi_J(j)dj \\
&= \int_0^\infty \max(f_{min} - (\lambda z + c), 0)\phi_{\chi^2_{k=1}(\delta)}(z)dz \\
&= \int_0^{\frac{f_{min}-c}{\lambda}} (f_{min} - \lambda z - c))\phi_{\chi^2_{k=1}(\delta)}(z)dz \\
&= (f_{min} - c)\int_0^{\frac{f_{min}-c}{\lambda}} \phi_{\chi^2_{k=1}(\delta)}(z)dz + \lambda\int_0^{\frac{f_{min}-c}{\lambda}} z\phi_{\chi^2_{k=1}(\delta)}(z)dz \\
&= (f_{min} - c)\Phi_{\chi^2_{k=1}(\delta)}\left(\frac{f_{min} - c}{\lambda}\right) + \lambda\int_0^{\frac{f_{min}-c}{\lambda}} z\phi_{\chi^2_{k=1}(\delta)}(z)dz
\end{aligned}
$$

The function $\Phi_{\chi^2_{k=1,\delta}}(\cdot)$ is the cumulative distribution function of $\chi^2_{k=1}(\delta)$, and is readily evaluated from off-the-shelf tools such as SciPy. Now we look at the integral in the second term.

$$
\int_0^{\frac{f_{min}-c}{\lambda}} z\phi_{\chi^2_{k=1}(\delta)}(z)dz \tag{1}
$$

where the non-central chi-square PDF $\phi_{\chi^2_{k=1}(\delta)}(z)$ is a Poisson-weighted mixture of central chi-square PDFs with increasing degrees of freedom:

$$
\phi_{\chi^2_k(\delta)}(z) = \sum_{m=0}^{\infty} \frac{e^{-\delta/2}(\delta/2)^m}{m!}\phi_{\chi^2_{k+2m}}(z)
$$

Multiplying by z and using the central chi-square relationship of $z\phi_{\chi_k^2}(z) = k \cdot \phi_{\chi_{k+2}^2}(z)$ freedom gives:

$$
\begin{aligned}
z \cdot \phi_{\chi_k^2(\delta)}(z) &= \sum_{m=0}^{\infty} \frac{e^{-\delta/2}(\delta/2)^m}{m!}(k+2m)\phi_{\chi_{k+2m+2}^2}(z) \\
&= k\sum_{m=0}^{\infty} \frac{e^{-\delta/2}(\delta/2)^m}{m!}\phi_{\chi_{k+2m+2}^2}(z) + 2\sum_{m=0}^{\infty} m \cdot \frac{e^{-\delta/2}(\delta/2)^m}{m!}\phi_{\chi_{k+2m+2}^2}(z)
\end{aligned}
$$

We simplify the first term with the non-central Chi-square identity:

$$
k \cdot \sum_{m=0}^{\infty} \frac{e^{-\delta/2}(\delta/2)^m}{m!}\phi_{\chi_{k+2m+2}^2}(z) = k\phi_{\chi_{k+2}^2(\delta)}(z)
$$

The second term can be simplified as a Poisson mixture equivalent to non-central chi-square distribution with $k+4$ degrees of freedom:

$$
\begin{aligned}
2\sum_{m=0}^{\infty} m \cdot \frac{e^{-\delta/2}(\delta/2)^m}{m!}\phi_{\chi_{k+2m+2}^2}(z) &= 2\sum_{m=0}^{\infty} m \cdot \frac{\delta}{2} \cdot \frac{e^{-\delta/2}(\delta/2)^{m-1}}{m \cdot (m-1)!}\phi_{\chi_{k+2m+2}^2}(z) \\
&= \delta\sum_{m=0}^{\infty} \frac{e^{-\delta/2}(\delta/2)^{m-1}}{(m-1)!}\phi_{\chi_{k+2m+2}^2}(z) \\
&= \delta\phi_{\chi_{k+4}^2(\delta)}(z)
\end{aligned}
$$

Therefore, we can write the integral in Eq (1) as follows:

$$
\begin{aligned}
\int_0^{\frac{f_{min}-c}{\lambda}} z\phi_{\chi_{k=1}^2(\delta)}(z)dz &= \int_0^{\frac{f_{min}-c}{\lambda}} k\phi_{\chi_{k=3}^2(\delta)}(z)dz + \int_0^{\frac{f_{min}-c}{\lambda}} \delta\phi_{\chi_{k=5}^2(\delta)}(z)dz \\
&= k\Phi_{\chi_{k=3}^2(\delta)}\left(\frac{f_{min}-c}{\lambda}\right) + \delta\Phi_{\chi_{k=5}^2(\delta)}\left(\frac{f_{min}-c}{\lambda}\right)
\end{aligned}
$$

And finally, the EI function as:

$$
EI(f_{min}, \lambda, \delta, c) = (f_{min} - c)\Phi_{\chi_{k=1}^2(\delta)}\left(\frac{f_{min}-c}{\lambda}\right) + \lambda\left[k\Phi_{\chi_{k=3}^2(\delta)}\left(\frac{f_{min}-c}{\lambda}\right) + \delta\Phi_{\chi_{k=5}^2(\delta)}\left(\frac{f_{min}-c}{\lambda}\right)\right]
$$