Exact Formulas for the Computation of Expected Tchebycheff Improvement

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Outline

Expected Tchebycheff Improvement (ETI)

- a popular acquisition function in expensive multiobjective optimization.

Existing methods for ETI computation

- approximation methods.

Our work

- exact formulas for the computation of ETI.

Expensive Multiobjective Optimization Problem (MOP):

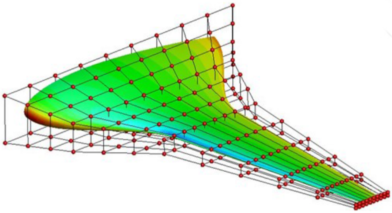
$$\begin{aligned} \text{minimize} \quad & F(x) = (f_1(x), \ldots, f_m(x))^T \\ \text{subject to} \quad & x \in \Omega \subseteq \mathbb{R}^d \end{aligned} \tag{1}$$

where

- evaluation of $F(x)$ is **very expensive**.
- evolutionary algorithms: difficult or impossible to directly use.

Efficient global optimization (EGO)

- ParEGO (J. Knowles, 2006)
- EHVI-EGO (Emmerich et al, 2006)
- MOEA/D-EGO (Zhang et al., 2009)
- ...



Aerodynamic shape optimization

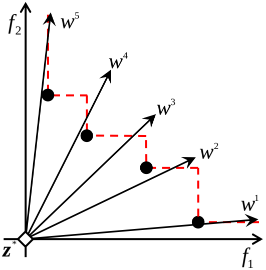
ParEGO VS MOEA/D-EGO

Decomposition

- Tchebycheff scalarization: $g^{te}(F(x)|\boldsymbol{w})$
- MOP -> single-objective subproblem

ParEGO

- randomly generates a weight vector $\boldsymbol{w}^i$
- Gaussian process (GP) model -> $g^{te}(F(x)|\boldsymbol{w}^i)$
- single-objective Expected Improvement (EI)
- select one query point: $x^* = \arg\max_{x\in\Omega} \mathrm{EI}(x)$



MOEA/D-EGO

- GP model -> $f_i(x)$
- Expected Tchebycheff Improvement (ETI): $\mathrm{EI}_T(x|\boldsymbol{w}^i), i = 1, \ldots, N$
- $Q = \arg\max_{x\in\Omega} \mathrm{EI}_T(x|\boldsymbol{w}^i), i = 1, \ldots, N$
- subset selection: select q query points from Q.

Advantages

- readily supports parallel expensive multiobjective optimization.
- achieves a good balance between convergence and diversity.

Disadvantages

- the computation of ETI is complex, due to the maximum of several Gaussians is not a Gaussian [1].

  Let $\eta_i := w_i(y_i - z_i^*)$. $p(\eta_i) = \mathcal{N}(w_i(\hat{\mu}_i(\boldsymbol{x}) - z_i^*), w_i^2\hat{\sigma}_i^2(\boldsymbol{x}))$.

$$\mathrm{EI}_T(x|\boldsymbol{w}) = \mathbb{E}_{\boldsymbol{y}\sim p(\boldsymbol{y}|x,\mathcal{D})}\left[\max(0, g^* - \max_{1\le i\le m}\{w_i(y_i - z_i^*)\})\right], \tag{2}$$

where $g^* = \min_{\boldsymbol{u}\in\mathcal{D}} g^{te}(\boldsymbol{u}|\boldsymbol{w})$, $\boldsymbol{y} = F(x)$, $\boldsymbol{w} = (w_1, \ldots, w_m)^T$.

[1] Nadarajah, S. and Kotz, S., 2008. Exact distribution of the max/min of two Gaussian random variables.

Approximation methods for the computation of ETI

- numerical integration (e.g., Gauss-Hermite quadrature)
- Monte Carlo methods (time-consuming)
- Moment Matching Approximation
  approximate $p(\max_{1 \leq i \leq m} \eta_i)$ with a Gaussian (Zhang et al., 2009)
- approximate $p(\max_{1 \leq i \leq m} \eta_i)$ with a Gumbel distribution (T. Chugh, 2022)

Limitation of approximation methods

- the estimation error of these methods cannot be fully determined without the aid of exact formulas.

Research Goal

- to derive an exact formula for the computation of ETI.
- to analyze the performance of the widely-used approximation method.

Outline

Similarity between Multi-point EI and ETI

- Multi-point EI (i.e., q-EI):

$$q\text{-}EI(X) = \mathbb{E}_{y^i \sim p(y^i|x^i,\mathcal{D})}\left[\max(0, f^* - \min_{1\leq i\leq q} y^i)\right], \quad (3)$$

  where f^* is the minimum of observed objective values.

- Expected Tchebycheff Improvement (ETI):

$$\mathrm{EI}_T(x|\boldsymbol{w}) = \mathbb{E}_{\boldsymbol{y}\sim p(\boldsymbol{y}|x,\mathcal{D})}\left[\max(0, g^* - \max_{1\leq i\leq m}\{w_i(y_i - z_i^*)\})\right], \quad (4)$$

  where g^* is the minimum of $g^{te}(F(x)|\boldsymbol{w})$ on observed samples.

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$$f^* - \min_{1\leq i\leq q} y^i = f^* + \max_{1\leq i\leq q}\{-y^i\}. \quad (5)$$

Exact Formula of ETI

Inspired by the exact computation method for multi-point EI [2]

$$\mathrm{EI}_T(x|\boldsymbol{w}) = \sum_{k=1}^{m} \mathbb{P}(\boldsymbol{Z}^{(k)} \leq \boldsymbol{b}^k)(g^* - \mathbb{E}[Z_k^{(k)}|\boldsymbol{Z}^{(k)} \leq \boldsymbol{b}^{(k)}]) \tag{6}$$

Proposition (Tallis formulas)

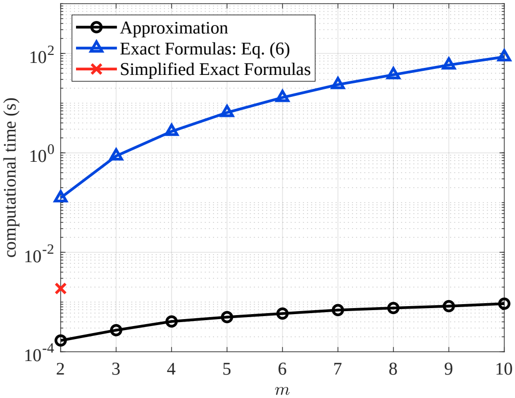
Let $\boldsymbol{Z} := (Z_1, \ldots, Z_m)$ *be a random vector obeying multivariate Gaussian distribution, i.e.,* $\boldsymbol{Z} \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$, *where* $\boldsymbol{\mu} = (\mu_1, \ldots, \mu_m)^T \in \mathbb{R}^m$ *and* $\boldsymbol{\Sigma} \in \mathbb{R}^{m \times m}$. *Let* $\boldsymbol{b} = (b_1, \ldots, b_m)^T \in \mathbb{R}^m$ *and* $\boldsymbol{Z} \leq \boldsymbol{b}$ *denotes* $\forall i, Z_i \leq b_i$. *For any* $k \in \{1, \ldots, m\}$, *the conditional expectation of* Z_k *given* $\boldsymbol{Z} \leq \boldsymbol{b}$ *is:*

$$\mathbb{E}(Z_k|\boldsymbol{Z} \leq \boldsymbol{b}) = \mu_k - \frac{1}{p} \sum_{i=1}^{m} \frac{\Sigma_{ik}}{\sqrt{\Sigma_{ii}}} \phi(\frac{b_i - \mu_i}{\sqrt{\Sigma_{ii}}}) p_i, \tag{7}$$

[2] C. Chevalier and D. Ginsbourger, 2013. Fast computation of the multi-points expected improvement with applications in batch selection.

Limitation

- relies on the specific technique to compute the multivariable Gaussian cumulative distribution function (cdf).
- is expensive to calculate



Computational time

- Moment Matching Approximation
- Exact formula, i.e., Eq. (6)
- Simplified exact formulas (independent assumption for $\eta_1, \ldots, \eta_m$)

Outline

Experimental settings

Compared methods

- MOEA/D-EGO-A (Moment Matching Approximation)
- MOEA/D-EGO-E (Exact formulas)

Test problems

- ZDT test suite
- F1-F4
- DTLZ test suite

General settings

- number of decision variables d: 8 for $m = 2$, 6 for $m = 3$
- number of initial samples: $11d - 1$
- maximal number of function evaluation: 200
- number of independent runs: 21

Mean IGD+ values ($m = 2$, Batch size: 5)

- perform similarly on the majority of test problems (13 out of 16).
- DTLZ2 and DTLZ5:MOEA/D-EGO-E outperforms MOEA/D-EGO-A.

Problem	m	d	MOEA/D-EGO-A	MOEA/D-EGO-E
ZDT1	2	8	9.9449e-3 (1.94e-3) $\approx$	1.0263e-2 (2.04e-3)
ZDT2	2	8	2.2673e-2 (1.11e-2) $\approx$	2.4315e-2 (7.31e-3)
ZDT3	2	8	1.2522e-2 (2.69e-3) $\approx$	2.1716e-2 (4.60e-2)
ZDT4	2	8	3.4847e+1 (1.14e+1) $+$	4.4925e+1 (1.76e+1)
ZDT6	2	8	4.3851e-1 (2.31e-1) $\approx$	3.8072e-1 (1.24e-1)
F1	2	8	5.5393e-3 (3.80e-4) $\approx$	5.3017e-3 (4.04e-4)
F2	2	8	2.0022e-2 (3.72e-3) $\approx$	2.1768e-2 (1.16e-2)
F3	2	8	1.7296e-2 (5.67e-3) $\approx$	2.4403e-2 (2.39e-2)
F4	2	8	1.8654e-2 (5.68e-3) $\approx$	1.8467e-2 (7.64e-3)
DTLZ1	2	8	9.0484e+1 (2.44e+1) $\approx$	8.9805e+1 (3.00e+1)
DTLZ2	2	8	1.4233e-2 (3.27e-3) $-$	9.7645e-3 (1.93e-3)
DTLZ3	2	8	2.0846e+2 (5.04e+1) $\approx$	2.1182e+2 (4.96e+1)
DTLZ4	2	8	2.6053e-1 (1.00e-1) $\approx$	2.9041e-1 (7.81e-2)
DTLZ5	2	8	1.3539e-2 (2.93e-3) $-$	9.8923e-3 (2.53e-3)
DTLZ6	2	8	8.0241e-1 (4.49e-1) $\approx$	1.0289e+0 (5.90e-1)
DTLZ7	2	8	1.0883e-1 (1.41e-1) $\approx$	7.6586e-2 (1.06e-1)
$+/-/\approx$			1/2/13	

Mean IGD+ values on DTLZ with different batch sizes

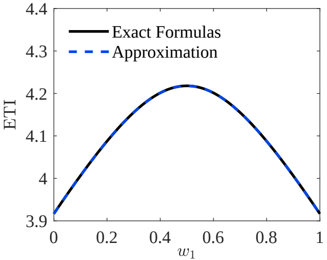
- perform similarly on the majority of test problems.
- DTLZ2 and DTLZ5:MOEA/D-EGO-E outperforms MOEA/D-EGO-A.

Problem	Batch Size	MOEA/D-EGO-A	MOEA/D-EGO-E
DTLZ1	1	9.0191e+1 (1.99e+1) ≈	7.9933e+1 (2.12e+1)
	2	9.1206e+1 (2.52e+1) ≈	8.9113e+1 (2.18e+1)
	5	9.0484e+1 (2.44e+1) ≈	8.9805e+1 (3.00e+1)
	8	9.1492e+1 (2.36e+1) ≈	8.9204e+1 (2.25e+1)
DTLZ2	1	8.9393e-3 (1.95e-3) −	6.3421e-3 (2.75e-3)
	2	9.4724e-3 (1.65e-3) −	7.6098e-3 (2.09e-3)
	5	1.4233e-2 (3.27e-3) −	9.7645e-3 (1.93e-3)
	8	1.3527e-2 (2.98e-3) −	9.7923e-3 (1.67e-3)
DTLZ3	1	2.0715e+2 (3.86e+1) ≈	1.9265e+2 (4.16e+1)
	2	2.0187e+2 (4.18e+1) ≈	2.0160e+2 (5.64e+1)
	5	2.0846e+2 (5.04e+1) ≈	2.1182e+2 (4.96e+1)
	8	2.0796e+2 (6.34e+1) ≈	1.9443e+2 (6.81e+1)
DTLZ4	1	2.0105e-1 (9.16e-2) ≈	2.1201e-1 (7.91e-2)
	2	2.3758e-1 (8.07e-2) ≈	2.2104e-1 (8.95e-2)
	5	2.6053e-1 (1.00e-1) ≈	2.9041e-1 (7.81e-2)
	8	2.9145e-1 (7.14e-2) ≈	3.2500e-1 (6.96e-2)
DTLZ5	1	8.0689e-3 (1.91e-3) −	6.5651e-3 (5.03e-3)
	2	1.0556e-2 (2.47e-3) −	7.2783e-3 (1.77e-3)
	5	1.3539e-2 (2.93e-3) −	9.8923e-3 (2.53e-3)
	8	1.4231e-2 (2.88e-3) −	9.5625e-3 (1.95e-3)
DTLZ6	1	1.1214e+0 (4.87e-1) ≈	1.2910e+0 (6.17e-1)
	2	8.4697e-1 (4.39e-1) ≈	1.1063e+0 (5.53e-1)
	5	8.0241e-1 (4.49e-1) ≈	1.0289e+0 (5.90e-1)
	8	7.8318e-1 (5.76e-1) ≈	1.2757e+0 (7.43e-1)
DTLZ7	1	6.2493e-2 (1.13e-2) ≈	7.0531e-2 (5.87e-2)
	2	9.1616e-2 (6.73e-2) ≈	9.3847e-2 (8.60e-2)
	5	1.0883e-1 (1.41e-1) ≈	7.6586e-2 (1.06e-1)
	8	3.8449e-2 (7.54e-2) ≈	3.2312e-2 (6.18e-2)
+/−/≈		0/8/20	

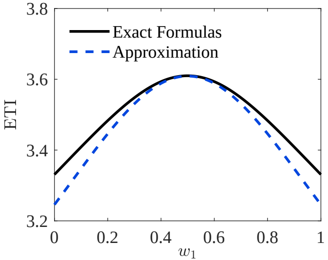
Discussion

Why the approximation method performs similarly with the exact formula on many of the test problems?

- (a) vs. (b): approximation error $\searrow$ as $\hat{\sigma}_i^2 \searrow$.
- predicted variances of the GP models get smaller during optimization.



(a) $\hat{\mu}_1 = 1, \hat{\mu}_2 = 1, \hat{\sigma}_1 = 1, \hat{\sigma}_2 = 1$



(b) $\hat{\mu}_1 = 1, \hat{\mu}_2 = 1, \hat{\sigma}_1 = 10, \hat{\sigma}_2 = 10$

Mean IGD+ values on DTLZ ($m = 3$, Batch size: 5)

- DTLZ2 and DTLZ5:MOEA/D-EGO-A outperforms MOEA/D-EGO-E.

Problem	m	d	MOEA/D-EGO-A	MOEA/D-EGO-E
DTLZ2	3	6	5.0246e-2 (3.53e-3) $+$	7.2728e-2 (1.82e-2)
DTLZ5	3	6	1.0300e-2 (1.35e-3) $+$	1.5099e-2 (4.68e-3)
DTLZ7	3	6	5.4108e-2 (4.88e-3) $\approx$	5.4427e-2 (3.86e-3)
$+/-/\approx$			2/0/1	

Discussion

Why does the approximation method outperform the exact formula?

- Exact formula relies on the specific technique to compute the multivariable Gaussian cumulative distribution function (cdf).
- Gaussian cdf: does not have a closed-form expression when $m \geq 3$.

Code

- https://github.com/mobo-d/MOEAD-EGO/ETI

```
for k=1:M
    L_k =  eye(M);    L_k(:,k)=-1;  L_k(k,k)= 1;
    mu_k = g_mu*L_k'; % The mean of Z^(k), n*m
    b_k = zeros(n,M); b_k(:,k) = Gbest;
    for j=1:1:n
        Sigma_k =L_k*diag(g_sig2(j,:))*L_k'; % The covariance matrix of Z^(k) for j-th query, m*m
        % P(Z^k<=b^k)
        p_k  =   qsimvnv(200*M,Sigma_k, -inf.*ones(M,1), (b_k(j,:)-mu_k(j,:))') ;
        ETI(j) =  ETI(j)+ p_k *(Gbest(j)-mu_k(j,k));

        temp_ci = (b_k(j,:) -mu_k(j,:))'./diag(Sigma_k);%m*1
        temp_Sigma_k_ii = sqrt(diag(Sigma_k));
        phi_ik =   Sigma_k(:,k).*normpdf((b_k(j,:) -mu_k(j,:))'./temp_Sigma_k_ii)./temp_Sigma_k_ii;%m*1
        for i=1:M
            % need c.i^(k) and Sigma.i^(k)
            cik =  b_k(j,:)'  - mu_k(j,:)' -Sigma_k(:,i).* temp_ci ; cik(i)=[]; % m-1*1
            sigmaik =  (Sigma_k - Sigma_k(:,i)*Sigma_k(i,:)./Sigma_k(i,i)) ;  sigmaik(i,:)=[]; sigmaik(:,i)=[]; % m-1*1
            Phi_ik =   qsimvnv(200*M,sigmaik ,-inf.*ones(M-1,1),cik ) ; %1*1
            ETI(j) =  ETI(j) +  phi_ik(i)*Phi_ik;
```

Outline

Conclusion and Future Work

Exact formulas VS Moment matching approximation

- Moment matching approximation: approximation error $\searrow$ as $\hat{\sigma}_i^2 \searrow$.
- Moment matching approximation is good enough in terms of both accuracy and computational time.

Future work

- Similarity between Multi-point EI and ETI:
  moment matching approximation -> multi-point EI

Thank you!

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