Integrated Formulation of Sequential Multiobjective Optimization Based on System Surrogate Model Learning Under L_∞-norm Error Constraints

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Abstract. This paper addresses expensive multiobjective optimization problems for black-box systems, where each evaluation requires costly experiments or high-fidelity simulations. In contrast to conventional methods that directly approximate objective functions, the proposed framework sequentially updates a surrogate model of the system response while enforcing componentwise ℓ_∞ error bounds. The resulting constrained learning problem is relaxed using an exterior penalty method, and the algorithm iterates through surrogate training, surrogate-based candidate search, and criterion-based sampling of new evaluation points. This response-modeling approach offers two practical advantages: the trained surrogate can be reused when objectives are modified or added, and componentwise error bounds enable physical design specifications to be expressed as allowable error margins per output component, thereby improving interpretability. Numerical experiments on a synthetic problem demonstrate that the proposed framework effectively approximates the Pareto front under a limited evaluation budget.

Keywords: Black-box system optimization · System response surrogate learning · Expensive multiobjective optimization · ℓ_∞-norm constraint.

1 Introduction

This paper addresses expensive multiobjective optimization problems (MOPs) for black-box systems whose input-output mappings are unknown. Such problems commonly arise in engineering applications, including design, operation, and control based on high-fidelity simulations or physical experiments [3, 8]. Since each evaluation may require substantial computational or experimental cost, efficient methods for approximating the Pareto optimal set under a limited evaluation budget are essential [5].

Surrogate-assisted evolutionary algorithms (SAEAs) are effective approaches for expensive MOPs [5, 8]. In a typical SAEA framework, surrogate models, including Gaussian processes and radial basis function networks, are combined with evolutionary multiobjective optimizers such as NSGA-II [6] and MOEA/D [14]. These surrogates are often constructed for objective vectors or scalarized functions [10, 15]. However, because such objective-level models are tied to the specified objectives, they often have to be rebuilt when the objectives are modified or new objectives are introduced during the design process.

To avoid this repeated modeling effort, we develop a framework that performs multiobjective optimization by sequentially learning a surrogate model of the system's input-output mapping (the system response) rather than the objective functions themselves. Modeling system responses instead of objective functions, a strategy recognized for its practicality in structural and computer-aided design optimization [7, 13], enables trained surrogate models to be reused when objectives are modified or added.

Conventional surrogate-assisted optimization typically trains surrogate models by minimizing an ℓ_2-type loss, such as the mean squared error [5, 8]. While this controls the average squared error, it provides no explicit bound on the maximum error of each output component. This is important in response-modeling settings, where response components represent distinct physical quantities and design specifications are naturally expressed as componentwise error tolerances. Motivated by this, the present study introduces an ℓ_∞ bounded-error formulation for surrogate learning [1, 4, 11], which enforces prescribed absolute error bounds for each response component at evaluated sample points. The surrogate is then combined with sequential candidate search and sampling to approximate the Pareto optimal set under a limited evaluation budget.

A related study has incorporated similar componentwise ℓ_∞ bounded-error response modeling into an sequential optimization framework [1], but it focuses on scalar optimization for worst-case risk management. In contrast, this study addresses expensive multiobjective optimization to obtain a uniform approximation of the Pareto front.

2 Problem Formulation and Proposed Solution Framework

2.1 Multiobjective Optimization of System Inputs

We consider a system with input $u \in \mathcal{U} \subset \mathbb{R}^n$ and output response $y \in \mathbb{R}^p$, represented by

$$y = S(u) = \begin{bmatrix} S_1(u) \cdots\ S_p(u) \end{bmatrix}^\top ,$$

where $S : \mathcal{U} \to \mathbb{R}^p$ is treated as a black-box mapping whose analytical form and derivative information are unavailable. Such conditions typically arise in scenarios where the output response to an input can only be observed through expensive evaluations, such as physical experiments or high-fidelity simulations.

The objective of this paper is to determine input variables that are optimal with respect to multiple evaluation criteria defined from the system response and the input. The objective function vector is given by a known mapping $\Phi : \mathbb{R}^p \times \mathcal{U} \to \mathbb{R}^m$ as

$$F(u) := \Phi(y, u) = \Phi(S(u), u).$$

The corresponding MOP is then formulated as

$$\underset{u\in\mathcal{U}}{\text{minimize}} \quad F(u) = \left[F_1(u) \cdots F_m(u)\right]^\top$$

For $u, v \in \mathcal{U}$, we write $F(u) \prec F(v)$ and say that u *dominates* v if $F_i(u) \le F_i(v)$ for all $i \in \{1, \dots, m\}$ and $F_j(u) < F_j(v)$ for some $j \in \{1, \dots, m\}$. A point $u^\star \in \mathcal{U}$ is *Pareto optimal* if no $u \in \mathcal{U}$ satisfies $F(u) \prec F(u^\star)$. The set $\mathcal{P}^\star$ of all Pareto optimal points is called the *Pareto optimal set*, and its image $F(\mathcal{P}^\star) \subset \mathbb{R}^m$ is called the *Pareto front*.

Our goal is to develop a method for efficiently approximating the Pareto set in the input space and the corresponding Pareto front of this expensive MOP.

2.2 ℓ_∞-Constrained Surrogate Model Learning

We formulate a surrogate model learning problem based on the evaluation dataset $\mathcal{D} = \{(u^{(s)}, y^{(s)})\}_{s=1}^N$, where $u^{(s)} \in \mathcal{U}$ is the s-th evaluated input and $y^{(s)} = S(u^{(s)}) = [y_1^{(s)} \cdots y_p^{(s)}]^\top \in \mathbb{R}^p$ is the corresponding observed response. The proposed approach learns a surrogate model of the system response, rather than the objective functions, and seeks to control its accuracy by imposing component-wise ℓ_∞ bounds on the approximation errors over the evaluated samples.

The surrogate model of the system response is denoted by

$$\widehat{S}(u; w) = \left[\widehat{S}_1(u; w_1) \cdots \widehat{S}_p(u; w_p)\right]^\top,$$

where $w = (w_1, \dots, w_p) \in \mathcal{W}_1 \times \cdots \times \mathcal{W}_p =: \mathcal{W}$ and $w_\ell \in \mathcal{W}_\ell \subset \mathbb{R}^{q_\ell}$ for $\ell = 1, \dots, p$. Here, $\widehat{S}_\ell(u; w_\ell)$ denotes the surrogate model for the ℓ-th component of the system response. The mapping $\widehat{S}(\cdot; w)$ represents a vector-valued surrogate model constructed component-wise from scalar surrogate models, such as polynomial models, radial basis function networks (RBFNs), or neural networks.

For the ℓ-th output component, let $e_\ell(w_\ell) \in \mathbb{R}^N$ denote the error vector whose s-th element is given by $e_\ell^{(s)}(w_\ell) = y_\ell^{(s)} - \widehat{S}_\ell(u^{(s)}; w_\ell)$. We impose an ℓ_∞ error bound on this component, requiring that the maximum absolute approximation error over the evaluated samples is bounded by ε_ℓ. To penalize model complexity, we incorporate a regularization term $R(w)$ and formulate the learning problem as selecting parameters $w \in \mathcal{W}$ that minimize $R(w)$ subject to these prescribed component-wise tolerances:

$$\begin{aligned} &\underset{w\in\mathcal{W}}{\text{minimize}} && R(w) \\ &\text{subject to} && \|e_\ell(w_\ell)\|_\infty = \max_{s=1,\dots,N} |e_\ell^{(s)}(w_\ell)| \le \varepsilon_\ell, \quad \ell = 1, \dots, p, \end{aligned} \tag{1}$$

where $\varepsilon = [\varepsilon_1 \cdots \varepsilon_p]^\top \in \mathbb{R}_{\ge 0}^p$ is the prescribed tolerance vector.

The ℓ_∞ constraint in problem (1) is equivalent to the Np pointwise constraints:

$$|e_\ell^{(s)}(w_\ell)| \le \varepsilon_\ell, \quad s = 1, \dots, N, \quad \ell = 1, \dots, p.$$

For practical implementation, we relax these constraints using the exterior penalty method. Defining the pointwise violation as

$$v_\ell^{(s)}(w_\ell) := \max\bigl\{|e_\ell^{(s)}(w_\ell)| - \varepsilon_\ell,\, 0\bigr\},$$

we obtain the following unconstrained optimization problem:

$$\underset{w\in\mathcal{W}}{\text{minimize}} \quad J(w) := R(w) + \rho \sum_{s=1}^{N} \sum_{\ell=1}^{p} \bigl(v_\ell^{(s)}(w_\ell)\bigr)^2, \tag{2}$$

where $\rho > 0$ is the penalty coefficient.

The resulting problem is unconstrained and, provided that the surrogate model $\widehat{S}_\ell(\cdot; w_\ell)$ and the regularizer R are continuously differentiable in w, the objective $J(w)$ is also continuously differentiable, allowing for standard gradient-based optimization with the penalty coefficient $\rho > 0$ controlling how strongly the prescribed tolerances are enforced.

2.3 Proposed Solution Framework

We embed the surrogate learning problem (2) into a sequential framework: at each iteration t, the surrogate is refined with newly evaluated samples, and the multiobjective search is conducted on the updated surrogate. To accommodate adaptive parameterizations (e.g., RBFNs whose centers are placed at the evaluated input points), the surrogate model and its parameter space are allowed to depend on t, denoted by $\widehat{S}_t$ and $\mathcal{W}_t$.

Let $\mathcal{D}_t = \{(u^{(s)}, y^{(s)})\}_{s=1}^{N_t}$ denote the dataset available at iteration t, where N_t is the number of evaluated samples. Solving the iteration-t instance of (2) (with $\widehat{S}, \mathcal{W}$ replaced by $\widehat{S}_t, \mathcal{W}_t$) on $\mathcal{D}_t$ yields optimal parameters $w_t^\star = (w_{t,1}^\star, \ldots, w_{t,p}^\star) \in \mathcal{W}_t$, and the resulting surrogate objective vector is

$$\widehat{F}_t(u) := \Phi\bigl(\widehat{S}_t(u; w_t^\star),\, u\bigr).$$

The framework has a natural bilevel structure: the lower level learns $w_t^\star$ from $\mathcal{D}_t$, and the upper level performs multiobjective search on $\widehat{F}_t$,

$$\begin{aligned} &\underset{u\in\mathcal{U}}{\text{minimize}} \quad \widehat{F}_t(u) \\ &\text{subject to} \quad w_t^\star \in \underset{w\in\mathcal{W}_t}{\operatorname{argmin}} \Biggl[R(w) + \rho \sum_{s=1}^{N_t} \sum_{\ell=1}^{p} \bigl(v_\ell^{(s)}(w_\ell)\bigr)^2\Biggr], \end{aligned}$$

where $v_{t,\ell}^{(s)}(w_\ell) := \max\bigl\{|y_\ell^{(s)} - \widehat{S}_{t,\ell}(u^{(s)}; w_\ell)| - \varepsilon_\ell, 0\bigr\}$ is the pointwise violation associated with the iteration-t surrogate.

The upper-level search at iteration t is realized by two mappings. A *search mapping* $\mathcal{Q}$ generates a candidate set $\mathcal{C}_t \subset \mathcal{U}$ by running a search algorithm—such as a multiobjective evolutionary algorithm (MOEA)—on $\widehat{F}_t$. A *selection* *mapping* $\mathcal{A}$ then chooses a subset $\mathcal{B}_t \subseteq \mathcal{C}_t$ with $|\mathcal{B}_t| = B$ for expensive evaluation by S, based on infill criteria [2, 12] that combine predicted values and distance metrics, or on filtering / pre-selection [9]. The newly evaluated samples are appended to $\mathcal{D}_t$ to form $\mathcal{D}_{t+1}$. The full cycle is

$$\mathcal{D}_t \xrightarrow{\text{Learn}} w_t^\star \xrightarrow{\text{Construct}} \widehat{F}_t \xrightarrow{\mathcal{Q}} \mathcal{C}_t \xrightarrow{\mathcal{A}} \mathcal{B}_t \xrightarrow{\text{Evaluate}} \mathcal{D}_{t+1},$$

and is summarized in Algorithm 1.

Algorithm 1: Sequential Multiobjective Optimization via ℓ_∞-Constrained Surrogate Models

Input: Initial dataset $\mathcal{D}_0$, tolerance ε, batch size B, max iterations T, regularization R, penalty coefficient ρ, search mapping $\mathcal{Q}$, and selection mapping $\mathcal{A}$.

Output: Final dataset $\mathcal{D}_T$, estimated Pareto set $\mathcal{P}_T$.

for $t = 0, 1, \ldots, T-1$ **do**

- **Step 1 (Learn):** Update parameters $w_t^\star \in \mathcal{W}_t$ by solving the iteration-t instance of (2) (with $\widehat{S}$ and $\mathcal{W}$ replaced by $\widehat{S}_t$ and $\mathcal{W}_t$) on $\mathcal{D}_t$;
- **Step 2 (Construct & Search):** Define $\widehat{F}_t(\cdot) = \Phi(\widehat{S}_t(\cdot; w_t^\star), \cdot)$ and generate candidates:
  $$\mathcal{C}_t \leftarrow \mathcal{Q}(\widehat{F}_t, \mathcal{D}_t);$$
- **Step 3 (Select):** Choose a batch of B points for expensive evaluation:
  $$\mathcal{B}_t \leftarrow \mathcal{A}(\mathcal{C}_t, \widehat{F}_t, \mathcal{D}_t);$$
- **Step 4 (Evaluate):** Observe $y = S(u)$ for all $u \in \mathcal{B}_t$ and update dataset:
  $$\mathcal{D}_{t+1} \leftarrow \mathcal{D}_t \cup \big\{(u, S(u)) \mid u \in \mathcal{B}_t\big\};$$
- **Step 5 (Update Pareto Set):** Compute true objective $F(u) = \Phi(y, u)$ for all $(u, y) \in \mathcal{D}_{t+1}$ and extract non-dominated points as $\mathcal{P}_{t+1}$;

3 Numerical Experiment

This section evaluates the effectiveness of Algorithm 1. We use a synthetic numerical example that mimics a typical performance–cost trade-off in physical systems. The experiment examines whether the proposed method can construct a system-response surrogate satisfying the prescribed ℓ_∞ error constraints and approximate the Pareto optimal set under a limited evaluation budget.

3.1 Experimental Setup

We employ a synthetic numerical example based on a smooth nonlinear input-output response model. The system is represented by the following single-input two-output function:

$$y = S(u) = \begin{bmatrix} 2\exp\bigl(-2(u-1)^2\bigr) \\ 1.5\exp\bigl(-0.8\,u^2\bigr) \end{bmatrix}, \quad u \in \mathcal{U} = [-2, 2].$$

The first response attains its maximum value of 2 at $u = 1.0$, whereas the second response attains its maximum value of 1.5 at $u = 0$.

For this system, we define a multiobjective optimization problem representing the trade-off between performance maximization and input-cost minimization:

$$\underset{u \in \mathcal{U}}{\text{minimize}} \quad F(u) = \begin{bmatrix} F_1(u) \\ F_2(u) \end{bmatrix} = \begin{bmatrix} -\bigl(S_1(u)/2.0 + S_2(u)/1.5\bigr) \\ u^2 \end{bmatrix}.$$

The first objective corresponds to maximizing the normalized total output, whereas the second objective represents the input cost. The true Pareto optimal set is $\mathcal{P}^\star = [0, u_\star]$, where $u_\star \approx 0.791$ is the maximizer of the normalized total output $S_1(u)/2.0 + S_2(u)/1.5$ over $\mathcal{U}$.

3.2 Implementation Details and Parameter Settings

The implementation and parameter settings for Algorithm 1 are as follows. The optimization is initiated with an initial dataset $\mathcal{D}_0$ of $N_0 = 3$ samples, whose input points are drawn uniformly at random from $\mathcal{U} = [-2, 2]$. The number of sequential iterations is set to $T = 5$ and the batch size per iteration to $B = 1$, giving a total evaluation budget of $N_0 + TB = 8$.

For the surrogate model $\widehat{S}(u; w)$ in the learning step (Step 1), which we keep fixed across iterations ($\widehat{S}_t \equiv \widehat{S}$, $\mathcal{W}_t \equiv \mathcal{W}$), we use an RBFN with Gaussian basis whose ℓ-th component is

$$\widehat{S}_\ell(u; w_\ell) = \sum_{j=1}^{M} w_{\ell j}\,\phi_j(u), \quad \phi_j(u) = \exp\left(-\frac{\|u - c_j\|^2}{2\sigma^2}\right), \quad \ell = 1, 2.$$

The number of basis functions is set to $M = 5$. The centers c_j are placed on a uniform grid over $\mathcal{U} = [-2, 2]$, and the width is set to $\sigma = 0.5$. The regularization term is taken as $R(w) = \lambda\|w\|_2^2$ with $\lambda = 0.001$, and the tolerance vector is set componentwise to $\varepsilon = [0.2, 0.1]^\top$. The learning problem (2) on $\mathcal{D}_t$ is approximately solved by steepest descent with learning rate $\eta = 0.05$, penalty coefficient $\rho = 10.0$, and 20 gradient updates per sequential iteration.

In the candidate-generation step (Step 2), we implement the search mapping $\mathcal{Q}(\cdot, \cdot)$ as an NSGA-II [6]-based search procedure operating on the surrogate objective vector $\widehat{F}_t$.[1] The internal population size is set to $N_{\text{pop}} = 10$, and the search is performed for 10 internal generations per sequential iteration. The final population is used as the candidate set $\mathcal{C}_t$.

[1] The non-dominated sorting and crowding-distance selection are retained; offspring are generated by Gaussian mutation projected onto $\mathcal{U}$.

In the sample-selection step (Step 3), the new evaluation point $u_{\mathrm{next}} \in \mathcal{C}_t$ is chosen by a diversity-oriented maximin criterion in the objective space [2]. Since the objective components may differ in scale, distances are measured after componentwise normalization: let $\bar{F}_t(u)$ and $\bar{F}(u_i)$ denote the normalized versions of $\widehat{F}_t(u)$ and $F(u_i)$, respectively. The next point is

$$u_{\mathrm{next}} = \arg\max_{u \in \mathcal{C}_t} \min_{(u_i, y_i) \in \mathcal{D}_t} \left\| \bar{F}_t(u) - \bar{F}(u_i) \right\|.$$

This maximin criterion selects a candidate far from the existing evaluated samples, promoting a diverse approximation of the Pareto front. After evaluating the true system response $y_{\mathrm{next}} = S(u_{\mathrm{next}})$, the dataset is updated as $\mathcal{D}_{t+1} = \mathcal{D}_t \cup \{(u_{\mathrm{next}}, y_{\mathrm{next}})\}$.

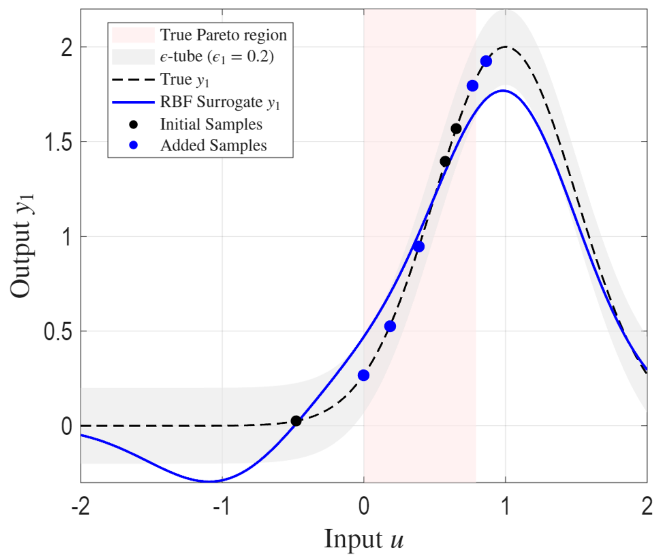
3.3 Results and Discussion

Fig. 1 shows the surrogate approximation results for the two system responses S_1 (Fig. 1(a)) and S_2 (Fig. 1(b)). In both subfigures, the approximation errors at the evaluated sample points lie within the prescribed ε-tube, confirming that the ℓ_∞-constrained learning step successfully enforces the componentwise tolerance specification. Around the Pareto-optimal region, where the evaluated samples are densely allocated, the surrogate accurately captures the underlying system responses. In contrast, in sparsely sampled regions away from the Pareto-optimal set, the surrogate deviates more noticeably from the true responses. This behavior reflects the sequential nature of the proposed method: expensive evaluations are not uniformly distributed over the entire design space but are gradually allocated to regions important for identifying Pareto optimal solutions.

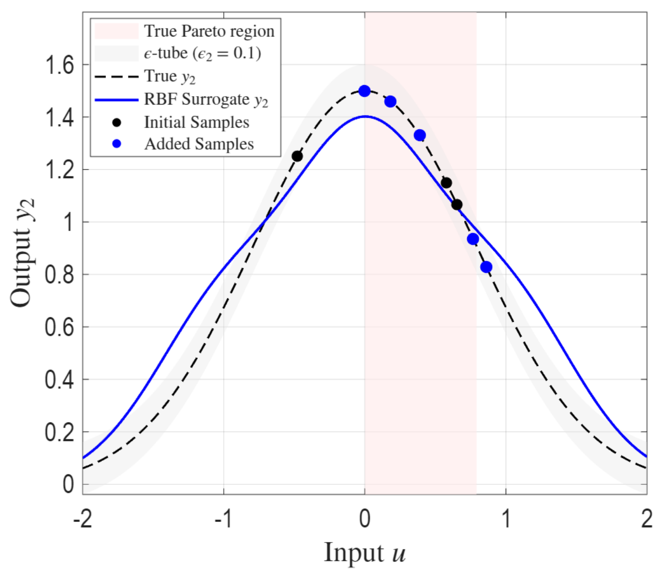
As shown in Fig. 2, even under a limited evaluation budget, the samples added by the sequential procedure are distributed near-uniformly along the Pareto-optimal region of the feasible objective space, although a few lie outside it. This near-uniform distribution is supported by two factors: the accurate surrogate approximation around the Pareto-optimal region observed in Fig. 1, which provides reliable predictions for candidate generation, and the diversity promotion by the NSGA-II-based candidate generation together with the maximin selection criterion in the normalized objective space. These results indicate that combining componentwise ℓ_∞-constrained surrogate learning with sequential candidate selection provides a practical surrogate-assisted approach for approximating the Pareto optimal set of an expensive black-box system.

4 Conclusion

This paper proposed a sequential multiobjective optimization framework using ℓ_∞-constrained surrogate models. By modeling the system response directly, the framework ensures high reusability when the objectives are modified or added, and allows the error tolerance ε to be specified as allowable error margins for each output component. Numerical results confirmed that integrating ℓ_∞-constrained



(a) Approximation result for the first system response S_1.



(b) Approximation result for the second system response S_2.

Fig. 1: Surrogate approximation results in the design space.

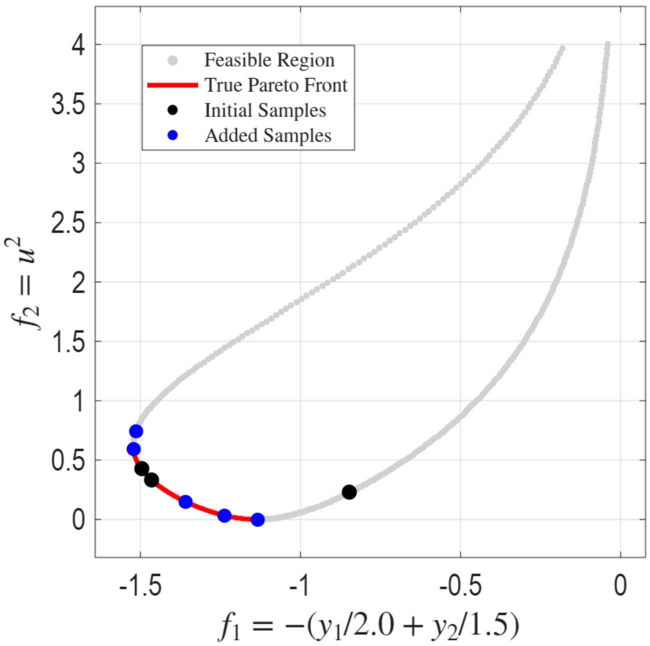


Fig. 2: Pareto search results in the objective space.

RBFN with NSGA-II enables efficient identification of the Pareto set within a limited evaluation budget. The framework adaptively allocates evaluations by prioritizing approximation accuracy within the Pareto-optimal region while controlling the approximation errors at the sampled points within the prescribed tolerance. Future work will focus on extending this method to high-dimensional input spaces and validating its robustness through application to real-world physical systems and high-fidelity simulations.

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