Efficient Region of Interest Detection under Guidance

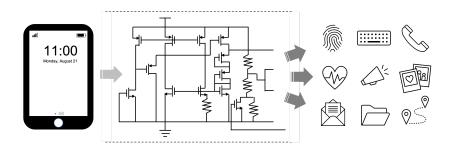
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Motivation

"Does this proposed design do what is intended?"



 \Rightarrow Design v.s. **Verification**

Circuit design

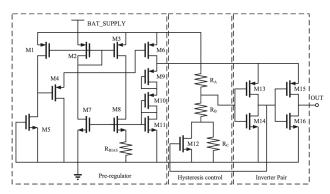


Figure: AMS design for a two-stage differential amplifier circuit diagram.

A figure of merit (FOM) is defined as a combination of four responses to quantify the performance of design.

Motivation

Verification:

- Configurations with extremely low failure rate is preferred
 - ▶ e.g. light intensity, the minimum intensity > some threshold?
- Difficulties
 - ► Large number of variables included
 - Unknown relationships between parameters and effects on the performance
 - Computationally expensive
 - ► Required extremely low failure rate

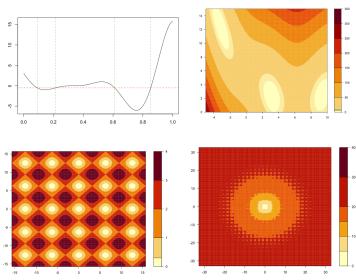
Background

Verification:

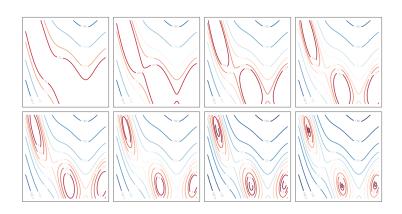
- Methods for failure rate estimation usually sampling-based and assume
 - ▶ The region of failure is somehow known
 - Both success and failure cases are observed

When failure is extremely rare, **failure detection** itself becomes a much more fundamental problem than failure rate estimation.

Synthetic Functions



Intuitive Idea



Problem Setting: Start with 1-dim response

Given a D-dimension parameter space $\Omega\subset\mathbb{R}^D$, the performance value $y(\mathbf{x})$ at $\mathbf{x}\in\Omega\subset\mathbb{R}^D$ can be determined by some hard-to-evaluate simulator/measurement.

A point can be regarded as a failure/success if

$$y(\mathbf{x}) < T, \mathbf{x} \in \Omega$$

where T is the targeted specification (the smaller the worse).

Properties of $y(\cdot)$:

- Highly nonlinear in high dimensional space
- Expensive in terms of simulation or measurement



Problem Setting

Goal: To detect the failure within a certain number of evaluations

- The smaller number of evaluations, the better (Better budget)
- The more, the better (Coverage of ROIs)
- The faster, the better (first hitting time for each region)

 \triangle If in each iteration: we can evaluate the location which is *of the highest potential* to have the "best" performance, we might be able to achieve this goal.

Problem Formulation

Define the specification of interest (SOI) x^* as a specification satisfying:

$$y(\mathbf{x}^*) < T$$
, with $\mathbf{x}^* \in \Omega$, (1)

if the lower range of the performance value is of interest. We can then define the complete set of SOIs of a response $y(\cdot)$ as

$$\Gamma_{y,T} = \{ \mathbf{x} \in \Omega : y(\mathbf{x}) < T \}.$$

$$= \bigcup_{k=1}^{n_r} \Gamma_T^{(k)}, \qquad (2)$$
where $\Gamma_T^{(i)} \cap \Gamma_T^{(j)} = \emptyset, \ \forall i \neq j \in \{1, \dots, n_r\}.$

 \Rightarrow Detect representative SOIs in disjoint regions as fast as more as possible under some constraints

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Potential Evaluation Metrics

| Notation | Description |
|-------------------------------------|--|
| ti | Average 1-st time hitting the <i>i</i> -th ROI or SOI |
| r _i | Average rate of detecting the <i>i</i> -th ROI |
| N_n^r , N_n | Average number of ROIs/SOIs until the <i>n</i> -th evaluation |
| A_n | Average length $(D=1)/\text{area}\ (D>1)$ of the convex hull generated by the SOIs in disjointed ROIs in the n -th iteration |
| y _{min} , y _{max} | \mid The optimal performance value achieved in n_b evaluations |

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- Excursion set: considers the exceedance probability for a given threshold T of the target function $f(\mathbf{x})$ with the corresponding excursion sets defined as

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However, most existing studies aim for the accurate estimation of excursion sets (e.g. [13–15]) and uncertainty quantification (e.g. [16]), both necessarily requiring a large sample size and with goals diverge from ours.

Bayesian Decision Making

- Specify the probability space of all the possible outcomes and decisions
- Determine the probability distribution of outcomes given each decision option
- Define a utility function mapping outcome onto real numbers
- Ompute the expected utility as a function of a given decision and choose the decision with the best expected utility.

Bayesian Optimization

A sequential learning strategy to globally optimize function

$$\min_{\mathbf{x} \in \Omega} f(\mathbf{x})$$
, or $\max_{\mathbf{x} \in \Omega} f(\mathbf{x})$

f typically have the following properties:

- Continuous
- Expensive to evaluate (time, computational resource, cost, etc)
- "Black box", lack known structure, hard to optimize
- Only observe (noisy) f(x), no first- or second-order derivatives

Bayesian Optimization: Algorithm

To solve this problem, the BO algorithm is as following:

Algorithm Bayesian Optimization for Rare Event Detection

Choose a surrogate model for modeling f;

while stopping criterion is not met do

Determine the next point to sample by acquisition function; /* inner optim. */

Add the newly sampled data to the set of observations;

Update model;

Compare $y_{\min} = \min_{t \in \{1,...,n_b\}} y_t$ with T to conclude.

Bayesian optimization: Surrogate model

Gaussian process regression is a typical choice of the surrogate statistical model. Assume $\mathbf{X}_{1:n} = [\mathbf{x}_1, \dots, \mathbf{x}_n], \mathbf{x}_i \in \mathbb{R}^D, i = 1, \dots, n$, and their corresponding function values are denoted as $\mathbf{f} = [f(\mathbf{x}_1), \dots, f(\mathbf{x}_n)]^T$.

$$\mathbf{f}(\mathbf{X}) \sim \mathcal{GP}(\mu_0(\mathbf{X}), \Sigma_0(\mathbf{X}, \mathbf{X}))$$

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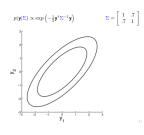
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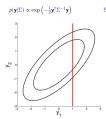
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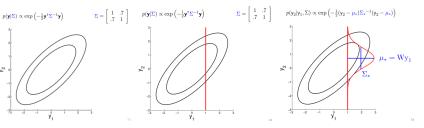
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Bayesian optimization: Acquisition function

Exploration v.s. Exploitation

(point with high uncertainty) (point with best expected value)

LCB:

$$LCB(\mathbf{x}|\mathcal{D}_n) = \mu(\mathbf{x}|\mathcal{D}_n) - \kappa\sigma(\mathbf{x}|\mathcal{D}_n)$$

• Expected Improvement (EI):

$$\mathsf{EI}(\mathbf{x}|\mathcal{D}_n) = E_n[(f^* - f(\mathbf{x}))_+|\mathcal{D}_n]$$

• Probability of Improvement (PI):

$$\mathsf{Pol}(\mathbf{x}|\mathcal{D}_n) = P(f(\mathbf{x}) < f^*|\mathcal{D}_n)$$

• (Maximal/Predicted) Entropy Search



Bayesian optimization: Acquisition function

• Expected Improvement (EI):

Suppose we have one additional evaluation to perform, then our choice after this evaluation will be either the newly evaluated point \mathbf{x} or the previously best point \mathbf{x}_n^* with function value f_n^* . The improvement of this point is

$$(f_n^* - f(\mathbf{x}))_+ = \begin{cases} f_n^* - f(\mathbf{x}), & \text{if } f(\mathbf{x}) < f_n^* \\ 0 & \text{if } f(\mathbf{x}) >= f_n^* \end{cases}$$

$$\implies \mathsf{EI}(\mathbf{x}|\mathcal{D}_n) = E_n[(f^* - f(\mathbf{x}))_+ | \mathcal{D}_n]$$

$$= \int (f^* - f(\mathbf{x}))_+ p(f(\mathbf{x})|\mathcal{D}_n) df(\mathbf{x})$$

$$= \sigma(\mathbf{x}) (z(\mathbf{x})\Phi(z) + \phi(z(\mathbf{x}))), \text{ where } z(\mathbf{x}) = \frac{f_n^* - \mu(\mathbf{x})}{\sigma(\mathbf{x})}$$

Overall goal: with a budget constraint, design an algorithm to detect as many ROIs as possible.

 Without the constraint of sample size, can we propose an algorithm to achieve a high coverage of ROIs through

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 - (possibly experimental design without an accurate recovery of excursion set, such as qMC with different discrepancy, shrinking level set, partition/reweighting different parts of space)
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- Multiple objectives: y being multivariate