Design of Computer Experiments for Optimization, Estimation of Function Contours, and Related Objectives by Bingham, Ranjan, and Welch

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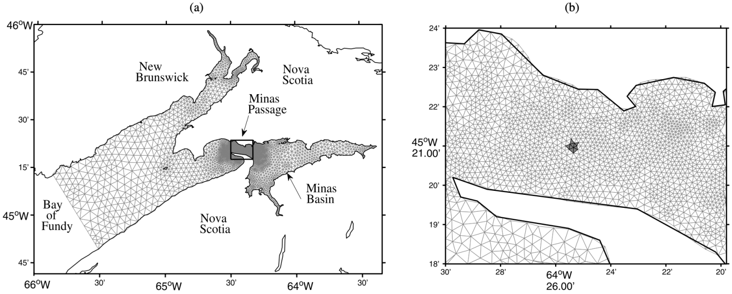
March 2, 2020

Example 1: Optimal Tidal Turbine Location

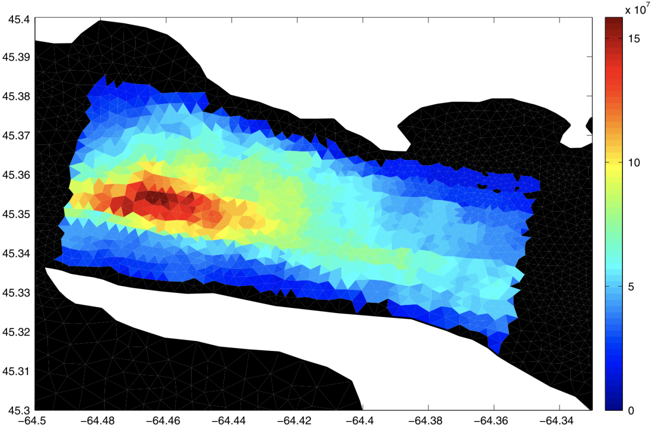


Source: Fig. 1 of Ranjan et al. 2011

Goal: To build a tidal turbine in the Minas Passage of the Bay of Fundy, Nova Scotia, Canada to maximize the extractable power averaged over a tidal cycle.

Tidal Turbine Example Cont'd

One can numerically simulate the tides (and hence the extractable power) using computer model (e.g., Finite-Volume Coastal Ocean Model (FVCOM)) but it is time consuming...



Source: Fig. 5 of Ranjan et al. 2011

Gaussian Process Emulation

$$Y(\boldsymbol{x}) = \mu(\boldsymbol{x}) + Z(\boldsymbol{x}), \quad \boldsymbol{x} \in \mathcal{X}$$

- $Y(\boldsymbol{x})$: extractable power at $\boldsymbol{x}$
- Usually assume $\mu(\boldsymbol{x}) = \mu$
- Assume $\{Z(\boldsymbol{x})\}_{\boldsymbol{x}\in\mathcal{X}}$ be a realization of a zero mean Gaussian process with some covariance structure (e.g., Cov$(\boldsymbol{x}, \boldsymbol{x}^{'}) = \sigma^2 \exp\left(-\sum_{j=1}^{d=2} \theta_j |x_j - x_j^{'}|^{p_j}\right)$, where $\theta_j > 0$ and $1 \leq p_j \leq 2$, $j = 1, \cdots, d$

Expected Improvement (EI) For Global Optimization

- Improvement function:

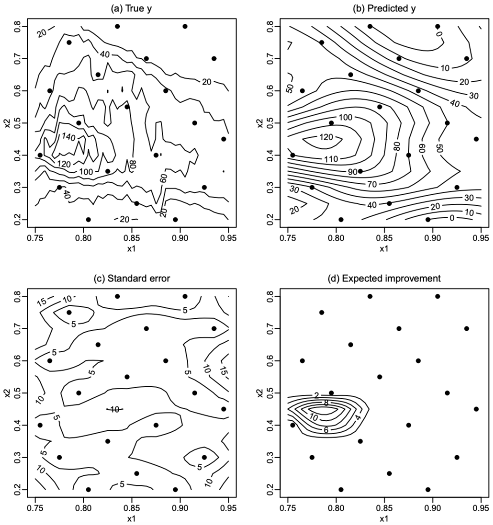
$$I(\boldsymbol{x}) = \max\left\{y_{min}^{(n)} - y(\boldsymbol{x}), 0\right\}$$

- Expected Improvement:

$$\mathbb{E}\left[I(\boldsymbol{x})\right] = \int I(\boldsymbol{x}) f(y|\boldsymbol{x})\, dy = s(\boldsymbol{x})\phi(u) + \left(y_{min}^{(n)} - \hat{y}(\boldsymbol{x})\right)\Phi(u),$$

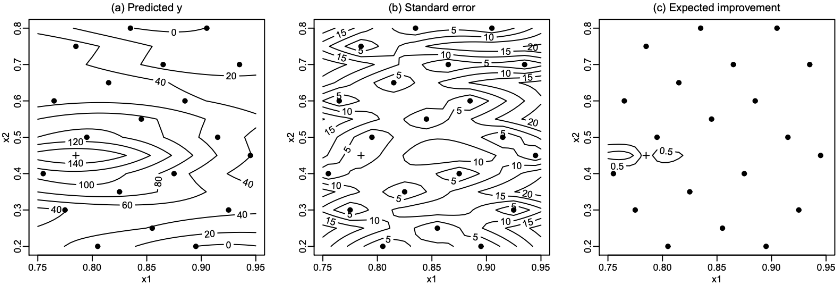
where $u = \frac{y_{min}^{(n)} - \hat{y}(\boldsymbol{x})}{s(\boldsymbol{x})}$.

GP Fit & EI



Source: Fig. 1 of Bingham et al. 2014

GP Fit & EI After Adding The New Run

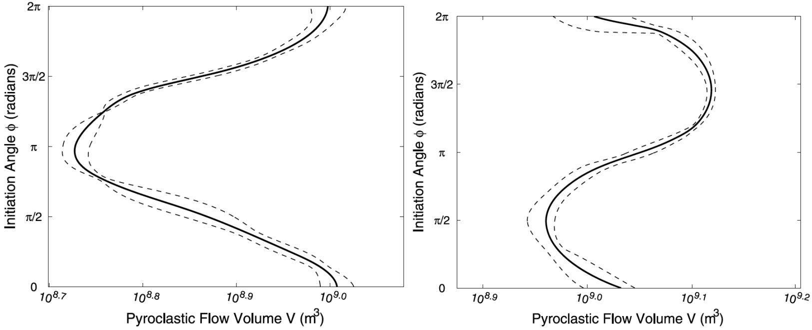


Source: Fig. 2 of Bingham et al. 2014

Example 2: Volcanic Eruption

Source: Bruce Pitman's slides on "Where You Gonna Go When the Volcano Blow".

The Problem: Contour Estimation



Source: Fig. 4 of Bayarri et al. 2009

Goal: To estimate the contour at level a:

$$S(a) = \{\boldsymbol{x} : y(\boldsymbol{x}) = a\}$$

EI For Contour Estimation

- Improvement function:

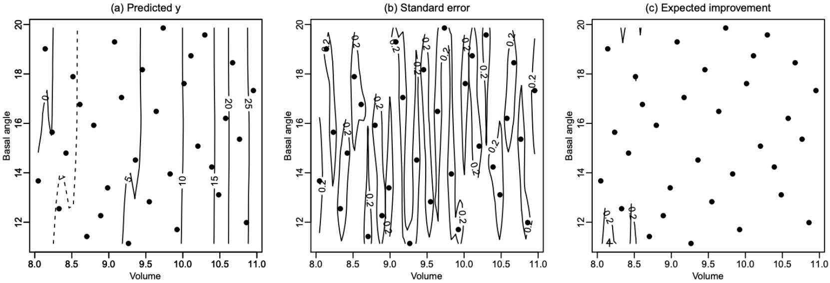
$$I(\boldsymbol{x}) = \epsilon^2(\boldsymbol{x}) - \min\left\{(y(\boldsymbol{x}) - a)^2, \epsilon^2(\boldsymbol{x})\right\}$$

- Expected Improvement:

$$\begin{aligned}\mathbb{E}\left[I(\boldsymbol{x})\right] = &\left[\epsilon^2(\boldsymbol{x}) - (\hat{y}(\boldsymbol{x}) - a)^2\right](\Phi(u_2) - \Phi(u_1)) \\ &+ s^2(\boldsymbol{x})\left[u_2\phi(u_2) - u_1\phi(u_2) - (\Phi(u_2) - \Phi(u_1))\right] \\ &+ 2\left(\hat{y}(\boldsymbol{x}) - a\right)s(\boldsymbol{x})\left(\phi(u_2) - \phi(u_1)\right),\end{aligned}$$

where $\epsilon(x) = \alpha s(\boldsymbol{x})$, $u_1 = \frac{(a - \hat{y}(\boldsymbol{x}) - \epsilon(\boldsymbol{x}))}{s(\boldsymbol{x})}$ and $u_2 = \frac{(a - \hat{y}(\boldsymbol{x}) + \epsilon(\boldsymbol{x}))}{s(\boldsymbol{x})}$

GP Fit & EI



Source: Fig. 3 of Bingham et al. 2014