Sequential Preference-Based Optimization

Ian Dewancker

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Sequential model-based (Bayesian) optimization techniques have demonstrated success as black box optimizers in low-dim spaces (hyperparams for ML models)

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$$\mathbf{x}_{opt} = \arg\max_{\mathbf{x} \in \mathcal{X}} f(\mathbf{x})$$

$$f(\boldsymbol{\lambda}) = \frac{1}{k} \sum_{i=1}^{k} \mathcal{L}(\boldsymbol{\lambda}, \mathcal{D}_{\text{train}}^{(i)}, \mathcal{D}_{\text{valid}}^{(i)})$$

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Open Source : SMAC, HyperOpt, Spearmint, MOE

Companies : Whetlab, SigOpt

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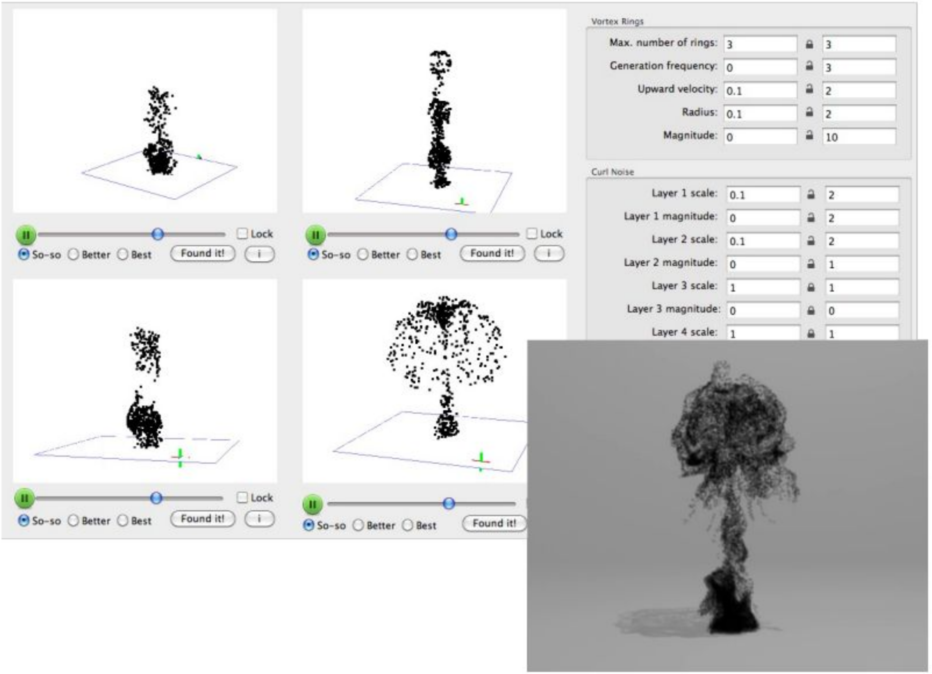
Approach : Interactive procedure to query user and guide optimization based on preference observations (bring human back into the loop!)

Prior Work

Tuning procedural animation parameters for particle simulations [1]



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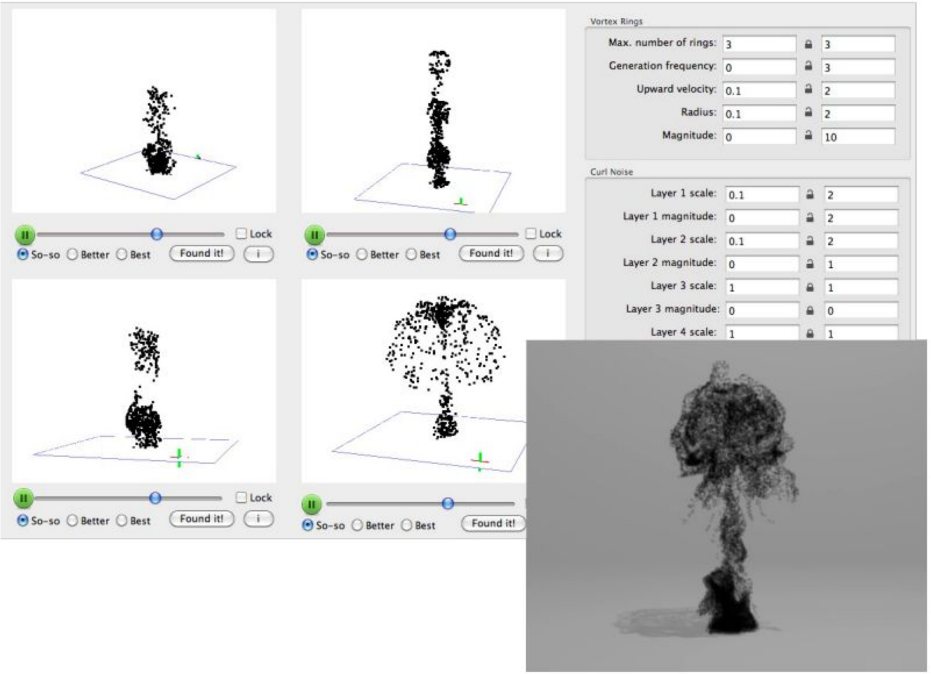

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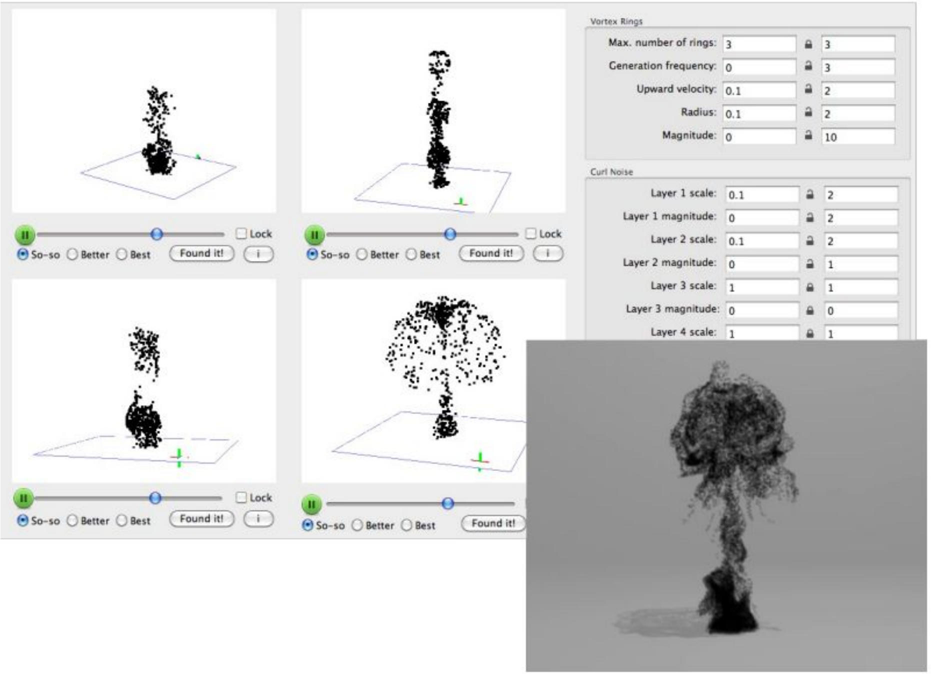

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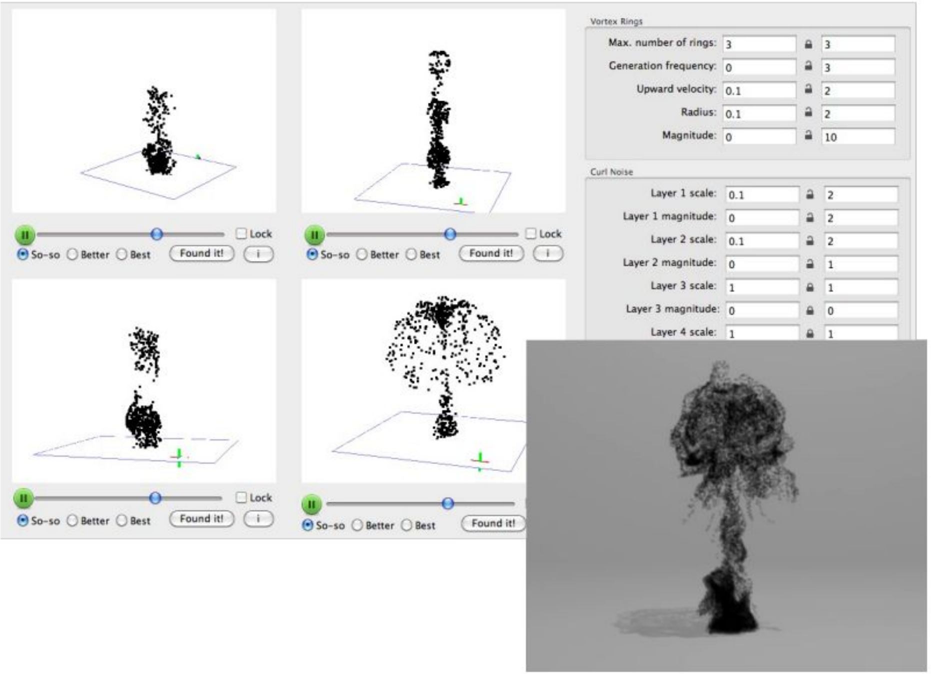

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3. Suggest new parameterizations that are expected to improve over best seen using latent utility

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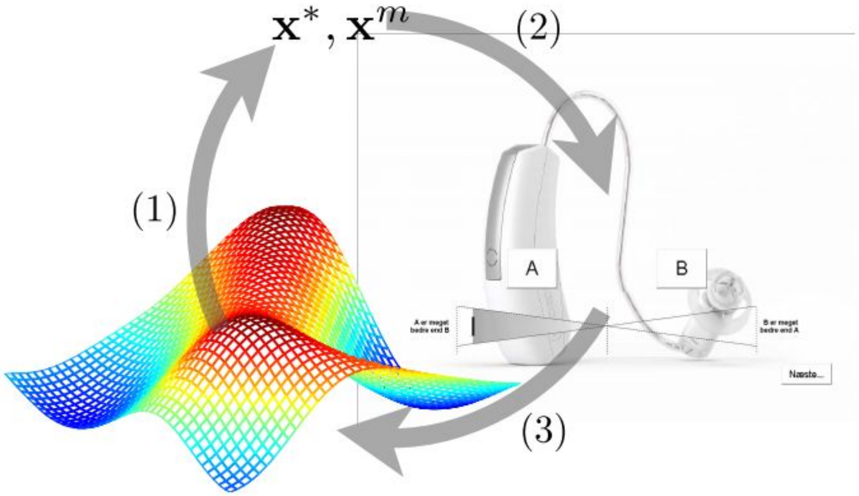
Tuning frequency-dependent hearing thresholds for hearing aid personalization [2]



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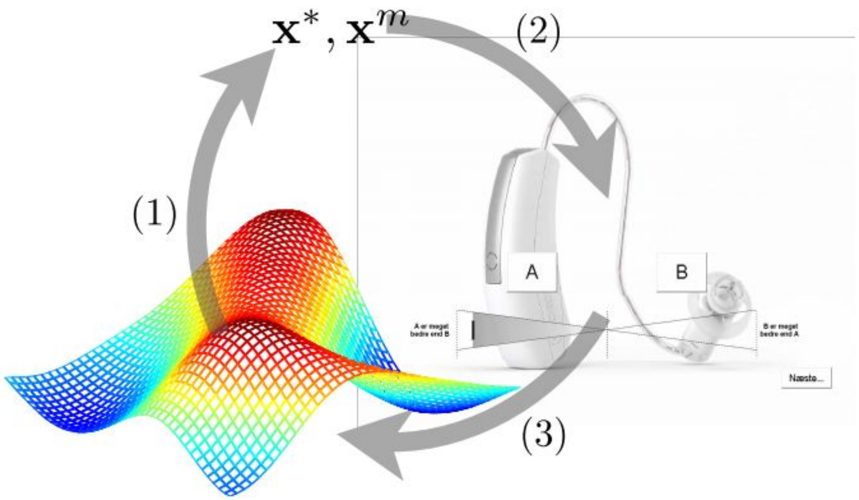

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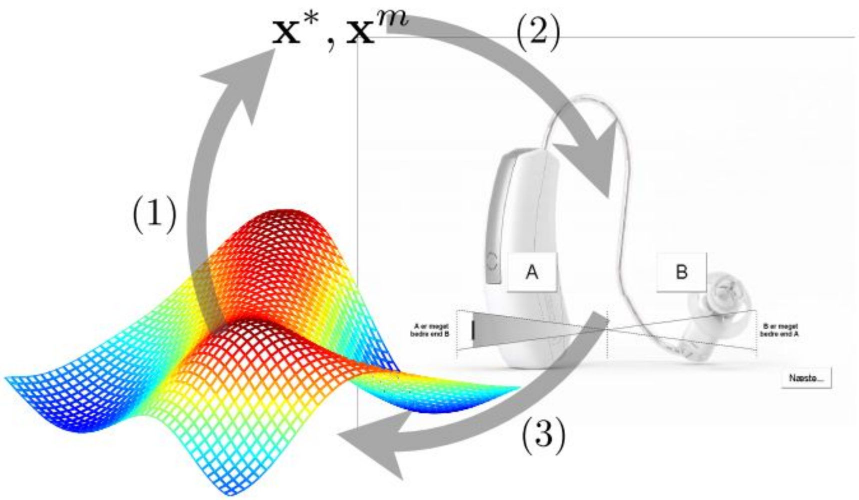

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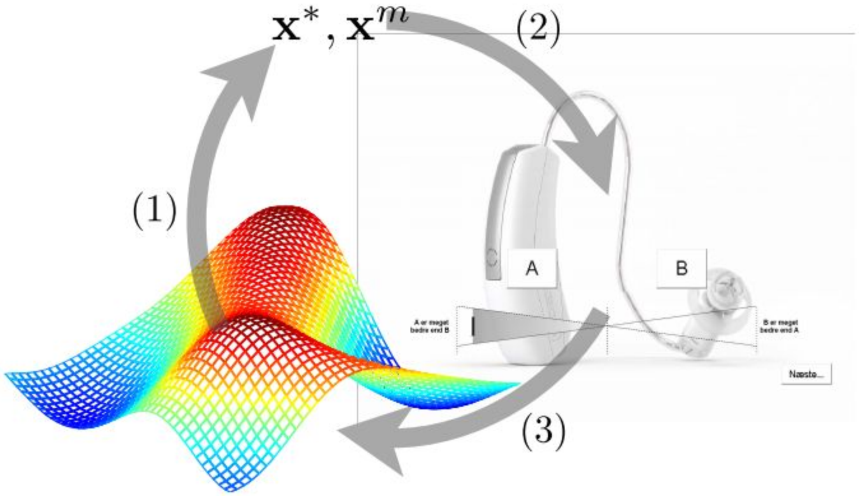

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Tuning feedback gains of a neuromuscular walking model [3]

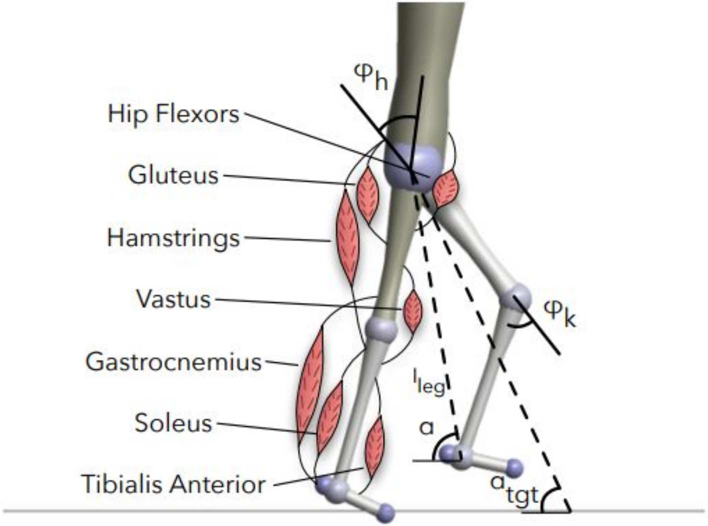

Fig. 2: Unimpaired human walking model with labeled muscles and definitions of hip and knee angles, leg length, and current and target swing leg angles.

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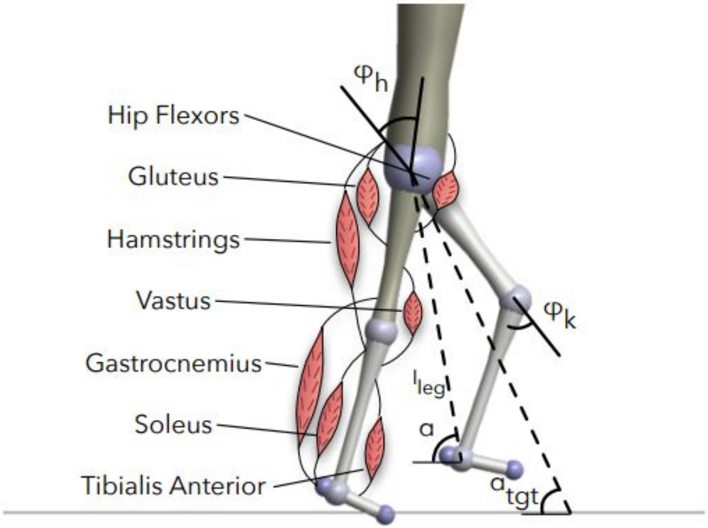

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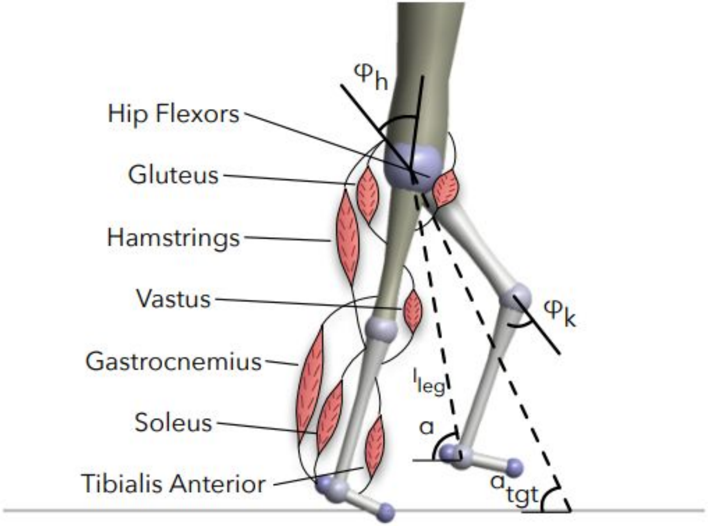

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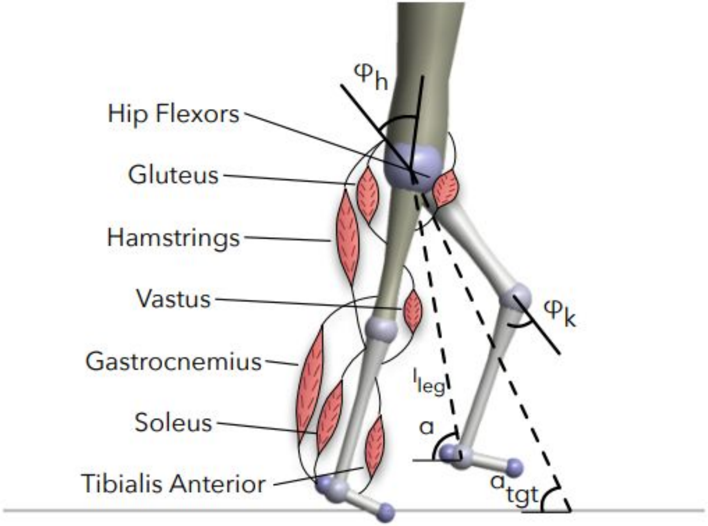

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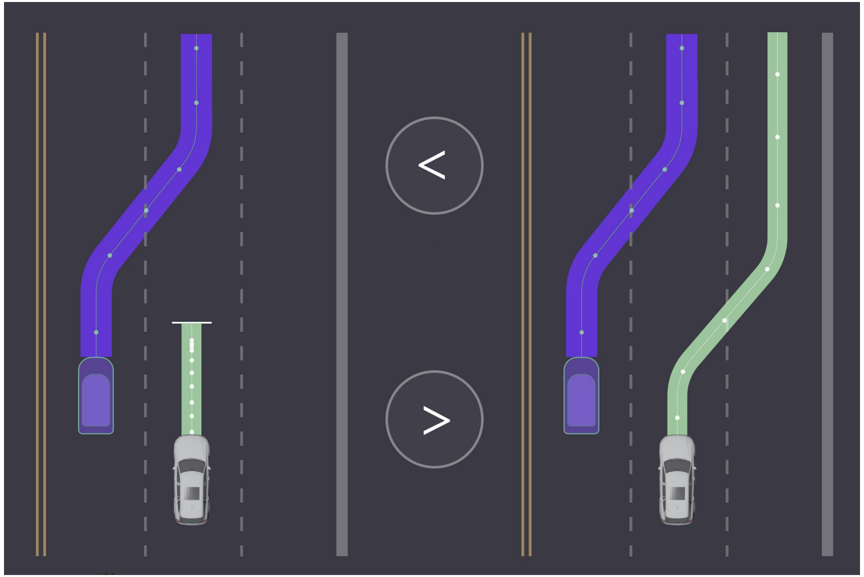

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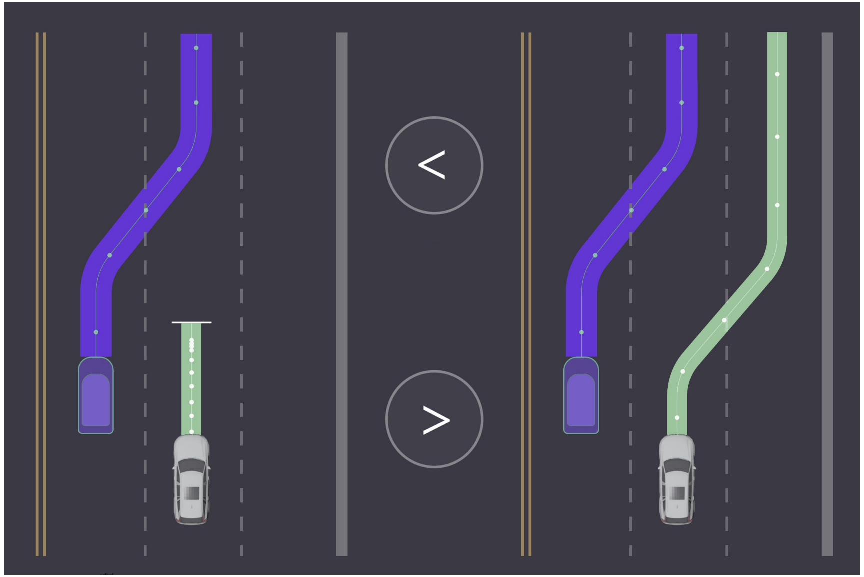

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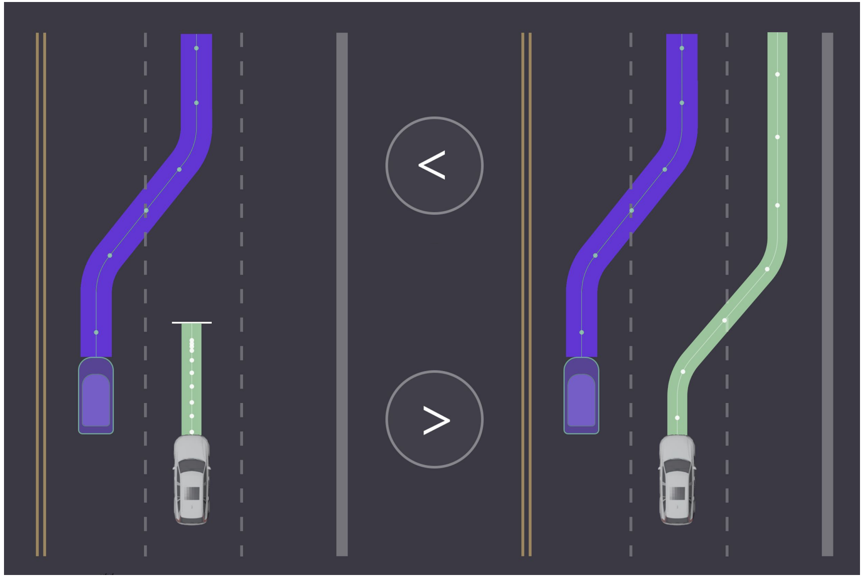

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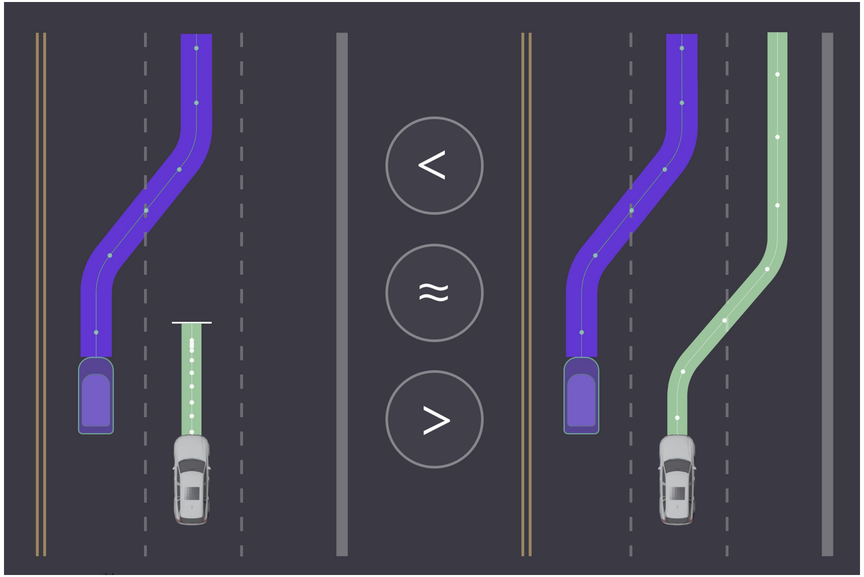

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Can we build on previous ideas to support observations having **equivalent** preference?

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Simple software interface to allow for extensions and rapid experiments

Gaussian Process Model Binary Preferences

M preference observations (**c**) are related to N unique query points (**X**) via a GP prior over latent function vectors (**f**) and a Bradley-Terry preference model [1,2,3]

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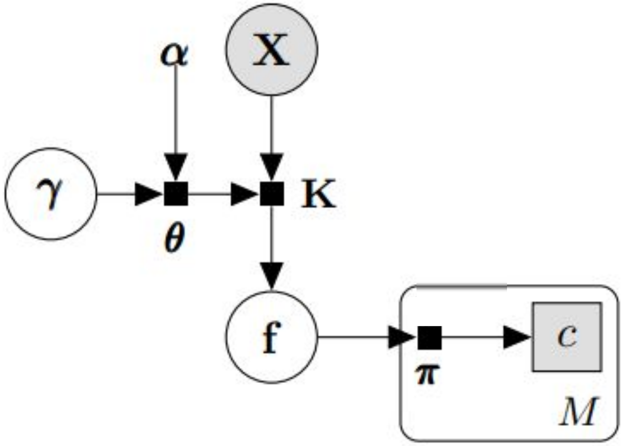


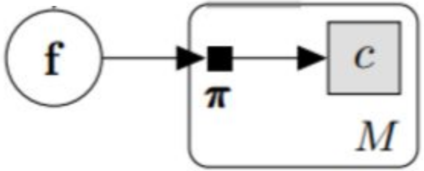
$$
\begin{aligned}
\gamma_d &\sim \mathbf{Normal}(0,1) \\
\theta_d &= S(\gamma_d)(\alpha_{d_U} - \alpha_{d_L}) + \alpha_{d_L} \\
K_{i,j} &= rbf(\mathbf{x}_i, \mathbf{x}_j, \boldsymbol{\theta}) \\
\mathbf{f} &\sim \mathbf{MVNormal}(\mathbf{0}, \mathbf{K}) \\
d_m &= \frac{f_m^1 - f_m^2}{\sqrt{2\sigma^2}} \\
\pi_m^{\succ} &= S(d_m), \quad \pi_m^{\prec} = 1 - S(d_m)
\end{aligned}
$$

$$
rbf(\mathbf{x}_i, \mathbf{x}_j, \boldsymbol{\theta}) = \sigma^2 \exp\left(-\tfrac{1}{2}\sum_{d=1}^{D} \tfrac{1}{\theta_d^2}(x_{i\,d} - x_{j\,d})^2\right) \qquad S(x) = \tfrac{1}{1+e^{-x}}
$$

Bradley-Terry Model Extension for Ties

The Bradley-Terry model relates the comparison points' latent function values to discrete binary preferences.

Binary



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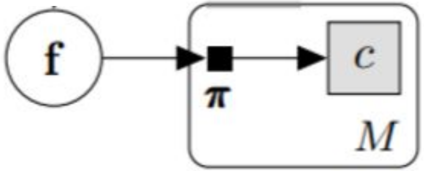

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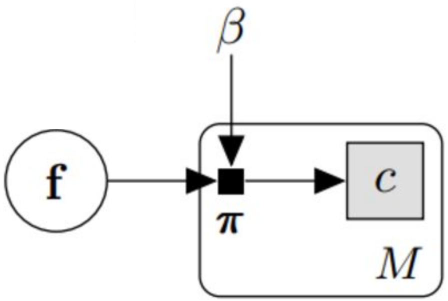
An extension to the BT model produces preference probabilities over 3 classes [4]

Ternary



$$d_m = \frac{f_m^1 - f_m^2}{\sqrt{2\sigma^2}}$$

$$z_m^1 = S(d_m), \quad z_m^2 = 1 - S(d_m)$$

$$\pi_m^{\prec} = \frac{z_m^2}{z_m^2 + \beta z_m^1}, \quad \pi_m^{\approx} = \frac{(\beta^2 - 1) z_m^1 z_m^2}{(z_m^1 + \beta z_m^2)(z_m^2 + \beta z_m^1)}$$

$$\pi_m^{\succ} = (1 - \pi_m^{\prec} - \pi_m^{\approx})$$

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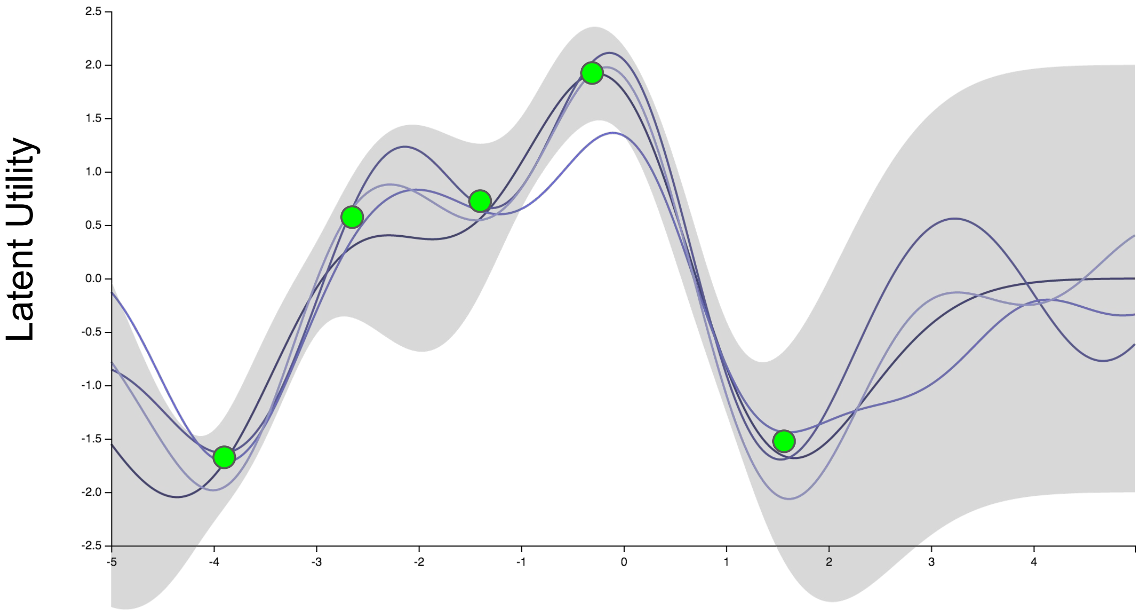

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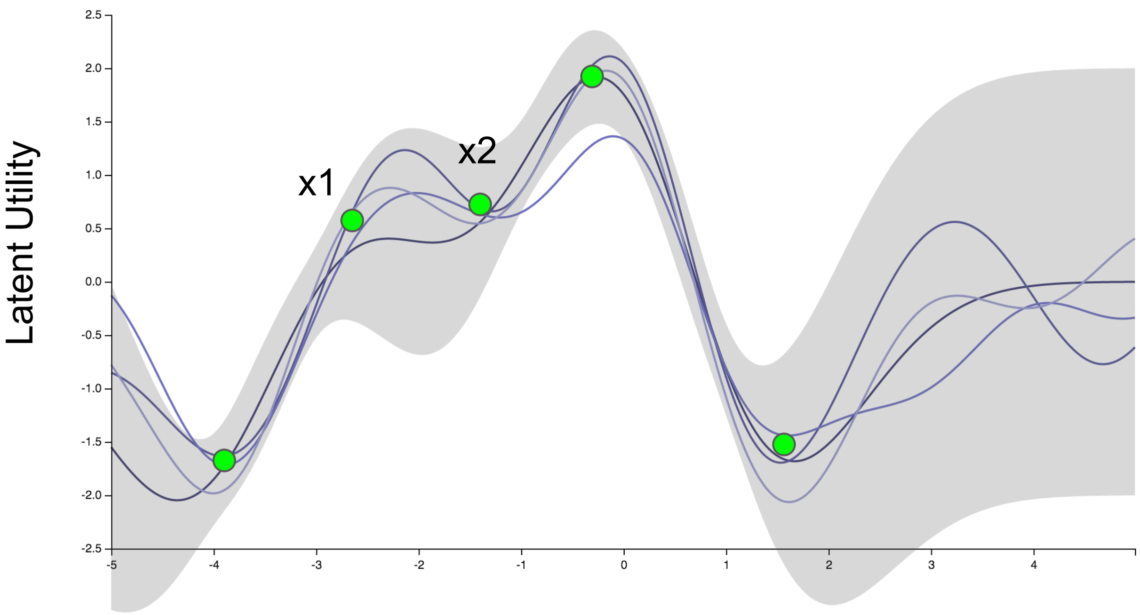

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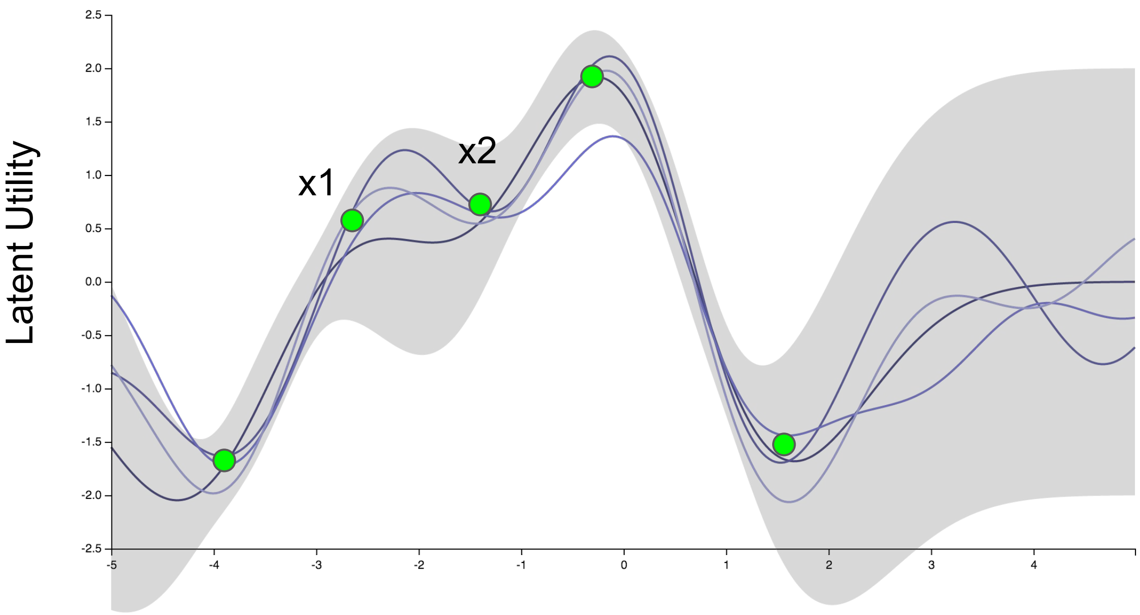

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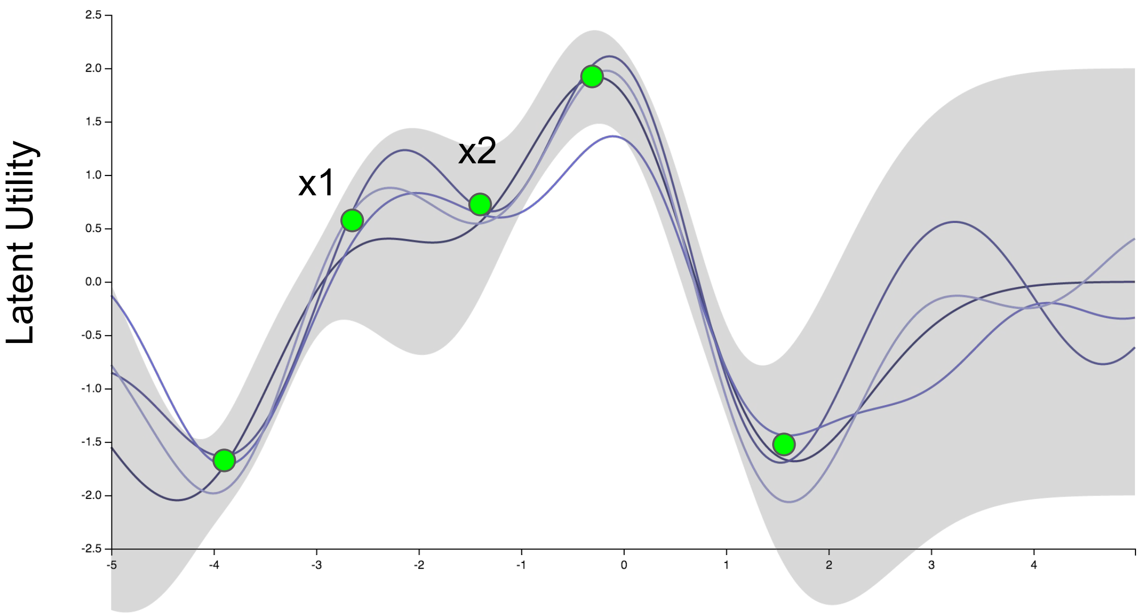

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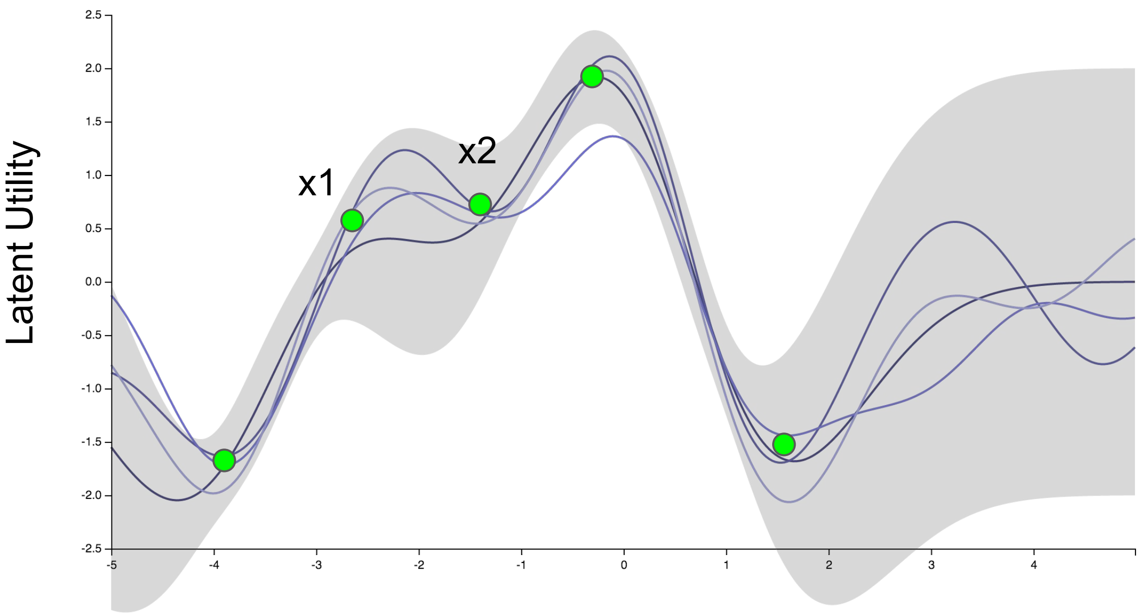

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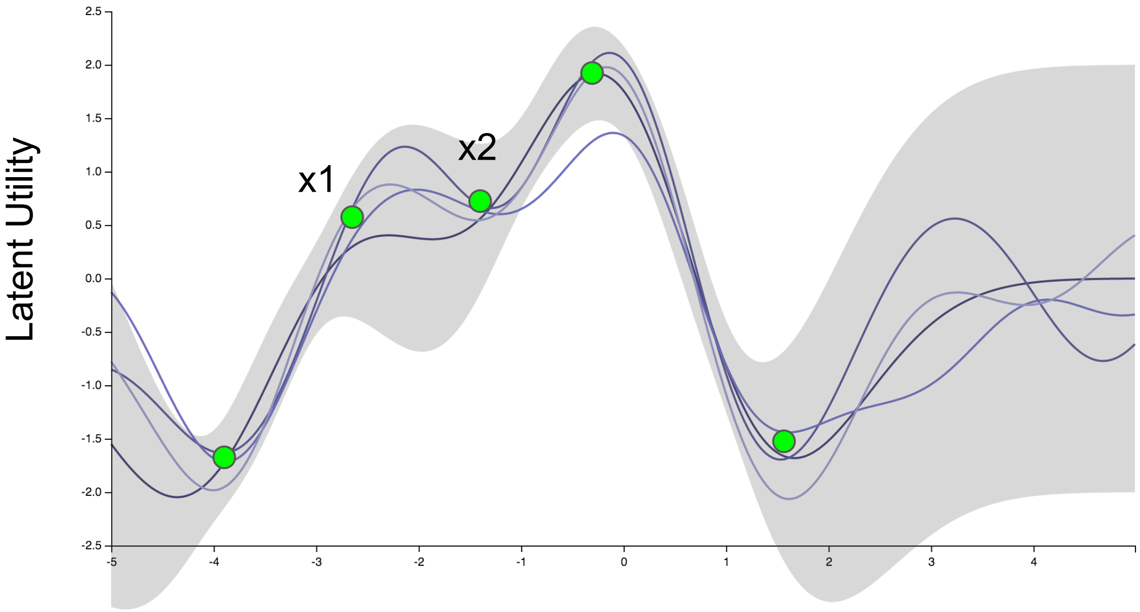

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Bradley-Terry with Ties (β = 2.5)

p = [0.28, 0.43, 0.29]

Inference

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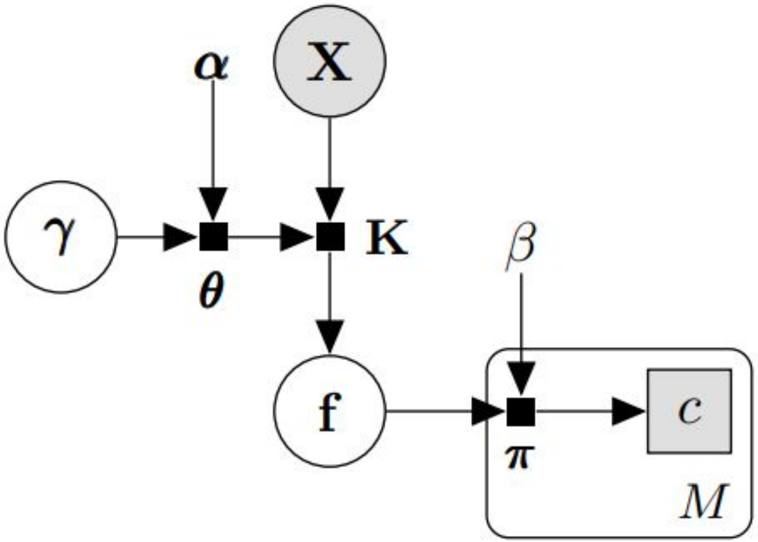

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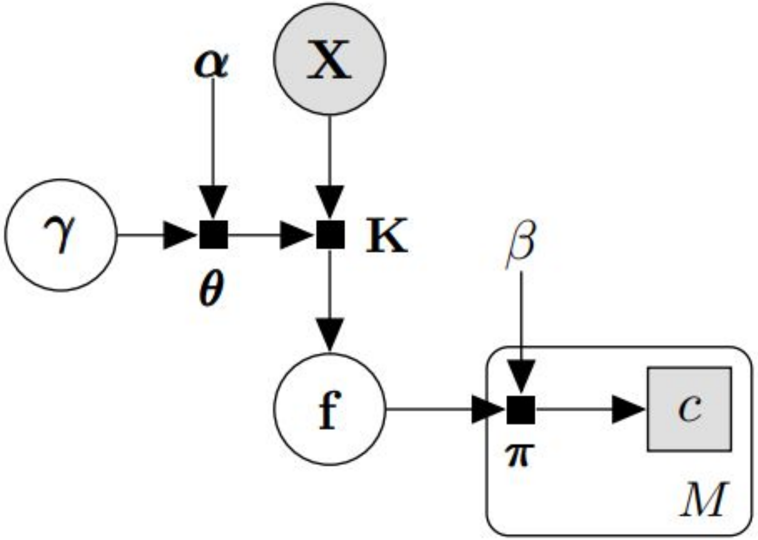

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Latent vars

x = {**X**, **c**}
Observed vars

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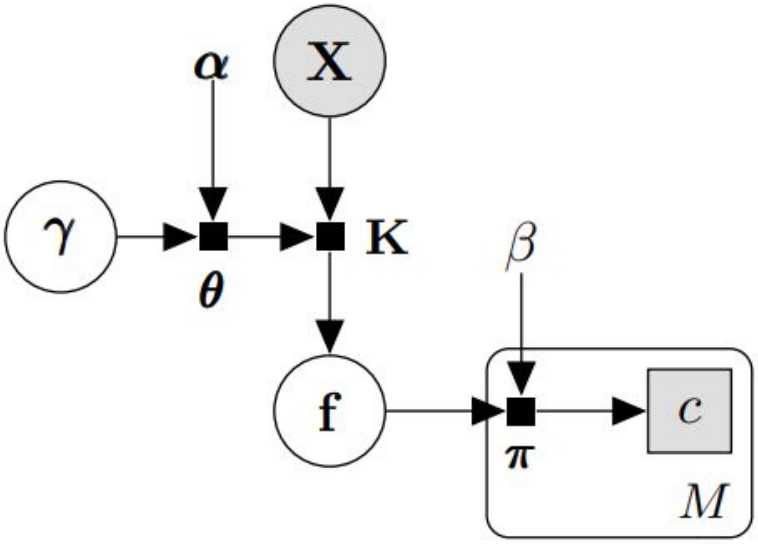
p(**x**, **z**) is fully defined (joint distribution) when we know **z**. However, we are interested in inferring the latent variables given only the observed preferences and the unique comparison points.



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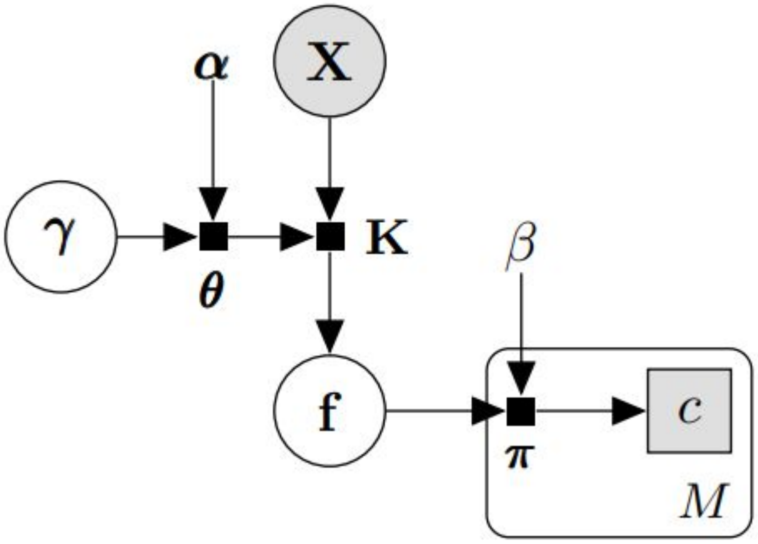
How to find (or approximate) the posterior p(**z** | **x**) ?



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Many strategies to approximate $p(z \mid x)$. One idea is to pick an approximating distribution $q(z)$ and minimize divergence between $p(z \mid x)$ and $q(z)$

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$$p(\mathbf{z} \mid \mathbf{x}) \approx q(\mathbf{z}\,;\,\boldsymbol{\lambda}) = \prod_{i=1}^{N} \mathcal{N}(z_i \mid \lambda_{\mu_i},\ \lambda_{\sigma i}) \prod_{k=1}^{D} \mathcal{N}(z_k \mid \lambda_{\mu_k},\ \lambda_{\sigma k})$$

One approximation strategy is to use the **mean-field approximation** that simply uses factorized gaussians for each of the latent random variables of interest.

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&= \arg\min_{\boldsymbol{\lambda}} \; \mathbb{E}_{\mathbf{z}\sim q(\mathbf{z};\boldsymbol{\lambda})} \left[\log q(\mathbf{z}\,;\,\boldsymbol{\lambda}) - \log p(\mathbf{z},\mathbf{x})\right]
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&= \arg\min_{\boldsymbol{\lambda}} \int q(\mathbf{z} \,;\, \boldsymbol{\lambda}) \log \frac{q(\mathbf{z} \,;\, \boldsymbol{\lambda})}{p(\mathbf{z}, \mathbf{x})} \, d\mathbf{z} \\
&= \arg\min_{\boldsymbol{\lambda}} \; \mathbb{E}_{\mathbf{z} \sim q(\mathbf{z};\boldsymbol{\lambda})} \left[\log q(\mathbf{z} \,;\, \boldsymbol{\lambda}) - \log p(\mathbf{z}, \mathbf{x})\right] \\
&= \arg\max_{\boldsymbol{\lambda}} \; \mathbb{E}_{\mathbf{z} \sim q(\mathbf{z};\boldsymbol{\lambda})} \left[\log p(\mathbf{z}, \mathbf{x}) - \log q(\mathbf{z} \,;\, \boldsymbol{\lambda})\right]
\end{aligned}
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Evidence Lower Bound (ELBO)

Variational Inference

Maximizing the ELBO is equivalent to minimizing KL(q || p). If we can estimate the gradient of this function we can optimize using gradient descent [6]

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&= \mathbb{E}_{\mathbf{z}\sim q(\mathbf{z};\boldsymbol{\lambda})}\left[\left(\log p(\mathbf{z},\mathbf{x}) - \log q(\mathbf{z}\,;\,\boldsymbol{\lambda})\right)\nabla_{\boldsymbol{\lambda}}\log q(\mathbf{z}\,;\,\boldsymbol{\lambda})\right]
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Monte Carlo Estimate

Acquisition Function for Preference-Based Opt.

With a model and inference algorithm selected, we still need to decide on mechanism to select next point to present to user to compare. Previous work has proposed use of expected improvement [1]

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$$\mathbf{k}_* = [rbf(\mathbf{x}^*, \mathbf{x}_1, \boldsymbol{\theta}) \ \cdots \ rbf(\mathbf{x}^*, \mathbf{x}_N, \boldsymbol{\theta})]$$

$$\mu(\mathbf{x}^*) = \mathbf{k}_*^{\mathsf{T}} \mathbf{K}^{-1} \mathbf{f}$$

$$s^2(\mathbf{x}^*) = rbf(\mathbf{x}^*, \mathbf{x}^*, \boldsymbol{\theta}) - \mathbf{k}_*^{\mathsf{T}} \mathbf{K}^{-1} \mathbf{k}_*$$

$$d = \mu(\mathbf{x}^*) - f_{best}$$

$$a_{\mathsf{EI}}(\mathbf{x}^*; \mathbf{z}) = \begin{cases} d\Phi(\frac{d}{s(\mathbf{x}^*)}) + s(\mathbf{x}^*)\phi(\frac{d}{s(\mathbf{x}^*)}), & \text{if } s(\mathbf{x}^*) > 0 \\ 0, & \text{if } s(\mathbf{x}^*) = 0 \end{cases}$$

$$\mathbf{x}^n = \arg\max_{\mathbf{x}^*} \int a_{\mathsf{EI}}(\mathbf{x}^*; \mathbf{z}) q(\mathbf{z} \ ; \ \boldsymbol{\lambda}) d\mathbf{z}$$

Experiments

Considered efficiency of method in minimizing synthetic test functions using only pairwise comparative observations

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At each iteration a query point (x_n) is selected by the algorithm and compared against the current best point (x_b) using a test function (f_test)

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The discrete preference observations are simulated in the following way :

$$\text{pref}(\mathbf{x}_1, \mathbf{x}_2) = \begin{cases} \mathbf{x}_1 \approx \mathbf{x}_2, & \text{if } |f_{\text{test}}(\mathbf{x}_1) - f_{\text{test}}(\mathbf{x}_2)| \leq \epsilon \\ \mathbf{x}_1 \succ \mathbf{x}_2, & \text{else if } f_{\text{test}}(\mathbf{x}_1) < f_{\text{test}}(\mathbf{x}_2) \\ \mathbf{x}_1 \prec \mathbf{x}_2, & \text{otherwise} \end{cases}$$

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Vary equivalent tolerance thresh under two settings (0.1, 0.001)

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Baselines search methods

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$$a_{\mathsf{PE}}(\mathbf{x}^*; \mathbf{z}) = rbf(\mathbf{x}^*, \mathbf{x}^*, \boldsymbol{\theta}) - \mathbf{k}_*^{\mathsf{T}} \mathbf{K}^{-1} \mathbf{k}_*$$

$$\mathbf{x}^n = \arg\max_{\mathbf{x}^*} \int a_{\mathsf{PE}}(\mathbf{x}^*; \mathbf{z}) q(\mathbf{z} \, ; \, \boldsymbol{\lambda}) d\mathbf{z}$$

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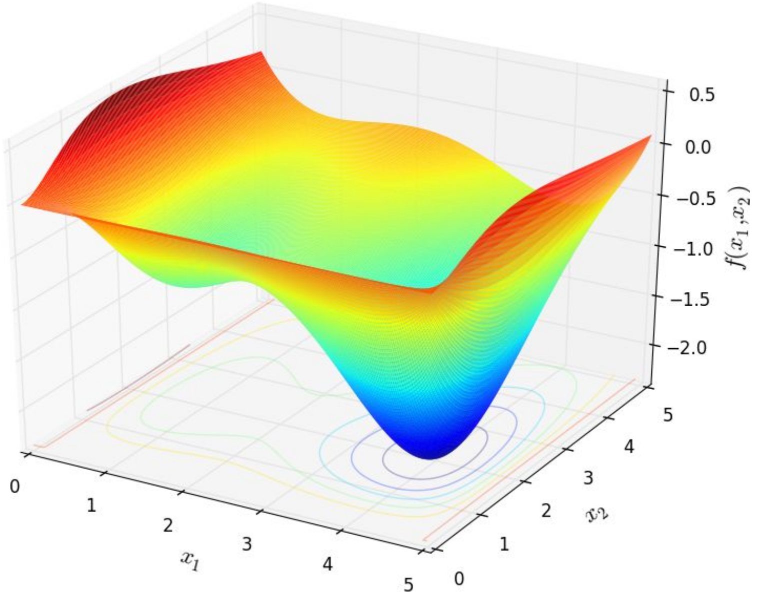
$$\mathbf{x}^n = \arg\max_{\mathbf{x}^*} \int a_{\mathsf{PE}}(\mathbf{x}^*; \mathbf{z}) q(\mathbf{z} \, ; \, \boldsymbol{\lambda}) dz$$

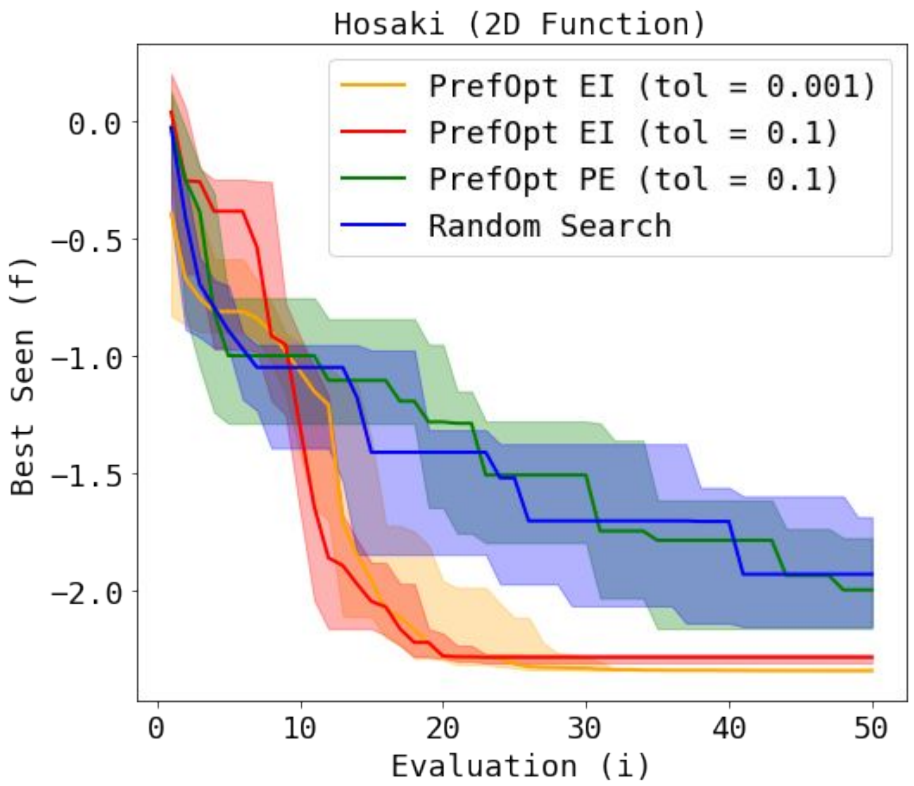
Run each strategy 10 times and record interquartile range

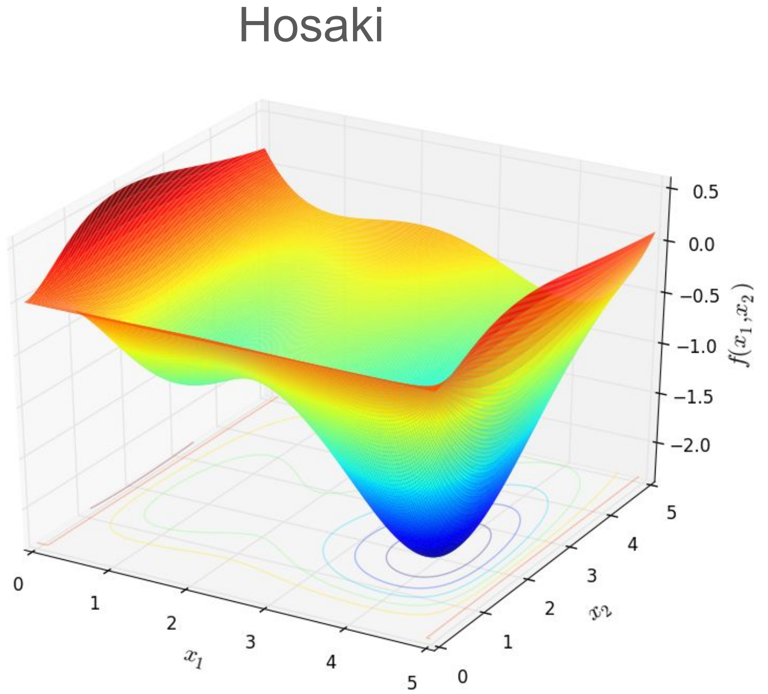
Experiments

Hosaki



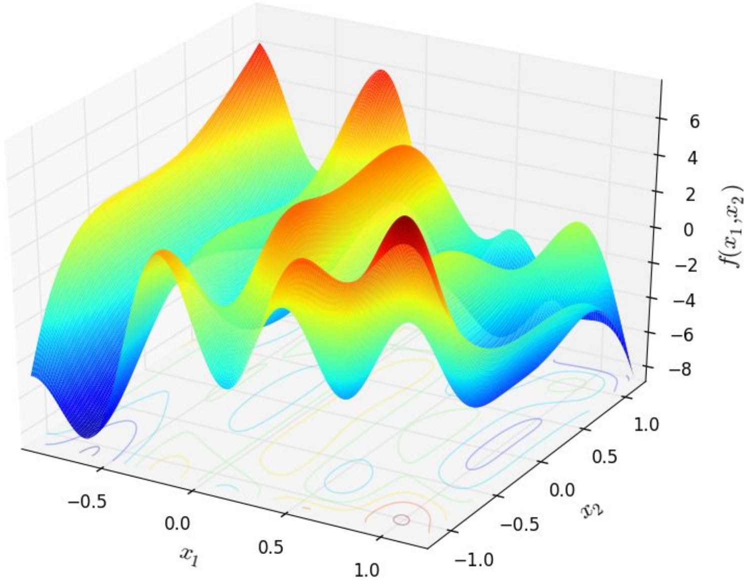
Experiments





Experiments

UrsemWaves



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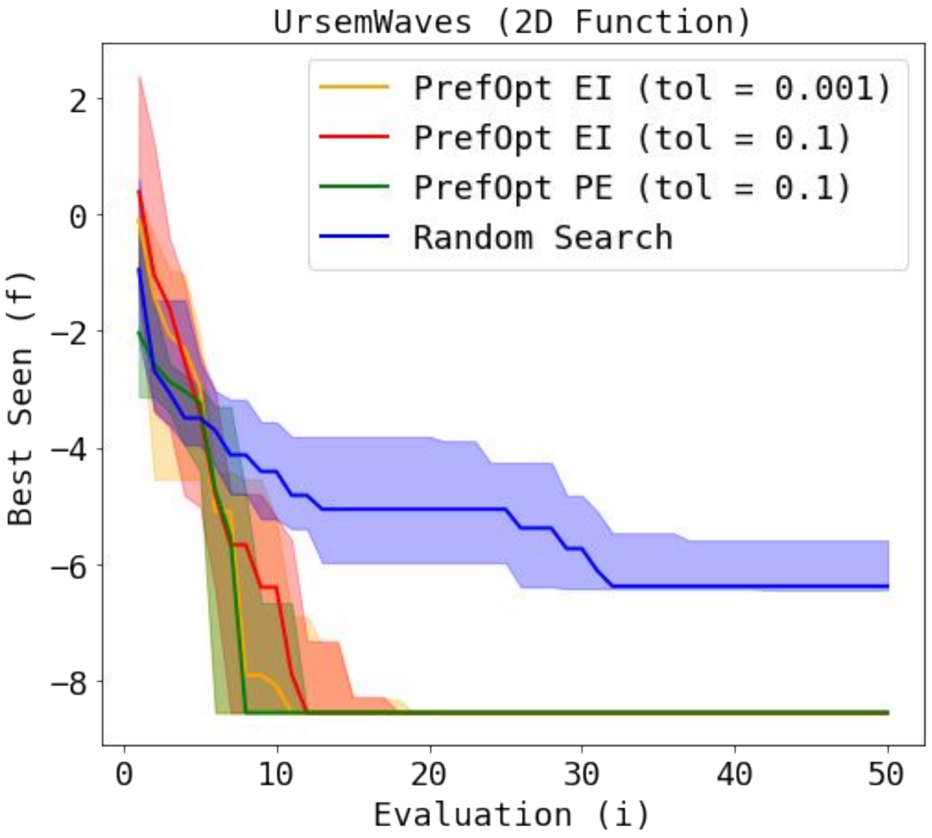

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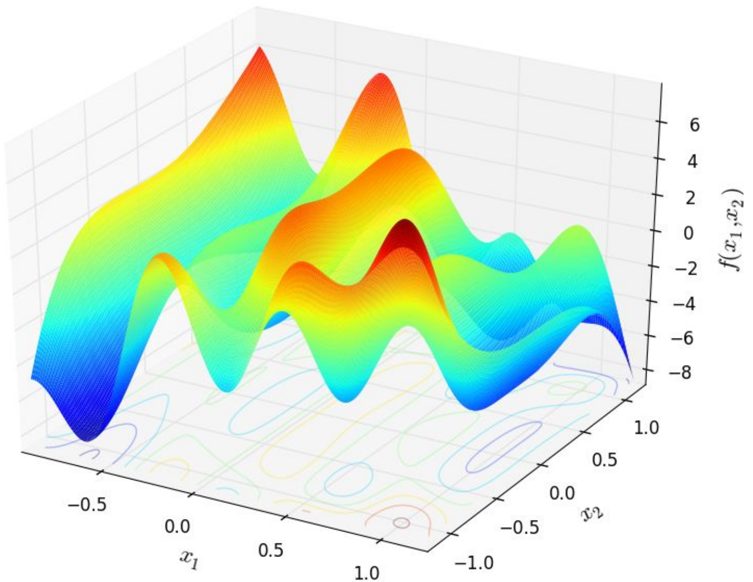

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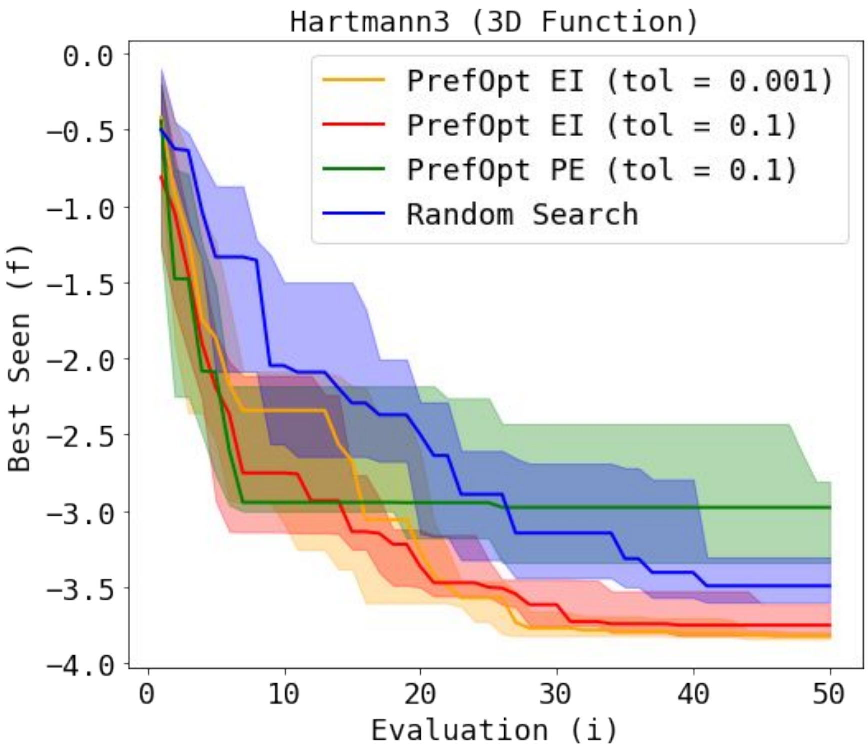
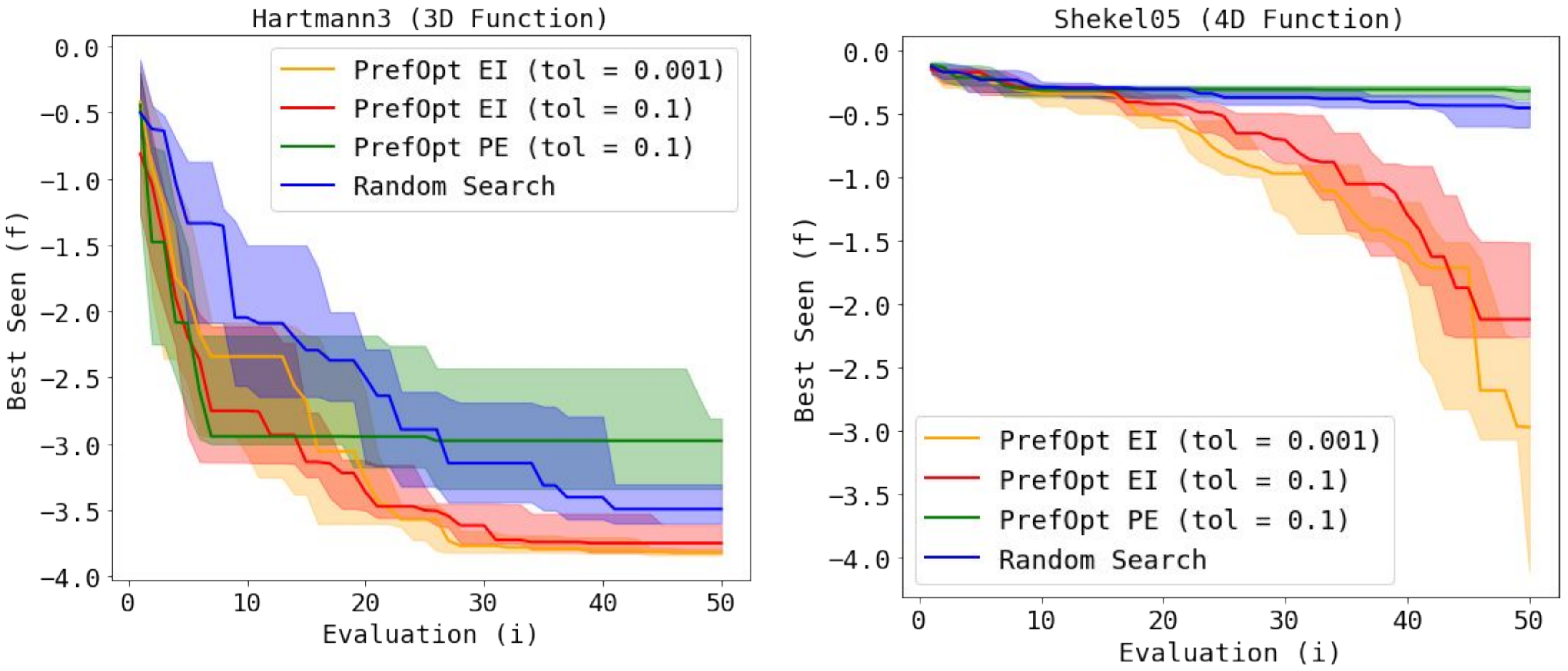


Experiments



PrefOpt Software

Open source python library built on top of Edward, TensorFlow

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Succinct interface to conduct preference-based optimizations

```
import prefopt
# define the domain of the search space
bounding_box = [[-5.0 , 5.0] , [0.0 , 10.0]]
exp = prefopt.PreferenceExperiment(bounding_box)
for i in xrange(1, N) :
    # search for the next points to compare
    X = exp.find_next()
    # get user preference : -1 denotes x1 < x2 , 0 denotes x1 = x2 , 1 denotes x1 > x2
    order = get_user_pref(X[0], X[1])
    # update model with new preference observation
    exp.prefer(X[0], X[1], order)
```

Future Work

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Beyond low dimensional spaces : How can we simplify building ML / RL systems via preferences? [7]

Questions / Comments

Thanks for Listening!

References

[1] Eric Brochu. *Interactive Bayesian Optimization: Learning Parameters for Graphics and Animation*.

[2] JB Nielsen, JN Widex, BS Jensen, J Larsen *Hearing Aid Personalization*

[3] Nitish Thatte, Helei Duan, Hartmut Geyer *A Sample-Efficient Black-Box Optimizer to Train Policies for Human-in-the-Loop Systems with User Preferences*

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