AutoML: Bayesian Optimization for HPO

The Tree-Parzen Estimator (TPE)

Bernd Bischl Frank Hutter Lars Kotthoff
Marius Lindauer Joaquin Vanschoren

Overview of TPE [Bergstra et al. 2011]

- Standard Bayesian optimization models the probability $p(y \mid \boldsymbol{\lambda})$ of observations y given configurations $\boldsymbol{\lambda}$
- Instead, TPE fits kernel density estimators (KDEs) $l(\boldsymbol{\lambda} \mid y \leq \gamma)$ and $g(\boldsymbol{\lambda} \mid y > \gamma)$
  - These KDEs are for "good configurations" (leading to objective function values below a threshold γ) and "bad configurations"
  - By default, γ is set to the 15% quantile of the observations

Overview of TPE [Bergstra et al. 2011]

- Standard Bayesian optimization models the probability $p(y \mid \boldsymbol{\lambda})$ of observations y given configurations $\boldsymbol{\lambda}$
- Instead, TPE fits kernel density estimators (KDEs) $l(\boldsymbol{\lambda} \mid y \leq \gamma)$ and $g(\boldsymbol{\lambda} \mid y > \gamma)$
  - These KDEs are for "good configurations" (leading to objective function values below a threshold γ) and "bad configurations"
  - By default, γ is set to the 15% quantile of the observations

- Optimizing $l(\boldsymbol{\lambda})/g(\boldsymbol{\lambda})$ is equivalent to optimizing standard expected improvement in Bayesian optimization [Bergstra et al. 2011]

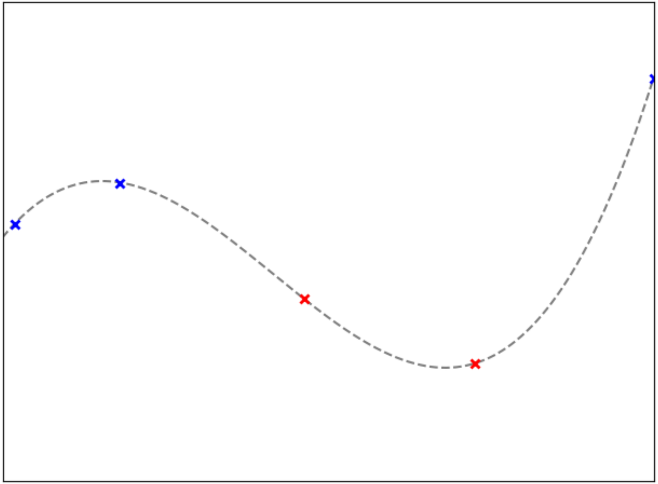
Overview of TPE [Bergstra et al. 2011]

- Standard Bayesian optimization models the probability $p(y \mid \boldsymbol{\lambda})$ of observations y given configurations $\boldsymbol{\lambda}$
- Instead, TPE fits kernel density estimators (KDEs) $l(\boldsymbol{\lambda} \mid y \leq \gamma)$ and $g(\boldsymbol{\lambda} \mid y > \gamma)$
  - These KDEs are for "good configurations" (leading to objective function values below a threshold γ) and "bad configurations"
  - By default, γ is set to the 15% quantile of the observations

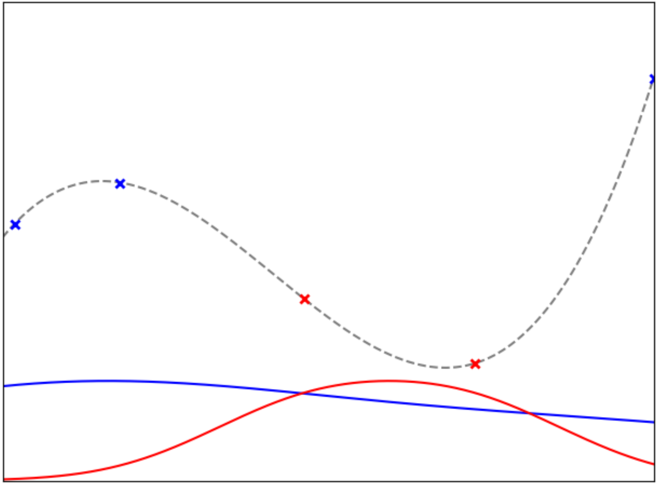
- Optimizing $l(\boldsymbol{\lambda})/g(\boldsymbol{\lambda})$ is equivalent to optimizing standard expected improvement in Bayesian optimization [Bergstra et al. 2011]

- Why is the technique called TPE?
  - The used KDEs are Parzen estimators
  - TPE can handle tree-structured search spaces

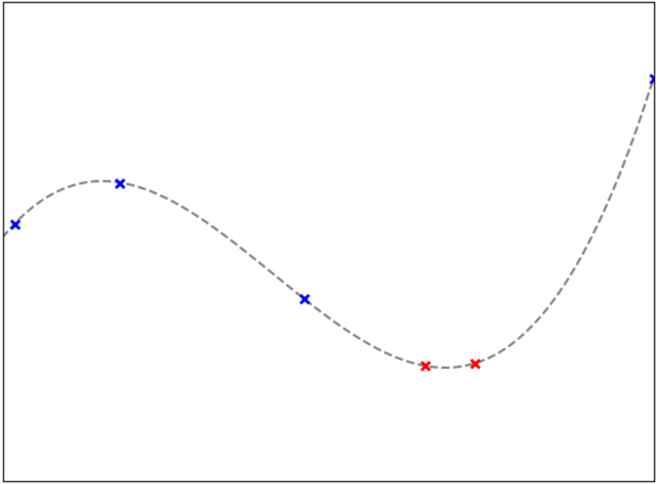
TPE Example



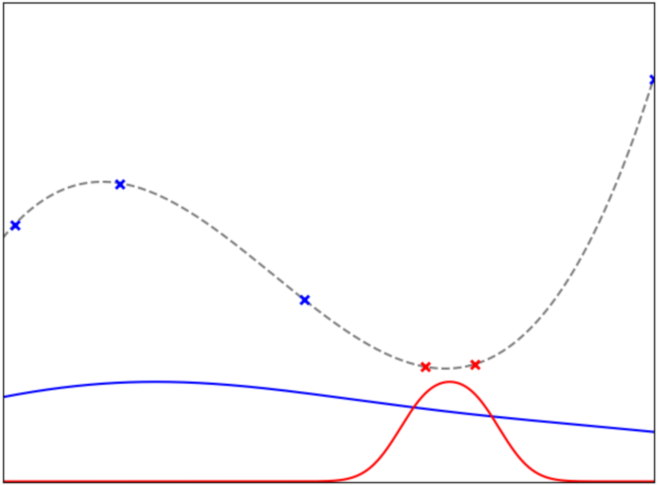
TPE Example



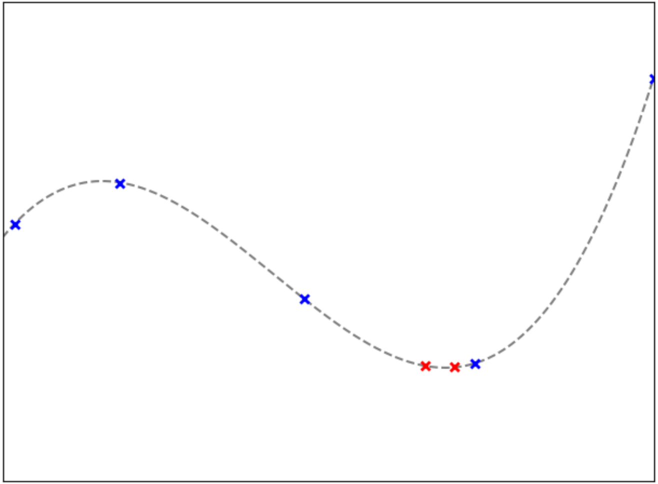
TPE Example



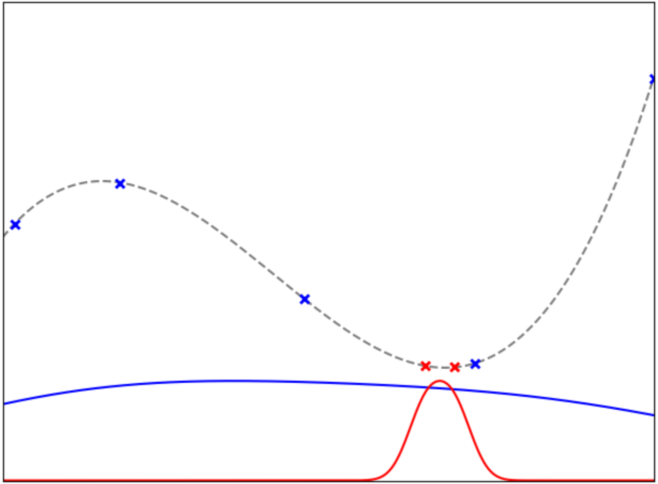
TPE Example



TPE Example



TPE Example



TPE Pseudocode

TPE loop

Require: Search space $\boldsymbol{\Lambda}$, cost function c, percentile γ, maximal number of function evaluations T

Result : Best observed configuration $\boldsymbol{\lambda}$ according to $\mathcal{D}^{(T)}$

Initialize data $\mathcal{D}^{(0)}$ with initial observations

for $t = 1$ **to** T **do**

  $\mathcal{D}_{\text{good}}, \mathcal{D}_{\text{bad}} \leftarrow$ split $\mathcal{D}^{(t-1)}$ according to quantile γ

  $l(\boldsymbol{\lambda})$, $g(\boldsymbol{\lambda}) \leftarrow$ fit KDE on $\mathcal{D}_{\text{good}}$, $\mathcal{D}_{\text{bad}}$ respectively

  $\boldsymbol{\Lambda}_{\text{cand}} \leftarrow$ draw samples from l;

  Select next query point: $\boldsymbol{\lambda}^{(t)} \in \arg\max_{\boldsymbol{\lambda} \in \boldsymbol{\Lambda}_{\text{cand}}} l(\boldsymbol{\lambda})/g(\boldsymbol{\lambda})$

  Query $c(\boldsymbol{\lambda}^{(t)})$

  $\mathcal{D}^{(t)} \leftarrow \mathcal{D}^{(t-1)} \cup \{\langle \boldsymbol{\lambda}^{(t)}, c(\boldsymbol{\lambda}^{(t)}) \rangle\}$

end

Further Details

Remarks:

- TPE models $p(\boldsymbol{\lambda}|c(\boldsymbol{\lambda}))$
  - we can multiply it with a prior to add expert knowledge

Further Details

Remarks:

- TPE models $p(\boldsymbol{\lambda}|c(\boldsymbol{\lambda}))$
  - we can multiply it with a prior to add expert knowledge
- Performance of TPE depends on:
  - setting of γ to trade-off exploration and exploitation
  - bandwidth of the KDEs

Further Details

Remarks:

- TPE models $p(\boldsymbol{\lambda}|c(\boldsymbol{\lambda}))$
  - we can multiply it with a prior to add expert knowledge
- Performance of TPE depends on:
  - setting of γ to trade-off exploration and exploitation
  - bandwidth of the KDEs
- A successful tool implementing TPE is Hyperopt [Bergstra et al.]

Summary

Advantages

- Computationally efficient: $O(Nd)$
- Parallelizable
- Robust
- Can handle complex search spaces with priors

Summary

Advantages

- Computationally efficient: $O(Nd)$
- Parallelizable
- Robust
- Can handle complex search spaces with priors

Disadvantages

- Less sample-efficient than GPs

Questions to Answer for Yourself / Discuss with Friends

- Disussion. Is TPE really Bayesian optimization?
- Disussion. How does γ impact the optimization procedure?
- Derivation. Go through the derivation that optimizing $l(\boldsymbol{\lambda})/g(\boldsymbol{\lambda})$ is equivalent to optimizing expected improvement; see Section 4.1 in [Bergstra et al. 2011].