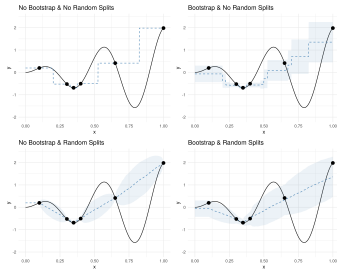


Optimization in Machine Learning

Bayesian Optimization Important Surrogate Models



Learning goals

- Search space / input data peculiarities in black box problems
- Gaussian process
- Random forest

SURROGATE MODELS

Desiderata:

- Regression model (there are also classification approaches)
- Non-linear local model
- Accurate predictions (especially for small sample sizes)
- Often: uncertainty estimates
- Robust, works often well without human modeler intervention

Depending on the application:

- Can handle different types of inputs (numerical and categorical)
- Can handle dependencies (i.e., hierarchical input)



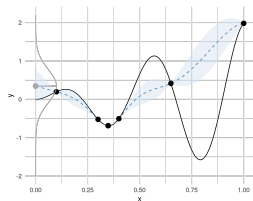
GAUSSIAN PROCESS

Posterior predictive distribution for test point $\mathbf{x} \in \mathcal{S}$:

$$Y(\mathbf{x}) \mid \mathbf{x}, \mathcal{D}^{[t]} \sim \mathcal{N} \left(\hat{f}(\mathbf{x}), \hat{s}^2(\mathbf{x}) \right)$$

with

$$\begin{aligned}\hat{f}(\mathbf{x}) &= \mathbf{k}(\mathbf{x})^\top \mathbf{K}^{-1} \mathbf{y} \\ \hat{s}^2(\mathbf{x}) &= k(\mathbf{x}, \mathbf{x}) - \mathbf{k}(\mathbf{x})^\top \mathbf{K}^{-1} \mathbf{k}(\mathbf{x})\end{aligned}$$



Kernel method, based on kernel / Gram matrix $\mathbf{K} := (k(\mathbf{x}^{[i]}, \mathbf{x}^{[j]}))_{i,j}$

GAUSSIAN PROCESS / 2

Example kernel functions:

- Radial basis function kernel (also known as Gauss kernel):

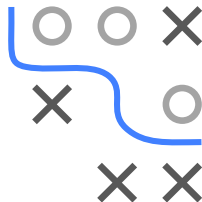
$$k(\mathbf{x}, \mathbf{x}') = \exp \left(-\frac{d(\mathbf{x}, \mathbf{x}')^2}{2l^2} \right)$$

- l length scale; $d(\cdot, \cdot)$ Euclidean distance
- infinitely differentiable - very “smooth”

- Matérn kernels:

$$k(\mathbf{x}, \mathbf{x}') = \frac{1}{\Gamma(\nu)2^{\nu-1}} \left(\frac{\sqrt{2\nu}}{l} d(\mathbf{x}, \mathbf{x}') \right)^\nu K_\nu \left(\frac{\sqrt{2\nu}}{l} d(\mathbf{x}, \mathbf{x}') \right)$$

- l length scale; $d(\cdot, \cdot)$ Euclidean distance; $K_\nu(\cdot)$ modified Bessel function; $\Gamma(\cdot)$ Gamma function
- for $\nu = 3/2$ once differentiable, for $\nu = 5/2$ twice differentiable
- Popular choice as a kernel function when using a GP as SM



GAUSSIAN PROCESS / 3

Pros:

- Smooth, local, powerful estimator, also for small data
- GPs yield well-calibrated uncertainty estimates
- The posterior predictive distribution under a GP is normal

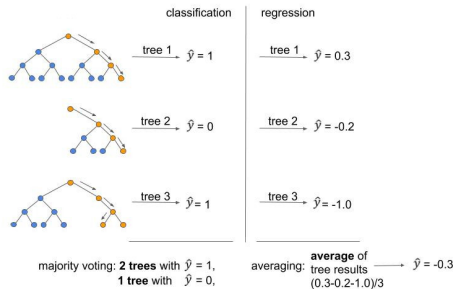
Cons:

- Vanilla GPs scale cubic in the number of data points
- Can natively only handle numeric features
Mixed inputs / dependencies require special kernels
- GPs aren't that robust; numerical problems can occur
- Can be sensitive to the choice of kernel and hyperparameters



RANDOM FOREST

- Bagging ensemble
- Fit B decision trees on bootstrap samples
- Feature subsampling

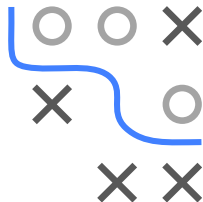


“extratrees” / random splits:

- Choose split location uniformly at random
- Results in a “smoother” mean prediction

RANDOM FOREST - MEAN AND VARIANCE

- Let $\hat{f}_b : \mathcal{S} \rightarrow \mathbb{R}$ be the mean prediction of a decision tree b (mean of all data points in the same node as observation $\mathbf{x} \in \mathcal{S}$)
- Let $\hat{s}_b^2 : \mathcal{S} \rightarrow \mathbb{R}$ be the variance prediction (variance of all data points in the same node as observation $\mathbf{x} \in \mathcal{S}$)
- Mean prediction of forest: $\hat{f} : \mathcal{S} \rightarrow \mathbb{R}, \mathbf{x} \mapsto \frac{1}{B} \sum_{b=1}^B \hat{f}_b(\mathbf{x})$
- Variance prediction of forest: $\hat{s}^2 : \mathcal{S} \rightarrow \mathbb{R},$
 $\mathbf{x} \mapsto \left(\frac{1}{B} \sum_{b=1}^B \hat{s}_b^2(\mathbf{x}) + \hat{f}_b(\mathbf{x})^2 \right) - \hat{f}(\mathbf{x})^2$
(law of total variance assuming a mixture of B models)
- Alternative variance estimator:
 - (infinitesimal) Jackknife
- Variance prediction derived from randomness of individual trees
 - Bagging / bootstrap samples
 - Features sampled at random
 - (randomized split locations in the case of “extratrees”)



RANDOM FOREST

Pros:

- Cheap(er) to train
- Scales well with the number of data points
- Scales well with the number of dimensions
- Can easily handle hierarchical mixed spaces. Either via imputation or directly respecting dependencies in the tree structure
- Robust

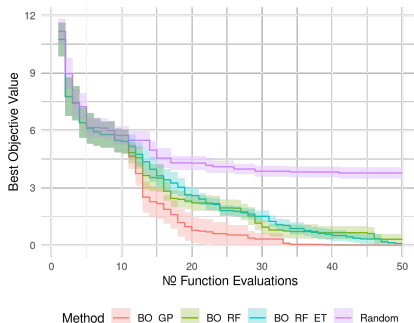
Cons:

- Suboptimal uncertainty estimates
- Not really Bayesian (no real posterior predictive distribution)
- Poor extrapolation



EXAMPLE

Minimize the 2D Ackley Function using BO_GP (GP with Matérn 3/2, EI), BO_RF (standard Random Forest, EI), BO_RF_ET (Random Forest with extratrees, EI) or a random search:



Strong BO_GP performance. BO_RF and BO_RF_ET not too bad either. BO_RF_ET maybe slightly better final performance than BO_RF.