

iML: Introduction into PDPs, SHAP and LIME

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Several groups, incl.

- ▶ Bernd Bischl, Giuseppe Casalicchio et al. at LMU (Munich)
- ▶ Marvin Wright at Univ. Bremen
- ▶ Avishek Anand at TU Delft
- ▶ Marius Lindauer at LUH (Hannover)

are jointly working on an upcoming MOOC on iML. The material is partially taken from that and should allow you to flawlessly dive deeper into it in the future.

Goals for today's lecture:

1. Global effects via **Partial Dependence Plots (PDPs)**
2. Contribution of a feature to a prediction via **SHAP**
3. Local explanation via **LIME**
4. Explaining the effects of hyperparameters (**AutoML**) via iML

Model-agnostic methods can be applied to all kinds of predictive models to explain them

Model-specific methods can only be applied to one model-class by making use of how the model is represented or constructed

~> I will focus on **model-agnostic methods** today

Model flexibility: Method can be applied to any predictive model, e.g., RFs or DNNs

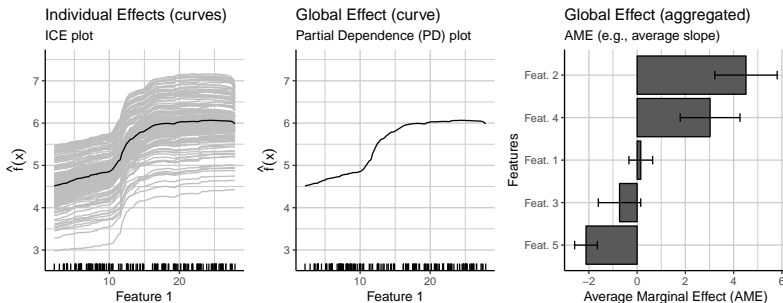
Explanation flexibility: Different explanations can be applied (based on the needs of the user)

Representation Flexibility: Different representations of features (e.g., tabular, images or text) should be applicable.

PDP: Partial Dependence Plots

Global Feature Effects visualize or quantify the (average) relationship between the features and the model predictions.

- Methods: PD Plots, ICE curves, ALE plots



Individual (curves) $\xrightarrow{\text{aggregate}}$ Global (curve) $\xrightarrow{\text{aggregate}}$ Global (number)

- ▶ each observation $x^{(i)}$ can be partitioned into $x_S^{(i)}$ and $x_C^{(i)}$
 - ▶ $x_S^{(i)}$ containing the features of interest
 - ▶ $x_C^{(i)}$ the remaining features

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ICE curves visualize how the model prediction of individual observations $x^{(i)}$ change by varying the feature values in x_S while keeping all other features in $x_C^{(i)}$ fixed:

$$\hat{f}_S^{(i)}(x_S) = \hat{f}(x_S, x_C^{(i)})$$

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In practice, x_S consists of one or two features.

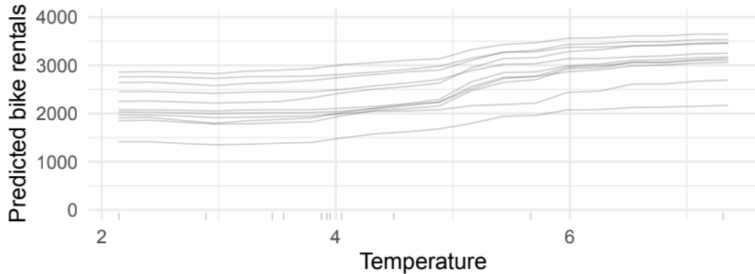
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Note: \hat{f} indicates we do this on our predictive model by simply querying it at different x_S .




- Each line displays the change in prediction for a single observation due to varying the feature temperature.

x_1	x_2	x_3
1	4	7
2	5	8
3	6	9

Sampling: Choose grid points along x_1 that will be used to intervene the data (here: all unique values 1, 2 and 3).

x_1	x_2	x_3
1	4	7
2	5	8
3	6	9




i	x_s	x_2	x_3
1	1	4	7
2	1	5	8
3	1	6	9

i	x_s	x_2	x_3
1	2	4	7
2	2	5	8
3	2	6	9

i	x_s	x_2	x_3
1	3	4	7
2	3	5	8
3	3	6	9

Intervention: Replace all observed values in x_1 for each observation with the previously sampled grid points.

x_1	x_2	x_3
1	4	7
2	5	8
3	6	9



i	x_s	x_2	x_3	\hat{f}
1	1	4	7	0.4
2	1	5	8	0.6
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i	x_s	x_2	x_3	\hat{f}
1	2	4	7	0.6
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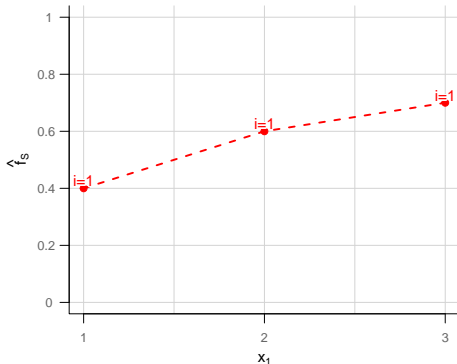
Prediction: Make predictions and plot $\hat{f}_1^{(i)}(x_1)$ vs. x_1 , where

$$\hat{f}_1^{(i)}(x_1) = \hat{f}(x_1, x_{2,3}^{(i)}).$$

i	x_1	x_2	x_3	\hat{f}
1	1	4	7	0.4
2	1	5	8	0.6
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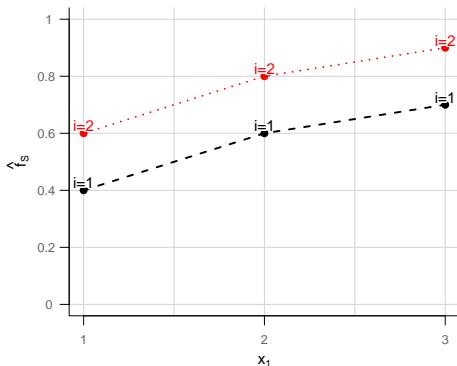


Visualization: ICE curve for observation $i = 1$ connects all predictions at the corresponding grid points associated to the i -th observation.

i	x_1	x_2	x_3	\hat{f}
1	1	4	7	0.4
2	1	5	8	0.6
3	1	6	9	0.1

i	x_1	x_2	x_3	\hat{f}
1	2	4	7	0.6
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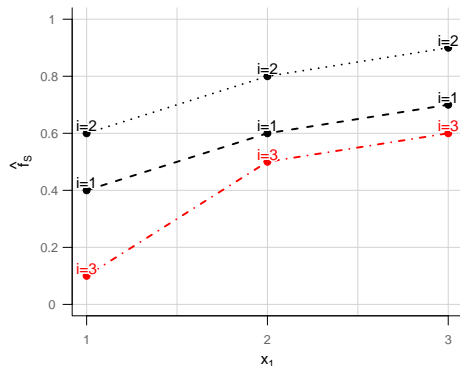


Visualization: ICE curve for observation $i = 2$ connects all predictions at the corresponding grid points associated to the i -th observation.

i	x_s	x_2	x_3	\hat{f}
1	1	4	7	0.4
2	1	5	8	0.6
3	1	6	9	0.1

i	x_s	x_2	x_3	\hat{f}
1	2	4	7	0.6
2	2	5	8	0.8
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Visualization: ICE curve for observation $i = 3$ connects all predictions at the corresponding grid points associated to the i -th observation.

The partial dependence (PD) plot is the expectation of the ICE curves w.r.t. the marginal distribution of complementary features x_C :

$$\mathbb{E}_{x_C} \left(\hat{f}(x_S, x_C) \right) = \int_{-\infty}^{\infty} \hat{f}(x_S, x_C) dP(x_C)$$

For a single x_S , it is estimated by the point-wise average of the ICE curves:

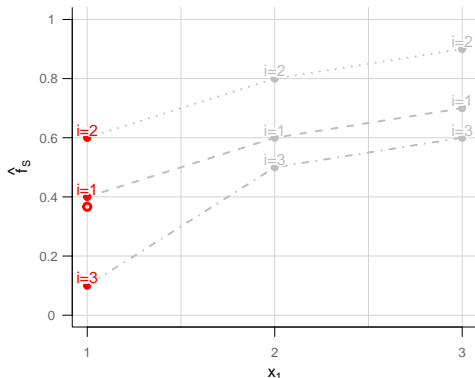
$$\text{PD}_S := \hat{f}_S(x_S) = \frac{1}{n} \sum_{i=1}^n \hat{f}(x_S, x_C^{(i)})$$

i	x_s	x_2	x_3	\hat{f}
1	1	4	7	0.4
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$\frac{1}{3} \sum_{i=1}^3 \hat{f}$
$\frac{1}{3} (0.4 + 0.6 + 0.1)$
$\frac{1}{3} (0.6 + 0.8 + 0.5)$
$\frac{1}{3} (0.7 + 0.9 + 0.6)$

i	x_s	x_2	x_3	\hat{f}
1	3	4	7	0.7
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3	3	6	9	0.6



Aggregation: Estimate partial dependence by the point-wise average of the ICE curves at

$x_s = x_1 = 1$:

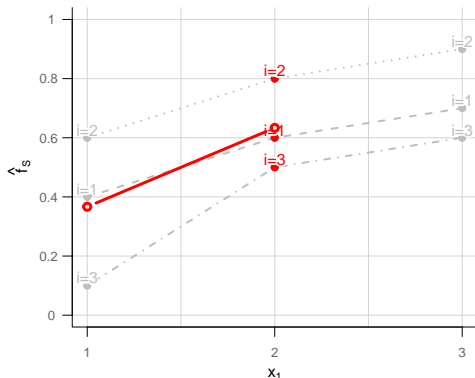
$$PD_1 = \hat{f}_1(x_1) = \frac{1}{n} \sum_{i=1}^n \hat{f}(x_1, x_{2,3}^{(i)})$$

i	x_s	x_2	x_3	\hat{f}
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Aggregation: Estimate partial dependence by the point-wise average of the ICE curves at

$x_s = x_1 = 2$:

$$PD_1 = \hat{f}_1(x_1) = \frac{1}{n} \sum_{i=1}^n \hat{f}(x_1, x_{2,3}^{(i)})$$

i	x_s	x_2	x_3	\hat{f}
1	1	4	7	0.4
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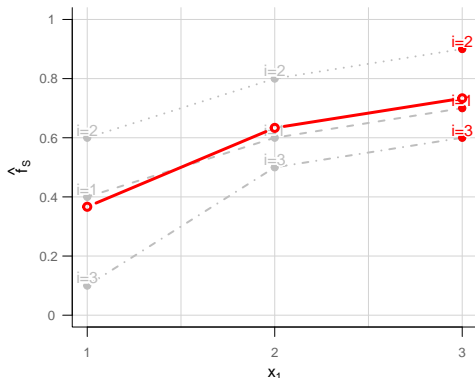
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$$PD_1 = \hat{f}_1(x_1) = \frac{1}{n} \sum_{i=1}^n \hat{f}(x_1, x_{2,3}^{(i)})$$

i	x_s	x_2	x_3	\hat{f}
1	1	4	7	0.4
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i	x_s	x_2	x_3	\hat{f}
1	2	4	7	0.6
2	2	5	8	0.8
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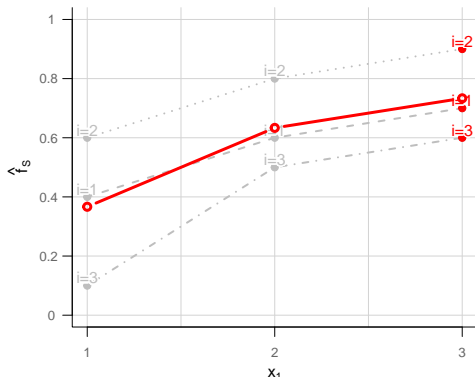
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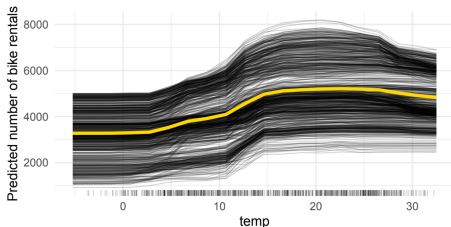
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- ▶ **ICE curve:** Visualize how the prediction of an **individual observation** changes if the feature value is changed.
⇒ ICE is a **local** interpretation method (black curves).
- ▶ **PD plot:** Visualizes the **average effect of a feature**, i.e., how the expected model prediction changes if the feature value is changed.
⇒ PD plot is a **global** interpretation method (yellow curve).

LIME: Local Interpretable Model-agnostic Explanations

Explaining the **local** behavior of a model.

- ▶ Some local methods provide insight into the driving factors for a **particular prediction**.
- ▶ Others, help to understand the model's decision making in a **local environment** of the input space.

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- ▶ Some local methods provide insight into the driving factors for a **particular prediction**.
- ▶ Others, help to understand the model's decision making in a **local environment** of the input space.
- ▶ Local Methods can address questions such as:
 - ▶ **Why** did the model decide y for input x ?
 - ▶ **How** decides the model for cases similar to x ?
 - ▶ **What** would the ML model have decided if x differed in \mathcal{X} ?
 - ▶ **Where** does the model fail?

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- ▶ In particular if algorithms make decisions in **socially/safety critical domains**, end users have justified interest in receiving explanations.
- ▶ Local Explanations can not only increase **user trust**, but also help to detect **critical local biases** in algorithmic decision making.
- ▶ European citizens have the legally binding **right to explanation** as given in the General Data Protection Regulation (GDPR; DSGVO in Germany).

Example: Husky or Wolf?

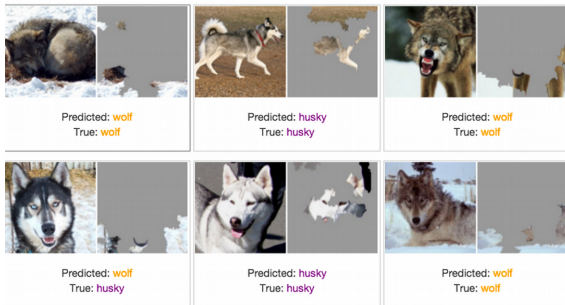
- ▶ Model to predict if an image shows a wolf or a husky
- ▶ Below the predictions on six test images
- ▶ Do you trust our predictor?



Source: [Sameer Singh. 2018]

Example: Husky or Wolf?

- ▶ We can use local explanations (in this case LIME) to highlight the parts of an image which led to the prediction.
- ▶ We can see that our predictor is actually a snow detector.



Source: [Sameer Singh. 2018]

Example: Stop or Right-of-Way?

Assume you work in a car company and are about to use an image classifier for autonomous driving. Then, you show your model the following image (an adversarial example). The classifier is 99% sure it describes a right-of-way sign.



Source: [Eykholt et. al. 2018]

Would you entrust other peoples lives into the hands of this software?

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- ▶ They should answer why a machine learning model predicted y for input x .
- ▶ Since they can be applied to any black-box model they are model-agnostic.

LIME provides a local explanation for a black-box model \hat{f} in form of a model $g \in \mathcal{G}$ with \mathcal{G} as the class of potential (interpretable) models. This model g should have two characteristics:

1. It should be **interpretable**, i.e. provide qualitative understanding between the input variables and the response that are easy to understand.
2. It should be **locally faithful**, i.e. it should behave similarly to \hat{f} in the vicinity of the instance being predicted. This characteristic is also called local fidelity.

Formally, we want to receive a model g with minimal complexity and maximal local-fidelity.

We can measure the complexity of a model g using $J(g)$.

Example: Linear model

Let $\mathcal{G} = \{g : \mathcal{X} \rightarrow \mathbb{R} \mid g(x) = s(w^\top x)\}$ be the class of linear models with $s(\cdot)$ being either the identity function for linear regression or the logistic sigmoid function for logistic regression. Then, $J(g) = \sum_{j=1}^p \mathbf{I}_{\{w_j \neq 0\}}$ could be the L_0 loss, i.e. the number of non-zero coefficients.

Example: Tree

Let $\mathcal{G} = \{g : \mathcal{X} \rightarrow \mathbb{R} \mid g(x) = \sum_{m=1}^M c_m \mathbf{I}_{\{x \in Q_m\}}\}$ be the class of trees (i.e., class of additive model over the leaf-rectangles) then $J(g)$ could measure the number of terminal/leaf nodes.

Local Model Fidelity

- ▶ A model g is locally faithful to \hat{f} w.r.t. a point x if for points $z \in \mathcal{Z} \subseteq \mathbb{R}^p$ close to x , the predictions of $g(z)$ are close to $\hat{f}(z)$.

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- ▶ In an optimization task: the closer z is to x , the closer $g(z)$ should be to $\hat{f}(z)$.
- ▶ For this definition we need two measures:
 1. A proximity measure $n(z)$ between z and x , e.g. the exponential kernel

$$n(z) = \exp(-d(x, z)^2 / \sigma^2)$$

with σ as the kernel width. d could be for example the Euclidean distance for numeric features.

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2. A distance measure or loss function $L(\hat{f}(z), g(z))$ to assess how close the predictions of $\hat{f}(z)$ and $g(z)$ are, e.g. the L2 loss/squared error

$$L(\hat{f}(z), g(z)) = (g(z) - \hat{f}(z))^2.$$

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$$L(\hat{f}(z), g(z)) = (g(z) - \hat{f}(z))^2.$$

- ▶ Given points z , we can measure local fidelity of g with respect to \hat{f} in terms of a weighted loss

$$L(\hat{f}, g, n) = \sum_{z \in \mathcal{Z}} n(z) L(\hat{f}(z), g(z)) \tag{1}$$

- ▶ Formally, an explanation produced by LIME is obtained by the following:

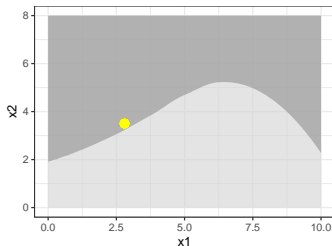
$$\arg \min_{g \in \mathcal{G}} L(\hat{f}, g, n) + J(g)$$

- ▶ In practice, LIME only optimizes $L(\hat{f}, g, n)$ (model-fidelity).
- ▶ The model complexity ($J(g)$) is determined by users beforehand by restricting the class \mathcal{G} . For example, users could only consider sparse linear models.
- ▶ Since we want a **model-agnostic** explainer, we need to optimize $L(\hat{f}, g, n)$ without making any assumptions about \hat{f} .
- ▶ Therefore, we learn g only approximately with the following algorithm.

For the algorithm, we need a pre-trained model \hat{f}, x whose prediction we want to explain and model class \mathcal{G} .

We illustrate the steps of the algorithm with a classification example:

- ▶ The light/dark background represents the prediction surface of a classifier $\hat{f} : \mathbb{R}^2 \rightarrow \{0, 1\}$.
- ▶ The yellow point displays x we are interested in.
- ▶ \mathcal{G} is restricted to the class of logistic regression models (\rightarrow classification).

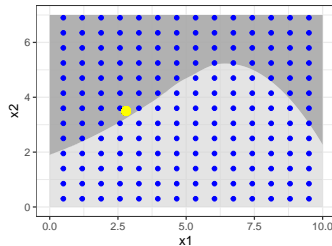
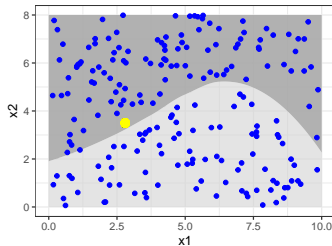


LIME Algorithm [Ribeiro et al. 2016]

1. Independently sample new points $z \in \mathcal{Z}$.
2. Retrieve predictions $\hat{f}(z)$ for obtained points z .

Strategies for sampling:

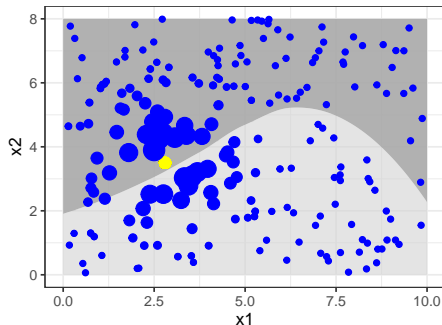
- ▶ Uniformly sample new points from the feasible feature range.
- ▶ Use the training data set with or without perturbations.
- ▶ Draw samples from the estimated univariate distribution of each feature.
- ▶ Create an equidistant grid over the supported feature range.



3. Weight $z \in \mathcal{Z}$ by their proximity $n(z)$.

In this example, we use the exponential kernel defined on the Euclidean distance d

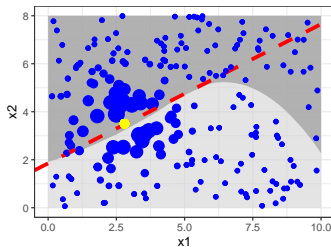
$$n(z) = \exp(-d(x, z)^2 / \sigma^2).$$



4. Train an interpretable model g on weighted data points $z \in \mathcal{Z}$. The obtained predictions $\hat{f}(z)$ is the target of this model.
5. Return the interpretable model g as the explainer.

Popular interpretable models are linear models, LASSO, classification/regression trees, decision rules. In our example, we fit a logistic regression model.

Consequently, $L(\hat{f}(z), g(z))$ is the Bernoulli loss in Eq. (1).



SHAP: Local Feature Importance via Shapley Values

- ▶ Exemplary model for predicting apartment price
- ▶ Inputs
 - ▶ Size (m²)
 - ▶ location (e.g., floor)
 - ▶ close by (e.g., train station)
 - ▶ pets allowed?
- ▶ Average apartment price is 310k

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- ▶ Average apartment price is 310k
- ▶ Query: 50m², 2nd floor, park close by, pets not allowed
- ▶ Prediction: 300k
- ~> Why?

Example (cont'd)

► Query: 50m², 2nd floor, park close by, pets not allowed

► Prediction: 300k

→ Why?

► Possible approaches: linear models or LIME

► **New question:** Under all possible subsets of features, how much would the set of features S contribute to the prediction?

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 - ▶ How much does a player contribute to the total payout (i.e., gain) under different coalitions with other players?

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- \rightsquigarrow Shapley value: Average marginal contribution of a feature value across all possible coalitions.

- ▶ For all possible subsets of features (i.e., coalition):
 1. add feature value under consideration to the coalition once and once a random value
 2. randomly change features not being in the coalition for both samples
 3. predict difference between both samples

↪ marginal contribution of feature to coalition

- ▶ Possible coalition for example if we consider **pet**:
 - ▶ \emptyset (no features)
 - ▶ size
 - ▶ location
 - ▶ close-by
 - ▶ size + location
 - ▶ size + close-by
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- ▶ Exemplary coalition: size
- ▶ Considered feature value: pets banned
- ▶ considered, randomly sampled feature vectors:
 1. size:50, pets:banned, location: 3rd, close-by:train-station
size:50, pets:allowed, location: 3rd, close-by:train-station
 2. size:50, pets:banned, location: 1st close-by:park
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 3. ...

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- ~> What would be properties of a fair distribution of the payout?

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Is there an attribution formula that adheres to all these axioms?

Shapley values solve the attribution problem and provide a unique solution given axioms of efficiency, symmetry, dummy and additivity.

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- ▶ $v(S \cup \{j\}) - v(S)$ is the marginal contribution of player j to coalition S .

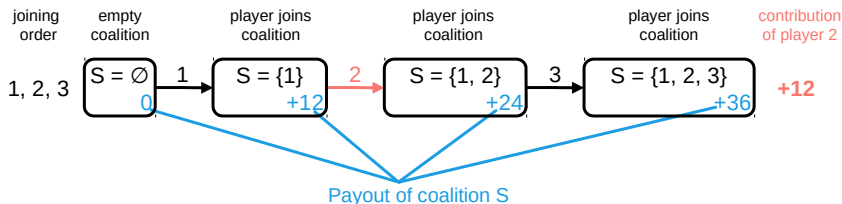
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- ▶ $v(S \cup \{j\}) - v(S)$ is the marginal contribution of player j to coalition S .
- ▶ To compute the Shapley payout for a player, we average, for all possible coalitions, how much the player would increase the value of the coalition (=marginal contribution).
- ▶ Shapley values are the *only* solution for the attribution with the specified axioms.

Shapley, Lloyd S. (August 21, 1951). "Notes on the n-Person Game – II: The Value of an n-Person Game" (PDF). Santa Monica, Calif.: RAND Corporation.

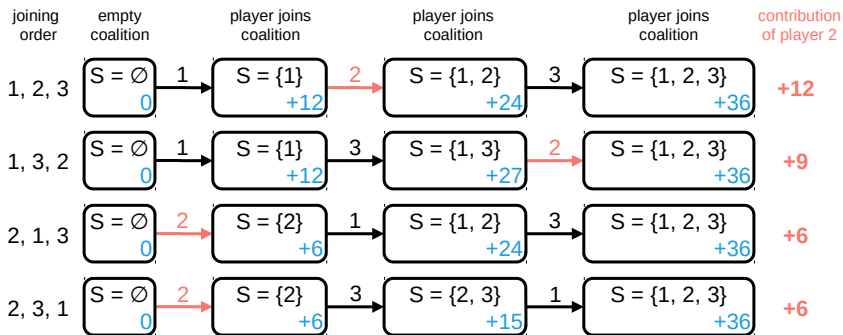
The Shapley value of a player $j = 2$ is the marginal contribution to the value function when Player 2 enters an arbitrary coalition.

Here, Player 2 enters the coalition after Player 1, resulting in a value change of $v(\{1, 2\}) - v(\{1\}) = 24 - 12 = 12$. Overall, the coalition has a value of $v(\{1, 2, 3\}) = 36$.



The Shapley value of a player $j = 2$ is the marginal contribution to the value function when Player 2 enters an arbitrary coalition.

We produce all possible orders of player coalitions and measure the value change if Player 2 enters the coalition.



- ▶ Game theory
- ▶ Economics (e.g., cost allocation) [Moulin. 1992]
- ▶ Marketing (e.g., social network analysis to discover influencers) [Naraynam et al. 2010]
- ▶ ...
- ▶ Machine learning
 - ▶ Feature selection: Attribute loss reduction to features. [Cohen et al. 2005]
 - ▶ Quantify data value: Attribute loss reduction to data points. [Ghorbani et al. 2019]
 - ▶ Algorithm Selection: Attribute loss reduction to algorithms of portfolios. [Fréchette et al. 2016]
 - ▶ Explain individual predictions \rightsquigarrow local explanation.

We can use Shapley values to explain individual predictions $\hat{f}(x^{(i)})$ of a machine learning model \hat{f} :

- ▶ Players $\hat{=}$ feature values of i-the observation $x_j^{(i)}, j \in \mathcal{P}$.
- ▶ Features cooperate to produce a prediction $\hat{f}(x_1^{(i)}, x_2^{(i)}, \dots, x_p^{(i)})$.

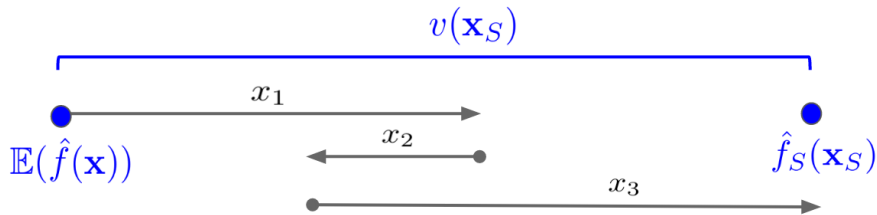
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- ▶ The value function / payout of coalition S for observation $x^{(i)}$ is

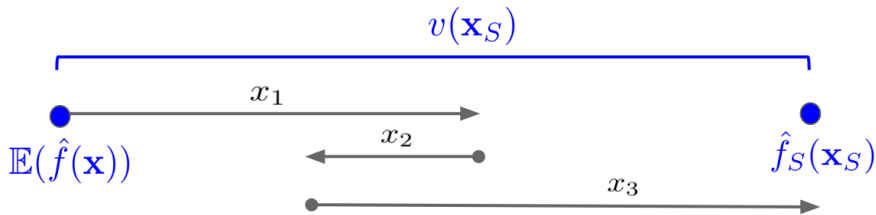
$$v(S) = \hat{f}_S(x_S^{(i)}) - \mathbb{E}[\hat{f}(x^{(i)})]$$

where $x_S^{(i)} = \{x_j^{(i)}\}_{j \in S}$ and $\hat{f}_S : \mathcal{X}_S \mapsto \mathcal{Y}$.

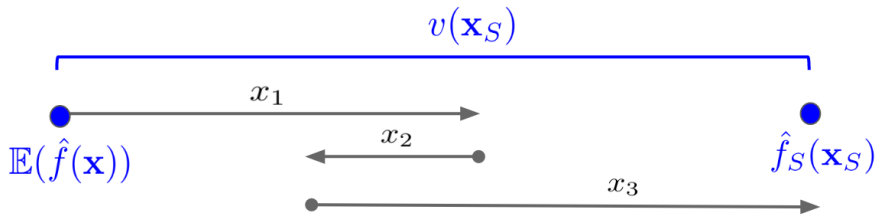
- ▶ The marginal prediction \hat{f}_S is defined as $\hat{f}_S(x_S^{(i)}) := \int_{\mathcal{X}_C} \hat{f}(x_S, X_C) dP_{X_C}$
 - ▶ Similar as in PDPs.
- ▶ Subtraction of $\mathbb{E}[\hat{f}(x^{(i)})]$ to achieve $v(\emptyset) = 0$.
- ▶ By using the marginal prediction, we have defined what it means for features to be **missing** for the prediction: We remove it by integrating over its distribution.



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- ▶ The sum of Shapley values over all features yields the difference between the average prediction of all data points (baseline) and the selected individual prediction.

Using the order definition, the Shapley value for feature j and a given data point $x^{(i)}$ can be computed as:

$$\phi_j^{(i)} = \frac{1}{p!} \sum_{S \cup \{j\}} \underbrace{\hat{f}_{S \cup \{j\}}(x_{S \cup \{j\}}) - \hat{f}_S(x_S)}_{\text{marginal contribution of feature } j}$$

- ▶ The term $\mathbb{E}[\hat{f}(x)]$ drops due to the subtraction of value functions.
- ▶ Interpretation of Shapley value $\phi_j^{(i)}$ for feature j and observation $x^{(i)}$: The feature value $x_j^{(i)}$ contributed $\phi_j^{(i)}$ towards the prediction $\hat{f}(x)$ compared to the average prediction for the dataset.

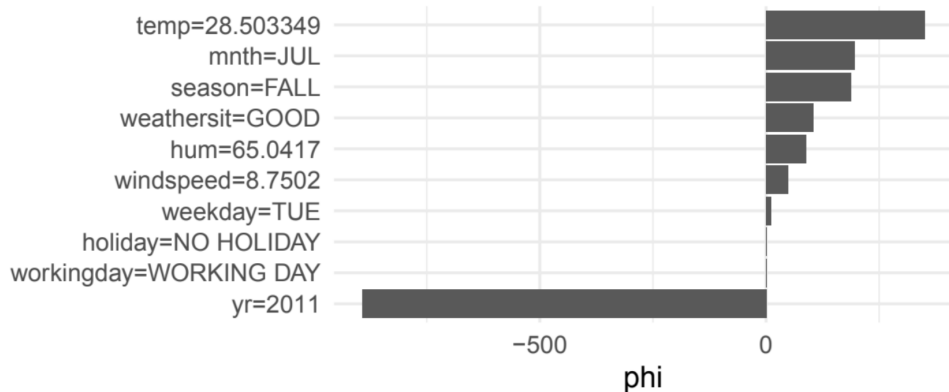
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- ▶ Note: Marginal contributions and Shapley values can be negative.

Shapley, Lloyd S. 1953. "A Value for N-Person Games."

Actual prediction: 4514.35
Average prediction: 4508.18



Explainable AutoML

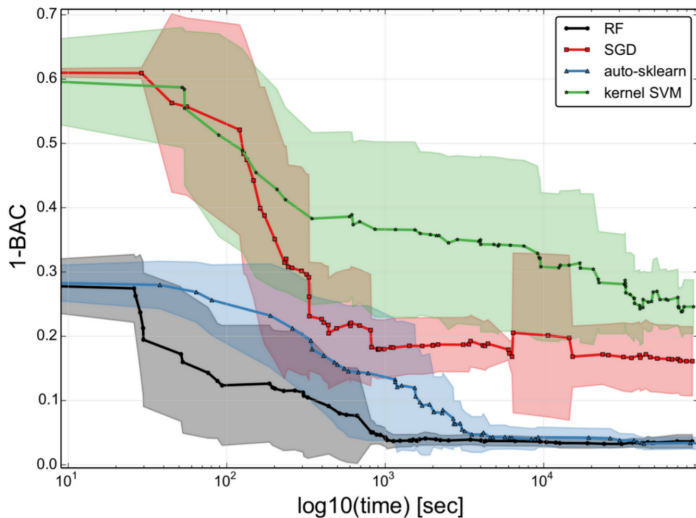
- ▶ ML algorithms have important hyperparameters
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- ↪ Can we automate this hyperparameter optimization (HPO)?

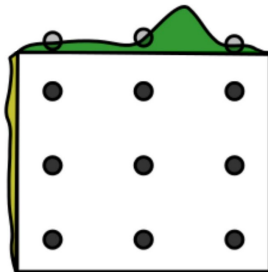
Effect of Hyperparameter Optimization



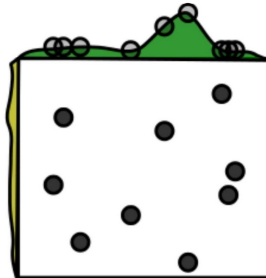
Grid Search vs. Random Search

- ▶ Let's tune 2 hyperparameters
- ▶ Plotting the samples of hyperparameter configurations for grid search and random search
- ▶ On each axis, we see the effect of each hyperparameter on the **validation loss**

Grid Layout



Random Layout



[Bergstra and Bengio 2012]

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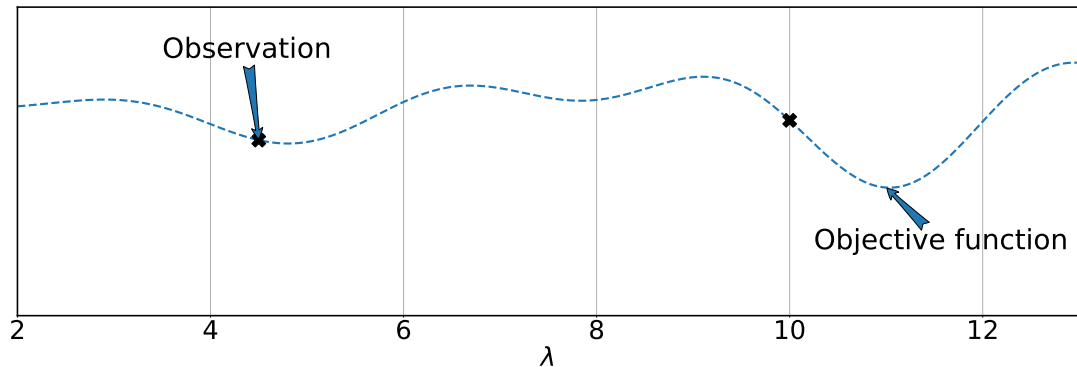
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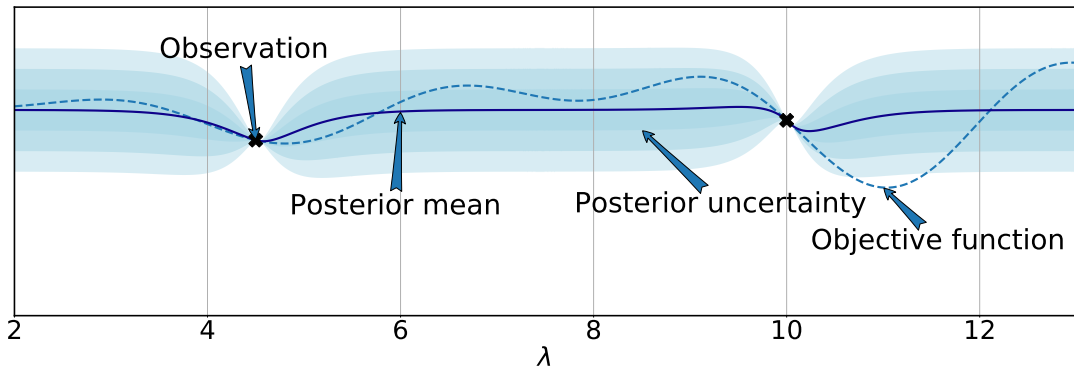
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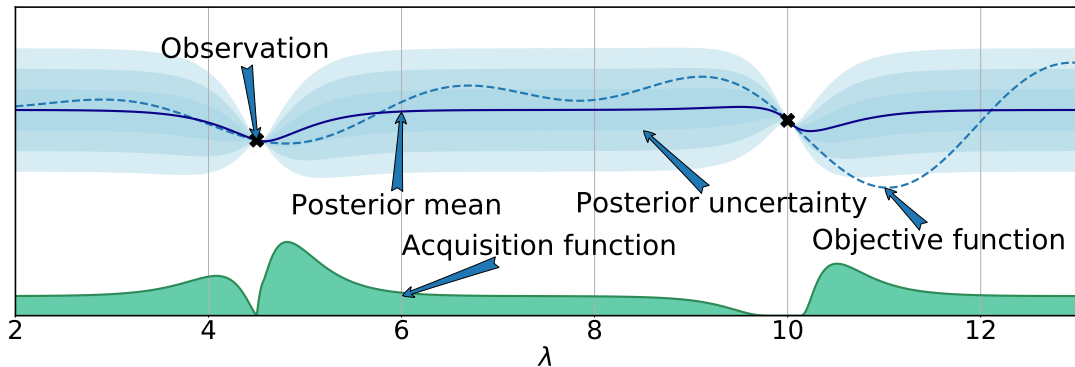
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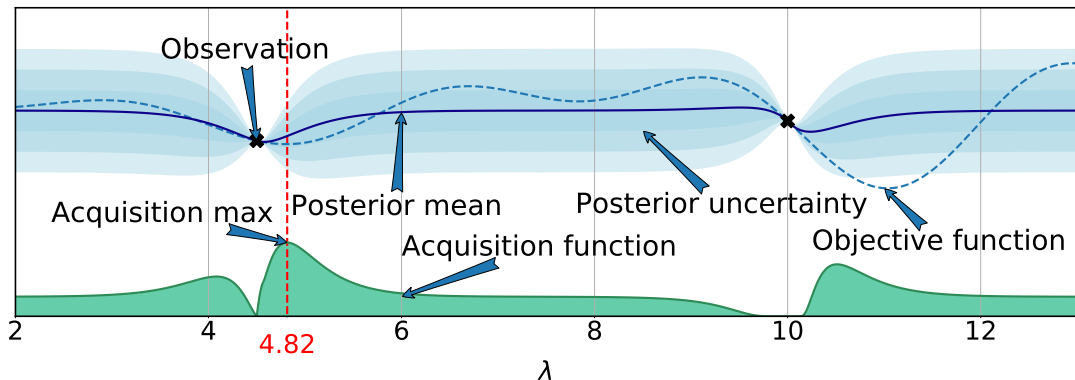
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- ▶ Blackbox optimization can be used for hyperparameter optimization (HPO)
 - ▶ Define $f(\lambda) := \mathcal{L}(\mathcal{A}_\lambda, \mathcal{D}_{train}, \mathcal{D}_{valid})$



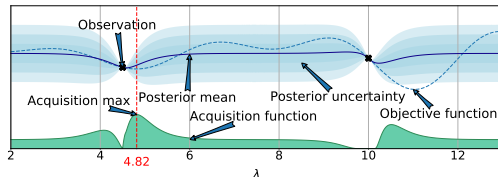






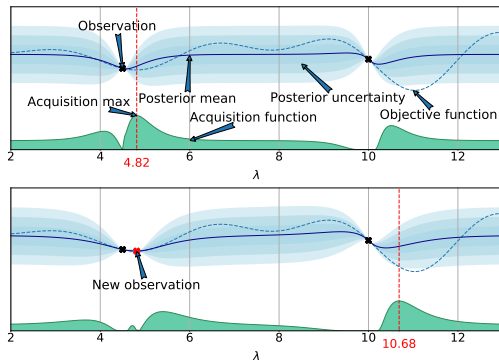
General approach

- Fit a **probabilistic model** to the collected function samples $\langle \lambda, c(\lambda) \rangle$
- Use the model to guide optimization, trading off **exploration vs exploitation**



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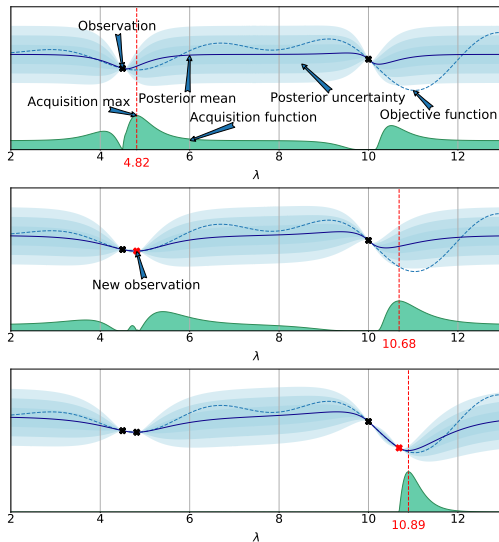
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Bayesian Optimization of a Blackbox Function in a Nutshell

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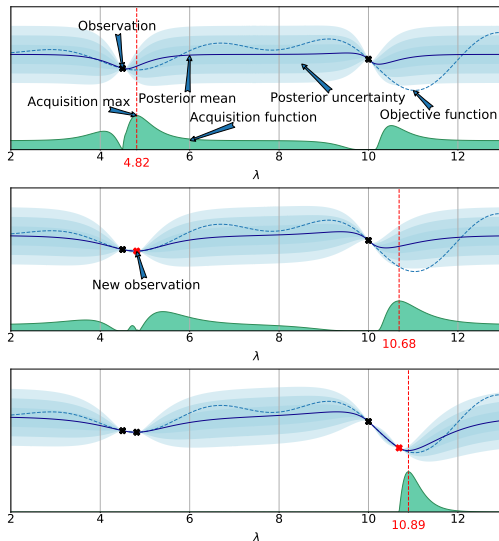


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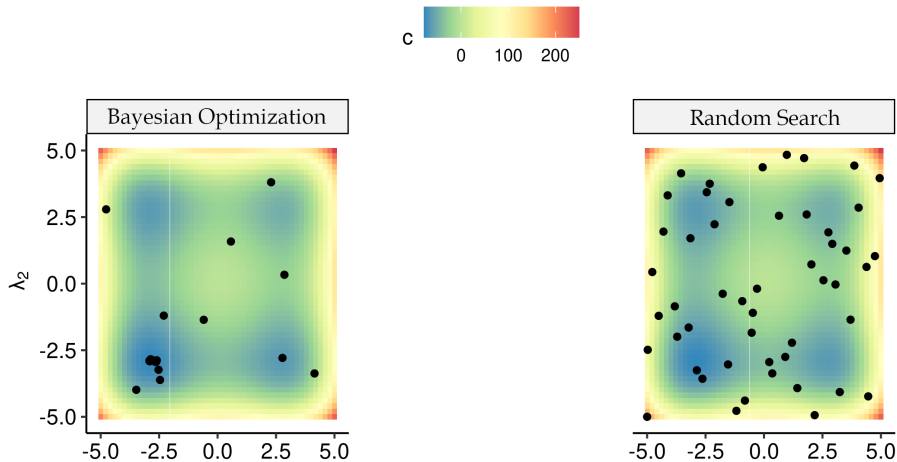
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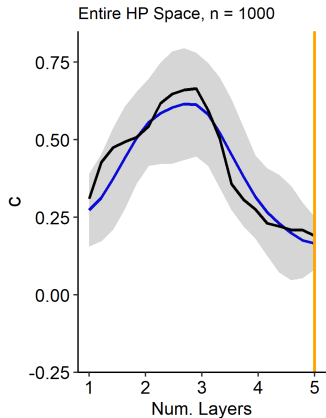
Popular approach in the statistics literature since [Mockus. 1975]

- ▶ Efficient in #function evaluations
- ▶ Works when objective is **nonconvex**, **noisy**, has **unknown derivatives**, etc.
- ▶ **Convergence** results
[Srinivas et al. 2009]; [Bull. 2011] [de Freitas et al. 2012]; [Kawaguchi et al. 2015]

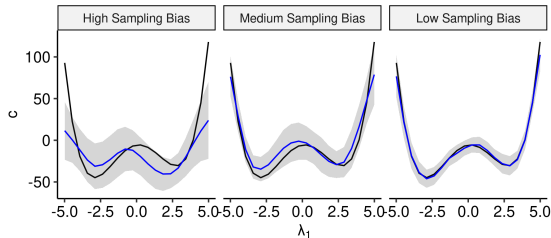
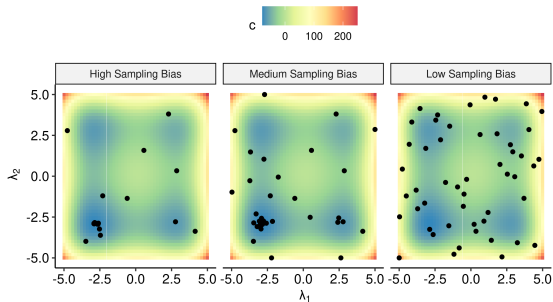


Bayesian Optimization vs Random Search





- ▶ How does changing one of the hyperparameters affect the performance (c) of the ML model?
- ← PDPs on the model of Bayesian Optimization can be used for these questions
- ▶ Can be extended to two hyperparameters and their interaction effects
- ▶ other iML techniques (such as LIME and SHAP) can also be applied
- ≈ improves understanding and trust into AutoML



- ▶ High sampling bias \rightsquigarrow Good optimization performance \rightsquigarrow Poor PDP estimates
- ▶ Low sampling bias \rightsquigarrow Good PDP estimates \rightsquigarrow Poor optimization performance

- ▶ [Moosbauer et al. 2021] identified regions with confident PDPs
- ▶ [Moosbauer et al. 2022] adapts the exploration in Bayesian Optimization to allow for globally well-estimated PDPs

Summary

1. Partial Dependence Plots (PDPs) show you the effect of hyperparameter(s)
2. LIME provide a local explanation of a single prediction
3. SHAP returns the feature importance of a prediction

1. Partial Dependence Plots (PDPs) show you the effect of hyperparameter(s)
2. LIME provide a local explanation of a single prediction
3. SHAP returns the feature importance of a prediction
4. iML can be applied to AutoML and HPO
5. But data distribution has to be taken into account