Interpretable Machine Learning

Partial Dependence Plots

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Prerequisites

Pemahaman mengenai

- Perbedaan masalah regresi & klasifikasi.
- Model *machine learning* seperti linear regression.
- Statistika $\Rightarrow$ distribusi marginal.

Github repository

The repository

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What is Interpretability?

- Interpretability is the degree to which a human can understand the cause of a decision (Miller, 2019).

- Interpretability is the degree to which a human can consistently predict the model's result (Kim et al., 2016).

The higher the interpretability of a machine learning model, the easier it is for someone to comprehend why certain decisions or predictions have been made.

- Christoph Molnar (a statistician, a machine learner)

A model is better interpretable than another model if its decisions are easier for a human to comprehend than decisions from the other model.

- Christoph Molnar

Taksonomi Teknik Interpretability[†]

- Berbagai taksonomi teknik *Interpretability* dapat dibaca di Molnar (2022).
- Kita berfokus pada taksonomi berdasarkan **model-specific** atau **model-agnostic**.

Teknik Interpretasi Model yang Spesifik (*Not Limited*)†

Algorithm	**Linear**	**Interaction**	**Task**
Linear regression	✓	✗	regr
Logistic regression	✗	✗	class
Decision trees	✗	✓	class, regr
RuleFit	✓	✓	class, regr
Naïve-Bayes	✗	✗	class
k-nearest neighbors	✗	✗	class, regr

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Metode Model-Agnostic

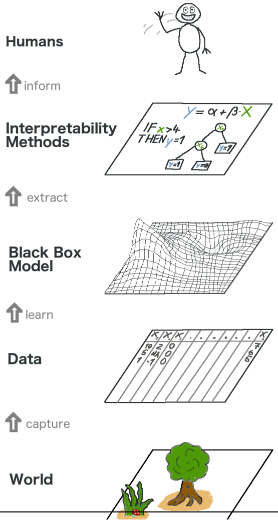
- Memisahkan penjelasan dari model machine learning mempunyai beberapa keuntungan (Ribeiro et al., 2016).
- Keuntungan terbesar metode ini adalah **fleksibilitas**nya.
- Pengembang model machine learning bebas menggunakan model machine learning apa saja.

Aspek yang Diinginkan†

Aspek yang diinginkan dari penjelasan model-agnostic (Ribeiro et al., 2016) adalah

- Model flexibility,
- Explanation flexibility, and
- Representation flexibility.

High Level Look (Molnar, 2022)†



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Global Methods

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- Contoh: $\hat{f}(x_1, x_2, x_3) =$ fungsi prediksi dengan 3 fitur.
  Untuk melihat efek x_1 pada fungsi prediksi, maka

$$\hat{g}(x_1) = \sum_{x_2} \sum_{x_3} \hat{f}(x_1, x_2, x_3).$$

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Partial Dependence Plot (PDP)†

- PDP menunjukkan **efek marginal satu atau dua fitur** pada hasil prediksi sebuah model machine learning (Friedman, 2001).
- PDP dapat menunjukkan hubungan antara target dan fitur apakah linier, monotonik atau lebih kompleks.

Definisi Fungsi Partial Dependence[†]

Bila
x_S = fitur-fitur yang akan diplot oleh fungsi partial dependence,
X_C = fitur-fitur lainnya dalam model machine learning $\hat{f}$, maka

$$\hat{f}_S(x_S) = E_{X_C}\left[\hat{f}(x_S, X_C)\right] = \int \hat{f}(x_S, X_C)\, d\mathbb{P}(X_C).$$

Estimasi Fungsi Partial Dependence[†]

Fungsi partial $\hat{f}_S$ diestimasi dengan menghitung rata-rata di *train set* (metode Monte Carlo):

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

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Asumsi: fitur di C tidak berkorelasi dengan fitur di S.

Bagaimana dengan fitur kategorikal?†

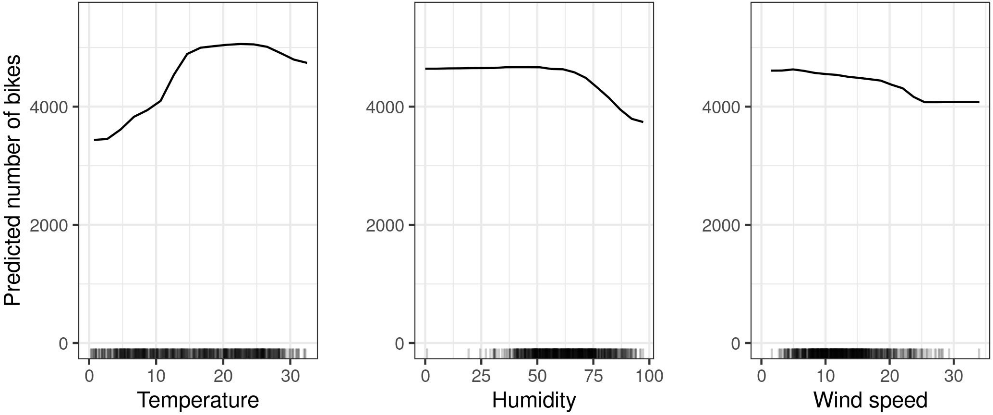
- Untuk setiap nilai kategori, kita hitung nilai PDP dengan "memaksa" semua instance data mempunyai nilai kategori yang sama.

- Hitung rata-rata dari semua nilai PDP yang sudah diperoleh.

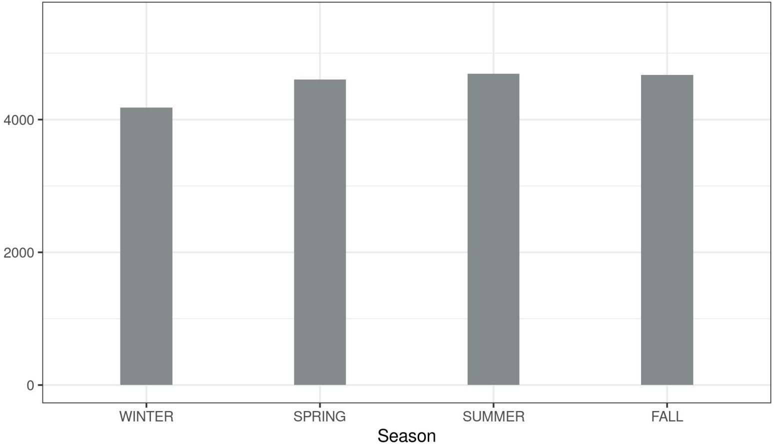
Contoh: #Sepeda yang dipinjam (1/3)

- Model machine learning, *random forest* dilatih.
- PDP plot $\Rightarrow$ visualisasi relationship yang model sudah pelajari.

Contoh: #Sepeda yang dipinjam (2/3)[†]



Contoh: #Sepeda yang dipinjam (3/3)†



Contoh: Prediksi Lead $\Rightarrow$ Customer[1]†

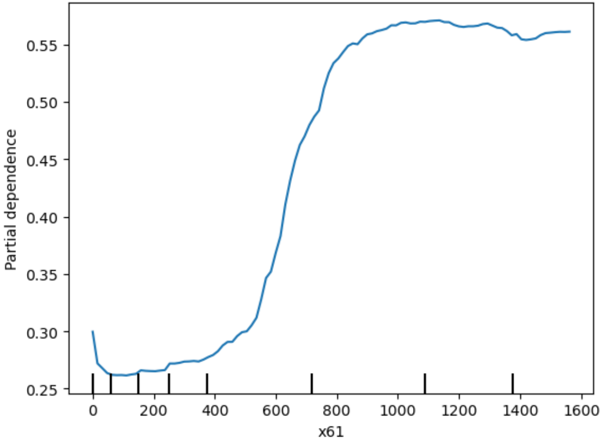
- Perusahaan edukasi (X Education) menjual online courses ke profesional industri.
- Perusahaan memasarkan course-course pada beberapa website dan search engines like Google.

[1]link dataset

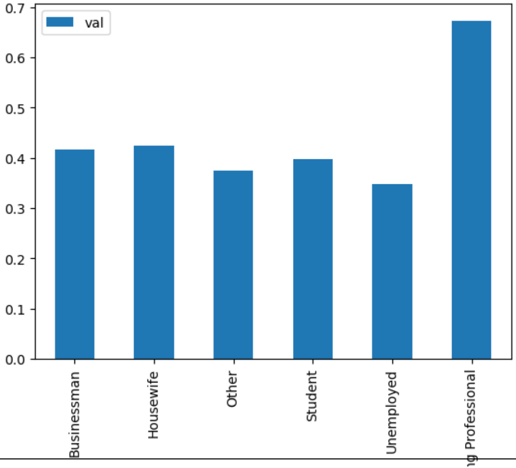
Contoh: Prediksi Lead $\Rightarrow$ Customer

- Lead origin
- Lead source
- Do Not Email
- Do Not Call
- Converted
- TotalVisits
- Total Time Spent on Website
- Page Views Per Visit
- Last activity
- Country
- Specialization
- How did you hear about X Education
- What is your current occupation
- What matters most to you in choosing this course
- Search

PDP for Model Prediksi Converted & Total Time Spent on Website



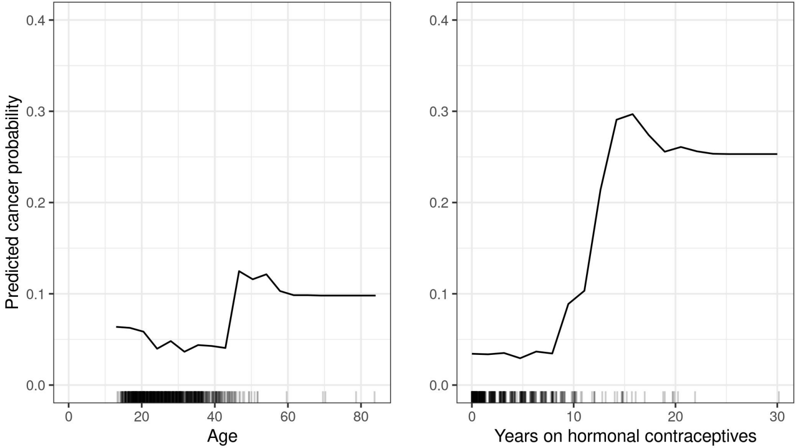
PDP for Model Prediksi Converted & What is Your Occupation



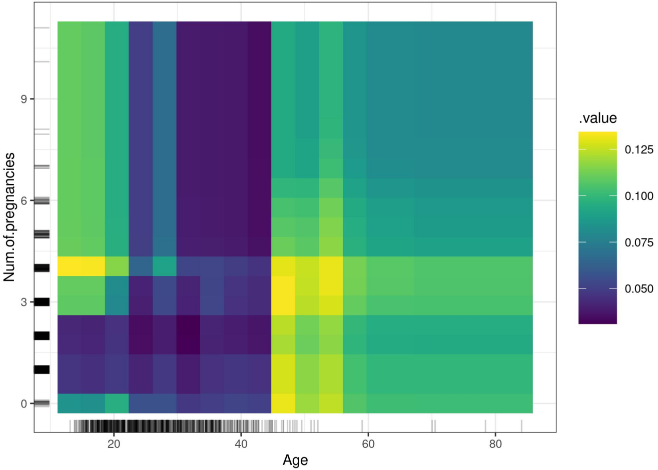
Contoh: Kanker Serviks (Fernandes and Fernandes, 2017)

- Age in years
- Number of sexual partners
- First sexual intercourse (age in years)
- Number of pregnancies
- Smoking yes or no
- Smoking (in years)
- Hormonal contraceptives yes or no
- Hormonal contraceptives (in years)
- Intrauterine device yes or no (IUD)
- Number of years with an intrauterine device (IUD)
- Has patient ever had a sexually transmitted disease (STD) yes or no
- Number of STD diagnoses
- Time since first STD diagnosis
- Time since last STD diagnosis
- The biopsy results : "Healthy" or "Cancer". Target outcome.

Contoh: Kanker Serviks[†] (1/2)



Contoh: Kanker Serviks† (2/2)



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Advantages†

- Perhitungan PDP *intuitif*.
- Dalam kasus tidak ada korelasi, interpretasi PDP jelas.
- PDP mudah untuk diimplementasi.
- Perhitungan PDPs mempunyai interpretasi *causal* (Zhao and Hastie, 2021).

Disadvantages[†]

- Jumlah maksimum fitur yang realistik dalam PDPs = 2.
- Beberapa PD plots tidak menampilkan distribusi dari fitur.
- Asumsi *independence* adalah masalah terbesar dengan PD plots $\Rightarrow$ *Accumulated Local Effect* (ALE) plots.
- Efek heterogeneous mungkin dapat tersembunyi $\Rightarrow$ kurva Individual Conditional Expectation (ICE).

Softwares

- R programming language: package `iml`, `pdp`, atau `DALEX`.
- Python programming language: `scikit-learn` atau library `PDPBox`

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