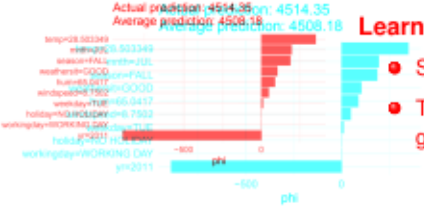
Interpretable Machine Learning

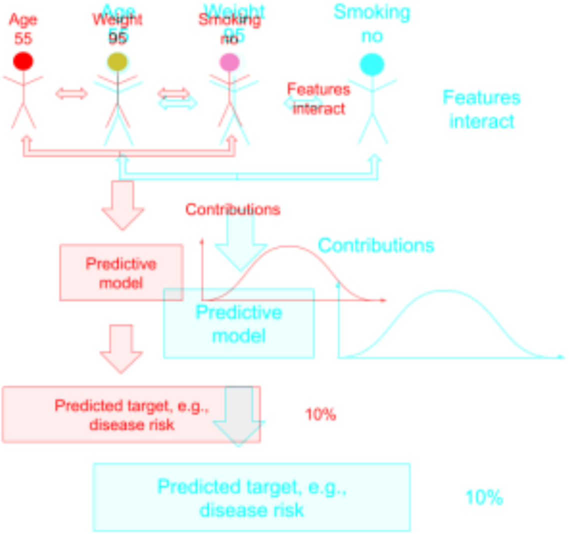
Shapley Values for Local Explanations



Learning goals

- See model predictions as a cooperative game
- Transfer the Shapley value concept from game theory to machine learning

FROM GAME THEORY TO MACHINE LEARNING



Age
55

Weight
95

Smoking
no

Features
interact

Contributions

Predictive
model

Predicted target, e.g.,
disease risk

10%

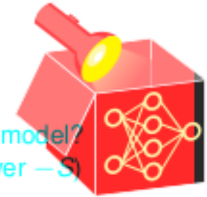
Interpretable Machine Learning – 1 / 9

FROM GAME THEORY TO MACHINE LEARNING

- Game: Make prediction $\hat{f}(x_1, x_2, \ldots, x_p)$ for a single observation $\mathbf{x}$

Interpretable Machine Learning – 2 / 9

FROM GAME THEORY TO MACHINE LEARNING



- Game: Make prediction $\hat{f}(x_1, x_2, \ldots, x_p)$ for a single observation $\mathbf{x}$
- Players: Features $x_j, j \in \{1, \ldots, p\}$ which cooperate to produce a prediction

  $\rightsquigarrow$ How can we make a prediction with a subset of features without changing the model?

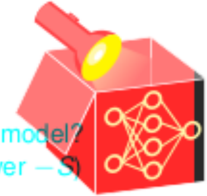
  $\rightsquigarrow$ PD function: $\hat{f}_S(\mathbf{x}_S) := \int_{X_{-S}} \hat{f}(\mathbf{x}_S, X_{-S}) d\mathbb{P}_{X_{-S}}$ ("removing" by marginalizing over $-S$)

- Game: Make prediction $\hat{f}(x_1, x_2, \ldots, x_p)$ for a single observation $\mathbf{x}$
- Players: Features $x_j, j \in \{1, \ldots, p\}$ which cooperate to produce a prediction

  $\rightsquigarrow$ How can we make a prediction with a subset of features without changing the model?

  $\rightsquigarrow$ PD function: $\hat{f}_S(\mathbf{x}_S) := \int_{X_{-S}} \hat{f}(\mathbf{x}_S, X_{-S}) d\mathbb{P}_{X_{-S}}$ ("removing" by marginalizing over $-S$)

FROM GAME THEORY TO MACHINE LEARNING



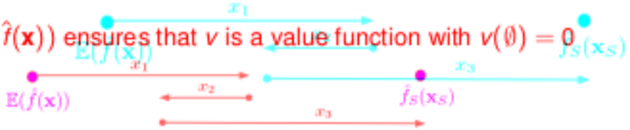
- Game: Make prediction $\hat{f}(x_1, x_2, \ldots, x_p)$ for a single observation $\mathbf{x}$
- Players: Features $x_j, j \in \{1, \ldots, p\}$, which cooperate to produce a prediction

  ⇝ How can we make a prediction with a subset of features without changing the model?

  ⇝ PD function: $\hat{f}_S(\mathbf{x}_S) := \int_{X_{-S}} \hat{f}(\mathbf{x}_S, X_{-S}) d\mathbb{P}_{X_{-S}}$ ("removing" by marginalizing over $-S$)
- Value function / payout of coalition $S \subseteq P$ for observation $\mathbf{x}$:

$$v(S) = \hat{f}_S(\mathbf{x}_S) - \mathbb{E}_{\mathbf{x}}(\hat{f}(\mathbf{x})), \text{ where } \hat{f}_S : \mathcal{X}_S \mapsto \mathcal{Y}$$

⇝ subtraction of $\mathbb{E}_{\mathbf{x}}(\hat{f}(\mathbf{x}))$ ensures that v is a value function with $v(\emptyset) = 0$



- Game: Make prediction $\hat{f}(x_1, x_2, \ldots, x_p)$ for a single observation $\mathbf{x}$
- Players: Features $x_j, j \in \{1, \ldots, p\}$, which cooperate to produce a prediction

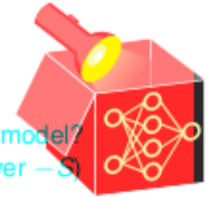
  ⇝ How can we make a prediction with a subset of features without changing the model?

  ⇝ PD function: $\hat{f}_S(\mathbf{x}_S) := \int_{X_{-S}} \hat{f}(\mathbf{x}_S, X_{-S}) d\mathbb{P}_{X_{-S}}$ ("removing" by marginalizing over $-S$)
- Value function / payout of coalition $S \subseteq P$ for observation $\mathbf{x}$:

$$v(S) = \hat{f}_S(\mathbf{x}_S) - \mathbb{E}_{\mathbf{x}}(\hat{f}(\mathbf{x})), \text{ where } \hat{f}_S : \mathcal{X}_S \mapsto \mathcal{Y}$$

⇝ subtraction of $\mathbb{E}_{\mathbf{x}}(\hat{f}(\mathbf{x}))$ ensures that v is a value function with $v(\emptyset) = 0$

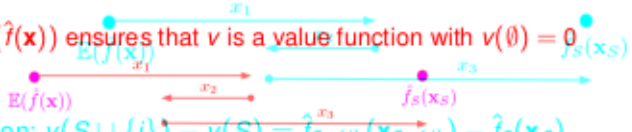
FROM GAME THEORY TO MACHINE LEARNING



- Game: Make prediction $\hat{f}(x_1, x_2, \ldots, x_p)$ for a single observation $\mathbf{x}$
- Players: Features $x_j, j \in \{1, \ldots, p\}$, which cooperate to produce a prediction
  ⇝ How can we make a prediction with a subset of features without changing the model?
  ⇝ PD function: $\hat{f}_S(\mathbf{x}_S) := \int_{X_{-S}} \hat{f}(\mathbf{x}_S, X_{-S}) d\mathbb{P}_{X_{-S}}$ ("removing" by marginalizing over $-S$)
- Value function / payout of coalition $S \subseteq P$ for observation $\mathbf{x}$:

$$v(S) = \hat{f}_S(\mathbf{x}_S) - \mathbb{E}_{\mathbf{x}}(\hat{f}(\mathbf{x})), \text{ where } \hat{f}_S : \mathcal{X}_S \mapsto \mathcal{Y}$$

  ⇝ subtraction of $\mathbb{E}_{\mathbf{x}}(\hat{f}(\mathbf{x}))$ ensures that v is a value function with $v(\emptyset) = 0$



- Marginal contribution: $v(S \cup \{j\}) - v(S) = \hat{f}_{S \cup \{j\}}(\mathbf{x}_{S \cup \{j\}}) - \hat{f}_S(\mathbf{x}_S)$
  ⇝ $\mathbb{E}_{\mathbf{x}}(\hat{f}(\mathbf{x}))$ cancels out due to the subtraction of value functions

- Game: Make prediction $\hat{f}(x_1, x_2, \ldots, x_p)$ for a single observation $\mathbf{x}$
- Players: Features $x_j, j \in \{1, \ldots, p\}$, which cooperate to produce a prediction
  ⇝ How can we make a prediction with a subset of features without changing the model?
  ⇝ PD function: $\hat{f}_S(\mathbf{x}_S) := \int_{X_{-S}} \hat{f}(\mathbf{x}_S, X_{-S}) d\mathbb{P}_{X_{-S}}$ ("removing" by marginalizing over $-S$)
- Value function / payout of coalition $S \subseteq P$ for observation $\mathbf{x}$:
  $v(S) = \hat{f}_S(\mathbf{x}_S) - \mathbb{E}_{\mathbf{x}}(\hat{f}(\mathbf{x}))$, where $\hat{f}_S : \mathcal{X}_S \mapsto \mathcal{Y}$
  ⇝ subtraction of $\mathbb{E}_{\mathbf{x}}(\hat{f}(\mathbf{x}))$ ensures that v is a value function with $v(\emptyset) = 0$
- Marginal contribution: $v(S \cup \{j\}) - v(S) = \hat{f}_{S \cup \{j\}}(\mathbf{x}_{S \cup \{j\}}) - \hat{f}_S(\mathbf{x}_S)$
  ⇝ $\mathbb{E}_{\mathbf{x}}(\hat{f}(\mathbf{x}))$ cancels out due to the subtraction of value functions

SHAPLEY VALUE - DEFINITION

▸ Shapley (1953) ▸ Strumbelj et al. (2014)

Shapley value ϕ_j of feature j for observation $\mathbf{x}$ via **order definition**:

$$\phi_j(\mathbf{x}) = \frac{1}{|P|!}\sum_{\tau\in\Pi}\underbrace{\hat f_{S_j^\tau\cup\{j\}}(\mathbf{x}_{S_j^\tau\cup\{j\}}) - \hat f_{S_j^\tau}(\mathbf{x}_{S_j^\tau})}_{\text{marginal contribution of feature } j}$$

- Interpretation: Feature x_j contributed ϕ_j to difference between $\hat f(\mathbf{x})$ and average prediction
  ⇝ Note: Marginal contributions and Shapley values can be negative
- For exact computation of $\phi_j(\mathbf{x})$, the PD function $\hat f_S(\mathbf{x}_S) = \frac{1}{n}\sum_{i=1}^n \hat f(\mathbf{x}_S, \mathbf{x}_{-S}^{(i)})$ for any set of features S can be used which yields

$$\phi_j(\mathbf{x}) = \frac{1}{|P|!\cdot n}\sum_{\tau\in\Pi}\sum_{i=1}^{n}\hat f(\mathbf{x}_{S_j^\tau\cup\{j\}}, \mathbf{x}^{(i)}_{-\{S_j^\tau\cup\{j\}\}}) - \hat f(\mathbf{x}_{S_j^\tau}, \mathbf{x}^{(i)}_{-S_j^\tau})$$

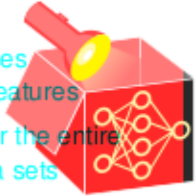
⇝ Note: $\hat f_S$ marginalizes over all other features $-S$ using all observations $i = 1, \dots, n$

ESTIMATION: A PRACTICAL PROBLEM

- Exact Shapley value computation is problematic for high-dimensional feature spaces
  $\leadsto$ For 10 features, there are already $|P|! = 10! \approx 3.6$ million possible orders of features

- Exact Shapley value computation is problematic for high-dimensional feature spaces
  $\leadsto$ For 10 features, there are already $|P|! = 10! \approx 3.6$ million possible orders of features

ESTIMATION: A PRACTICAL PROBLEM



- Exact Shapley value computation is problematic for high-dimensional feature spaces
  $\leadsto$ For 10 features, there are already $|P|! = 10! \approx 3.6$ million possible orders of features
- Additional problem due to estimation of the marginal prediction $\hat{f}_{S_j^\tau}$: Averaging over the entire data set for each coalition S_j^τ introduced by τ can be very expensive for large data sets

ESTIMATION: A PRACTICAL PROBLEM

- Exact Shapley value computation is problematic for high-dimensional feature spaces
  $\leadsto$ For 10 features, there are already $|P|! = 10! \approx 3.6$ million possible orders of features
- Additional problem due to estimation of the marginal prediction $\hat{f}_{S_j^\tau}$: Averaging over the entire data set for each coalition S_j^τ introduced by τ can be very expensive for large data sets

ESTIMATION: A PRACTICAL PROBLEM

- Exact Shapley value computation is problematic for high-dimensional feature spaces
  $\rightsquigarrow$ For 10 features, there are already $|P|! = 10! \approx 3.6$ million possible orders of features
- Additional problem due to estimation of the marginal prediction $\hat{f}_{S_j^\tau}$: Averaging over the entire data set for each coalition S_j^τ introduced by τ can be very expensive for large data sets
- Solution to both problems is sampling: Instead of averaging over $|P|! \cdot n$ terms, we approximate it using a limited amount of M random samples of τ to build coalitions S_j^τ

ESTIMATION: A PRACTICAL PROBLEM

- Exact Shapley value computation is problematic for high-dimensional feature spaces
  $\rightsquigarrow$ For 10 features, there are already $|P|! = 10! \approx 3.6$ million possible orders of features
- Additional problem due to estimation of the marginal prediction $\hat{f}_{S_j^\tau}$: Averaging over the entire data set for each coalition S_j^τ introduced by τ can be very expensive for large data sets
- Solution to both problems is sampling: Instead of averaging over $|P|! \cdot n$ terms, we approximate it using a limited amount of M random samples of τ to build coalitions S_j^τ

ESTIMATION: A PRACTICAL PROBLEM

- Exact Shapley value computation is problematic for high-dimensional feature spaces
  ⇝ For 10 features, there are already $|P|! = 10! \approx 3.6$ million possible orders of features
- Additional problem due to estimation of the marginal prediction $\hat{f}_{S_j^\tau}$: Averaging over the entire data set for each coalition S_j^τ introduced by τ can be very expensive for large data sets
- Solution to both problems is sampling: Instead of averaging over $|P|! \cdot n$ terms, we approximate it using a limited amount of M random samples of τ to build coalitions S_j^τ
- M is a tradeoff between accuracy of the Shapley value and computational costs
  ⇝ The higher M, the closer to the exact Shapley values, but the more costly the computation

ESTIMATION: A PRACTICAL PROBLEM

- Exact Shapley value computation is problematic for high-dimensional feature spaces
  ⇝ For 10 features, there are already $|P|! = 10! \approx 3.6$ million possible orders of features
- Additional problem due to estimation of the marginal prediction $\hat{f}_{S_j^\tau}$: Averaging over the entire data set for each coalition S_j^τ introduced by τ can be very expensive for large data sets
- Solution to both problems is sampling: Instead of averaging over $|P|! \cdot n$ terms, we approximate it using a limited amount of M random samples of τ to build coalitions S_j^τ
- M is a tradeoff between accuracy of the Shapley value and computational costs
  ⇝ The higher M, the closer to the exact Shapley values, but the more costly the computation

APPROXIMATION ALGORITHM

▸ Strumbelj et al. (2014)

Estimation of ϕ_j for observation $\mathbf{x}$ of model $\hat{f}$ fitted on data $\mathcal{D}$ using sample size M:

1. For $m = 1, \ldots, M$ do:

APPROXIMATION ALGORITHM

Štrumbelj et al. (2014)

Estimation of ϕ_j for observation $\mathbf{x}$ of model $\hat{f}$ fitted on data $\mathcal{D}$ using sample size M:

```
1. For $m = 1, \ldots, M$ do:
    1. Select random order / perm. of feature indices $\tau = (\tau^{(1)}, \ldots, \tau^{(p)}) \in \Pi$
```

APPROXIMATION ALGORITHM

Strumbelj et al. (2014)

Estimation of ϕ_j for observation $\mathbf{x}$ of model $\hat{f}$ fitted on data $\mathcal{D}$ using sample size M:

1. For $m = 1, \dots, M$ **do**:
    1. Select random order / perm. of feature indices $\tau = (\tau^{(1)}, \dots, \tau^{(p)}) \in \Pi$
    2. Determine coalition $S_m = S_j^\tau$, i.e., the set of feat. before feat. j in order τ

Estimation of ϕ_j for observation $\mathbf{x}$ of model $\hat{f}$ fitted on data $\mathcal{D}$ using sample size M:

1. For $m = 1, \dots, M$ **do**:
    1. Select random order / permutation of feature indices $\tau = (\tau^{(1)}, \dots, \tau^{(p)}) \in \Pi$
    2. Determine coalition $S_m := S_j^\tau$, i.e., the set of features before feature j in order τ

APPROXIMATION ALGORITHM

Strumbelj et al. (2014)

Estimation of ϕ_j for observation $\mathbf{x}$ of model $\hat{f}$ fitted on data $\mathcal{D}$ using sample size M:

1. For $m = 1, \ldots, M$ do:
   1. Select random order / perm. of feature indices $\tau = (\tau^{(1)}, \ldots, \tau^{(p)}) \in \Pi$
   2. Determine coalition $S_m = S_j^\tau$, i.e., the set of feat. before feat. j in order τ
   3. Select random data point $\mathbf{z}^{(m)} \in \mathcal{D}$

Interpretable Machine Learning – 5 / 9

APPROXIMATION ALGORITHM

Štrumbelj et al. (2014)

Estimation of ϕ_j for observation $\mathbf{x}$ of model $\hat{f}$ fitted on data $\mathcal{D}$ using sample size M:

1. For $m = 1, \dots, M$ **do**:
   1. Select random order / perm. of feature indices $\tau = (\tau^{(1)}, \dots, \tau^{(p)}) \in \Pi$
   2. Determine coalition $S_m = S_j^\tau$, i.e., the set of feat. before feat. j in order τ
   3. Select random data point $\mathbf{z}^{(m)} \in \mathcal{D}$
   4. Construct two artificial obs. by replacing feature values from $\mathbf{x}$ with $\mathbf{z}^{(m)}$:

APPROXIMATION ALGORITHM

Štrumbelj et al. (2014)

Estimation of ϕ_j for observation $\mathbf{x}$ of model $\hat{f}$ fitted on data $\mathcal{D}$ using sample size M:

1. For $m = 1, \dots, M$ **do**:
   1. Select random order / permutation of feature indices $\tau = (\tau^{(1)}, \dots, \tau^{(p)}) \in \Pi$
   2. Determine coalition $S_m := S_j^\tau$, i.e., the set of features before feature j in order τ
   3. Select random data point $\mathbf{z}^{(m)} \in \mathcal{D}$
   4. Construct two artificial observations by replacing feature values from $\mathbf{x}$ with $\mathbf{z}^{(m)}$:

APPROXIMATION ALGORITHM

▸ Strumbelj et al. (2014)

Estimation of ϕ_j for observation $\mathbf{x}$ of model $\hat{f}$ fitted on data $\mathcal{D}$ using sample size M:

```
1. For $m = 1, \ldots, M$ do:
    1. Select random order / perm. of feature indices $\tau = (\tau^{(1)}, \ldots, \tau^{(p)}) \in \Pi$
    2. Determine coalition $S_m := S_j^{\tau}$, i.e., the set of feat. before feat. $j$ in order $\tau$
    3. Select random data point $\mathbf{z}^{(m)} \in \mathcal{D}$
    4. Construct two artificial obs. by replacing feature values from $\mathbf{x}$ with $\mathbf{z}^{(m)}$:
        - $\mathbf{x}_{+j}^{(m)} = (\underbrace{x_{\tau^{(1)}}, \ldots, x_{\tau^{(|S_m|-1)}}, x_j}_{\mathbf{x}_{S_m \cup \{j\}}}, \underbrace{z^{(m)}_{\tau^{(|S_m|+1)}}, \ldots, z^{(m)}_{\tau^{(p)}}}_{\mathbf{z}^{(m)}_{-\{S_m \cup \{j\}\}}})$ takes features $S_m \cup \{j\}$ from $\mathbf{x}$
```

APPROXIMATION ALGORITHM

▸ Strumbelj et al. (2014)

Estimation of ϕ_j for observation **x** of model $\hat{f}$ fitted on data $\mathcal{D}$ using sample size M:

1. For $m = 1, \dots, M$ **do**:
   1. Select random order / perm. of feature indices $\tau = (\tau^{(1)}, \dots, \tau^{(p)}) \in \Pi$
   2. Determine coalition $S_m := S_j^\tau$, i.e., the set of feat. before feat. j in order τ
   3. Select random data point $\mathbf{z}^{(m)} \in \mathcal{D}$
   4. Construct two artificial obs. by replacing feature values from **x** with $\mathbf{z}^{(m)}$:
      - $\mathbf{x}_{+j}^{(m)} = (\underbrace{x_{\tau^{(1)}}, \dots, x_{\tau^{(|S_m|-1)}}, x_j}_{\mathbf{x}_{S_m \cup \{j\}}}, \underbrace{z^{(m)}_{\tau^{(|S_m|+1)}}, \dots, z^{(m)}_{\tau^{(p)}}}_{\mathbf{z}^{(m)}_{-\{S_m \cup \{j\}\}}})$ takes features $S_m \cup \{j\}$ from **x**
      - $\mathbf{x}_{-j}^{(m)} = (\underbrace{x_{\tau^{(1)}}, \dots, x_{\tau^{(|S_m|-1)}}}_{\mathbf{x}_{S_m}}, \underbrace{z_j^{(m)}, z^{(m)}_{\tau^{(|S_m|+1)}}, \dots, z^{(m)}_{\tau^{(p)}}}_{\mathbf{z}^{(m)}_{-S_m}})$ takes features S_m from **x**

Estimation of ϕ_j for observation **x** of model $\hat{f}$ fitted on data $\mathcal{D}$ using sample size M:

1. For $m = 1, \dots, M$ **do**:
   1. Select random order / permutation of feature indices $\tau = (\tau^{(1)}, \dots, \tau^{(p)}) \in \Pi$
   2. Determine coalition $S_m := S_j^\tau$, i.e., the set of features before feature j in order τ
   3. Select random data point $\mathbf{z}^{(m)} \in \mathcal{D}$
   4. Construct two artificial observations by replacing feature values from **x** with $\mathbf{z}^{(m)}$:
      - $\mathbf{x}_{+j}^{(m)} = (\underbrace{x_{\tau^{(1)}}, \dots, x_{\tau^{(|S_m|-1)}}, x_j}_{\mathbf{x}_{S_m \cup \{j\}}}, \underbrace{z^{(m)}_{\tau^{(|S_m|+1)}}, \dots, z^{(m)}_{\tau^{(p)}}}_{\mathbf{z}^{(m)}_{-\{S_m \cup \{j\}\}}})$ takes features $S_m \cup \{j\}$ from **x**
      - $\mathbf{x}_{-j}^{(m)} = (\underbrace{x_{\tau^{(1)}}, \dots, x_{\tau^{(|S_m|-1)}}}_{\mathbf{x}_{S_m}}, \underbrace{z_j^{(m)}, z^{(m)}_{\tau^{(|S_m|+1)}}, \dots, z^{(m)}_{\tau^{(p)}}}_{\mathbf{z}^{(m)}_{-S_m}})$ takes features S_m from **x**

APPROXIMATION ALGORITHM

▸ Štrumbelj et al. (2014)

Estimation of ϕ_j for observation $\mathbf{x}$ of model $\hat{f}$ fitted on data $\mathcal{D}$ using sample size M:

1. For $m = 1, \ldots, M$ **do**:
   1. Select random order / perm. of feature indices $\tau = (\tau^{(1)}, \ldots, \tau^{(p)}) \in \Pi$
   2. Determine coalition $S_m := S_j^\tau$, i.e., the set of feat. before feat. j in order τ
   3. Select random data point $\mathbf{z}^{(m)} \in \mathcal{D}$
   4. Construct two artificial obs. by replacing feature values from $\mathbf{x}$ with $\mathbf{z}^{(m)}$:
      - $\mathbf{x}_{+j}^{(m)} = (\underbrace{x_{\tau^{(1)}}, \ldots, x_{\tau^{(|S_m|-1)}}, x_j}_{\mathbf{x}_{S_m \cup \{j\}}}, \underbrace{z^{(m)}_{\tau^{(|S_m|+1)}}, \ldots, z^{(m)}_{\tau^{(p)}}}_{\mathbf{z}^{(m)}_{-\{S_m \cup \{j\}\}}})$ takes features $S_m \cup \{j\}$ from $\mathbf{x}$
      - $\mathbf{x}_{-j}^{(m)} = (\underbrace{x_{\tau^{(1)}}, \ldots, x_{\tau^{(|S_m|-1)}}}_{\mathbf{x}_{S_m}}, \underbrace{z_j^{(m)}, z^{(m)}_{\tau^{(|S_m|+1)}}, \ldots, z^{(m)}_{\tau^{(p)}}}_{\mathbf{z}^{(m)}_{-S_m}})$ takes features S_m from $\mathbf{x}$
   5. Compute difference $\phi_j^m = \hat{f}(\mathbf{x}_{+j}^{(m)}) - \hat{f}(\mathbf{x}_{-j}^{(m)})$

$\rightsquigarrow$ $\hat{f}_{S_m}(\mathbf{x}_{S_m})$ is approximated by $\hat{f}(\mathbf{x}_{-j}^{(m)})$ and $\hat{f}_{S_m \cup \{j\}}(\mathbf{x}_{S_m \cup \{j\}})$ by $\hat{f}(\mathbf{x}_{+j}^{(m)})$ over M iters.

APPROXIMATION ALGORITHM ▸ Štrumbelj et al. (2014)

Estimation of ϕ_j for observation $\mathbf{x}$ of model $\hat{f}$ fitted on data $\mathcal{D}$ using sample size M:

1. For $m = 1, \ldots, M$ **do**:
   1. Select random order / permutation of feature indices $\tau = (\tau^{(1)}, \ldots, \tau^{(p)}) \in \Pi$
   2. Determine coalition $S_m := S_j^\tau$, i.e., the set of features before feature j in order τ
   3. Select random data point $\mathbf{z}^{(m)} \in \mathcal{D}$
   4. Construct two artificial observations by replacing feature values from $\mathbf{x}$ with $\mathbf{z}^{(m)}$:
      - $\mathbf{x}_{+j}^{(m)} = (\underbrace{x_{\tau^{(1)}}, \ldots, x_{\tau^{(|S_m|-1)}}, x_j}_{\mathbf{x}_{S_m \cup \{j\}}}, \underbrace{z^{(m)}_{\tau^{(|S_m|+1)}}, \ldots, z^{(m)}_{\tau^{(p)}}}_{\mathbf{z}^{(m)}_{-\{S_m \cup \{j\}\}}})$ takes features $S_m \cup \{j\}$ from $\mathbf{x}$
      - $\mathbf{x}_{-j}^{(m)} = (\underbrace{x_{\tau^{(1)}}, \ldots, x_{\tau^{(|S_m|-1)}}}_{\mathbf{x}_{S_m}}, \underbrace{z_j^{(m)}, z^{(m)}_{\tau^{(|S_m|+1)}}, \ldots, z^{(m)}_{\tau^{(p)}}}_{\mathbf{z}^{(m)}_{-S_m}})$ takes features S_m from $\mathbf{x}$
   5. Compute difference $\phi_j^m = \hat{f}(\mathbf{x}_{+j}^{(m)}) - \hat{f}(\mathbf{x}_{-j}^{(m)})$

$\rightsquigarrow$ $\hat{f}_{S_m}(\mathbf{x}_{S_m})$ is approximated by $\hat{f}(\mathbf{x}_{-j}^{(m)})$ and $\hat{f}_{S_m \cup \{j\}}(\mathbf{x}_{S_m \cup \{j\}})$ by $\hat{f}(\mathbf{x}_{+j}^{(m)})$ over M iters

APPROXIMATION ALGORITHM ▸ Štrumbelj et al. (2014)

Estimation of ϕ_j for observation $\mathbf{x}$ of model $\hat{f}$ fitted on data $\mathcal{D}$ using sample size M:

1. For $m = 1, \ldots, M$ **do**:
   1. Select random order / perm. of feature indices $\tau = (\tau^{(1)}, \ldots, \tau^{(p)}) \in \Pi$
   2. Determine coalition $S_m := S_j^{\tau}$, i.e., the set of feat. before feat. j in order τ
   3. Select random data point $\mathbf{z}^{(m)} \in \mathcal{D}$
   4. Construct two artificial obs. by replacing feature values from $\mathbf{x}$ with $\mathbf{z}^{(m)}$:
      - $\mathbf{x}_{+j}^{(m)} = (\underbrace{x_{\tau^{(1)}}, \ldots, x_{\tau^{(|S_m|-1)}}, x_j}_{\mathbf{x}_{S_m \cup \{j\}}}, \underbrace{z_{\tau^{(|S_m|+1)}}^{(m)}, \ldots, z_{\tau^{(p)}}^{(m)}}_{\mathbf{z}_{-\{S_m \cup \{j\}\}}^{(m)}})$ takes features $S_m \cup \{j\}$ from $\mathbf{x}$
      - $\mathbf{x}_{-j}^{(m)} = (\underbrace{x_{\tau^{(1)}}, \ldots, x_{\tau^{(|S_m|-1)}}}_{\mathbf{x}_{S_m}}, \underbrace{z_j^{(m)}, z_{\tau^{(|S_m|+1)}}^{(m)}, \ldots, z_{\tau^{(p)}}^{(m)}}_{\mathbf{z}_{-S_m}^{(m)}})$ takes features S_m from $\mathbf{x}$
   5. Compute difference $\phi_j^m = \hat{f}(\mathbf{x}_{+j}^{(m)}) - \hat{f}(\mathbf{x}_{-j}^{(m)})$

   $\rightsquigarrow$ $\hat{f}_{S_m}(\mathbf{x}_{S_m})$ is approximated by $\hat{f}(\mathbf{x}_{-j}^{(m)})$ and $\hat{f}_{S_m \cup \{j\}}(\mathbf{x}_{S_m \cup \{j\}})$ by $\hat{f}(\mathbf{x}_{+j}^{(m)})$ over M iters.
2. Compute Shapley value $\phi_j = \frac{1}{M} \sum_{m=1}^{M} \phi_j^m$

APPROXIMATION ALGORITHM ▸ Štrumbelj et al. (2014)

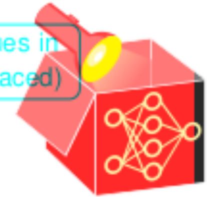
Estimation of ϕ_j for observation $\mathbf{x}$ of model $\hat{f}$ fitted on data $\mathcal{D}$ using sample size M:

1. For $m = 1, \ldots, M$ **do**:
   1. Select random order / permutation of feature indices $\tau = (\tau^{(1)}, \ldots, \tau^{(p)}) \in \Pi$
   2. Determine coalition $S_m := S_j^{\tau}$, i.e., the set of features before feature j in order τ
   3. Select random data point $\mathbf{z}^{(m)} \in \mathcal{D}$
   4. Construct two artificial observations by replacing feature values from $\mathbf{x}$ with $\mathbf{z}^{(m)}$:
      - $\mathbf{x}_{+j}^{(m)} = (\underbrace{x_{\tau^{(1)}}, \ldots, x_{\tau^{(|S_m|-1)}}, x_j}_{\mathbf{x}_{S_m \cup \{j\}}}, \underbrace{z_{\tau^{(|S_m|+1)}}^{(m)}, \ldots, z_{\tau^{(p)}}^{(m)}}_{\mathbf{z}_{-\{S_m \cup \{j\}\}}^{(m)}})$ takes features $S_m \cup \{j\}$ from $\mathbf{x}$
      - $\mathbf{x}_{-j}^{(m)} = (\underbrace{x_{\tau^{(1)}}, \ldots, x_{\tau^{(|S_m|-1)}}}_{\mathbf{x}_{S_m}}, \underbrace{z_j^{(m)}, z_{\tau^{(|S_m|+1)}}^{(m)}, \ldots, z_{\tau^{(p)}}^{(m)}}_{\mathbf{z}_{-S_m}^{(m)}})$ takes features S_m from $\mathbf{x}$
   5. Compute difference $\phi_j^m = \hat{f}(\mathbf{x}_{+j}^{(m)}) - \hat{f}(\mathbf{x}_{-j}^{(m)})$

   $\rightsquigarrow$ $\hat{f}_{S_m}(\mathbf{x}_{S_m})$ is approximated by $\hat{f}(\mathbf{x}_{-j}^{(m)})$ and $\hat{f}_{S_m \cup \{j\}}(\mathbf{x}_{S_m \cup \{j\}})$ by $\hat{f}(\mathbf{x}_{+j}^{(m)})$ over M iters
2. Compute Shapley value $\phi_j = \frac{1}{M} \sum_{m=1}^{M} \phi_j^m$

Interpretable Machine Learning – 5 / 9

SHAPLEY VALUE APPROXIMATION - ILLUSTRATION



Definition

$\mathbf{x}$: obs. of interest

$\mathbf{x}$ with feature values in S_m (other are replaced)

$$\phi_j(\mathbf{x}) = \frac{1}{M}\sum_{m=1}^{M}\left[\hat{f}(\mathbf{x}_{+j}{}^{(m)}) - \hat{f}(\mathbf{x}_{-j}{}^{(m)})\right]$$

$\mathbf{x}$ with feature values in $S_m \cup \{j\}$

	Temperature	Humidity	Windspeed	Year
x	10.66	56	11	2012
x_{+j}	10.66	56	$random : z_{windspeed}^{(m)}$	2012
x_{-j}	10.66	56	$random : z_{windspeed}^{(m)}$	$random : z_{year}^{(m)}$

$$\underbrace{}_{j}$$

SHAPLEY VALUE APPROXIMATION - ILLUSTRATION

Definition

$\mathbf{x}$: obs. of interest

$\mathbf{x}$ with feature values in S_m (other are replaced)

$$\phi_j(\mathbf{x}) = \frac{1}{M}\sum_{m=1}^{M}\left[\hat{f}(\mathbf{x}_{+j}{}^{(m)}) - \hat{f}(\mathbf{x}_{-j}{}^{(m)})\right]$$

$\mathbf{x}$ with feature values in $S_m \cup \{j\}$

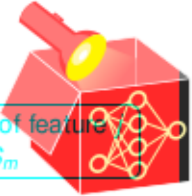
	Temperature	Humidity	Windspeed	Year
x	10.66	56	11	2012
x_{+j}	10.66	56	$random : z_{windspeed}^{(m)}$	2012
x_{-j}	10.66	56	$random : z_{windspeed}^{(m)}$	$random : z_{year}^{(m)}$

j

SHAPLEY VALUE APPROXIMATION - ILLUSTRATION

Definition

Contribution of feature j to coalition S_m



$$\phi_j(\mathbf{x}) = \frac{1}{M}\sum_{m=1}^{M} \underbrace{\left[\hat{f}(\mathbf{x}_{+j}{}^{(m)}) - \hat{f}(\mathbf{x}_{-j}{}^{(m)})\right]}_{:=\Delta(j,S_m)}$$

- $\Delta(j, S_m) = \hat{f}(\mathbf{x}_{+j}^{(m)}) - \hat{f}(\mathbf{x}_{-j}^{(m)})$ is the marginal contribution of feature j to coalition S_m
- Here: Feature *year* contributes +700 bike rentals if it joins coalition $S_m = \{temp, hum\}$

	Temperature	Humidity	Windspeed	Year	Count
x	10.66	56	11	2012	
x_{+j}	10.66	56	$random: z^{(m)}_{windspeed}$	2012	5600
x_{-j}	10.66	56	$random: z^{(m)}_{windspeed}$	$random: z^{(m)}_{year}$	4900

j

$\hat{f}$

700

$\Delta(j, S_m)$ marginal contribution

Definition

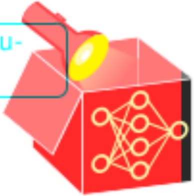
Contribution of feature j to coalition S_m

$$\phi_j(\mathbf{x}) = \frac{1}{M}\sum_{m=1}^{M} \underbrace{\left[\hat{f}(\mathbf{x}_{+j}{}^{(m)}) - \hat{f}(\mathbf{x}_{-j}{}^{(m)})\right]}_{:=\Delta(j,S_m)}$$

- $\Delta(j, S_m) = \hat{f}(\mathbf{x}_{+j}^{(m)}) - \hat{f}(\mathbf{x}_{-j}^{(m)})$ is the marginal contribution of feature j to coalition S_m
- Here: Feature *year* contributes +700 bike rentals if it joins coalition $S_m = \{temp, hum\}$

j $\hat{f}$ 5600 4900 700 $\Delta(j, S_m)$ marginal contribution

SHAPLEY VALUE APPROXIMATION - ILLUSTRATION

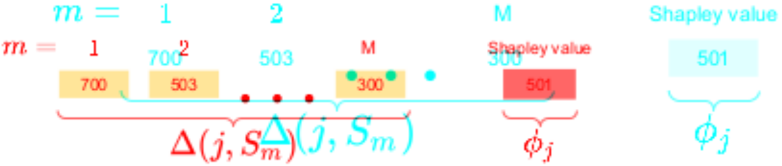


Definition

average the contributions of feature j

$$\phi_j(\mathbf{x}) = \frac{1}{M}\sum_{m=1}^{M}\left[\hat{f}(\mathbf{x}_{+j}{}^{(m)}) - \hat{f}(\mathbf{x}_{-j}{}^{(m)})\right]$$

- Compute marginal contribution of feature j towards the prediction across all randomly drawn feature coalitions $S_1, \dots, S_m$
- Average all M marginal contributions of feature j
- Shapley value ϕ_j is the payout of feature j, i.e., how much feature *year* contributed to the overall prediction in bicycle counts of a specific observation $\mathbf{x}$



average the contributions of feature j

- Compute marginal contribution of feature j towards the prediction across all randomly drawn feature coalitions $S_1, \dots, S_m$
- Average all M marginal contributions of feature j
- Shapley value ϕ_j is the payout of feature j, i.e., how much feature *year* contributed to the overall prediction in bicycle counts of a specific observation $\mathbf{x}$

REVISITED: AXIOMS FOR FAIR ATTRIBUTIONS

We take the general axioms for Shapley Values and apply it to predictions:

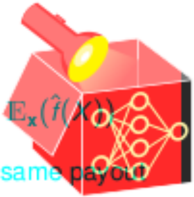
- **Efficiency:** Shapley values add up to the (centered) prediction: $\sum_{j=1}^{p} \phi_j = \hat{f}(\mathbf{x}) - \mathbb{E}_{\mathbf{x}}(\hat{f}(X))$

REVISITED: AXIOMS FOR FAIR ATTRIBUTIONS

We take the general axioms for Shapley Values and apply it to predictions:

- **Efficiency:** Shapley values add up to the (centered) prediction: $\sum_{j=1}^{p} \phi_j = \hat{f}(\mathbf{x}) - \mathbb{E}_{\mathbf{x}}(\hat{f}(X))$

REVISITED: AXIOMS FOR FAIR ATTRIBUTIONS



We take the general axioms for Shapley Values and apply it to predictions:

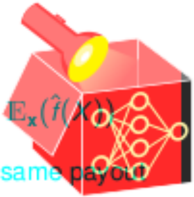
- **Efficiency:** Shapley values add up to the (centered) prediction: $\sum_{j=1}^{p} \phi_j = \hat{f}(\mathbf{x}) - \mathbb{E}_{\mathbf{x}}(\hat{f}(X))$
- **Symmetry:** Two features j and k that contribute the same to the prediction get the same payout
  $\leadsto$ interaction effects between features are fairly divided
  $\hat{f}_{S\cup\{j\}}(\mathbf{x}_{S\cup\{j\}}) = \hat{f}_{S\cup\{k\}}(\mathbf{x}_{S\cup\{k\}})$ for all $S \subseteq P \setminus \{j, k\}$ then $\phi_j = \phi_k$

REVISITED: AXIOMS FOR FAIR ATTRIBUTIONS

We take the general axioms for Shapley Values and apply it to predictions:

- **Efficiency:** Shapley values add up to the (centered) prediction: $\sum_{j=1}^{p} \phi_j = \hat{f}(\mathbf{x}) - \mathbb{E}_{\mathbf{x}}(\hat{f}(X))$
- **Symmetry:** Two features j and k that contribute the same to the prediction get the same payout
  $\leadsto$ interaction effects between features are fairly divided
  $\hat{f}_{S\cup\{j\}}(\mathbf{x}_{S\cup\{j\}}) = \hat{f}_{S\cup\{k\}}(\mathbf{x}_{S\cup\{k\}})$ for all $S \subseteq P \setminus \{j, k\}$ then $\phi_j = \phi_k$

REVISITED: AXIOMS FOR FAIR ATTRIBUTIONS



We take the general axioms for Shapley Values and apply it to predictions:

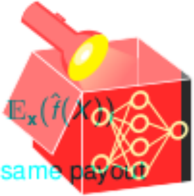
- **Efficiency**: Shapley values add up to the (centered) prediction: $\sum_{j=1}^{p} \phi_j = \hat{f}(\mathbf{x}) - \mathbb{E}_{\mathbf{x}}(\hat{f}(X))$
- **Symmetry**: Two features j and k that contribute the same to the prediction get the same payout
  ⇝ interaction effects between features are fairly divided
  $\hat{f}_{S\cup\{j\}}(\mathbf{x}_{S\cup\{j\}}) = \hat{f}_{S\cup\{k\}}(\mathbf{x}_{S\cup\{k\}})$ for all $S \subseteq P \setminus \{j, k\}$ then $\phi_j = \phi_k$
- **Dummy / Null Player**: Shapley value of a feature that does not influence the prediction is zero ⇝ if a feature was not selected by the model (e.g., tree or LASSO), its Shapley value is zero
  $\hat{f}_{S\cup\{j\}}(\mathbf{x}_{S\cup\{j\}}) = \hat{f}_S(\mathbf{x}_S)$ for all $S \subseteq P$ then $\phi_j = 0$

REVISITED: AXIOMS FOR FAIR ATTRIBUTIONS

We take the general axioms for Shapley Values and apply it to predictions:

- **Efficiency**: Shapley values add up to the (centered) prediction: $\sum_{j=1}^{p} \phi_j = \hat{f}(\mathbf{x}) - \mathbb{E}_{\mathbf{x}}(\hat{f}(X))$
- **Symmetry**: Two features j and k that contribute the same to the prediction get the same payout
  ⇝ interaction effects between features are fairly divided
  $\hat{f}_{S\cup\{j\}}(\mathbf{x}_{S\cup\{j\}}) = \hat{f}_{S\cup\{k\}}(\mathbf{x}_{S\cup\{k\}})$ for all $S \subseteq P \setminus \{j, k\}$ then $\phi_j = \phi_k$
- **Dummy / Null Player**: Shapley value of a feature that does not influence the prediction is zero
  ⇝ if a feature was not selected by the model (e.g., tree or LASSO), its Shapley value is zero
  $\hat{f}_{S\cup\{j\}}(\mathbf{x}_{S\cup\{j\}}) = \hat{f}_S(\mathbf{x}_S)$ for all $S \subseteq P$ then $\phi_j = 0$

REVISITED: AXIOMS FOR FAIR ATTRIBUTIONS



We take the general axioms for Shapley Values and apply it to predictions:

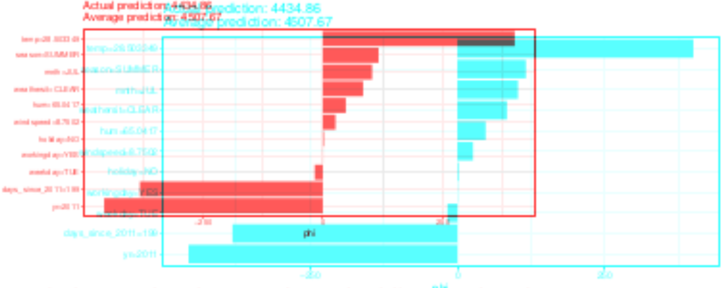
- **Efficiency**: Shapley values add up to the (centered) prediction: $\sum_{j=1}^{p} \phi_j = \hat{f}(\mathbf{x}) - \mathbb{E}_{\mathbf{x}}(\hat{f}(X))$
- **Symmetry**: Two features j and k that contribute the same to the prediction get the same payout ⇝ interaction effects between features are fairly divided $\hat{f}_{S \cup \{j\}}(\mathbf{x}_{S \cup \{j\}}) = \hat{f}_{S \cup \{k\}}(\mathbf{x}_{S \cup \{k\}})$ for all $S \subseteq P \setminus \{j, k\}$ then $\phi_j = \phi_k$
- **Dummy / Null Player**: Shapley value of a feature that does not influence the prediction is zero ⇝ if a feature was not selected by the model (e.g., tree or LASSO), its Shapley value is zero $\hat{f}_{S \cup \{j\}}(\mathbf{x}_{S \cup \{j\}}) = \hat{f}_S(\mathbf{x}_S)$ for all $S \subseteq P$ then $\phi_j = 0$
- **Additivity**: For a prediction with combined payouts, the payout is the sum of payouts: $\phi_j(v_1) + \phi_j(v_2)$ ⇝ Shapley values for model ensembles can be combined

REVISITED: AXIOMS FOR FAIR ATTRIBUTIONS

We take the general axioms for Shapley Values and apply it to predictions:

- **Efficiency**: Shapley values add up to the (centered) prediction: $\sum_{j=1}^{p} \phi_j = \hat{f}(\mathbf{x}) - \mathbb{E}_{\mathbf{x}}(\hat{f}(X))$
- **Symmetry**: Two features j and k that contribute the same to the prediction get the same payout
  ⇝ interaction effects between features are fairly divided
  $\hat{f}_{S \cup \{j\}}(\mathbf{x}_{S \cup \{j\}}) = \hat{f}_{S \cup \{k\}}(\mathbf{x}_{S \cup \{k\}})$ for all $S \subseteq P \setminus \{j, k\}$ then $\phi_j = \phi_k$
- **Dummy / Null Player**: Shapley value of a feature that does not influence the prediction is zero
  ⇝ if a feature was not selected by the model (e.g., tree or LASSO), its Shapley value is zero
  $\hat{f}_{S \cup \{j\}}(\mathbf{x}_{S \cup \{j\}}) = \hat{f}_S(\mathbf{x}_S)$ for all $S \subseteq P$ then $\phi_j = 0$
- **Additivity**: For a prediction with combined payouts, the payout is the sum of payouts: $\phi_j(v_1) + \phi_j(v_2)$ ⇝ Shapley values for model ensembles can be combined

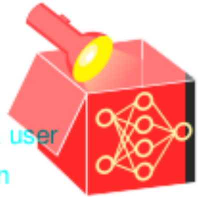
BIKE SHARING DATASET



- Shapley values of observation $i = 200$ from the bike sharing data
- Difference between model prediction of this observation and the average prediction of the data is fairly distributed among the features (i.e., $4434 - 4507 \approx -73$)
- Feature value temp = 28.5 has the most positive effect, with a contribution (increase of prediction) of about +400

- Shapley values of observation $i = 200$ from the bike sharing data
- Difference between model prediction of this observation and the average prediction of the data is fairly distributed among the features (i.e., $4434 - 4507 \approx -73$)
- Feature value temp = 28.5 has the most positive effect, with a contribution (increase of prediction) of about +400

ADVANTAGES AND DISADVANTAGES



Advantages:

- **Solid theoretical foundation** in game theory
- Prediction is **fairly distributed** among the feature values → easy to interpret for a user
- **Contrastive explanations** that compare the prediction with the average prediction

Disadvantages:

- Without sampling, Shapley values need a lot of computing time to inspect all possible coalitions
- Like many other IML methods, Shapley values suffer from the inclusion of unrealistic data observations when features are correlated

ADVANTAGES AND DISADVANTAGES

Advantages:

- Solid theoretical foundation in game theory
- Prediction is fairly distributed among the feature values → easy to interpret for a user
- Contrastive explanations that compare the prediction with the average prediction

Disadvantages:

- Without sampling, Shapley values need a lot of computing time to inspect all possible coalitions
- Like many other IML methods, Shapley values suffer from the inclusion of unrealistic data observations when features are correlated