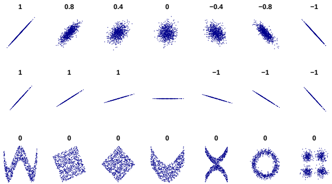
# Interpretable Machine Learning

## Intro to IML
## Correlation and Dependencies



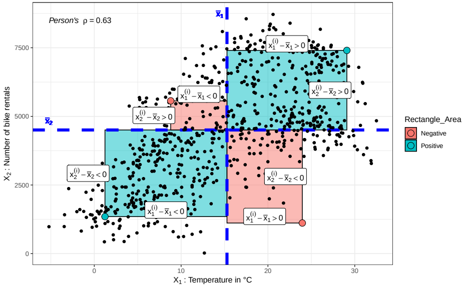

**Learning goals**

- Pearson correlation
- Coefficient of determination $R^2$
- Mutual information
- Correlation vs. dependence

# PEARSON'S CORRELATION COEFFICIENT $\rho$

**Correlation** often refers to Pearson's correlation (measures only **linear relationship**)

$$\rho(X_1, X_2) = \frac{\sum_{i=1}^{n} (x_1^{(i)} - \bar{x}_1) \cdot (x_2^{(i)} - \bar{x}_2)}{\sqrt{\sum_{i=1}^{n} (x_1^{(i)} - \bar{x}_1)^2 \sum_{i=1}^{n} (x_2^{(i)} - \bar{x}_2)^2}} \in [-1, 1]$$




Geometric interpretation of $\rho$:

- Numerator is sum of rectangle's area with width $x_1^{(i)} - \bar{x}_1$ and height $x_2^{(i)} - \bar{x}_2$
- Areas enter numerator with positive (**+**) or negative (**-**) sign, depending on position
- Denominator scales the sum into the range $[-1, 1]$

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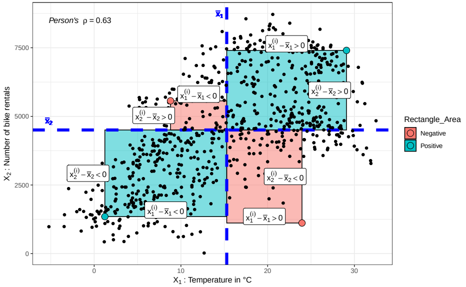


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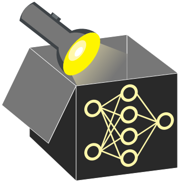
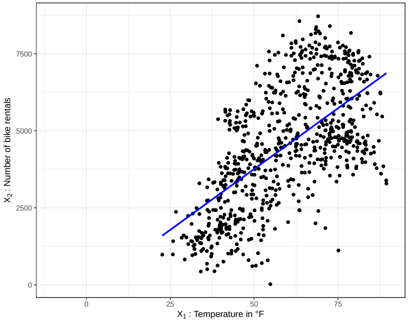
- $\rho > 0$ if positive areas dominate negative areas $\rightsquigarrow X_1, X_2$ positive correlated
- $\rho < 0$ if negative areas dominate positive areas $\rightsquigarrow X_1, X_2$ negative correlated
- $\rho = 0$ if area of rectangles cancels out $\rightsquigarrow X_1, X_2$ linearly uncorrelated

# COEFFICIENT OF DETERMINATION $R^2$



Another method to evaluate **linear dependency** between features is $R^2$




- Fit a linear model:
  $\hat{x}_2 = \hat{f}_{LM}(x_1) = \theta_0 + \theta_1 x_1$

$\rightsquigarrow$ Slope $\theta_1 = 0 \Rightarrow$ no dependence

$\rightsquigarrow$ Large slope $\Rightarrow$ strong dependence

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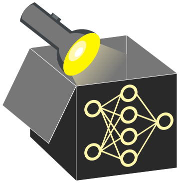

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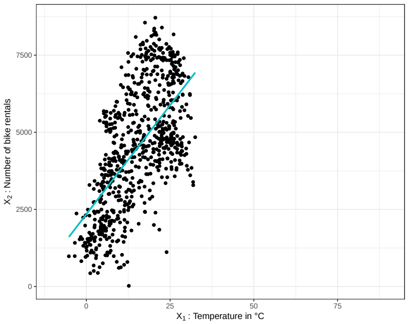


- Fit a linear model: $\hat{x}_2 = \hat{f}_{LM}(x_1) = \theta_0 + \theta_1 x_1$
- $\leadsto$ Slope $\theta_1 = 0 \Rightarrow$ no dependence
- $\leadsto$ Large slope $\Rightarrow$ strong dependence
- Exact $\theta_1$ score problematic
- $\leadsto$ Re-scaling of $x_1$ or $x_2$ changes $\theta_1$
- $\leadsto$ °F $\longrightarrow$ °C $\Rightarrow \theta_1 = 78 \longrightarrow \theta_1^* = 141$

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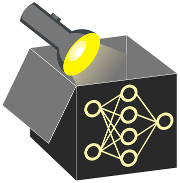

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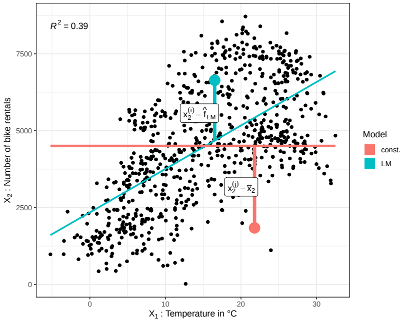


- Fit a linear model:
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  - ⇝ Large slope $\Rightarrow$ strong dependence
- Exact $\theta_1$ score problematic
  - ⇝ Re-scaling of $x_1$ or $x_2$ changes $\theta_1$
- Set $SSE_{LM}$ in relation to $SSE$ of a constant model $\hat{f}_c = \bar{x}_2$

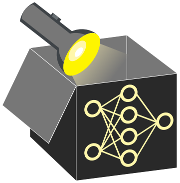
  $SSE_{LM} = \sum_{i=1}^{n}(x_2^{(i)} - \hat{f}_{LM}(x_1^{(i)}))^2$

  $SSE_c = \sum_{i=1}^{n}(x_2^{(i)} - \bar{x}_2)^2$

$\Rightarrow$ Measure of fitting quality of LM: $R^2 = 1 - \frac{SSE_{LM}}{SSE_c} \in [0, 1]$

$\Rightarrow \rho(X_1, X_2) = R$

# JOINT, MARGINAL AND CONDITIONAL DISTRIBUTION



For two discrete random variables $X_1, X_2$:

**Joint distribution**

$$p_{X_1,X_2}(x_1, x_2) = \mathbb{P}(X_1 = x_1, X_2 = x_2)$$

| $p_{X_1,X_2}$ | $\mathbb{P}(X_2 = 0)$ | $\mathbb{P}(X_2 = 1)$ | $p_{X_1}$ |
|---|---|---|---|
| $\mathbb{P}(X_1 = 0)$ | 0.2 | 0.3 | 0.5 |
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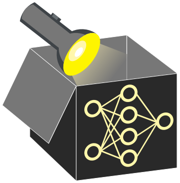

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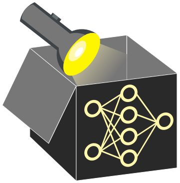
**Conditional distribution**

$$p_{X_1|X_2}(x_1|x_2) = \mathbb{P}(X_1 = x_1|X_2 = x_2) = \frac{p_{X_1,X_2}(x_1, x_2)}{p_{X_2}(x_2)}$$

| | $x_2 = 0$ | $x_2 = 1$ |
|---|---|---|
| $\mathbb{P}(X_1 = 0\|X_2 = x_2)$ | 0.67 | 0.43 |
| $\mathbb{P}(X_1 = 1\|X_2 = x_2)$ | 0.33 | 0.57 |
| $\sum$ | 1 | 1 |

# DEPENDENCE



**Dependence:** Describes general dependence structure (e.g., non-lin. relationships)

- Definition: $X_j$, $X_k$ independent $\Leftrightarrow$ joint distribution is product of marginals:

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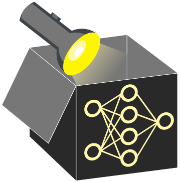

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  $\mathbb{P}(X_j|X_k) = \mathbb{P}(X_j)$ and $\mathbb{P}(X_k|X_j) = \mathbb{P}(X_k)$ (follows from cond. probability)

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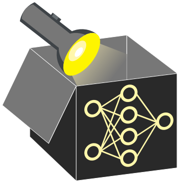

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- Measuring complex dependencies is difficult but different measures exist
  Examples
  $\leadsto$ Spearman correlation (measures monotonic dependencies via ranks)
  $\leadsto$ Information-theoretical measures like mutual information
  $\leadsto$ Kernel-based measures like Hilbert-Schmidt Independence Criterion (HSIC)

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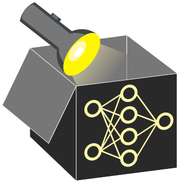

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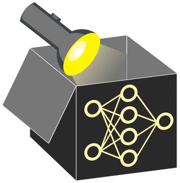
- **N.B.:** $X_j$, $X_k$ indep. $\Rightarrow \rho(X_j, X_k) = 0$ **but** $\rho(X_j, X_k) = 0 \nRightarrow X_j$, $X_k$ indep.
  Equivalency holds if distribution is jointly normal

# MUTUAL INFORMATION

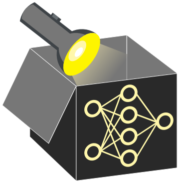


- MI describes expected amount of information shared by two RVs:

$$MI(X_1, X_2) = \mathbb{E}_{p(x_1, x_2)}\left[log\left(\frac{p(x_1, x_2)}{p(x_1)p(x_2)}\right)\right]$$

- MI measures amount of "dependence" between features by looking how different the joint distribution is from pure indep. $p(x_1, x_2) = p(x_1)p(x_2)$
  $\rightsquigarrow MI(X_1, X_2) = \mathbb{E}_{p(x_1, x_2)}\left[log\left(\frac{p(x_1, x_2)}{p(x_1, x_2)}\right)\right] = \mathbb{E}_{p(x_1, x_2)}[log(1)] = 0$
  $\rightsquigarrow MI(X_j, X_k) = 0$ if and only if the features are independent
- Unlike (Pearson) correlation, MI is also defined for categorical features

# MUTUAL INFORMATION: EXAMPLE



For two discrete RV $X_1$ and $Y$:

$$MI(X_1; Y) = \mathbb{E}_{p(x_1,y)}\left[log\left(\frac{p(x_1,y)}{p(x_1)p(y)}\right)\right] = \sum_{x_1\in\mathcal{X}_1}\sum_{y\in\mathcal{Y}} p(x_1,y) log\left(\frac{p(x_1,y)}{p(x_1)p(y)}\right)$$

| **$X_1$** | ... | **Y** |
|---|---|---|
| yes | ... | yes |
| yes | ... | no |
| no | ... | yes |
| no | ... | no |

| | $\mathbb{P}(X_1 = \text{yes})$ | $\mathbb{P}(X_1 = \text{no})$ | $p_Y$ |
|---|---|---|---|
| $\mathbb{P}(Y = \text{yes})$ | 0.25 | 0.25 | 0.5 |
| $\mathbb{P}(Y = \text{no})$ | 0.25 | 0.25 | 0.5 |
| $p_{X_1}$ | 0.5 | 0.5 | 1 |

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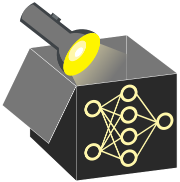

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| $\mathbf{X_1}$ | ... | **Y** |
|---|---|---|
| yes | ... | yes |
| yes | ... | no |
| no | ... | yes |
| no | ... | no |

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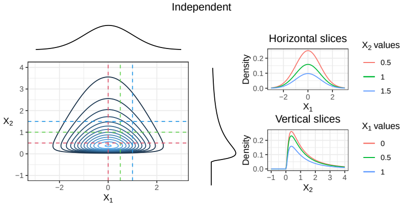
$$\begin{aligned} MI(X_1;Y) &= 0.25\, log\left(\frac{0.25}{0.5\cdot 0.5}\right) + 0.25\, log\left(\frac{0.25}{0.5\cdot 0.5}\right) \\ &\quad + 0.25\, log\left(\frac{0.25}{0.5\cdot 0.5}\right) + 0.25\, log\left(\frac{0.25}{0.5\cdot 0.5}\right) \\ &= 0.25\, log\left(\frac{0.25}{0.25}\right)\cdot 4 \\ &= 0.25\, log\left(1\right)\cdot 4 = 0 \end{aligned}$$

# DEPENDENCE AND INDEPENDENCE

**Example:**




Conditional distributions at different vertical and horizontal slices (after normalizing area to 1) match their marginal distributions

$$\Rightarrow \mathbb{P}(X_1|X_2) = \mathbb{P}(X_1)$$
$$\mathbb{P}(X_2|X_1) = \mathbb{P}(X_2)$$

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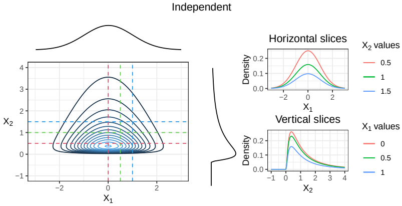


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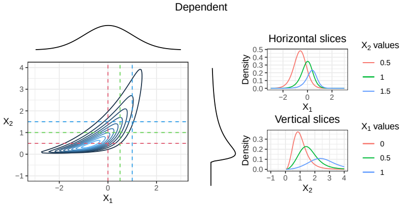


Conditional distributions do not match their marginal distributions

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# CORRELATION VS. DEPENDENCE

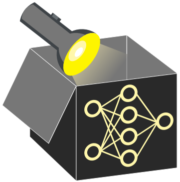
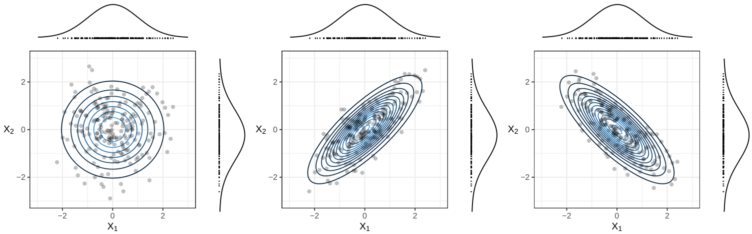


Illustration of bivariate normal distribution with different correlations
$X_1, X_2 \sim N(0,1)$

$\rho(X_1, X_2) = 0$ (independent) $\quad \rho(X_1, X_2) = 0.8 \quad \rho(X_1, X_2) = -0.8$



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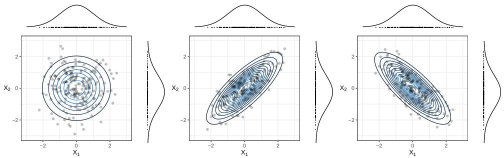


Examples with Pearson's corr. $\rho \approx 0$ but non-linear dependencies (MI $\neq 0$):