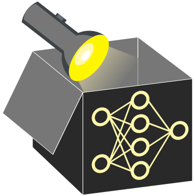
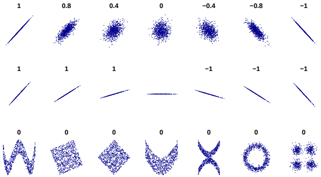
Interpretable Machine Learning



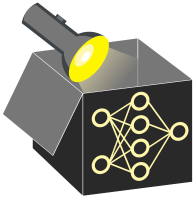
Correlation and Dependencies



Learning goals

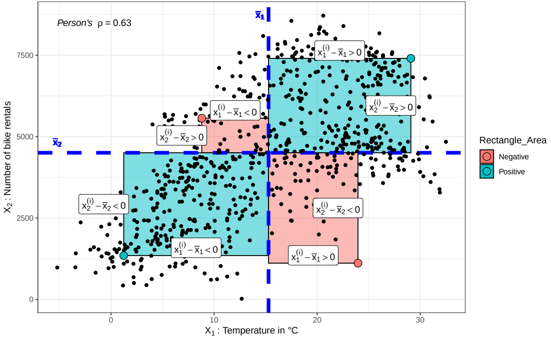
- Pearson correlation
- Coefficient of determination R^2
- Mutual Information
- Correlation vs. dependence

PEARSON'S CORRELATION COEFFICIENT ρ



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 ρ:

- 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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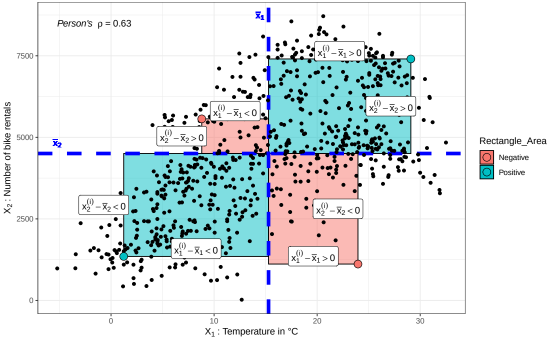

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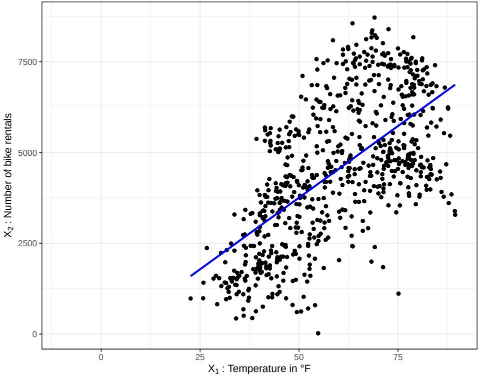
- $\rho > 0$ if positive areas dominate negative areas $\rightsquigarrow X_1, X_2$ positive correlated
- $\rho < 0$ if negative areas dominate positive areas $\rightsquigarrow X_1, X_2$ negative correlated
- $\rho = 0$ if area of rectangles cancels out $\rightsquigarrow X_1, X_2$ linearly uncorrelated

COEFFICIENT OF DETERMINATION R^2

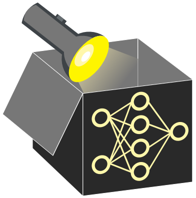
Another method to evaluate **linear dependency** between features is R^2



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

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

⇝ Large slope $\Rightarrow$ strong dependence



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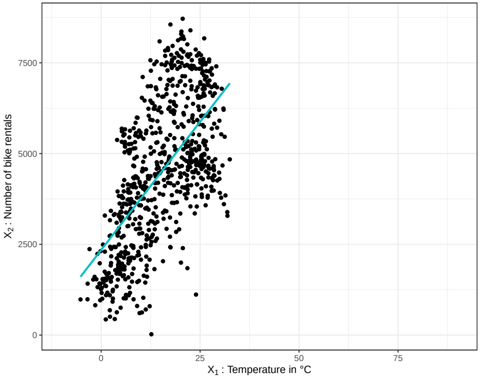
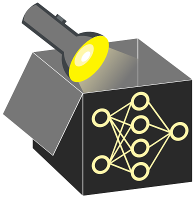


- Fit a linear model: $\hat{x}_2 = \hat{f}_{LM}(x_1) = \theta_0 + \theta_1 x_1$
- ⇝ Slope $\theta_1 = 0 \Rightarrow$ no dependence
- ⇝ Large slope $\Rightarrow$ strong dependence
- Exact θ_1 score problematic
- ⇝ Re-scaling of x_1 or x_2 changes θ_1
- ⇝ °F $\rightarrow$ °C $\Rightarrow \theta_1 = 78 \rightarrow \theta_1^* = 141$



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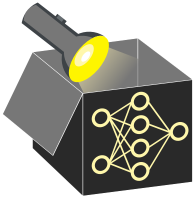

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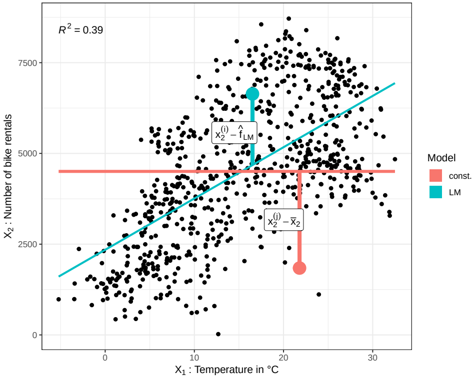

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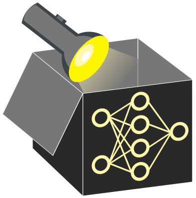
- ⇝ Large slope $\Rightarrow$ strong dependence
- Exact θ_1 score problematic
- ⇝ Re-scaling of x_1 or x_2 changes θ_1
- Set SSE_{LM} in relation to SSE of a constant model $\hat{f}_c = \bar{x}_2$
  $SSE_{LM} = \sum_{i=1}^{n}(x_2^{(i)} - \hat{f}_{LM}(x_1^{(i)}))^2$
  $SSE_c = \sum_{i=1}^{n}(x_2^{(i)} - \bar{x}_2)^2$

$\Rightarrow$ 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
$\mathbb{P}(X_1 = 1)$	0.1	0.4	0.5
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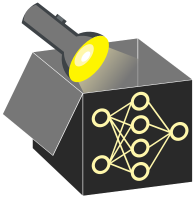

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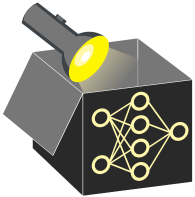

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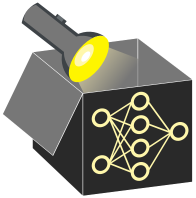
Conditional distribution

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

	$x_2 = 0$	$x_2 = 1$
$\mathbb{P}(X_1 = 0 \vert X_2 = x_2)$	0.67	0.43
$\mathbb{P}(X_1 = 1 \vert X_2 = x_2)$	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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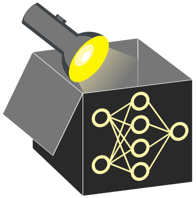

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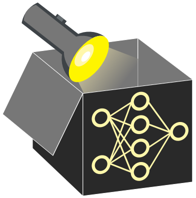

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- Measuring complex dependencies is difficult but different measures exist, e.g.,
  $\rightsquigarrow$ Spearman correlation (measures monotonic dependencies via ranks)
  $\rightsquigarrow$ Information-theoretical measures like mutual information
 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

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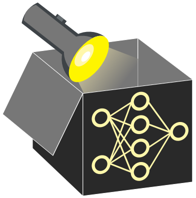

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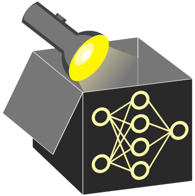
  $\leadsto$ Spearman correlation (measures monotonic dependencies via ranks)
  $\leadsto$ Information-theoretical measures like mutual information
  $\leadsto$ Kernel-based measures like Hilbert-Schmidt Independence Criterion (HSIC)
- **N.B.:** X_j, X_k independent $\Rightarrow \rho(X_j, X_k) = 0$ **but** $\rho(X_j, X_k) = 0 \not\Rightarrow X_j$, X_k indep.
  Equivalency holds if distribution is jointly normal

MUTUAL INFORMATION



- MI describes expected amount of information shared by two random variables:

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

- MI measures amount of "dependence" between features by looking how different the joint distribution is from pure independence $p(x_1, x_2) = p(x_1)p(x_2)$
  $\rightsquigarrow MI(X_1, X_2) = \mathbb{E}_{p(x_1,x_2)}\left[log\left(\frac{p(x_1,x_2)}{p(x_1,x_2)}\right)\right] = \mathbb{E}_{p(x_1,x_2)}[log(1)] = 0$
  $\rightsquigarrow MI(X_j, X_k) = 0$ if and only if the features are independent
- Unlike (Pearson) correlation, MI is not limited to continuous random variables

MUTUAL INFORMATION: EXAMPLE

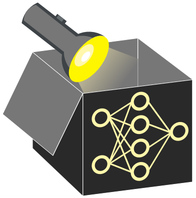
For two discrete RV X_1 and Y:

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

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

MUTUAL INFORMATION: EXAMPLE



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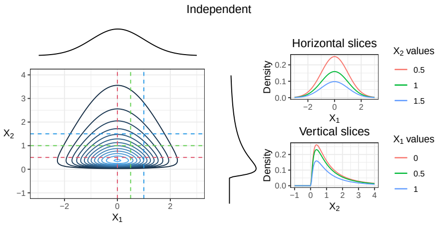
$$\begin{aligned} MI(X_1;Y) &= 0.25\, log\left(\frac{0.25}{0.5\cdot 0.5}\right) + 0.25\, log\left(\frac{0.25}{0.5\cdot 0.5}\right) \\ &\quad + 0.25\, log\left(\frac{0.25}{0.5\cdot 0.5}\right) + 0.25\, log\left(\frac{0.25}{0.5\cdot 0.5}\right) \\ &= 0.25\, log\left(\frac{0.25}{0.25}\right)\cdot 4 \\ &=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

DEPENDENCE AND INDEPENDENCE

Example:



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

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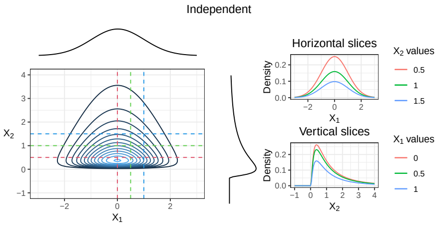

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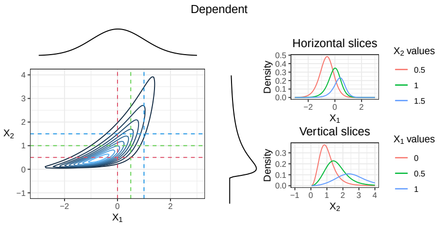
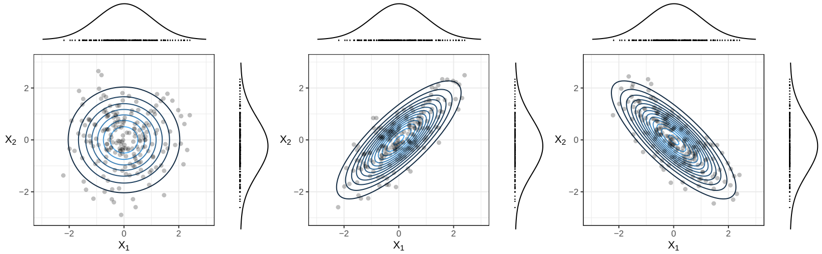


Conditional distributions do not match their marginal distributions

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) | $\rho(X_1, X_2) = 0.8$ | $\rho(X_1, X_2) = -0.8$



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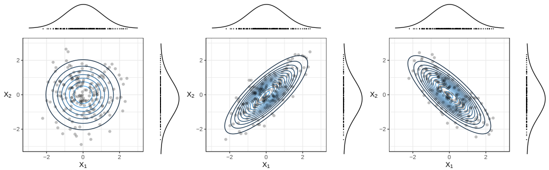

Examples with Pearson's correlation $\rho \approx 0$ but non-linear dependencies (MI $\neq 0$):

$\rho(X_1, X_2) = 0$, $MI(X_1, X_2) = 0.52 \qquad \rho(X_1, X_2) = 0.01$, $MI(X_1, X_2) = 0.37 \qquad \rho(X_1, X_2) = -0.06$, $MI(X_1, X_2) = 0.61$