### Linear Regression: Explained Variance

Probability and Statistics for Data Science

Carlos Fernandez-Granda

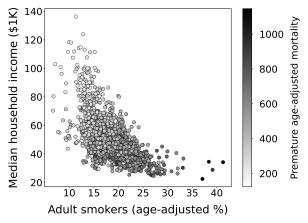




These slides are based on the book Probability and Statistics for Data Science by Carlos Fernandez-Granda, available for purchase here. A free preprint, videos, code, slides and solutions to exercises are available at https://www.ps4ds.net

### Regression

### Goal: Estimate response from features



#### Response:

Premature mortality (deaths < age 75 per 10<sup>4</sup> people)

#### Features:

(1) Fraction of adult smokers (2) Median household income

### Linear regression

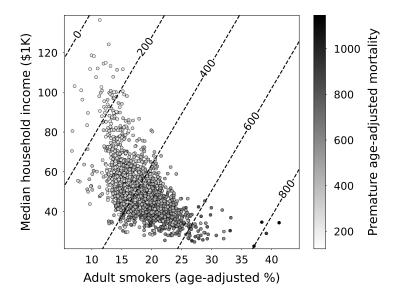
Linear minimum MSE estimator of response  $\tilde{y}$  given features  $\tilde{x}$ 

$$\ell_{\mathsf{MMSE}}(\tilde{\mathbf{x}}) = \mathbf{\Sigma}_{\tilde{\mathbf{x}}\tilde{\mathbf{y}}}^{\mathsf{T}} \mathbf{\Sigma}_{\tilde{\mathbf{x}}}^{-1} \left( \tilde{\mathbf{x}} - \mu_{\tilde{\mathbf{x}}} \right) + \mu_{\tilde{\mathbf{y}}}$$

Ordinary-least-squares estimator from dataset  $(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)$ 

$$\ell_{\mathsf{OLS}}(x_i) = \Sigma_{XY}^T \Sigma_X^{-1} (x_i - m(X)) + m(Y)$$

## $15.7 x_{\text{tobacco}} - 3.04 x_{\text{income}} + 281$



Goal: Evaluate the estimator

#### One feature $\tilde{a}$

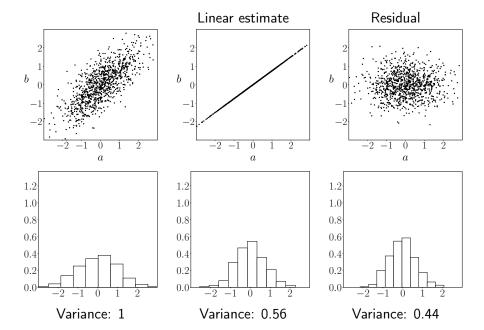
$$ilde{y} = \underbrace{\ell_{\mathsf{MMSE}}( ilde{a})}_{\mathsf{Linear}\ \mathsf{MMSE}\ \mathsf{estimate}} + \underbrace{ ilde{y} - \ell_{\mathsf{MMSE}}( ilde{a})}_{\mathsf{Residual}}$$

Residual uncorrelated with  $\ell_{\mathsf{MMSE}}(\tilde{a})$ 

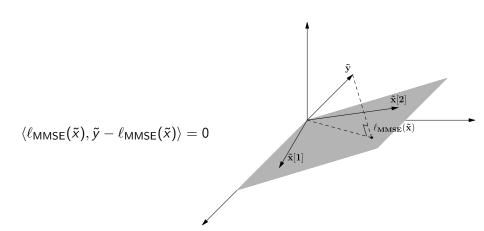
$$\operatorname{Var}\left[\tilde{y}\right] = \operatorname{Var}\left[\ell_{\mathsf{MMSE}}(\tilde{a})\right] + \operatorname{Var}\left[\tilde{y} - \ell_{\mathsf{MMSE}}(\tilde{a})\right]$$

$$\operatorname{Var}\left[\ell_{\mathsf{MMSE}}(\tilde{\boldsymbol{a}})\right] = \rho_{\tilde{\boldsymbol{a}},\tilde{\boldsymbol{y}}}^{2} \operatorname{Var}\left[\tilde{\boldsymbol{y}}\right] = R^{2} \operatorname{Var}\left[\tilde{\boldsymbol{y}}\right]$$

 $\rho_{\tilde{a},\tilde{y}} = 0.75, R^2 = 0.56$ 



### Geometric intuition



### Uncorrelated residual

$$\begin{aligned} &\operatorname{Cov}\left[\ell_{\operatorname{\mathsf{MMSE}}}\left(\tilde{x}\right),\tilde{y}-\ell_{\operatorname{\mathsf{MMSE}}}\left(\tilde{x}\right)\right]\\ &=\operatorname{E}\left[\operatorname{ct}\left(\ell_{\operatorname{\mathsf{MMSE}}}\left(\tilde{x}\right)\right)\operatorname{ct}\left(\tilde{y}-\ell_{\operatorname{\mathsf{MMSE}}}\left(\tilde{x}\right)\right)\right]\\ &=\operatorname{E}\left[\beta_{\operatorname{\mathsf{MMSE}}}^{T}\operatorname{ct}\left(\tilde{x}\right)\left(\operatorname{ct}\left(\tilde{y}\right)-\operatorname{ct}\left(\tilde{x}\right)^{T}\beta_{\operatorname{\mathsf{MMSE}}}\right)\right]\\ &=\beta_{\operatorname{\mathsf{MMSE}}}^{T}\operatorname{E}\left[\operatorname{ct}\left(\tilde{x}\right)\operatorname{ct}\left(\tilde{y}\right)\right]-\beta_{\operatorname{\mathsf{MMSE}}}^{T}\operatorname{E}\left[\operatorname{ct}\left(\tilde{x}\right)\operatorname{ct}\left(\tilde{x}\right)^{T}\right]\beta_{\operatorname{\mathsf{MMSE}}}\\ &=\Sigma_{\tilde{x}\tilde{y}}^{T}\Sigma_{\tilde{x}}^{-1}\Sigma_{\tilde{x}\tilde{y}}-\Sigma_{\tilde{x}\tilde{y}}^{T}\Sigma_{\tilde{x}}^{-1}\Sigma_{\tilde{x}\tilde{y}}\Sigma_{\tilde{x}}^{-1}\Sigma_{\tilde{x}\tilde{y}}\\ &=\Sigma_{\tilde{x}\tilde{y}}^{T}\Sigma_{\tilde{x}}^{-1}\Sigma_{\tilde{x}\tilde{y}}-\Sigma_{\tilde{x}\tilde{y}}^{T}\Sigma_{\tilde{x}}^{-1}\Sigma_{\tilde{x}\tilde{y}}\\ &=0\end{aligned}$$

$$\begin{split} \operatorname{ct}\left(\ell_{\mathsf{MMSE}}\left(\tilde{x}\right)\right) &= \ell_{\mathsf{MMSE}}\left(\tilde{x}\right) - \operatorname{E}\left[\ell_{\mathsf{MMSE}}\left(\tilde{x}\right)\right] \\ &= \beta_{\mathsf{MMSE}}^{T}\tilde{x} + \alpha_{\mathsf{MMSE}} - \beta_{\mathsf{MMSE}}^{T}\mu_{\tilde{x}} - \alpha_{\mathsf{MMSE}} \\ &= \beta_{\mathsf{MMSE}}^{T}\operatorname{ct}\left(\tilde{x}\right) \end{split}$$

## Decomposition of variance

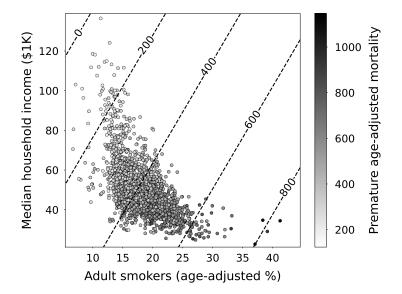
$$\begin{split} \operatorname{Var}\left[\tilde{y}\right] &= \operatorname{Var}\left[\ell_{\mathsf{MMSE}}(\tilde{x}) + \tilde{y} - \ell_{\mathsf{MMSE}}(\tilde{x})\right] \\ &= \operatorname{Var}\left[\ell_{\mathsf{MMSE}}(\tilde{x})\right] + \operatorname{Var}\left[\tilde{y} - \ell_{\mathsf{MMSE}}(\tilde{x})\right] \\ &= \operatorname{Var}\left[\ell_{\mathsf{MMSE}}(\tilde{x})\right] + \mathsf{MSE} \end{split}$$

$$\begin{split} \mathbf{E}\left[\tilde{\mathbf{y}} - \ell_{\mathsf{MMSE}}\left(\tilde{\mathbf{x}}\right)\right] &= \mathbf{E}\left[\tilde{\mathbf{y}} - \beta_{\mathsf{MMSE}}^{\mathsf{T}}\tilde{\mathbf{x}} - \alpha_{\mathsf{MMSE}}\right] \\ &= \mathbf{E}\left[\tilde{\mathbf{y}}\right] - \beta_{\mathsf{MMSE}}^{\mathsf{T}}\mathbf{E}\left[\tilde{\mathbf{x}}\right] - \alpha_{\mathsf{MMSE}} \\ &= \mathbf{0} \end{split}$$

### Coefficient of determination

$$\begin{aligned} \operatorname{Var}\left[\tilde{y}\right] &= \operatorname{Var}\left[\ell_{\mathsf{MMSE}}(\tilde{x})\right] + \mathsf{MSE} \\ R^2 &:= \frac{\operatorname{Var}\left[\ell_{\mathsf{MMSE}}(\tilde{x})\right]}{\operatorname{Var}\left[\tilde{y}\right]} \\ &= \frac{\operatorname{Var}\left[\tilde{y}\right] - \mathsf{MSE}}{\operatorname{Var}\left[\tilde{y}\right]} \\ &= 1 - \frac{\mathsf{MSE}}{\operatorname{Var}\left[\tilde{y}\right]} \end{aligned}$$

## $15.7 x_{\text{tobacco}} - 3.04 x_{\text{income}} + 281$



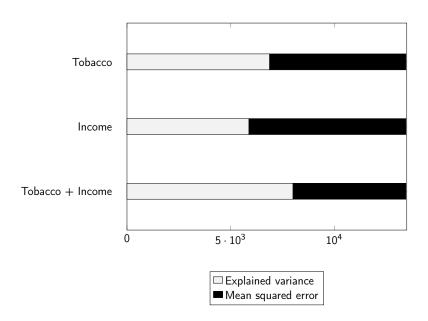
#### Counties in the United States

$$\ell_{ ext{OLS}}\left(x_{ ext{tobacco}}, x_{ ext{income}}\right) = 15.7 \, x_{ ext{tobacco}} - 3.04 \, x_{ ext{income}} + 281$$

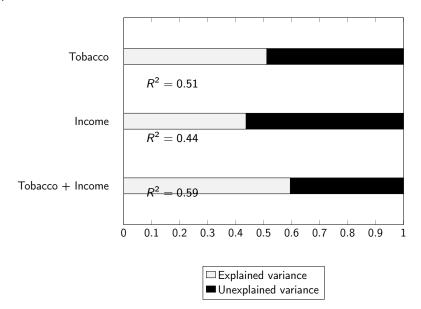
$$\ell_{ ext{OLS}}\left(x_{ ext{tobacco}}\right) = 22.52 \, x_{ ext{tobacco}} + 2$$

$$\ell_{ ext{OLS}}\left(x_{ ext{income}}\right) = -5.57 \, x_{ ext{income}} + 692$$

# Variance of the response: $1.35 \cdot 10^4$



### Explained variance



Sample correlation coefficient between tobacco and income: -0.6

