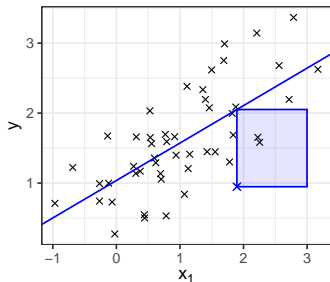


Introduction to Machine Learning

Supervised Regression: Linear Models with L_2 Loss



Learning goals

- Grasp the overall concept of linear regression
- Understand how L_2 loss optimization results in SSE-minimal model
- Understand this as a general template for ERM in ML

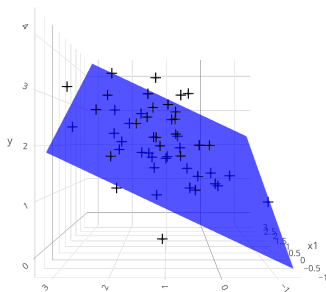
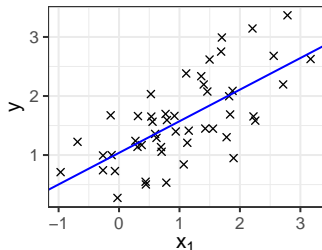
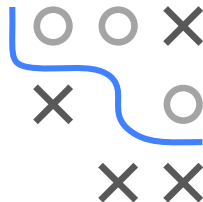
LINEAR REGRESSION

- Idea: predict $y \in \mathbb{R}$ as **linear** combination of features¹:

$$\hat{y} = f(\mathbf{x}) = \boldsymbol{\theta}^\top \mathbf{x} = \theta_0 + \theta_1 x_1 + \cdots + \theta_p x_p$$

\rightsquigarrow find loss-optimal params to describe relation $y|\mathbf{x}$

- Hypothesis space: $\mathcal{H} = \{f(\mathbf{x}) = \boldsymbol{\theta}^\top \mathbf{x} \mid \boldsymbol{\theta} \in \mathbb{R}^{p+1}\}$



¹ Actually, special case of linear model, which is linear combo of *basis functions* of features \rightsquigarrow Polynomial Regression Models

DESIGN MATRIX

- Mismatch: $\theta \in \mathbb{R}^{p+1}$ vs $\mathbf{x} \in \mathbb{R}^p$ due to intercept term
- Trick: pad feature vectors with leading 1, s.t.
 - $\mathbf{x} \mapsto \mathbf{x} = (1, x_1, \dots, x_p)^\top$, and
 - $\theta^\top \mathbf{x} = \theta_0 \cdot 1 + \theta_1 x_1 + \dots + \theta_p x_p$
- Collect all observations in **design matrix** $\mathbf{X} \in \mathbb{R}^{n \times (p+1)}$
 \rightsquigarrow more compact: single param vector incl. intercept
- Resulting linear model:

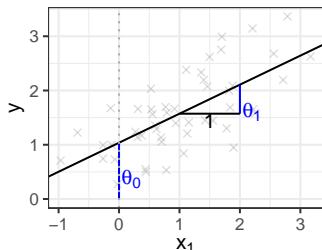
$$\hat{\mathbf{y}} = \mathbf{X}\theta = \begin{pmatrix} 1 & x_1^{(1)} & \dots & x_p^{(1)} \\ 1 & x_1^{(2)} & \dots & x_p^{(2)} \\ \vdots & \vdots & & \vdots \\ 1 & x_1^{(n)} & \dots & x_p^{(n)} \end{pmatrix} \begin{pmatrix} \theta_0 \\ \theta_1 \\ \vdots \\ \theta_p \end{pmatrix} = \begin{pmatrix} \theta_0 + \theta_1 x_1^{(1)} + \dots + \theta_p x_p^{(1)} \\ \theta_0 + \theta_1 x_1^{(2)} + \dots + \theta_p x_p^{(2)} \\ \vdots \\ \theta_0 + \theta_1 x_1^{(n)} + \dots + \theta_p x_p^{(n)} \end{pmatrix}$$

- We will make use of this notation in other contexts



EFFECT INTERPRETATION

- Big plus of LM: immediately **interpretable** feature effects
- "Marginally increasing x_j by 1 unit increases y by θ_j units"
 \rightsquigarrow *ceteris paribus* assumption: $x_1, \dots, x_{j-1}, x_{j+1}, \dots, x_p$ fixed



Call:

```
lm(formula = y ~ x_1, data = dt_univ)
```

Residuals:

	Min	1Q	Median	3Q	Max
	-1.10346	-0.34727	-0.00766	0.31500	1.04284

Coefficients:

	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	1.03727	0.11360	9.131	4.55e-12 ***
x_1	0.53521	0.08219	6.512	4.13e-08 ***

Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 0.5327 on 48 degrees of freedom

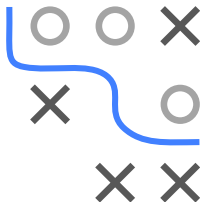
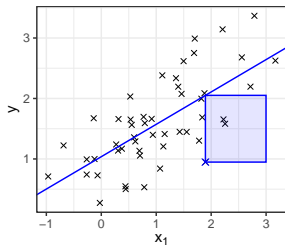
Multiple R-squared: 0.469, Adjusted R-squared: 0.458

F-statistic: 42.4 on 1 and 48 DF, p-value: 4.129e-08

MODEL FIT

- How to determine LM fit? \rightsquigarrow define risk & optimize
- Popular: **L_2 loss** / **quadratic loss** / **squared error**

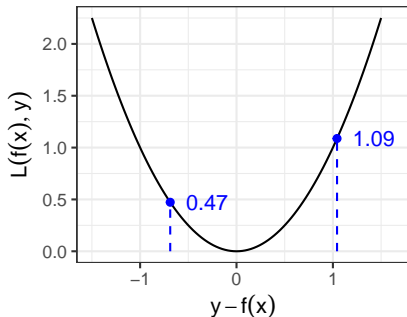
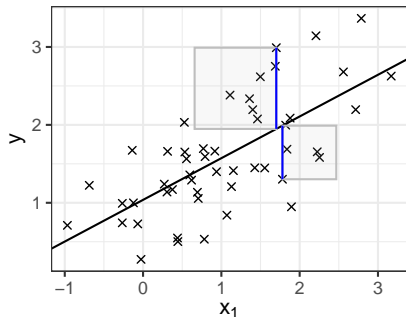
$$L(y, f(\mathbf{x})) = (y - f(\mathbf{x}))^2 \text{ or } L(y, f(\mathbf{x})) = 0.5 \cdot (y - f(\mathbf{x}))^2$$



- Why penalize **residuals** $r = y - f(\mathbf{x})$ quadratically?
 - Easy to optimize (convex, differentiable)
 - Theoretically appealing (connection to classical stats LM)

LOSS PLOTS

We will often visualize loss effects like this:



- Data as $y \sim x_1$
- Prediction hypersurface
 \rightsquigarrow here: line
- Residuals $r = y - f(x)$
 \rightsquigarrow squares to illustrate loss

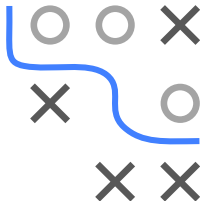
- Loss as function of residuals
 \rightsquigarrow strength of penalty?
 \rightsquigarrow symmetric?
- Highlighted: loss for residuals shown on LHS

OPTIMIZATION

- Resulting risk equivalent to **sum of squared errors (SSE)**:

$$\mathcal{R}_{\text{emp}}(\boldsymbol{\theta}) = \sum_{i=1}^n \left(y^{(i)} - \boldsymbol{\theta}^\top \mathbf{x}^{(i)} \right)^2$$

- Consider example with $n = 5 \rightsquigarrow$ different models with varying SSE

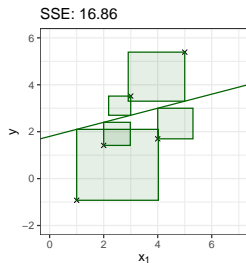


OPTIMIZATION

- Resulting risk equivalent to **sum of squared errors (SSE)**:

$$\mathcal{R}_{\text{emp}}(\boldsymbol{\theta}) = \sum_{i=1}^n \left(y^{(i)} - \boldsymbol{\theta}^\top \mathbf{x}^{(i)} \right)^2$$

- Consider example with $n = 5 \rightsquigarrow$ different models with varying SSE

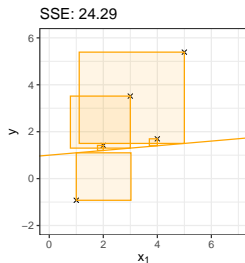
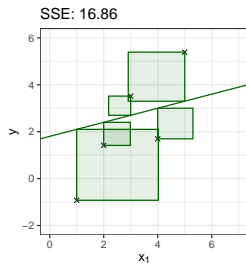


OPTIMIZATION

- Resulting risk equivalent to **sum of squared errors (SSE)**:

$$\mathcal{R}_{\text{emp}}(\theta) = \sum_{i=1}^n \left(y^{(i)} - \theta^\top \mathbf{x}^{(i)} \right)^2$$

- Consider example with $n = 5$ \rightsquigarrow different models with varying SSE

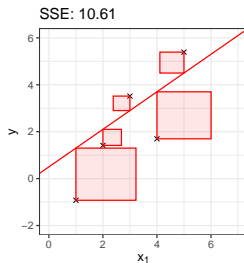
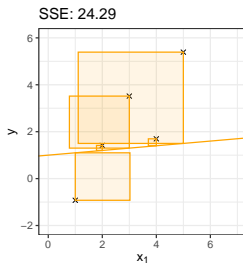
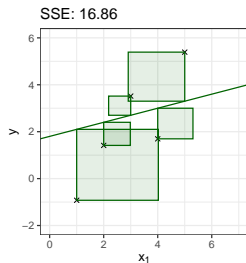


OPTIMIZATION

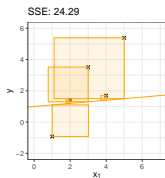
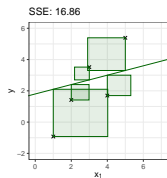
- Resulting risk equivalent to **sum of squared errors (SSE)**:

$$\mathcal{R}_{\text{emp}}(\theta) = \sum_{i=1}^n \left(y^{(i)} - \theta^\top \mathbf{x}^{(i)} \right)^2$$

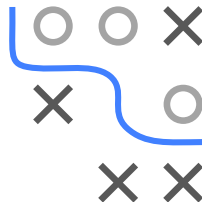
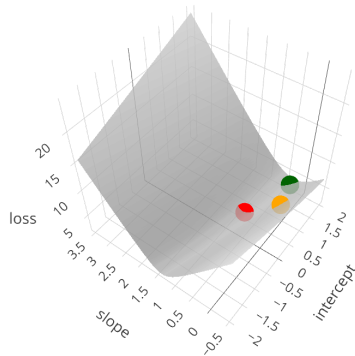
- Consider example with $n = 5$ \rightsquigarrow different models with varying SSE



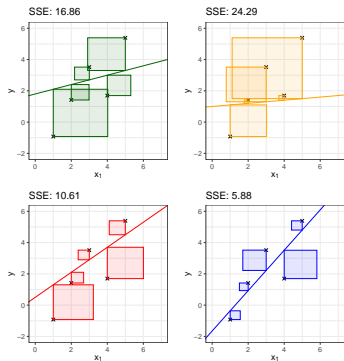
OPTIMIZATION



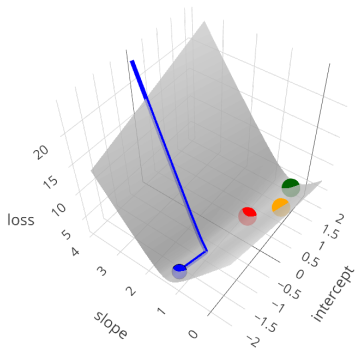
Intercept θ_0	Slope θ_1	SSE
1.80	0.30	16.86
1.00	0.10	24.29
0.50	0.80	10.61



OPTIMIZATION



Intercept θ_0	Slope θ_1	SSE
1.80	0.30	16.86
1.00	0.10	24.29
0.50	0.80	10.61
-1.65	1.29	5.88



Instead of guessing, of course, use **optimization**!

ANALYTICAL OPTIMIZATION

- Special property of LM with L_2 loss: **analytical solution** available

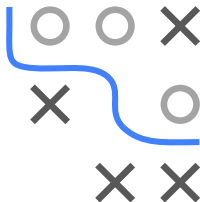
$$\begin{aligned}\hat{\boldsymbol{\theta}} \in \arg \min_{\boldsymbol{\theta}} \mathcal{R}_{\text{emp}}(\boldsymbol{\theta}) &= \arg \min_{\boldsymbol{\theta}} \sum_{i=1}^n \left(y^{(i)} - \boldsymbol{\theta}^\top \mathbf{x}^{(i)} \right)^2 \\ &= \arg \min_{\boldsymbol{\theta}} \|\mathbf{y} - \mathbf{X}\boldsymbol{\theta}\|_2^2\end{aligned}$$

- Find via **normal equations**

$$\frac{\partial \mathcal{R}_{\text{emp}}(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}} = 0$$

- Solution: **ordinary-least-squares (OLS)** estimator

$$\hat{\theta} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y}$$



STATISTICAL PROPERTIES

- LM with $L2$ loss intimately related to classical stats LM
- Assumptions
 - $\mathbf{x}^{(i)}$ iid for $i \in \{1, \dots, n\}$
 - **Homoskedastic** (equivariant) **Gaussian** errors

$$\mathbf{y} = \mathbf{X}\boldsymbol{\theta} + \boldsymbol{\epsilon}, \boldsymbol{\epsilon} \sim \mathcal{N}(0, \sigma^2 \mathbf{I})$$

$\rightsquigarrow y_i$ conditionally independent & normal: $\mathbf{y}|\mathbf{X} \sim \mathcal{N}(\mathbf{X}\boldsymbol{\theta}, \sigma^2 \mathbf{I})$

- Uncorrelated features
 - \rightsquigarrow multicollinearity destabilizes effect estimation
 - If assumptions hold: statistical **inference** applicable
 - Hypothesis tests on significance of effects, incl. p -values
 - Confidence & prediction intervals via student- t distribution
 - Goodness-of-fit measure $R^2 = 1 - \text{SSE} / \underbrace{\text{SST}}_{\sum_{i=1}^n (y^{(i)} - \bar{y})^2}$
- \rightsquigarrow SSE = part of data variance *not* explained by model

