Machine Learning

A. Supervised Learning: Linear Models & Fundamentals

A.3. Regularization

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Syllabus

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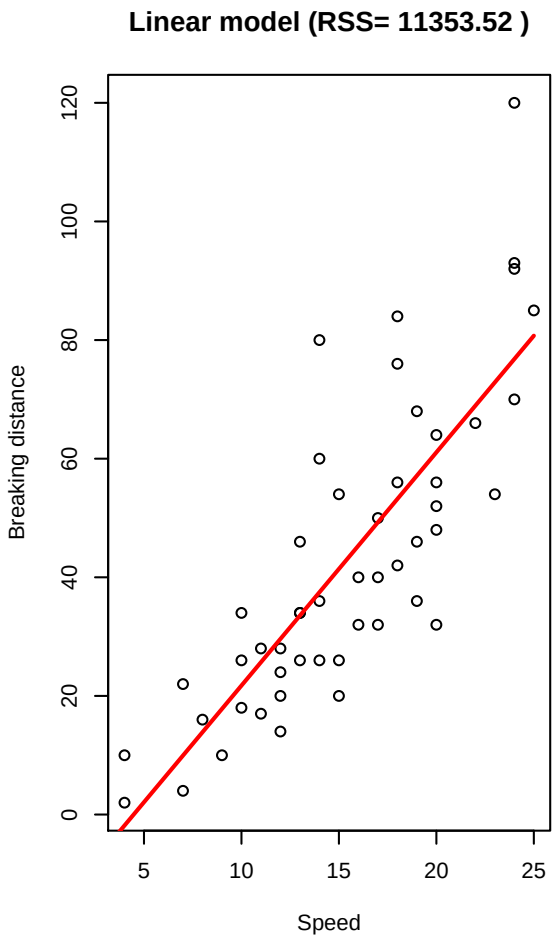
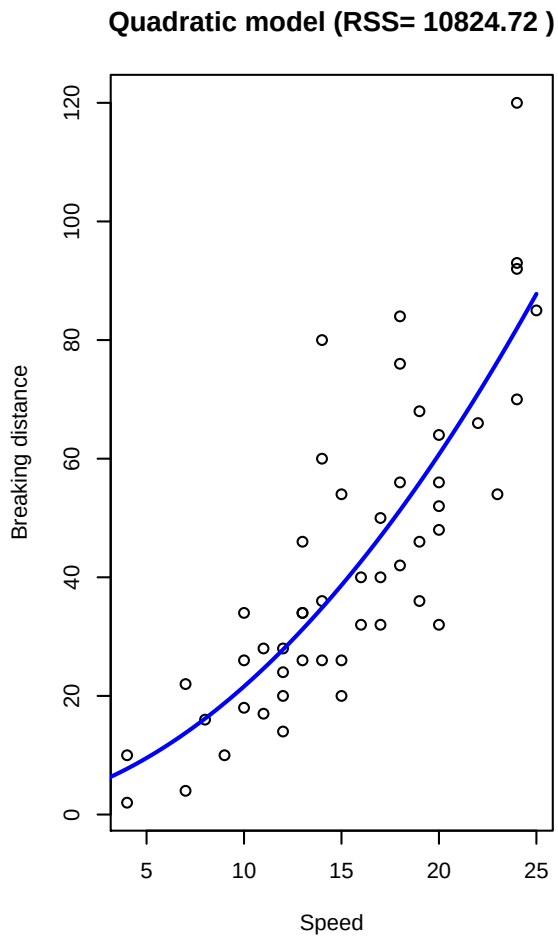
Outline

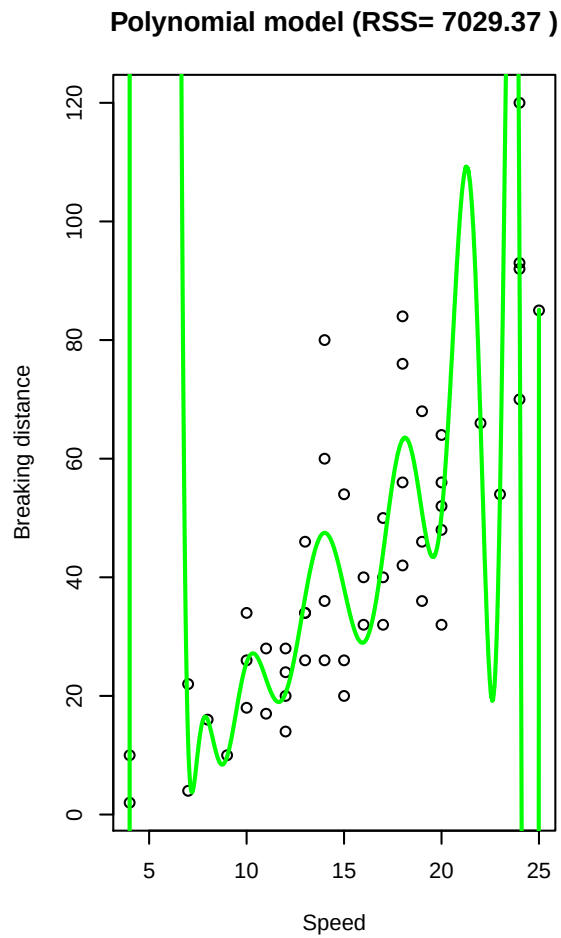
1. The Problem of Overfitting
2. Model Selection
3. Regularization
4. Hyperparameter Optimization

Outline

Fitting of models







Underfitting/Overfitting

- **Underfitting:**
  - the model is not complex enough to explain the data well.
  - results in poor predictive performance.
- **Overfitting:**
  - the model is too complex, it describes the
    - noise, inherent random variations of the data generating process, instead of the
    - signal, the underlying relationship between target and predictors.
  - results in poor predictive performance as well.
- Overfitting is easy: given N points (x_n, y_n) without repeated measurements (i.e. $x_n \neq x_m,\ n \neq m$), there exists a polynomial of degree $N-1$ with RSS equal to 0.

$$\hat{y}(x) := \sum_{n=1}^{N} y_n \prod_{\substack{m=1 \\ m \neq n}}^{N} \frac{x - x_m}{x_n - x_m}$$

Outline

Losses and Fit Measures

	loss	**fit/quality measure**
semantics	the smaller, the better	the larger, the better
goal	minimize	maximize
regression	$\text{RSS}(y, \hat{y}) := \|\|y - \hat{y}\|\|_2^2 := \sum_{n=1}^{N}(y_n - \hat{y}_n)^2$ $\text{L2}(y, \hat{y}) := \frac{1}{N}\sum_{n=1}^{N}(y_n - \hat{y}_n)^2$ $\text{RMSE}(y, \hat{y}) := (\frac{1}{N}\sum_{n=1}^{N}(y_n - \hat{y}_n)^2)^{\frac{1}{2}}$ $\text{MAE}(y, \hat{y}) := \frac{1}{N}\|\|y - \hat{y}\|\|_1 := \frac{1}{N}\sum_{n=1}^{N}\|y_n - \hat{y}_n\|$	$\log L_{\mathcal{N}}(y, \hat{y}) := \sum_{n=1}^{N} -\frac{1}{2\sigma_y^2}(y_n - \hat{y}_n)^2$
classification	$\text{MR}(y, \hat{y}) := \sum_{n=1}^{N}\mathbb{I}(y_n \neq \hat{y}_n)$	$\text{ACC}(y, \hat{y}) := \frac{1}{N}\sum_{n=1}^{N}\mathbb{I}(y_n = \hat{y}_n)$ $\log L_{\text{binomial}}(y, \hat{y}) := \sum_{n=1}^{N}\hat{y}_n\mathbb{I}(y_n = 1) + (1 - \hat{y}_n)\mathbb{I}(y_n = 0)$

Model Selection Measures

- **Model selection**:
  - given a set of models
    indexed by p, one model for each value of p

$$\hat{y}_p(x) = \sum_{m=0}^{p-1} \hat{\beta}_m x_m$$

  - make a choice which model **describes** the data best.

- If we just look at **losses** / **fit measures** such as RSS, then

  the larger p, the better the fit

  or equivalently

  the larger p, the lower the loss

  as the model with p parameters can be **reparametrized** in a model with $p' > p$ parameters by setting

$$\hat{\beta}'_m = \begin{cases} \hat{\beta}_m, & \text{for } m \leq p \\ 0, & \text{for } m > p \end{cases}$$

Model Selection Measures

- One uses **model selection measures** of type

$$\text{model selection measure} = \text{fit} - \text{complexity} \quad \text{(max!)}$$

or equivalently

$$\text{model selection measure} = \text{loss} + \text{complexity} \quad \text{(min!)}$$

- The smaller the loss (= lack of fit), the better the model.
- The smaller the complexity, the simpler and thus better the model.
- The model selection measure tries to find a trade-off between
  - fit/loss and
  - complexity.

Model Selection Measures

Akaike Information Criterion (AIC):

(maximize)

$$\text{AIC} := \log L - p$$

or (minimize)

$$\text{AIC} := -2 \log L + 2p$$

Bayes Information Criterion (BIC) / Bayes-Schwarz Information Criterion: (maximize)

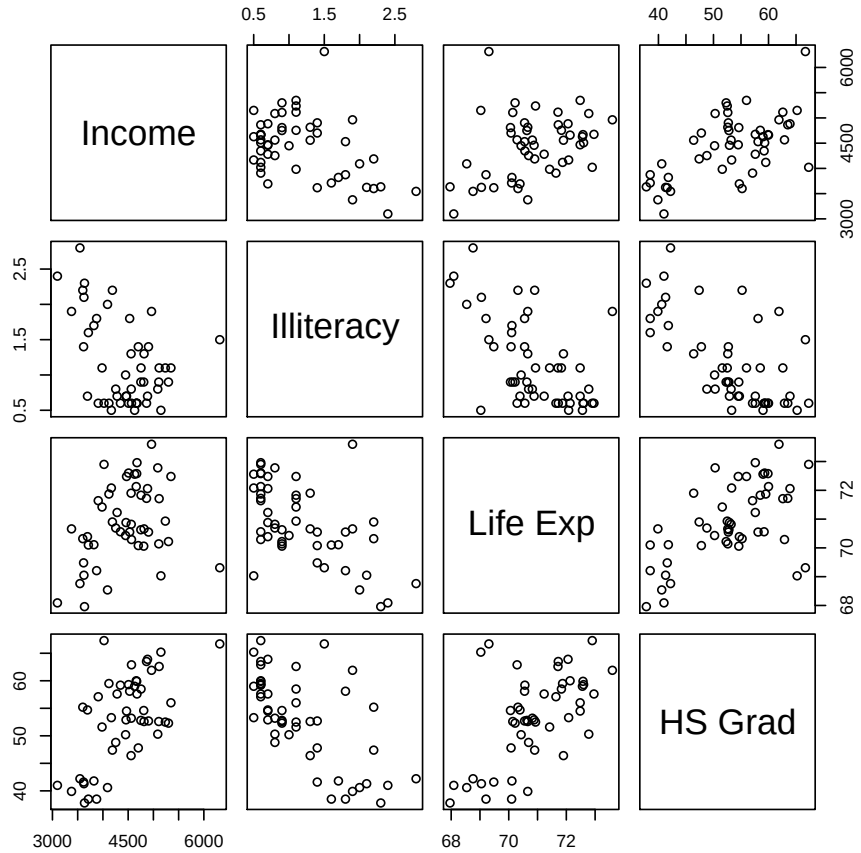
$$\text{BIC} := \log L - \frac{p}{2} \log N$$

where L denotes the likelihood
p the number of parameters
N the number of samples

Example: Predicting Murder Rate

sociographic data of the 50 US states in 1977:

- x_A land area in square miles
- x_F mean number of days with minimum temperature below freezing (1931–1960) in capital or large city
- x_H percent high-school graduates (1970).
- x_I illiteracy (percent of population, 1970),
- x_J income (per capita, 1974),
- x_L life expectancy (in years, 1969–71),
- x_P population (July 1, 1975)
- y_M murder rate per 100,000 population (1976)

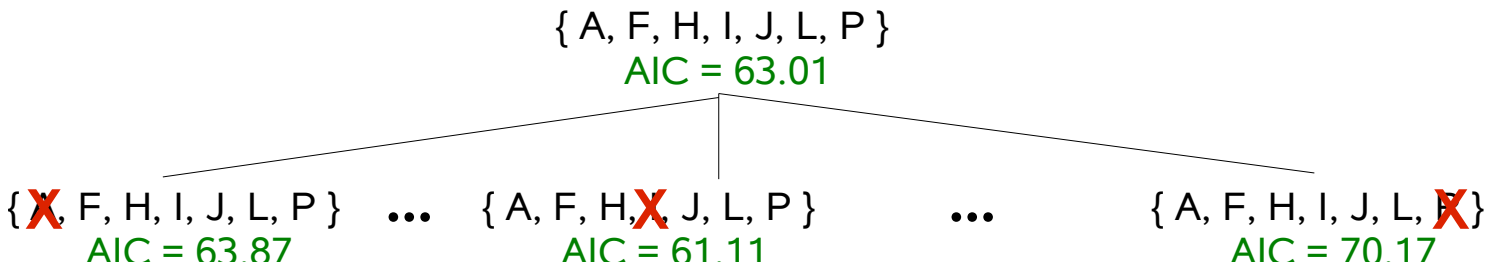


$$y_M = \beta_0 + \beta_A x_A + \beta_F x_F + \beta_H x_H + \beta_I x_I + \beta_J x_J + \beta_L x_L + \beta_P x_P$$

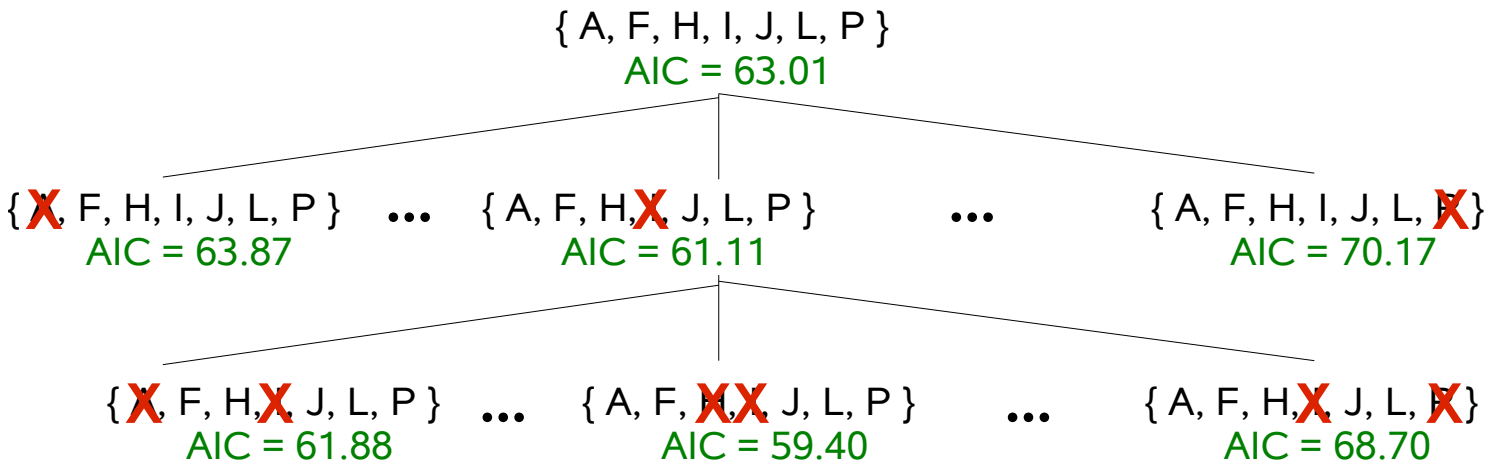
Variable Backward Selection

{ A, F, H, I, J, L, P }
AIC = 63.01

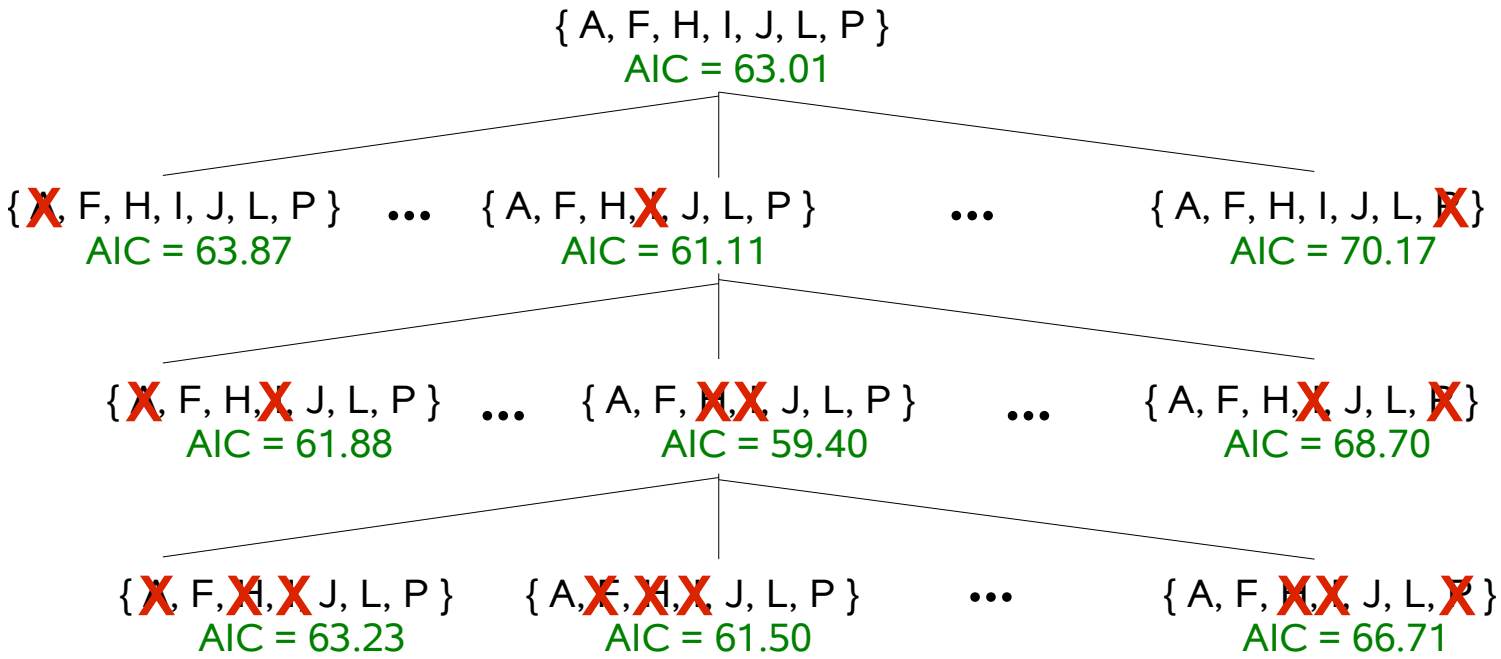
Variable Backward Selection



Variable Backward Selection



Variable Backward Selection



Outline

Shrinkage

- **Model selection** operates by
  1. fitting model instances for a set of models with varying complexity
  2. picking the "best one" in hindsight,
- **Variable Selection**
  - = model selection applied to models with different predictor subsets
  - for models $\hat{y}$ that factor through a linear combination of the predictors,

$$\hat{y}(x; \hat{\beta}) = f(\sum_{m=1}^{M} \hat{\beta}_m x_m) \quad \text{for a suitable } f$$

    - dropping a variable x_m from the model is equivalent to
    - forcing its model parameter $\hat{\beta}_m$ to be 0.

Note: "Fitting a model instance" = "Learning model parameters",
for models having parameters such as linear regression, logistic regression etc.

Shrinkage

- **Variable Selection**
  - ...
    - forcing its model parameter $\hat{\beta}_m$ to be 0.

- **Shrinkage** follows a similar idea:
  - smaller parameters mean a simpler hypothesis/less complex model.
  - hence, small parameters should be prefered in general.
  - a term is added to the objective function to
    - favor small parameters or equivalently
    - **penalize large parameters** or
    - **shrink them towards 0**

    instead of forcing them to be 0.

Shrinkage / Regularization Penalties

There are various types of shrinkage techniques for different problem settings.

L1/Lasso Regularization: $\lambda \sum_{m=1}^{M} |\hat{\beta}_m| = \lambda \|\hat{\beta}\|_1$

L2/Tikhonov Regularization: $\lambda \sum_{m=1}^{M} \hat{\beta}_m^2 = \lambda \|\hat{\beta}\|_2^2$

Elastic Net: $\lambda_1 \|\hat{\beta}\|_1 + \lambda_2 \|\hat{\beta}\|_2^2$

Ridge Regression

Ridge regression is a combination of

$$\underbrace{f(\hat{\beta}; \lambda, \mathcal{D})}_{\text{objective function}} := \underbrace{\frac{1}{N}\sum_{n=1}^{N}(y_n - \hat{y}_n(x_n; \hat{\beta}))^2}_{\text{L2 loss}} + \underbrace{\lambda \sum_{m=1}^{M} \hat{\beta}_m^2}_{\lambda \text{ L2 regularization}}$$

Learning Ridge Regression (Closed Form)

Ridge regression: minimize

$$f(\hat{\beta}; \lambda, \mathcal{D}) = \mathrm{L2}(\hat{\beta}) + \lambda \sum_{m=1}^{M} \hat{\beta}_m^2 = \frac{1}{N} \langle \mathbf{y} - \mathbf{X}\hat{\beta}, \mathbf{y} - \mathbf{X}\hat{\beta} \rangle + \lambda \langle \hat{\beta}, \hat{\beta} \rangle$$

$$\Rightarrow \hat{\beta} = \left(\frac{1}{N} \mathbf{X}^T \mathbf{X} + \lambda I \right)^{-1} \mathbf{X}^T \mathbf{y}, \quad I := \begin{pmatrix} 1 & 0 & \cdots & 0 \\ 0 & 1 & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & 1 \end{pmatrix}$$

with $\lambda \geq 0$ a **complexity hyperparameter** / **regularization weight**.

Beware: ridge regression parameter estimates are not equivariant under scaling of the predictors

$\rightsquigarrow$ data should be normalized before parameter estimation:

$$x'_{n,m} := \frac{x_{n,m} - \bar{x}_{.,m}}{\hat{\sigma}(x_{.,m})}$$

Learning Ridge Regression (Gradient Descent)

learn-ridgereg-GD$(\mathcal{D}^{\text{train}} := \{(x_1, y_1), \ldots, (x_N, y_N)\}, \lambda, \mu, i_{\max} \in \mathbb{N}, \epsilon \in \mathbb{R}^+)$:

$X := (x_1, x_2, \ldots, x_N)^T$

$y := (y_1, y_2, \ldots, y_N)^T$

$\hat{\beta}_0 := (0, \ldots, 0)$

$\hat{\beta} :=$ **minimize-GD**$($ $f(\hat{\beta}) := \frac{1}{N}(y - X\hat{\beta})^T(y - X\hat{\beta}) + \lambda \hat{\beta}^T \hat{\beta}$, $\hat{\beta}_0, \mu, i_{\max}, \epsilon)$

return $\hat{\beta}$

Learning Ridge Regression (Gradient Descent; elementary operations)

learn-ridgereg-GD$(\mathcal{D}^{\text{train}} := \{(x_1, y_1), \ldots, (x_N, y_N)\}, \lambda, \mu, i_{\max} \in \mathbb{N}, \epsilon \in \mathbb{R}^+)$:

$X := (x_1, x_2, \ldots, x_N)^T$

$y := (y_1, y_2, \ldots, y_N)^T$

$\hat{\beta} := 0_M$

$\ell := \frac{1}{N}||y - X\hat{\beta}||^2$

for $t = 1, \ldots, i_{\max}$:

  $\hat{\beta} := \hat{\beta} - \mu(-\frac{2}{N} \cdot X^T(y - X\hat{\beta}) + 2\lambda\hat{\beta})$

  $\ell^{\text{old}} := \ell$

  $\ell := \frac{1}{N}||y - X\hat{\beta}||^2$

  if $\ell - \ell^{\text{old}} < \epsilon$:

    return $\hat{\beta}$

raise exception "not converged in $i_{\max}$ iterations"

L2-Regularized Update Rule

$$\hat{\beta}^{(t)} := (1 - 2\mu\lambda)\hat{\beta}^{(t-1)} + \frac{2\mu}{N} X^T(y - X\hat{\beta}^{(t-1)})$$

Tikhonov Regularization Derivation (1/2)

Treat the true parameters θ_j as random variables Θ_j with the following distribution (**prior**):

$$\Theta_j \sim \mathcal{N}(0, \sigma_\Theta), \quad j = 1, \ldots, p$$

Then the **joint likelihood of the data and the parameters** is

$$L_{\mathcal{D},\Theta}(\theta) := \left(\prod_{n=1}^{N} p(x_n, y_n \,|\, \theta) \right) \prod_{j=1}^{p} p(\Theta_j = \theta_j)$$

and the conditional joint log likelihood of the data and the parameters

$$\log L^{\text{cond}}_{\mathcal{D},\Theta}(\theta) := \left(\sum_{n=1}^{N} \log p(y_n \,|\, x_n, \theta) \right) + \sum_{j=1}^{p} \log p(\Theta_j = \theta_j)$$

and

$$\log p(\Theta_j = \theta_j) = \log \frac{1}{\sqrt{2\pi}\sigma_\Theta} e^{-\frac{\theta_j^2}{2\sigma_\Theta^2}} = -\log(\sqrt{2\pi}\sigma_\Theta) - \frac{\theta_j^2}{2\sigma_\Theta^2}$$

Tikhonov Regularization Derivation (2/2)

Dropping the terms that do not depend on θ_j yields:

$$\log L^{\text{cond}}_{\mathcal{D},\Theta}(\theta) := \left(\sum_{n=1}^{N} \log p(y_n \mid x_n, \theta)\right) + \sum_{j=1}^{p} \log p(\Theta_j = \theta_j)$$

$$\propto \left(\sum_{n=1}^{N} \log p(y_n \mid x_n, \theta)\right) - \frac{1}{2\sigma^2_\Theta} \sum_{j=1}^{p} \theta_j^2$$

This also gives a semantics to the complexity / regularization weight λ:

$$\lambda = \frac{1}{2\sigma^2_\Theta}$$

but σ^2_Θ is unknown. (We will see methods to estimate λ soon.)

The parameters θ that maximize the joint likelihood of

- the data and
- the parameters

are called **Maximum Aposteriori Estimators (MAP estimators)**.

L2-Regularized Logistic Regression (Gradient Descent)

learn-reglogreg-GA$(\mathcal{D}^{\text{train}} := \{(x_1, y_1), \ldots, (x_N, y_N)\}, \lambda, \mu, t_{\max} \in \mathbb{N}, \epsilon \in \mathbb{R}^+)$:

$\ell := \frac{1}{N} \log L_{\mathcal{D}}^{\text{cond}}(\hat{\beta}) := \frac{1}{N} \sum_{n=1}^{N} y_n \langle x_n, \hat{\beta} \rangle - \log(1 + e^{\langle x_n, \hat{\beta} \rangle}) + \lambda \hat{\beta}^T \hat{\beta}$

$\hat{\beta} := \text{maximize-GA}(\ell, 0_M, \mu, t_{\max}, \epsilon)$

return $\hat{\beta}$

L2-Regularized Logistic Regression (Gradient Descent)

learn-logreg-GA$(\mathcal{D}^{\text{train}} := \{(x_1, y_1), \ldots, (x_N, y_N)\}, \lambda, \mu, t_{\max} \in \mathbb{N}, \epsilon \in \mathbb{R}^+)$:

$X := (x_1, x_2, \ldots, x_N)^T$

$y := (y_1, y_2, \ldots, y_N)^T$

$\hat{\beta} := 0_M$

$\ell := \frac{1}{N} \sum_{n=1}^{N} y_n \langle x_n, \hat{\beta} \rangle - \log(1 + e^{\langle x_n, \hat{\beta} \rangle})$

for $t = 1, \ldots, t_{\max}$:

$\hat{y} := (1/(1 + e^{-\hat{\beta}^T x_n})_{n \in 1:N}$

$\hat{\beta} := \hat{\beta} + \mu \cdot (\frac{1}{N} X^T (y - \hat{y}) - 2\lambda\hat{\beta})$

$\ell^{\text{old}} := \ell$

$\ell := \frac{1}{N} \sum_{n=1}^{N} y_n \langle x_n, \hat{\beta} \rangle - \log(1 + e^{\langle x_n, \hat{\beta} \rangle})$

if $\ell - \ell^{\text{old}} < \epsilon$:

return $\hat{\beta}$

raise exception "not converged in $t_{\max}$ iterations"

L2-Regularized Logistic Regression (Newton)

Newton update rule:

$$\hat{\beta}^{(t+1)} := \hat{\beta}^{(t)} + \mu (H^{(t)})^{-1} \nabla_{\hat{\beta}} (L_{\mathcal{D}}^{\text{cond}})^{(t)}$$

$$(\nabla_{\hat{\beta}} L_{\mathcal{D}}^{\text{cond}})^{(t)} = \begin{pmatrix} \sum_{n=1}^{N} \left(y_n - \hat{y}_n^{(t)} \right) \\ \sum_{n=1}^{N} x_{n,1} \left(y_n - \hat{y}_n^{(t)} \right) - 2\lambda \hat{\beta}_1^{(t)} \\ \vdots \\ \sum_{n=1}^{N} x_{n,M} \left(y_n - \hat{y}_n^{(t)} \right) - 2\lambda \hat{\beta}_M^{(t)} \end{pmatrix}$$

$$H^{(t)} = \sum_{n=1}^{N} -\hat{y}_n^{(t)} \left(1 - \hat{y}_n^{(t)} \right) x_n x_n^T - 2\lambda I$$

Outline

What is Hyperparameter Optimization?

- Most models and learning algorithms have parameters that cannot be learned by minimizing the objective function, because either
  - the objective function would be minimized for a trivial value, e.g., $\lambda = 0$, or
  - the parameters affect the learning algorithm, e.g., learning rate.

- These parameters are called **hyperparameters** λ and they parametrize a **learning algorithm** $\mathcal{A}_\lambda$.
  - choose suitable hyperparameters λ
  - use $\mathcal{A}_\lambda$ to map the training data $\mathcal{D}_{\text{train}}$ to a prediction function $\hat{y}$ by minimizing some loss $\mathcal{L}(\mathcal{D}, \hat{y})$ over the training data.

What is Hyperparameter Optimization?

- Identifying good values for the hyperparameters λ is called **hyperparameter optimization**.
  - hyperparameter optimization is a second level optimization

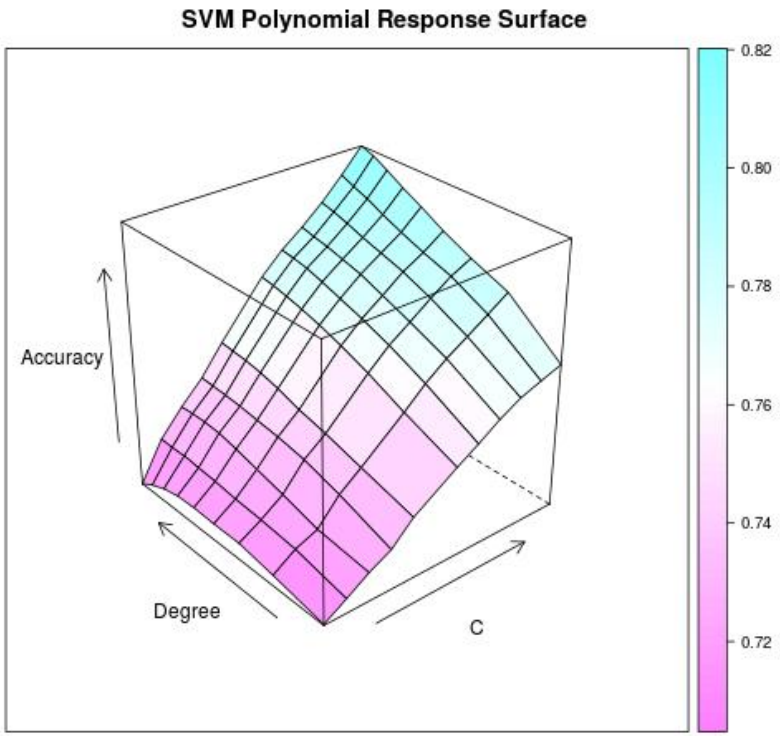
$$\arg\min_{\lambda \in \Lambda} \mathcal{L}(\mathcal{D}_{\text{valid}}, \mathcal{A}_\lambda(\mathcal{D}_{\text{train}})) = \arg\min_{\lambda \in \Lambda} \Psi(\lambda)$$

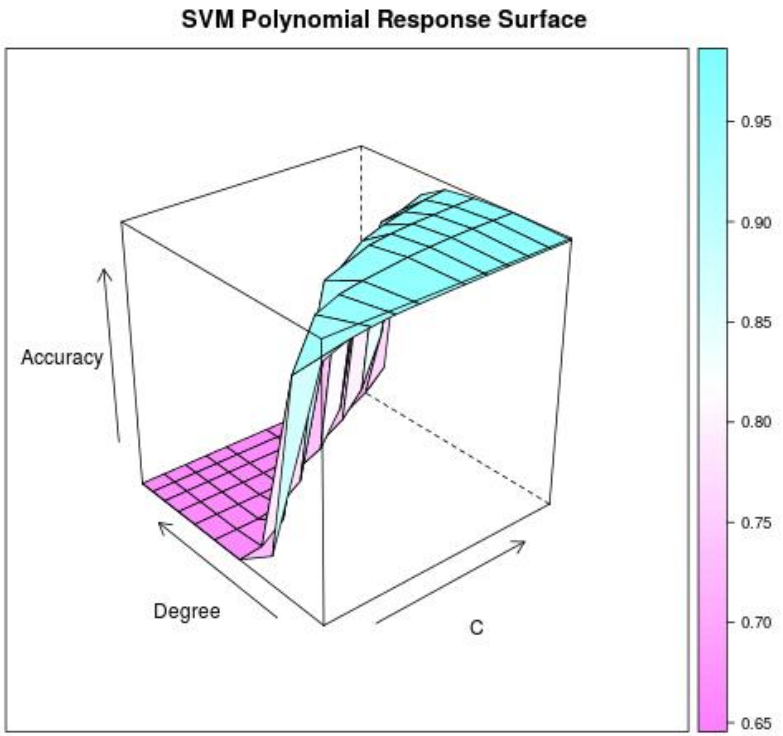
where

- Ψ is the **hyperparameter response function** and
- $\mathcal{D}_{\text{valid}}$ a **validation data** (aka **calibration data** and **holdout data**).

Why Hyperparameter Optimization

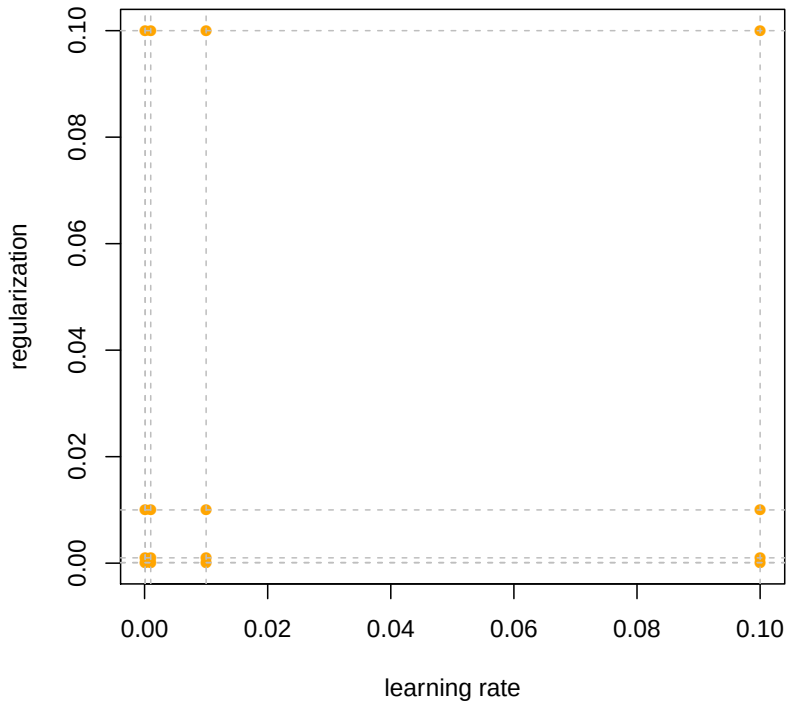
- So far only model parameters were optimized.
- Values for hyperparameters (such as regularization λ and learning rate μ) came "out of the blue".
- Hyperparameters can have a big impact on the prediction quality.





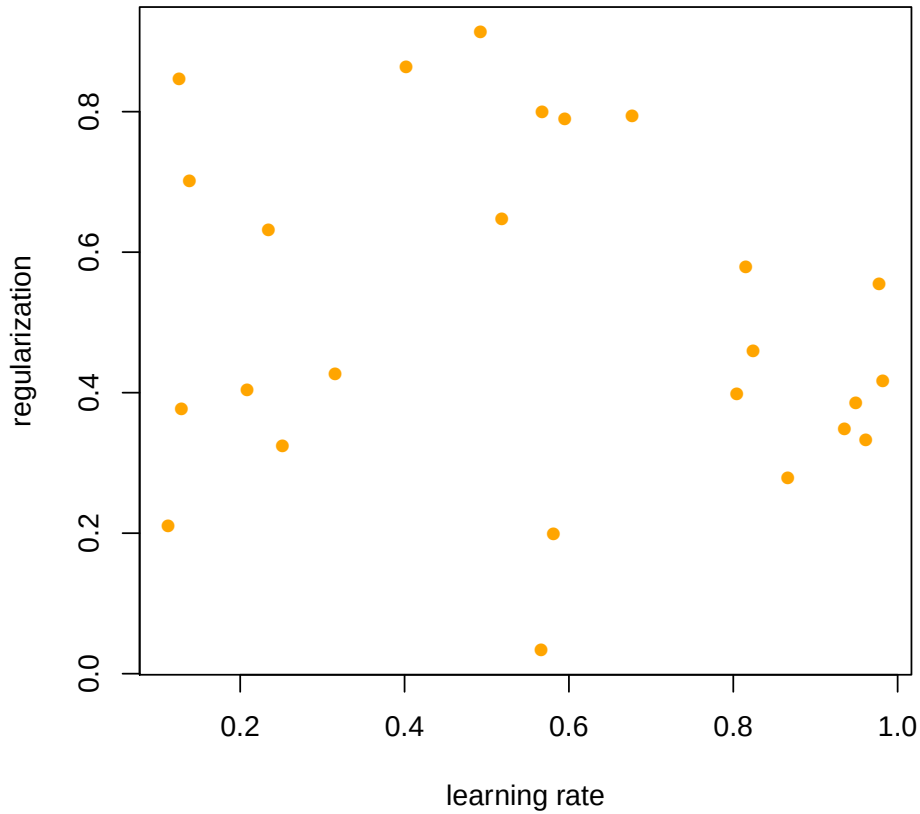
Grid Search

- Assume we have Q hyperparameters $\lambda_1, \ldots, \lambda_Q$
- Choose for each hyperparameter λ_q a set of values Λ_q.
- $\Lambda := \prod_{q=1}^{Q} \Lambda_q$ is then a grid of hyperparameters.
- Choose the hyperparameter combination $\lambda \in \Lambda$ with best performance on $\mathcal{D}_{\text{valid}}$.



Random Search

- Instead of trying hyperparameter combinations on a grid, try random hyperparameter combinations λ for Λ (within a reasonable range).
- Usually slightly better results than grid search.



What is the Validation Data?

- Whenever a learning process depends on a hyperparameter, the hyperparameter can be estimated by picking the value with the lowest error.
- If this is done on test data, one actually uses test data in the training process (**"train on test"**), thereby lessen its usefulness for estimating the test error.
- Therefore, one splits the training data again in
  - **(proper) training data** and
  - **validation data**.
- The validation data figures as test data during the training process.

Cross Validation

Instead of a single split into

training data, (validation data,) and test data

K-fold cross validation splits the data in K parts (of roughly equal size)

$$\mathcal{D} = \mathcal{D}_1 \cup \mathcal{D}_2 \cup \cdots \cup \mathcal{D}_K, \quad \mathcal{D}_k \text{ pairwise disjoint}$$

and averages performance over K learning problems

$$\mathcal{D}^{(k)}_{\text{train}} := \mathcal{D} \setminus \mathcal{D}_k, \quad \mathcal{D}^{(k)}_{\text{test}} := \mathcal{D}_k, \quad k = 1, \ldots, K$$

Common is 5- and 10-fold cross validation.

N-fold cross validation is also known as **leave one out**.

Cross Validation

How many folds to use in K-fold cross validation?

$K = N$ / leave one out:

- approximately unbiased for the true prediction error.
- high variance as the N training sets are very similar.
- in general computationally costly
  as N different models have to be learnt.

$K = 5$:

- lower variance.
- bias could be a problem,
  due to smaller training set size the prediction error could be overestimated.

Summary

- The problem of **underfitting** can be overcome by using more complex models, e.g., having
  - variable interactions as in polynomial models.
- The problem of **overfitting** can be overcome by
  - **model selection** / variable selection as well as by
  - (parameter) **shrinkage**.
- Applying L2-regularization to Linear and Logistic Regression requires only few changes in the learning algorithms.
- Shrinkage introduces a **hyperparameter** λ that cannot be learned by direct loss minimization.
- Estimating the best hyperparameters can be considered as a **meta-learning problem**. They can be estimated e.g. by
  - **Grid Search** or
  - Random Search — both using **validation data**.

Further Readings

- [James et al., 2013, chapter 3], [Murphy, 2012, chapter 7], [Hastie et al., 2005, chapter 3].

References

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