



Supervised Learning

All slides

July 20, 2021

INTRODUCTION TO MACHINE LEARNING

Advanced Risk Minimization

Multiclass Classification

Information Theory

Curse of Dimensionality

Hypothesis Space

Regularization

Linear Support Vector Machine

Nonlinear Support Vector Machine

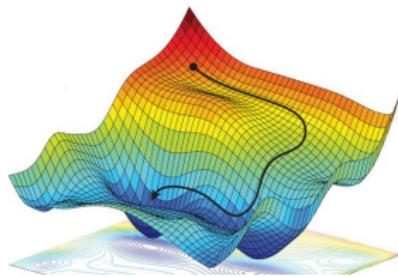
Gaussian Processes

Boosting

Introduction to Machine Learning

Risk Minimizers

Learning goals



- Know the concepts of the Bayes optimal model (also: risk minimizer, population minimizer)
- Bayes risk
- Consistent learners
- Bayes regret, estimation and approximation error
- Optimal constant model
- Proper scoring rules

RISK MINIMIZER

Our goal is to minimize the risk

$$\mathcal{R}_L(f) := \mathbb{E}_{xy}[L(y, f(\mathbf{x}))] = \int L(y, f(\mathbf{x})) d\mathbb{P}_{xy}.$$

for a certain hypothesis $f(\mathbf{x}) \in \mathcal{H}$ and a loss $L(y, f(\mathbf{x}))$.

NB: As \mathcal{R}_L depends on loss L , we sometimes make this explicit with a subscript if needed, and omit in other cases.

Let us assume we are in an “ideal world”:

- The hypothesis space \mathcal{H} is unrestricted. We can choose any $f : \mathcal{X} \rightarrow \mathbb{R}^g$.
- We also assume an ideal optimizer; the risk minimization can always be solved perfectly and efficiently.
- We know \mathbb{P}_{xy} .

How should f be chosen?

RISK MINIMIZER

The f with minimal risk across all (measurable) functions is called the **risk minimizer, population minimizer or Bayes optimal model**.

$$\begin{aligned} f^* &= \arg \min_{f: \mathcal{X} \rightarrow \mathbb{R}^g} \mathcal{R}_L(f) = \arg \min_{f: \mathcal{X} \rightarrow \mathbb{R}^g} \mathbb{E}_{xy} [L(y, f(\mathbf{x}))] \\ &= \arg \min_{f: \mathcal{X} \rightarrow \mathbb{R}^g} \int L(y, f(\mathbf{x})) d\mathbb{P}_{xy}. \end{aligned}$$

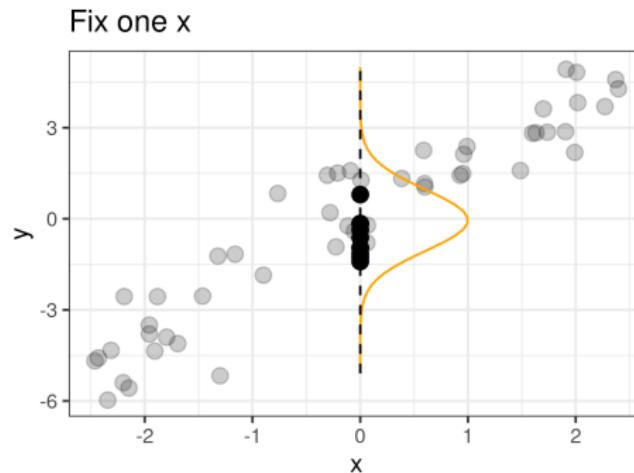
The resulting risk is called **Bayes risk**

$$\mathcal{R}_L^* = \inf_{f: \mathcal{X} \rightarrow \mathbb{R}^g} \mathcal{R}_L(f)$$

OPTIMAL POINT-WISE PREDICTIONS

To derive the risk minimizer we usually make use of the following trick:

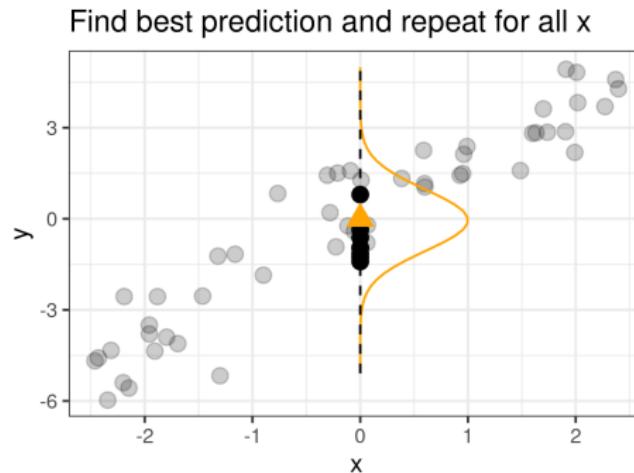
- We can choose $f(\mathbf{x})$ as we want (unrestricted hypothesis space, no assumed functional form)
- Consequently, for a fixed value $\mathbf{x} \in \mathcal{X}$ we can select **any** value c we want to predict
- So we construct the **point-wise optimizer** for every $\mathbf{x} \in \mathcal{X}$.



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- So we construct the **point-wise optimizer** for every $\mathbf{x} \in \mathcal{X}$.



THEORETICAL AND EMPIRICAL RISK

The risk minimizer is mainly a theoretical tool:

- In practice we need to restrict the hypothesis space \mathcal{H} such that we can efficiently search over it.
- In practice we (usually) do not know \mathbb{P}_{xy} . Instead of $\mathcal{R}(f)$, we are optimizing the empirical risk

$$\hat{f} = \arg \min_{f \in \mathcal{H}} \mathcal{R}_{\text{emp}}(f) = \arg \min_{f \in \mathcal{H}} \sum_{i=1}^n L\left(y^{(i)}, f\left(\mathbf{x}^{(i)}\right)\right)$$

Note that according to the **law of large numbers** (LLN), the empirical risk converges to the true risk (but beware of overfitting!):

$$\bar{\mathcal{R}}_{\text{emp}}(f) = \frac{1}{n} \sum_{i=1}^n L\left(y^{(i)}, f\left(\mathbf{x}^{(i)}\right)\right) \xrightarrow{n \rightarrow \infty} \mathcal{R}(f).$$

ESTIMATION AND APPROXIMATION ERROR

Goal of learning: Train a model \hat{f} for which the true risk $\mathcal{R}_L(\hat{f})$ is close to the Bayes risk \mathcal{R}_L^* . In other words, we want the **Bayes regret**

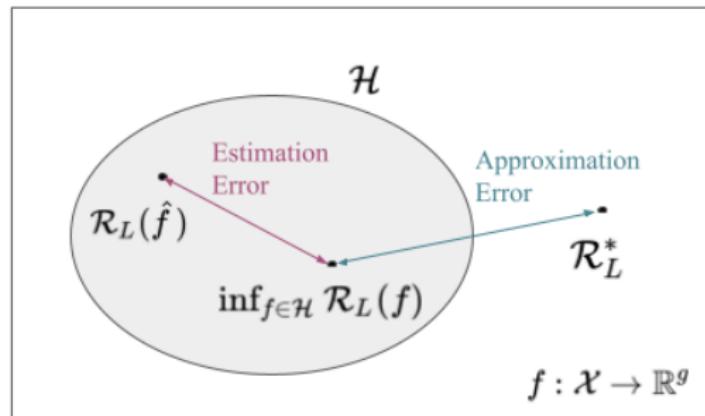
$$\mathcal{R}_L(\hat{f}) - \mathcal{R}_L^*$$

to be as low as possible.

The Bayes regret can be decomposed as follows:

$$\mathcal{R}_L(\hat{f}) - \mathcal{R}_L^* = \underbrace{\left[\mathcal{R}_L(\hat{f}) - \inf_{f \in \mathcal{H}} \mathcal{R}_L(f) \right]}_{\text{estimation error}} + \underbrace{\left[\inf_{f \in \mathcal{H}} \mathcal{R}_L(f) - \mathcal{R}_L^* \right]}_{\text{approximation error}}$$

ESTIMATION AND APPROXIMATION ERROR



- $\mathcal{R}_L(\hat{f}) - \inf_{f \in \mathcal{H}} \mathcal{R}_L(f)$ is the **estimation error**. We fit \hat{f} via empirical risk minimization and (usually) use approximate optimization, so we usually do not find the optimal $f \in \mathcal{H}$.
- $\inf_{f \in \mathcal{H}} \mathcal{R}_L(f) - \mathcal{R}_L^*$ is the **approximation error**. We need to restrict to a hypothesis space \mathcal{H} which might not even contain the Bayes optimal model f^* .

(UNIVERSALLY) CONSISTENT LEARNERS

Consistency is an asymptotic property of a learning algorithm, which ensures the algorithm returns **the correct model** when given **unlimited data**.

Let $\mathcal{I} : \mathbb{D} \times \Lambda \rightarrow \mathcal{H}$ be a learning algorithm^(*) that takes a training set $\mathcal{D}_{\text{train}} \sim \mathbb{P}_{xy}$ of size n_{train} and estimates a model $\hat{f} : \mathcal{X} \rightarrow \mathbb{R}^g$.

The learning method \mathcal{I} is said to be **consistent** w.r.t. a certain distribution \mathbb{P}_{xy} if the risk of the estimated model \hat{f} converges in probability (" \xrightarrow{p} ") to the Bayes risk \mathcal{R}^* when n_{train} goes to ∞ :

$$\mathcal{R}(\mathcal{I}(\mathcal{D}_{\text{train}}, \lambda)) \xrightarrow{p} \mathcal{R}_L^* \quad \text{for } n_{\text{train}} \rightarrow \infty.$$

(*) $\lambda \in \Lambda$ denotes hyperparameters of the learning algorithm.

(UNIVERSALLY) CONSISTENT LEARNERS

Consistency is defined w.r.t. a particular distribution \mathbb{P}_{xy} . But since we usually do not know \mathbb{P}_{xy} , consistency does not offer much help to choose an algorithm for a particular task.

More interesting is the stronger concept of **universal consistency**: An algorithm is universally consistent if it is consistent for **any** distribution.

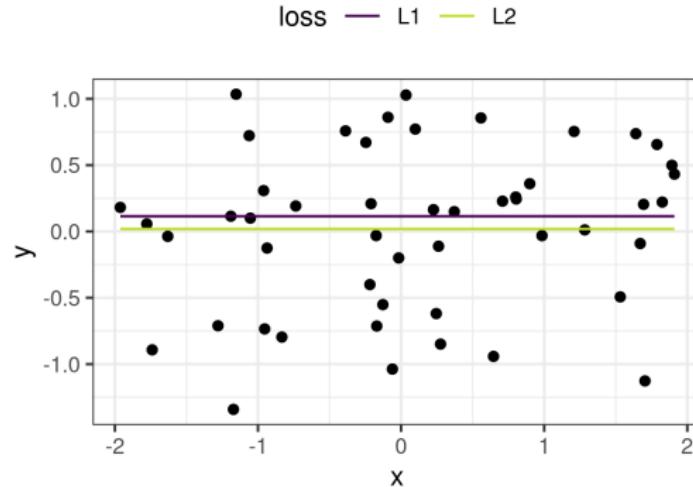
In Stone's famous consistency theorem from 1977, the universal consistency of a weighted average estimator as KNN was proven. Many other ML models have since then been proven to be universally consistent (SVMs, ANNs, etc.).

Note that universal consistency is obviously a desirable property - however, (universal) consistency does not tell us anything about convergence rates ...

OPTIMAL CONSTANT MODEL

While the risk minimizer gives us the (theoretical) optimal solution, the **optimal constant model** (also: featureless predictor) gives us an computable empirical lower baseline solution.

The constant model is the model $f(\mathbf{x}) = \theta$ that optimizes the empirical risk $\mathcal{R}_{\text{emp}}(\theta)$.



RISK MINIMIZER AND OPTIMAL CONSTANT

Later, we will derive risk minimizers for various losses.

Name	Risk Minimizer	Optimal Constant
L2	$f^*(\mathbf{x}) = \mathbb{E}_{y \mathbf{x}} [y \mathbf{x}]$	$\hat{f}(\mathbf{x}) = \frac{1}{n} \sum_{i=1}^n y^{(i)}$
L1	$f^*(\mathbf{x}) = \text{med}_{y \mathbf{x}} [y \mathbf{x}]$	$\hat{f}(\mathbf{x}) = \text{med}(y^{(i)})$
0-1	$h^*(\mathbf{x}) = \arg \max_{l \in \mathcal{Y}} \mathbb{P}(y = l \mathbf{x})$	$\hat{h}(\mathbf{x}) = \text{mode} \left\{ y^{(i)} \right\}$
Brier	$\pi^*(\mathbf{x}) = \mathbb{P}(y = 1 \mathbf{x} = \mathbf{x})$	$\hat{\pi}(\mathbf{x}) = \frac{1}{n} \sum_{i=1}^n y^{(i)}$
Bernoulli (on probs)	$\pi^*(\mathbf{x}) = \mathbb{P}(y = 1 \mathbf{x} = \mathbf{x})$	$\hat{\pi}(\mathbf{x}) = \frac{1}{n} \sum_{i=1}^n y^{(i)}$
Bernoulli (on scores)	$f^*(\mathbf{x}) = \log \left(\frac{\mathbb{P}(y=1 \mathbf{x})}{1 - \mathbb{P}(y=1 \mathbf{x})} \right)$	$\hat{f}(\mathbf{x}) = \log \frac{n+1}{n-1}$

We see: For regression, the RMs model the conditional expectation and median of the underlying distribution. This makes intuitive sense, depending on your concept of how to best estimate central location / how robust this location should be.

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For the 0-1 loss, we use the risk minimizer to construct the **optimal Bayes decision rule**: We predict the class with maximal posterior probability.

RISK MINIMIZER AND OPTIMAL CONSTANT

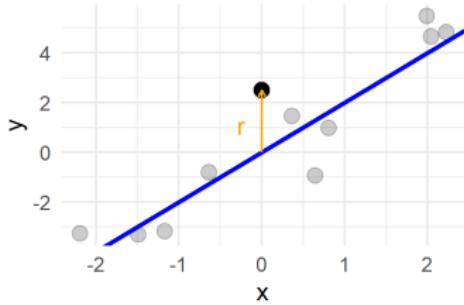
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For Brier and Bernoulli, we predict the posterior probabilities (of the true DGP!). Losses that have this desirable property are called **proper scoring (rules)**.

Introduction to Machine Learning

Pseudo-Residuals and Gradient Descent



Learning goals

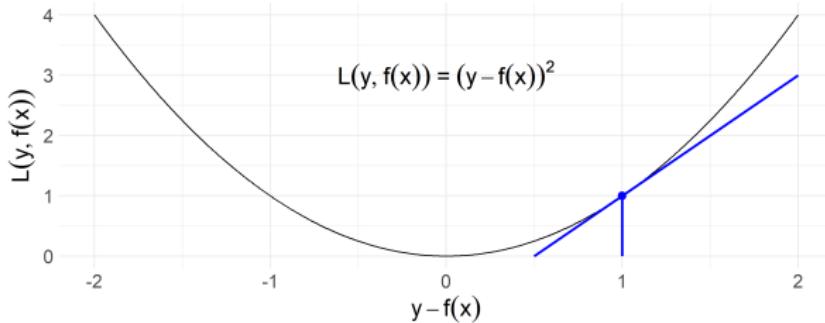
- Know the concept of pseudo-residuals
- Understand the relationship between pseudo-residuals and gradient descent

PSEUDO-RESIDUALS

- In regression, residuals are defined as $r := y - f(\mathbf{x})$.
- We further define **pseudo-residuals** as the negative first derivatives of loss functions w.r.t. $f(\mathbf{x})$

$$\tilde{r} := -\frac{\partial L(y, f(\mathbf{x}))}{\partial f(\mathbf{x})}.$$

- This definition also holds for score / probability based classifiers.
- Note that \tilde{r} depends on y and $f(\mathbf{x})$ and L .

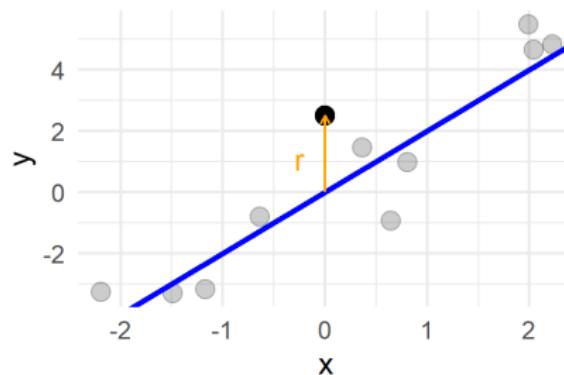


BEST POINT-WISE UPDATE

Assume we have (partially) fitted a model $f(\mathbf{x})$ to data \mathcal{D} .

Assume we could update $f(\mathbf{x})$ point-wise as we like. For a fixed $\mathbf{x} \in \mathcal{X}$, the best point-wise update is the direction of the residual $r = y - f(\mathbf{x})$

$$f(\mathbf{x}) \leftarrow f(\mathbf{x}) + r$$



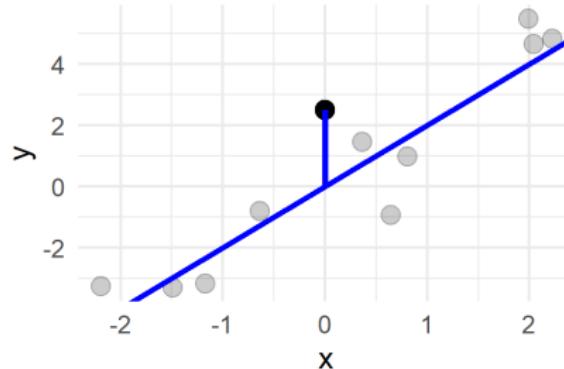
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$$f(\mathbf{x}) \leftarrow f(\mathbf{x}) + r$$

The point-wise error at this specific \mathbf{x} becomes 0.



APPROXIMATE BEST POINT-WISE UPDATE

When applying gradient descent to compute a point-wise update of $f(\mathbf{x})$, we would go a step into the direction of the negative gradient

$$f(\mathbf{x}) \leftarrow f(\mathbf{x}) - \frac{\partial L(y, f(\mathbf{x}))}{\partial f(\mathbf{x})}.$$

which is the direction of the pseudo-residual

$$f(\mathbf{x}) \leftarrow f(\mathbf{x}) + \tilde{r}$$

Iteratively stepping towards the direction of the pseudo-residuals is the underlying idea of gradient boosting, which is a learning algorithm that will be covered in a later chapter.

GD IN ML AND PSEUDO-RESIDUALS

- In GD, we move in the direction of the negative gradient by updating the parameters:

$$\boldsymbol{\theta}^{[t+1]} = \boldsymbol{\theta}^{[t]} - \alpha^{[t]} \cdot \nabla_{\boldsymbol{\theta}} \mathcal{R}_{\text{emp}}(\boldsymbol{\theta})|_{\boldsymbol{\theta}=\boldsymbol{\theta}^{[t]}}$$

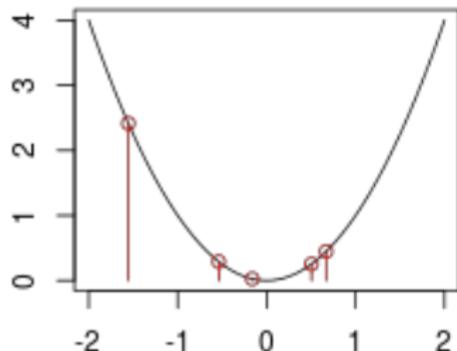
- This can be seen as approximating the unexplained information (measured by the loss) through a model update.
- Using the chain rule:

$$\begin{aligned}\nabla_{\boldsymbol{\theta}} \mathcal{R}_{\text{emp}}(\boldsymbol{\theta}) &= \sum_{i=1}^n \frac{\partial L(y^{(i)}, f)}{\partial f} \Bigg|_{f=f(\mathbf{x}^{(i)} | \boldsymbol{\theta})} \cdot \nabla_{\boldsymbol{\theta}} f(\mathbf{x}^{(i)} | \boldsymbol{\theta}) \\ &= - \sum_{i=1}^n \tilde{r}^{(i)} \cdot \nabla_{\boldsymbol{\theta}} f(\mathbf{x}^{(i)} | \boldsymbol{\theta}).\end{aligned}$$

- Hence the update is determined by a loss-optimal directional change of the model output and a loss-independent derivate of f . This is a very flexible, nearly loss-independent formulation of GD.

Introduction to Machine Learning

Regression Losses: L2-loss



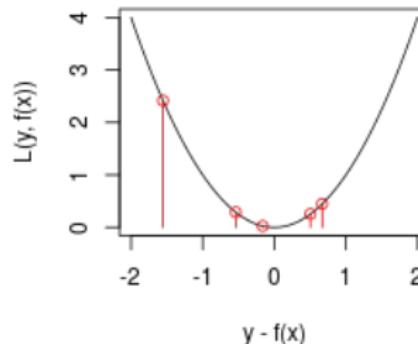
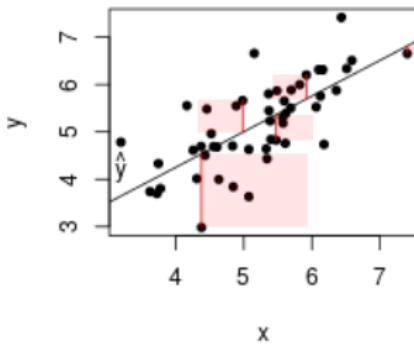
Learning goals

- Derive the risk minimizer of the L2-loss
- Derive the optimal constant model for the L2-loss

L2-LOSS

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

- Tries to reduce large residuals (if residual is twice as large, loss is 4 times as large), hence outliers in y can become problematic
- Analytic properties: convex, differentiable (gradient no problem in loss minimization)
- Residuals = Pseudo-residuals: $\tilde{r} = -\frac{\partial 0.5(y-f(\mathbf{x}))^2}{\partial f(\mathbf{x})} = y - f(\mathbf{x}) = r$



L2-LOSS: RISK MINIMIZER

Let us consider the (true) risk for $\mathcal{Y} = \mathbb{R}$ and the L2-Loss

$L(y, f(\mathbf{x})) = (y - f(\mathbf{x}))^2$ with unrestricted $\mathcal{H} = \{f : \mathcal{X} \rightarrow \mathbb{R}^g\}$.

- By the law of total expectation

$$\begin{aligned}\mathcal{R}(f) &= \mathbb{E}_{xy} [L(y, f(\mathbf{x}))] \\ &= \mathbb{E}_x [\mathbb{E}_{y|x} [L(y, f(\mathbf{x})) \mid \mathbf{x} = \mathbf{x}]] \\ &= \mathbb{E}_x [\mathbb{E}_{y|x} [(y - f(\mathbf{x}))^2 \mid \mathbf{x} = \mathbf{x}]].\end{aligned}$$

- Since \mathcal{H} is unrestricted we can choose f as we wish: At any point $\mathbf{x} = \mathbf{x}$ we can predict any value c we want. The best point-wise prediction is the conditional mean

$$\hat{f}(\mathbf{x}) = \operatorname{argmin}_c \mathbb{E}_{y|x} [(y - c)^2 \mid \mathbf{x} = \mathbf{x}] \stackrel{(*)}{=} \mathbb{E}_{y|x} [y \mid \mathbf{x}].$$

L2-LOSS: RISK MINIMIZER

(*) follows from:

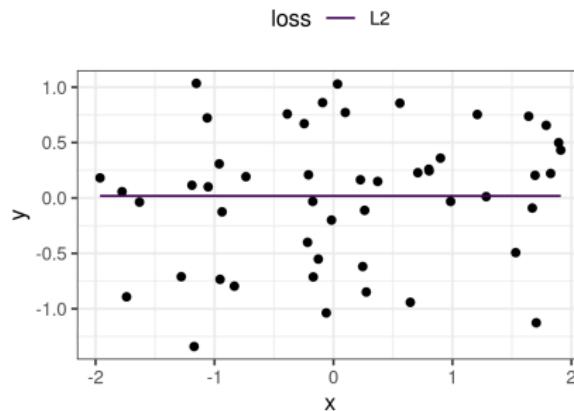
$$\begin{aligned}\operatorname{argmin}_c \mathbb{E} [(y - c)^2] &= \operatorname{argmin}_c \underbrace{\mathbb{E} [(y - c)^2] - (\mathbb{E}[y] - c)^2}_{=\text{Var}[y-c]=\text{Var}[y]} + (\mathbb{E}[y] - c)^2 \\ &= \operatorname{argmin}_c \text{Var}[y] + (\mathbb{E}[y] - c)^2 = \mathbb{E}[y].\end{aligned}$$

L2-LOSS: OPTIMAL CONSTANT MODEL

The optimal constant model in terms of the (theoretical) risk for the L2 loss is the expected value over y :

$$f(\mathbf{x}) = \mathbb{E}_{y | \mathbf{x}} [y | \mathbf{x}] \stackrel{\text{drop } \mathbf{x}}{=} \mathbb{E}_y [y]$$

The optimizer of the empirical risk is \bar{y} (the empirical mean over $y^{(i)}$), which is the empirical estimate for $\mathbb{E}_y [y]$.



L2-LOSS: OPTIMAL CONSTANT MODEL

Proof:

For the optimal constant model $f(\mathbf{x}) = \theta$ for the L2-loss $L(y, f(\mathbf{x})) = (y - f(\mathbf{x}))^2$ we solve the optimization problem

$$\arg \min_{f \in \mathcal{H}} \mathcal{R}_{\text{emp}}(f) = \arg \min_{c \in \mathbb{R}} \sum_{i=1}^n (y^{(i)} - \theta)^2.$$

We calculate the first derivative of \mathcal{R}_{emp} w.r.t. θ and set it to 0:

$$\frac{\partial \mathcal{R}_{\text{emp}}(\theta)}{\partial \theta} = 2 \sum_{i=1}^n (y^{(i)} - \theta) \stackrel{!}{=} 0$$

$$\sum_{i=1}^n y^{(i)} - n\theta = 0$$

$$\hat{\theta} = \frac{1}{n} \sum_{i=1}^n y^{(i)} =: \bar{y}.$$

L2 LOSS MEANS MINIMIZING VARIANCE

Rethinking what we just did: We optimized for the constant, whose squared distance to all data points is minimal (in sum, or on average). This turned out to be the mean.

What happens if we calculate the incurred loss of $\hat{\theta} = \bar{y}$

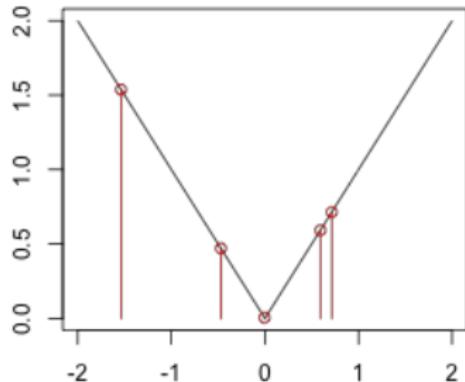
That's obviously $\mathcal{R}_{\text{emp}} = \sum_{i=1}^n (y^{(i)} - \bar{y})^2$.

Average this sum by $\frac{1}{n}$ or $\frac{1}{n-1}$, and we get the empirical variance.

The same holds true for the pointwise construction / conditional distribution as considered in the slides before.

Introduction to Machine Learning

Regression Losses: L1-loss



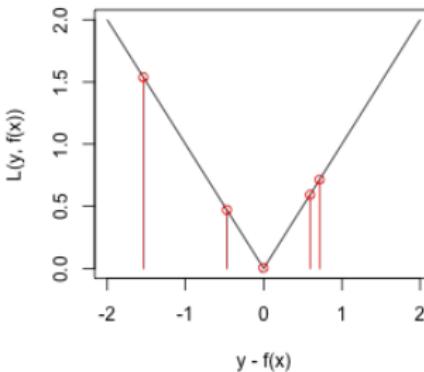
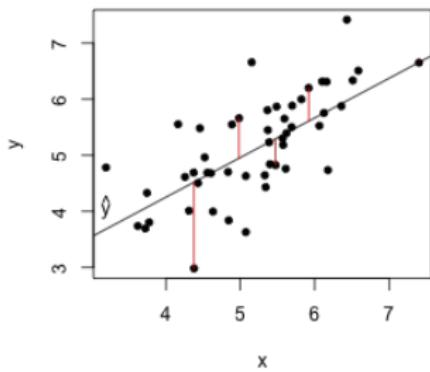
Learning goals

- Derive the risk minimizer of the L1-loss
- Derive the optimal constant model for the L1-loss

L1-LOSS

$$L(y, f(\mathbf{x})) = |y - f(\mathbf{x})|$$

- More robust than L_2 , outliers in y are less problematic.
- Analytical properties: convex, not differentiable for $y = f(\mathbf{x})$ (optimization becomes harder).



L1-LOSS: RISK MINIMIZER

We calculate the (true) risk for the L1-Loss $L(y, f(\mathbf{x})) = |y - f(\mathbf{x})|$ with unrestricted $\mathcal{H} = \{f : \mathcal{X} \rightarrow \mathcal{Y}\}$.

- We use the law of total expectation

$$\mathcal{R}(f) = \mathbb{E}_{\mathbf{x}} [\mathbb{E}_{y|\mathbf{x}} [|y - f(\mathbf{x})| \mid \mathbf{x} = \mathbf{x}]] .$$

- As the functional form of f is not restricted, we can just optimize point-wise at any point $\mathbf{x} = \mathbf{x}$. The best prediction at $\mathbf{x} = \mathbf{x}$ is then

$$\hat{f}(\mathbf{x}) = \operatorname{argmin}_c \mathbb{E}_{y|\mathbf{x}} [|y - c|] = \operatorname{med}_{y|\mathbf{x}} [y \mid \mathbf{x}] .$$

L1-LOSS: RISK MINIMIZER

Proof: Let $p(y)$ be the density function of y . Then:

$$\begin{aligned} \operatorname{argmin}_c \mathbb{E}[|y - c|] &= \operatorname{argmin}_c \int_{-\infty}^{\infty} |y - c| p(y) dy \\ &= \operatorname{argmin}_c \int_{-\infty}^c -(y - c) p(y) dy + \int_c^{\infty} (y - c) p(y) dy \end{aligned}$$

We now compute the derivative of the above term and set it to 0

$$\begin{aligned} 0 &= \frac{\partial}{\partial c} \left(\int_{-\infty}^c -(y - c) p(y) dy + \int_c^{\infty} (y - c) p(y) dy \right) \\ &\stackrel{* \text{ Leibniz}}{=} \int_{-\infty}^c p(y) dy - \int_c^{\infty} p(y) dy = \mathbb{P}_y(y \leq c) - (1 - \mathbb{P}_y(y \leq c)) \\ &= 2 \cdot \mathbb{P}_y(y \leq c) - 1 \\ \Leftrightarrow 0.5 &= \mathbb{P}_y(y \leq c), \end{aligned}$$

which yields $c = \operatorname{med}_y(y)$.

L1-LOSS: RISK MINIMIZER

* Note that since we are computing the derivative w.r.t. the integration boundaries, we need to use Leibniz integration rule

$$\begin{aligned}\frac{\partial}{\partial c} \left(\int_a^c g(c, y) dy \right) &= g(c, c) + \int_a^c \frac{\partial}{\partial c} g(c, y) dy \\ \frac{\partial}{\partial c} \left(\int_c^a g(c, y) dy \right) &= -g(c, c) + \int_c^a \frac{\partial}{\partial c} g(c, y) dy\end{aligned}$$

We get

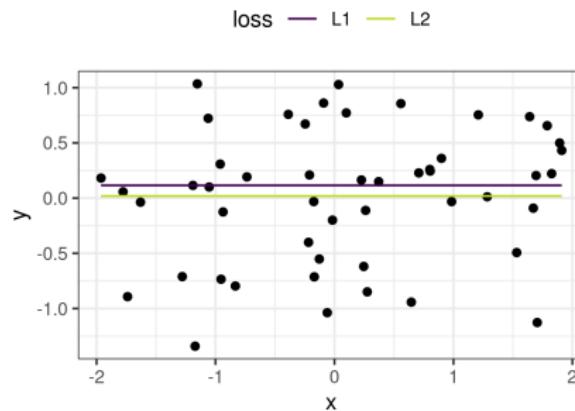
$$\begin{aligned}& \frac{\partial}{\partial c} \left(\int_{-\infty}^c -(y - c) p(y) dy + \int_c^{\infty} (y - c) p(y) dy \right) \\&= \frac{\partial}{\partial c} \left(\int_{-\infty}^c \underbrace{-(y - c) p(y)}_{g_1(c, y)} dy \right) + \frac{\partial}{\partial c} \left(\int_c^{\infty} \underbrace{(y - c) p(y)}_{g_2(c, y)} dy \right) \\&= \underbrace{g_1(c, c)}_{=0} + \int_{-\infty}^c \frac{\partial}{\partial c}(-(y - c)) p(y) dy - \underbrace{g_2(c, c)}_{=0} + \int_c^{\infty} \frac{\partial}{\partial c}(y - c) p(y) dy \\&= \int_{-\infty}^c p(y) dy + \int_c^{\infty} -p(y) dy.\end{aligned}$$

L1-LOSS: OPTIMAL CONSTANT MODEL

The optimal constant model in terms of the theoretical risk for the L1 loss is the median over y :

$$f(\mathbf{x}) = \text{med}_{y|x} [y | \mathbf{x}] \stackrel{\text{drop } \mathbf{x}}{=} \text{med}_y [y]$$

The optimizer of the empirical risk is $\text{med}(y^{(i)})$ over $y^{(i)}$, which is the empirical estimate for $\text{med}_y [y]$.



L1-LOSS: OPTIMAL CONSTANT MODEL

Proof:

- Firstly note that for $n = 1$ the median $\hat{\theta} = \text{med}(y^{(i)}) = y^{(1)}$ obviously minimizes the empirical risk \mathcal{R}_{emp} associated to the L1 loss L .
- Hence let $n > 1$ in the following: Let

$$S_{a,b} : \mathbb{R} \rightarrow \mathbb{R}_0^+, \theta \mapsto |a - \theta| + |b - \theta|$$

for $a, b \in \mathbb{R}$. It holds that

$$S_{a,b}(\theta) = \begin{cases} |a - b|, & \text{for } \theta \in [a, b] \\ |a - b| + 2 \cdot \min\{|a - \theta|, |b - \theta|\}, & \text{otherwise.} \end{cases}$$

Thus, any $\hat{\theta} \in [a, b]$ minimizes $S_{a,b}$.

L1-LOSS: OPTIMAL CONSTANT MODEL

W.l.o.g. assume now that all $y^{(i)}$ are sorted in increasing order.

Let us define $i_{\max} = n/2$ for n even and $i_{\max} = (n - 1)/2$ for n odd and consider the intervals

$$\mathcal{I}_i := [y^{(i)}, y^{(n+1-i)}], i \in \{1, \dots, i_{\max}\}.$$

By construction $\mathcal{I}_{j+1} \subseteq \mathcal{I}_j$ for $j \in \{1, \dots, i_{\max} - 1\}$ and $\mathcal{I}_{i_{\max}} \subseteq \mathcal{I}_i$. With this, \mathcal{R}_{emp} can be expressed as

$$\begin{aligned}\mathcal{R}_{\text{emp}}(\theta) &= \sum_{i=1}^n L(y^{(i)}, \theta) = \sum_{i=1}^n |y^{(i)} - \theta| \\ &= \underbrace{|y^{(1)} - \theta| + |y^{(n)} - \theta|}_{=S_{y^{(1)}, y^{(n)}}(\theta)} + \underbrace{|y^{(2)} - \theta| + |y^{(n-1)} - \theta| + \dots}_{=S_{y^{(2)}, y^{(n-1)}}(\theta)} + \dots \\ &= \begin{cases} \sum_{i=1}^{i_{\max}} S_{y^{(i)}, y^{(n+1-i)}}(\theta) & \text{for } n \text{ is even} \\ \sum_{i=1}^{i_{\max}} (S_{y^{(i)}, y^{(n+1-i)}}(\theta)) + |y^{((n+1)/2)} - \theta| & \text{for } n \text{ is odd.} \end{cases}\end{aligned}$$

L1-LOSS: OPTIMAL CONSTANT MODEL

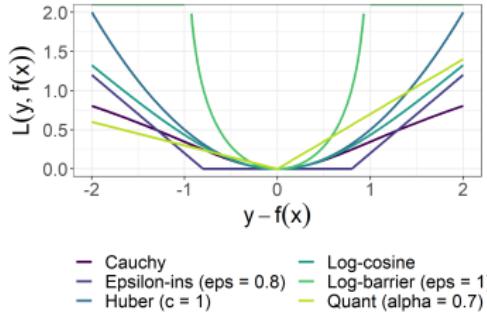
From this follows that

- for “ n is even”: $\hat{\theta} \in \mathcal{I}_{i_{\max}} = [y^{(n/2)}, y^{(n/2+1)}]$ minimizes S_i for all $i \in \{1, \dots, i_{\max}\}$ \Rightarrow it minimizes \mathcal{R}_{emp} ,
- for “ n is odd”: $\hat{\theta} = y^{((n+1)/2)} \in \mathcal{I}_{i_{\max}}$ minimizes S_i for all $i \in \{1, \dots, i_{\max}\}$ and its minimal for $|y^{((n+1)/2)} - \theta|$ \Rightarrow it minimizes \mathcal{R}_{emp} ,

Since the median fulfills these conditions, we can conclude that it minimizes the $L1$ loss.

Introduction to Machine Learning

Advanced Regression Losses



Learning goals

- Know the Huber loss
- Know the log-cosh loss
- Know the Cauchy loss
- Know the log-barrier loss
- Know the ϵ -insensitive loss
- Know the quantile loss

ADVANCED LOSS FUNCTIONS

Special loss functions can be used to estimate non-standard posterior components, to measure errors in a custom way or are designed to have special properties like robustness.

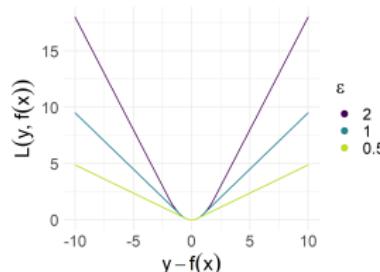
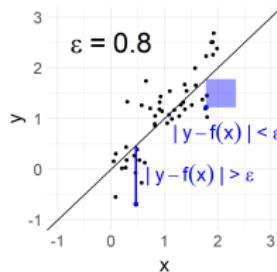
Examples:

- Quantile loss: Overestimating a clinical parameter might not be as bad as underestimating it.
- Log-barrier loss: Extremely under- or overestimating demand in production would put company profit at risk.
- ϵ -insensitive loss: A certain amount of deviation in production does no harm, larger deviations do.

HUBER LOSS

$$L(y, f(\mathbf{x})) = \begin{cases} \frac{1}{2}(y - f(\mathbf{x}))^2 & \text{if } |y - f(\mathbf{x})| \leq \epsilon \\ \epsilon|y - f(\mathbf{x})| - \frac{1}{2}\epsilon^2 & \text{otherwise} \end{cases}, \quad \epsilon > 0$$

- Piece-wise combination of $L1/L2$ to have robustness/smoothness
- Analytic properties: convex, differentiable (once)

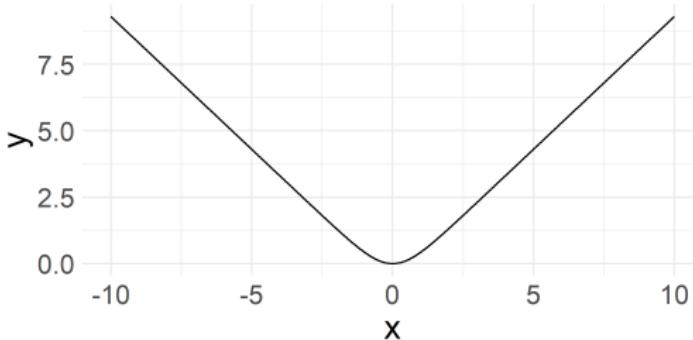


- Risk minimizer and optimal constant do not have a closed-form solution. To fit a model numerical optimization is necessary.
- Solution behaves like **trimmed mean**: a (conditional) mean of two (conditional) quantiles.

LOG-COSH LOSS

$$L(y, f(\mathbf{x})) = \log(\cosh(|y - f(\mathbf{x})|))$$

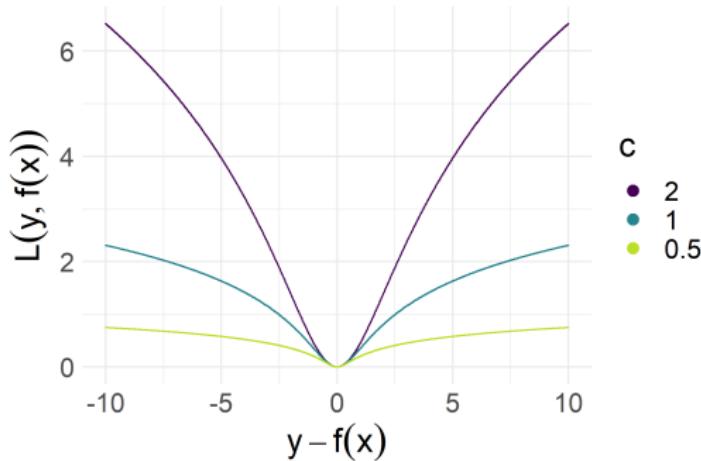
- Logarithm of the hyperbolic cosine of the residual.
- Approximately equal to $0.5(|y - f(\mathbf{x})|)^2$ for small \mathbf{x} and to $|y - f(\mathbf{x})| - \log 2$ for large \mathbf{x} , meaning it works mostly like $L2$ loss but is less outlier-sensitive.
- Has all the advantages of Huber loss and is, moreover, twice differentiable everywhere.



CAUCHY LOSS

$$L(y, f(\mathbf{x})) = \frac{c^2}{2} \log \left(1 + \left(\frac{|y - f(\mathbf{x})|}{c} \right)^2 \right), \quad c \in \mathbb{R}$$

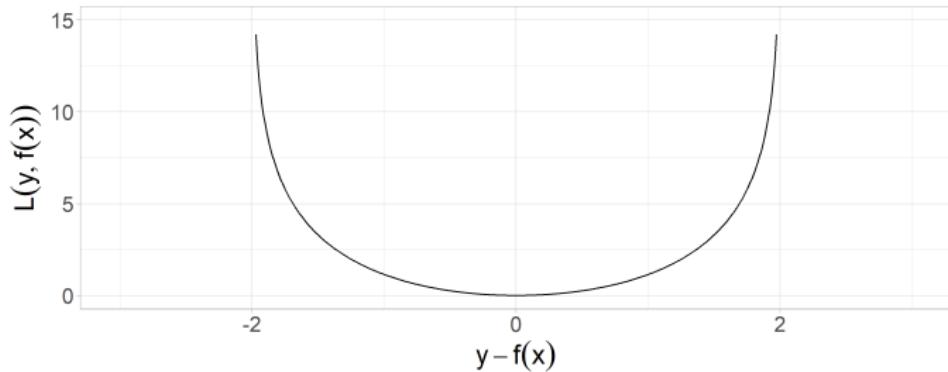
- Particularly robust toward outliers (controllable via c).
- Analytic properties: differentiable, but not convex!



LOG-BARRIER LOSS

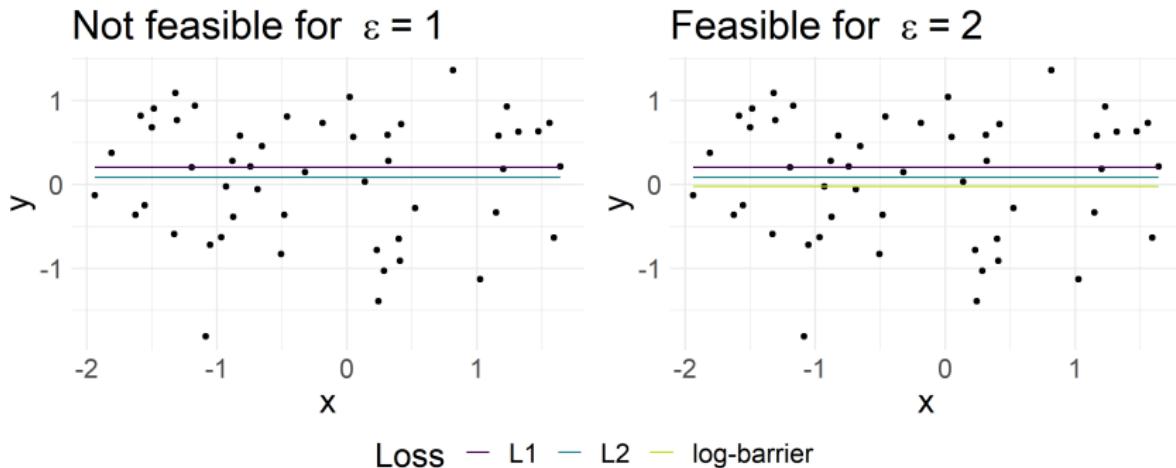
$$L(y, f(\mathbf{x})) = \begin{cases} -\epsilon^2 \cdot \log\left(1 - \left(\frac{|y-f(\mathbf{x})|}{\epsilon}\right)^2\right) & \text{if } |y - f(\mathbf{x})| \leq \epsilon \\ \infty & \text{if } |y - f(\mathbf{x})| > \epsilon \end{cases}$$

- Behaves like L_2 loss for small residuals.
- We use this if we don't want residuals larger than ϵ at all.
- No guarantee that the risk minimization problem has a solution.
- Plot shows log-barrier loss for $\epsilon = 2$:



LOG-BARRIER LOSS

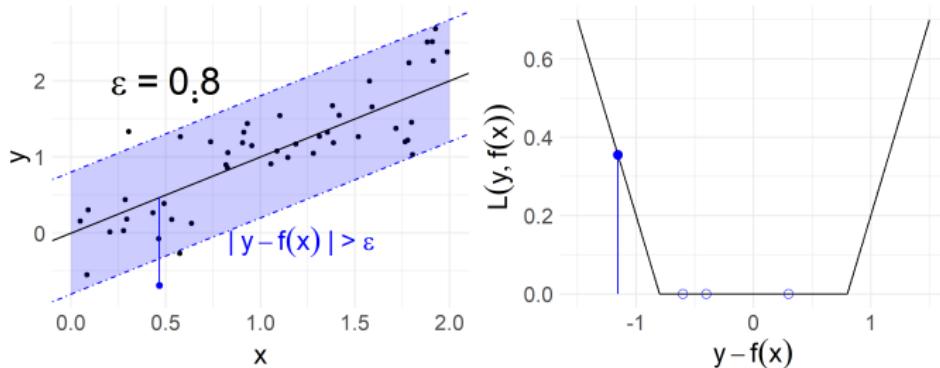
- Note that the optimization problem has no (finite) solution if there is no way to fit a constant where all residuals are smaller than a .



ϵ -INSENSITIVE LOSS

$$L(y, f(\mathbf{x})) = \begin{cases} 0 & \text{if } |y - f(\mathbf{x})| \leq \epsilon \\ |y - f(\mathbf{x})| - \epsilon & \text{otherwise} \end{cases}, \quad \epsilon \in \mathbb{R}_+$$

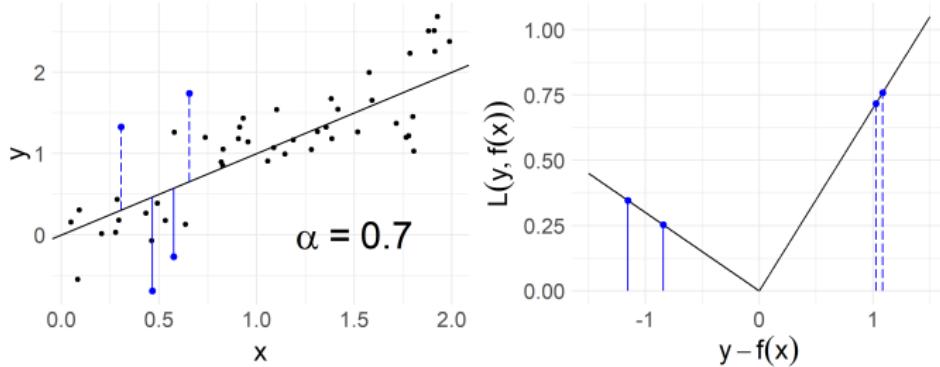
- Modification of L_1 loss, errors below ϵ accepted without penalty.
- Used in SVM regression.
- Properties: convex and not differentiable for $y - f(\mathbf{x}) \in \{-\epsilon, \epsilon\}$.



QUANTILE LOSS / PINBALL LOSS

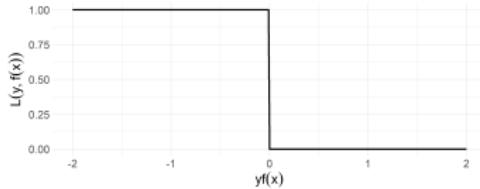
$$L(y, f(\mathbf{x})) = \begin{cases} (1 - \alpha)(f(\mathbf{x}) - y) & \text{if } y < f(\mathbf{x}) \\ \alpha(y - f(\mathbf{x})) & \text{if } y \geq f(\mathbf{x}) \end{cases}, \quad \alpha \in (0, 1)$$

- Extension of L_1 loss (equal to L_1 for $\alpha = 0.5$).
- Weights either positive or negative residuals more strongly.
- $\alpha < 0.5$ ($\alpha > 0.5$) penalty to over-estimation (under-estimation)
- Risk minimizer is (conditional) α -quantile (median for $\alpha = 0.5$).



Introduction to Machine Learning

0-1-Loss



Learning goals

- Derive the risk minimizer of the 0-1-loss
- Derive the optimal constant model for the 0-1-loss

0-1-LOSS

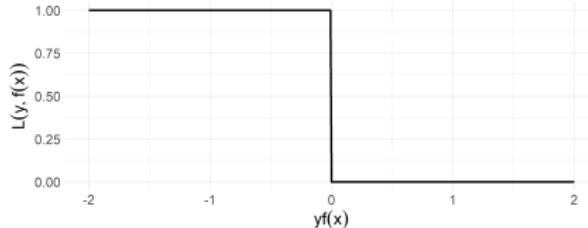
- Let us first consider a discrete classifier $h(\mathbf{x}) : \mathcal{X} \rightarrow \mathcal{Y}$.
- The most natural choice for $L(y, h(\mathbf{x}))$ is the 0-1-loss

$$L(y, h(\mathbf{x})) = \mathbb{1}_{\{y \neq h(\mathbf{x})\}} = \begin{cases} 1 & \text{if } y \neq h(\mathbf{x}) \\ 0 & \text{if } y = h(\mathbf{x}) \end{cases}$$

- For the binary case ($g = 2$) we can express the 0-1-loss for a scoring classifier $f(\mathbf{x})$ based on the margin $\nu := yf(\mathbf{x})$

$$L(y, f(\mathbf{x})) = \mathbb{1}_{\{\nu < 0\}} = \mathbb{1}_{\{yf(\mathbf{x}) < 0\}}.$$

- Analytic properties: Not continuous, even for linear f the optimization problem is NP-hard and close to intractable.



0-1-LOSS: RISK MINIMIZER

By the law of total expectation we can in general rewrite the risk as
(this all works for the multiclass case with 0-1)

$$\begin{aligned}\mathcal{R}(f) &= \mathbb{E}_{xy} [L(y, f(\mathbf{x}))] = \mathbb{E}_{\mathbf{x}} [\mathbb{E}_{y|x}[L(y, f(\mathbf{x}))]] \\ &= \mathbb{E}_{\mathbf{x}} \left[\sum_{k \in \mathcal{Y}} L(k, f(\mathbf{x})) \mathbb{P}(y = k \mid \mathbf{x} = \mathbf{x}) \right],\end{aligned}$$

with $\mathbb{P}(y = k \mid \mathbf{x} = \mathbf{x})$ the posterior probability for class k . For the binary case we denote $\eta(\mathbf{x}) := \mathbb{P}(y = 1 \mid \mathbf{x} = \mathbf{x})$ and the expression becomes

$$\mathcal{R}(f) = \mathbb{E}_{\mathbf{x}} [L(1, \pi(\mathbf{x})) \cdot \eta(\mathbf{x}) + L(0, \pi(\mathbf{x})) \cdot (1 - \eta(\mathbf{x}))].$$

0-1-LOSS: RISK MINIMIZER

We compute the point-wise optimizer of the above term for the 0-1-loss (defined on a discrete classifier $h(\mathbf{x})$):

$$\begin{aligned} h^*(\mathbf{x}) &= \arg \min_{l \in \mathcal{Y}} \sum_{k \in \mathcal{Y}} L(k, l) \cdot \mathbb{P}(y = k \mid \mathbf{x} = \mathbf{x}) \\ &= \arg \min_{l \in \mathcal{Y}} \sum_{k \neq l} \mathbb{P}(y = k \mid \mathbf{x} = \mathbf{x}) \\ &= \arg \min_{l \in \mathcal{Y}} 1 - \mathbb{P}(y = l \mid \mathbf{x} = \mathbf{x}) \\ &= \arg \max_{l \in \mathcal{Y}} \mathbb{P}(y = l \mid \mathbf{x} = \mathbf{x}), \end{aligned}$$

which corresponds to predicting the most probable class.

Note that sometimes $h^*(\mathbf{x}) = \arg \max_{l \in \mathcal{Y}} \mathbb{P}(y = l \mid \mathbf{x} = \mathbf{x})$ is referred to as the **Bayes optimal classifier** (without closer specification of the loss function used).

0-1-LOSS: RISK MINIMIZER

The Bayes risk for the 0-1-loss (also: Bayes error rate) is

$$\mathcal{R}^* = 1 - \mathbb{E}_x \left[\max_{l \in \mathcal{Y}} \mathbb{P}(y = l \mid \mathbf{x} = \mathbf{x}) \right].$$

In the binary case ($g = 2$) we can write risk minimizer and Bayes risk as follows:

$$h^*(\mathbf{x}) = \begin{cases} 1 & \eta(\mathbf{x}) \geq \frac{1}{2} \\ 0 & \eta(\mathbf{x}) < \frac{1}{2} \end{cases}$$

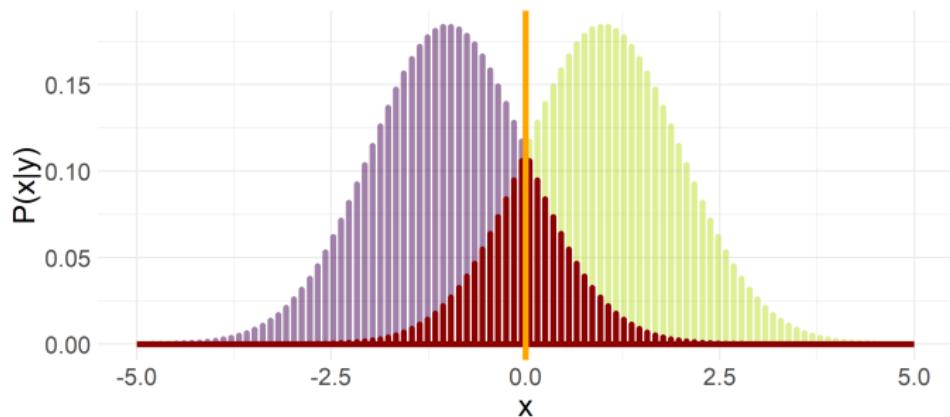
$$\mathcal{R}^* = \mathbb{E}_x [\min(\eta(\mathbf{x}), 1 - \eta(\mathbf{x}))] = \mathbb{E}_x [\max(\eta(\mathbf{x}), 1 - \eta(\mathbf{x}))].$$

0-1-LOSS: RISK MINIMIZER

Example: Assume that $\mathbb{P}(y = 1) = \frac{1}{2}$ and

$$\mathbb{P}(x | y) = \begin{cases} \phi_{\mu_1, \sigma^2}(x) & \text{for } y = 0 \\ \phi_{\mu_2, \sigma^2}(x) & \text{for } y = 1 \end{cases}$$

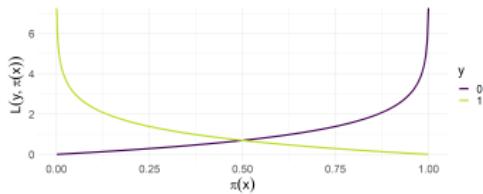
The decision boundary of the Bayes optimal classifier is shown in orange and the Bayes error rate is highlighted as red area.



Introduction to Machine Learning

Bernoulli Loss

Learning goals



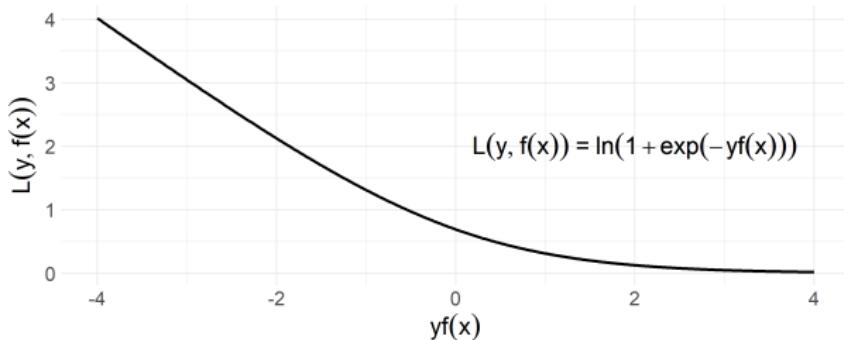
- Know the Bernoulli loss and related losses (log-loss, logistic loss, Binomial loss)
- Derive the risk minimizer
- Derive the optimal constant model
- Understand the connection between log-loss and entropy splitting

BERNOULLI LOSS

$$L(y, f(\mathbf{x})) = \ln(1 + \exp(-y \cdot f(\mathbf{x}))) \quad \text{for } y \in \{-1, +1\}$$

$$L(y, f(\mathbf{x})) = -y \cdot f(\mathbf{x}) + \log(1 + \exp(f(\mathbf{x}))) \quad \text{for } y \in \{0, 1\}$$

- Two equivalent formulations for different label encodings
- Negative log-likelihood of Bernoulli model, e.g., logistic regression
- Convex, differentiable
- Pseudo-residuals (0/1 case): $\tilde{r} = y - \frac{1}{1+\exp(-f(\mathbf{x}))}$
Interpretation: L_1 distance between 0/1-labels and posterior prob!

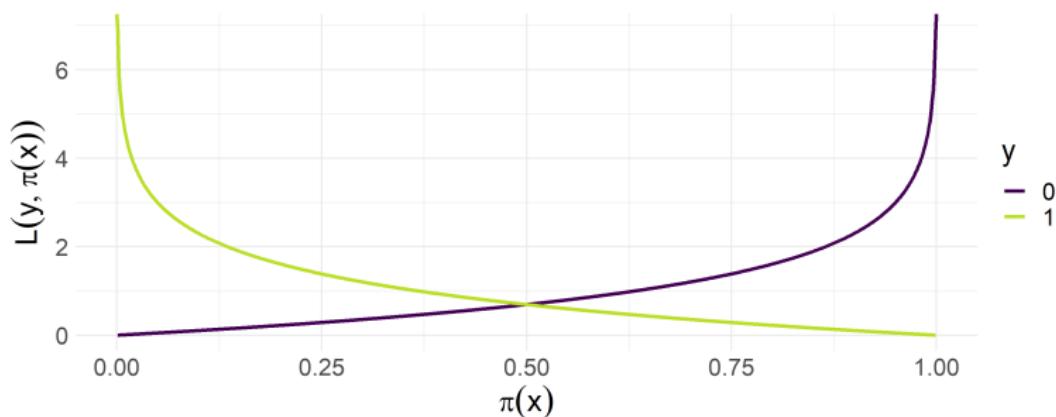


BERNOULLI LOSS ON PROBABILITIES

If scores are transformed into probabilities by the logistic function

$\pi(\mathbf{x}) = (1 + \exp(-f(\mathbf{x})))^{-1}$ (or equivalently if $f(x) = \log\left(\frac{\pi(\mathbf{x})}{1-\pi(\mathbf{x})}\right)$ are the log-odds of $\pi(\mathbf{x})$), we arrive at another equivalent formulation of the loss, where y is again encoded as $\{0, 1\}$:

$$L(y, \pi(\mathbf{x})) = -y \log(\pi(\mathbf{x})) - (1 - y) \log(1 - \pi(\mathbf{x})).$$



BERNOULLI LOSS: RISK MINIMIZER

The risk minimizer for the Bernoulli loss defined for probabilistic classifiers $\pi(\mathbf{x})$ and on $y \in \{0, 1\}$ is

$$\pi^*(\mathbf{x}) = \eta(\mathbf{x}) = \mathbb{P}(y = 1 \mid \mathbf{x} = \mathbf{x}).$$

Proof: We can write the risk for binary y as follows:

$$\mathcal{R}(f) = \mathbb{E}_{\mathbf{x}} [L(1, \pi(\mathbf{x})) \cdot \eta(\mathbf{x}) + L(0, \pi(\mathbf{x})) \cdot (1 - \eta(\mathbf{x}))],$$

with $\eta(\mathbf{x}) = \mathbb{P}(y = 1 \mid \mathbf{x} = \mathbf{x})$ (see chapter on the 0-1-loss for more details).

For a fixed \mathbf{x} we compute the point-wise optimal value c by setting the derivative to 0:

$$\begin{aligned}\frac{\partial}{\partial c} (-\log c \cdot \eta(\mathbf{x}) - \log(1 - c) \cdot (1 - \eta(\mathbf{x}))) &= 0 \\ -\frac{\eta(\mathbf{x})}{c} + \frac{1 - \eta(\mathbf{x})}{1 - c} &= 0 \\ \frac{-\eta(\mathbf{x}) + \eta(\mathbf{x})c + c - \eta(\mathbf{x})c}{c(1 - c)} &= 0 \\ c &= \eta(\mathbf{x}).\end{aligned}$$

BERNOULLI LOSS: RISK MINIMIZER

The risk minimizer for the Bernoulli loss defined on $y \in \{-1, 1\}$ and scores $f(\mathbf{x})$ is the point-wise log-odds:

$$f^*(\mathbf{x}) = \ln\left(\frac{\mathbb{P}(y | \mathbf{x} = \mathbf{x})}{1 - \mathbb{P}(y | \mathbf{x} = \mathbf{x})}\right).$$

The function is undefined when $\mathbb{P}(y | \mathbf{x} = \mathbf{x}) = 1$ or $\mathbb{P}(y | \mathbf{x} = \mathbf{x}) = 0$, but predicts a smooth curve which grows when $\mathbb{P}(y | \mathbf{x} = \mathbf{x})$ increases and equals 0 when $\mathbb{P}(y | \mathbf{x} = \mathbf{x}) = 0.5$.

Proof: As before we minimize

$$\begin{aligned}\mathcal{R}(f) &= \mathbb{E}_{\mathbf{x}} [L(1, f(\mathbf{x})) \cdot \eta(\mathbf{x}) + L(-1, f(\mathbf{x})) \cdot (1 - \eta(\mathbf{x}))] \\ &= \ln(1 + \exp(-f(\mathbf{x})))\eta(\mathbf{x}) + \ln(1 + \exp(f(\mathbf{x}))) (1 - \eta(\mathbf{x})).\end{aligned}$$

BERNOULLI LOSS: RISK MINIMIZER

For a fixed \mathbf{x} we compute the point-wise optimal value c by setting the derivative to 0:

$$\frac{\partial}{\partial c} \ln(1 + \exp(-c))\eta(\mathbf{x}) + \ln(1 + \exp(c))(1 - \eta(\mathbf{x})) = 0$$

$$-\frac{\exp(-c)}{1 + \exp(-c)}\eta(\mathbf{x}) + \frac{\exp(c)}{1 + \exp(c)}(1 - \eta(\mathbf{x})) = 0$$

$$-\frac{\exp(-c)}{1 + \exp(-c)}\eta(\mathbf{x}) + \frac{1}{1 + \exp(-c)}(1 - \eta(\mathbf{x})) = 0$$

$$-\eta(\mathbf{x}) + \frac{1}{1 + \exp(-c)} = 0$$

$$\eta(\mathbf{x}) = \frac{1}{1 + \exp(-c)}$$

$$c = \ln \left(\frac{\eta(\mathbf{x})}{1 - \eta(\mathbf{x})} \right)$$

BERNOULLI: OPTIMAL CONSTANT MODEL

The optimal constant probability model $\pi(\mathbf{x}) = \theta$ w.r.t. the Bernoulli loss for labels from $\mathcal{Y} = \{0, 1\}$ is:

$$\hat{\theta} = \arg \min_{\theta} \mathcal{R}_{\text{emp}}(\theta) = \frac{1}{n} \sum_{i=1}^n y^{(i)}$$

Again, this is the fraction of class-1 observations in the observed data. We can simply prove this again by setting the derivative of the risk to 0 and solving for θ .

BERNOULLI: OPTIMAL CONSTANT MODEL

The optimal constant score model $f(\mathbf{x}) = \theta$ w.r.t. the Bernoulli loss labels from $\mathcal{Y} = \{-1, +1\}$ or $\mathcal{Y} = \{0, 1\}$ is:

$$\hat{\theta} = \arg \min_{\theta} \mathcal{R}_{\text{emp}}(\theta) = \ln \frac{n_+}{n_-} = \ln \frac{n_+/n}{n_-/n}$$

where n_- and n_+ are the numbers of negative and positive observations, respectively.

This again shows a tight (and unsurprising) connection of this loss to log-odds.

Proving this is also a (quite simple) exercise.

BERNOULLI-LOSS: NAMING CONVENTION

We have seen three loss functions that are closely related. In the literature, there are different names for the losses:

$$L(y, f(\mathbf{x})) = \ln(1 + \exp(-yf(\mathbf{x}))) \quad \text{for } y \in \{-1, +1\}$$

$$L(y, f(\mathbf{x})) = -y \cdot f(\mathbf{x}) + \log(1 + \exp(f(\mathbf{x}))) \quad \text{for } y \in \{0, 1\}$$

are referred to as Bernoulli, Binomial or logistic loss.

$$L(y, \pi(\mathbf{x})) = -y \log(\pi(\mathbf{x})) - (1 - y) \log(1 - \pi(\mathbf{x})) \quad \text{for } y \in \{0, 1\}$$

is referred to as cross-entropy or log-loss.

We usually refer to all of them as **Bernoulli loss**, and rather make clear whether they are defined on labels $y \in \{0, 1\}$ or $y \in \{-1, +1\}$ and on scores $f(\mathbf{x})$ or probabilities $\pi(\mathbf{x})$.

BERNOULLI LOSS MIN = ENTROPY SPLITTING

When fitting a tree we minimize the risk within each node \mathcal{N} by risk minimization and predict the optimal constant. Another approach that is common in literature is to minimize the average node impurity $\text{Imp}(\mathcal{N})$.

Claim: Entropy splitting $\text{Imp}(\mathcal{N}) = \sum_{k=1}^g \pi_k^{(\mathcal{N})} \log \pi_k^{(\mathcal{N})}$ is equivalent to minimize risk measured by the Bernoulli loss.

Note that $\pi_k^{(\mathcal{N})} := \frac{1}{n_{\mathcal{N}}} \sum_{(\mathbf{x}, y) \in \mathcal{N}} [y = k]$.

Proof: To prove this we show that the risk related to a subset of observations $\mathcal{N} \subseteq \mathcal{D}$ fulfills

$$\mathcal{R}(\mathcal{N}) = n_{\mathcal{N}} \text{Imp}(\mathcal{N}),$$

where I is the entropy criterion $\text{Imp}(\mathcal{N})$ and $\mathcal{R}(\mathcal{N})$ is calculated w.r.t. the (multiclass) Bernoulli loss

$$L(y, \pi_k(\mathbf{x})) = \sum_{k=1}^g [y = k] \log (\pi_k(\mathbf{x})).$$

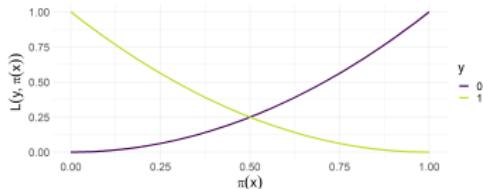
BERNOULLI LOSS MIN = ENTROPY SPLITTING

$$\begin{aligned}\mathcal{R}(\mathcal{N}) &= \sum_{(\mathbf{x},y) \in \mathcal{N}} \sum_{k=1}^g [y = k] \log \pi_k(\mathbf{x}) \stackrel{(*)}{=} \sum_{k=1}^g \sum_{(\mathbf{x},y) \in \mathcal{N}} [y = k] \log \pi_k^{(\mathcal{N})} \\ &= \sum_{k=1}^g \log \pi_k^{(\mathcal{N})} \underbrace{\sum_{(\mathbf{x},y) \in \mathcal{N}} [y = k]}_{n_{\mathcal{N}} \cdot \pi_k^{(\mathcal{N})}} \\ &= n_{\mathcal{N}} \sum_{k=1}^g \pi_k^{(\mathcal{N})} \log \pi_k^{(\mathcal{N})} = n_{\mathcal{N}} \text{Imp}(\mathcal{N}),\end{aligned}$$

where in $(*)$ the optimal constant per node $\pi_k^{(\mathcal{N})} = \frac{1}{n_{\mathcal{N}}} \sum_{(\mathbf{x},y) \in \mathcal{N}} [y = k]$ was plugged in.

Introduction to Machine Learning

Brier Score



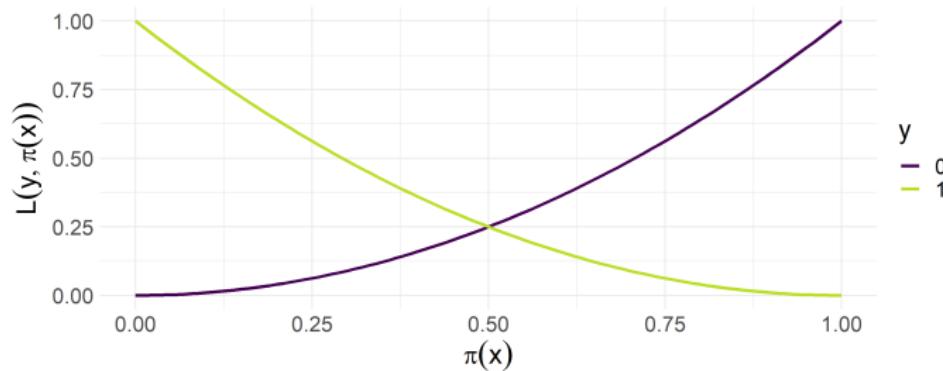
Learning goals

- Know the Brier score
- Derive the risk minimizer
- Derive the optimal constant model
- Understand the connection between Brier score and Gini splitting

BRIER SCORE

The binary Brier score is defined on probabilities $\pi(\mathbf{x}) \in [0, 1]$ and 0-1-encoded labels $y \in \{0, 1\}$ and measures their squared distance (L2 loss on probabilities).

$$L(y, \pi(\mathbf{x})) = (\pi(\mathbf{x}) - y)^2$$



BRIER SCORE: RISK MINIMIZER

The risk minimizer for the (binary) Brier score is

$$\pi^*(\mathbf{x}) = \eta(\mathbf{x}) = \mathbb{P}(y | \mathbf{x} = \mathbf{x}),$$

which means that the Brier score will reach its minimum if the prediction equals the “true” probability of the outcome.

The risk minimizer for the multiclass Brier score is

$$\pi^*(\mathbf{x}) = \mathbb{P}(y = k | \mathbf{x} = \mathbf{x}).$$

Proof: We only show the proof for the binary case. We need to minimize

$$\mathbb{E}_{\mathbf{x}} [L(1, \pi(\mathbf{x})) \cdot \eta(\mathbf{x}) + L(0, \pi(\mathbf{x})) \cdot (1 - \eta(\mathbf{x}))],$$

BRIER SCORE: RISK MINIMIZER

which we do point-wise for every \mathbf{x} . We plug in the Brier score

$$\begin{aligned} & \arg \min_c L(1, c)\eta(\mathbf{x}) + L(0, c)(1 - \eta(\mathbf{x})) \\ = & \arg \min_c (c - 1)^2\eta(\mathbf{x}) + c^2(1 - \eta(\mathbf{x})) \\ = & \arg \min_c (c - \eta(\mathbf{x}))^2. \end{aligned}$$

The expression is minimal if $c = \eta(\mathbf{x}) = \mathbb{P}(y = 1 \mid \mathbf{x} = \mathbf{x})$.

BRIER SCORE: OPTIMAL CONSTANT MODEL

The optimal constant probability model $\pi(\mathbf{x}) = \theta$ w.r.t. the Brier score for labels from $\mathcal{Y} = \{0, 1\}$ is:

$$\begin{aligned}\min_{\theta} \mathcal{R}_{\text{emp}}(\theta) &= \min_{\theta} \sum_{i=1}^n (y^{(i)} - \theta)^2 \\ \Leftrightarrow \frac{\partial \mathcal{R}_{\text{emp}}(\theta)}{\partial \theta} &= -2 \cdot \sum_{i=1}^n (y^{(i)} - \theta) = 0 \\ \hat{\theta} &= \frac{1}{n} \sum_{i=1}^n y^{(i)}.\end{aligned}$$

This is the fraction of class-1 observations in the observed data.
(This also directly follows from our L_2 proof for regression).

Similarly, for the multiclass brier score the optimal constant is

$$\hat{\theta}_k = \frac{1}{n} \sum_{i=1}^n [y = k].$$

BRIER SCORE MINIMIZATION = GINI SPLITTING

When fitting a tree we minimize the risk within each node \mathcal{N} by risk minimization and predict the optimal constant. Another approach that is common in literature is to minimize the average node impurity $\text{Imp}(\mathcal{N})$.

Claim: Gini splitting $\text{Imp}(\mathcal{N}) = \sum_{k=1}^g \pi_k^{(\mathcal{N})} (1 - \pi_k^{(\mathcal{N})})$ is equivalent to the Brier score minimization.

Note that $\pi_k^{(\mathcal{N})} := \frac{1}{n_{\mathcal{N}}} \sum_{(\mathbf{x}, y) \in \mathcal{N}} [y = k]$

Proof: We show that the risk related to a subset of observations $\mathcal{N} \subseteq \mathcal{D}$ fulfills

$$\mathcal{R}(\mathcal{N}) = n_{\mathcal{N}} \text{Imp}(\mathcal{N}),$$

where Imp is the Gini impurity and $\mathcal{R}(\mathcal{N})$ is calculated w.r.t. the (multiclass) Brier score

$$L(y, \pi(\mathbf{x})) = \sum_{k=1}^g ([y = k] - \pi_k(\mathbf{x}))^2.$$

BRIER SCORE MINIMIZATION = GINI SPLITTING

$$\mathcal{R}(\mathcal{N}) = \sum_{(\mathbf{x}, y) \in \mathcal{N}} \sum_{k=1}^g ([y = k] - \pi_k(\mathbf{x}))^2 = \sum_{k=1}^g \sum_{(\mathbf{x}, y) \in \mathcal{N}} \left([y = k] - \frac{n_{\mathcal{N}, k}}{n_{\mathcal{N}}} \right)^2,$$

by plugging in the optimal constant prediction w.r.t. the Brier score ($n_{\mathcal{N}, k}$ is defined as the number of class k observations in node \mathcal{N}):

$$\hat{\pi}_k(\mathbf{x}) = \pi_k^{(\mathcal{N})} = \frac{1}{n_{\mathcal{N}}} \sum_{(\mathbf{x}, y) \in \mathcal{N}} [y = k] = \frac{n_{\mathcal{N}, k}}{n_{\mathcal{N}}}.$$

We split the inner sum and further simply the expression

$$\begin{aligned} &= \sum_{k=1}^g \left(\sum_{(\mathbf{x}, y) \in \mathcal{N}: y=k} \left(1 - \frac{n_{\mathcal{N}, k}}{n_{\mathcal{N}}} \right)^2 + \sum_{(\mathbf{x}, y) \in \mathcal{N}: y \neq k} \left(0 - \frac{n_{\mathcal{N}, k}}{n_{\mathcal{N}}} \right)^2 \right) \\ &= \sum_{k=1}^g n_{\mathcal{N}, k} \left(1 - \frac{n_{\mathcal{N}, k}}{n_{\mathcal{N}}} \right)^2 + (n_{\mathcal{N}} - n_{\mathcal{N}, k}) \left(\frac{n_{\mathcal{N}, k}}{n_{\mathcal{N}}} \right)^2, \end{aligned}$$

since for $n_{\mathcal{N}, k}$ observations the condition $y = k$ is met, and for the remaining $(n_{\mathcal{N}} - n_{\mathcal{N}, k})$ observations it is not.

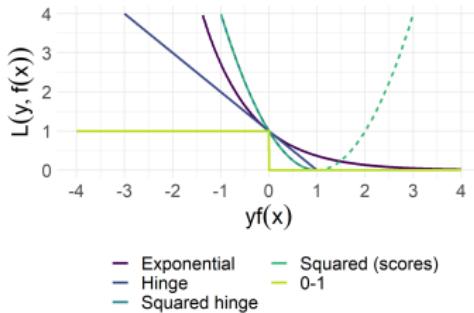
BRIER SCORE MINIMIZATION = GINI SPLITTING

We further simplify the expression to

$$\begin{aligned}\mathcal{R}(\mathcal{N}) &= \sum_{k=1}^g n_{\mathcal{N},k} \left(\frac{n_{\mathcal{N}} - n_{\mathcal{N},k}}{n_{\mathcal{N}}} \right)^2 + (n_{\mathcal{N}} - n_{\mathcal{N},k}) \left(\frac{n_{\mathcal{N},k}}{n_{\mathcal{N}}} \right)^2 \\ &= \sum_{k=1}^g \frac{n_{\mathcal{N},k}}{n_{\mathcal{N}}} \frac{n_{\mathcal{N}} - n_{\mathcal{N},k}}{n_{\mathcal{N}}} (n_{\mathcal{N}} - n_{\mathcal{N},k} + n_{\mathcal{N},k}) \\ &= n_{\mathcal{N}} \sum_{k=1}^g \pi_k^{(\mathcal{N})} \cdot \left(1 - \pi_k^{(\mathcal{N})} \right) = n_{\mathcal{N}} \text{Imp}(\mathcal{N}).\end{aligned}$$

Introduction to Machine Learning

Advanced Classification Losses



Learning goals

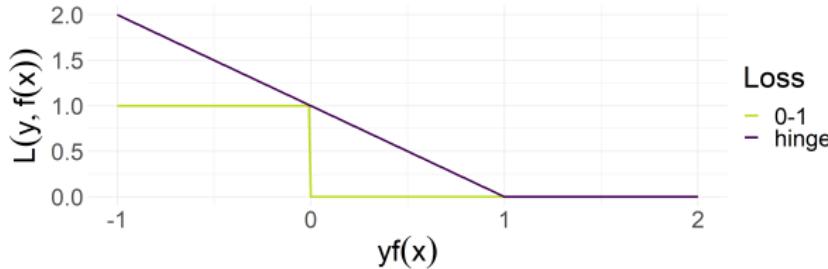
- Know the (squared) hinge loss
- Know the L_2 loss defined on scores
- Know the exponential loss
- Know the AUC loss

HINGE LOSS

- The intuitive appeal of the 0-1-loss is set off by its analytical properties ill-suited to direct optimization.
- The **hinge loss** is a continuous relaxation that acts as a convex upper bound on the 0-1-loss (for $y \in \{-1, +1\}$):

$$L(y, f(\mathbf{x})) = \max\{0, 1 - yf(\mathbf{x})\}.$$

- Note that the hinge loss only equals zero for a margin ≥ 1 , encouraging confident (correct) predictions.
- It resembles a door hinge, hence the name:

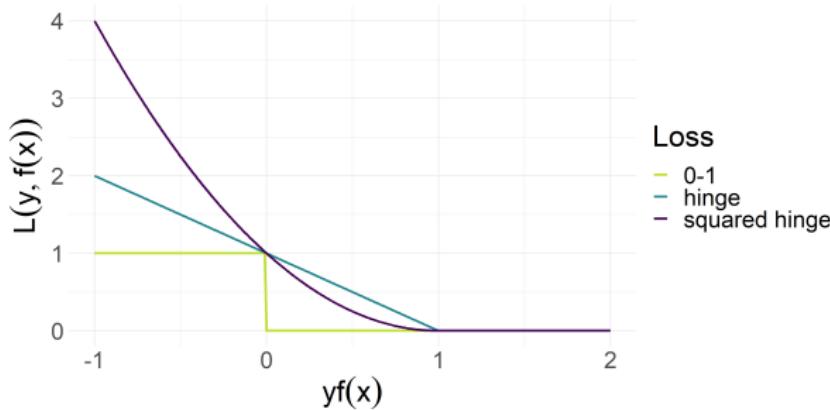


SQUARED HINGE LOSS

- We can also specify a **squared** version for the hinge loss:

$$L(y, f(\mathbf{x})) = \max\{0, (1 - yf(\mathbf{x}))^2\}.$$

- The *L2* form punishes margins $yf(\mathbf{x}) \in (0, 1)$ less severely but puts a high penalty on more confidently wrong predictions.
- Therefore, it is smoother yet more outlier-sensitive than the non-squared hinge loss.

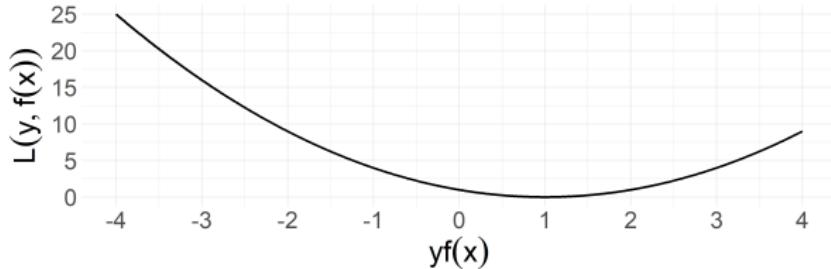


SQUARED LOSS ON SCORES

- Analogous to the Brier score defined on probabilities we can specify a **squared loss on classification scores** (again, $y \in \{-1, +1\}$, using that $y^2 \equiv 1$):

$$\begin{aligned} L(y, f(\mathbf{x})) &= (y - f(\mathbf{x}))^2 = y^2 - 2yf(\mathbf{x}) + (f(\mathbf{x}))^2 = \\ &= 1 - 2yf(\mathbf{x}) + (yf(\mathbf{x}))^2 = (1 - yf(\mathbf{x}))^2 \end{aligned}$$

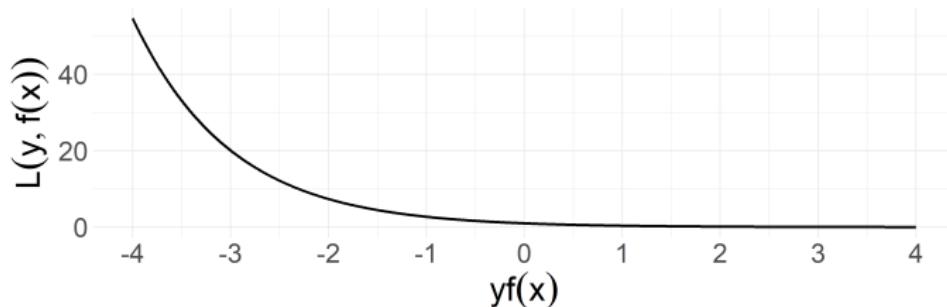
- This loss behaves just like the squared hinge loss for $yf(\mathbf{x}) < 1$, but is zero only for $yf(\mathbf{x}) = 1$ and actually increases again for larger margins (which is in general not desirable!)



CLASSIFICATION LOSSES: EXPONENTIAL LOSS

Another possible choice for a (binary) loss function that is a smooth approximation to the 0-1-loss is the **exponential loss**:

- $L(y, f(\mathbf{x})) = \exp(-yf(\mathbf{x}))$, used in AdaBoost.
- Convex, differentiable (thus easier to optimize than 0-1-loss).
- The loss increases exponentially for wrong predictions with high confidence; if the prediction is right with a small confidence only, there, loss is still positive.
- No closed-form analytic solution to (empirical) risk minimization.



CLASSIFICATION LOSSES: AUC-LOSS

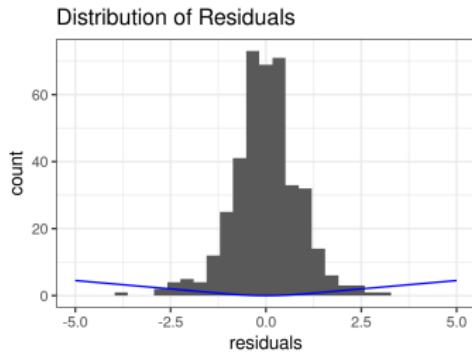
- Often AUC is used as an evaluation criterion for binary classifiers.
- Let $y \in \{-1, +1\}$ with n_- negative and n_+ positive samples.
- The AUC can then be defined as

$$AUC = \frac{1}{n_+} \frac{1}{n_-} \sum_{i:y^{(i)}=1} \sum_{j:y^{(j)}=-1} [f^{(i)} > f^{(j)}]$$

- This is not differentiable w.r.t f due to $[f^{(i)} > f^{(j)}]$.
- But the indicator function can be approximated by the distribution function of the triangular distribution on $[-1, 1]$ with mean 0.
- However, direct optimization of the AUC is numerically more difficult, and might not work as well as using a common loss and tuning for AUC in practice.

Introduction to Machine Learning

Maximum Likelihood Estimation vs. Empirical Risk Minimization



Learning goals

- Understand the connection between maximum likelihood and risk minimization
- Learn the correspondence between a Gaussian error distribution and the L2 loss

MAXIMUM LIKELIHOOD

Let us approach regression from a maximum likelihood perspective. In the following we assume that

$$y \mid \mathbf{x} \sim p(y \mid \mathbf{x}, \theta),$$

For example, we commonly consider a true underlying relationship f_{true} with additive noise:

$$y = f_{\text{true}}(\mathbf{x}) + \epsilon,$$

where f_{true} is a function that is parameterized by θ and ϵ being a RV that follows some distribution \mathbb{P}_ϵ , with $\mathbb{E}[\epsilon] = 0$. Further, we assume ϵ to be independent of \mathbf{x} .

MAXIMUM LIKELIHOOD

From a statistics / maximum-likelihood perspective, we assume (or we pretend) we know the underlying distribution $p(y | \mathbf{x}, \theta)$.

- Then, given data

$$\mathcal{D} = \left(\left(\mathbf{x}^{(1)}, y^{(1)} \right), \dots, \left(\mathbf{x}^{(n)}, y^{(n)} \right) \right)$$

the maximum-likelihood principle is to maximize the **likelihood**

$$\mathcal{L}(\theta) = \prod_{i=1}^n p\left(y^{(i)} | \mathbf{x}^{(i)}, \theta\right)$$

or to minimize the **negative log-likelihood**

$$-\ell(\theta) = - \sum_{i=1}^n \log p\left(y^{(i)} | \mathbf{x}^{(i)}, \theta\right).$$

MAXIMUM LIKELIHOOD

Let us take a machine learning perspective and assume our hypothesis space corresponds to the space of the (parameterized) f_{true} .

- Let us now simply define the negative log-likelihood as **loss function**

$$L(y, f(\mathbf{x} \mid \theta)) := -\log p(y \mid \mathbf{x}, \theta)$$

- Maximum-likelihood optimization can be formulated as an empirical risk minimization problem

$$\mathcal{R}_{\text{emp}}(\theta) = \sum_{i=1}^n L\left(y^{(i)}, f\left(\mathbf{x}^{(i)} \mid \theta\right)\right)$$

- We can even disregard multiplicative or additive constants in the loss as they do not change the minimizer.

MAXIMUM LIKELIHOOD

- For every error distribution \mathbb{P}_ϵ we can derive an equivalent loss function, which leads to the same point estimator for the parameter vector θ as maximum-likelihood.
- **NB:** The other way around does not always work: We cannot derive a probability density function or error distribution corresponding to every loss function – the Hinge loss is a prominent example.

GAUSSIAN ERRORS - L2-LOSS

Let us assume $y = f_{\text{true}}(\mathbf{x}) + \epsilon$ with additive Gaussian errors are Gaussian, i.e. $\epsilon^{(i)} \sim \mathcal{N}(0, \sigma^2)$. Then

$$y \mid \mathbf{x} \sim N(f_{\text{true}}(\mathbf{x}), \sigma^2).$$

The likelihood is then

$$\begin{aligned}\mathcal{L}(\boldsymbol{\theta}) &= \prod_{i=1}^n p\left(y^{(i)} \mid f\left(\mathbf{x}^{(i)} \mid \boldsymbol{\theta}\right), \sigma^2\right) \\ &\propto \exp\left(-\frac{1}{2\sigma^2} \sum_{i=1}^n \left(y^{(i)} - f\left(\mathbf{x}^{(i)} \mid \boldsymbol{\theta}\right)\right)^2\right).\end{aligned}$$

GAUSSIAN ERRORS - L2-LOSS

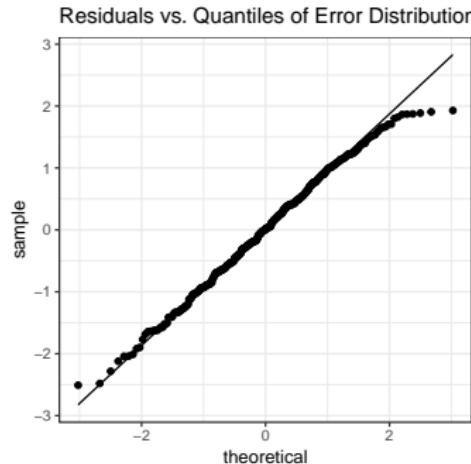
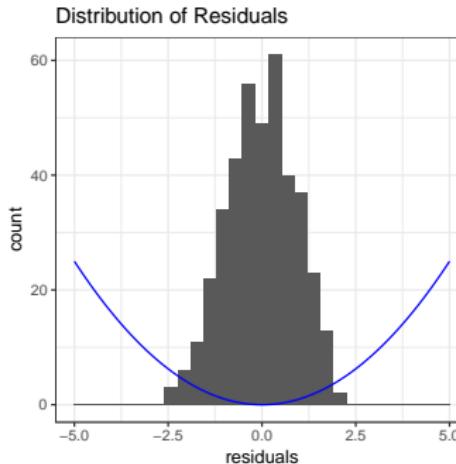
It is easy to see that minimizing the negative log-likelihood is equivalent to the $L2$ -loss minimization approach since

$$\begin{aligned}-\ell(\boldsymbol{\theta}) &= -\log (\mathcal{L}(\boldsymbol{\theta})) \\&= -\log \left(\exp \left(-\frac{1}{2\sigma^2} \sum_{i=1}^n \left(y^{(i)} - f(\mathbf{x}^{(i)} | \boldsymbol{\theta}) \right)^2 \right) \right) \\&\propto \sum_{i=1}^n \left(y^{(i)} - f(\mathbf{x}^{(i)} | \boldsymbol{\theta}) \right)^2.\end{aligned}$$

Note: We use \propto as “proportional to ... up to multiplicative and additive constants”.

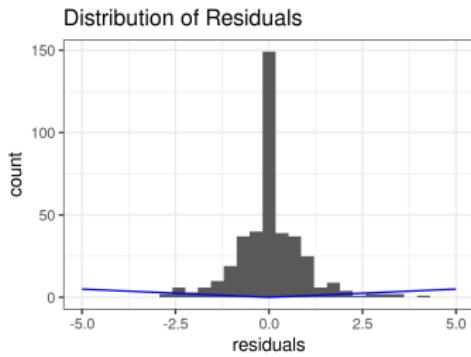
GAUSSIAN ERRORS - L2-LOSS

- We simulate data $y \mid \mathbf{x} \sim \mathcal{N}(f_{\text{true}}(\mathbf{x}), 1)$ with $f_{\text{true}} = 0.2 \cdot \mathbf{x}$.
- We can plot the empirical error distribution, i.e. the distribution of the residuals after fitting a regression model w.r.t. L2-loss.
- With the help of a Q-Q-plot we can compare the empirical residuals vs. the theoretical quantiles of a Gaussian distribution.



Introduction to Machine Learning

Maximum Likelihood Estimation vs. Empirical Risk Minimization



Learning goals

- Learn the correspondence between a Laplacian error distribution and the L1 loss
- Learn that there is no error distribution for the Huber loss
- Learn the correspondence between Bernoulli-distributed targets and the Bernoulli loss

LAPLACE ERRORS - L1-LOSS

Let us assume that errors are Laplacian, i.e. ϵ follows a Laplace distribution which has the density

$$\frac{1}{2\sigma} \exp\left(-\frac{|x|}{\sigma}\right), \sigma > 0.$$

Then

$$y = f_{\text{true}}(\mathbf{x}) + \epsilon$$

follows a Laplace distribution with mean $f(\mathbf{x}^{(i)} | \theta)$ and scale parameter σ .

LAPLACE ERRORS - L1-LOSS

The likelihood is then

$$\begin{aligned}\mathcal{L}(\boldsymbol{\theta}) &= \prod_{i=1}^n p\left(y^{(i)} \mid f\left(\mathbf{x}^{(i)} \mid \boldsymbol{\theta}\right), \sigma\right) \\ &\propto \exp\left(-\frac{1}{\sigma} \sum_{i=1}^n |y^{(i)} - f\left(\mathbf{x}^{(i)} \mid \boldsymbol{\theta}\right)|\right).\end{aligned}$$

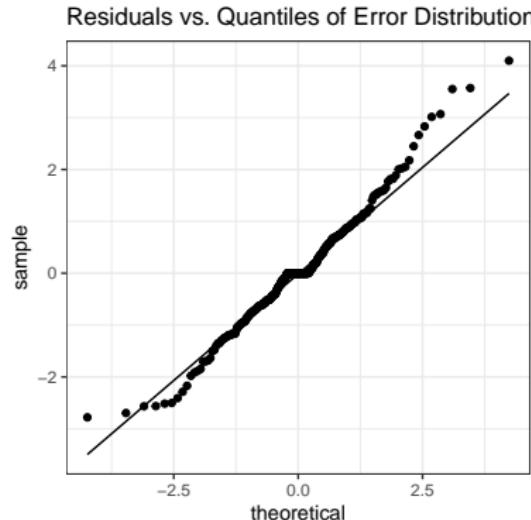
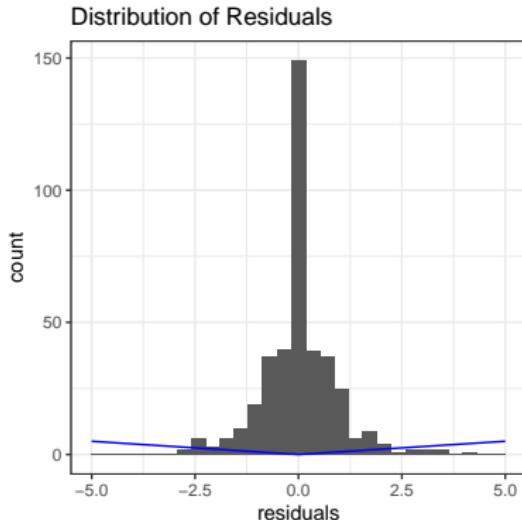
The negative log-likelihood is

$$-\ell(\boldsymbol{\theta}) \propto -\sum_{i=1}^n |y^{(i)} - f\left(\mathbf{x}^{(i)} \mid \boldsymbol{\theta}\right)|.$$

Minimizing the negative log-likelihood for Laplacian error terms corresponds to empirical risk minimization with L1-loss.

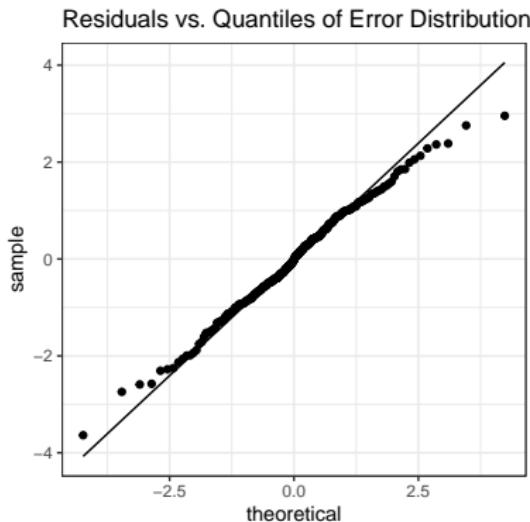
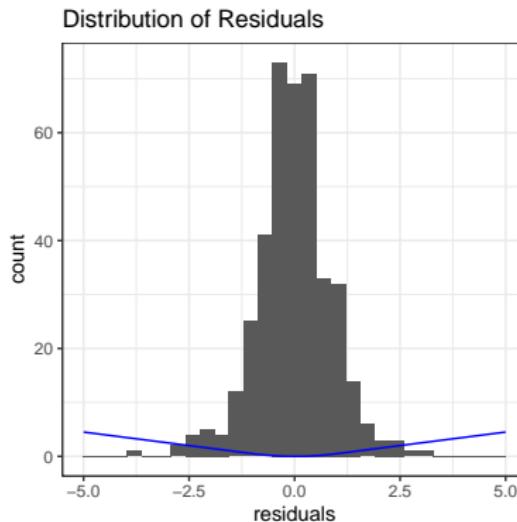
LAPLACE ERRORS - L1-LOSS

- We simulate data $y \mid \mathbf{x} \sim \text{Laplacian}(f_{\text{true}}(\mathbf{x}), 1)$ with $f_{\text{true}} = 0.2 \cdot \mathbf{x}$.
- We can plot the empirical error distribution, i.e. the distribution of the residuals after fitting a regression model w.r.t. $L1$ -loss.
- With the help of a Q-Q-plot we can compare the empirical residuals vs. the theoretical quantiles of a Laplacian distribution.



OTHER ERROR DISTRIBUTIONS

- There are losses that do not correspond to “real” error densities, like the Huber loss. (In the QQ-plot below we show residuals against quantiles of a normal.)



MAXIMUM LIKELIHOOD IN CLASSIFICATION

Let us assume the outputs y to be Bernoulli-distributed, i.e.

$$y \mid \mathbf{x} \sim \text{Ber}(\pi_{\text{true}}(\mathbf{x})).$$

The negative log likelihood is

$$\begin{aligned}-\ell(\boldsymbol{\theta}) &= -\sum_{i=1}^n \log p(y^{(i)} \mid \mathbf{x}^{(i)}, \boldsymbol{\theta}) \\&= -\sum_{i=1}^n \log \left[\pi(\mathbf{x}^{(i)})^{y^{(i)}} \cdot (1 - \pi(\mathbf{x}^{(i)}))^{(1-y^{(i)})} \right] \\&= \sum_{i=1}^n -y^{(i)} \log[\pi(\mathbf{x}^{(i)})] - (1 - y^{(i)}) \log[1 - \pi(\mathbf{x}^{(i)})].\end{aligned}$$

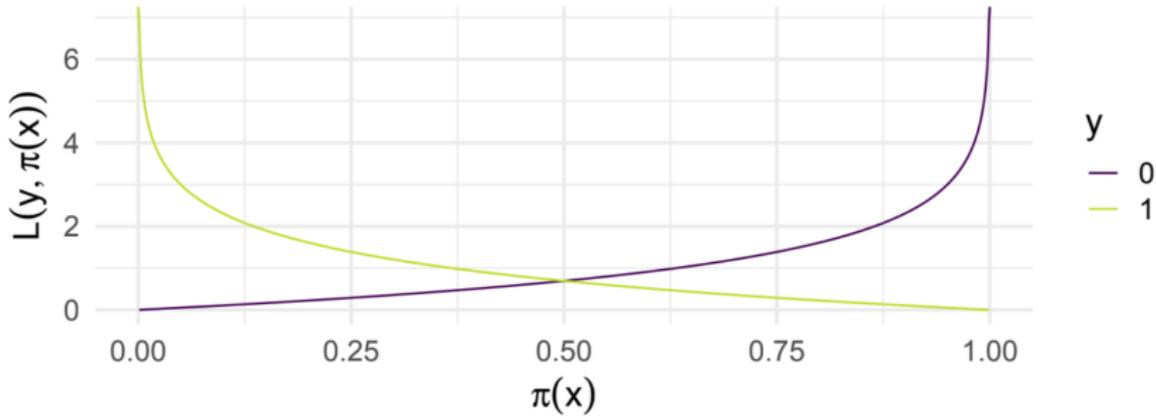
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MAXIMUM LIKELIHOOD IN CLASSIFICATION

This gives rise to the following loss function

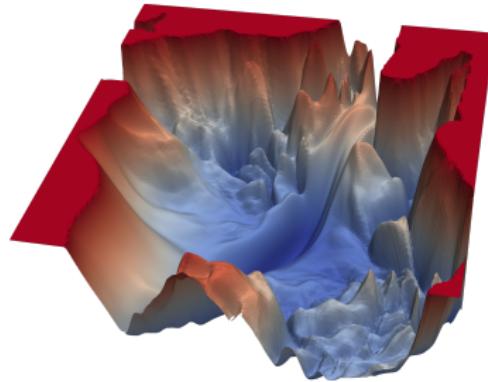
$$L(y, \pi(\mathbf{x})) = -y \ln(\pi(\mathbf{x})) - (1 - y) \ln(1 - \pi(\mathbf{x})), \quad y \in \{0, 1\}$$

which we introduced as **Bernoulli** loss.



Introduction to Machine Learning

Properties of Loss Functions



Learning goals

- Know the concept of robustness
- Learn about analytical and computational properties of loss functions
- Understand that the loss function may influence convergence of the optimizer

THE ROLE OF LOSS FUNCTIONS

Why should we care about how to choose the loss function $L(y, f(\mathbf{x}))$?

- **Statistical** properties: Choice of loss implies statistical assumptions on the distribution of $y \mid \mathbf{x} = \mathbf{x}$ (see *Maximum Likelihood Estimation vs. Empirical Risk Minimization*).
- **Robustness** properties: Some loss functions are more robust towards outliers than others.
- **Analytical** properties: The computational / optimization complexity of the problem.

$$\arg \min_{\theta \in \Theta} \mathcal{R}_{\text{emp}}(\theta)$$

is influenced by the choice of the loss function.

BASIC TYPES OF REGRESSION LOSSES

- Regression losses usually only depend on the **residuals**

$$r := y - f(\mathbf{x})$$

- A loss is called **distance-based** if
 - it can be written in terms of the residual

$$L(y, f(\mathbf{x})) = \psi(r) \text{ for some } \psi : \mathbb{R} \rightarrow \mathbb{R}$$

- $\psi(r) = 0 \Leftrightarrow r = 0$.
- A loss is **translation-invariant**, if $L(y + a, f(\mathbf{x}) + a) = L(y, f(\mathbf{x}))$.
- Losses are called **symmetric** if $L(y, f(\mathbf{x})) = L(f(\mathbf{x}), y)$.

@BB: This slide is a bit without context imo. We are also not saying anything about classification losses - should we?

ROBUSTNESS

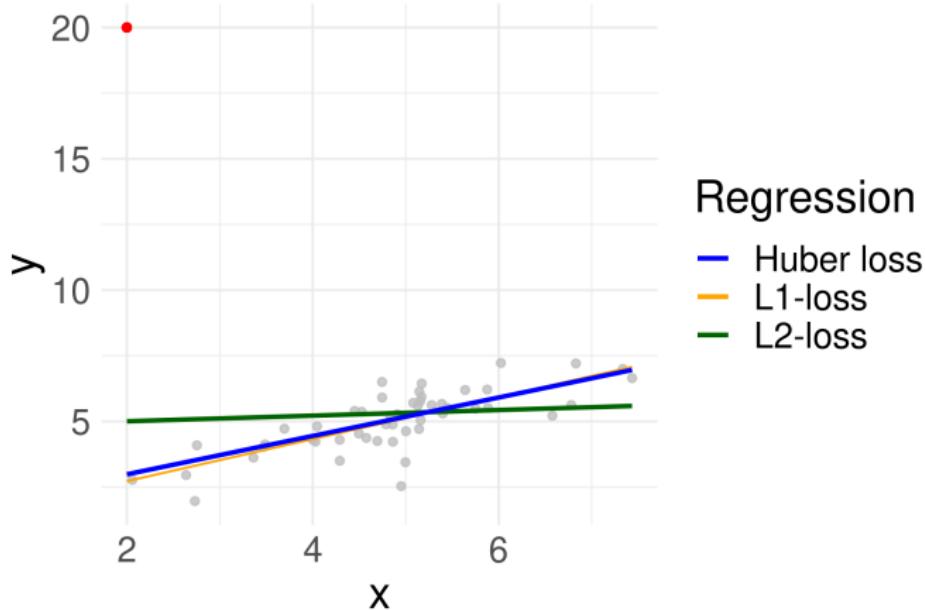
Outliers (in y) have large residuals $r = y - f(\mathbf{x})$. For some losses large residuals have a much bigger impact on the risk much more than for other losses.

y	$\hat{f}(\mathbf{x})$	L1	L2	Huber ($\epsilon = 5$)
1	0	1	1	0.5
5	0	5	25	12.5
10	0	10	100	37.5
50	0	50	2500	237.5

As a consequence, a model is less influenced by outliers than by inliers if the loss is robust.

ROBUSTNESS

The L2 loss is an example for a loss function that is not very robust towards outliers. It penalizes large residuals more than the L1 or the Huber loss. The L1 and the Huber loss are thus regarded robust.

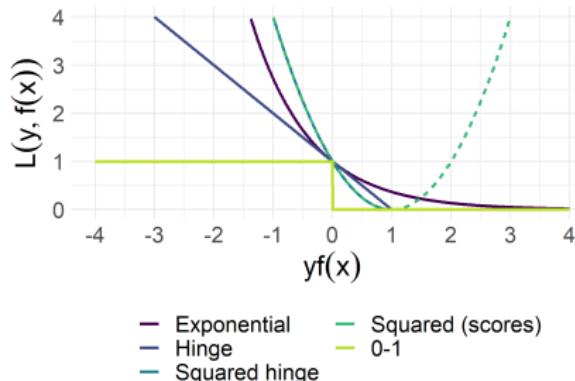


ANALYTICAL PROPERTIES: SMOOTHNESS

- **Smoothness** of a function is a property that is measured by the number of continuous derivatives it has.
- A function is said to be \mathcal{C}^k if it is k times continuously differentiable. A function is \mathcal{C}^∞ if it is continuously differentiable for all orders k .
- In contrast to derivative-free methods, derivative-based methods require a certain level of smoothness of the risk function $\mathcal{R}_{\text{emp}}(\theta)$.
- Example: Gradient descent requires differentiability of the $\mathcal{R}_{\text{emp}}(\theta)$ (existence of $\nabla \mathcal{R}_{\text{emp}}(\theta)$), Newton-Raphson requires $\mathcal{R}_{\text{emp}}(\theta)$ to be twice differentiable (existence of Hessian $\nabla^2 \mathcal{R}_{\text{emp}}(\theta)$).

ANALYTICAL PROPERTIES: SMOOTHNESS

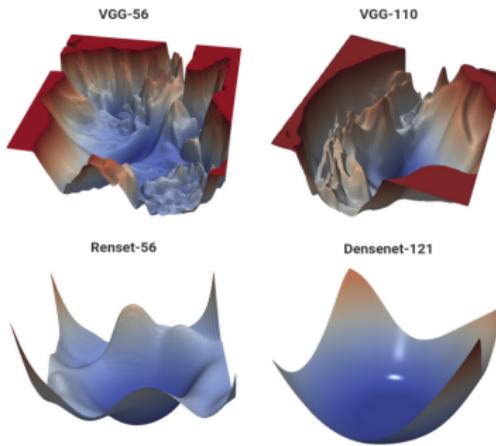
- If the loss function is not smooth, the risk minimization problem is in general not smooth either.
- Instead, derivative-free optimization need to be used (which might not be desirable)



Squared loss, exponential loss, and squared hinge loss are continuously differentiable. The hinge loss is continuous but not differentiable. The 0-1-loss is not even continuous.

ANALYTICAL PROPERTIES: CONVEXITY

- In optimization, convex optimization problems are desirable because they have a number of convenient properties. In particular, it holds for convex problems: A local minimum of a convex function is also a global minimum. A strictly convex function has at most **one** global minimum (uniqueness).



Li et al., 2018, Visualizing the Loss Landscape of Neural Nets. The problem on the bottom right is convex, the others are not.

ANALYTICAL PROPERTIES: CONVEXITY

- In practical terms complexity means that we do not need to worry to get stuck in a local minimum during risk minimization.
- Note that convexity of $\mathcal{R}_{\text{emp}}(\theta)$ does not only depend on convexity of the loss function: Convexity of $\mathcal{R}_{\text{emp}}(\theta)$ is also determined by the choice of the hypothesis space!
- For example, if $L(y, f(\mathbf{x}))$ is convex in its second argument, and $f(\mathbf{x} | \theta)$ is linear in θ , then $\mathcal{R}_{\text{emp}}(\theta)$ is convex. If L is not convex, $\mathcal{R}_{\text{emp}}(\theta)$ might have multiple local minima (bad!).

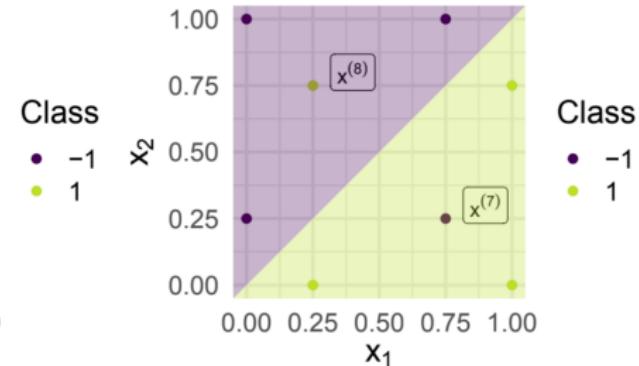
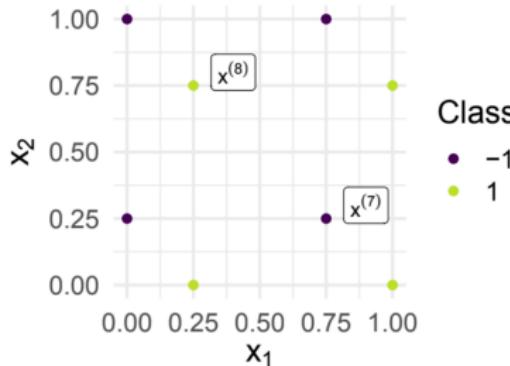
ANALYTICAL PROPERTIES: CONVERGENCE

@BB: Do we want to cover this case here in such a detailed manner?

The choice of the loss function may also imply convergence behavior of the optimization problem.

Example: Gradient descent will not converge if we minimize the Bernoulli loss for linearly separable data.

First, we take a look at logistic regression for an almost linearly separable dataset consisting of the observations $\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(8)}$.



ANALYTICAL PROPERTIES: CONVERGENCE

Note: WLOG we estimate the model without intercept, s.t. we can visualize the regression coefficient θ in 2D. Also, the symmetry of the data does not influence the generality of our conclusions.

Because of the symmetry of the data, the direction¹ of θ is
 $\tilde{\theta} := (\frac{1}{\sqrt{2}}, -\frac{1}{\sqrt{2}})^\top$.

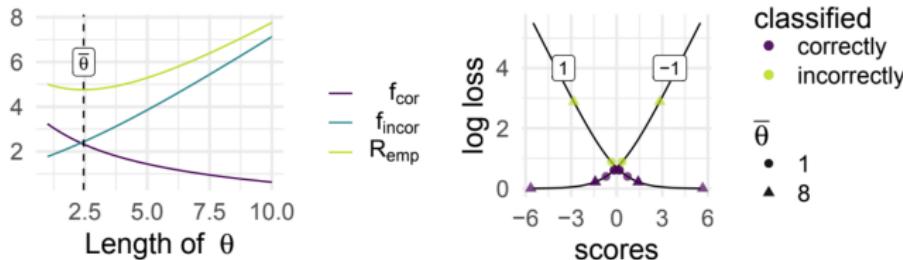
To find $\bar{\theta} := \|\theta\|_2$, we consider the empirical risk \mathcal{R}_{emp} along $\tilde{\theta}$:

$$\begin{aligned}\mathcal{R}_{\text{emp}} &= \sum_{i=1}^8 \log \left[1 + \exp \left(-y^{(i)} \theta^\top \mathbf{x}^{(i)} \right) \right] \\ &= \underbrace{\sum_{i=1}^6 \log \left[1 + \exp \left(-\bar{\theta} |\tilde{\theta}^\top \mathbf{x}^{(i)}| \right) \right]}_{=: f_{\text{cor}}(\bar{\theta}) \text{ (correctly classified)}} + \underbrace{\sum_{i=7}^8 \log \left[1 + \exp \left(\bar{\theta} |\tilde{\theta}^\top \mathbf{x}^{(i)}| \right) \right]}_{=: f_{\text{incor}}(\bar{\theta}) \text{ (incorrectly classified)}}.\end{aligned}$$

¹ θ is perpendicular to the decision boundary and points to the "1"-space

ANALYTICAL PROPERTIES: CONVERGENCE

Clearly, $f_{\text{cor}} / f_{\text{incor}}$ are monotonically decreasing/increasing with rising length of θ :



- By removing obs. 7 and 8, we get a linearly separable dataset.
- This also means that we lose our "counterweight", i.e., if a parameter vector θ is able to classify the samples perfectly, the vector 2θ also classifies the samples perfectly, with decreased risk.
- Therefore, an iterative optimizer such as gradient descent will continually increase θ and never halt (in theory).
- In such cases, regularization can guarantee convergence (see chapter on regularization).

INTRODUCTION TO MACHINE LEARNING

Advanced Risk Minimization

Multiclass Classification

Information Theory

Curse of Dimensionality

Hypothesis Space

Regularization

Linear Support Vector Machine

Nonlinear Support Vector Machine

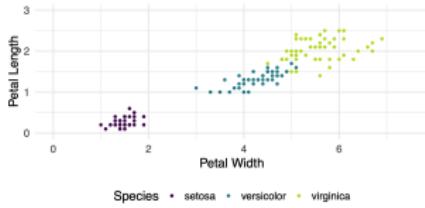
Gaussian Processes

Boosting

Introduction to Machine Learning

Multiclass Classification and Losses

Learning goals



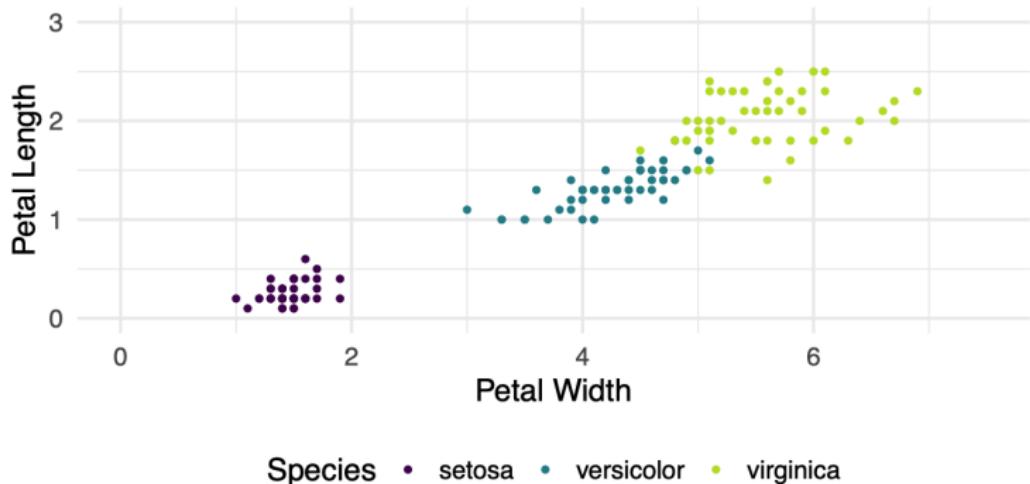
- Know what multiclass means and which types of classifier exist
- Know the MC 0-1-loss
- Know the MC brier score
- Know the MC logarithmic loss

MULTICLASS CLASSIFICATION

Scenario: Multiclass classification with $g > 2$ classes

$$\mathcal{D} \subset (\mathcal{X} \times \mathcal{Y})^n, \mathcal{Y} = \{1, \dots, g\}$$

Example: Iris dataset with $g = 3$



REVISION: RISK FOR CLASSIFICATION

Goal: Find a model $f : \mathcal{X} \rightarrow \mathbb{R}^g$, where g is the number of classes, that minimizes the expected loss over random variables $(\mathbf{x}, y) \sim \mathbb{P}_{xy}$

$$\mathcal{R}(f) = \mathbb{E}_{xy}[L(y, f(\mathbf{x}))] = \mathbb{E}_x \left[\sum_{k \in \mathcal{Y}} L(k, f(\mathbf{x})) \mathbb{P}(y = k | \mathbf{x} = \mathbf{x}) \right]$$

The optimal model for a loss function $L(y, f(\mathbf{x}))$ is

$$\hat{f}(\mathbf{x}) = \arg \min_{f \in \mathcal{H}} \sum_{k \in \mathcal{Y}} L(k, f(\mathbf{x})) \mathbb{P}(y = k | \mathbf{x} = \mathbf{x}).$$

Because we usually do not know \mathbb{P}_{xy} , we minimize the **empirical risk** as an approximation to the **theoretical** risk

$$\hat{f} = \arg \min_{f \in \mathcal{H}} \mathcal{R}_{\text{emp}}(f) = \arg \min_{f \in \mathcal{H}} \sum_{i=1}^n L\left(y^{(i)}, f\left(\mathbf{x}^{(i)}\right)\right).$$

TYPES OF CLASSIFIERS

- We already saw losses for binary classification tasks. Now we will consider losses for **multiclass classification** tasks.
- For multiclass classification, loss functions will be defined on
 - vectors of scores

$$f(\mathbf{x}) = (f_1(\mathbf{x}), \dots, f_g(\mathbf{x}))$$

- vectors of probabilities

$$\pi(\mathbf{x}) = (\pi_1(\mathbf{x}), \dots, \pi_g(\mathbf{x}))$$

- hard labels

$$h(\mathbf{x}) = k, k \in \{1, 2, \dots, g\}$$

ONE-HOT ENCODING

- Multiclass outcomes y with classes $1, \dots, g$ are often transformed to g binary (1/0) outcomes using

$$\text{with } \mathbb{1}_{\{y=k\}} = \begin{cases} 1 & \text{if } y = k \\ 0 & \text{otherwise} \end{cases}$$

- One-hot encoding does not lose any information contained in the outcome.

Example: Iris

Species	Species.setosa	Species.versicolor	Species.virginica
versicolor	0	1	0
virginica	0	0	1
versicolor	0	1	0
versicolor	0	1	0
setosa	1	0	0
setosa	1	0	0

0-1-Loss

0-1-LOSS

We have already seen that optimizer $\hat{h}(\mathbf{x})$ of the theoretical risk using the 0-1-loss

$$L(y, h(\mathbf{x})) = \mathbb{1}_{\{y \neq h(\mathbf{x})\}}$$

is the Bayes optimal classifier, with

$$\hat{h}(\mathbf{x}) = \arg \max_{l \in \mathcal{Y}} \mathbb{P}(y = l \mid \mathbf{x} = \mathbf{x})$$

and the optimal constant model (featureless predictor)

$$h(\mathbf{x}) = k, k \in \{1, 2, \dots, g\}$$

is the classifier that predicts the most frequent class $k \in \{1, 2, \dots, g\}$ in the data

$$h(\mathbf{x}) = \text{mode} \left\{ y^{(i)} \right\}.$$

MC Brier Score

MC BRIER SCORE

The (binary) Brier score generalizes to the multiclass Brier score that is defined on a vector of class probabilities $(\pi_1(\mathbf{x}), \dots, \pi_g(\mathbf{x}))$

$$L(y, \pi(\mathbf{x})) = \sum_{k=1}^g (\mathbb{1}_{\{y=k\}} - \pi_k(\mathbf{x}))^2.$$

The optimal constant model $\pi(\mathbf{x}) = (\theta_1, \dots, \theta_g)$ (outputting a vector of constant class probabilities) is

$$\pi_k(\mathbf{x}) = \arg \min_{\theta_k} \mathcal{R}_{\text{emp}}(\theta) = \arg \min_{\theta_k} \left(\sum_{i=1}^n \sum_{k=1}^g (\mathbb{1}_{\{y^{(i)}=k\}} - \theta_k)^2 \right)$$

We solve this by setting the derivative w.r.t. θ_k to 0

$$\frac{\partial \mathcal{R}_{\text{emp}}(\theta)}{\partial \theta_k} = -2 \cdot \sum_{i=1}^n (\mathbb{1}_{\{y^{(i)}=k\}} - \theta_k) = 0$$

$$\hat{\pi}_k(\mathbf{x}) = \hat{\theta}_k = \frac{1}{n} \sum_{i=1}^n \mathbb{1}_{\{y^{(i)}=k\}},$$

being the fraction of class- k observations.

MC BRIER SCORE

Claim: For $g = 2$ the MC Brier score is exactly twice as high as the binary Brier score, defined as $(\pi_1(\mathbf{x}) - y)^2$.

Proof:

$$L(y, \pi(x)) = \sum_{k=0}^1 (\mathbb{1}_{\{y=k\}} - \pi_k(\mathbf{x}))^2$$

For $y = 0$:

$$\begin{aligned} L(y, \pi(x)) &= (1 - \pi_0(\mathbf{x}))^2 + (0 - \pi_1(\mathbf{x}))^2 = (1 - (1 - \pi_1(\mathbf{x})))^2 + \pi_1(\mathbf{x})^2 \\ &= \pi_1(\mathbf{x})^2 + \pi_1(\mathbf{x})^2 = 2 \cdot \pi_1(\mathbf{x})^2 \end{aligned}$$

For $y = 1$:

$$\begin{aligned} L(y, \pi(x)) &= (0 - \pi_0(\mathbf{x}))^2 + (1 - \pi_1(\mathbf{x}))^2 = (-(1 - \pi_1(\mathbf{x})))^2 + (1 - \pi_1(\mathbf{x}))^2 \\ &= 1 - 2 \cdot \pi_1(\mathbf{x}) + \pi_1(\mathbf{x})^2 + 1 - 2 \cdot \pi_1(\mathbf{x}) + \pi_1(\mathbf{x})^2 \\ &= 2 \cdot (1 - 2 \cdot \pi_1(\mathbf{x}) + \pi_1(\mathbf{x})^2) = 2 \cdot (1 - \pi_1(\mathbf{x}))^2 = 2 \cdot (\pi_1(\mathbf{x}) - 1)^2 \end{aligned}$$

$$L(y, \pi(x)) = \begin{cases} 2 \cdot \pi_1(\mathbf{x})^2 & \text{for } y = 0 \\ 2 \cdot (\pi_1(\mathbf{x}) - 1)^2 & \text{for } y = 1 \end{cases} = 2 \cdot (\pi_1(\mathbf{x}) - y)^2$$

Logarithmic Loss

LOGARITHMIC LOSS (LOG-LOSS)

The generalization of the Binomial loss (logarithmic loss) for two classes is the multiclass **logarithmic loss / cross-entropy loss**:

$$L(y, \pi(x)) = - \sum_{k=1}^g \mathbb{1}_{\{y=k\}} \log (\pi_k(\mathbf{x})) ,$$

with $\pi_k(\mathbf{x})$ denoting the predicted probability for class k .

The optimal constant model $\pi(\mathbf{x}) = (\theta_1, \dots, \theta_g)$ (outputting a vector of constant class probabilities) is

$$\pi_k(\mathbf{x}) = \hat{\theta}_k = \frac{1}{n} \sum_{i=1}^n \mathbb{1}_{\{y^{(i)}=k\}},$$

being the fraction of class- k observations.

Proof: Exercise.

In the upcoming section we will see how this corresponds to the (multinomial) **softmax regression**.

LOGARITHMIC LOSS (LOG-LOSS)

Claim: For $g = 2$ the log-loss is equal to the Bernoulli loss, defined as

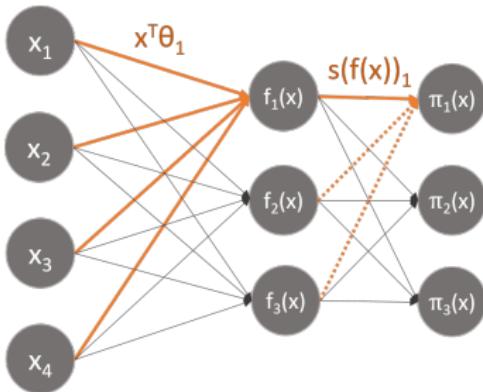
$$L_{0,1}(y, \pi_1(\mathbf{x})) = -y\log(\pi_1(\mathbf{x})) - (1-y)\log(1-\pi_1(\mathbf{x}))$$

Proof:

$$\begin{aligned} L_{0,1}(y, \pi_1(\mathbf{x})) &= -y\log(\pi_1(\mathbf{x})) - (1-y)\log(1-\pi_1(\mathbf{x})) \\ &= -y\log(\pi_1(\mathbf{x})) - (1-y)\log(\pi_0(\mathbf{x})) \\ &= -\mathbb{1}_{\{y=1\}}\log(\pi_1(\mathbf{x})) - \mathbb{1}_{\{y=0\}}\log(\pi_0(\mathbf{x})) \\ &= -\sum_{k=0}^1 \mathbb{1}_{\{y=k\}} \log(\pi_k(\mathbf{x})) = L(y, \pi(\mathbf{x})) \end{aligned}$$

Introduction to Machine Learning

Softmax Regression



Learning goals

- Know softmax regression
- Understand that softmax regression is a generalization of logistic regression

FROM LOGISTIC REGRESSION ...

Remember **logistic regression** ($\mathcal{Y} = \{0, 1\}$): We combined the hypothesis space of linear functions, transformed by the logistic function $s(z) = \frac{1}{1+\exp(-z)}$, i.e.

$$\mathcal{H} = \left\{ \pi : \mathcal{X} \rightarrow \mathbb{R} \mid \pi(\mathbf{x}) = s(\boldsymbol{\theta}^\top \mathbf{x}) \right\},$$

with the Bernoulli (logarithmic) loss:

$$L(y, \pi(\mathbf{x})) = -y \log(\pi(\mathbf{x})) - (1 - y) \log(1 - \pi(\mathbf{x})).$$

Remark: We suppress the intercept term for better readability. The intercept term can be easily included via $\boldsymbol{\theta}^\top \tilde{\mathbf{x}}$, $\boldsymbol{\theta} \in \mathbb{R}^{p+1}$, $\tilde{\mathbf{x}} = (1, \mathbf{x})$.

... TO SOFTMAX REGRESSION

There is a straightforward generalization to the multiclass case:

- Instead of a single linear discriminant function we have g linear discriminant functions

$$f_k(\mathbf{x}) = \boldsymbol{\theta}_k^\top \mathbf{x}, \quad k = 1, 2, \dots, g,$$

each indicating the confidence in class k .

- The g score functions are transformed into g probability functions by the **softmax** function $s : \mathbb{R}^g \rightarrow \mathbb{R}^g$

$$\pi_k(\mathbf{x}) = s(f(\mathbf{x}))_k = \frac{\exp(\boldsymbol{\theta}_k^\top \mathbf{x})}{\sum_{j=1}^g \exp(\boldsymbol{\theta}_j^\top \mathbf{x})},$$

instead of the **logistic** function for $g = 2$. The probabilities are well-defined: $\sum \pi_k(\mathbf{x}) = 1$ and $\pi_k(\mathbf{x}) \in [0, 1]$ for all k .

... TO SOFTMAX REGRESSION

- The softmax function is a generalization of the logistic function.
For $g = 2$, the logistic function and the softmax function are equivalent.
- Instead of the **Bernoulli** loss, we use the multiclass **logarithmic loss**

$$L(y, \pi(\mathbf{x})) = - \sum_{k=1}^g \mathbb{1}_{\{y=k\}} \log (\pi_k(\mathbf{x})).$$

- Note that the softmax function is a “smooth” approximation of the arg max operation, so $s((1, 1000, 2)^T) \approx (0, 1, 0)^T$ (picks out 2nd element!).
- Furthermore, it is invariant to constant offsets in the input:

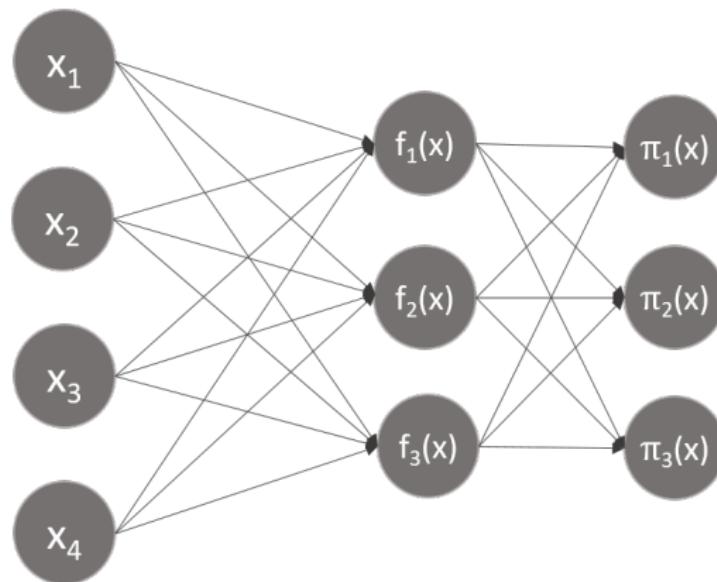
$$s(f(\mathbf{x}) + \mathbf{c}) = \frac{\exp(\theta_k^\top \mathbf{x} + c)}{\sum_{j=1}^g \exp(\theta_j^\top \mathbf{x} + c)} = \frac{\exp(\theta_k^\top \mathbf{x}) \cdot \exp(c)}{\sum_{j=1}^g \exp(\theta_j^\top \mathbf{x}) \cdot \exp(c)} = s(f(\mathbf{x}))$$

LOGISTIC VS. SOFTMAX REGRESSION

	Logistic Regression	Softmax Regression
\mathcal{Y}	$\{0, 1\}$	$\{1, 2, \dots, g\}$
Discriminant fun.	$f(\mathbf{x}) = \boldsymbol{\theta}^\top \mathbf{x}$	$f_k(\mathbf{x}) = \boldsymbol{\theta}_k^\top \mathbf{x}, k = 1, 2, \dots, g$
Probabilities	$\pi(\mathbf{x}) = \frac{1}{1 + \exp(-\boldsymbol{\theta}^\top \mathbf{x})}$	$\pi_k(\mathbf{x}) = \frac{\exp(\boldsymbol{\theta}_k^\top \mathbf{x})}{\sum_{j=1}^g \exp(\boldsymbol{\theta}_j^\top \mathbf{x})}$
$L(y, \pi(\mathbf{x}))$	Bernoulli / logarithmic loss $-y \log(\pi(\mathbf{x})) - (1 - y) \log(1 - \pi(\mathbf{x}))$	Multiclass logarithmic loss $-\sum_{k=1}^g [y = k] \log(\pi_k(\mathbf{x}))$

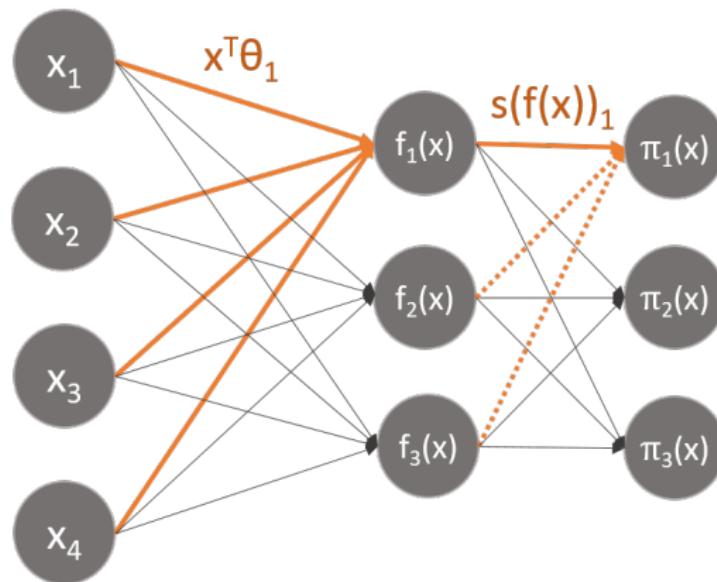
LOGISTIC VS. SOFTMAX REGRESSION

We can schematically depict softmax regression as follows:



LOGISTIC VS. SOFTMAX REGRESSION

We can schematically depict softmax regression as follows:



LOGISTIC VS. SOFTMAX REGRESSION

Further comments:

- We can now, for instance, calculate gradients and optimize this with standard numerical optimization software.
- Softmax regression has an unusual property in that it has a “redundant” set of parameters. If we subtract a fixed vector from all θ_k , the predictions do not change at all. Hence, our model is “over-parameterized”. For any hypothesis we might fit, there are multiple parameter vectors that give rise to exactly the same hypothesis function. This also implies that the minimizer of $\mathcal{R}_{\text{emp}}(\theta)$ above is not unique (but $\mathcal{R}_{\text{emp}}(\theta)$ is convex)! Hence, a numerical trick is to set $\theta_g = 0$ and only optimize the other θ_k .
- A similar approach is used in many ML models: multiclass LDA, naive Bayes, neural networks and boosting.

SOFTMAX: LINEAR DISCRIMINANT FUNCTIONS

Softmax regression gives us a **linear classifier**.

- The softmax function $s(\mathbf{z})_k = \frac{\exp(\mathbf{z}_k)}{\sum_{j=1}^g \exp(\mathbf{z}_j)}$ is
 - a rank-preserving function, i.e. the ranks among the elements of the vector \mathbf{z} are the same as among the elements of $s(\mathbf{z})$. This is because softmax transforms all scores by taking the $\exp(\cdot)$ (rank-preserving) and divides each element by **the same** normalizing constant.

Thus, the softmax function has a unique inverse function $s^{-1} : \mathbb{R}^g \rightarrow \mathbb{R}^g$ that is also monotonic and rank-preserving.

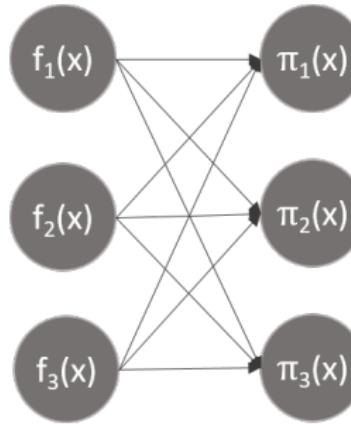
Applying s_k^{-1} to $\pi_k(\mathbf{x}) = \frac{\exp(\theta_k^\top \mathbf{x})}{\sum_{j=1}^n \exp(\theta_j^\top \mathbf{x})}$ gives us $f_k(\mathbf{x}) = \theta_k^\top \mathbf{x}$. Thus, softmax regression is a linear classifier.

GENERALIZING SOFTMAX REGRESSION

Instead of simple linear discriminant functions we could use **any** model that outputs g scores

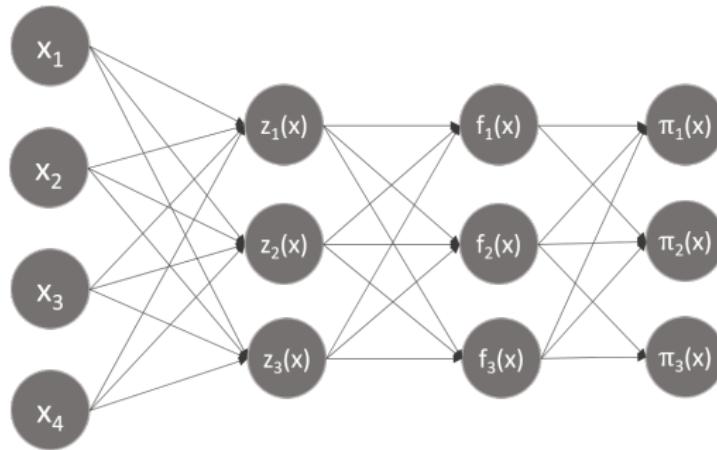
$$f_k(\mathbf{x}) \in \mathbb{R}, k = 1, 2, \dots, g$$

We can choose a multiclass loss and optimize the score functions $f_k, k \in \{1, \dots, g\}$ by multivariate minimization. The scores can be transformed to probabilities by the **softmax** function.



GENERALIZING SOFTMAX REGRESSION

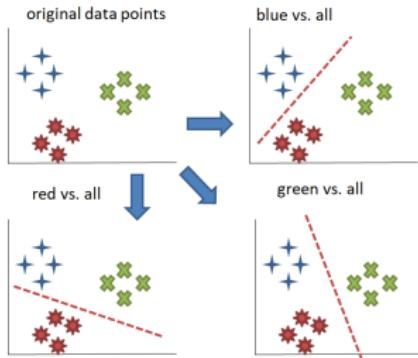
For example for a **neural network** (note that softmax regression is also a neural network with no hidden layers):



Remark: For more details about neural networks please refer to the lecture **Deep Learning**.

Introduction to Machine Learning

One-vs-Rest and One-vs-One



Learning goals

- Reduce a multiclass problem to multiple binary problems in a model-agnostic way
- Know one-vs-rest reduction
- Know one-vs-one reduction

MULTICLASS TO BINARY REDUCTION

- Assume we have a way to train binary classifiers, either outputting class labels $h(\mathbf{x})$, scores $f(\mathbf{x})$ or probabilities $\pi(\mathbf{x})$.
- We are now looking for a model-agnostic reduction principle to reduce a multiclass problem to the problem of solving **multiple binary problems**.
- Two common approaches are **one-vs-rest** and **one-vs-one** reductions.

CODEBOOKS

How binary problems are generated can be defined by a codebook.

Example:

Class	$f_1(\mathbf{x})$	$f_2(\mathbf{x})$	$f_3(\mathbf{x})$
1	1	-1	-1
2	-1	1	1
3	0	1	-1

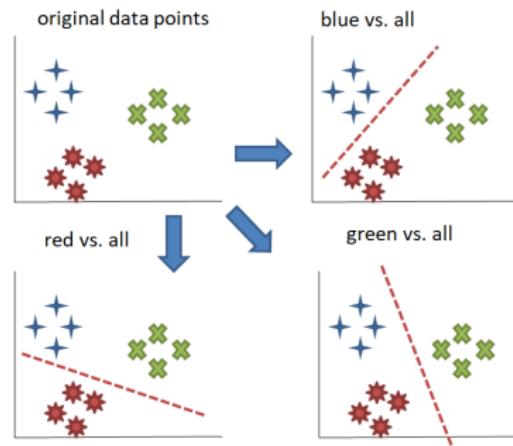
- The k -th column defines how classes of all observations are encoded in the binary subproblem / for binary classifier $f_k(\mathbf{x})$.
- Entry (m, l) takes values $\in \{-1, 0, +1\}$
 - if 0, observations of class $y^{(i)} = m$ are ignored.
 - if 1, observations of class $y^{(i)} = m$ are encoded as 1.
 - if -1, observations of class $y^{(i)} = m$ are encoded as -1.

One-vs-Rest

ONE-VS-REST

Create g binary subproblems, where in each the k -th original class is encoded as $+1$, and all other classes (the **rest**) as -1 .

Class	$f_1(\mathbf{x})$	$f_2(\mathbf{x})$	$f_3(\mathbf{x})$
1	1	-1	-1
2	-1	1	-1
3	-1	-1	1



ONE-VS-REST

- Making decisions means applying all classifiers to a sample $\mathbf{x} \in \mathcal{X}$ and predicting the label k for which the corresponding classifier reports the highest confidence:

$$\hat{y} = \arg \max_{k \in \{1, 2, \dots, g\}} \hat{f}_k(\mathbf{x}).$$

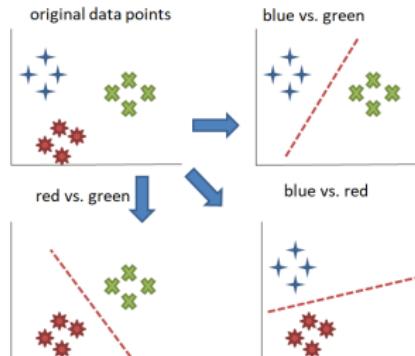
- Obtaining calibrated posterior probabilities is not completely trivial, we could fit a second-stage, multinomial logistic regression model on our output scores, so with inputs $(\hat{f}_1(\mathbf{x}^{(i)}), \dots, \hat{f}_g(\mathbf{x}^{(i)}))$ and outputs $y^{(i)}$ as training data.

One-vs-One

ONE-VS-ONE

We create $\frac{g(g-1)}{2}$ binary sub-problems, where each $\mathcal{D}_{k,\tilde{k}} \subset \mathcal{D}$ only considers observations from a class-pair $y^{(i)} \in \{k, \tilde{k}\}$, other observations are omitted.

Class	$f_1(\mathbf{x})$	$f_2(\mathbf{x})$	$f_3(\mathbf{x})$
1	1	-1	0
2	-1	0	1
3	0	1	-1



ONE-VS-ONE

- Label prediction is done via **majority voting**. We predict the label of a new \mathbf{x} with all classifiers and select the class that occurred most often.
- **Pairwise coupling** (see *Hastie, T. and Tibshirani, R. (1998). Classification by Pairwise Coupling*) is a heuristic to transform scores obtained by a one-vs-one reduction to probabilities.

COMPARISON ONE-VS-ONE AND ONE-VS-REST

- Note that each binary problem has now much less than n observations!
- For classifiers that scale (at least) quadratically with the number of observations, this means that one-vs-one usually does not create quadratic extra effort in g , but often only approximately linear extra effort in g .
- We experimentally investigate the train times of the one-vs-rest and one-vs-one approaches for an increasing number of classes g .
- We train a support vector machine classifier (SVMs will be covered later in the lecture) on an artificial dataset with $n = 1000$.

COMPARISON ONE-VS-ONE AND ONE-VS-REST

We see that the computational effort for one-vs-one is much higher than for one-vs-rest, but it does not scale proportionally to the (quadratic) number of trained classifiers.

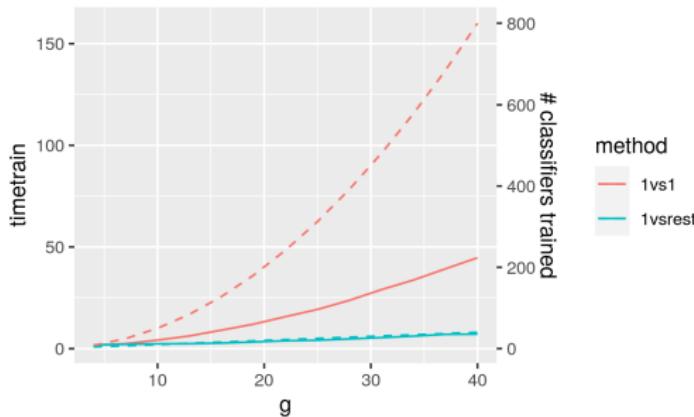
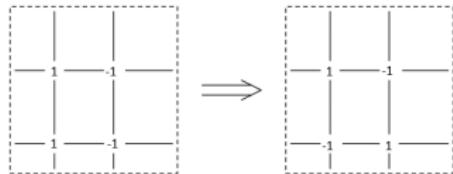


Figure: The number of classes vs. the training time (solid lines, left axis) and number of learners (dashed lines, right axis) for each of the two approaches.

Introduction to Machine Learning

Designing Codebooks and ECOC

Learning goals



- Know what a codebook is
- Understand that codebooks generalize one-vs-one and one-vs-rest
- Know how to define a good codebook and error-correcting output codes (ECOC)
- Know how randomized hill-climbing algorithm is used to find good codebooks

Designing Codebooks

CODEBOOKS

- We have already seen that we can write down principles like one-vs-rest and one-vs-one reduction compactly by so-called **codebooks**.
- During training, a scoring classifier is trained for each column.
- The k -th row is called **codeword** for class k .
- Knowing the principle of **codebooks**, we can define multiclass-to-binary reductions quite flexibly.
- We can now ask ourselves, how to create optimal codebooks.

Class	$f_1(\mathbf{x})$	$f_2(\mathbf{x})$	$f_3(\mathbf{x})$
1	1	-1	-1
2	-1	1	-1
3	-1	-1	1

Class	$f_1(\mathbf{x})$	$f_2(\mathbf{x})$	$f_3(\mathbf{x})$
1	1	-1	0
2	-1	0	1
3	0	1	-1

Left: one-vs-rest codebook. Right: one-vs-one codebook.

CODEBOOKS: DECIDING LABELS

For a general codebook, once we trained the classifiers, how to predict the class \hat{y} for a new input \mathbf{x} ?

- When a new sample \mathbf{x} is going to be classified, all classifiers f_k are applied to \mathbf{x} , scores are potentially transformed and turned into binary labels by $\text{sgn}(f_k(\mathbf{x}))$.

Class	$f_1(\mathbf{x})$	$f_2(\mathbf{x})$	$f_3(\mathbf{x})$
1	1	1	0
2	-1	1	1
3	0	-1	-1
$\text{sgn}(\hat{f}(\mathbf{x}))$	-1	1	-1

- We obtain a code for the observation \mathbf{x} for which we can calculate the distance to the codewords of the other classes. This can be done by **Hamming distance** (counting the number of bits that differ) or by L_1 -distance.

CODEBOOKS: DECIDING LABELS

- For example, the L_1 -distance between $\text{sgn}(\hat{f}(\mathbf{x})) = (-1, 1, -1)$ and the class 1 codeword $(1, 1, 0)$ is 3.
- We can do so for all the classes to obtain respective distances:

Classes	Dist
1	3
2	2
3	3

The distance for class 2 is minimal, therefore we predict class 2 for the input \mathbf{x} .

DEFINING GOOD CODEBOOKS

Question: How to define a good codebook?

- Assume we are given a test observation (\mathbf{x}, y) with $y = 2$.
- Assume classifier $f_2(\mathbf{x})$ produces a false prediction:

Class	$f_1(\mathbf{x})$	$f_2(\mathbf{x})$	$f_3(\mathbf{x})$	Dist
1	1	-1	0	3
2	-1	1	1	2
3	0	-1	-1	3
$ \hat{f}(\mathbf{x}) $	-1	-1	1	

- Even though $f_2(\mathbf{x})$ is wrong, the overall prediction will be correct in the above case, if we pick the best codeword w.r.t. distance from the predicted codeword.
- We effectively **corrected** for the error.
- This motivates a desirable characteristic of a codebook: we want to have codes that can correct for as many errors as possible.
- Which is called **error-correcting output codes** (ECOC).

Error-Correcting Codes (ECOC)

ERROR-CORRECTING CODES (ECOC)

The power of a code to correct errors is related to the **row separation**:

- Each codeword should be well-separated in Hamming distance from each of the other codewords.
- Otherwise, if the class codewords are very similar, a prediction error in a single binary classifier easily results in an “overall” error.
- If the minimum distance between any pair of codewords is d , the code can correct at least $\left\lfloor \frac{d-1}{2} \right\rfloor$ single bit errors.

ERROR-CORRECTING CODES (ECOC)

Another desirable property is **column separation**:

- Columns should be uncorrelated.
- If two columns k and l are similar or identical, a learning algorithm will make similar (correlated) mistakes in learning f_k and f_l .
- Error-correcting codes only succeed if the errors made in the individual classifiers are relatively uncorrelated, so that the number of simultaneous errors in many classifiers is small.
- Errors in classifiers f_k and f_l will also be highly correlated if the bits in those columns are complementary.
- Try to ensure that columns are neither identical nor complementary.

→ **We want to maximize distances between rows, and want the distances between columns to not be too small (identical columns) or too high (complementary columns).**

ERROR-CORRECTING CODES (ECOC)

Remark:

- In general, if there are k classes, there will be at most $2^{k-1} - 1$ usable binary columns.
- For example for $k = 3$, there are only $2^3 = 8$ possible columns. Of these, half are complements of the other half. The columns that only contain 1s or the one that only contains -1s are also not usable.

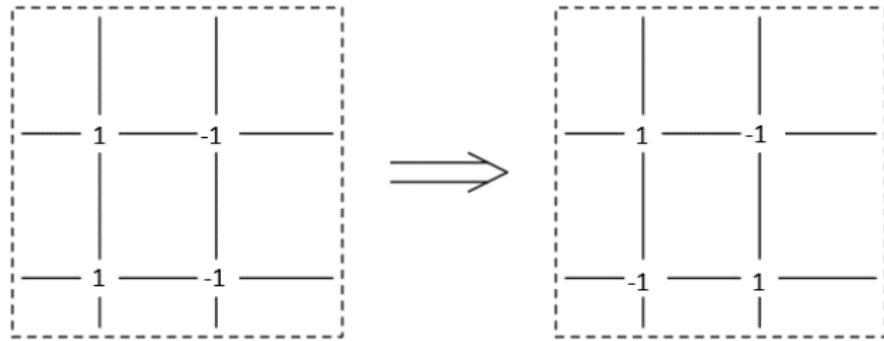
Class	$f_1(\mathbf{x})$	$f_2(\mathbf{x})$	$f_3(\mathbf{x})$	$f_4(\mathbf{x})$	$f_5(\mathbf{x})$	$f_6(\mathbf{x})$	$f_7(\mathbf{x})$	$f_8(\mathbf{x})$
1	-1	-1	-1	-1	1	1	1	1
2	-1	-1	1	1	-1	-1	1	1
3	-1	1	-1	1	-1	1	-1	1

ERROR-CORRECTING CODES (ECOC)

Assume we have the budget to train L binary classifiers and now want to find an error-correcting code with maximal row and column separation.

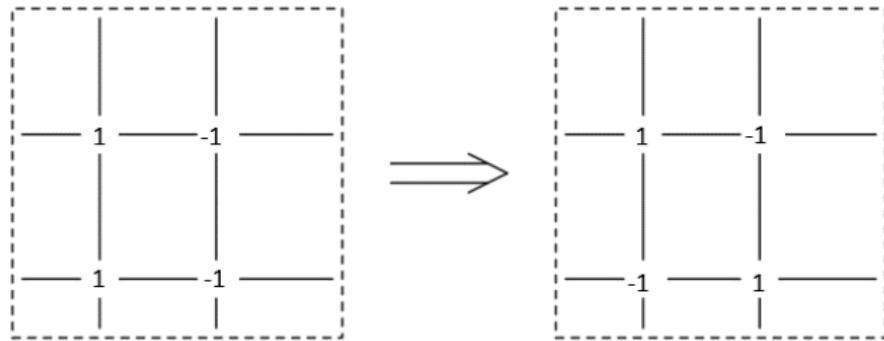
- For only few classes $g \leq 11$, exhaustive search can be performed and a codebook that has good row and column separation is chosen.
- However, for many classes $g > 11$, it becomes more and more challenging to find the optimal codebook with codewords of length L .
- *Dietterich et al.* employed a randomized hill-climbing algorithm for this task.

ECOC: RANDOMIZED HILL-CLIMBING ALGORITHM



- g codewords of length L are randomly drawn.
- Any pair of such random strings will be separated by a Hamming distance that is binomially distributed with mean $\frac{L}{2}$.
- The algorithm now iteratively improves the code: The algorithm repeatedly finds the pair of rows closest together (in Hamming distance or any other distance) and the pair of columns that have the “most extreme” distance (i.e. too close, or too far apart).

ECOC: RANDOMIZED HILL-CLIMBING ALGORITHM



- The algorithm then computes the four codeword bits where these rows and columns intersect and changes them to improve the row and column separations
- When the procedure reaches a local maximum, the algorithm randomly chooses pairs of rows and columns and tries to improve their separation.

INTRODUCTION TO MACHINE LEARNING

Advanced Risk Minimization

Multiclass Classification

Information Theory

Curse of Dimensionality

Hypothesis Space

Regularization

Linear Support Vector Machine

Nonlinear Support Vector Machine

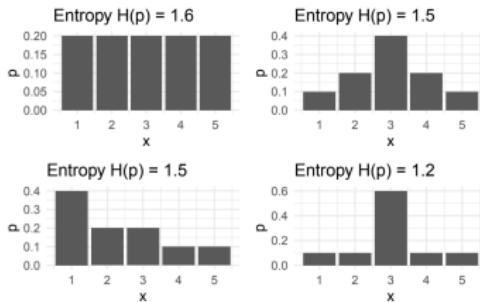
Gaussian Processes

Boosting

Introduction to Machine Learning

Entropy

Learning goals



- Know that the entropy expresses expected information for discrete RVs
- Entropy for a single RV
- Joint entropy for two RVs
- Understand that the uniqueness theorem justifies the choice for the formula of the entropy

INFORMATION THEORY

- **Information Theory** is a field of study based on probability theory.
- The foundation of the field was laid by Claude Shannon in 1948 and it has since found applications in areas as diverse as communication theory, computer science, optimization, cryptography, machine learning and statistical inference.
- In addition to quantifying information, it also deals with efficiently storing and transmitting the information.
- Information theory tries to quantify the "amount" of information gained or uncertainty reduced when a random variable is observed.

INFORMATION THEORY

- We introduce the basic concepts from a probabilistic perspective, without referring too much to communication, channels or coding.
- We will show some proofs, but not for everything. We recommend *Elements of Information Theory* by Cover and Thomas as a reference for more.
- The application of information theory to the concepts of statistics and ML can sometimes be confusing, we will try to make the connection as clear as possible.

ENTROPY

- We develop in this unit entropy as a measure of uncertainty.
- Entropy is often introduced in IT as a measure of expected information or in terms of bits needed for efficient coding, but for us in stats and ML the first type of intuition seems most useful.

For a discrete random variable X with domain $x \in \mathcal{X}$ and pmf $p(x)$:

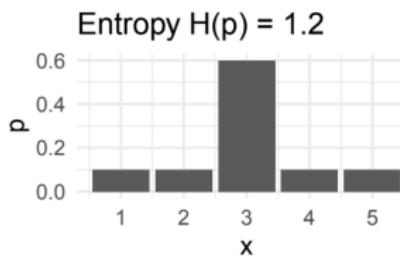
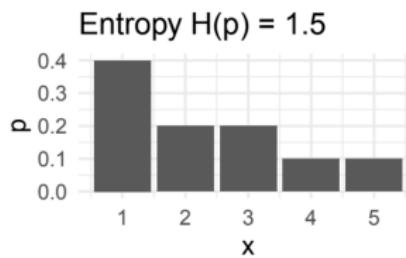
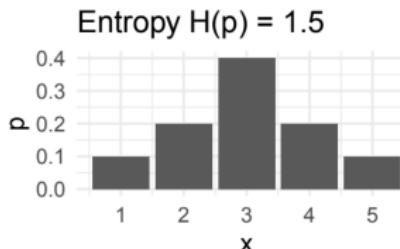
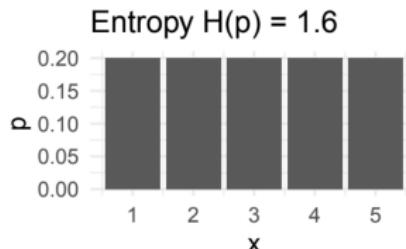
$$\begin{aligned} H(X) := H(p) &= -\mathbb{E}[\log_2(p(X))] = -\sum_{x \in \mathcal{X}} p(x) \log_2 p(x) \\ &= \mathbb{E} \left[\log_2 \left(\frac{1}{p(X)} \right) \right] = \sum_{x \in \mathcal{X}} p(x) \log_2 \frac{1}{p(x)} \end{aligned}$$

- **Definition:** Base 2 means the information is measured in bits, but you can use any number > 1 as base of the logarithm.
- **Note:** Because $\lim_{p \rightarrow 0} p \log_2 p = 0$, if $p(x) = 0$, $p(x) \log_2 p(x)$ is taken to be zero for $x = 0$.

ENTROPY

- We have encountered various other measures of spread or uncertainty in statistics before.
- Furthermore, the formula does not seem to make intuitive sense?
- We will now do the following:
 - Approach it by various simple examples.
 - Note some basic properties - which seem desirable for an uncertainty measure.
 - Note that if we require these measures axiomatically, entropy drops out automatically as the result.
 - Note even more nice properties.

ENTROPY EXAMPLES

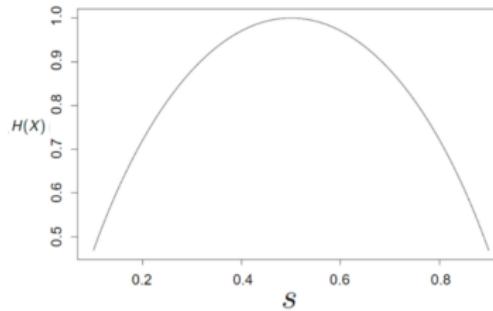


Naive observations: Uniform seems maximal, re-ordering does not matter, and the more peaked, the less entropy.

ENTROPY OF BERNOULLI DISTRIBUTION

Let X be Bernoulli / a coin with $\mathbb{P}(X = 1) = s$ and $\mathbb{P}(X = 0) = 1 - s$.

$$H(X) = -s \cdot \log_2(s) - (1 - s) \cdot \log_2(1 - s).$$

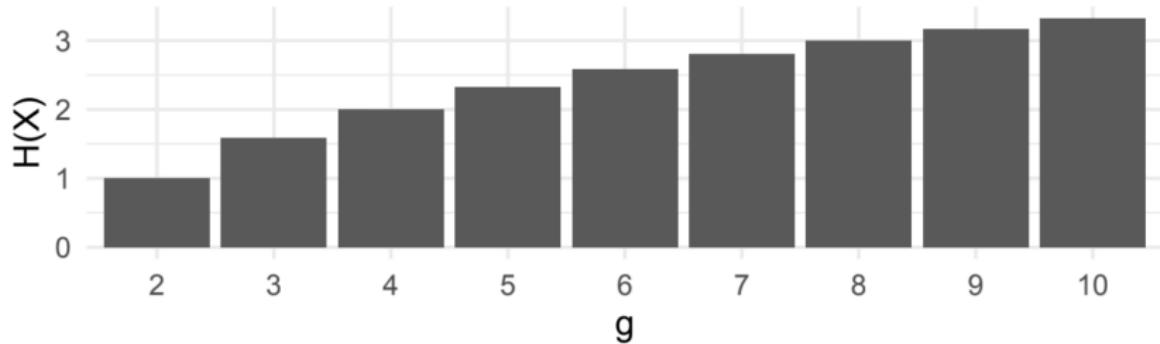


We note: If the coin is deterministic, so $s = 1$ or $s = 0$, then $H(s) = 0$; $H(s)$ is maximal for $s = 0.5$, a fair coin. $H(s)$ becomes monotonically larger the closer we get to $s = 0.5$. This all seems plausible.

ENTROPY OF UNIFORM DISTRIBUTIONS

Let X be a uniform, discrete RV with g outcomes (g -sided fair die).

$$H(X) = - \sum_{i=1}^g \frac{1}{g} \log_2 \left(\frac{1}{g} \right) = \log_2 g$$



The more sides a die has, the harder it is to predict the outcome.
Unpredictability grows *monotonically* with the number of potential outcomes

PROPERTIES OF DISCRETE ENTROPY

- ① Entropy is non-negative, so $H(X) \geq 0$.
- ② If one event has probability $p(x) = 1$, then $H(X) = 0$.
- ③ Symmetry. If the values $p(x)$ in the pmf are re-ordered, entropy does not change.
- ④ Adding or removing an event with $p(x) = 0$ does not change entropy.
- ⑤ $H(X)$ is continuous in probabilities $p(x)$.
- ⑥ Entropy is additive for independent RVs.
- ⑦ Entropy is maximal for a uniform distribution, so for a domain with g elements: $H(X) \leq -g\frac{1}{g} \log_2(\frac{1}{g}) = \log_2(g)$.

All properties except the last 2 follow trivially from the definition.

JOINT ENTROPY

- The **joint entropy** of two discrete random variables X and Y is:

$$H(X, Y) = H(p_{X,Y}) = - \sum_{x \in \mathcal{X}} \sum_{y \in \mathcal{Y}} p(x, y) \log_2(p(x, y))$$

- Intuitively, the joint entropy is a measure of the total uncertainty in the two variables X and Y . In other words, it is simply the entropy of the joint distribution $p(x, y)$.
- There is nothing really new in this definition because $H(X, Y)$ can be considered to be a single vector-valued random variable.
- More generally:

$$H(X_1, X_2, \dots, X_n) = - \sum_{x_1 \in \mathcal{X}_1} \dots \sum_{x_n \in \mathcal{X}_n} p(x_1, x_2, \dots, x_n) \log_2(p(x_1, x_2, \dots, x_n))$$

ENTROPY IS ADDITIVE UNDER INDEPENDENCE

Let X and Y be two independent RVs. Then:

$$\begin{aligned} H(X, Y) &= - \sum_{x \in \mathcal{X}} \sum_{y \in \mathcal{Y}} p(x, y) \log_2(p(x, y)) \\ &= - \sum_{x \in \mathcal{X}} \sum_{y \in \mathcal{Y}} p_X(x)p_Y(y) \log_2(p_X(x)p_Y(y)) \\ &= - \sum_{x \in \mathcal{X}} \sum_{y \in \mathcal{Y}} p_X(x)p_Y(y) \log_2(p_X(x)) + p_X(x)p_Y(y) \log_2(p_Y(y)) \\ &= - \sum_{x \in \mathcal{X}} \sum_{y \in \mathcal{Y}} p_X(x)p_Y(y) \log_2(p_X(x)) - \sum_{y \in \mathcal{Y}} \sum_{x \in \mathcal{X}} p_X(x)p_Y(y) \log_2(p_Y(y)) \\ &= - \sum_{x \in \mathcal{X}} p_X(x) \log_2(p_X(x)) - \sum_{y \in \mathcal{Y}} p_Y(y) \log_2(p_Y(y)) = H(X) + H(Y) \end{aligned}$$

ENTROPY OF UNIFORM DISTRIBUTIONS

Claim: The entropy of a discrete random variable X which takes on values in $\{x_1, x_2, \dots, x_g\}$ with associated probabilities $\{p_1, p_2, \dots, p_g\}$ is maximal when the distribution over X is uniform.

Proof: The entropy $H(X)$ is $-\sum_{i=1}^g p_i \log_2 p_i$ and our goal is to find:

$$\operatorname{argmax}_{p_1, p_2, \dots, p_g} - \sum_{i=1}^g p_i \log_2 p_i$$

subject to

$$\sum_{i=1}^g p_i = 1.$$

ENTROPY OF UNIFORM DISTRIBUTIONS

The Lagrangian $L(p_1, \dots, p_g, \lambda)$ is :

$$L(p_1, \dots, p_g, \lambda) = - \sum_{i=1}^g p_i \log_2(p_i) - \lambda \left(\sum_{i=1}^g p_i - 1 \right)$$

Solving for $\nabla L = 0$,

$$\begin{aligned} \frac{\partial L(p_1, \dots, p_g, \lambda)}{\partial p_i} &= 0 = -\log_2(p_i) - 1 - \lambda \\ \implies p_i &= 2^{(-1-\lambda)} \implies p_i = \frac{1}{g}, \end{aligned}$$

where the last step follows from the fact that all p_i are equal and the constraint.

THE UNIQUENESS THEOREM

Khinchin (1957) showed that the only family of functions satisfying

- $H(p)$ is continuous in probabilities $p(x)$
- adding or removing an event with $p(x) = 0$ does not change it
- is additive for independent RVs
- is maximal for a uniform distribution.

is of the following form:

$$H(p) = -\lambda \sum_{x \in \mathcal{X}} p(x) \log p(x)$$

where λ is a positive constant. Setting $\lambda = 1$ and using the binary logarithm gives us the Shannon entropy.

Introduction to Machine Learning

Differential Entropy

Learning goals



- Know that the entropy expresses expected information for continuous RVs
- Know the basic properties of the differential entropy

DIFFERENTIAL ENTROPY

- For a continuous random variable X with density function $f(x)$ and support \mathcal{X} , the analogue of entropy is **differential entropy**:

$$h(X) := h(f) := - \int_{\mathcal{X}} f(x) \log(f(x)) dx$$

- The base of the log is again somewhat arbitrary, and we could either use 2 (and measure in bits) or e (to measure in nats).
- The integral above does not necessarily exist for all densities.
- Differential entropy lacks some properties of discrete entropy.
- $h(X) < 0$ is possible because $f(x) > 1$ is possible.

DIFF. ENTROPY OF UNIFORM DISTRIBUTION

Let X be a uniform random variable on $[0, a]$.

$$\begin{aligned} h(X) &= - \int_0^a f(x) \log(f(x)) dx \\ &= - \int_0^a \frac{1}{a} \log\left(\frac{1}{a}\right) dx = \log(a) \end{aligned}$$

- For $a < 1$, $h(X) < 0$.

DIFF. ENTROPY OF GAUSSIAN

Let X be a Gaussian random variable $X \sim \mathcal{N}(\mu, \sigma^2)$ and let us measure in nats:

$$\begin{aligned} h(X) &= - \int_{\mathbb{R}} f(x) \ln(f(x)) dx \\ &= - \int_{\mathbb{R}} f(x) \ln \left(\frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}} \right) dx \\ &= - \int_{\mathbb{R}} f(x) \ln \left(\frac{1}{\sqrt{2\pi\sigma^2}} \right) dx + \int_{\mathbb{R}} f(x) \frac{(x-\mu)^2}{2\sigma^2} dx \\ &= - \underbrace{\ln \left(\frac{1}{\sqrt{2\pi\sigma^2}} \right)}_{=1} \underbrace{\int_{\mathbb{R}} f(x) dx}_{=} + \frac{1}{2\sigma^2} \underbrace{\int_{\mathbb{R}} f(x)(x-\mu)^2 dx}_{=: \sigma^2} \\ &= \frac{1}{2} \ln(2\pi\sigma^2) + \frac{1}{2} = \ln(\sigma\sqrt{2\pi e}) \end{aligned}$$

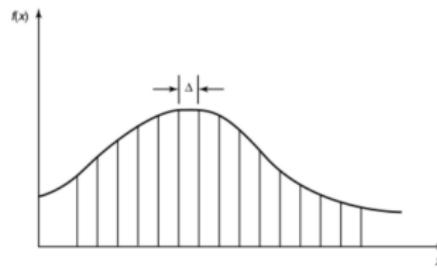
DIFF. ENTROPY OF GAUSSIAN

- $h(X)$ is not a function of μ (see translation invariance).
- As σ^2 increases, the differential entropy also increases.
- For $\sigma^2 < \frac{1}{2\pi e}$, it is negative.

DIFF. ENTROPY VS. DISCRETE

It is not so simple as to characterize $h(X)$ as a straightforward generalization of $H(X)$ of a limiting process. Consider the quantized random variable X^Δ , which is defined by

$$X^\Delta = x_i \quad \text{if} \quad i\Delta \leq X < (i+1)\Delta$$



If the density $f(x)$ of the random variable X is Riemann-integrable, then

$$H(X^\Delta) + \log(\Delta) \rightarrow h(X) \text{ as } \Delta \rightarrow 0.$$

Thus, the entropy of an n -bit quantization of a continuous random variable X is approximately $h(X) + n$.

JOINT DIFFERENTIAL ENTROPY

- For a continuous random vector X with density function $f(x)$ and support \mathcal{X} , differential entropy is also defined as:

$$h(X) = h(X_1, \dots, X_n) = h(f) = - \int_{\mathcal{X}} f(x) \log(f(x)) dx$$

- Hence this also defines the joint differential entropy for a set of continuous RVs.

Entropy of a multivariate normal distribution: If $X \sim N(\mu, \Sigma)$ is multivariate Gaussian, then

$$h(X) = \frac{1}{2} \ln(2\pi e)^n |\Sigma| \quad (\text{nats})$$

PROPERTIES OF DIFFERENTIAL ENTROPY

- ① $h(f)$ can be negative.
- ② $h(f)$ is additive for independent RVs.
- ③ $h(f)$ is maximized by the multivariate normal, if we restrict to all distributions with the same (co)variance, so $h(X) \leq \frac{1}{2} \ln(2\pi e)^n |\Sigma|$.
- ④ Translation-invariant, $h(X + a) = h(X)$.
- ⑤ $h(aX) = h(X) + \log |a|$.
- ⑥ $h(AX) = h(X) + \log |A|$ for random vectors and matrix A.

Introduction to Machine Learning

Entropy and Optimal Code Length

Learning goals

0 0 0 1 0 0 1 1	encoded string
00 01 00 11	codewords
dog cat dog bird	source symbols

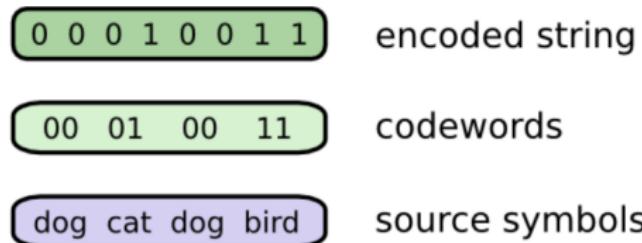
- Know that source coding is about encoding messages efficiently
- Know how to compute the average length of a code
- Know that the entropy of the source distribution is the lower bound for the average code length

SOURCE CODING

- There is an interesting connection between entropy and a subfield of information theory known as **source coding**.
- Abstractly, a source is any system or process that generates messages or information.
- A code is simply a way to represent the message so that it can be stored or transmitted over a communication channel (such as radio or fiber-optic cables).
- For example, one could use binary strings (0's and 1's) to encode messages.
- Because it may be expensive to transmit or store information, an important problem addressed by source coding is efficient coding schemes of minimal average length.

SOURCE CODING

- Formally, given a discrete alphabet/dictionary X of message symbols, a **binary code** is a mapping from symbols in X to a set of codewords of binary strings.
- For example, if our dictionary only consists of the words "dog", "cat", "fish" and "bird", each word can be encoded as a binary string of length 2 : "dog" → **00**, "cat" → **01**, "fish" → **10** and "bird" → **11**.
- For this code, a binary string can be decoded by replacing each successive pair of digits with the associated word.

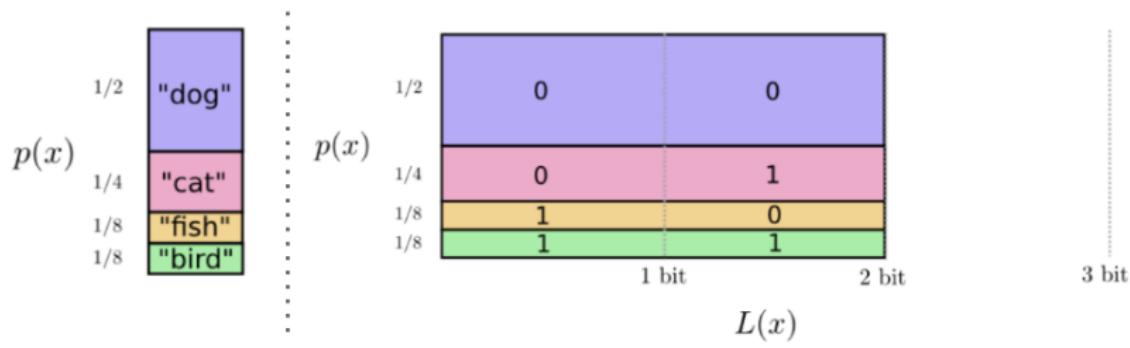


Credit: Chris Olah

Chris Olah (2015): Visual Information Theory. <http://colah.github.io/posts/2015-09-Visual-Information/>

SOURCE CODING

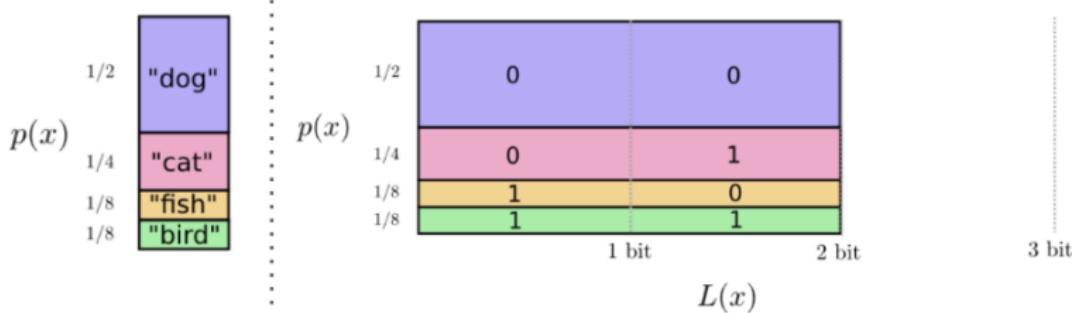
- Encoded messages are emitted by a source which can be modeled as a probability distribution over the message symbols in the dictionary.
- Let X be a random variable that represents a symbol from our data source and let $p(x) = \mathbb{P}(X = x)$, for symbol x in our dictionary.



Credit: Chris Olah

- The length $L(x)$ is simply the number of bits in the corresponding codeword. In this example, all codewords have length 2.

SOURCE CODING



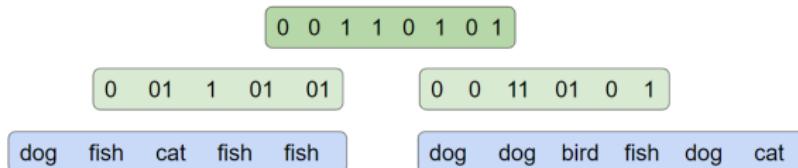
- For this code, the expected length of a message emitted by the source is, naturally:

$$\mathbb{E}[L(X)] = \frac{1}{2} \cdot 2 + \frac{1}{4} \cdot 2 + \frac{1}{8} \cdot 2 + \frac{1}{8} \cdot 2 = 2 \text{ bits.}$$

- The area of a rectangle in the image on the right reflects the size of the corresponding term in the expectation.

SOURCE CODING

- Maybe we can create better average-length coding schemes with **variable-length** codes by assigning shorter codes to more likely messages and longer one to less likely messages.
- However, this can be problematic because we want the receiver to be able to unambiguously decode the encoded string.
- Let us say the words in our dictionary are encoded in this way: "dog" → **0**, "cat" → **1**, "fish" → **01** and "bird" → **11**.
- In this case, the string 00110101 can be decoded in multiple ways.



- One way to make variable-length messages unambiguous is by ensuring that no codeword is a prefix (initial segment) of any other codeword. Such a code is known as a **prefix code**.

SOURCE CODING

- In general, the number of possible codewords grows exponentially in length L .
- For binary codes, there are two possible words of length one, four possible words of length two and 2^L possible words of length L .

0	0	0
		1
1	1	0
		1
1	0	0
		1
1	1	0
		1

bit 1 bit 2 bit 3

- In total, there are $(2^{L+1} - 2)$ codewords of length $\leq L$.

SOURCE CODING

0	0	0	$\frac{1}{2^L} = \frac{1}{4}$
	1	1	
1	0	0	$\frac{1}{2^L} = \frac{1}{4}$
	1	1	

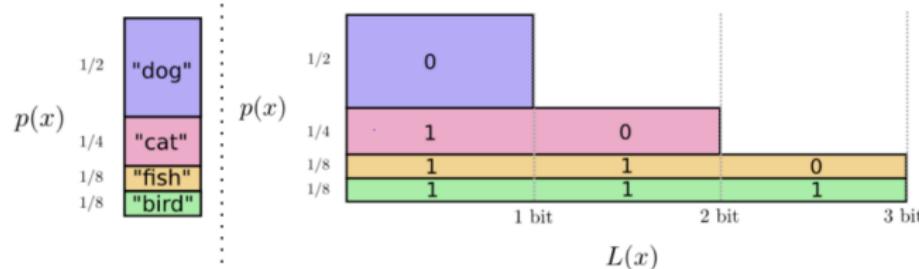
bit 1 bit 2 bit 3

- Here, if the codeword **01** is assigned to a symbol, then **010** and **011** cannot be assigned to any other symbol because that would break the prefix property.
- If a codeword of length L is assigned to a symbol, then $\frac{1}{2^L}$ of the possible codewords of length $> L$ must be discarded.
- If some symbols are assigned short codewords, due to the prefix property, many marginally longer codewords cannot be assigned to other symbols.

SOURCE CODING

- An example of prefix code:

"dog" → 0, "cat" → 10, "fish" → 110 and "bird" → 111.



- Here, the expected code length is :

$$\begin{aligned} \mathbb{E}[L(X)] &= \frac{1}{2} \cdot 1 + \frac{1}{4} \cdot 2 + \frac{1}{8} \cdot 3 + \frac{1}{8} \cdot 3 \\ &= -\frac{1}{2} \cdot \log_2 \left(\frac{1}{2} \right) - \frac{1}{4} \cdot \log_2 \left(\frac{1}{4} \right) - \frac{1}{8} \cdot \log_2 \left(\frac{1}{8} \right) - \frac{1}{8} \cdot \log_2 \left(\frac{1}{8} \right) \\ &= H(X) = 1.75 \text{ bits. } (< 2 \text{ bits}) \end{aligned}$$

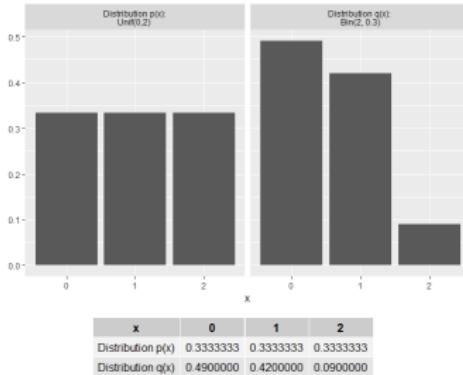
- Actually, this coding scheme is the most efficient way to store and transmit these messages. It is simply not possible to do better!

SOURCE CODING

- In fact, Shannon's **source coding theorem** (or **noiseless coding theorem**) tells us that the optimal trade-off is made when the code length of a symbol with probability p is $\log(1/p)$.
- In other words, the entropy of the source distribution is the theoretical lower bound on the average code length.
- If it is any lower, some information will be distorted or lost.
- In practice, algorithms such as Huffman Coding can be used to find variable-length codes that are close (in terms of expected length) to the theoretical limit.

Introduction to Machine Learning

Kullback-Leibler Divergence



Learning goals

- Know the KL divergence as distance between distributions
- Understand KL as expected log-difference
- Understand how KL can be used as loss
- Understand that KL is equivalent to the expected likelihood ratio

KULLBACK-LEIBLER DIVERGENCE

We now want to establish a measure of distance between (discrete or continuous) distributions with the same support:

$$D_{KL}(p\|q) = \mathbb{E}_p \left[\log \frac{p(X)}{q(X)} \right] = \sum_{x \in \mathcal{X}} p(x) \cdot \log \frac{p(x)}{q(x)},$$

or:

$$D_{KL}(p\|q) = \mathbb{E}_p \left[\log \frac{p(X)}{q(X)} \right] = \int_{x \in \mathcal{X}} p(x) \cdot \log \frac{p(x)}{q(x)}.$$

In the above definition, we use the convention that $0 \log(0/0) = 0$ and the convention (based on continuity arguments) that $0 \log(0/q) = 0$ and $p \log(p/0) = \infty$. Thus, if there is any symbol $x \in \mathcal{X}$ such that $p(x) > 0$ and $q(x) = 0$, then $D_{KL}(p\|q) = \infty$.

KULLBACK-LEIBLER DIVERGENCE

$$D_{KL}(p\|q) = \mathbb{E}_p \left[\log \frac{p(X)}{q(X)} \right]$$

- What is the intuition behind this formula?
- We will soon see that KL has quite some value in measuring “differences” but is not a true distance.
- We already see that the formula is not symmetric and it often makes sense to think of p as the first or original form of the data, and q as something that we want to measure the quality of with reference to p .

INFORMATION INEQUALITY

$D_{KL}(p\|q) \geq 0$ holds always true for any pair of distributions, and holds with equality if and only if $p = q$.

We use Jensen's inequality. Let A be the support of p :

$$\begin{aligned}-D_{KL}(p\|q) &= - \sum_{x \in A} p(x) \log \frac{p(x)}{q(x)} \\&= \sum_{x \in A} p(x) \log \frac{q(x)}{p(x)} \\&\leq \log \sum_{x \in A} p(x) \frac{q(x)}{p(x)} \\&\leq \log \sum_{x \in \mathcal{X}} q(x) = \log(1) = 0\end{aligned}$$

As \log is strictly concave, Jensen also tells us that equality can only happen if $q(x)/p(x)$ is constant everywhere. That implies $p = q$.

KL AS LOG-DIFFERENCE

Suppose that data is being generated from an unknown distribution $p(x)$. Suppose we modeled $p(x)$ using an approximating distribution $q(x)$.

First, we could simply see KL as the expected log-difference between $p(x)$ and $q(x)$:

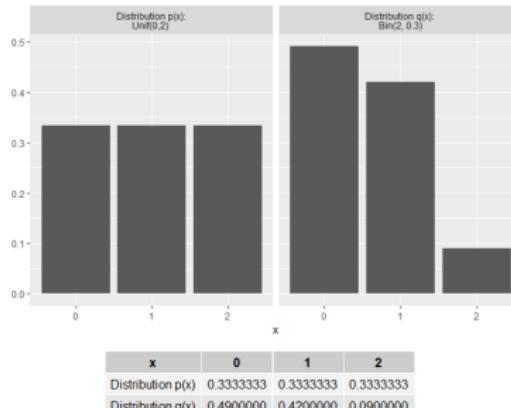
$$D_{KL}(p\|q) = \mathbb{E}_p(\log(p(x)) - \log(q(x))).$$

This is why we integrate out with respect to the data distribution p . A “good” approximation $q(x)$ should minimize the difference to $p(x)$.

KL AS LOG-DIFFERENCE

In machine learning, KL divergence is commonly used to quantify how different one distribution is from another.

Example: Let $q(x)$ be a binomial distribution with $N = 2$ and $p = 0.3$ and let $p(x)$ be a discrete uniform distribution. Both distributions have the same support $\mathcal{X} = \{0, 1, 2\}$.



KL AS LOG-DIFFERENCE

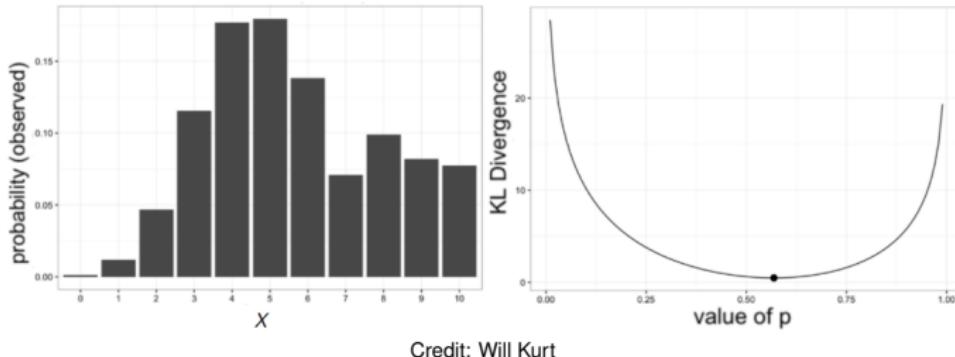
$$\begin{aligned} D_{KL}(p\|q) &= \sum_{x \in \mathcal{X}} p(x) \ln \left(\frac{p(x)}{q(x)} \right) \\ &= 0.333 \ln \left(\frac{0.333}{0.49} \right) + 0.333 \ln \left(\frac{0.333}{0.42} \right) + 0.333 \ln \left(\frac{0.333}{0.09} \right) \\ &= 0.23099 \text{ (nats)} \end{aligned}$$

$$\begin{aligned} D_{KL}(q\|p) &= \sum_{x \in \mathcal{X}} q(x) \ln \left(\frac{q(x)}{p(x)} \right) \\ &= 0.49 \ln \left(\frac{0.49}{0.333} \right) + 0.42 \ln \left(\frac{0.42}{0.333} \right) + 0.09 \ln \left(\frac{0.09}{0.333} \right) \\ &= 0.16801 \text{ (nats)} \end{aligned}$$

Again, note that $D_{KL}(p\|q) \neq D_{KL}(q\|p)$.

KL IN FITTING

Because KL quantifies the difference between distributions, it can be used as a loss function to find a good fit for the observed data.



Credit: Will Kurt

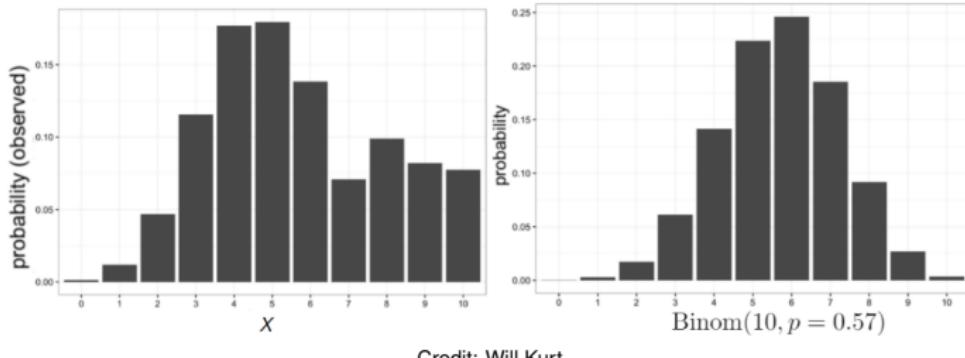
Figure: Left: Histogram of observed frequencies of a random variable X which takes values between 0 and 10. Right: The KL divergence between the observed data and $\text{Binom}(10, p)$ is minimized when $p \approx 0.57$.

Will Kurt (2017): Kullback-Leibler Divergence Explained.

<https://www.countbayesie.com/blog/2017/5/9/kullback-leibler-divergence-explained>

KL IN FITTING

Because KL quantifies the difference between distributions, it can be used as a loss function to find a good fit for the observed data.



Credit: Will Kurt

Figure: Left: Histogram of observed frequencies of a random variable which takes values between 0 and 10. Right: Fitted Binomial distribution ($p \approx 0.57$).

On the right is the Binomial distribution that minimizes the KL divergence.

KL AS LIKELIHOOD RATIO

- Let us assume we have some data and want to figure out whether $p(x)$ or $q(x)$ matches it better.
- How do we usually do that in stats? Likelihood ratio!

$$LR = \frac{p(x)}{q(x)}$$

In the above, if for x we have $LR > 1$, then p seems better, for $LR < 1$ q seems better.

KL AS LIKELIHOOD RATIO

Or we can compute LR for a complete set of data (as always, logs make our life easier):

$$LR = \prod_i \frac{p(\mathbf{x}^{(i)})}{q(\mathbf{x}^{(i)})} \quad LLR = \sum_i \log \frac{p(\mathbf{x}^{(i)})}{q(\mathbf{x}^{(i)})}$$

Now let us assume that our data already come from p . It does not really make sense anymore to ask whether p or q fit the data better.

But maybe we want to pose the question "How different is q from p ?" by formulating it as: "If we sample many data from p , how easily can we see that p is better than q through LR, on average?"

$$\mathbb{E}_p \left[\log \frac{p(x)}{q(x)} \right]$$

That expected LR is really KL!

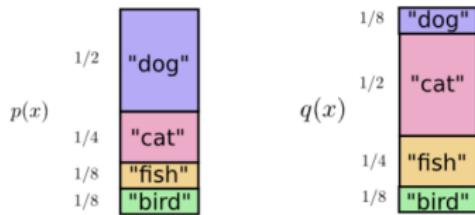
KL AS LIKELIHOOD RATIO

In summary we could say for KL:

- It measures how much "evidence" each sample provides on average to distinguish p from q , if you sample from p .
- If p and q are very similar, most samples will not help much, and vice versa for very different distributions.
- In practice, we often want to make the approximation q as indistinguishable from the real p (our data) as possible. We already did that when we fitted (in our log-difference perspective).

Introduction to Machine Learning

Cross-Entropy, KL and Source Coding

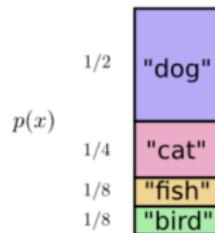


Learning goals

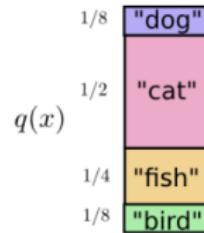
- Know the cross-entropy
- Understand the connection between entropy, cross-entropy, and KL divergence

CROSS-ENTROPY - DISCRETE CASE

- For a random source / distribution p , the minimal number of bits to optimally encode messages from is the entropy $H(p)$.
- If the optimal code for a different distribution $q(x)$ is instead used to encode messages from $p(x)$, expected code length will grow.



$$H(p) = H_p(p) = 1.75 \text{ bits}$$



$$H_q(p) = 2.375 \text{ bits}$$

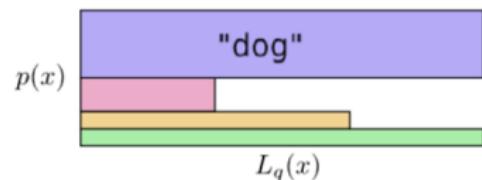
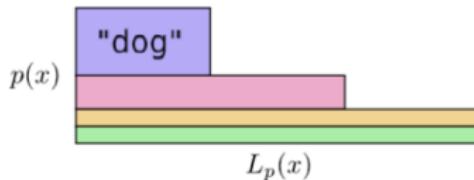


Figure: $L_p(x)$, $L_q(x)$ are the optimal code lengths for $p(x)$ and $q(x)$

CROSS-ENTROPY - DISCRETE CASE

Cross-entropy is the average length of communicating an event from one distribution with the optimal code for another distribution (assume they have the same domain \mathcal{X} as in KL).

$$H_q(p) = \sum_{x \in \mathcal{X}} p(x) \log \left(\frac{1}{q(x)} \right) = - \sum_{x \in \mathcal{X}} p(x) \log (q(x))$$

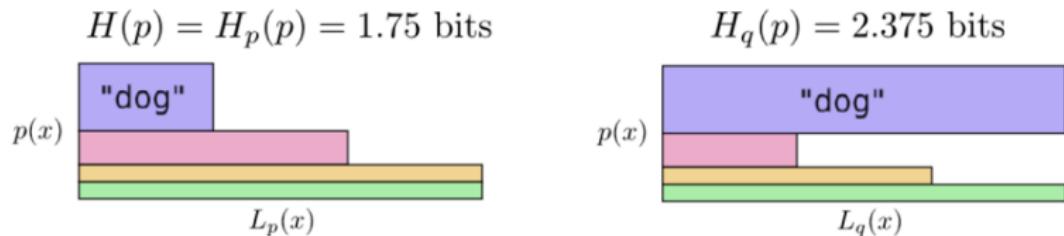
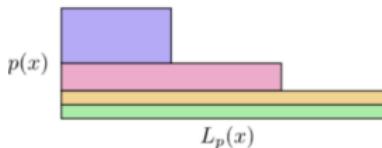


Figure: $L_p(x)$, $L_q(x)$ are the optimal code lengths for $p(x)$ and $q(x)$

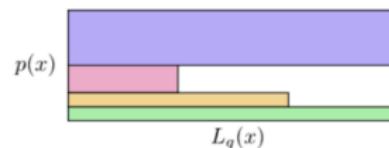
We directly see: cross-entropy of p with itself is entropy: $H_p(p) = H(p)$.

CROSS-ENTROPY - DISCRETE CASE

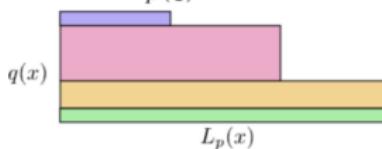
$$H(p) = H_p(p) = 1.75 \text{ bits}$$



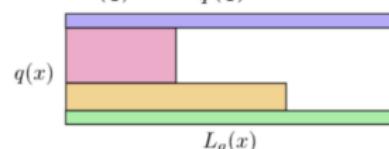
$$H_q(p) = 2.375 \text{ bits}$$



$$H_p(q) = 2.25 \text{ bits}$$



$$H(q) = H_q(q) = 1.75 \text{ bits}$$

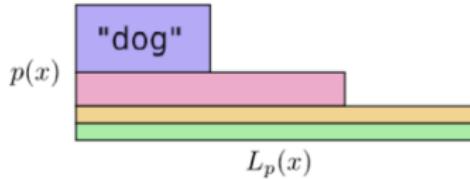


Credit: Chris Olah

- In top, $H_q(p)$ is greater than $H(p)$ primarily because the blue event that is very likely under p has a very long codeword in q .
- Same, in bottom, for pink when we go from q to p .
- Note that $H_q(p) \neq H_p(q)$.

CROSS-ENTROPY - DISCRETE CASE

$$H(p) = H_p(p) = 1.75 \text{ bits}$$



$$H_q(p) = 2.375 \text{ bits}$$

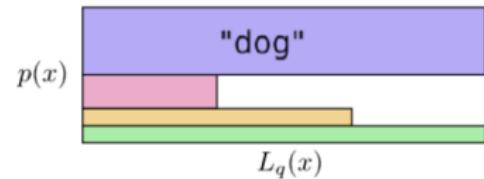


Figure: $L_p(x), L_q(x)$ are the optimal code lengths for $p(x)$ and $q(x)$

- Let x' denote the symbol "dog". The difference in code lengths is:

$$\log\left(\frac{1}{q(x')}\right) - \log\left(\frac{1}{p(x')}\right) = \log \frac{p(x')}{q(x')}$$

- If $p(x') > q(x')$, this is positive, if $p(x') < q(x')$, it is negative.
- The expected difference is KL, if we encode symbols from p :

$$D_{KL}(p\|q) = \sum_{x \in \mathcal{X}} p(x) \cdot \log \frac{p(x)}{q(x)}$$

CROSS-ENTROPY - DISCRETE CASE

- Entropy = Avg. nr. of bits if we optimally encode p
- Cross-Entropy = Avg. nr. of bits if we suboptimally encode p with q
- $D_{KL}(p\|q)$: Difference in bits between the two

We can summarize this also through this identity:

$$H_q(p) = H(p) + D_{KL}(p\|q)$$

This is because:

$$\begin{aligned} H(p) + D_{KL}(p\|q) &= - \sum_{x \in \mathcal{X}} p(x) \log p(x) + \sum_{x \in \mathcal{X}} p(x) \log \frac{p(x)}{q(x)} \\ &= \sum_{x \in \mathcal{X}} p(x)(-\log p(x) + \log p(x) - \log q(x)) \\ &= - \sum_{x \in \mathcal{X}} p(x) \log q(x) = H_q(p) \end{aligned}$$

CROSS-ENTROPY - CONTINUOUS CASE

For continuous density functions $p(x)$ and $q(x)$:

$$H_p(q) = \int q(x) \ln \left(\frac{1}{p(x)} \right) dx = - \int q(x) \ln(p(x)) dx$$

- It is not symmetric.
- As for the discrete case, $H_p(q) = h(q) + D_{KL}(q||p)$ holds.
- Can now become negative, as the $h(q)$ can be negative!

PROOF: MAXIMUM OF DIFFERENTIAL ENTROPY

Claim: For a given variance, the distribution that maximizes differential entropy is the Gaussian.

Proof: Let $g(x)$ be a Gaussian with mean μ and variance σ^2 and $f(x)$ an arbitrary density function with the same variance. Since differential entropy is translation invariant, we can assume $f(x)$ and $g(x)$ have the same mean.

The KL divergence (which is non-negative) between $f(x)$ and $g(x)$ is:

$$\begin{aligned} 0 \leq D_{KL}(f\|g) &= -h(f) + H_g(f) \\ &= -h(f) - \int_{-\infty}^{\infty} f(x) \ln(g(x)) dx \end{aligned} \tag{1}$$

PROOF: MAXIMUM OF DIFFERENTIAL ENTROPY

The second term in (1) is,

$$\begin{aligned} \int_{-\infty}^{\infty} f(x) \log(g(x)) dx &= \int_{-\infty}^{\infty} f(x) \log\left(\frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}\right) dx \\ &= \int_{-\infty}^{\infty} f(x) \log\left(\frac{1}{\sqrt{2\pi\sigma^2}}\right) dx + \log(e) \int_{-\infty}^{\infty} f(x) \left(-\frac{(x-\mu)^2}{2\sigma^2}\right) dx \\ &= -\frac{1}{2} \log(2\pi\sigma^2) - \log(e) \frac{\sigma^2}{2\sigma^2} = -\frac{1}{2} (\log(2\pi\sigma^2) + \log(e)) \\ &= -\frac{1}{2} \log(2\pi e \sigma^2) = -h(g), \end{aligned} \tag{2}$$

where the last equality follows from the normal distribution example of the entropy chapter. Combining (1) and (2) results in

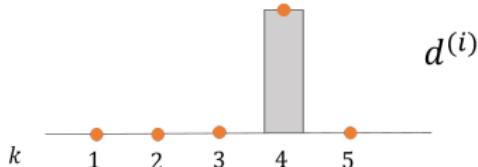
$$h(g) - h(f) \geq 0$$

with equality when $f(x) = g(x)$ (following from the properties of Kullback-Leibler divergence).

Introduction to Machine Learning

Information Theory for Machine Learning

Learning goals



- Minimizing KL is equivalent to maximizing the log-likelihood
- Minimizing KL is equivalent to minimizing cross-entropy
- Minimizing cross-entropy between modeled and observed probabilities is equivalent to log-loss minimization

KL VS MAXIMUM LIKELIHOOD

Minimizing KL between the true distribution $p(x)$ and approximating model $q(x|\theta)$ is equivalent to maximizing the log-likelihood.

$$\begin{aligned} D_{KL}(p\|q_\theta)) &= \mathbb{E}_{x \sim p} \left[\log \frac{p(x)}{q(x|\theta)} \right] \\ &= \mathbb{E}_{x \sim p} \log p(x) - \mathbb{E}_{x \sim p} \log q(x|\theta) \end{aligned}$$

The first term above does not depend on θ . Therefore,

$$\begin{aligned} \arg \min_{\theta} D_{KL}(p\|q_\theta) &= \arg \min_{\theta} -\mathbb{E}_{x \sim p} \log q(x|\theta) \\ &= \arg \max_{\theta} \mathbb{E}_{x \sim p} \log q(x|\theta) \end{aligned}$$

For a finite dataset of n samples from p , this is approximated as

$$\arg \max_{\theta} \mathbb{E}_{x \sim p} \log q(x|\theta) \approx \arg \max_{\theta} \frac{1}{n} \sum_{i=1}^n \log q(\mathbf{x}^{(i)}|\theta).$$

KL VS CROSS-ENTROPY

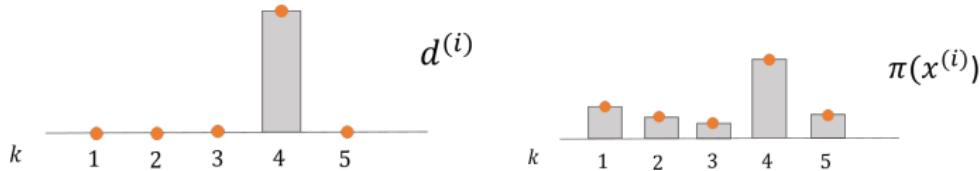
From this here we can actually see much more:

$$\arg \min_{\theta} D_{KL}(p \| q_{\theta}) = \arg \min_{\theta} -\mathbb{E}_{x \sim p} \log q(x | \theta) = H_{q_{\theta}}(p)$$

- So minimizing with respect to KL is the same as minimizing with respect to cross-entropy!
- That implies minimizing with respect to cross-entropy is the same as maximum likelihood!
- Remember, how we only characterized cross-entropy through source coding / bits? We could now motivate cross-entropy as the "relevant" term that you have to minimize, when you minimize KL - after you drop $\mathbb{E}_p \log p(x)$, which is simply the entropy $H(p)$!
- Or we could say: Cross-entropy between p and q is simply the expected negative log-likelihood of q , when our data comes from p !

CROSS-ENTROPY VS. LOG-LOSS

- Consider a multi-class classification task with dataset $\mathcal{D} = ((\mathbf{x}^{(1)}, y^{(1)}), \dots, (\mathbf{x}^{(n)}, y^{(n)}))$.
- For g classes, each $y^{(i)}$ can be one-hot-encoded as a vector $d^{(i)}$ of length g . $d^{(i)}$ can be interpreted as a categorical distribution which puts all its probability mass on the true label $y^{(i)}$ of $\mathbf{x}^{(i)}$.
- $\pi(\mathbf{x}^{(i)}|\theta)$ is the probability output vector of the model, and also a categorical distribution over the classes.



CROSS-ENTROPY VS. LOG-LOSS

To train the model, we minimize KL between $d^{(i)}$ and $\pi(\mathbf{x}^{(i)}|\boldsymbol{\theta})$:

$$\arg \min_{\boldsymbol{\theta}} \sum_{i=1}^n D_{KL}(d^{(i)} \| \pi(\mathbf{x}^{(i)}|\boldsymbol{\theta})) = \arg \min_{\boldsymbol{\theta}} \sum_{i=1}^n H_{\pi(\mathbf{x}^{(i)}|\boldsymbol{\theta})}(d^{(i)})$$

We see that this is equivalent to log-loss risk minimization!

$$\begin{aligned} R &= \sum_{i=1}^n H_{\pi_k(\mathbf{x}^{(i)}|\boldsymbol{\theta})}(d^{(i)}) \\ &= \sum_{i=1}^n \left(- \sum_k d_k^{(i)} \log \pi_k(\mathbf{x}^{(i)}|\boldsymbol{\theta}) \right) \\ &= \sum_{i=1}^n \underbrace{\left(- \sum_{k=1}^g [y^{(i)} = k] \log \pi_k(\mathbf{x}^{(i)}|\boldsymbol{\theta}) \right)}_{\text{log loss}} \\ &= \sum_{i=1}^n (-\log \pi_{y^{(i)}}(\mathbf{x}^{(i)}|\boldsymbol{\theta})) \end{aligned}$$

CROSS-ENTROPY VS. BERNOULLI LOSS

For completeness sake:

Let us use the Bernoulli loss for binary classification:

$$L(y, \pi(\mathbf{x})) = -y \ln(\pi(\mathbf{x})) - (1 - y) \ln(1 - \pi(\mathbf{x}))$$

If p represents a $\text{Ber}(y)$ distribution (so deterministic, where the true label receives probability mass 1) and we also interpret $\pi(\mathbf{x})$ as a Bernoulli distribution $\text{Ber}(\pi(\mathbf{x}))$, the Bernoulli loss $L(y, \pi(\mathbf{x}))$ is the cross-entropy $H_{\pi(\mathbf{x})}(p)$.

ENTROPY AS PREDICTION LOSS

Assume log-loss for a situation where you only model with a constant probability vector π . We know the optimal model under that loss:

$$\pi_k = \frac{n_k}{n} = \frac{\sum_{i=1}^n [y^{(i)} = 1]}{n}$$

What is the (average) risk of that minimal constant model?

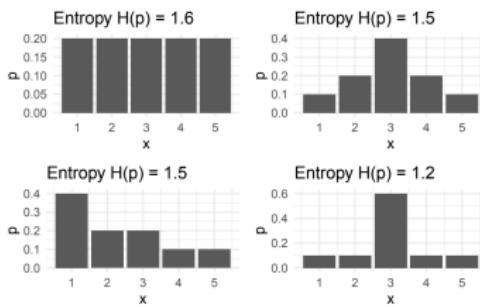
ENTROPY AS PREDICTION LOSS

$$\begin{aligned}\mathcal{R} &= \frac{1}{n} \sum_{i=1}^n \left(- \sum_{k=1}^g [y^{(i)} = k] \log \pi_k \right) \\ &= -\frac{1}{n} \sum_{k=1}^g \sum_{i=1}^n [y^{(i)} = k] \log \pi_k \\ &= -\sum_{k=1}^g \frac{n_k}{n} \log \pi_k \\ &= -\sum_{k=1}^g \pi_k \log \pi_k = H(\pi)\end{aligned}$$

So entropy is the (average) risk of the optimal "observed class frequency" model under log-loss!

Introduction to Machine Learning

Joint Entropy and Mutual Information



Learning goals

- Know the joint entropy
- Know conditional entropy as remaining uncertainty
- Know mutual information as the amount of information of an RV obtained by another

JOINT ENTROPY

- The **joint entropy** of two discrete random variables X and Y with a joint distribution $p(x, y)$ is:

$$H(X, Y) = - \sum_{x \in \mathcal{X}} \sum_{y \in \mathcal{Y}} p(x, y) \log(p(x, y)),$$

which can also be expressed as

$$H(X, Y) = -\mathbb{E} [\log(p(X, Y))].$$

- For continuous random variables X and Y with joint density $p(x, y)$, the differential joint entropy is:

$$h(X, Y) = - \int_{\mathcal{X}, \mathcal{Y}} p(x, y) \ln p(x, y) dx dy$$

For the rest of the section we will stick to the discrete case. Pretty much everything we show and discuss works in a completely analogous manner for the continuous case - if you change sums to integrals.

CONDITIONAL ENTROPY

- The **conditional entropy** $H(Y|X)$ quantifies the uncertainty of Y that remains if the outcome of X is given.
- $H(Y|X)$ is defined as the expected value of the entropies of the conditional distributions, averaged over the conditioning RV.
- If $(X, Y) \sim p(x, y)$, the conditional entropy $H(Y|X)$ is defined as

$$\begin{aligned} H(Y|X) &= \mathbb{E}_x[H(Y|X = x)] = \sum_{x \in \mathcal{X}} p(x)H(Y|X = x) \\ &= -\sum_{x \in \mathcal{X}} p(x) \sum_{y \in \mathcal{Y}} p(y|x) \log p(y|x) \\ &= -\sum_{x \in \mathcal{X}} \sum_{y \in \mathcal{Y}} p(x, y) \log p(y|x) \\ &= -\mathbb{E}[\log p(Y|X)]. \end{aligned}$$

- For the continuous case with density f we have

$$h(Y|X) = - \int f(x, y) \log f(x|y) dx dy.$$

CHAIN RULE FOR ENTROPY

The **chain rule for entropy** is analogous to the chain rule for probability and, in fact, derives directly from it.

$$H(X, Y) = H(X) + H(Y|X)$$

Proof:

$$\begin{aligned} H(X, Y) &= - \sum_{x \in \mathcal{X}} \sum_{y \in \mathcal{Y}} p(x, y) \log p(x, y) \\ &= - \sum_{x \in \mathcal{X}} \sum_{y \in \mathcal{Y}} p(x, y) \log p(x)p(y|x) \\ &= - \sum_{x \in \mathcal{X}} \sum_{y \in \mathcal{Y}} p(x, y) \log p(x) - \sum_{x \in \mathcal{X}} \sum_{y \in \mathcal{Y}} p(x, y) \log p(y|x) \\ &= - \sum_{x \in \mathcal{X}} p(x) \log p(x) - \sum_{x \in \mathcal{X}} \sum_{y \in \mathcal{Y}} p(x, y) \log p(y|x) \\ &= H(X) + H(Y|X) \end{aligned}$$

n-Variable version:

$$H(X_1, X_2, \dots, X_n) = \sum_{i=1}^n H(X_i | X_{i-1}, \dots, X_1).$$

JOINT AND CONDITIONAL ENTROPY

The following relations hold:

$$H(X, X) = H(X)$$

$$H(X|X) = 0$$

$$H(X, Y|Z) = H(X|Z) + H(Y|X, Z)$$

Which can all be trivially derived from the previous considerations.

Furthermore, if $H(X|Y) = 0$, then X is a function of Y , so for all x with $p(x) > 0$, there is only one y with $p(x, y) > 0$. Proof is not hard, but also not completely trivial.

MUTUAL INFORMATION

- The MI describes the amount of information about one random variable obtained through the other one or how different the joint distribution is from pure independence.
- Consider two random variables X and Y with a joint probability mass function $p(x, y)$ and marginal probability mass functions $p(x)$ and $p(y)$. The MI $I(X; Y)$ is the Kullback-Leibler distance between the joint distribution and the product distribution $p(x)p(y)$:

$$\begin{aligned} I(X; Y) &= \sum_{x \in \mathcal{X}} \sum_{y \in \mathcal{Y}} p(x, y) \log \frac{p(x, y)}{p(x)p(y)} \\ &= D_{KL}(p(x, y) || p(x)p(y)) \\ &= \mathbb{E}_{p(x, y)} \left[\log \frac{p(X, Y)}{p(X)p(Y)} \right]. \end{aligned}$$

- For two continuous random variables with joint density $f(x, y)$:

$$I(X; Y) = \int f(x, y) \log \frac{f(x, y)}{f(x)f(y)} dx dy.$$

MUTUAL INFORMATION

We can rewrite the definition of mutual information $I(X; Y)$ as

$$\begin{aligned} I(X; Y) &= \sum_{x,y} p(x, y) \log \frac{p(x, y)}{p(x)p(y)} \\ &= \sum_{x,y} p(x, y) \log \frac{p(x|y)}{p(x)} \\ &= - \sum_{x,y} p(x, y) \log p(x) + \sum_{x,y} p(x, y) \log p(x|y) \\ &= - \sum_x p(x) \log p(x) - \left(- \sum_{x,y} p(x, y) \log p(x|y) \right) \\ &= H(X) - H(X|Y). \end{aligned}$$

Thus, mutual information $I(X; Y)$ is the reduction in the uncertainty of X due to the knowledge of Y .

MUTUAL INFORMATION

The following relations hold:

$$I(X; Y) = H(X) - H(X|Y)$$

$$I(X; Y) = H(Y) - H(Y|X)$$

$$I(X; Y) = H(X) + H(Y) - H(X, Y)$$

$$I(X; Y) = I(Y; X)$$

$$I(X; X) = H(X)$$

All of the above are trivial to prove.

MUTUAL INFORMATION - EXAMPLE

Let X, Y have the following joint distribution:

	X_1	X_2	X_3	X_4
Y_1	$\frac{1}{8}$	$\frac{1}{16}$	$\frac{1}{32}$	$\frac{1}{32}$
Y_2	$\frac{1}{16}$	$\frac{1}{8}$	$\frac{1}{32}$	$\frac{1}{32}$
Y_3	$\frac{1}{16}$	$\frac{1}{16}$	$\frac{1}{16}$	$\frac{1}{16}$
Y_4	$\frac{1}{4}$	0	0	0

The marginal distribution of X is $(\frac{1}{2}, \frac{1}{4}, \frac{1}{8}, \frac{1}{8})$ and the marginal distribution of Y is $(\frac{1}{4}, \frac{1}{4}, \frac{1}{4}, \frac{1}{4})$, and hence $H(X) = \frac{7}{4}$ bits and $H(Y) = 2$ bits.

MUTUAL INFORMATION - EXAMPLE

The conditional entropy $H(X|Y)$ is given by:

$$\begin{aligned} H(X|Y) &= \sum_{i=1}^4 p(Y=i)H(X|Y=i) \\ &= \frac{1}{4}H\left(\frac{1}{2}, \frac{1}{4}, \frac{1}{8}, \frac{1}{8}\right) + \frac{1}{4}H\left(\frac{1}{4}, \frac{1}{2}, \frac{1}{8}, \frac{1}{8}\right) \\ &\quad + \frac{1}{4}H\left(\frac{1}{4}, \frac{1}{4}, \frac{1}{4}, \frac{1}{4}\right) + \frac{1}{4}H(1, 0, 0, 0) \\ &= \frac{1}{4} \cdot \frac{7}{4} + \frac{1}{4} \cdot \frac{7}{4} + \frac{1}{4} \cdot 2 + \frac{1}{4} \cdot 0 \\ &= \frac{11}{8} \text{ bits.} \end{aligned}$$

Similarly, $H(Y|X) = \frac{13}{8}$ bits and $H(X, Y) = \frac{27}{8}$ bits.

MUTUAL INFORMATION - COROLLARIES

Non-negativity of mutual information: For any two random variables, X , Y , $I(X; Y) \geq 0$, with equality if and only if X and Y are independent.

Proof: $I(X; Y) = D_{KL}(p(x, y) \| p(x)p(y)) \geq 0$, with equality if and only if $p(x, y) = p(x)p(y)$ (i.e., X and Y are independent).

Conditioning reduces entropy (information can't hurt):

$$H(X|Y) \leq H(X),$$

with equality if and only if X and Y are independent.

Proof: $0 \leq I(X; Y) = H(X) - H(X|Y)$

Intuitively, the theorem says that knowing another random variable Y can only reduce the uncertainty in X . Note that this is true only on the average.

MUTUAL INFORMATION - COROLLARIES

Independence bound on entropy: Let X_1, X_2, \dots, X_n be drawn according to $p(x_1, x_2, \dots, x_n)$. Then

$$H(X_1, X_2, \dots, X_n) \leq \sum_{i=1}^n H(X_i),$$

with equality if and only if the X_i are independent.

Proof: With the chain rule for entropies,

$$H(X_1, X_2, \dots, X_n) = \sum_{i=1}^n H(X_i | X_{i-1}, \dots, X_1) \leq \sum_{i=1}^n H(X_i),$$

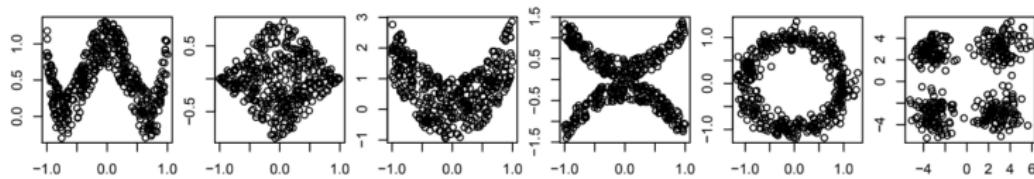
where the inequality follows directly from above. We have equality if and only if X_i is independent of X_{i-1}, \dots, X_1 for all i (i.e., if and only if the X_i 's are independent).

MUTUAL INFORMATION PROPERTIES

- MI is a measure of the amount of "dependence" between variables. It is zero if and only if the variables are independent.
- On the other hand, if one of the variables is a deterministic function of the other, the mutual information is maximal, i.e. entropy of the first.
- Unlike (Pearson) correlation, mutual information is not limited to real-valued random variables.
- Mutual information can be used to perform **feature selection**.
Quite simply, each variable X_i is rated according to $I(X_i; Y)$, this is sometime called information gain.
- The same principle can also be used in decision trees to select a feature to split on. Splitting on MI/IG is then equivalent to risk reduction with log-loss.

MUTUAL INFORMATION VS. CORRELATION

- If two variables are independent, their correlation is 0.
- However, the reverse is not necessarily true. It is possible for two dependent variables to have 0 correlation because correlation only measures linear dependence.



- The figure above shows various scatterplots where, in each case, the correlation is 0 even though the two variables are strongly dependent, and MI is large.
- Mutual information can therefore be seen as a more general measure of dependence between variables than correlation.

MUTUAL INFORMATION - EXAMPLE

Let X, Y be two correlated Gaussian random variables.

$(X, Y) \sim \mathcal{N}(0, K)$ with correlation ρ and covariance matrix K :

$$K = \begin{pmatrix} \sigma^2 & \rho\sigma^2 \\ \rho\sigma^2 & \sigma^2 \end{pmatrix}$$

Then $h(X) = h(Y) = \frac{1}{2} \log(2\pi e)\sigma^2$, and

$h(X, Y) = \log(2\pi e)^2 |K| = \log(2\pi e)^2 \sigma^4 (1 - \rho^2)$, and thus

$$I(X; Y) = h(X) + h(Y) - h(X, Y) = -\frac{1}{2} \log(1 - \rho^2).$$

For $\rho = 0$, X and Y are independent and $I(X; Y) = 0$.

For $\rho = \pm 1$, X and Y are perfectly correlated and $I(X; Y) \rightarrow \infty$.

INTRODUCTION TO MACHINE LEARNING

Advanced Risk Minimization

Multiclass Classification

Information Theory

Curse of Dimensionality

Hypothesis Space

Regularization

Linear Support Vector Machine

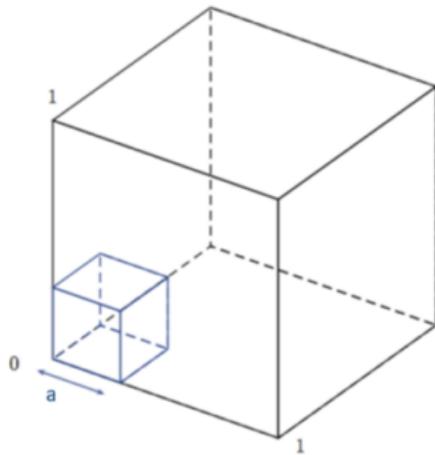
Nonlinear Support Vector Machine

Gaussian Processes

Boosting

Introduction to Machine Learning

Curse of Dimensionality



Learning goals

- Understand that our intuition about geometry fails in high-dimensional spaces
- Understand the effects of the curse of dimensionality

CURSE OF DIMENSIONALITY

- The phenomenon of data becoming sparse in high-dimensional spaces is one effect of the **curse of dimensionality**.
- The **curse of dimensionality** refers to various phenomena that arise when analyzing data in high-dimensional spaces that do not occur in low-dimensional spaces.
- Our intuition about the geometry of a space is formed in two and three dimensions.
- We will see: This intuition is often misleading in high-dimensional spaces.

CURSE OF DIMENSIONALITY: EXAMPLE

To illustrate one of the problematic phenomena of data in high dimensional data, we look at an introductory example:

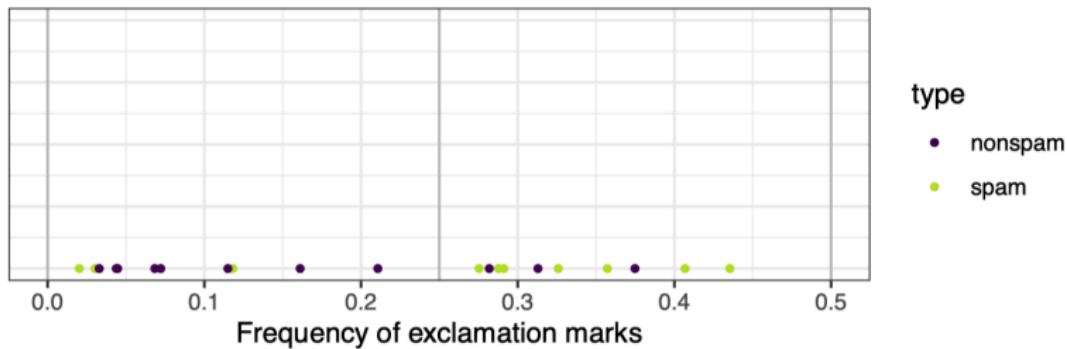
We are given 20 emails, 10 of them are spam and 10 are not. Our goal is to predict if a new incoming mail is spam or not.

For each email, we extract the following features:

- frequency of exclamation marks (in %)
- the length of the longest sequence of capital letters
- the frequency of certain words, e.g., “free” (in %)
- ...

... and we could extract many more features!

CURSE OF DIMENSIONALITY: EXAMPLE

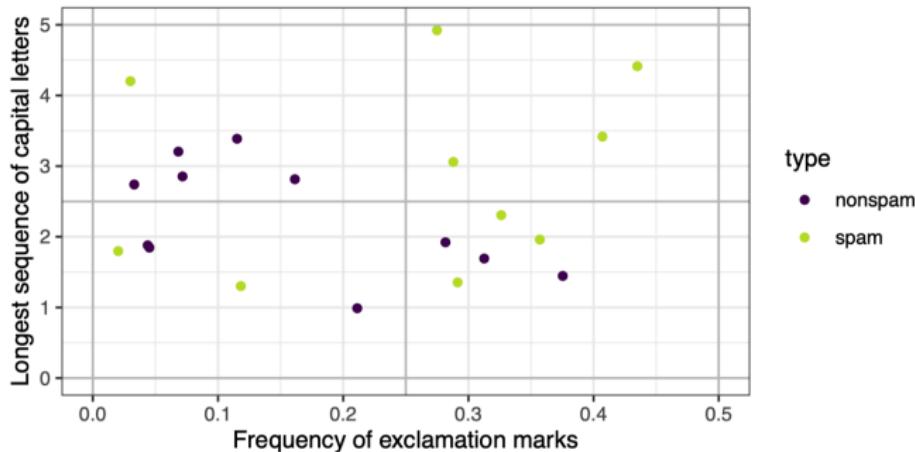


Based on the frequency of exclamation marks, we train a very simple classifier (a decision stump with split point $x = 0.25$):

- We divide the input space into 2 equally sized regions.
- In the second region $[0.25, 0.5]$, 7 out of 10 are spam.
- Given that at least 0.25% of all letters are exclamation marks, an email is spam with a probability of $\frac{7}{10} = 0.7$.

CURSE OF DIMENSIONALITY: EXAMPLE

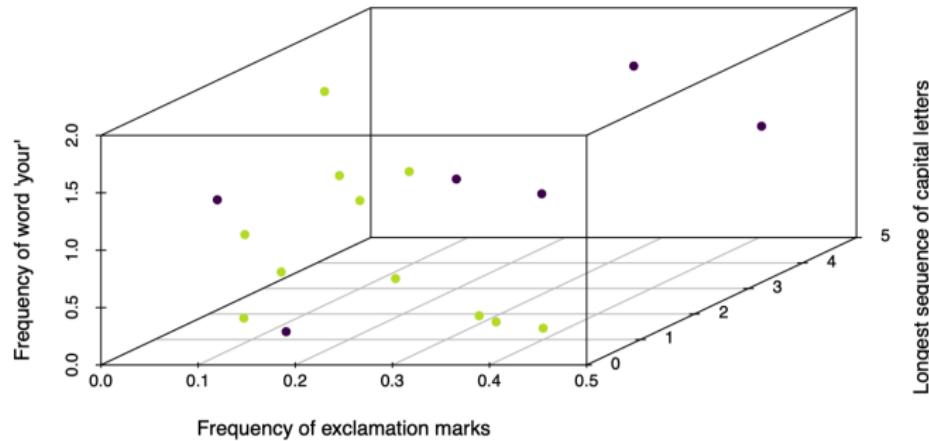
Let us feed more information into our classifier. We include a feature that contains the length of the longest sequence of capital letters.



- In the 1D case we had 20 observations across 2 regions.
- The same number is now spread across 4 regions.

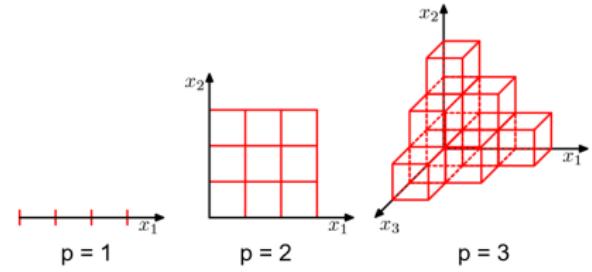
CURSE OF DIMENSIONALITY: EXAMPLE

Let us further increase the dimensionality to 3 by using the frequency of the word “your” in an email.



CURSE OF DIMENSIONALITY: EXAMPLE

- When adding a third dimension, the same number of observations is spread across 8 regions.
- In 4 dimensions the data points are spread across 16 cells, in 5 dimensions across 32 cells and so on ...
- As dimensionality increases, the data become **sparse**; some of the cells become empty.
- There might be too few data in each of the blocks to understand the distribution of the data and to model it.

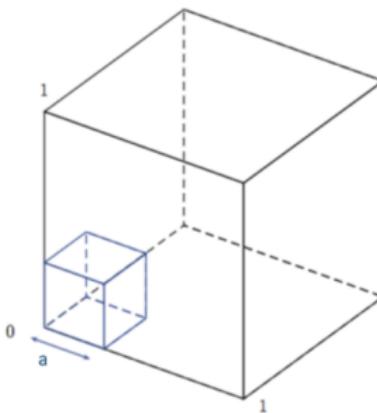


Bishop, Pattern Recognition and Machine Learning, 2006

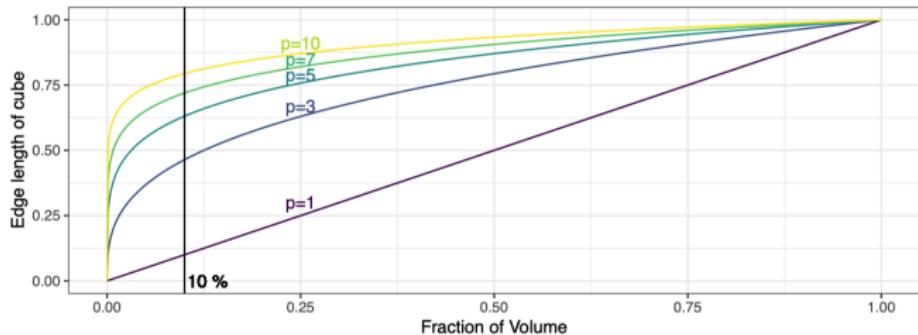
Geometry of High-Dimensional Spaces

THE HIGH-DIMENSIONAL CUBE

- We embed a small cube with edge length a inside a unit cube.
- How long does the edge length a of this small hypercube have to be so that the hypercube covers 10%, 20%, ... of the volume of the unit cube (volume 1)?



THE HIGH-DIMENSIONAL CUBE



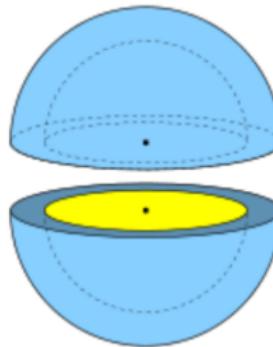
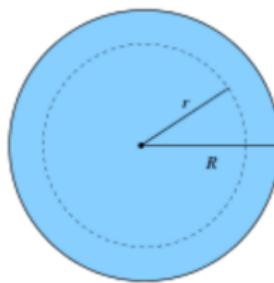
$$a^p = \frac{1}{10} \Leftrightarrow a = \frac{1}{\sqrt[p]{10}}$$

- So: covering 10% of total volume in a cell requires cells with almost 50% of the entire range in 3 dimensions, 80% in 10 dimensions.

THE HIGH-DIMENSIONAL SPHERE

Another manifestation of the **curse of dimensionality** is that the majority of data points are close to the outer edges of the sample. Consider a hypersphere of radius 1. The fraction of volume that lies in the ϵ -“edge”, $\epsilon := R - r$, of this hypersphere can be calculated by the formula

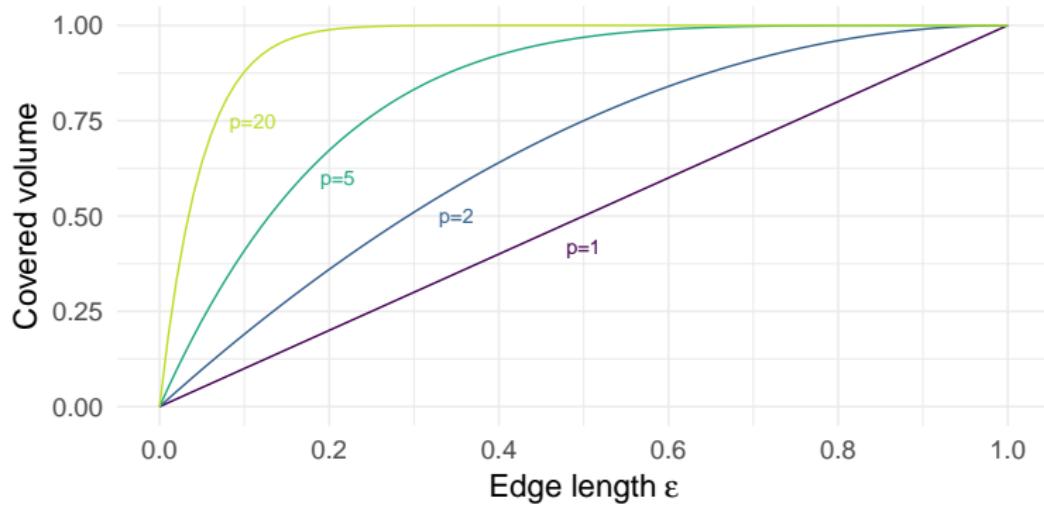
$$1 - \left(1 - \frac{\epsilon}{R}\right)^p.$$



If we peel a high-dimensional orange, there is almost nothing left.

THE HIGH-DIMENSIONAL SPHERE

Consider a 20-dimensional sphere. Nearly all of the volume lies in its outer shell of thickness 0.2:

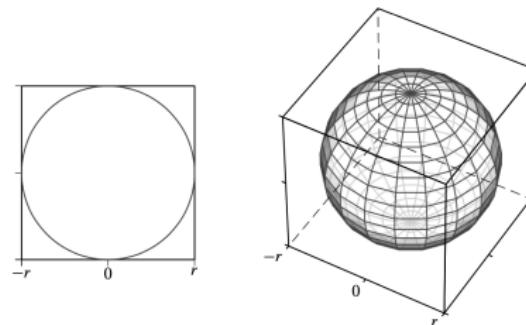


HYPERSPHERE WITHIN HYPERCUBE

Consider a p-dimensional hypersphere of radius r and volume $S_p(r)$ inscribed in a p-dimensional hypercube with sides of length $2r$ and volume $C_p(r)$. Then it holds that

$$\lim_{p \rightarrow \infty} \frac{S_p(r)}{C_p(r)} = \lim_{p \rightarrow \infty} \frac{\left(\frac{\pi^{\frac{p}{2}}}{\Gamma(\frac{p}{2}+1)} \right) r^p}{(2r)^p} = \lim_{p \rightarrow \infty} \frac{\pi^{\frac{p}{2}}}{2^p \Gamma(\frac{p}{2} + 1)} = 0,$$

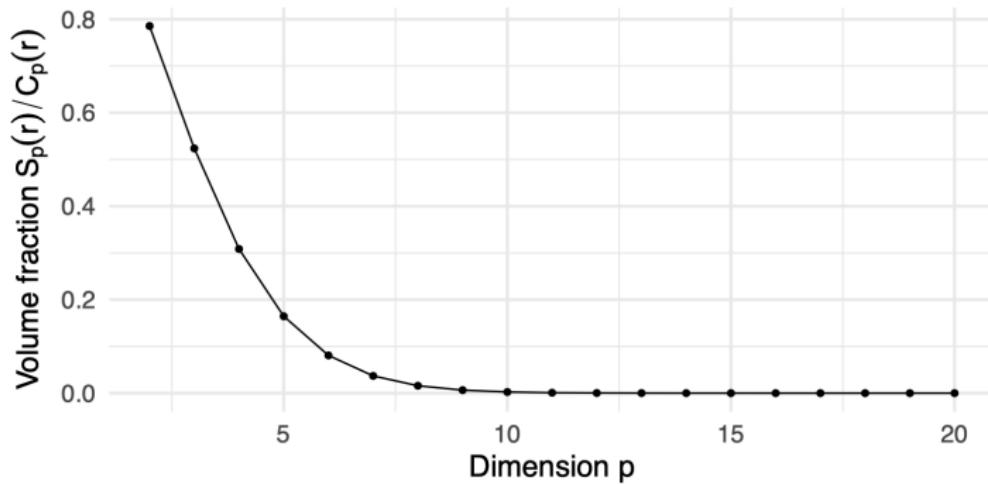
i.e., as the dimensionality increases, most of the volume of the hypercube can be found in its corners.



Mohammed J. Zaki, Wagner Meira, Jr., Data Mining and Analysis: Fundamental Concepts and Algorithms, 2014

HYPERSPHERE WITHIN HYPERCUBE

Consider a 10-dimensional sphere inscribed in a 10-dimensional cube.
Nearly all of the volume lies in the corners of the cube:



Note: For $r > 0$, the volume fraction $\frac{S_p(r)}{C_p(r)}$ is independent of r .

UNIFORMLY DISTRIBUTED DATA

The consequences of the previous results for uniformly distributed data in the high-dimensional hypercube are:

- Most of the data points will lie on the boundary of the space.
- The points will be mainly scattered on the large number of corners of the hypercube, which themselves will become very long spikes.
- Hence the higher the dimensionality, the more similar the minimum and maximum distances between points will become.
- This degrades the effectiveness of most distance functions.
- Neighborhoods of points will not be local anymore.

GAUSSIANS IN HIGH DIMENSIONS

A further manifestation of the **curse of dimensionality** appears if we consider a standard Gaussian $N_p(\mathbf{0}, \mathbf{I}_p)$ in p dimensions.

- After transforming from Cartesian to polar coordinates and integrating out the directional variables, we obtain an expression for the density $p(r)$ as a function of the radius r (i.e., the point's distance from the origin), s.t.

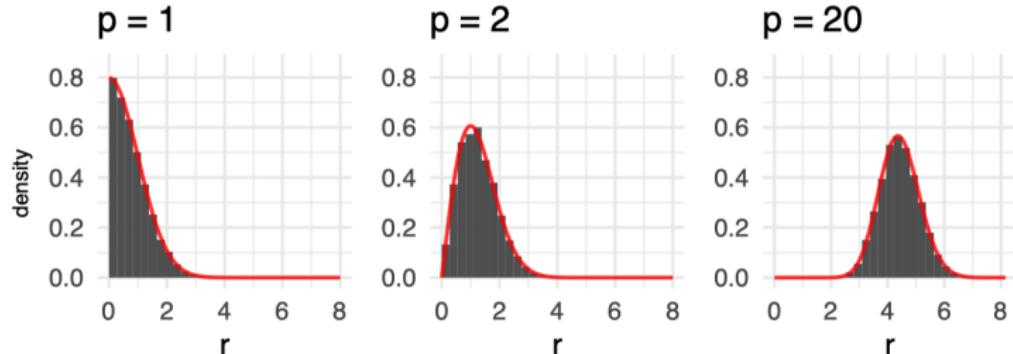
$$p(r) = \frac{S_p(r)r^{p-1}}{(2\pi\sigma^2)^{p/2}} \exp\left(-\frac{r^2}{2\sigma^2}\right),$$

where $S_p(r)$ is the surface of the p -dimensional hypersphere of radius r .

- Thus $p(r)\delta r$ is the approximate probability mass inside a thin shell of thickness δr located at radius r .

GAUSSIANS IN HIGH DIMENSIONS

- To verify this functional relationship empirically, we draw 10^4 points from the p -dimensional standard normal distribution and plot $p(r)$ over the histogram of the points' distances to the origin:



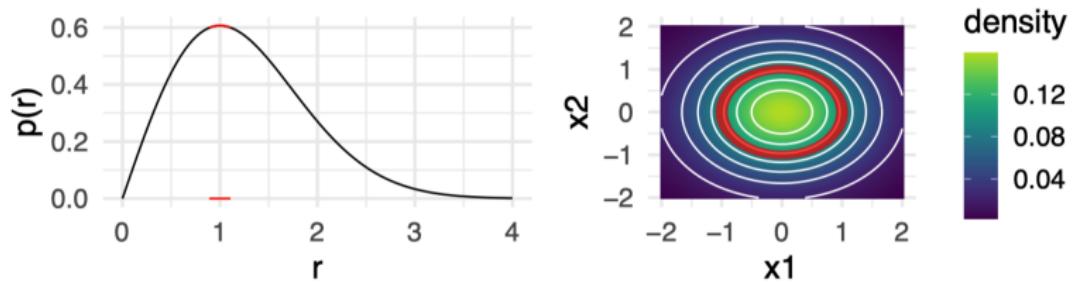
- We can see that for large p the probability mass of the Gaussian is concentrated in a fairly thin “shell” rather far away from the origin. This may seem counterintuitive, but:

GAUSSIANS IN HIGH DIMENSIONS

- For the probability mass of a hyperspherical shell it follows that

$$\int_{r-\frac{\delta r}{2}}^{r+\frac{\delta r}{2}} p(\tilde{r}) d\tilde{r} = \int_{r-\frac{\delta r}{2}}^{r+\frac{\delta r}{2}} f_p(\tilde{\mathbf{x}}) d\tilde{\mathbf{x}},$$

where $f_p(\mathbf{x})$ is the density of the p -dimensional standard normal distribution and $p(r)$ the associated radial density.



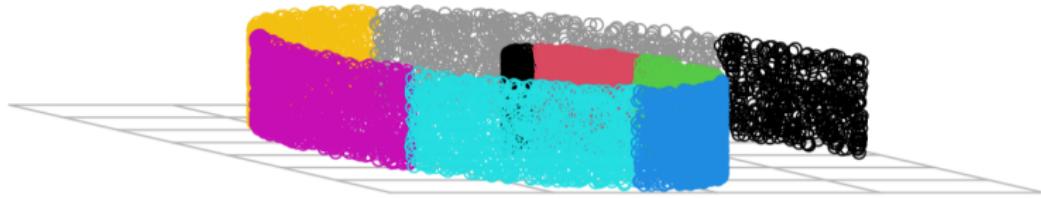
Example: 2D normal distribution

- While f_p becomes smaller with increasing r , the region of the integral -the hyperspherical shell- becomes bigger.

INTERMEDIATE REMARKS

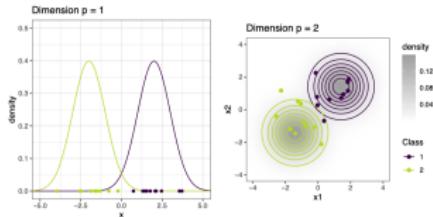
However, we can find effective techniques applicable to high-dimensional spaces if we exploit these properties of real data:

- Often the data is restricted to a manifold of a lower dimension.
(Or at least the directions in the feature space over which significant changes in the target variables occur may be confined.)
- At least locally small changes in the input variables usually will result in small changes in the target variables.



Introduction to Machine Learning

Curse of Dimensionality - Examples Learning Algorithms



Learning goals

- See how the performance of k-NN and the linear model deteriorates in high-dimensional spaces

EXAMPLE: K-NN

Let us look at the performance of algorithms for increasing dimensionality. First, we consider the k-NN algorithm:

- In a high dimensional space, data points are spread across a huge space.
- The distance to the **next neighbor** $d_{NN1}(\mathbf{x})$ becomes extremely large.
- The distance might even get so large that all points are **equally far** away - we cannot really determine the nearest neighbor anymore.

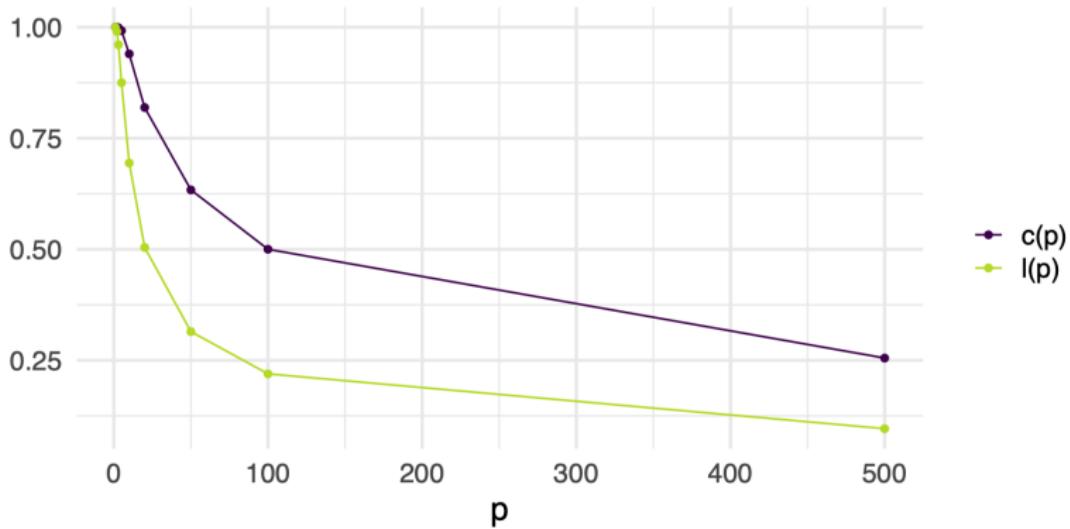
EXAMPLE: K-NN

Minimal, mean and maximal (NN)-distances of 10^4 points uniformly distributed in the hypercube $[0, 1]^p$:

p	$\min(d(\mathbf{x}, \tilde{\mathbf{x}}))$	$\overline{d(\mathbf{x}, \tilde{\mathbf{x}})}$	$\max(d(\mathbf{x}, \tilde{\mathbf{x}}))$	$d_{NN1}(\mathbf{x})$	$\max(d_{NN1}(\mathbf{x}))$
1	0.000000012	0.33	1	0.00005	0.00042
2	0.00011	0.52	1.4	0.0051	0.02
3	0.0021	0.66	1.7	0.026	0.073
5	0.016	0.88	2	0.11	0.23
10	0.15	1.3	2.5	0.39	0.63
20	0.55	1.8	3	0.9	1.2
50	1.5	2.9	4.1	2	2.4
100	2.7	4.1	5.4	3.2	3.5
500	7.8	9.1	10	8.2	8.6

EXAMPLE: K-NN

We see a decrease of relative contrast¹ $c := \frac{\max(d(\mathbf{x}, \tilde{\mathbf{x}})) - \min(d(\mathbf{x}, \tilde{\mathbf{x}}))}{\max(d(\mathbf{x}, \tilde{\mathbf{x}}))}$ and
“locality”² $l := \frac{d(\mathbf{x}, \tilde{\mathbf{x}}) - d_{NN1}(\mathbf{x})}{d(\mathbf{x}, \tilde{\mathbf{x}})}$ with increasing number of dimensions p :



EXAMPLE: K-NN

The consequences for the k-nearest neighbors approach can be summarized as follows:

- At constant sample size n and growing p , the distance between the observations increases
 - the coverage of the p -dimensional space decreases,
 - every point becomes isolated / far way from all other points.
- The size of the neighborhood $N_k(x)$ also “increases”
(at constant k)
 - it is no longer a “local” method.
- Reducing k dramatically does not help much either, since the fewer observations we average, the higher the variance of our fit.
 - k-NN estimates get more inaccurate with increasing dimensionality of the data.

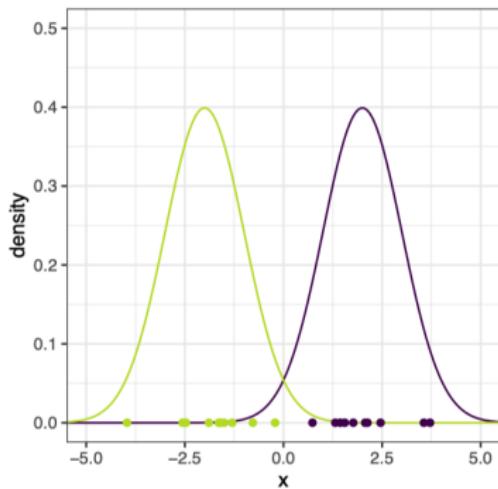
EXAMPLE: K-NN

To demonstrate this, we generate an artificial data set of dimension p as follows: We define $a = \frac{2}{\sqrt{p}}$ and

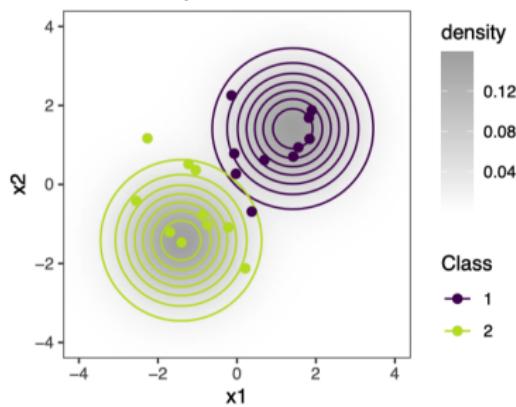
- with probability $\frac{1}{2}$ we generate a sample from class 1 by sampling from a Gaussian with mean $\mu = (a, a, \dots, a)$ and unit covariance matrix
- with probability $\frac{1}{2}$ we generate a sample from class 2 by sampling from a Gaussian with mean $-\mu = (-a, -a, \dots, -a)$ and unit covariance matrix

EXAMPLE: K-NN

Dimension p = 1



Dimension p = 2



EXAMPLE: K-NN

This example is constructed such that the Bayes error is always constant and does not depend on the dimension p .

The Bayes optimal classifiers predicts $\hat{y} = 1$ iff

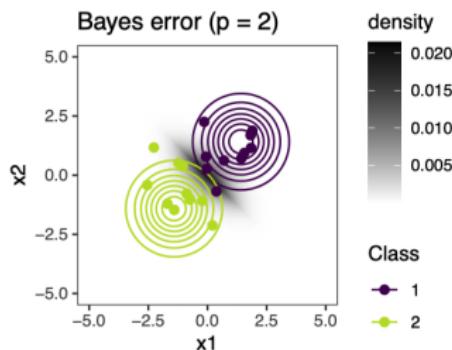
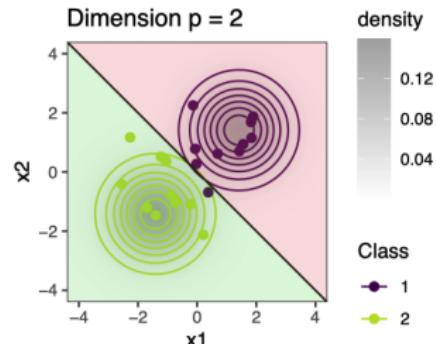
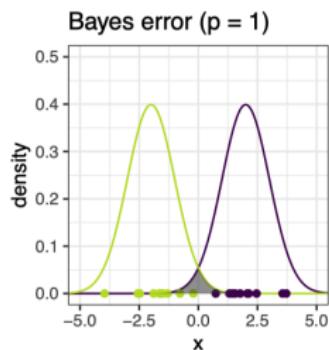
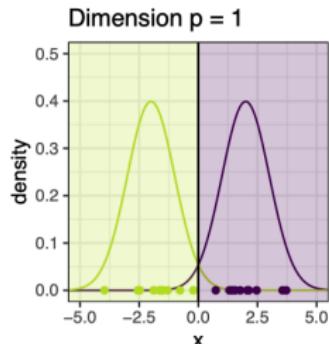
$$\begin{aligned}\mathbb{P}(y = 1 \mid \mathbf{x}) &= \frac{p(\mathbf{x} \mid y = 1)\mathbb{P}(y = 1)}{p(\mathbf{x})} = \frac{1}{2} \cdot \frac{p(\mathbf{x} \mid y = 1)}{p(\mathbf{x})} \\ &\geq \frac{1}{2} \cdot \frac{p(\mathbf{x} \mid y = 2)}{p(\mathbf{x})} \\ &= \frac{p(\mathbf{x} \mid y = 2)\mathbb{P}(y = 2)}{p(\mathbf{x})} = \mathbb{P}(y = 2 \mid \mathbf{x}).\end{aligned}$$

This is equivalent to

$$\begin{aligned}\hat{y} = 1 &\Leftrightarrow \exp\left(-\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu})^\top(\mathbf{x} - \boldsymbol{\mu})\right) \geq \exp\left(-\frac{1}{2}(\mathbf{x} + \boldsymbol{\mu})^\top(\mathbf{x} + \boldsymbol{\mu})\right) \\ &\Leftrightarrow \mathbf{x}^\top \boldsymbol{\mu} \geq 0.\end{aligned}$$

EXAMPLE: K-NN

Optimal Bayes classifier and Bayes error (shaded area):



EXAMPLE: K-NN

We can calculate the corresponding expected misclassification error (Bayes error)

$$\begin{aligned} & p(\hat{y} = 1 \mid y = 2) \mathbb{P}(y = 2) + p(\hat{y} = 2 \mid y = 1) \mathbb{P}(y = 1) \\ = & \frac{1}{2} \cdot p(\mathbf{x}^\top \boldsymbol{\mu} \geq 0 \mid y = 2) + \frac{1}{2} \cdot p(\mathbf{x}^\top \boldsymbol{\mu} \leq 0 \mid y = 1) \\ \stackrel{\text{symm.}}{=} & p(\mathbf{x}^\top \boldsymbol{\mu} \leq 0 \mid y = 1) = p\left(\sum_{i=1}^p a \mathbf{x}_i \leq 0 \mid y = 1\right) \\ = & p\left(\sum_{i=1}^p \mathbf{x}_i \leq 0 \mid y = 1\right). \end{aligned}$$

$\sum_{i=1}^p \mathbf{x}_i \mid y = 1 \sim \mathcal{N}(p \cdot a, p)$, because it is the sum of independent normal random variables $\mathbf{x}_i \mid y = 1 \sim \mathcal{N}(a, 1)$ (the vector $\mathbf{x} \mid y = 1$ follows a $\mathcal{N}(\boldsymbol{\mu}, \mathbf{I})$ distribution with $\boldsymbol{\mu} = (a, \dots, a)$).

EXAMPLE: K-NN

We get for the Bayes error:

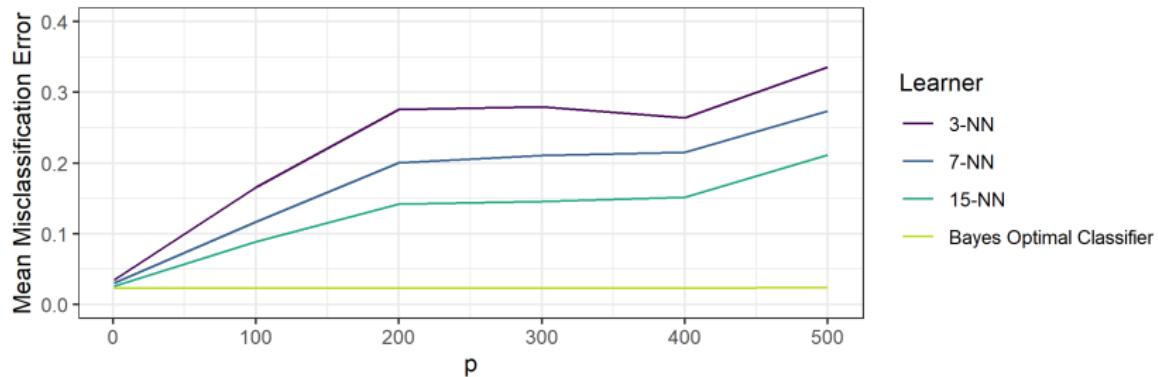
$$\begin{aligned} &= p \left(\frac{\sum_{i=1}^p \mathbf{x}_i - p \cdot \mathbf{a}}{\sqrt{p}} \leq \frac{-p \cdot \mathbf{a}}{\sqrt{p}} \mid y = 1 \right) \\ &= \Phi(-\sqrt{p}a) \stackrel{a=\frac{2}{\sqrt{p}}}{=} \Phi(-2) \approx 0.0228, \end{aligned}$$

where Φ is the distribution function of a standard normal random variable.

We see that the Bayes error is independent of p .

EXAMPLE: K-NN

We also train a k-NN classifier for $k = 3, 7, 15$ for increasing dimensions and monitor its performance (evaluated by 10 times repeated 10-fold CV).



→ k-NN deteriorates quickly with increasing dimension

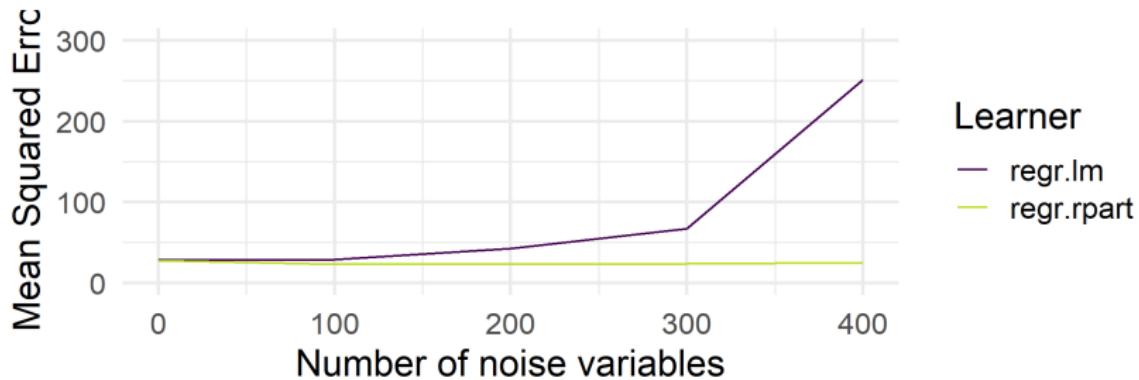
EXAMPLE: LINEAR MODEL

We also investigate how the linear model behaves in high dimensional spaces.

- We take the Boston Housing data set, where the value of houses in the area around Boston is predicted based on 13 features describing the region (e.g., crime rate, status of the population, etc.).
- We train a linear model on the data consisting of 506 observations.
- We artificially create a high-dimensional dataset by adding 100, 200, 300, ... noise variables (containing no information at all) and look at the performance of a linear model trained on this modified data (10 times repeated 10-fold CV).

EXAMPLE: LINEAR MODEL

We compare the performance of an LM to that of a regression tree.



→ The unregularized LM struggles with the added noise features, while our tree seems to nicely filter them out.

Note: Trees automatically perform feature selection as only one feature at a time is considered for splitting (the smaller the depth of the tree, the less features are selected). Thus, they often perform well in high-dimensional settings.

EXAMPLE: LINEAR MODEL

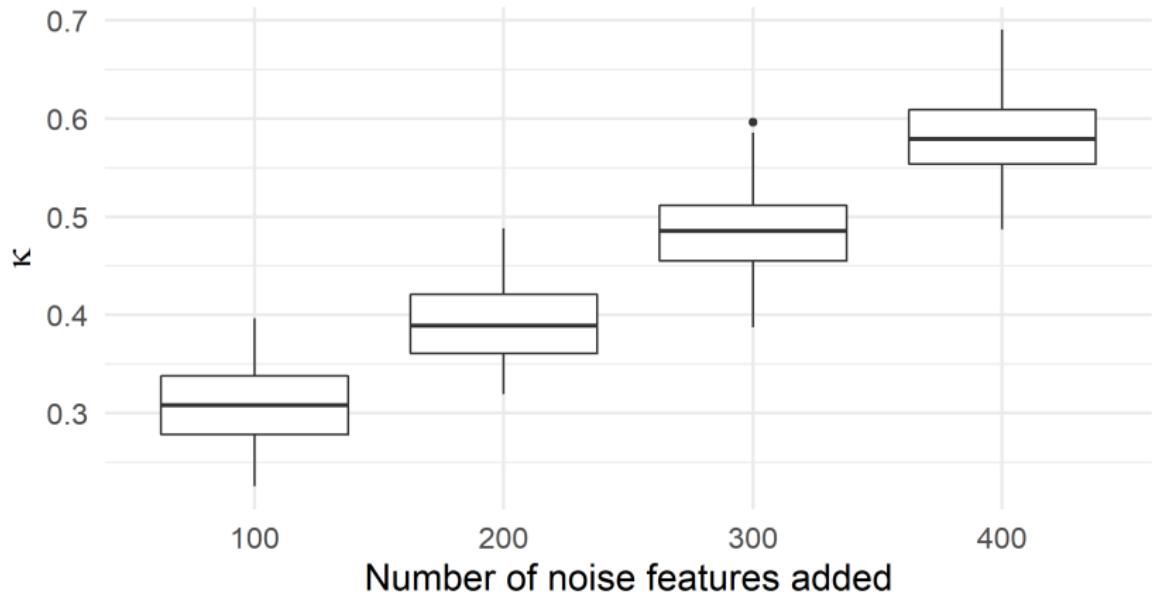
- The regression coefficients of the noise features can not be estimated precisely as zero in the unregularized LM due to small random correlations.
- With an increasing number of these noise features, the prediction error rises.
- To see this, we can quantify the influence of the noise features on the prediction of each iteration.

Therefore we decompose the response $\hat{y}^{(i)}$ of each iterations' test set into $\hat{y}_{\text{true}}^{(i)}$ (predicted with noise features set to 0) and $\hat{y}_{\text{noise}}^{(i)}$ (predicted with true features set to 0), s.t.

$$\hat{y}^{(i)} = \hat{y}_{\text{true}}^{(i)} + \hat{y}_{\text{noise}}^{(i)} + \text{intercept}.$$

With this, we can define the “average proportional influence of the noise features” $\kappa := \overline{\left(\frac{|\hat{y}_{\text{noise}}^{(i)}|}{|\hat{y}_{\text{true}}^{(i)}| + |\hat{y}_{\text{noise}}^{(i)}|} \right)}$.

EXAMPLE: LINEAR MODEL



When we add 400 noise features to the model, most of the time, on average, over 50% of the flexible part of the prediction ($\hat{y}^{(i)} - \text{intercept}$) is determined by the noise features.

COD: WAYS OUT

Many methods besides k-NN struggle with the curse of dimensionality. A large part of ML is concerned with dealing with this problem and finding ways around it.

Possible approaches are:

- Increasing the space coverage by gathering more observations (not always viable in practice!)
- Reducing the number of dimensions before training (e.g. by using domain knowledge, PCA or feature selection)
- Regularization

INTRODUCTION TO MACHINE LEARNING

Advanced Risk Minimization

Multiclass Classification

Information Theory

Curse of Dimensionality

Hypothesis Space

Regularization

Linear Support Vector Machine

Nonlinear Support Vector Machine

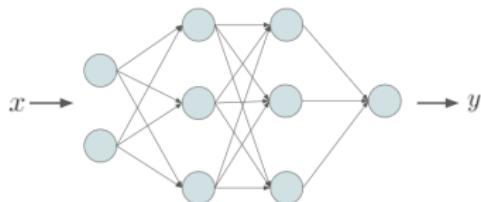
Gaussian Processes

Boosting

Introduction to Machine Learning

Examples of Hypothesis Spaces

Learning goals



- Recall that the hypothesis space is the set of all admissible functions
- Know the hypothesis space for: linear regression, separating hyperplanes, decision trees, ensembles, and neural networks

HYPOTHESIS SPACES

Recall, the **hypothesis space** is the set of all admissible functions, that we have to pick a certain element from during learning / risk minimization.

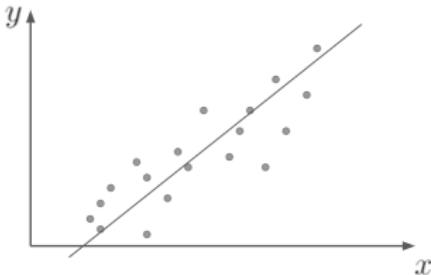
$$\mathcal{H} := \{f : \mathcal{X} \rightarrow \mathbb{R}^g \mid f \text{ has a specific form}\}.$$

Often f is parameterized by $\theta \in \Theta$. We write $f(\mathbf{x}) = f(\mathbf{x} \mid \theta)$.

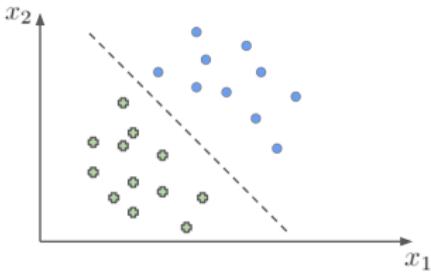
Note: If we are explicitly talking about hard classifiers outputting a discrete class, we write h instead of f .

LINEAR MODELS

- **Linear regression:** $f(\mathbf{x} \mid \theta_0, \boldsymbol{\theta}) = \mathbf{x}^T \boldsymbol{\theta} + \theta_0$ with $\boldsymbol{\theta} \in \mathbb{R}^p, \theta_0 \in \mathbb{R}$

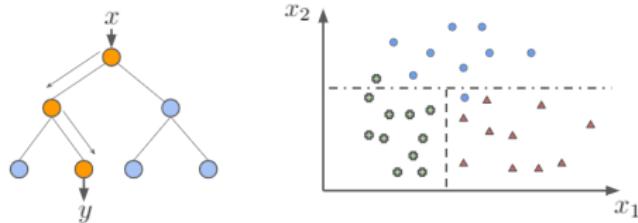


- **Separating hyperplanes:** $h(\mathbf{x} \mid \theta_0, \boldsymbol{\theta}) = \mathbb{I}[\mathbf{x}^T \boldsymbol{\theta} - \theta_0 > 0]$

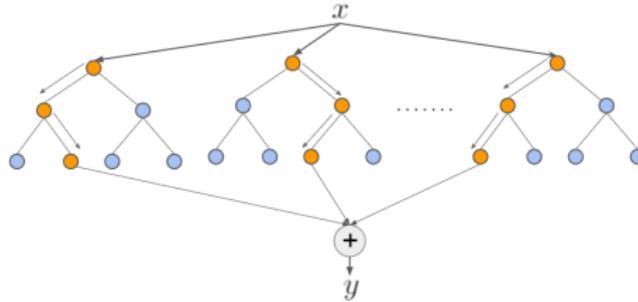


TREES AND ENSEMBLES

- **Decision trees:** $f(\mathbf{x}) = \sum_{i=1}^m c_i \mathbb{I}(\mathbf{x} \in Q_i)$ Where the Q_i are an axis-aligned, rectangular partitioning of the input space

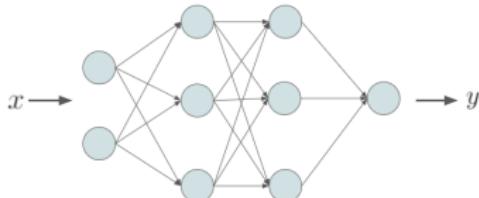


- **Simple Ensembles:** $f(\mathbf{x} | \beta^{[j]}) = \sum_{j=1}^m \beta^{[j]} b^{[j]}(\mathbf{x})$ Where the $b^{[j]}(\mathbf{x})$ come from some base learner space \mathcal{B} .



NEURAL NETWORKS

$$f(\mathbf{x}) = \tau \circ \phi \circ \sigma^{(h)} \circ \phi^{(h)} \circ \sigma^{(h-1)} \circ \phi^{(h-1)} \circ \dots \circ \sigma^{(1)} \circ \phi^{(1)}(\mathbf{x})$$



- Consists of layers of simple computational “neurons”
- Each neuron in a given layer performs a two-step computation: an affine linear transformation of its inputs, then a scalar non-linear activation. We can write this in vector notation for a complete layer:

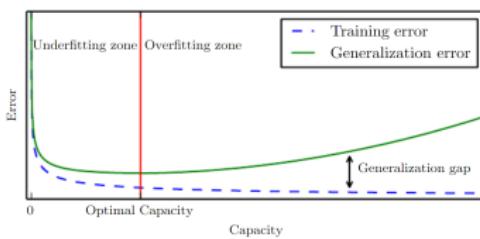
$$\phi^{(j)}(\mathbf{z}) = \mathbf{W}_j^\top \mathbf{z} + \mathbf{b}_j$$

The activation $\sigma^{(j)}$ applies componentwise the same non-linear function to its vector inputs (e.g. logistic or ReLU), while τ simply rescales for the final output (e.g. softmax). Usually, σ and τ contain no learnable parameters.

Introduction to Machine Learning

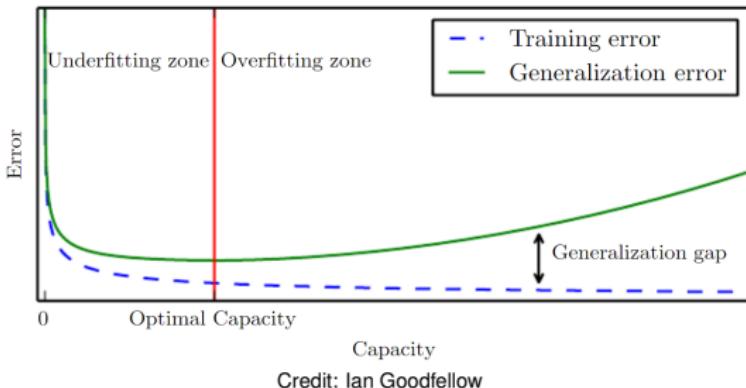
Capacity & Overfitting

Learning goals



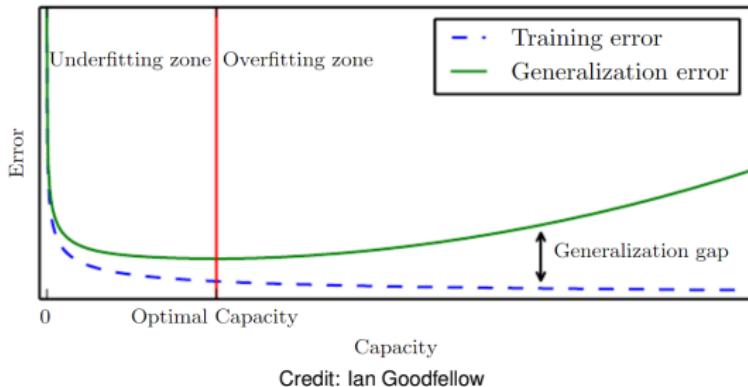
- Know that the capacity of a hypothesis space impacts generalization
- Know that low capacity carries the risk of underfitting
- Know that too high capacity carries the risk of overfitting

CAPACITY



- The performance of a learner depends on its ability to:
 - Minimize the training error
 - Generalize well to new data
- Failure to obtain a sufficiently low training error is known as **underfitting**.
- On the other hand, if there is a large difference in training and test error, this is known as **overfitting**.

CAPACITY



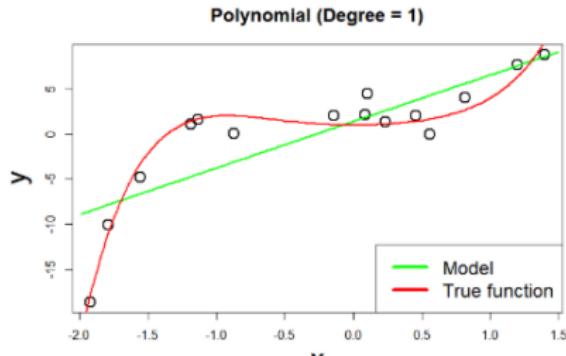
- The tendency of a model to over-/underfit is a function of its **capacity**, determined by the type of hypotheses it can learn.
- Loosely speaking, a model with low capacity can only learn a few simple hypotheses, whereas a model with large capacity can learn many, possibly complex, hypotheses.
- As the figure shows, the test error is minimized when the model neither underfits nor overfits, that is, when it has the right capacity.

OVERFITTING

- The capacity (or “complexity”) of a model can be increased by increasing the size of the hypothesis space.
- This (usually) also increases the number of learnable parameters.
- Examples: Increasing the degree of the polynomial in linear regression, increasing the depth of a decision tree or a neural network, adding additional predictors, etc.
- As the size of the hypothesis space increases, the tendency of a model to overfit also increases.
- Such a model might fit even the random quirks in the training data, thereby failing to generalize.

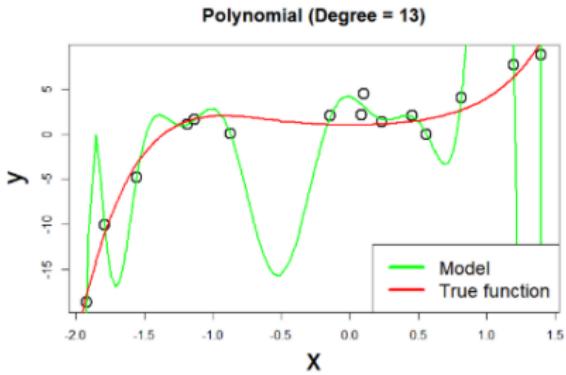
OVERFITTING: POLYNOMIAL REGRESSION

Degree = 1
(highest degree of a term in the polynomial)



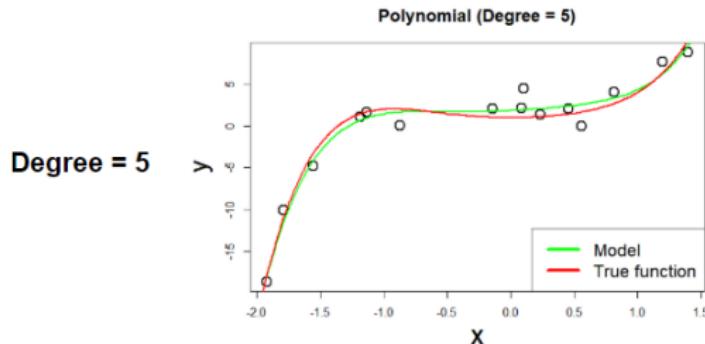
Underfitting
(Low Capacity)

Degree = 13



Overfitting
(High Capacity)

OVERFITTING: POLYNOMIAL REGRESSION

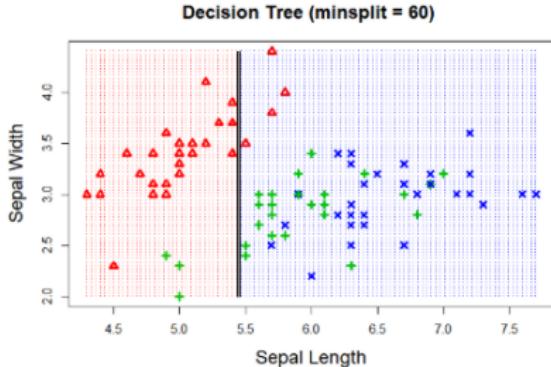


Good fit
(Appropriate capacity)

	Degree = 1	Degree = 5	Degree = 13
Training error (RMSE)	3.87	1.23	0.48
Test error (RMSE)	4.11	1.55	148.5

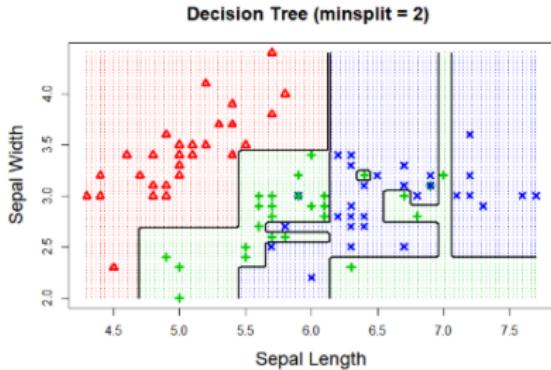
OVERFITTING: DECISION TREES

minsplit = 60
(minimum number of samples in a node being split)



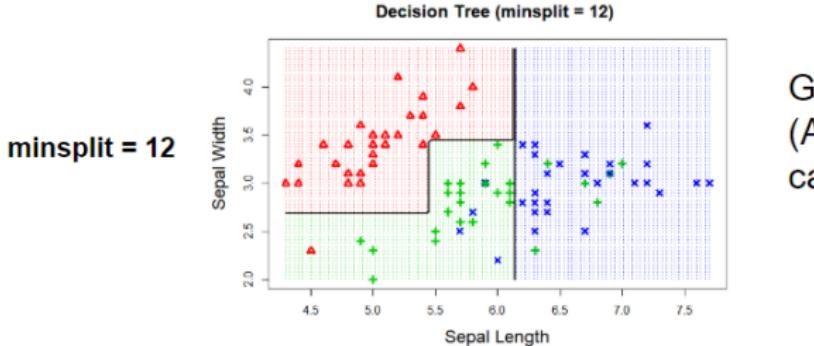
Underfitting
(Low Capacity)

minsplit = 2



Overfitting
(High Capacity)

OVERFITTING: DECISION TREES

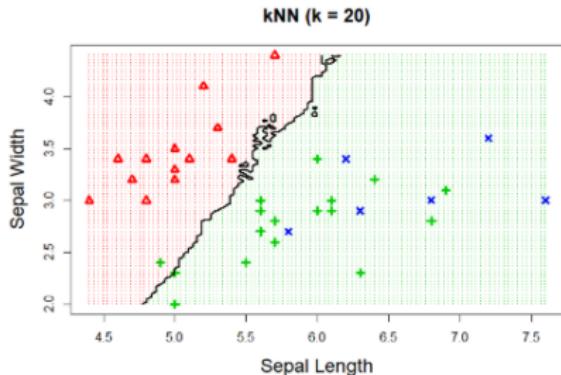


Good fit
(Appropriate capacity)

	minsplit = 60	minsplit = 12	minsplit = 2
Training error (Misclassification)	0.36	0.12	0.02
Test error (Misclassification)	0.40	0.32	0.35

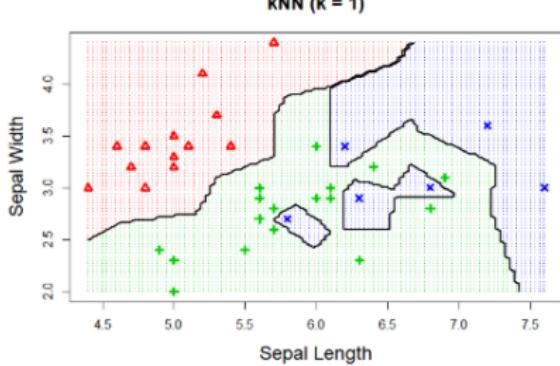
OVERFITTING: K-NEAREST NEIGHBORS

k = 20
(number of
neighbours)



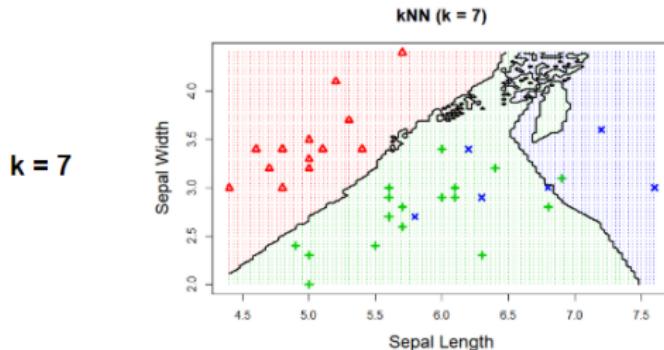
Underfitting
(Low Capacity)

k = 1



Overfitting
(High Capacity)

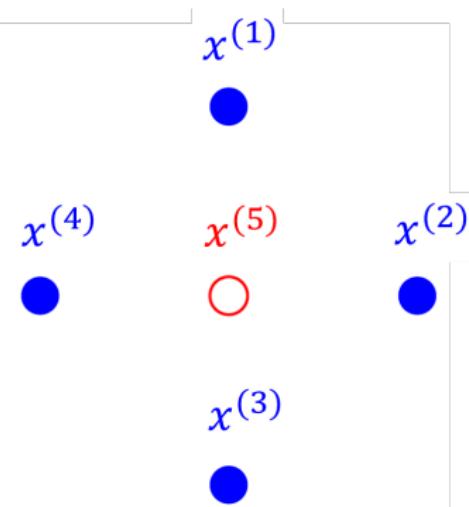
OVERFITTING: K-NEAREST NEIGHBORS



	k = 20	k = 7	k = 1
Training error (Misclassification)	0.22	0.13	0
Test error (Misclassification)	0.40	0.25	0.33

Introduction to Machine Learning

PAC Learning and VC Dimension



Learning goals

- Know PAC learning
- Know that there is no "universal" learner which works on every task (no free lunch)
- Know that complexity of a hypothesis space can be measured by VC dimension
- Know that a hypothesis space is PAC learnable iff it has finite VC dimension

PAC LEARNING

A hypothesis space \mathcal{H} over a data space $\mathcal{X} \times \mathcal{Y}$ is agnostic PAC learnable, if there exists a function $n_{\mathcal{H}} : (0, 1)^2 \rightarrow \mathbb{N}$ and a learning algorithm with the following property:

For every ϵ, δ and for **every data distribution** \mathbb{P}_{xy} , when running the algorithm on $n \geq n_{\mathcal{H}}(\epsilon, \delta)$ i.i.d. examples from \mathbb{P}_{xy} , the learner returns a model \hat{f} such that, which probability at least $1 - \delta$ (over the choice of the n training examples), it holds

$$\mathcal{R}(\hat{f}) \leq \min_{f \in \mathcal{H}} \mathcal{R}(f) + \epsilon$$

- PAC = Probably (δ) Approximately (ϵ) Correct learning.
- It implies that our learner, given enough samples, always return an "approximately" correct function.
- $n_{\mathcal{H}}(\epsilon, \delta)$ is the sample complexity of our learner, how many samples do we need to obtain a PAC solution.
- PAC gives us finite-sample bounds on **arbitrary** data distributions!

FINITE SPACES ARE AGNOSTIC PAC LEARNABLE

Every finite hypothesis space is agnostic PAC learnable, using empirical risk minimization, with sample complexity

$$n_{\mathcal{H}}(\epsilon, \delta) \leq \lceil \frac{2 \log(2|\mathcal{H}|/\delta)}{\epsilon^2} \rceil$$

- Proof: See "Understanding Machine Learning", chapter 4.
- While many spaces \mathcal{H} are infinite, we can discretize them to get a certain impression of their sample complexity.
 - Assume that parameters are floats on a 32bit machine, then there are at most 2^{32} different values for each parameter.
 - If we have d parameters, that's 2^{32d} functions in \mathcal{H} .
 - That gives us $n_{\mathcal{H}} \leq \frac{64d + \log 2/\delta}{\epsilon^2}$
 - For 10 parameters and $\epsilon = \delta = 0.05$ that is ca. $n = 250.000$.

NO FREE LUNCH

Let \mathcal{I} be any learning algorithm for binary classification, with respect to 0-1 loss over domain \mathcal{X} . Let the training set size $n \leq |\mathcal{X}|/2$. Then a data distribution \mathbb{P}_{xy} exists, such that

- ① There exists a function f with $\mathcal{R}_{\mathbb{P}}(f) = 0$
 - ② With probability at least $1/7$ (over the choice of \mathcal{D}_n) we have that $\mathcal{R}_{\mathbb{P}}(I(\mathcal{D}_n)) \geq 1/8$.
-
- Proof: See "Understanding Machine Learning", chapter 5.
 - This implies that for every learner, there is a task on which it fails, even though it could be learned by another learner. So there is no "universal" learner.
 - This implies that if \mathcal{X} is infinite, the space \mathcal{H} of all functions is not PAC learnable. Learning without any assumptions does not work.

VC DIMENSION

A general measure of the complexity of a function space is the **Vapnik-Chervonenkis (VC)** dimension.

The **VC dimension** of a class of binary-valued functions

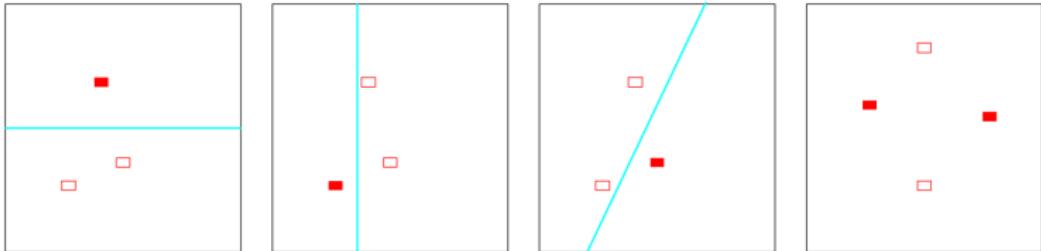
$\mathcal{H} = \{h : \mathcal{X} \rightarrow \{0, 1\}\}$ is defined to be the largest number of points in \mathcal{X} (in some configuration) that can be “shattered” by members of \mathcal{H} .

We write $VC_p(\mathcal{H})$, where p denotes the dimension of the input space.

A set of points is said to be **shattered** by a class of functions if a member of this class can perfectly separate them no matter how we assign binary labels to the points.

Note: If the VC dimension of a hypothesis class is d , it does not mean that **all** sets of size d can be shattered. Rather, it simply means that there is at least **one** such set which can be shattered and **no** set of size $d + 1$ which can be shattered.

VC DIMENSION OF HYPERPLANES



For $\mathbf{x} \in \mathbb{R}^2$, the class of linear indicator functions

$$\mathcal{H} = \{h : \mathbb{R}^2 \rightarrow \{0, 1\} \mid h(\mathbf{x} \mid \theta_0, \boldsymbol{\theta}) = \mathbb{I}[\mathbf{x}^T \boldsymbol{\theta} - \theta_0 > 0]\}$$

- can shatter 3 points: No matter how we assign labels to the configuration of three points shown above, we can find a linear line separating them perfectly;
- cannot shatter a configuration of 4 points.

Hence, $VC_2(\mathcal{H}) = 3$.

VC DIMENSION OF HYPERPLANES

Theorem: The VC dimension of the class of homogeneous halfspaces, $\mathcal{H} = \{h : \mathbb{R}^p \rightarrow \{-1, 1\} \mid h(\mathbf{x}) = \text{sign}(\mathbf{x}^T \boldsymbol{\theta})\}$, in \mathbb{R}^p is p .

Proof: p as a lower bound:

Consider the set of standard basis vectors $\mathbf{e}^{(1)}, \mathbf{e}^{(2)}, \dots, \mathbf{e}^{(p)}$ in \mathbb{R}^p . For every possible labeling $y^{(1)}, y^{(2)}, \dots, y^{(p)} \in \{-1, +1\}$, if we set $\boldsymbol{\theta} = (y^{(1)}, y^{(2)}, \dots, y^{(p)})^\top$, then $h(\mathbf{e}^{(i)}) = \text{sgn}(\boldsymbol{\theta}^\top \mathbf{e}^{(i)}) = \text{sgn}(y^{(i)}) = y^{(i)}$ for all i . Therefore, the p points are shattered.

p as an upper bound:

- Let $\mathbf{x}^{(1)}, \mathbf{x}^{(2)}, \dots, \mathbf{x}^{(p+1)}$ be a set of $p+1$ vectors in \mathbb{R}^p .
- Because any set of $p+1$ vectors in \mathbb{R}^p is linearly dependent, there must exist real numbers $a_1, a_2, \dots, a_{p+1} \in \mathbb{R}$, not all of them zero, such that $\sum_{i=1}^{p+1} a_i \mathbf{x}^{(i)} = 0$.

VC DIMENSION OF HYPERPLANES

Let $I = \{i : a_i > 0\}$ and $J = \{j : a_j < 0\}$. Either I or J is nonempty. If we assume both I and J are nonempty, then:

- $\sum_{i \in I} a_i \mathbf{x}^{(i)} = \sum_{j \in J} |a_j| \mathbf{x}^{(j)}$
- Let us assume $\mathbf{x}^{(1)}, \mathbf{x}^{(2)}, \dots, \mathbf{x}^{(p+1)}$ are shattered by \mathcal{H} .
- There must exist a vector $\theta \in \mathbb{R}^p$ such that

$$h(\mathbf{x}^{(i)} | \theta) = 1 \Leftrightarrow \theta^\top \mathbf{x}^{(i)} > 0 \quad \text{for all } i \in I$$
$$h(\mathbf{x}^{(j)} | \theta) = -1 \Leftrightarrow \theta^\top \mathbf{x}^{(j)} < 0 \quad \text{for all } j \in J$$

VC DIMENSION OF HYPERPLANES

- This implies

$$\begin{aligned} 0 < \sum_{i \in I} a_i \cdot \boldsymbol{\theta}^\top \mathbf{x}^{(i)} &= \left(\sum_{i \in I} a_i \mathbf{x}^{(i)} \right)^\top \boldsymbol{\theta} \\ &= \left(\sum_{j \in J} |a_j| \mathbf{x}^{(j)} \right)^\top \boldsymbol{\theta} = \sum_{j \in J} |a_j| \cdot \boldsymbol{\theta}^\top \mathbf{x}^{(j)} < 0 \end{aligned}$$

which is a contradiction.

On the other hand, if we assume J (respectively, I) is empty, then the rightmost (respectively, leftmost) inequality should be replaced by an equality, which is still a contradiction.

□

VC DIMENSION OF HYPERPLANES

Theorem: The VC dimension of the class of non-homogeneous halfspaces, $\mathcal{H} = \{h : \mathbb{R}^p \rightarrow \{-1, 1\} \mid h(\mathbf{x} \mid \boldsymbol{\theta}) = \text{sgn}(\mathbf{x}^\top \boldsymbol{\theta} + \theta_0)\}$, in \mathbb{R}^p is $p + 1$.

Proof: $p + 1$ as a lower bound: Similar to the proof of the previous theorem, the set of basis vectors and the origin, that is, $0, \mathbf{e}^{(1)}, \dots, \mathbf{e}^{(p)}$ can be shattered by non-homogenous halfspaces.

$p + 1$ as an upper bound:

- Assume that $p + 2$ vectors $\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(p+2)}$ are shattered.
- If we denote $\tilde{\boldsymbol{\theta}} = (\theta_0, \dots, \theta_p)^\top \in \mathbb{R}^{p+1}$, where θ_0 is the bias/intercept, and $\tilde{\mathbf{x}} = (1, x_1, \dots, x_p)^\top \in \mathbb{R}^{p+1}$, then $h(\mathbf{x} \mid \boldsymbol{\theta}) = \text{sgn}(\mathbf{x}^\top \boldsymbol{\theta} + \theta_0) = \text{sgn}(\tilde{\mathbf{x}}^\top \tilde{\boldsymbol{\theta}})$. Any affine function in \mathbb{R}^p can be rewritten as a homogeneous linear function in \mathbb{R}^{p+1} .
- By the previous theorem, the set of homogeneous halfspaces in \mathbb{R}^{p+1} cannot shatter any $p + 2$ points. Contradiction.

VC DIMENSION OF RECTANGLES

Example: Let \mathcal{H} be the class of axis-aligned rectangles in \mathbb{R}^2

$$\mathcal{H} = \{h_{(a_1, a_2, b_1, b_2)} : \mathbb{R}^2 \rightarrow \{0, 1\} : a_1 \leq a_2 \text{ and } b_1 \leq b_2\}$$

where

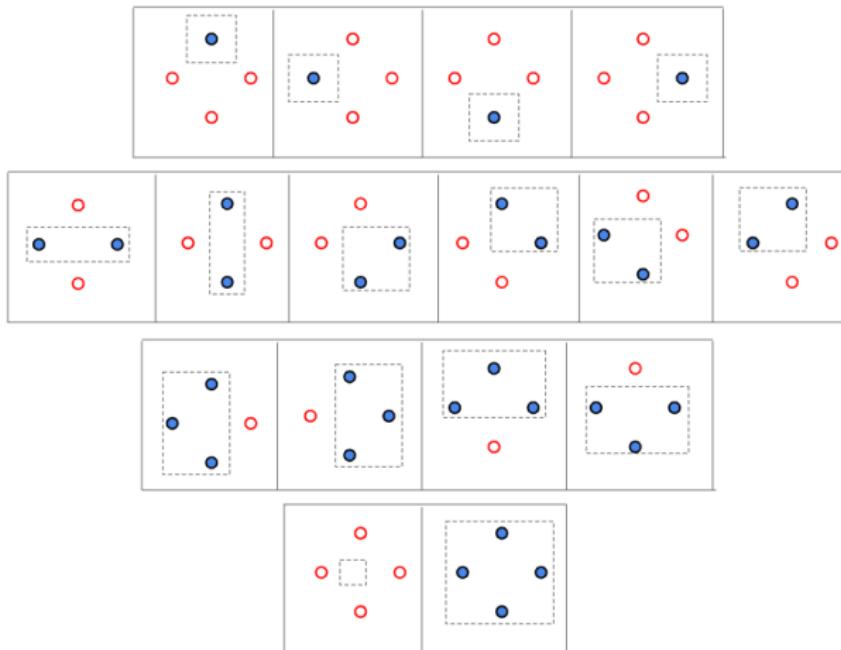
$$h_{(a_1, a_2, b_1, b_2)}(\mathbf{x}) = \begin{cases} 1 & a_1 \leq x_1 \leq a_2 \text{ and } b_1 \leq x_2 \leq b_2 \\ 0 & \text{otherwise} \end{cases}$$

Claim: $VC_2(\mathcal{H}) = 4$

Proof: (next slide)

VC DIMENSION OF RECTANGLES

4 as a lower bound: There exists a set of 4 points that can be shattered.

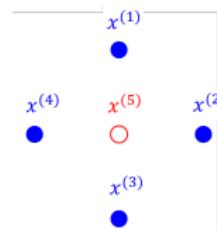


VC DIMENSION OF RECTANGLES

4 as an upper bound: For any set of 5 points

$$\mathbf{x}^{(1)}, \mathbf{x}^{(2)}, \mathbf{x}^{(3)}, \mathbf{x}^{(4)}, \mathbf{x}^{(5)} \in \mathbb{R}^2:$$

- Assign the leftmost point (lowest x_1), rightmost point (highest x_1), highest point (highest x_2), and lowest point (lowest x_2) to class 1.
- The point not chosen, $\mathbf{x}^{(5)}$, is assigned to class 0.
- The rectangle must contain $\mathbf{x}^{(1)}, \mathbf{x}^{(2)}, \mathbf{x}^{(3)}$ and $\mathbf{x}^{(4)}$.
- $\mathbf{x}^{(5)}$ is classified as 1 as well since its coordinates are within the intervals defined by the other 4.



Credit: Shalev-Shwartz, Ben-David. Understanding Machine Learning.

Therefore, the VC dimension of axis-aligned rectangles is 4. □

INFINITE VC DIMENSION

- We can show that if \mathcal{H} has a VC dimension of $2n$, we cannot reliably learn \mathcal{H} from only n examples. Similar to our first statement of the NFL theorem, we can now show that an adversarial data distribution exists, on which our learner fails. But also a function with risk 0 exists, but because of the shattering, this will be in \mathcal{H} .
- This directly implies that spaces of infinite VC dimension are not PAC learnable.

FUNDAMENTAL THEOREM OF PAC LEARNING

Assume hypothesis space \mathcal{H} , classification, and 0-1 loss. Then:

- \mathcal{H} is agnostic PAC learnable if and only if \mathcal{H} has finite VC dimension.
- Any ERM algorithm is a successful agnostic PAC learner for \mathcal{H} .
- For finite VC dimension d , the sample complexity is

$$C_1 \frac{d + \log(1/\delta)}{\epsilon} \leq n_{\mathcal{H}}(\epsilon, \delta) \leq C_2 \frac{d \log(1/\epsilon) + \log(1/\delta)}{\epsilon}$$

with positive, absolute constants C_1 and C_2 .

PROBABILISTIC BOUND ON TEST ERROR

Recall that the training error is an optimistic estimate of the generalization (or test) error. For a classification model with VC dimension d , 0-1-loss, and a training set of size n , the VC dimension can predict a probabilistic upper bound on the test error (with probability $1 - \delta$):

$$\mathcal{R}(f) \leq \mathcal{R}_{\text{emp}}(f) + \sqrt{\frac{1}{n} \left[d \left(\log \frac{2n}{d} + 1 \right) - \log \frac{\delta}{4} \right]}$$

if the training data set is large enough ($d < n$ required).

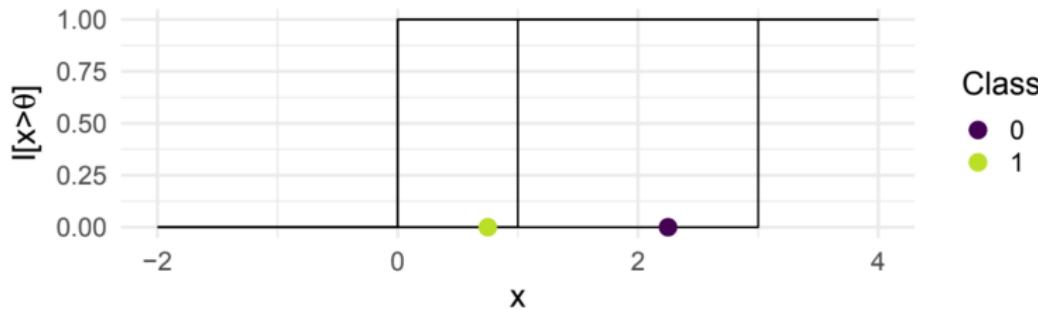
- So for finite VC dimension we could increase our sample size n so much, that the training error would give a close estimate of the test error, with high probability.
- Usually such a bound is too loose for practical relevance, and we would have to use an enormous amount of data.

VC DIMENSION VS NR OF PARAMETERS

Often, VC dimension of a hypothesis space increases with the number of learnable parameters. However, there are counterexamples.

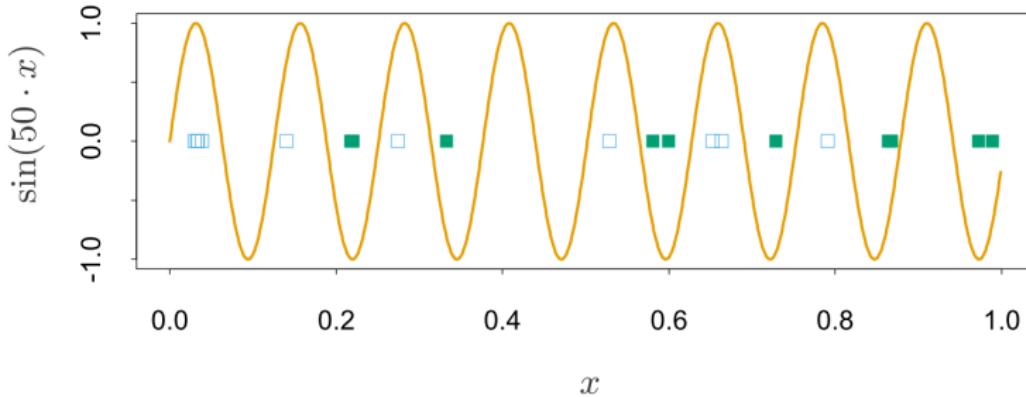
Example: A single-parametric threshold classifier ($h(x) = \mathbb{I}[x \geq \theta]$) has VC dimension 1:

- It can shatter a single point.
- It cannot shatter any set of 2 points (for every set of 2 numbers, if the smaller is labeled 1, the larger must also be labeled 1).



VC DIMENSION VS NR OF PARAMETERS

A single-parametric sine classifier $h(x) = \mathbb{I}[\sin(\theta x) > 0]$, for $x \in \mathbb{R}$, however, has infinite VC dimension, since it can shatter any set of points if the frequency θ is chosen large enough.

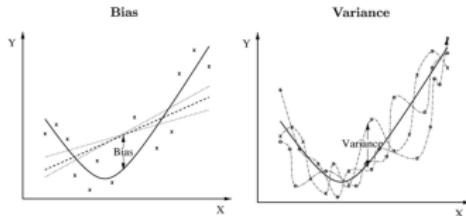


Credit: Trevor Hastie (2019). The Elements of Statistical Learning.

Introduction to Machine Learning

Bias-Variance Decomposition

Learning goals



- Understand how to decompose the generalization error of an inducer into
 - Bias of the inducer
 - Variance of the inducer
 - Noise in the data

BIAS-VARIANCE DECOMPOSITION

Let us take a closer look at the generalization error of a learning algorithm $\mathcal{I}_{L,O}$. This is the expected error an induced model, on trainings sets of size n , when this is applied to a fresh, random test observation.

$$GE_n(\mathcal{I}_{L,O}) = \mathbb{E}_{\mathcal{D}_n \sim \mathbb{P}_{xy}, (\mathbf{x}, y) \sim \mathbb{P}_{xy}} \left(L \left(y, \hat{f}_{\mathcal{D}_n}(\mathbf{x}) \right) \right) = \mathbb{E}_{\mathcal{D}_n, xy} \left(L \left(y, \hat{f}_{\mathcal{D}_n}(\mathbf{x}) \right) \right)$$

We therefore need to take the expectation over all training sets of size n , as well as the independent test observation.

We assume that the data is generated by

$$y = f_{\text{true}}(\mathbf{x}) + \epsilon,$$

with normally distributed error $\epsilon \sim \mathcal{N}(0, \sigma^2)$ independent of \mathbf{x} .

BIAS-VARIANCE DECOMPOSITION

By plugging in the $L2$ loss $L(y, f(\mathbf{x})) = (y - f(\mathbf{x}))^2$ we get

$$\begin{aligned} GE_n(\mathcal{I}_{L,O}) &= \mathbb{E}_{\mathcal{D}_n,xy} \left(L \left(y, \hat{f}_{\mathcal{D}_n}(\mathbf{x}) \right) \right) = \mathbb{E}_{\mathcal{D}_n,xy} \left((y - \hat{f}_{\mathcal{D}_n}(\mathbf{x}))^2 \right) \\ &= \mathbb{E}_{xy} \underbrace{\left[\mathbb{E}_{\mathcal{D}_n} \left((y - \hat{f}_{\mathcal{D}_n}(\mathbf{x}))^2 \mid \mathbf{x}, y \right) \right]}_{(*)} \end{aligned}$$

Let us consider the error $(*)$ conditioned on one fixed test observation (\mathbf{x}, y) first. (We omit the $\mid \mathbf{x}, y$ for better readability for now.)

$$\begin{aligned} (*) &= \mathbb{E}_{\mathcal{D}_n} \left((y - \hat{f}_{\mathcal{D}_n}(\mathbf{x}))^2 \right) \\ &= \underbrace{\mathbb{E}_{\mathcal{D}_n} (y^2)}_{=y^2} + \underbrace{\mathbb{E}_{\mathcal{D}_n} (\hat{f}_{\mathcal{D}_n}(\mathbf{x})^2)}_{(1)} - 2 \underbrace{\mathbb{E}_{\mathcal{D}_n} (y \hat{f}_{\mathcal{D}_n}(\mathbf{x}))}_{(2)} \end{aligned}$$

by using the linearity of the expectation.

BIAS-VARIANCE DECOMPOSITION

$$\mathbb{E}_{\mathcal{D}_n} \left((y - \hat{f}_{\mathcal{D}_n}(\mathbf{x}))^2 \right) = y^2 + \underbrace{\mathbb{E}_{\mathcal{D}_n} \left(\hat{f}_{\mathcal{D}_n}(\mathbf{x})^2 \right)}_{(1)} - 2 \underbrace{\mathbb{E}_{\mathcal{D}_n} \left(y \hat{f}_{\mathcal{D}_n}(\mathbf{x}) \right)}_{(2)} =$$

By using that $\mathbb{E}(z^2) = \text{Var}(z) + \mathbb{E}^2(z)$, we see that

$$= y^2 + \text{Var}_{\mathcal{D}_n} \left(\hat{f}_{\mathcal{D}_n}(\mathbf{x}) \right) + \mathbb{E}_{\mathcal{D}_n}^2 \left(\hat{f}_{\mathcal{D}_n}(\mathbf{x}) \right) - 2y \mathbb{E}_{\mathcal{D}_n} \left(\hat{f}_{\mathcal{D}_n}(\mathbf{x}) \right)$$

Plug in the definition of y

$$= f_{\text{true}}(\mathbf{x})^2 + 2\epsilon f_{\text{true}}(\mathbf{x}) + \epsilon^2 + \text{Var}_{\mathcal{D}_n} \left(\hat{f}_{\mathcal{D}_n}(\mathbf{x}) \right) + \mathbb{E}_{\mathcal{D}_n}^2 \left(\hat{f}_{\mathcal{D}_n}(\mathbf{x}) \right) - 2(f_{\text{true}}(\mathbf{x}) + \epsilon) \mathbb{E}_{\mathcal{D}_n} \left(\hat{f}_{\mathcal{D}_n}(\mathbf{x}) \right)$$

Reorder terms and use the binomial formula

$$= \epsilon^2 + \text{Var}_{\mathcal{D}_n} \left(\hat{f}_{\mathcal{D}_n}(\mathbf{x}) \right) + \left(f_{\text{true}}(\mathbf{x}) - \mathbb{E}_{\mathcal{D}_n} \left(\hat{f}_{\mathcal{D}_n}(\mathbf{x}) \right) \right)^2 + 2\epsilon \left(f_{\text{true}}(\mathbf{x}) - \mathbb{E}_{\mathcal{D}_n} \left(\hat{f}_{\mathcal{D}_n}(\mathbf{x}) \right) \right)$$

BIAS-VARIANCE DECOMPOSITION

$$(*) = \epsilon^2 + \text{Var}_{\mathcal{D}_n}(\hat{f}_{\mathcal{D}_n}(\mathbf{x})) + \left(f_{\text{true}}(\mathbf{x}) - \mathbb{E}_{\mathcal{D}_n}(\hat{f}_{\mathcal{D}_n}(\mathbf{x})) \right)^2 + 2\epsilon \left(f_{\text{true}}(\mathbf{x}) - \mathbb{E}_{\mathcal{D}_n}(\hat{f}_{\mathcal{D}_n}(\mathbf{x})) \right)$$

Let us come back to the generalization error by taking the expectation over all fresh test observations $(\mathbf{x}, y) \sim \mathbb{P}_{xy}$:

$$\begin{aligned} GE_n(\mathcal{I}_{L,O}) &= \underbrace{\sigma^2}_{\text{Variance of the data}} + \mathbb{E}_{xy} \left[\underbrace{\text{Var}_{\mathcal{D}_n}(\hat{f}_{\mathcal{D}_n}(\mathbf{x}) | \mathbf{x}, y)}_{\text{Variance of inducer at } (\mathbf{x}, y)} \right] \\ &\quad + \underbrace{\mathbb{E}_{xy} \left[\left(f_{\text{true}}(\mathbf{x}) - \mathbb{E}_{\mathcal{D}_n}(\hat{f}_{\mathcal{D}_n}(\mathbf{x})) \right)^2 | \mathbf{x}, y \right]}_{\text{Squared bias of inducer at } (\mathbf{x}, y)} + \underbrace{0}_{\text{As } \epsilon \text{ is zero-mean and independent}} \end{aligned}$$

BIAS-VARIANCE DECOMPOSITION

$$GE_n(\mathcal{I}_{L,O}) =$$

$$\underbrace{\sigma^2}_{\text{Variance of the data}} + \mathbb{E}_{xy} \left[\underbrace{\text{Var}_{\mathcal{D}_n} \left(\hat{f}_{\mathcal{D}_n}(\mathbf{x}) \mid \mathbf{x}, y \right)}_{\text{Variance of inducer at } (\mathbf{x},y)} \right] + \mathbb{E}_{xy} \left[\underbrace{\left(f_{\text{true}}(\mathbf{x}) - \mathbb{E}_{\mathcal{D}_n} \left(\hat{f}_{\mathcal{D}_n}(\mathbf{x}) \right)^2 \mid \mathbf{x}, y \right)}_{\text{Squared bias of inducer at } (\mathbf{x},y)} \right]$$

- ① The first term expresses the variance of the data. This is **noise** present in the data. Also called Bayes, intrinsic or unavoidable error. No matter what we do, we will never get below this error.
- ② The second term expresses how the predictions fluctuate on test-points on average, if we vary the training data. Expresses also the learner's tendency to learn random things irrespective of the real signal (overfitting).
- ③ The third term says how much we are "off" on average at test locations (underfitting). Models with high capacity have low **bias** and models with low capacity have high **bias**.

BIAS-VARIANCE DECOMPOSITION

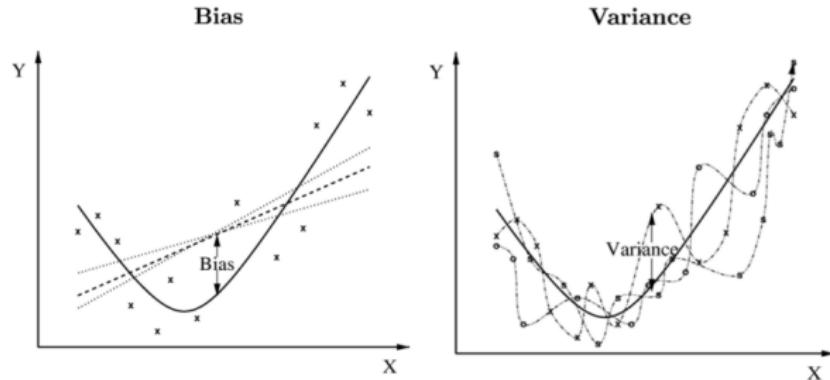


Figure: *Left:* A model with high bias is unable to fit the curved relationship present in the data. *Right:* A model with no bias and high variance can, in principle, learn the true pattern in the data. However, in practice, the learner outputs wildly different hypotheses for different training sets.

INTRODUCTION TO MACHINE LEARNING

Advanced Risk Minimization

Multiclass Classification

Information Theory

Curse of Dimensionality

Hypothesis Space

Regularization

Linear Support Vector Machine

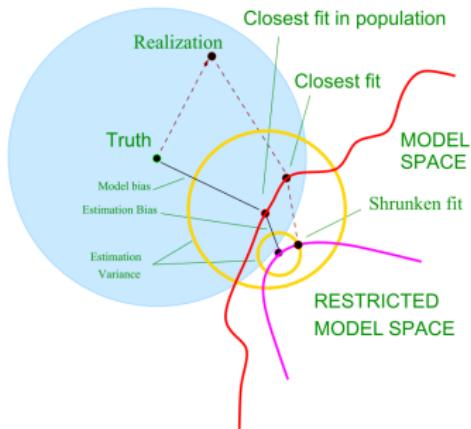
Nonlinear Support Vector Machine

Gaussian Processes

Boosting

Introduction to Machine Learning

Introduction to Regularization



Learning goals

- Understand why overfitting happens
- Know how overfitting can be avoided
- Know regularized empirical risk minimization

Motivation for Regularization

EXAMPLE: OVERFITTING

- Assume we want to predict the daily maximum **ozone level** in LA given a data set containing 50 observations.
- The data set contains 12 features describing time conditions (e.g., weekday, month), the weather (e.g., temperature at different weather stations, humidity, wind speed) or geographic variables (e.g., the pressure gradient).
- We fit a linear regression model using **all** of the features

$$f(\mathbf{x} \mid \boldsymbol{\theta}) = \boldsymbol{\theta}^T \mathbf{x} = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \dots + \theta_{12} x_{12}$$

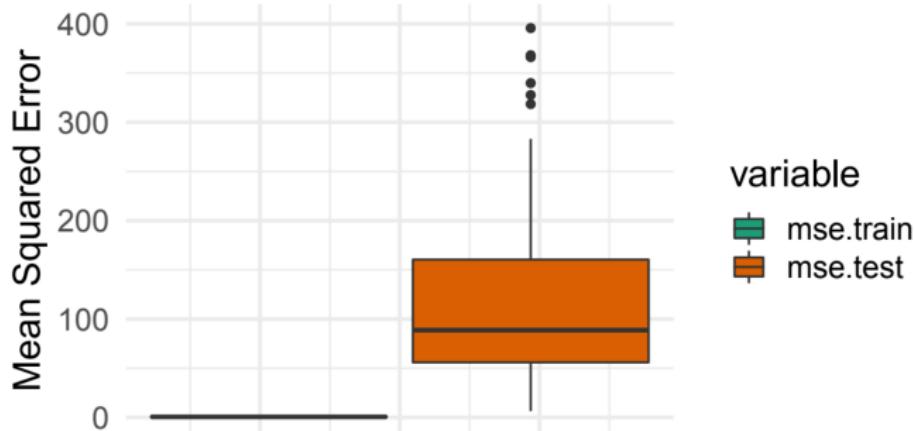
with the *L2* loss.

- We evaluate the performance with 10 times 10-fold CV.

We use (a subset of) the Ozone data set from the mlbench package. This way, we artificially create a “high-dimensional” dataset by reducing the number of observations drastically while keeping the number of features fixed.

EXAMPLE: OVERFITTING

While our model fits the training data almost perfectly (left), it generalizes poorly to new test data (right). We overfitted.



AVOID OVERFITTING

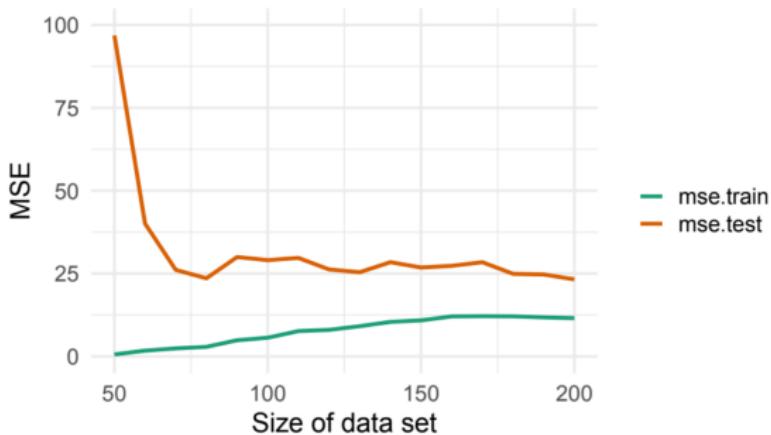
Why can **overfitting** happen? And how to avoid it?

- ➊ Not enough data
→ collect **more data**
- ➋ Data is noisy
→ collect **better data** (reduce noise)
- ➌ Models are too complex
→ use **less complex models**
- ➍ Aggressive loss optimization
→ **optimize less**

AVOID OVERFITTING

Approach 1: Collect more data

We explore our results for increased dataset size by 10 times 10-fold CV. The fit worsens slightly, but the test error decreases.



Good idea, but often not feasible in practice.

AVOID OVERFITTING

Approach 3: Reduce complexity

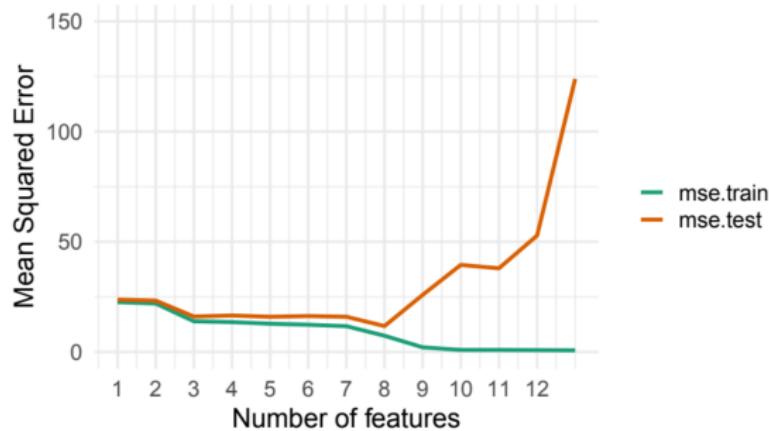
We try the simplest model we can think of: the constant model. For the L_2 loss, the optimal constant model is

$$f(\mathbf{x} \mid \boldsymbol{\theta}) = \frac{1}{n} \sum_{i=1}^n y^{(i)}$$

We then increase the complexity of the model step-by-step by adding one feature at a time.

AVOID OVERFITTING

We can control the complexity of the model by including/excluding features. We can try out all feature combinations and investigate the model fit.



Note: For simplicity, we added the features in one specific (clever) order, so we cheated a bit. Also note there are $2^{12} = 4096$ potential feature combinations.

AVOID OVERFITTING

Approach 4: Optimize less

Now we use polynomial regression with temperature as the only feature to predict the ozone level, i.e.,

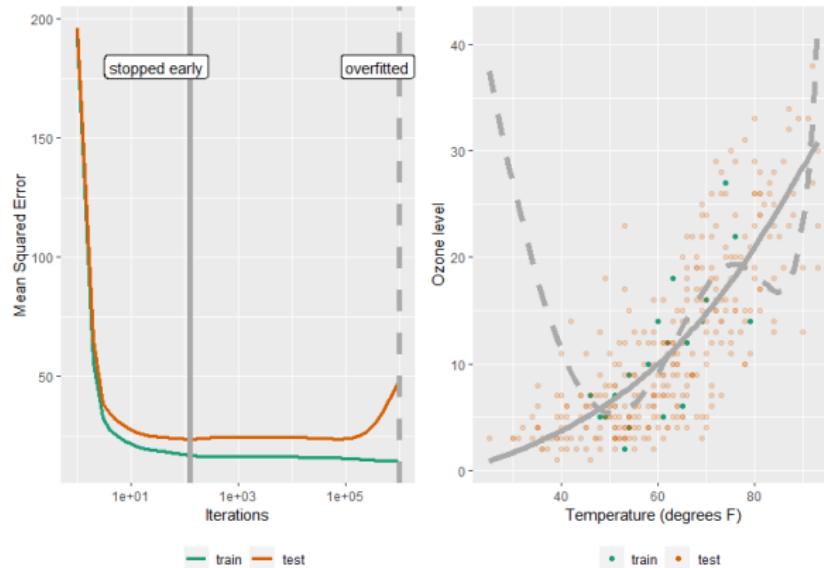
$$f(\mathbf{x} \mid \boldsymbol{\theta}) = \sum_{i=0}^d \theta_i (x_T)^i.$$

We choose $d = 15$, for which we get a very flexible model, which can be prone to overfitting for small data sets.

In this example, we don't solve for $\hat{\boldsymbol{\theta}}$ directly, but instead, we use the gradient descent algorithm to find $\hat{\boldsymbol{\theta}}$ stepwise.

AVOID OVERFITTING

We want to stop the optimization early when the generalization error starts to degrade.



Note: For polynomial regression, gradient descent usually needs many iterations before it starts to overfit. Hence a very small training set was chosen to accelerate this effect.

AVOID OVERFITTING

We have contradictory goals

- **maximizing the fit** (minimizing the train loss)
- **minimizing the complexity** of the model.

We need to find the “sweet spot”.



AVOID OVERFITTING

Until now, we can either add a feature completely or not at all.

Instead of controlling the complexity in a discrete way by specifying the number of features, we might prefer to control the complexity **on a continuum** from simple to complex.



Regularized Empirical Risk Minimization

REGULARIZED EMPIRICAL RISK MINIMIZATION

Recall, empirical risk minimization with a complex hypothesis set tends to overfit. A major tool to handle overfitting is **regularization**.

In the broadest sense, regularization refers to any modification made to a learning algorithm that is intended to reduce its generalization error but not its training error.

Explicitly or implicitly, such modifications represent the preferences we have regarding the elements of the hypothesis set.

REGULARIZED EMPIRICAL RISK MINIMIZATION

Commonly, regularization takes the following form:

$$\mathcal{R}_{\text{reg}}(f) = \mathcal{R}_{\text{emp}}(f) + \lambda \cdot J(f) = \sum_{i=1}^n L\left(y^{(i)}, f\left(\mathbf{x}^{(i)}\right)\right) + \lambda \cdot J(f)$$

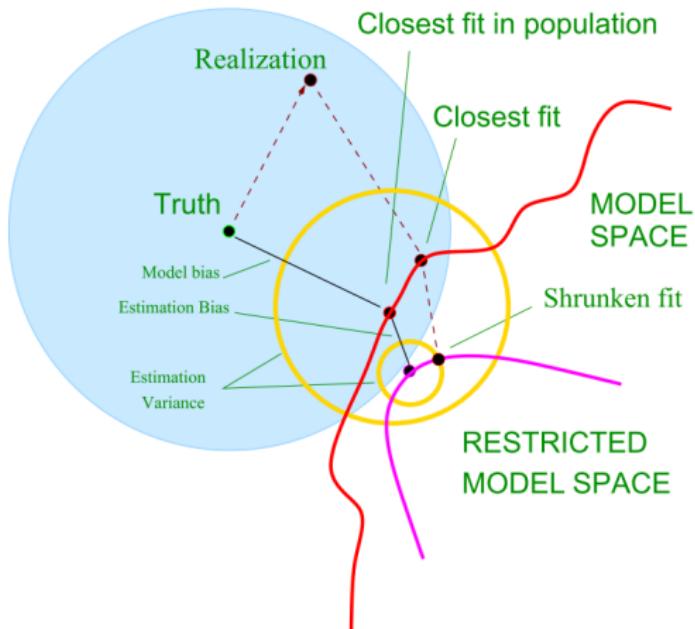
- $J(f)$ is called **complexity penalty**, **roughness penalty** or **regularizer**.
- $\lambda > 0$ is called **complexity control** parameter.
- It measures the “complexity” of a model and penalizes it in the fit.
- As for \mathcal{R}_{emp} , often \mathcal{R}_{reg} and J are defined on θ instead of f , so $\mathcal{R}_{\text{reg}}(\theta) = \mathcal{R}_{\text{emp}}(\theta) + \lambda \cdot J(\theta)$.

REGULARIZED EMPIRICAL RISK MINIMIZATION

Remarks:

- Note that we now face an optimization problem with two criteria:
 - ➊ models should fit well (low empirical risk),
 - ➋ but not be too complex (low $J(f)$).
- We decide to combine the two in a weighted sum and to control the trade-off via the complexity control parameter λ .
- λ is hard to set manually and is usually selected via cross-validation (see later).
- $\lambda = 0$: The regularized risk $\mathcal{R}_{\text{reg}}(f)$ reduces to the simple empirical $\mathcal{R}_{\text{emp}}(f)$.
- If λ goes to infinity, we stop caring about the loss/fit and models become as “simple” as possible.

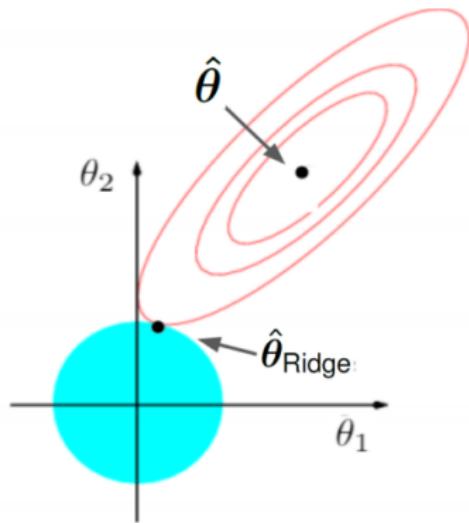
REGULARIZED EMPIRICAL RISK MINIMIZATION



Hastie, The Elements of Statistical Learning, 2009 (p. 225)

Introduction to Machine Learning

Lasso and Ridge Regression



Learning goals

- Know the regularized linear model
- Know Ridge regression (L_2 penalty)
- Know Lasso regression (L_1 penalty)

REGULARIZATION IN THE LINEAR MODEL

- Linear models can also overfit if we operate in a high-dimensional space with not that many observations.
- OLS usually require a full-rank design matrix.
- When features are highly correlated, the least-squares estimate becomes highly sensitive to random errors in the observed response, producing a large variance in the fit.
- We now add a complexity penalty to the loss:

$$\mathcal{R}_{\text{reg}}(\boldsymbol{\theta}) = \sum_{i=1}^n \left(y^{(i)} - \boldsymbol{\theta}^\top \mathbf{x}^{(i)} \right)^2 + \lambda \cdot J(\boldsymbol{\theta}).$$

- Intuitive to measure model complexity as deviation from the 0-origin, as the 0-model is empty and contains no effects. Models close to this either have few active features or only weak effects.
- So we measure $J(\boldsymbol{\theta})$ through a vector norm. This shrinks coefficients closer 0, hence the term **shrinkage methods**.

RIDGE REGRESSION

Ridge regression uses a simple $L2$ penalty:

$$\begin{aligned}\hat{\boldsymbol{\theta}}_{\text{Ridge}} &= \arg \min_{\boldsymbol{\theta}} \sum_{i=1}^n \left(y^{(i)} - \boldsymbol{\theta}^T \mathbf{x}^{(i)} \right)^2 + \lambda \|\boldsymbol{\theta}\|_2^2 \\ &= \arg \min_{\boldsymbol{\theta}} (\mathbf{y} - \mathbf{X}\boldsymbol{\theta})^\top (\mathbf{y} - \mathbf{X}\boldsymbol{\theta}) + \lambda \boldsymbol{\theta}^\top \boldsymbol{\theta}.\end{aligned}$$

Optimization is possible (as in the normal LM) in analytical form:

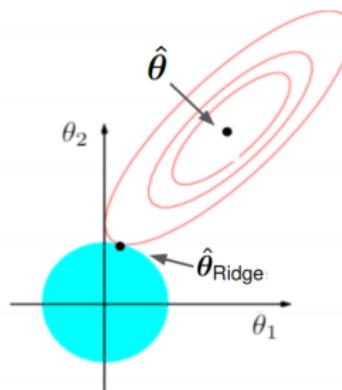
$$\hat{\boldsymbol{\theta}}_{\text{Ridge}} = (\mathbf{X}^T \mathbf{X} + \lambda \mathbf{I})^{-1} \mathbf{X}^T \mathbf{y}$$

Name comes from the fact that we add positive entries along the diagonal "ridge" $\mathbf{X}^T \mathbf{X}$.

RIDGE REGRESSION

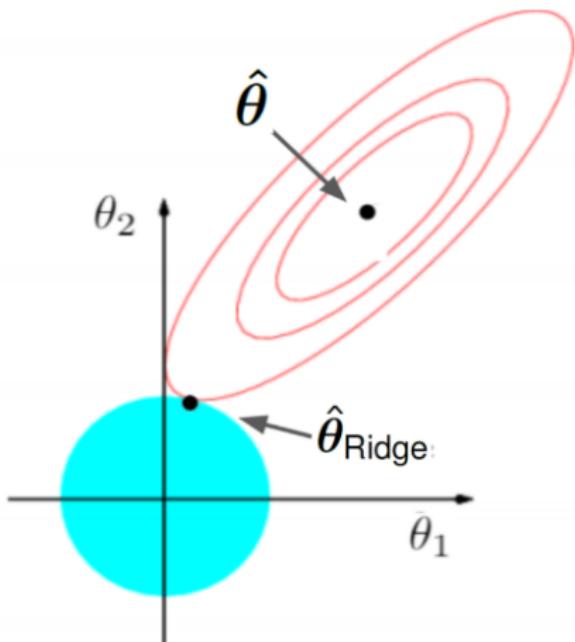
We understand the geometry of these 2 mixed components in our regularized risk objective much better, if we formulate the optimization as a constrained problem (see this a Lagrange multipliers in reverse).

$$\begin{aligned} \min_{\theta} \quad & \sum_{i=1}^n \left(y^{(i)} - f(\mathbf{x}^{(i)} | \theta) \right)^2 \\ \text{s.t.} \quad & \|\theta\|_2^2 \leq t \end{aligned}$$



NB: Relationship between λ and t will be explained later.

RIDGE REGRESSION



- We still optimize the $\mathcal{R}_{\text{emp}}(\theta)$, but cannot leave a ball around the origin.
- $\mathcal{R}_{\text{emp}}(\theta)$ grows monotonically if we move away from $\hat{\theta}$.
- Inside constraints perspective: From origin, jump from contour line to contour line (better) until you become infeasible, stop before.
- Outside constraints perspective: From $\hat{\theta}$, jump from contour line to contour line (worse) until you become feasible, stop then.
- So our new optimum will lie on the boundary of that ball.

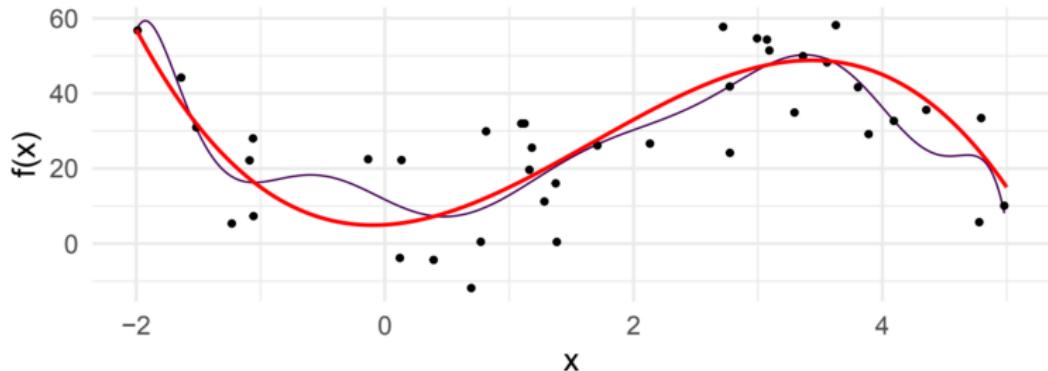
EXAMPLE: POLYNOMIAL RIDGE REGRESSION

True (unknown) function is $f(x) = 5 + 2x + 10x^2 - 2x^3 + \epsilon$ (in red).

Let us consider a d th-order polynomial

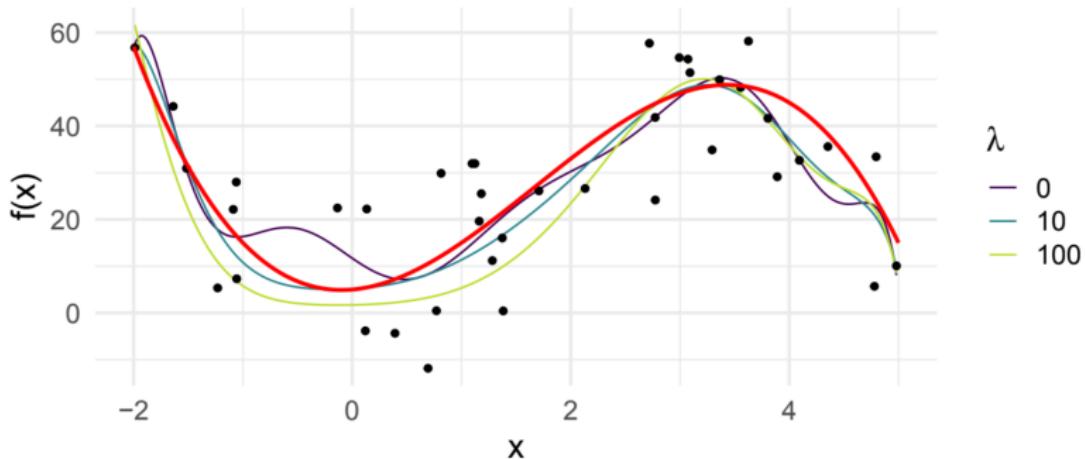
$$f(x) = \theta_0 + \theta_1 x + \cdots + \theta_d x^d = \sum_{j=0}^d \theta_j x^j.$$

Using model complexity $d = 10$ overfits:



EXAMPLE: POLYNOMIAL RIDGE REGRESSION

With an $L2$ penalty we can now select d "too large" but regularize our model by shrinking its coefficients. Otherwise we have to optimize over the discrete d .



λ	β_0	β_1	β_2	β_3	β_4	β_5	β_6	β_7	β_8	β_9	β_{10}
0.00	12.00	-16.00	4.80	23.00	-5.40	-9.30	4.20	0.53	-0.63	0.13	-0.01
10.00	5.20	1.30	3.70	0.69	1.90	-2.00	0.47	0.20	-0.14	0.03	-0.00
100.00	1.70	0.46	1.80	0.25	1.80	-0.94	0.34	-0.01	-0.06	0.02	-0.00

LASSO REGRESSION

Another shrinkage method is the so-called **Lasso regression**, which uses an $L1$ penalty on θ :

$$\begin{aligned}\hat{\theta}_{\text{Lasso}} &= \arg \min_{\theta} \sum_{i=1}^n \left(y^{(i)} - \theta^T \mathbf{x}^{(i)} \right)^2 + \lambda \|\theta\|_1 \\ &= \arg \min_{\theta} (\mathbf{y} - \mathbf{X}\theta)^T (\mathbf{y} - \mathbf{X}\theta) + \lambda \|\theta\|_1.\end{aligned}$$

Note that optimization now becomes much harder. $\mathcal{R}_{\text{reg}}(\theta)$ is still convex, but we have moved from an optimization problem with an analytical solution towards a non-differentiable problem.

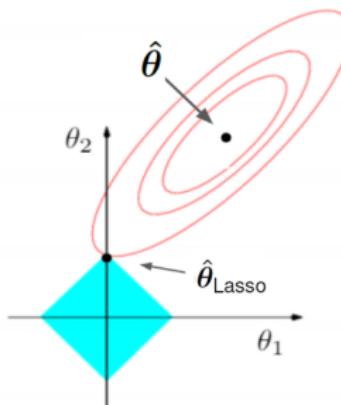
Name: least absolute shrinkage and selection operator.

LASSO REGRESSION

We can also rewrite this as a constrained optimization problem. The penalty results in the constrained region to look like a diamond shape.

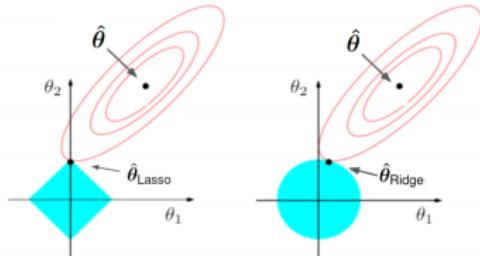
$$\min_{\theta} \quad \sum_{i=1}^n \left(y^{(i)} - f(\mathbf{x}^{(i)} | \theta) \right)^2$$

subject to: $\|\theta\|_1 \leq t$



Introduction to Machine Learning

Lasso vs. Ridge Regression

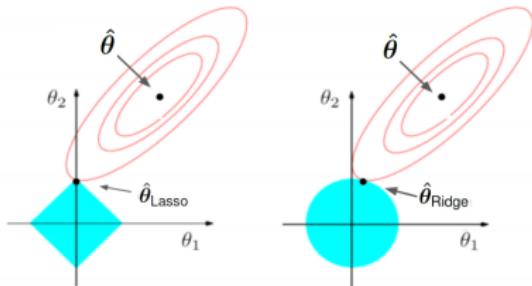


Learning goals

- Know the geometry of Ridge vs. Lasso regularization
- Understand the effects of the methods on model coefficients
- Understand that Lasso creates sparse solutions

LASSO VS. RIDGE GEOMETRY

$$\min_{\theta} \sum_{i=1}^n \left(y^{(i)} - f(\mathbf{x}^{(i)} | \theta) \right)^2 \quad \text{s.t. } \|\theta\|_p^p \leq t$$

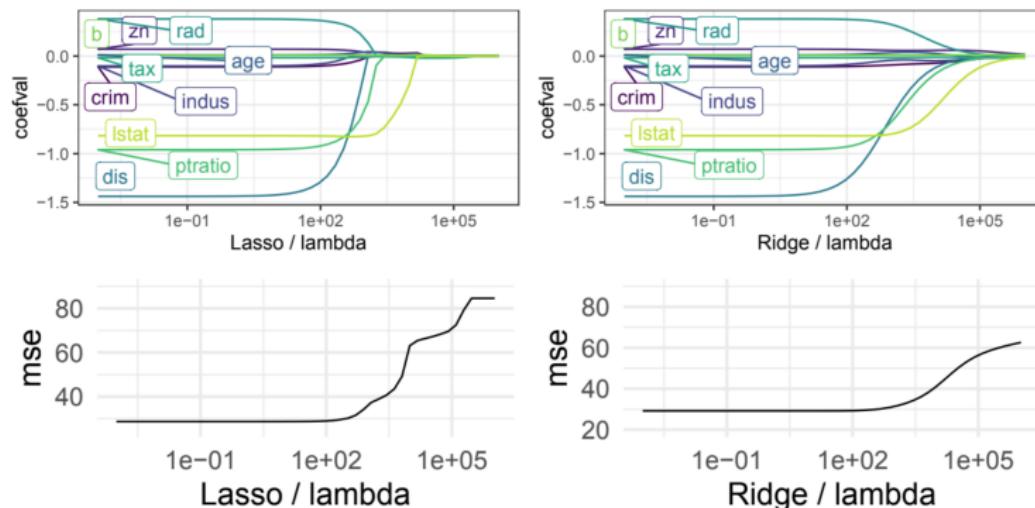


- In both cases, the solution which minimizes $\mathcal{R}_{\text{reg}}(\theta)$ is always a point on the boundary of the feasible region (for sufficiently large λ).
- As expected, $\hat{\theta}_{\text{Lasso}}$ and $\hat{\theta}_{\text{Ridge}}$ have smaller parameter norms than $\hat{\theta}$.
- For Lasso, the solution likely touches vertices of the constraint region. This induces sparsity and is a form of variable selection.
- In the $p > n$ case, the Lasso selects at most n features (due to the nature of the convex optimization problem).

COEFFICIENT PATHS AND 0-SHRINKAGE

Example 1: Boston Housing (few features removed for readability)

We cannot overfit here with an unregularized linear model as the task is so low-dimensional. But we see how only Lasso shrinks to sparsely 0.



Coef paths and cross-val. MSE for λ values for Ridge and Lasso.

COEFFICIENT PATHS AND 0-SHRINKAGE

Example 2: High-dimensional simulated data

We simulate a continuous, correlated dataset with 50 features, 100 observations $\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(100)} \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(\mathbf{0}, \Sigma)$ and

$$y = 10 \cdot (x_1 + x_2) + 5 \cdot (x_3 + x_4) + \sum_{j=5}^{14} x_j + \epsilon$$

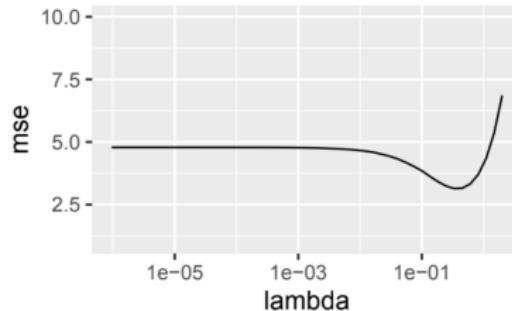
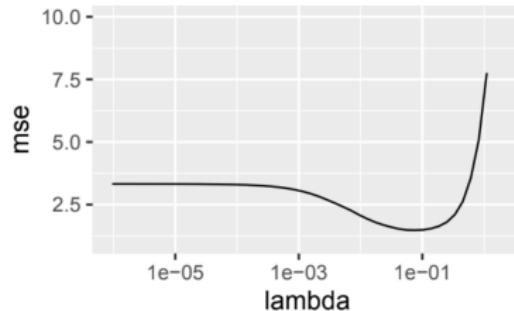
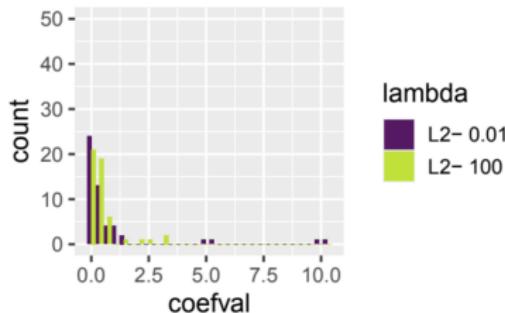
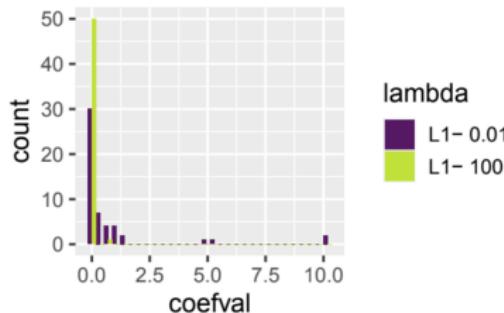
where $\epsilon \sim \mathcal{N}(0, 1)$ and $\forall k, l \in \{1, \dots, 50\}$:

$$\text{Cov}(x_k, x_l) = \begin{cases} 0.7^{|k-l|} & \text{for } k \neq l \\ 1 & \text{else} \end{cases}.$$

Note that 36 of the 50 features are noise variables.

COEFFICIENT PATHS AND 0-SHRINKAGE

Coefficient histograms for different λ values for Ridge and Lasso, on high-dimensional data along with the cross-validated MSE.



REGULARIZATION AND FEATURE SCALING

- Note that very often we do not include θ_0 in the penalty term $J(\theta)$ (but this can be implementation-dependent).
- These methods are typically not equivariant under scaling of the inputs, so one usually standardizes the features.
- Note that for a normal LM, if you scale some features, we can simply "anti-scale" the coefficients the same way. The risk does not change. For regularized models this is not so simple. If you scale features to smaller values, coefficients have to become larger to counteract. They now are penalized more heavily in $J(\theta)$. Such a scaling would make some features less attractive without changing anything relevant in the data.

REGULARIZATION AND FEATURE SCALING

Example:

- Let the true data generating process be

$$y = x_1 + \epsilon, \quad \epsilon \sim \mathcal{N}(0, 1).$$

- Let there be 5 features $x_1, \dots, x_5 \sim \mathcal{N}(0, 1)$.
- Using the Lasso (package `glmnet`), we get

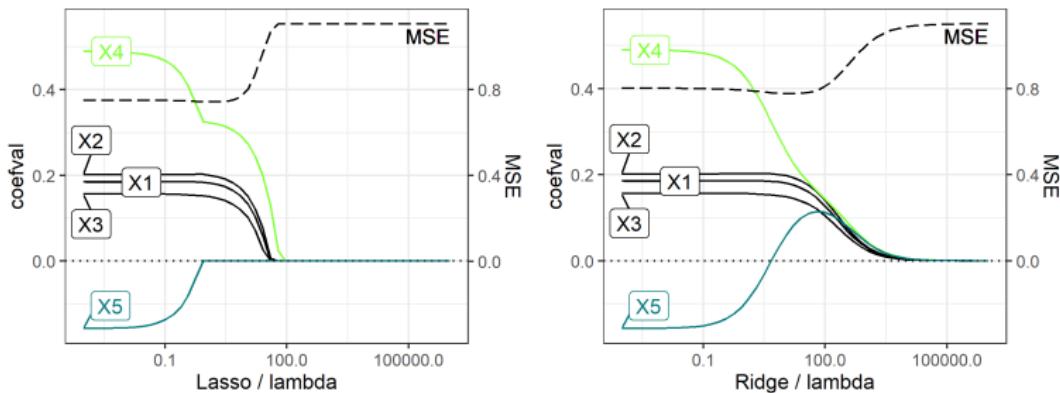
	(Intercept)	x1	x2	x3	x4
	-0.056	0.489	0.000	0.000	0.000

- But if we rescale any of the noise features, say $x_2 = 10000 \cdot x_2$ and don't use standardization, we get

	(Intercept)	x1	x2	x3	x4
	-0.106830	0.000000	-0.000013	0.000000	0.000000

- This is due to the fact, that the coefficient of x_2 will live on a very small scale as the covariate itself is large. The feature will thus get less penalized by the L_1 -norm and is favored by Lasso.

CORRELATED FEATURES



Fictional example for the model

$y = 0.2X_1 + 0.2X_2 + 0.2X_3 + 0.2X_4 + 0.2X_5 + \epsilon$ of 100 observations,
 $\epsilon \sim \mathcal{N}(0, 1)$. X_1 - X_4 are independently drawn from different normal distributions: $X_1, X_2, X_3, X_4 \sim \mathcal{N}(0, 2)$. While X_1 - X_4 have pairwise correlation coefficients of 0, X_4 and X_5 are nearly perfectly correlated: $X_5 = X_4 + \delta, \delta \sim \mathcal{N}(0, 0.3), \rho(X_4, X_5) = 0.98$.

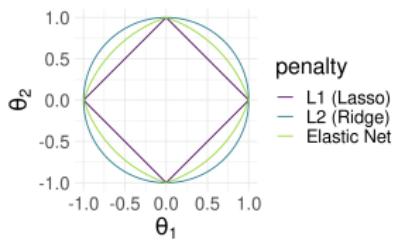
We see that Lasso shrinks the coefficient for X_5 to zero early on, while Ridge assigns similar coefficients to X_4, X_5 for larger λ .

SUMMARIZING COMMENTS

- Neither one can be classified as overall better.
- Lasso is likely better if the true underlying structure is sparse, so if only few features influence y . Ridge works well if there are many influential features.
- Lasso can set some coefficients to zero, thus performing variable selection, while Ridge regression usually leads to smaller estimated coefficients, but still dense θ vectors.
- Lasso has difficulties handling correlated predictors. For high correlation Ridge dominates Lasso in performance.
- For Lasso one of the correlated predictors will have a larger coefficient, while the rest are (nearly) zeroed. The respective feature is, however, selected randomly.
- For Ridge the coefficients of correlated features are similar.

Introduction to Machine Learning

Elastic Net and Regularization for GLMs



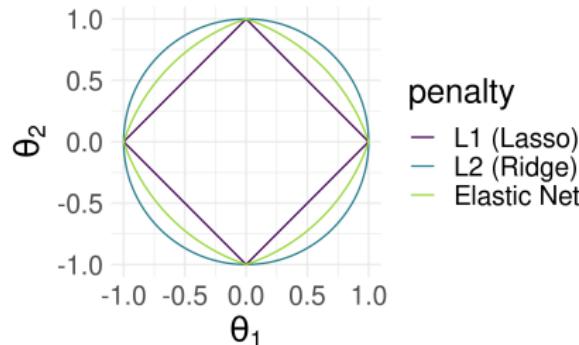
Learning goals

- Know the elastic net as compromise between Ridge and Lasso regression
- Know regularized logistic regression

ELASTIC NET

Elastic Net combines the L_1 and L_2 penalties:

$$\mathcal{R}_{\text{elnet}}(\boldsymbol{\theta}) = \sum_{i=1}^n (y^{(i)} - \boldsymbol{\theta}^\top \mathbf{x}^{(i)})^2 + \lambda_1 \|\boldsymbol{\theta}\|_1 + \lambda_2 \|\boldsymbol{\theta}\|_2^2.$$



- Correlated predictors tend to be either selected or zeroed out together.
- Selection of more than n features possible for $p > n$.

ELASTIC NET

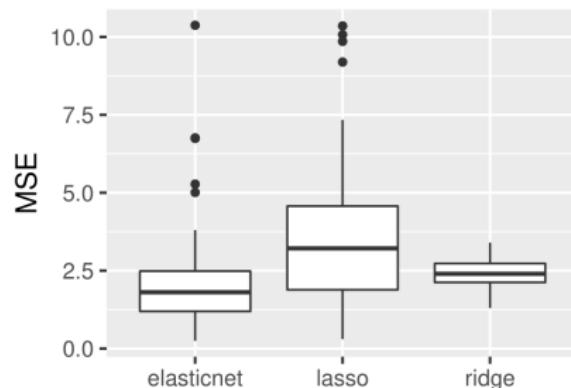
Simulating two examples with each 50 data sets and 100 observations each:

$$\mathbf{y} = \mathbf{X}\beta + \sigma\epsilon, \quad \epsilon \sim N(0, 1), \quad \sigma = 1$$

Ridge performs better for:

$$\beta = (\underbrace{2, \dots, 2}_{5}, \underbrace{0, \dots, 0}_{5})$$

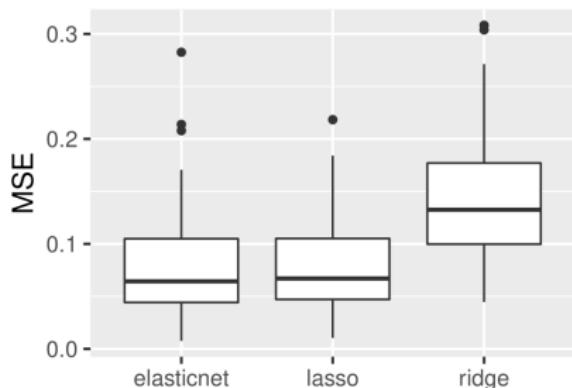
$$\text{corr}(\mathbf{X}_i, \mathbf{X}_j) = 0.8^{|i-j|} \text{ for all } i \text{ and } j$$



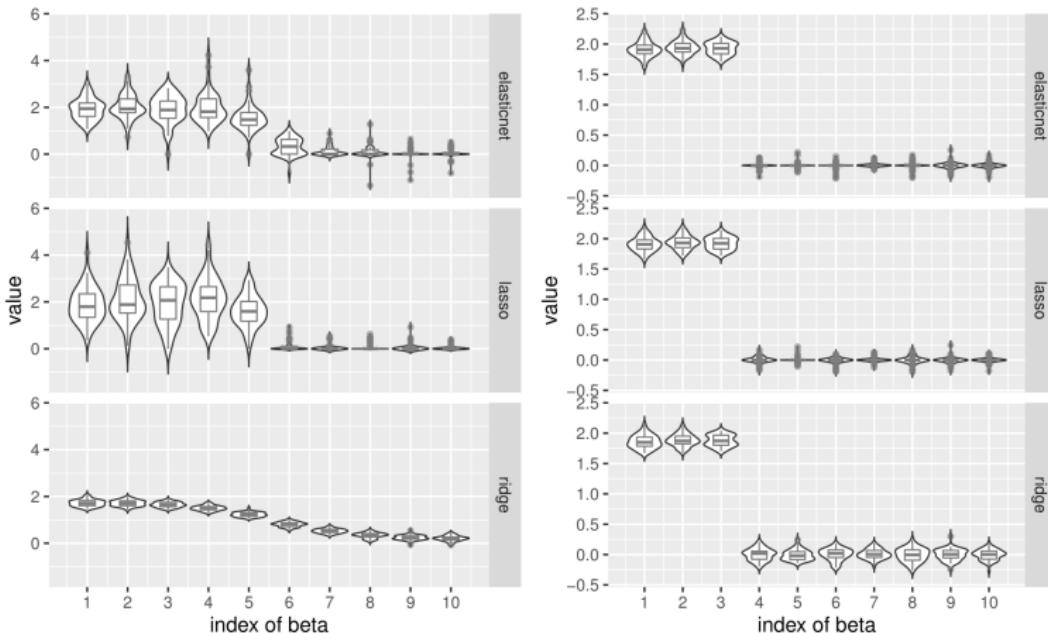
Lasso performs better for:

$$\beta = (2, 2, 2, \underbrace{0, \dots, 0}_{7})$$

$$\text{corr}(\mathbf{X}_i, \mathbf{X}_j) = 0 \text{ for all } i \neq j, \text{ otherwise } 1$$



ELASTIC NET



Since Elastic Net offers a compromise between Ridge and Lasso, it is suitable for both data situations.

REGULARIZED LOGISTIC REGRESSION

Regularizers can be added very flexibly to basically any model which is based on ERM.

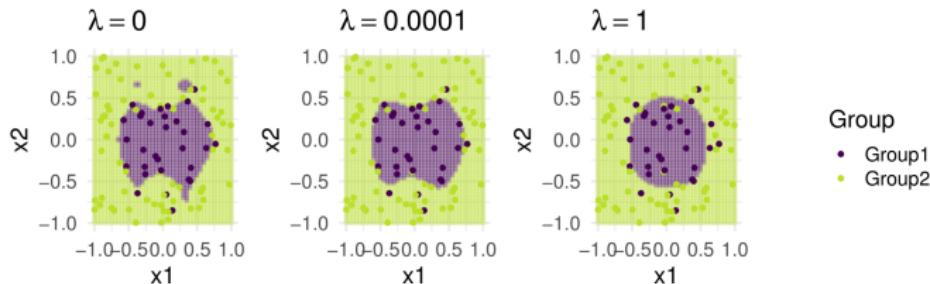
Hence, we can, e.g., construct L_1 - or L_2 -penalized logistic regression to enable coefficient shrinkage and variable selection in this model.

$$\begin{aligned}\mathcal{R}_{\text{reg}}(\boldsymbol{\theta}) &= \mathcal{R}_{\text{emp}}(\boldsymbol{\theta}) + \lambda \cdot J(\boldsymbol{\theta}) \\ &= \sum_{i=1}^n \log \left[1 + \exp \left(-2y^{(i)} f \left(\mathbf{x}^{(i)} \mid \boldsymbol{\theta} \right) \right) \right] + \lambda \cdot J(\boldsymbol{\theta})\end{aligned}$$

REGULARIZED LOGISTIC REGRESSION

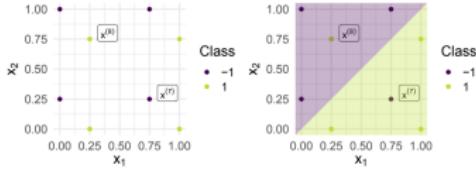
We fit a logistic regression model using polynomial features for x_1 and x_2 with maximum degree of 7. We add an L_2 penalty. We see for

- $\lambda = 0$: The unregularized model seems to overfit.
- $\lambda = 0.0001$: Regularization helps to learn the underlying mechanism.
- $\lambda = 1$: The real data-generating process is captured very well.



Introduction to Machine Learning

Regularization for Underdetermined Problems



Learning goals

- Understand that regularization is used to make ill-posed problems well defined
- Know that regularization can guarantee convergence for logistic regression on a linearly separable dataset

UNDERDETERMINED PROBLEMS

Regularization can also be motivated from a numerical perspective:

- Regularization can sometimes be necessary to make certain ill-posed problems well defined. Linear models such as (linear) regression and PCA depend "inverting" / solving a linear system, which not always works.
- When we solve linear systems like $\mathbf{X}\theta = \mathbf{y}$, there are 3 cases:
 - ① \mathbf{X} is of square form and has full rank. This is normal linear system solving and irrelevant for us here, now.
 - ② \mathbf{X} has more rows than columns. The system is "overdetermined". We now try to solve $\mathbf{X}\theta \approx \mathbf{y}$, by minimizing $||\mathbf{X}\theta - \mathbf{y}||$. Ideally, this difference would be zero, but due to the too many rows this is often not possible. This is equivalent to linear regression!
 - ③ \mathbf{X} has more columns than rows / linear dependence between columns exists. Now there are usually an infinite number of solutions. We have to define a "preference" for them to make the problem well-defined (sounds familiar?). Such problems are called "underdetermined".

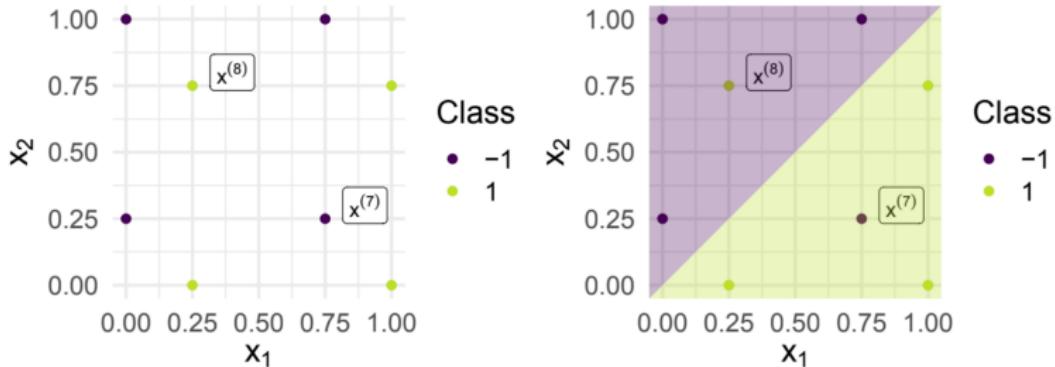
UNDERDETERMINED PROBLEMS

- A very old and well-known approach in underdetermined cases is to still reduce the problem to optimization by minimizing $\|\mathbf{X}\boldsymbol{\theta} - \mathbf{y}\|$, but adding a small positive constant to the diagonal of $\mathbf{X}^T\mathbf{X}$.
- In optimization / numerical analysis this is known as **Tikhonov** regularization.
- But as you should be able to see now: This is completely equivalent to Ridge regression!

UNDERDETERMINED PROBLEMS

We now study not the normal LM (which we could), but logistic regression applied to a linearly separable dataset for a more subtle example:

First, we take a look at logistic regression for an almost linearly separable dataset consisting of the observations $\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(8)}$.



Note: WLOG we estimate the model without intercept, s.t. we can visualize the regression coefficient θ in 2D. Also, the symmetry of the data does not influence the generality of our conclusions.

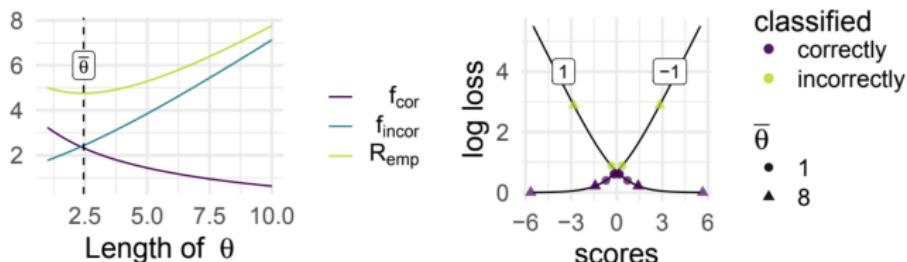
UNDERDETERMINED PROBLEMS

Because of the symmetry of the data, the direction¹ of θ is $\tilde{\theta} := (\frac{1}{\sqrt{2}}, -\frac{1}{\sqrt{2}})^\top$.

To find $\bar{\theta} := \|\theta\|_2$, we consider the empirical risk \mathcal{R}_{emp} along $\tilde{\theta}$:

$$\begin{aligned}\mathcal{R}_{\text{emp}} &= \sum_{i=1}^8 \log \left[1 + \exp \left(-y^{(i)} \theta^\top \mathbf{x}^{(i)} \right) \right] \\ &= \underbrace{\sum_{i=1}^6 \log \left[1 + \exp \left(-\bar{\theta} |\tilde{\theta}^\top \mathbf{x}^{(i)}| \right) \right]}_{=: f_{\text{cor}}(\bar{\theta}) \text{ (correctly classified)}} + \underbrace{\sum_{i=7}^8 \log \left[1 + \exp \left(\bar{\theta} |\tilde{\theta}^\top \mathbf{x}^{(i)}| \right) \right]}_{=: f_{\text{incor}}(\bar{\theta}) \text{ (incorrectly classified)}}.\end{aligned}$$

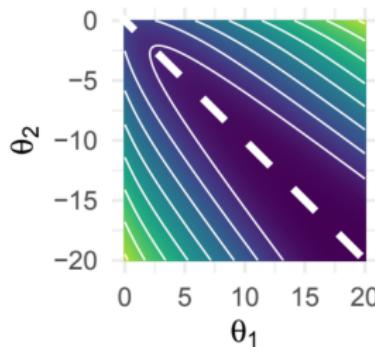
Clearly, $f_{\text{cor}} / f_{\text{incor}}$ are monotonically decreasing/increasing with rising length of θ :



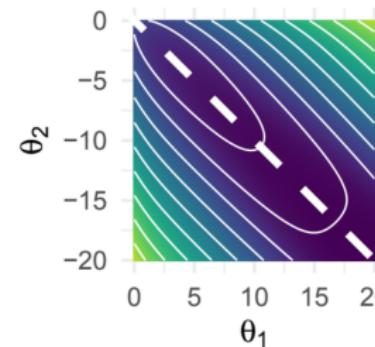
¹ θ is perpendicular to the decision boundary and points to the "1"-space

UNDERCONSTRAINED PROBLEMS

- By removing the 7th and 8th observation, we get a linearly separable dataset.
- This also means that we lose our "counterweight", i.e., if a parameter vector θ is able to classify the samples perfectly, the vector 2θ also classifies the samples perfectly, with decreased risk.
- Therefore, an iterative optimizer such as stochastic gradient descent (SGD) will continually increase θ and never halt (in theory).
- In such cases, regularization can guarantee convergence:



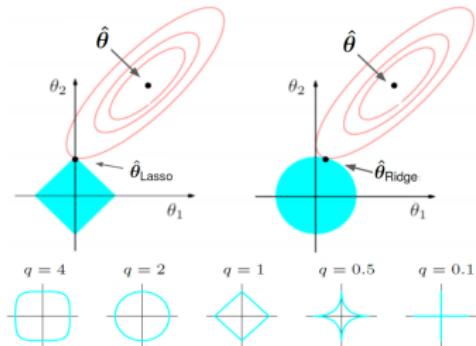
non-regularized R_{emp}



L2 regularized R_{emp}

Introduction to Machine Learning

L0 Regularization



Learning goals

- Know LQ norm regularization
- Understand that L0 norm regularization simply counts the number of non-zero parameters

LQ NORM REGULARIZATION

Besides L_1 and L_2 norm we could use any L_q norm for regularization.

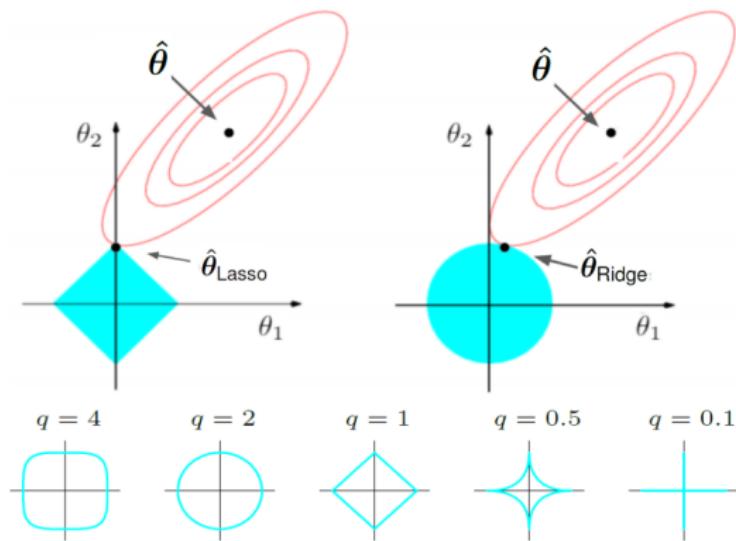


Figure: Top: Ridge and Lasso loss contours and feasible regions. Bottom: Different feasible region shapes for L_q norms $\sum_j |\theta_j|^q$.

L0 REGULARIZATION

- Consider the L_0 -regularized risk of a model $f(\mathbf{x} \mid \theta)$

$$\mathcal{R}_{\text{reg}}(\theta) = \mathcal{R}_{\text{emp}}(\theta) + \lambda \|\theta\|_0 := \mathcal{R}_{\text{emp}}(\theta) + \lambda \sum_j |\theta_j|^0.$$

- Unlike the L_1 and L_2 norms, the L_0 "norm" simply counts the number of non-zero parameters in the model.

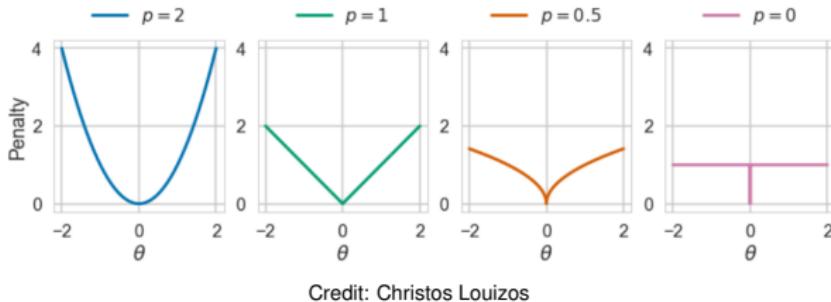


Figure: L_p norm penalties for a parameter θ according to different values of p .

L₀ REGULARIZATION

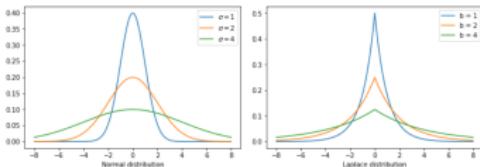
- For any parameter θ , the L_0 penalty is zero for $\theta = 0$ (defining $0^0 := 0$) and is constant for any $\theta \neq 0$, no matter how large or small it is.
- L_0 regularization induces sparsity in the parameter vector more aggressively than L_1 regularization, but does not shrink concrete parameter values as L1 and L2 does.
- Model selection criteria such as Akaike Information Criterion (AIC) and Bayesian Information Criterion (BIC) are special cases of L_0 regularization (corresponding to specific values of λ).
- The L_0 -regularized risk is neither continuous, differentiable or convex.
- It is computationally hard to optimize (NP-hard) and likely intractable. For smaller n and p we might be able to solve this nowadays directly, for larger scenarios efficient approximations of the L_0 are still topic of current research.

Introduction to Machine Learning

Regularization in Non-Linear Models and Bayesian Priors

Learning goals

- Understand that regularization and parameter shrinkage can be applied to non-linear models
- Know structural risk minimization
- Know how regularization risk minimization is the same as MAP in a Bayesian perspective, where the penalty corresponds to parameter prior.



SUMMARY: REGULARIZED RISK MINIMIZATION

If we should define ML in only one line, this might be it:

$$\mathcal{R}_{\text{reg}}(\theta) = \min_{\theta} \sum_{i=1}^n L\left(y^{(i)}, f\left(\mathbf{x}^{(i)} \mid \theta\right)\right) + \lambda \cdot J(\theta)$$

We can choose for a task at hand:

- the **hypothesis space** of f , which determines how features can influence the predicted y
- the **loss** function L , which measures how errors should be treated
- the **regularization** $J(\theta)$, which encodes our inductive bias and preference for certain simpler models

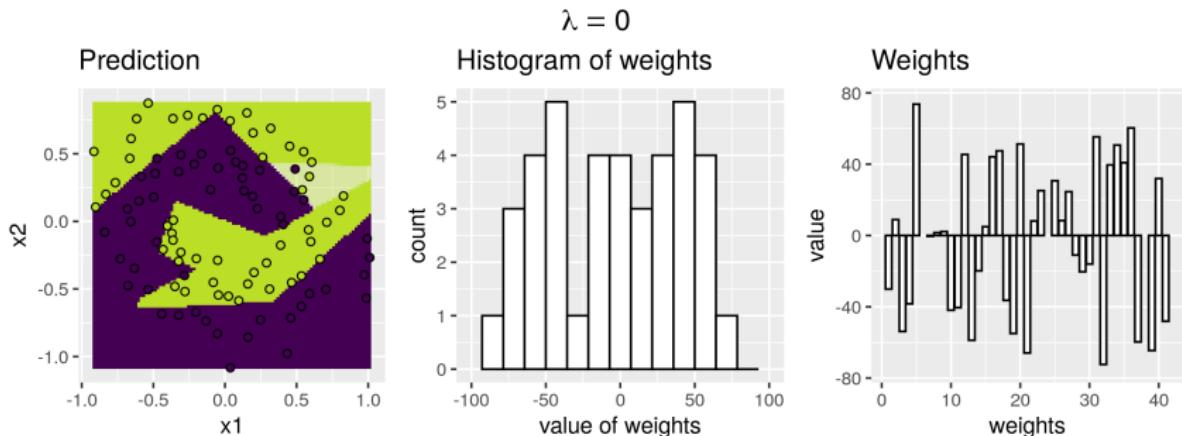
By varying these choices one can construct a huge number of different ML models. Many ML models follow this construction principle or can be interpreted through the lens of regularized risk minimization.

REGULARIZATION IN NONLINEAR MODELS

- So far we have mainly considered regularization in LMs.
- Can also be applied to non-linear models (with numeric parameters), where it is often important to prevent overfitting.
- Here, we typically use L_2 regularization, which still results in parameter shrinkage and weight decay.
- By adding regularization, prediction surfaces in regression and classification become smoother.
- Note: In the chapter on non-linear SVMs we will study the effects of regularization on a non-linear model in detail.

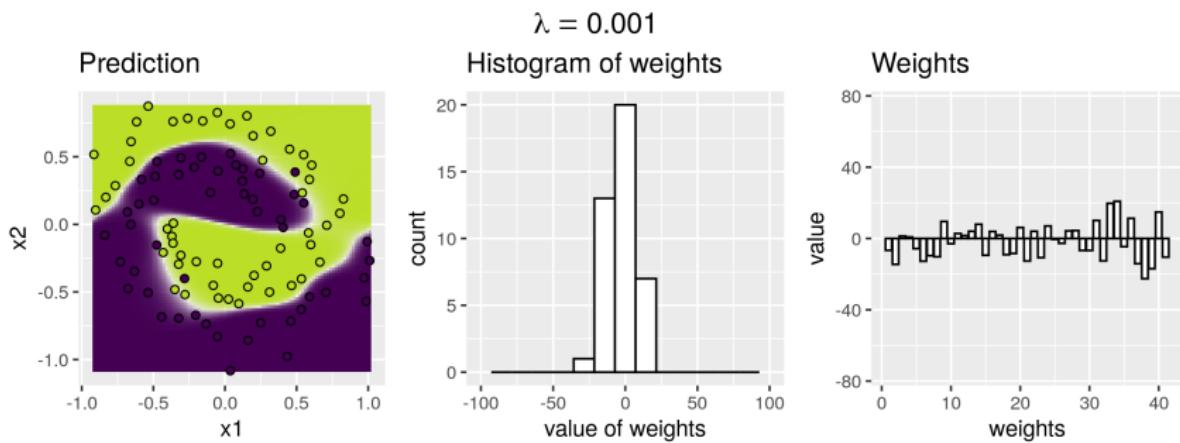
REGULARIZATION IN NONLINEAR MODELS

Setting: Classification for the spirals data. Neural network with single hidden layer containing 10 neurons and logistic output activation, regularized with L_2 penalty term for $\lambda > 0$. Varying λ affects smoothness of the decision boundary and magnitude of network weights:



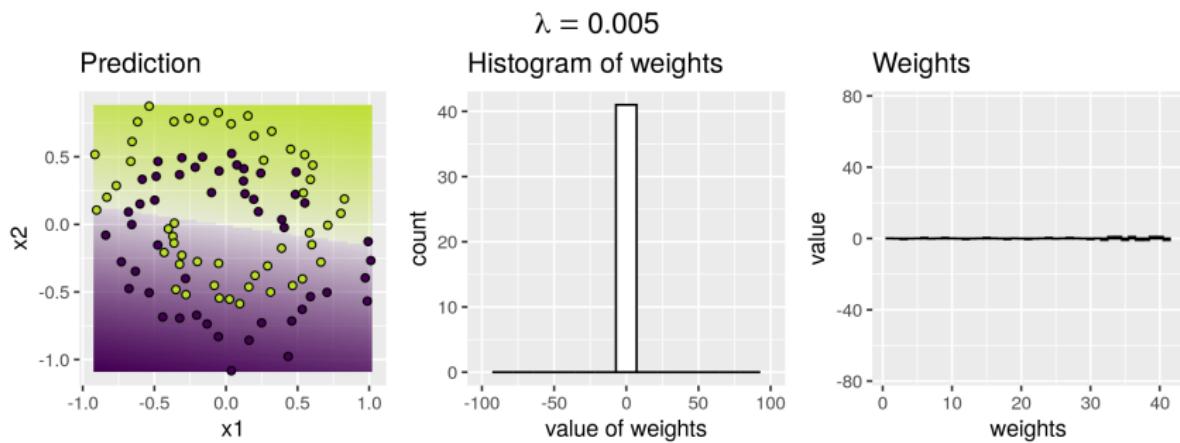
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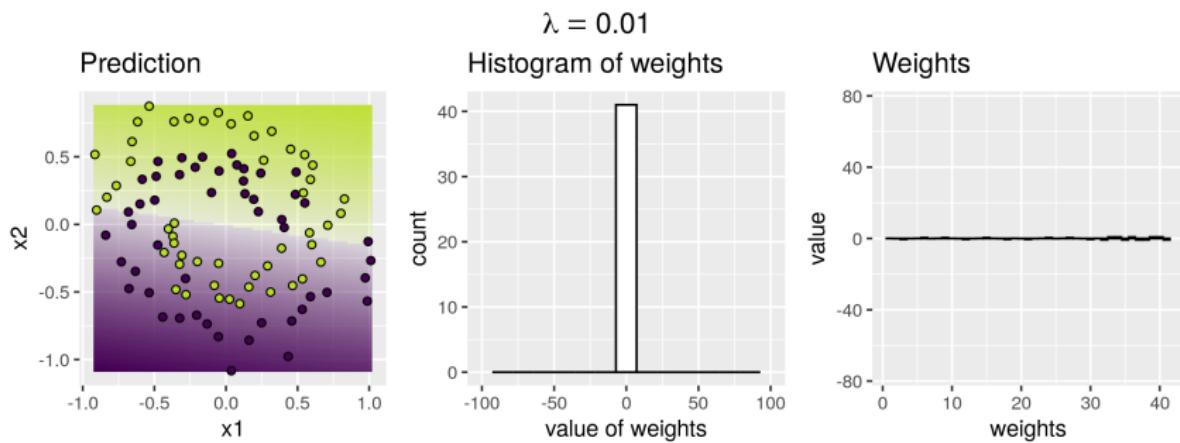
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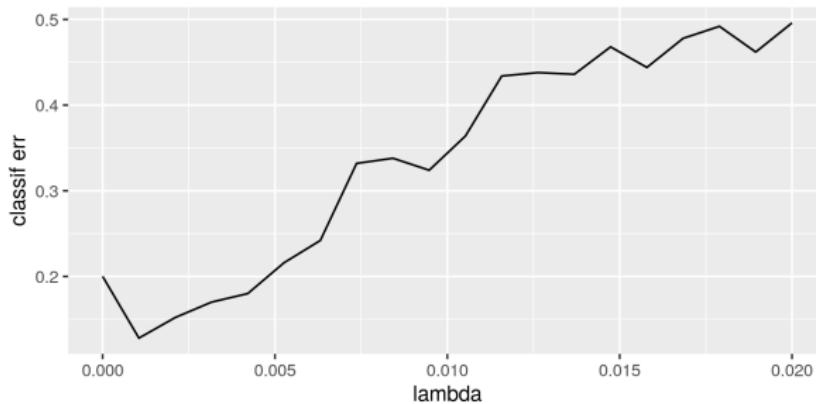
REGULARIZATION IN NONLINEAR MODELS

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REGULARIZATION IN NONLINEAR MODELS

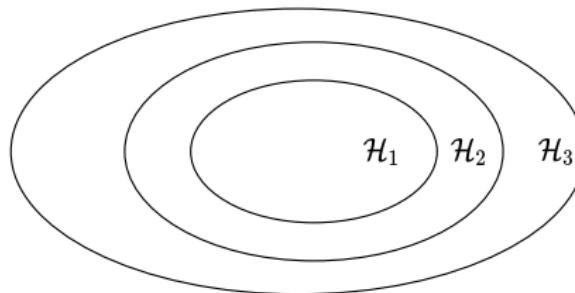
The prevention of overfitting can also be seen in CV. Same settings as before, but each λ is evaluated with repeated CV (10 folds, 5 reps).



We see the typical U-shape with the sweet spot between overfitting (LHS, low λ) and underfitting (RHS, high λ) in the middle.

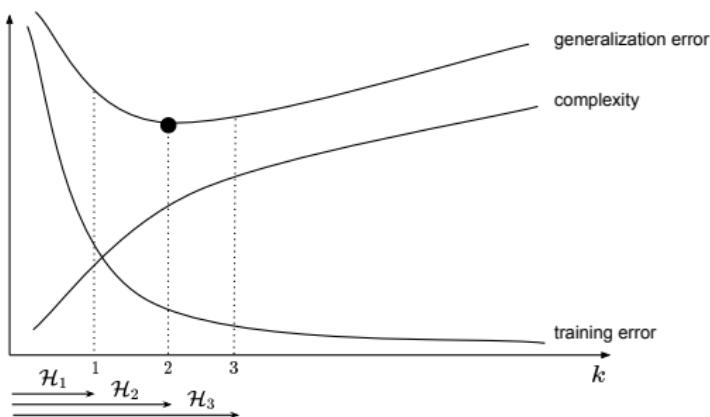
STRUCTURAL RISK MINIMIZATION

- Thus far, we only considered adding a complexity penalty to empirical risk minimization.
- Instead, structural risk minimization (SRM) assumes that the hypothesis space \mathcal{H} can be decomposed into increasingly complex hypotheses (size or capacity): $\mathcal{H} = \cup_{k \geq 1} \mathcal{H}_k$.
- Complexity parameters can be the, e.g. the degree of polynomials in linear models or the size of hidden layers in neural networks.



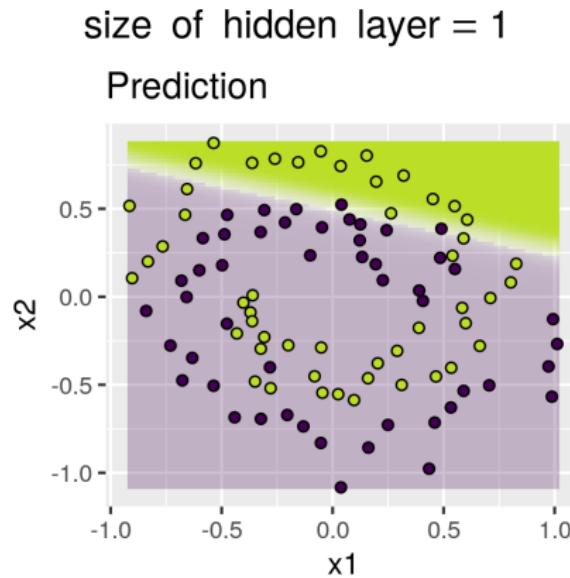
STRUCTURAL RISK MINIMIZATION

- SRM chooses the smallest k such that the optimal model from \mathcal{H}_k found by ERM or RRM cannot significantly be outperformed by a model from a \mathcal{H}_m with $m > k$.
- By this, the simplest model can be chosen, which minimizes the generalization bound.
- One challenge might be choosing an adequate complexity measure, as for some models, multiple complexity measures exist.



STRUCTURAL RISK MINIMIZATION

Setting: Classification for the spirals data. Neural network with single hidden layer containing k neurons and logistic output activation, L2 regularized with $\lambda = 0.001$. So here SRM and RRM are both used. Varying the size of the hidden layer affects smoothness of the decision boundary:

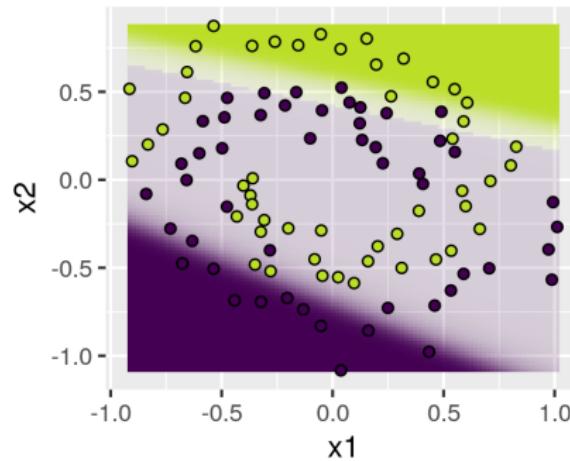


STRUCTURAL RISK MINIMIZATION

Setting: Classification for the spirals data. Neural network with single hidden layer containing k neurons and logistic output activation, L2 regularized with $\lambda = 0.001$. So here SRM and RRM are both used. Varying the size of the hidden layer affects smoothness of the decision boundary:

size of hidden layer = 2

Prediction

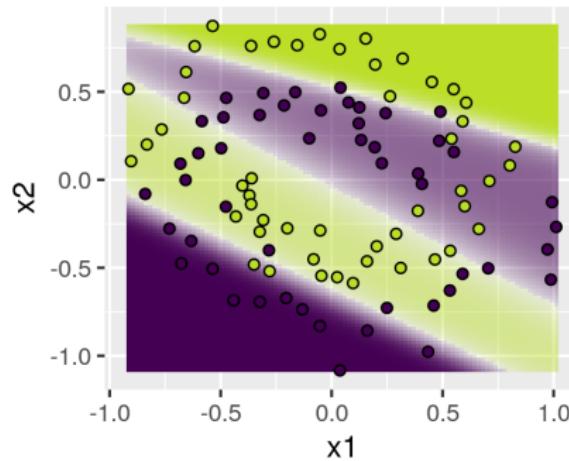


STRUCTURAL RISK MINIMIZATION

Setting: Classification for the spirals data. Neural network with single hidden layer containing k neurons and logistic output activation, L2 regularized with $\lambda = 0.001$. So here SRM and RRM are both used. Varying the size of the hidden layer affects smoothness of the decision boundary:

size of hidden layer = 3

Prediction

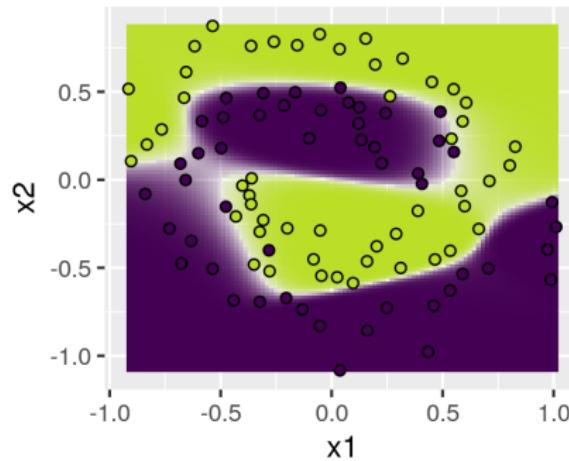


STRUCTURAL RISK MINIMIZATION

Setting: Classification for the spirals data. Neural network with single hidden layer containing k neurons and logistic output activation, L2 regularized with $\lambda = 0.001$. So here SRM and RRM are both used. Varying the size of the hidden layer affects smoothness of the decision boundary:

size of hidden layer = 5

Prediction

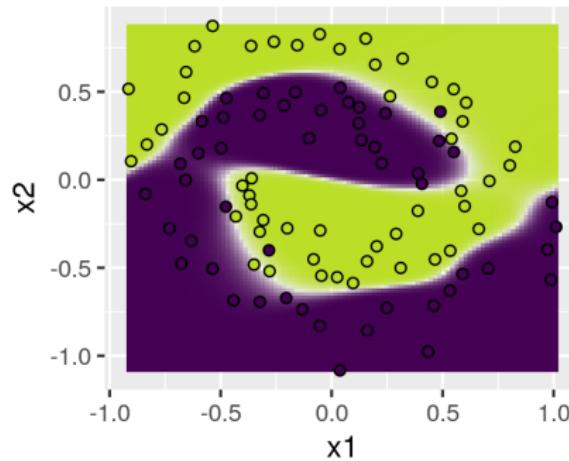


STRUCTURAL RISK MINIMIZATION

Setting: Classification for the spirals data. Neural network with single hidden layer containing k neurons and logistic output activation, L2 regularized with $\lambda = 0.001$. So here SRM and RRM are both used. Varying the size of the hidden layer affects smoothness of the decision boundary:

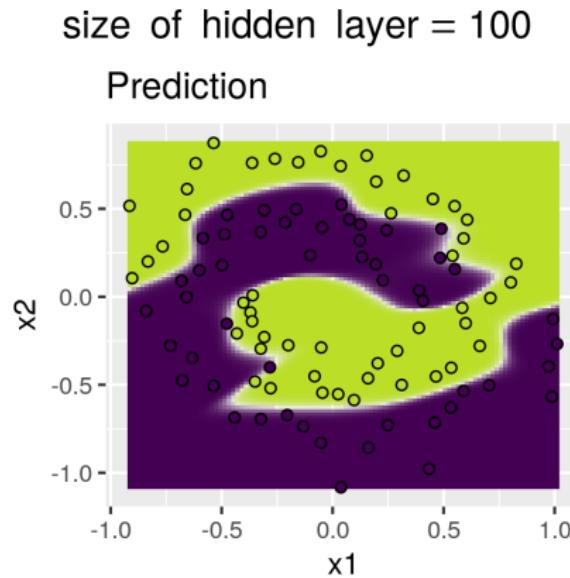
size of hidden layer = 10

Prediction



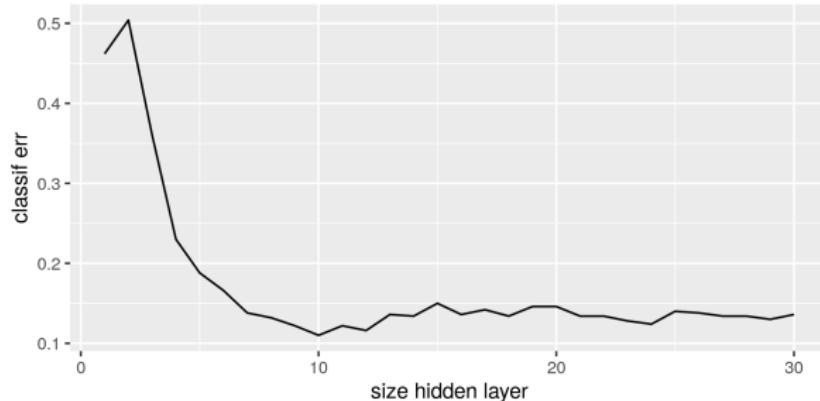
STRUCTURAL RISK MINIMIZATION

Setting: Classification for the spirals data. Neural network with single hidden layer containing k neurons and logistic output activation, L2 regularized with $\lambda = 0.001$. So here SRM and RRM are both used. Varying the size of the hidden layer affects smoothness of the decision boundary:



STRUCTURAL RISK MINIMIZATION

Again, complexity vs CV score.

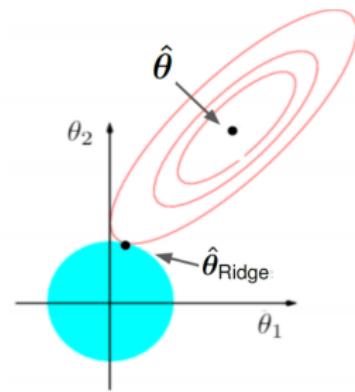


A minimal model with good generalization seems to have ca. 6-8 hidden neurons.

STRUCTURAL RISK MINIMIZATION AND RRM

Note that normal RRM can also be interpreted through SRM, if we rewrite the penalized ERM as constrained ERM.

$$\begin{aligned} \min_{\theta} \quad & \sum_{i=1}^n L(y^{(i)}, f(\mathbf{x}^{(i)} | \theta)) \\ \text{s.t.} \quad & \|\theta\|_2^2 \leq t \end{aligned}$$



We can interpret going through λ from large to small as through t from small to large. This constructs a series of ERM problems with hypothesis spaces \mathcal{H}_λ , where we constrain the norm of θ to unit balls of growing size.

RRM VS. BAYES

We already created a link between max. likelihood estimation and ERM.

Now we will generalize this for RRM.

Assume we have a parameterized distribution $p(y|\theta, \mathbf{x})$ for our data and a prior $q(\theta)$ over our parameter space, all in the Bayesian framework.

From the Bayes theorem we know:

$$p(\theta|\mathbf{x}, y) = \frac{p(y|\theta, \mathbf{x})q(\theta)}{p(y|\mathbf{x})} \propto p(y|\theta, \mathbf{x})q(\theta)$$

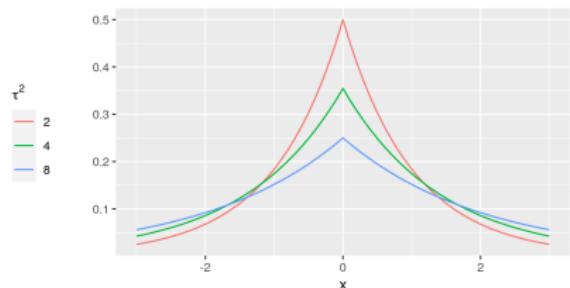
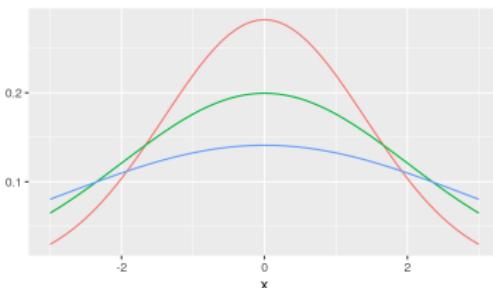
RRM VS. BAYES

The maximum a posteriori (MAP) estimator of θ is now the minimizer of

$$-\log p(y | \theta, \mathbf{x}) - \log q(\theta).$$

- Again, we identify the loss $L(y, f(\mathbf{x} | \theta))$ with $-\log(p(y|\theta, \mathbf{x}))$.
- If $q(\theta)$ is constant (i.e., we used a uniform, non-informative prior), the second term is irrelevant and we arrive at ERM.
- If not, we can identify $J(\theta) \propto -\log(q(\theta))$, i.e., the log-prior corresponds to the regularizer, and the additional λ , which controls the strength of our penalty, usually influences the peakedness / inverse variance / strength of our prior.

RRM VS. BAYES



- L_2 regularization corresponds to a zero-mean Gaussian prior with constant variance on our parameters: $\theta_j \sim \mathcal{N}(0, \tau^2)$
- L_1 corresponds to a zero-mean Laplace prior: $\theta_j \sim \text{Laplace}(0, b)$. $\text{Laplace}(\mu, b)$ has density $\frac{1}{2b} \exp\left(-\frac{|\mu-x|}{b}\right)$, with scale parameter b , mean μ and variance $2b^2$.
- In both cases, regularization strength increases as the variance of the prior decreases: a prior probability mass more narrowly concentrated around 0 encourages shrinkage.

EXAMPLE: BAYESIAN L2 REGULARIZATION

We can easily see the equivalence of $L2$ regularization and a Gaussian prior:

- We define a Gaussian prior with uncorrelated components for θ :

$$q(\theta) = \mathcal{N}_d(\mathbf{0}, \text{diag}(\tau^2)) = \prod_{j=1}^d \mathcal{N}(0, \tau^2) = (2\pi\tau^2)^{-\frac{d}{2}} \exp\left(-\frac{1}{2\tau^2} \sum_{j=1}^d \theta_j^2\right).$$

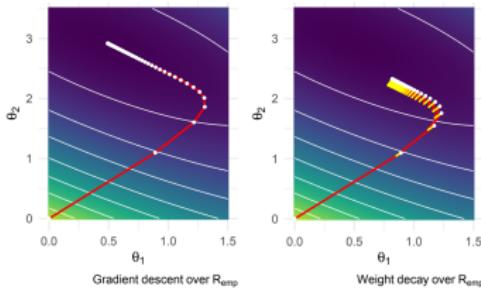
- With this, the MAP estimator becomes

$$\begin{aligned}\hat{\theta}^{\text{MAP}} &= \arg \min_{\theta} (-\log p(y | \theta, \mathbf{x}) - \log q(\theta)) \\ &= \arg \min_{\theta} \left(-\log p(y | \theta, \mathbf{x}) + \frac{d}{2} \log(2\pi\tau^2) + \frac{1}{2\tau^2} \sum_{j=1}^d \theta_j^2 \right) \\ &= \arg \min_{\theta} \left(-\log p(y | \theta, \mathbf{x}) + \frac{1}{2\tau^2} \|\theta\|_2^2 \right).\end{aligned}$$

- We see how the inverse variance (precision) $1/\tau^2$ controls shrinkage.

Introduction to Machine Learning

Geometric Analysis of L2 Regularization and Weight Decay



Learning goals

- Have a geometric understanding of $L2$ regularization
- Understand why $L2$ regularization in combination with gradient descent is called weight decay

WEIGHT DECAY VS. L2 REGULARIZATION

Let us optimize the $L2$ -regularized risk of a model $f(\mathbf{x} \mid \theta)$

$$\min_{\theta} \mathcal{R}_{\text{reg}}(\theta) = \min_{\theta} \mathcal{R}_{\text{emp}}(\theta) + \frac{\lambda}{2} \|\theta\|_2^2$$

by gradient descent. The gradient is

$$\nabla_{\theta} \mathcal{R}_{\text{reg}}(\theta) = \nabla_{\theta} \mathcal{R}_{\text{emp}}(\theta) + \lambda \theta.$$

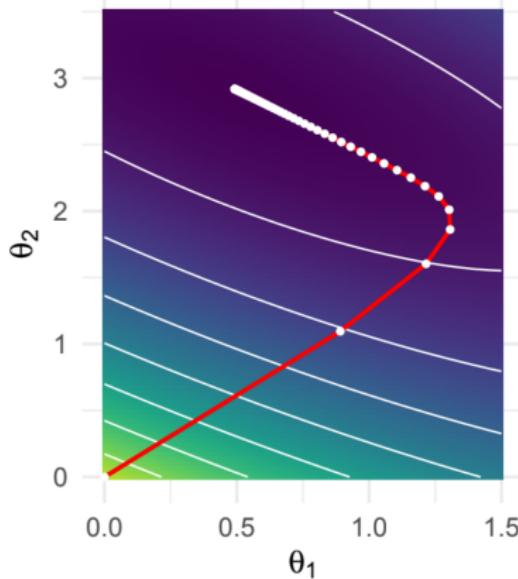
We iteratively update θ by step size α times the negative gradient

$$\begin{aligned}\theta^{[\text{new}]} &= \theta^{[\text{old}]} - \alpha \left(\nabla_{\theta} \mathcal{R}_{\text{emp}}(\theta^{[\text{old}]}) + \lambda \theta^{[\text{old}]} \right) \\ &= \theta^{[\text{old}]} (1 - \alpha \lambda) - \alpha \nabla_{\theta} \mathcal{R}_{\text{emp}}(\theta^{[\text{old}]}).\end{aligned}$$

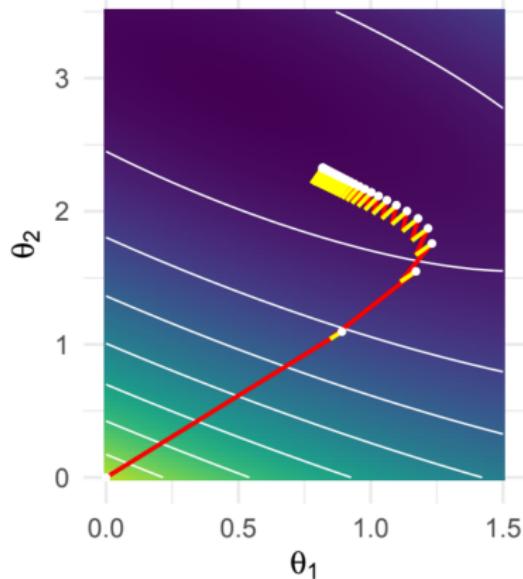
The term $\lambda \theta^{[\text{old}]}$ causes the parameter (**weight**) to **decay** in proportion to its size. This is a very well-known technique in deep learning - and simply $L2$ regularization in disguise.

WEIGHT DECAY VS. L2 REGULARIZATION

When we use weight decay, we follow the steepest slope of \mathcal{R}_{emp} as for gradient descent, but in every step, we are pulled back to the origin.



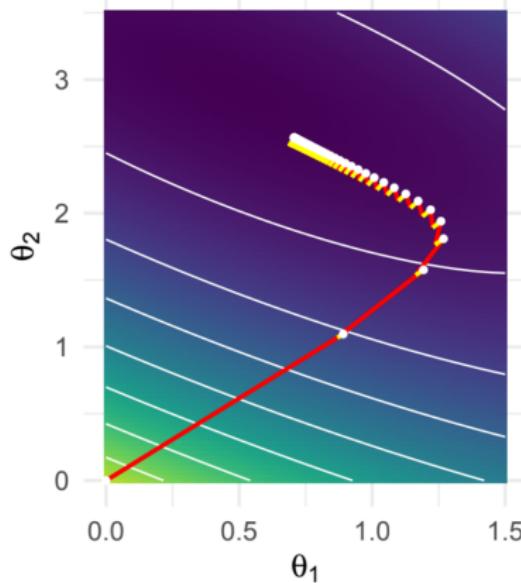
Gradient descent over \mathcal{R}_{emp}



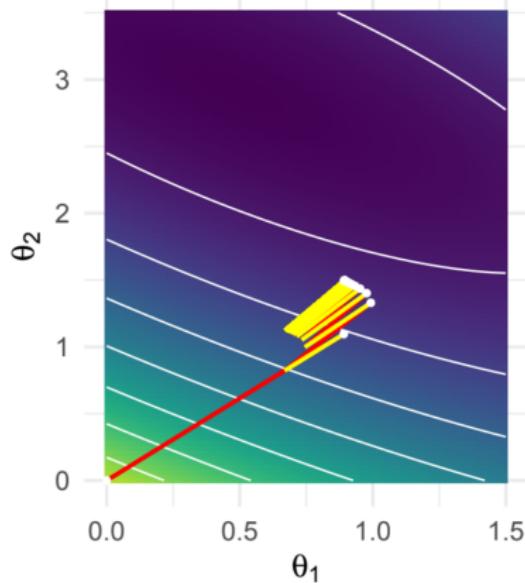
Weight decay over \mathcal{R}_{emp}

WEIGHT DECAY VS. L2 REGULARIZATION

How strongly we are pulled back to the origin for a fixed stepsize α depends only on λ (as long as the procedure converges):



Weight decay (small λ) over R_{emp}



Weight decay (large λ) over R_{emp}

WEIGHT DECAY VS. L2 REGULARIZATION

Weight decay can be interpreted **geometrically**.

Let's use a quadratic Taylor approximation of the unregularized objective $\mathcal{R}_{\text{emp}}(\theta)$ in the neighborhood of its minimizer $\hat{\theta}$,

$$\tilde{\mathcal{R}}_{\text{emp}}(\theta) = \mathcal{R}_{\text{emp}}(\hat{\theta}) + \nabla_{\theta} \mathcal{R}_{\text{emp}}(\hat{\theta}) \cdot (\theta - \hat{\theta}) + \frac{1}{2}(\theta - \hat{\theta})^T \mathbf{H}(\theta - \hat{\theta}),$$

where \mathbf{H} is the Hessian matrix of $\mathcal{R}_{\text{emp}}(\theta)$ evaluated at $\hat{\theta}$.

- The first-order term is 0 in the expression above because the gradient is 0 at the minimizer.
- \mathbf{H} is positive semidefinite.

WEIGHT DECAY VS. L2 REGULARIZATION

The minimum of $\tilde{\mathcal{R}}_{\text{emp}}(\theta)$ occurs where $\nabla_{\theta} \tilde{\mathcal{R}}_{\text{emp}}(\theta) = \mathbf{H}(\theta - \hat{\theta})$ is 0.

Now we *L2*-regularize $\tilde{\mathcal{R}}_{\text{emp}}(\theta)$, such that

$$\tilde{\mathcal{R}}_{\text{reg}}(\theta) = \tilde{\mathcal{R}}_{\text{emp}}(\theta) + \frac{\lambda}{2} \|\theta\|_2^2$$

and solve this approximation of \mathcal{R}_{reg} for the minimizer $\hat{\theta}_{\text{Ridge}}$:

$$\begin{aligned}\nabla_{\theta} \tilde{\mathcal{R}}_{\text{reg}}(\theta) &= 0, \\ \lambda \theta + \mathbf{H}(\theta - \hat{\theta}) &= 0, \\ (\mathbf{H} + \lambda \mathbf{I})\theta &= \mathbf{H}\hat{\theta}, \\ \hat{\theta}_{\text{Ridge}} &= (\mathbf{H} + \lambda \mathbf{I})^{-1} \mathbf{H}\hat{\theta},\end{aligned}$$

This give us a formula to see how the minimizer of the *L2*-regularized version is a transformation of the minimizer of the unpenalized version.

WEIGHT DECAY VS. L2 REGULARIZATION

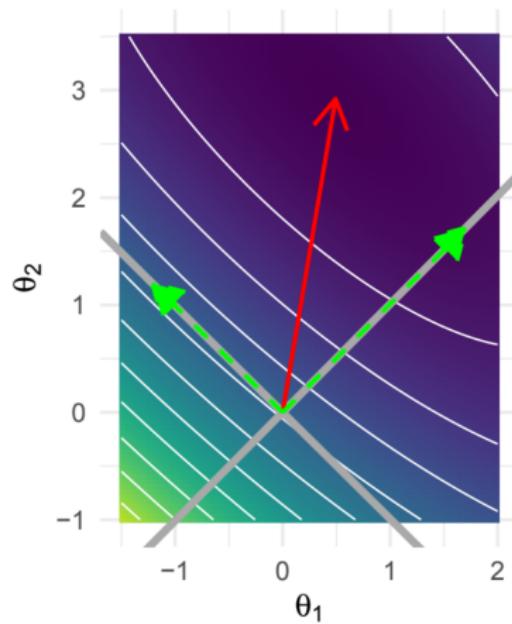
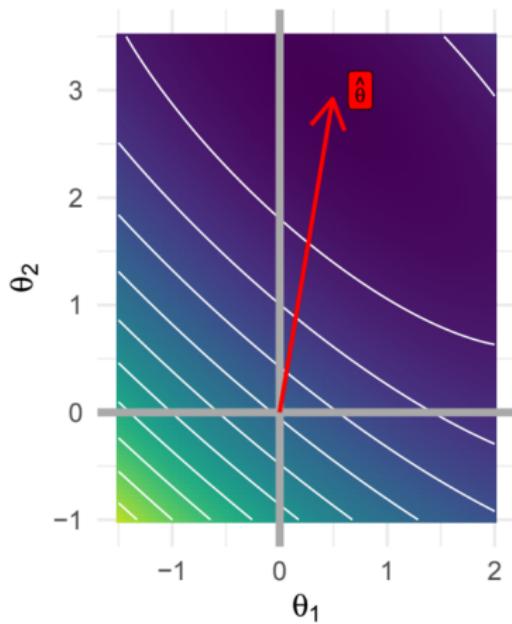
- As λ approaches 0, the regularized solution $\hat{\theta}_{\text{Ridge}}$ approaches $\hat{\theta}$. What happens as λ grows?
- Because H is a real symmetric matrix, it can be decomposed as $H = Q\Sigma Q^T$, where Σ is a diagonal matrix of eigenvalues and Q is an orthonormal basis of eigenvectors.
- Rewriting the transformation formula with this:

$$\begin{aligned}\hat{\theta}_{\text{Ridge}} &= \left(Q\Sigma Q^T + \lambda I\right)^{-1} Q\Sigma Q^T \hat{\theta} \\ &= \left[Q(\Sigma + \lambda I)Q^T\right]^{-1} Q\Sigma Q^T \hat{\theta} \\ &= Q(\Sigma + \lambda I)^{-1} \Sigma Q^T \hat{\theta}\end{aligned}$$

- Therefore, weight decay rescales $\hat{\theta}$ along the axes defined by the eigenvectors of H . The component of $\hat{\theta}$ that is aligned with the j -th eigenvector of H is rescaled by a factor of $\frac{\sigma_j}{\sigma_j + \lambda}$, where σ_j is the corresponding eigenvalue.

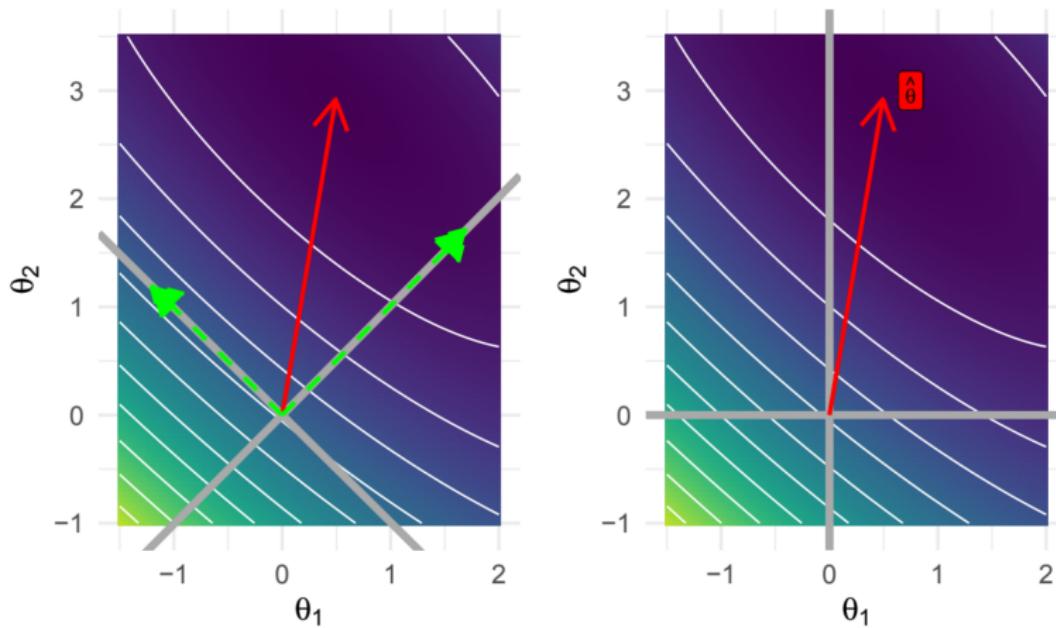
WEIGHT DECAY VS. L2 REGULARIZATION

Firstly, $\hat{\theta}$ is rotated by \mathbf{Q}^T , which we can interpret as a projection of $\hat{\theta}$ on the rotated coordinate system defined by the principal directions of \mathbf{H} :



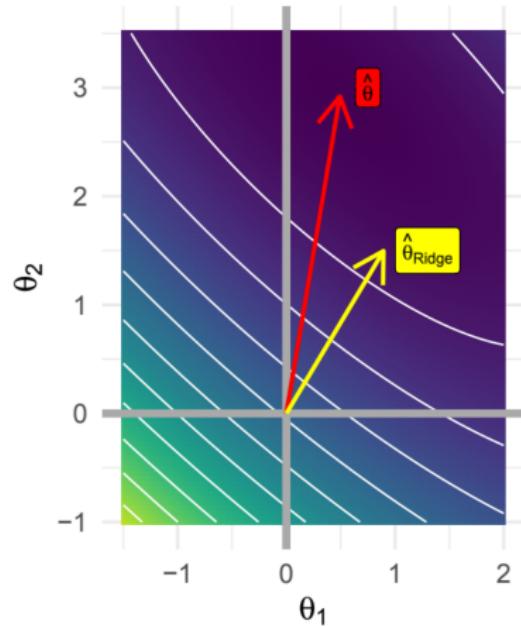
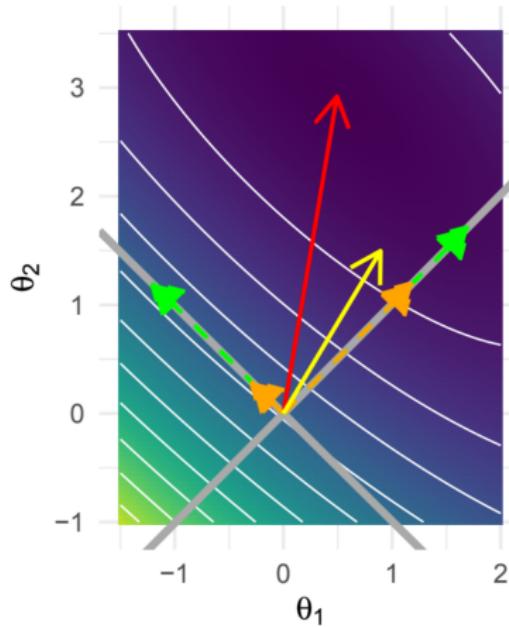
WEIGHT DECAY VS. L2 REGULARIZATION

Since, for $\lambda = 0$, the transformation matrix $(\Sigma + \lambda I)^{-1}\Sigma = \Sigma^{-1}\Sigma = I$, we simply arrive at $\hat{\theta}$ again after projecting back.



WEIGHT DECAY VS. L2 REGULARIZATION

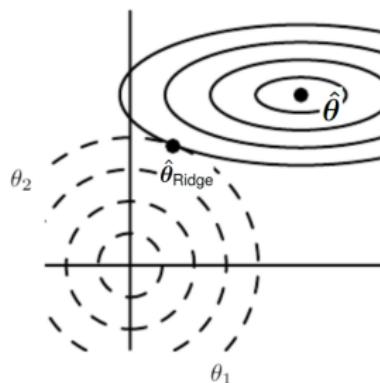
If $\lambda > 0$, the component projected on the j -th axis gets rescaled by $\frac{\sigma_j}{\sigma_j + \lambda}$ before $\hat{\theta}_{\text{Ridge}}$ is rotated back.



WEIGHT DECAY VS. L2 REGULARIZATION

- Along directions where the eigenvalues of H are relatively large, for example, where $\sigma_j \gg \lambda$, the effect of regularization is quite small.
- On the other hand, components with $\sigma_j \ll \lambda$ will be shrunk to have nearly zero magnitude.
- In other words, only directions along which the parameters contribute significantly to reducing the objective function are preserved relatively intact.
- In the other directions, a small eigenvalue of the Hessian means that moving in this direction will not significantly increase the gradient. For such unimportant directions, the corresponding components of θ are decayed away.

WEIGHT DECAY VS. L2 REGULARIZATION

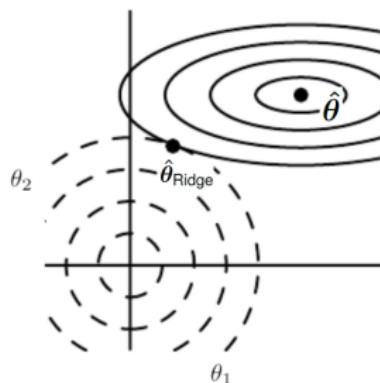


Credit: Goodfellow et al. (2016), ch. 7

Figure: The solid ellipses represent the contours of the unregularized objective and the dashed circles represent the contours of the $L2$ penalty. At $\hat{\theta}_{\text{Ridge}}$, the competing objectives reach an equilibrium.

In the first dimension, the eigenvalue of the Hessian of $\mathcal{R}_{\text{emp}}(\theta)$ is small. The objective function does not increase much when moving horizontally away from $\hat{\theta}$. Therefore, the regularizer has a strong effect on this axis and θ_1 is pulled close to zero.

WEIGHT DECAY VS. L2 REGULARIZATION



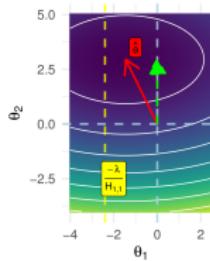
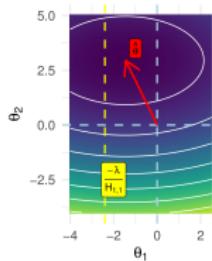
Credit: Goodfellow et al. (2016), ch. 7

Figure: The solid ellipses represent the contours of the unregularized objective and the dashed circles represent the contours of the $L2$ penalty. At $\hat{\theta}_{\text{Ridge}}$, the competing objectives reach an equilibrium.

In the second dimension, the corresponding eigenvalue is large indicating high curvature. The objective function is very sensitive to movement along this axis and, as a result, the position of θ_2 is less affected by the regularization.

Introduction to Machine Learning

Geometric Analysis of L1-regularization



Learning goals

- Have a geometric understanding of L1-regularization
- Understand geometrically how L1-regularization induces sparsity

L1-REGULARIZATION

- The L1-regularized risk of a model $f(\mathbf{x} \mid \boldsymbol{\theta})$ is

$$\min_{\boldsymbol{\theta}} \mathcal{R}_{\text{reg}}(\boldsymbol{\theta}) = \mathcal{R}_{\text{emp}}(\boldsymbol{\theta}) + \lambda \|\boldsymbol{\theta}\|_1$$

and the (sub-)gradient is:

$$\nabla_{\boldsymbol{\theta}} \mathcal{R}_{\text{reg}}(\boldsymbol{\theta}) = \lambda \text{sign}(\boldsymbol{\theta}) + \nabla_{\boldsymbol{\theta}} \mathcal{R}_{\text{emp}}(\boldsymbol{\theta})$$

- Note that, unlike in the case of L2, the contribution of the L1 penalty to the gradient doesn't scale linearly with each θ_j .
- Let us now make (again) a quadratic Taylor approximation of $\mathcal{R}_{\text{emp}}(\boldsymbol{\theta})$ around its minimizer $\hat{\boldsymbol{\theta}}$. To get a clean algebraic expression, we further assume the Hessian of $\mathcal{R}_{\text{emp}}(\boldsymbol{\theta})$ is diagonal, i.e. $\mathbf{H} = \text{diag}([H_{1,1}, \dots, H_{d,d}])$, where each $H_{j,j} \geq 0$.
- This assumption holds, for example, if the input features for a linear regression task have been decorrelated using PCA.

L1-REGULARIZATION

- If we plug this approximation into $\mathcal{R}_{\text{reg}}(\theta)$, the result nicely decomposes into a sum over the parameters:

$$\tilde{\mathcal{R}}_{\text{reg}}(\theta) = \mathcal{R}_{\text{emp}}(\hat{\theta}) + \sum_j \left[\frac{1}{2} H_{j,j} (\theta_j - \hat{\theta}_j)^2 \right] + \sum_j \lambda |\theta_j|$$

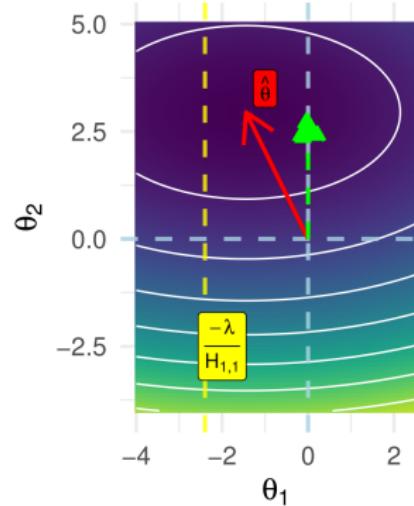
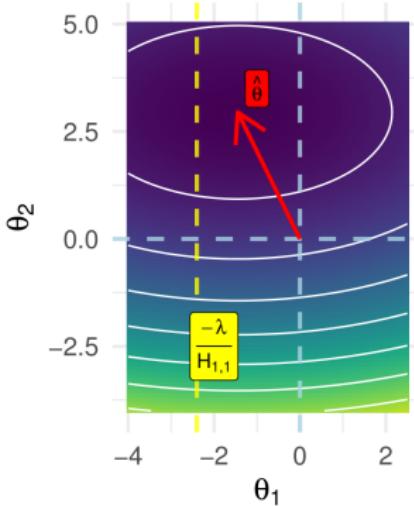
- We can minimize analytically:

$$\begin{aligned}\hat{\theta}_{\text{Lasso},j} &= \text{sign}(\hat{\theta}_j) \max \left\{ |\hat{\theta}_j| - \frac{\lambda}{H_{j,j}}, 0 \right\} \\ &= \begin{cases} \hat{\theta}_j + \frac{\lambda}{H_{j,j}} & , \text{if } \hat{\theta}_j < -\frac{\lambda}{H_{j,j}} \\ 0 & , \text{if } \hat{\theta}_j \in [-\frac{\lambda}{H_{j,j}}, \frac{\lambda}{H_{j,j}}] \\ \hat{\theta}_j - \frac{\lambda}{H_{j,j}} & , \text{if } \hat{\theta}_j > \frac{\lambda}{H_{j,j}} \end{cases}\end{aligned}$$

- If $H_{j,j} = 0$ exactly, $\hat{\theta}_{\text{Lasso},j} = 0$.

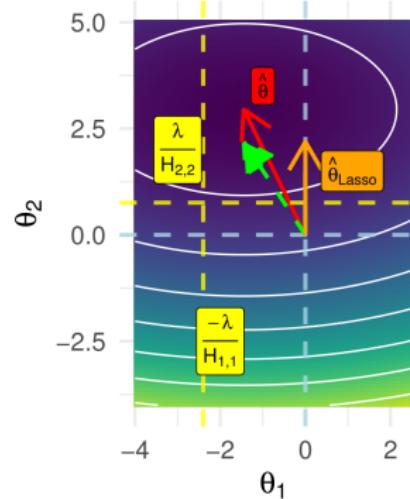
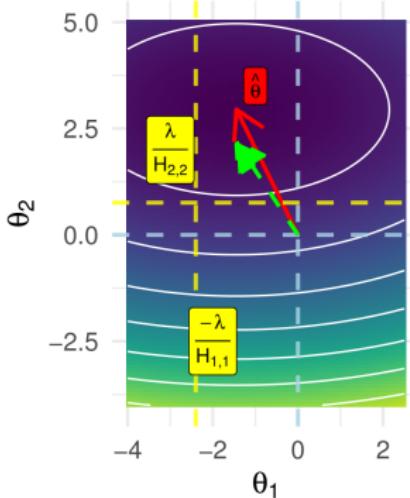
L1-REGULARIZATION

- If $0 < \hat{\theta}_j \leq \frac{\lambda}{H_{j,j}}$ or $0 > \hat{\theta}_j \geq -\frac{\lambda}{H_{j,j}}$, the optimal value of θ_j (for the regularized risk) is 0 because the contribution of $\mathcal{R}_{\text{emp}}(\theta)$ to $\mathcal{R}_{\text{reg}}(\theta)$ is overwhelmed by the L1 penalty, which forces it to be 0.



L1-REGULARIZATION

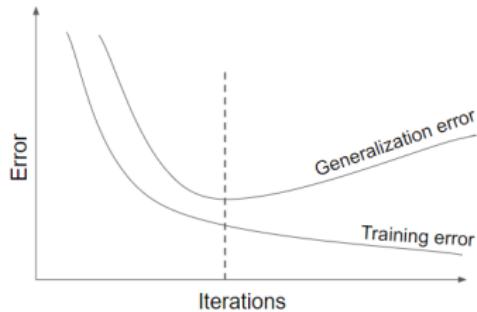
- If $0 < \frac{\lambda}{H_{j,j}} < \hat{\theta}_j$ or $0 > -\frac{\lambda}{H_{j,j}} > \hat{\theta}_j$, the L1 penalty shifts the optimal value of θ_j toward 0 by the amount $\frac{\lambda}{H_{j,j}}$.



- Therefore, the L1 penalty induces sparsity in the parameter vector.

Introduction to Machine Learning

Early Stopping



Learning goals

- Know how early stopping works
- Understand how early stopping acts as a regularizer

EARLY STOPPING

- When training with an iterative optimizer such as SGD, it is commonly the case that, after a certain number of iterations, generalization error begins to increase even though training error continues to decrease.
- Early stopping** refers to stopping the algorithm early before the generalization error increases.

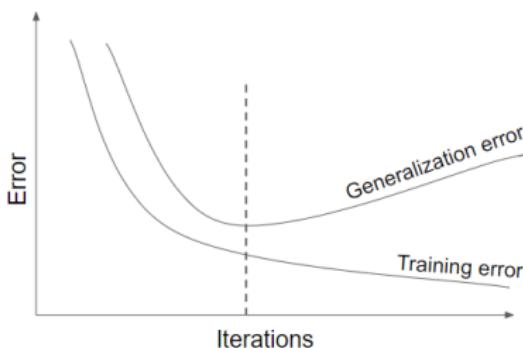


Figure: After a certain number of iterations, the algorithm begins to overfit.

EARLY STOPPING

How early stopping works:

- ❶ Split training data $\mathcal{D}_{\text{train}}$ into $\mathcal{D}_{\text{subtrain}}$ and \mathcal{D}_{val} (e.g. with a ratio of 2:1).
- ❷ Train on $\mathcal{D}_{\text{subtrain}}$ and evaluate model using the validation set \mathcal{D}_{val} .
- ❸ Stop training when validation error stops decreasing (after a range of “patience” steps).
- ❹ Use parameters of the previous step for the actual model.

More sophisticated forms also apply cross-validation.

EARLY STOPPING

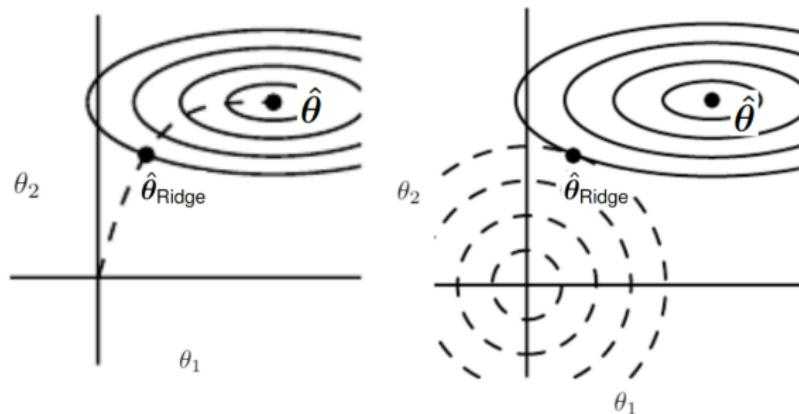
Strengths	Weaknesses
Effective and simple	Periodical evaluation of validation error
Applicable to almost any model without adjustment	Temporary copy of θ (we have to save the whole model each time validation error improves)
Combinable with other regularization methods	Less data for training \rightarrow include \mathcal{D}_{val} afterwards

- Relation between optimal early-stopping iteration T_{stop} and weight-decay penalization parameter λ for step-size α (see Goodfellow et al. (2016) page 251-252 for proof):

$$T_{\text{stop}} \approx \frac{1}{\alpha \lambda} \Leftrightarrow \lambda \approx \frac{1}{T_{\text{stop}} \alpha}$$

- Small λ (low penalization) \Rightarrow high T_{stop} (complex model / lots of updates).

EARLY STOPPING



Credit: Goodfellow et al. (2016)

Figure: An illustration of the effect of early stopping. *Left:* The solid contour lines indicate the contours of the negative log-likelihood. The dashed line indicates the trajectory taken by SGD beginning from the origin. Rather than stopping at the point $\hat{\theta}$ that minimizes the risk, early stopping results in the trajectory stopping at an earlier point $\hat{\theta}_{\text{Ridge}}$. *Right:* An illustration of the effect of L_2 regularization for comparison. The dashed circles indicate the contours of the L_2 penalty which causes the minimum of the total cost to lie closer to the origin than the minimum of the unregularized cost.

INTRODUCTION TO MACHINE LEARNING

Advanced Risk Minimization

Multiclass Classification

Information Theory

Curse of Dimensionality

Hypothesis Space

Regularization

Linear Support Vector Machine

Nonlinear Support Vector Machine

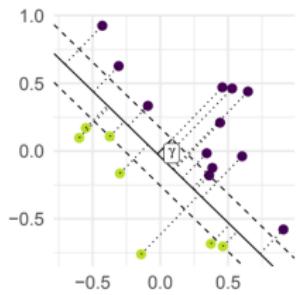
Gaussian Processes

Boosting

Introduction to Machine Learning

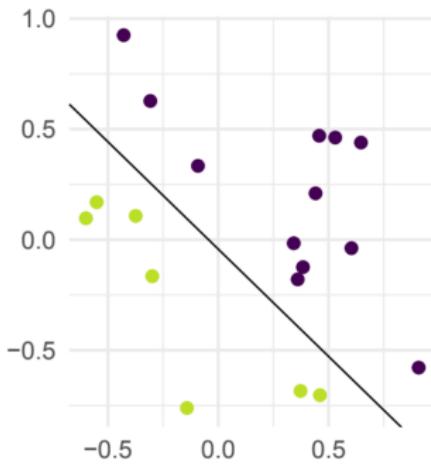
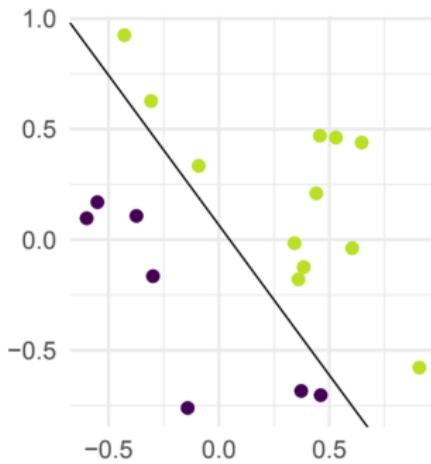
Linear Hard Margin SVM

Learning goals



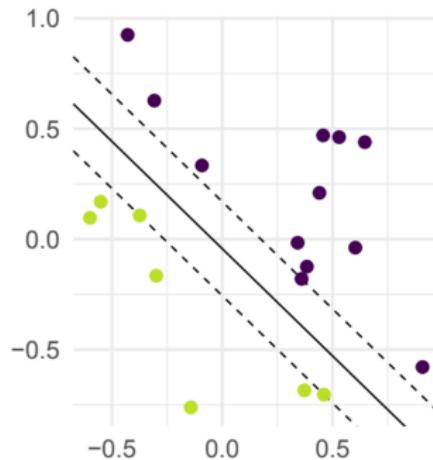
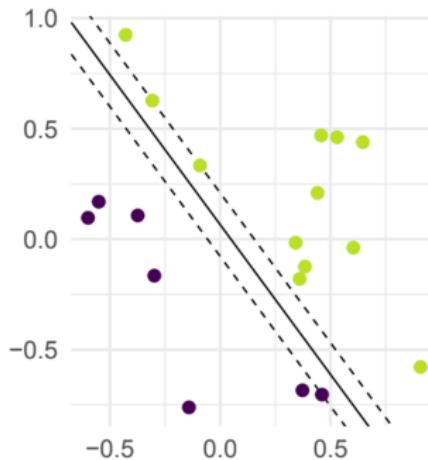
- Know that the hard-margin SVM maximizes the margin between data points and hyperplane
- Know that this is a quadratic program
- Know that support vectors are the data points closest to the separating hyperplane

LINEAR CLASSIFIERS



- We want study how to build a binary, linear classifier from solid geometrical principles.
- Which of these two classifiers is “better”?

LINEAR CLASSIFIERS



- We want study how to build a binary, linear classifier from solid geometrical principles.
- Which of these two classifiers is “better”?
 - The decision boundary on the right has a larger **safety margin**.

SUPPORT VECTOR MACHINES: GEOMETRY

For labeled data $\mathcal{D} = ((\mathbf{x}^{(1)}, y^{(1)}), \dots, (\mathbf{x}^{(n)}, y^{(n)}))$, with $y^{(i)} \in \{-1, +1\}$:

- Assume linear separation by $f(\mathbf{x}) = \boldsymbol{\theta}^\top \mathbf{x} + \theta_0$, such that all $+$ -observations are in the positive halfspace

$$\{\mathbf{x}^{(i)} \in \mathcal{X} : f(\mathbf{x}) > 0\}$$

and all $-$ -observations are in the negative halfspace

$$\{\mathbf{x} \in \mathcal{X} : f(\mathbf{x}) < 0\}.$$

- For a linear separating hyperplane, we have

$$y^{(i)} \underbrace{\left(\boldsymbol{\theta}^\top \mathbf{x}^{(i)} + \theta_0 \right)}_{=f(\mathbf{x}^{(i)})} > 0 \quad \forall i \in \{1, 2, \dots, n\}.$$

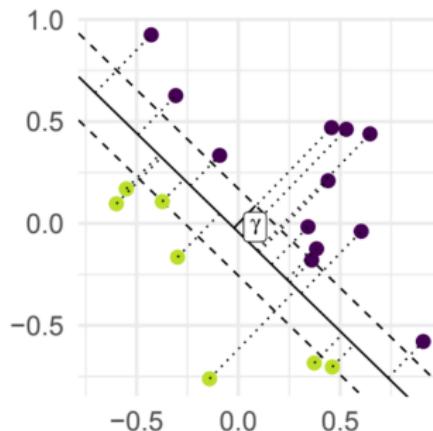
SUPPORT VECTOR MACHINES: GEOMETRY

-

$$d(f, \mathbf{x}^{(i)}) = \frac{y^{(i)} f(\mathbf{x}^{(i)})}{\|\boldsymbol{\theta}\|} = y^{(i)} \frac{\boldsymbol{\theta}^T \mathbf{x}^{(i)} + \theta_0}{\|\boldsymbol{\theta}\|}$$

computes the (signed) distance to the separating hyperplane $f(\mathbf{x})$,
positive for correct classifications, negative for incorrect.

- This expression becomes negative for misclassified points.

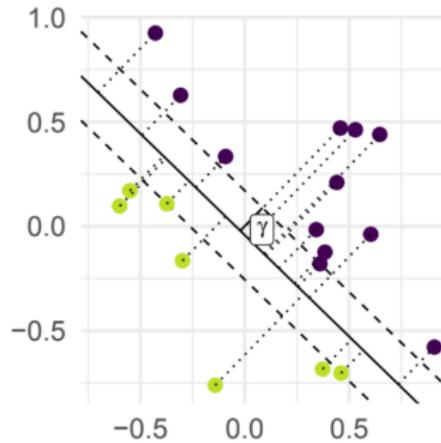


SUPPORT VECTOR MACHINES: GEOMETRY

- The distance of f to the whole dataset \mathcal{D} is the smallest distance

$$\gamma = \min_i \left\{ d(f, \mathbf{x}^{(i)}) \right\}.$$

- This represents the “safety margin”, it is positive if f separates and we want to maximize it.



MAXIMUM MARGIN SEPARATION

We formulate the desired property of a large “safety margin” as an optimization problem:

$$\max_{\theta, \theta_0} \gamma$$

$$\text{s.t. } d(f, \mathbf{x}^{(i)}) \geq \gamma \quad \forall i \in \{1, \dots, n\}.$$

- The constraints mean: We require that any instance i should have a “safety” distance of at least γ from the decision boundary defined by $f = \theta^T + \theta_0 \mathbf{x}$.
- Our objective is to maximize the “safety” distance.

MAXIMUM MARGIN SEPARATION

We reformulate the problem:

$$\begin{aligned} & \max_{\theta, \theta_0} \quad \gamma \\ \text{s.t.} \quad & \frac{y^{(i)} (\langle \theta, \mathbf{x}^{(i)} \rangle + \theta_0)}{\|\theta\|} \geq \gamma \quad \forall i \in \{1, \dots, n\}. \end{aligned}$$

- The inequality is rearranged by multiplying both sides with $\|\theta\|$:

$$\begin{aligned} & \max_{\theta, \theta_0} \quad \gamma \\ \text{s.t.} \quad & y^{(i)} (\langle \theta, \mathbf{x}^{(i)} \rangle + \theta_0) \geq \|\theta\| \gamma \quad \forall i \in \{1, \dots, n\}. \end{aligned}$$

MAXIMUM MARGIN SEPARATION

- Note that the same hyperplane does not have a unique representation:

$$\{\mathbf{x} \in \mathcal{X} \mid \boldsymbol{\theta}^\top \mathbf{x} = 0\} = \{\mathbf{x} \in \mathcal{X} \mid \mathbf{c} \cdot \boldsymbol{\theta}^\top \mathbf{x} = 0\}$$

for arbitrary $\mathbf{c} \neq 0$.

- To ensure uniqueness of the solution, we make a reference choice
 - we only consider hyperplanes with $\|\boldsymbol{\theta}\| = 1/\gamma$:

$$\begin{aligned} & \max_{\boldsymbol{\theta}, \theta_0} \quad \gamma \\ \text{s.t.} \quad & y^{(i)} \left(\langle \boldsymbol{\theta}, \mathbf{x}^{(i)} \rangle + \theta_0 \right) \geq 1 \quad \forall i \in \{1, \dots, n\}. \end{aligned}$$

MAXIMUM MARGIN SEPARATION

- Substituting $\gamma = 1/\|\theta\|$ in the objective yields:

$$\begin{aligned} \max_{\theta, \theta_0} \quad & \frac{1}{\|\theta\|} \\ \text{s.t.} \quad & y^{(i)} (\langle \theta, \mathbf{x}^{(i)} \rangle + \theta_0) \geq 1 \quad \forall i \in \{1, \dots, n\}. \end{aligned}$$

- Maximizing $1/\|\theta\|$ is the same as minimizing $\|\theta\|$, which is the same as minimizing $\frac{1}{2}\|\theta\|^2$:

$$\begin{aligned} \min_{\theta, \theta_0} \quad & \frac{1}{2}\|\theta\|^2 \\ \text{s.t.} \quad & y^{(i)} (\langle \theta, \mathbf{x}^{(i)} \rangle + \theta_0) \geq 1 \quad \forall i \in \{1, \dots, n\}. \end{aligned}$$

QUADRATIC PROGRAM

We derived the following optimization problem:

$$\begin{aligned} \min_{\theta, \theta_0} \quad & \frac{1}{2} \|\theta\|^2 \\ \text{s.t.} \quad & y^{(i)} (\langle \theta, \mathbf{x}^{(i)} \rangle + \theta_0) \geq 1 \quad \forall i \in \{1, \dots, n\}. \end{aligned}$$

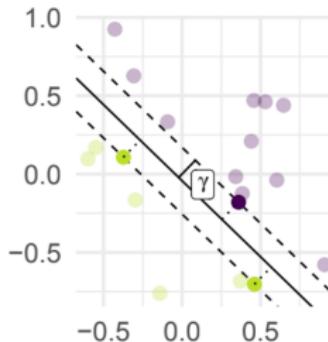
This turns out to be a **convex optimization problem** – particularly, a **quadratic program**: The objective function is quadratic, and the constraints are linear inequalities.

This is called the **primal** problem. We will later show that we can also derive a dual problem from it.

We will call this the **linear hard-margin SVM**.

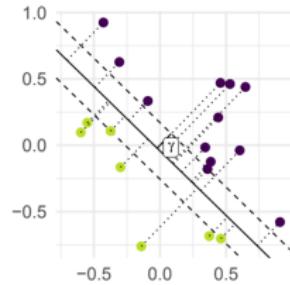
SUPPORT VECTORS

- There exist instances $(\mathbf{x}^{(i)}, y^{(i)})$ with minimal margin $y^{(i)} f(\mathbf{x}^{(i)}) = 1$, fulfilling the inequality constraints with equality.
- They are called **support vectors (SVs)**. They are located exactly at a distance of $\gamma = 1/\|\theta\|$ from the separating hyperplane.
- It is already geometrically obvious that the solution does not depend on the non-SVs! We could delete them from the data and would arrive at the same solution.



Introduction to Machine Learning

Hard-Margin SVM Dual



Learning goals

- Know how to derive the SVM dual problem

HARD MARGIN SVM DUAL

We have derived the primal quadratic program for the hard margin SVM. We could directly solve this, but traditionally the SVM is solved in the dual and this has some advantages. In any case, many algorithms and derivations are based on it, so we need to know it.

$$\begin{aligned} \min_{\theta, \theta_0} \quad & \frac{1}{2} \|\theta\|^2 \\ \text{s.t.} \quad & y^{(i)} (\langle \theta, \mathbf{x}^{(i)} \rangle + \theta_0) \geq 1 \quad \forall i \in \{1, \dots, n\}. \end{aligned}$$

The Lagrange function of the SVM optimization problem is

$$\begin{aligned} L(\theta, \theta_0, \alpha) = \quad & \frac{1}{2} \|\theta\|^2 - \sum_{i=1}^n \alpha_i [y^{(i)} (\langle \theta, \mathbf{x}^{(i)} \rangle + \theta_0) - 1] \\ \text{s.t.} \quad & \alpha_i \geq 0 \quad \forall i \in \{1, \dots, n\}. \end{aligned}$$

The **dual** form of this problem is

$$\max_{\alpha} \min_{\theta, \theta_0} L(\theta, \theta_0, \alpha).$$

HARD MARGIN SVM DUAL

Notice how the $(p+1)$ decision variables (θ, θ_0) have become n decisions variables α , as constraints turned into variables and vice versa. Now every data point has an associated non-negative weight.

$$\begin{aligned} L(\theta, \theta_0, \alpha) = & \frac{1}{2} \|\theta\|^2 - \sum_{i=1}^n \alpha_i \left[y^{(i)} (\langle \theta, \mathbf{x}^{(i)} \rangle + \theta_0) - 1 \right] \\ \text{s.t.} \quad & \alpha_i \geq 0 \quad \forall i \in \{1, \dots, n\}. \end{aligned}$$

We find the stationary point of $L(\theta, \theta_0, \alpha)$ w.r.t. θ, θ_0 and obtain

$$\begin{aligned} \theta &= \sum_{i=1}^n \alpha_i y^{(i)} \mathbf{x}^{(i)}, \\ 0 &= \sum_{i=1}^n \alpha_i y^{(i)} \quad \forall i \in \{1, \dots, n\}. \end{aligned}$$

HARD MARGIN SVM DUAL

By inserting these expressions & simplifying we obtain the dual problem

$$\begin{aligned} \max_{\alpha \in \mathbb{R}^n} \quad & \sum_{i=1}^n \alpha_i - \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n \alpha_i \alpha_j y^{(i)} y^{(j)} \langle \mathbf{x}^{(i)}, \mathbf{x}^{(j)} \rangle \\ \text{s.t.} \quad & \sum_{i=1}^n \alpha_i y^{(i)} = 0, \\ & \alpha_i \geq 0 \quad \forall i \in \{1, \dots, n\}, \end{aligned}$$

or, equivalently, in matrix notation:

$$\begin{aligned} \max_{\alpha \in \mathbb{R}^n} \quad & \mathbf{1}^T \alpha - \frac{1}{2} \alpha^T \text{diag}(\mathbf{y}) \mathbf{K} \text{diag}(\mathbf{y}) \alpha \\ \text{s.t.} \quad & \alpha^T \mathbf{y} = 0, \\ & \alpha \geq 0, \end{aligned}$$

with $\mathbf{K} := \mathbf{X} \mathbf{X}^T$.

HARD MARGIN SVM DUAL

If $(\theta, \theta_0, \alpha)$ fulfills the KKT conditions (stationarity, primal/dual feasibility, complementary slackness), it solves both the primal and dual problem (strong duality).

Under these conditions, and if we solve the dual problem and obtain $\hat{\alpha}$, we know that θ is a linear combination of our data points:

$$\hat{\theta} = \sum_{i=1}^n \hat{\alpha}_i y^{(i)} \mathbf{x}^{(i)}$$

Complementary slackness means:

$$\hat{\alpha}_i \left[y^{(i)} \left(\langle \theta, \mathbf{x}^{(i)} \rangle + \theta_0 \right) - 1 \right] = 0 \quad \forall i \in \{1, \dots, n\}.$$

HARD MARGIN SVM DUAL

$$\hat{\boldsymbol{\theta}} = \sum_{i=1}^n \hat{\alpha}_i y^{(i)} \mathbf{x}^{(i)}$$

$$\hat{\alpha}_i \left[y^{(i)} (\langle \boldsymbol{\theta}, \mathbf{x}^{(i)} \rangle + \theta_0) - 1 \right] = 0 \quad \forall i \in \{1, \dots, n\}.$$

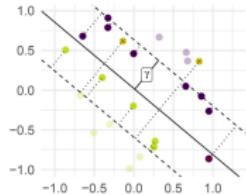
- So either $\hat{\alpha}_i = 0$, and is not active in the linear combination, or $\hat{\alpha}_i > 0$, then $y^{(i)} (\langle \boldsymbol{\theta}, \mathbf{x}^{(i)} \rangle + \theta_0) = 1$, and $(\mathbf{x}^{(i)}, y^{(i)})$ has minimal margin and is a support vector!
- We see that we can directly extract the support vectors from the dual variables and the $\boldsymbol{\theta}$ solution only depends on them.
- We can reconstruct the bias term θ_0 from any support vector:

$$\theta_0 = y^{(i)} - \langle \boldsymbol{\theta}, \mathbf{x}^{(i)} \rangle.$$

Introduction to Machine Learning

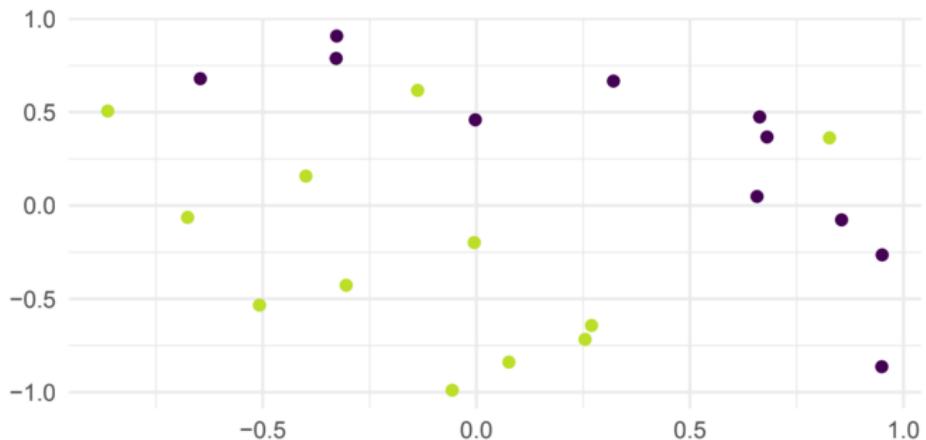
Soft-Margin SVM

Learning goals



- Understand that the hard-margin SVM problem is not solvable for linearly separable data
- Know that the soft-margin SVM problem therefore allows margin violations
- The degree to which margin violations are tolerated is controlled by a hyperparameter

NON-SEPARABLE DATA



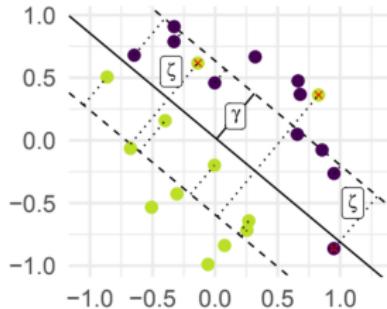
- Assume that dataset \mathcal{D} is not linearly separable.
- Margin maximization becomes meaningless because the hard-margin SVM optimization problem has contradictory constraints and thus an empty **feasible region**.

MARGIN VIOLATIONS

- We still want a large margin for most of the examples.
- We allow violations of the margin constraints via slack vars $\zeta^{(i)} \geq 0$

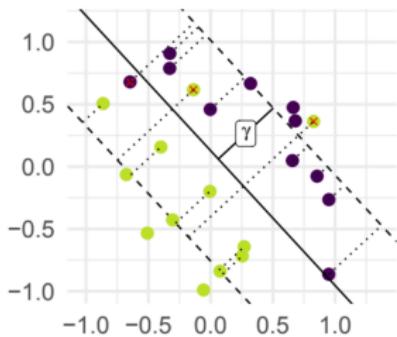
$$y^{(i)} \left(\langle \theta, \mathbf{x}^{(i)} \rangle + \theta_0 \right) \geq 1 - \zeta^{(i)}$$

- Even for separable data, a decision boundary with a few violations and a large average margin may be preferable to one without any violations and a small average margin ...

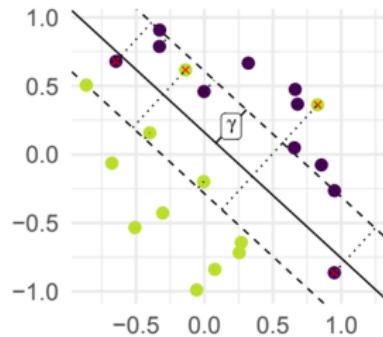


MARGIN VIOLATIONS

- Now we have two distinct and contradictory goals:
 - Maximize the margin.
 - Minimize margin violations.
- Let's minimize a weighted sum of them: $\frac{1}{2} \|\theta\|^2 + C \sum_{i=1}^n \zeta^{(i)}$
- Constant $C > 0$ controls the relative importance of the two parts.



$C = 0.5$



$C = 100$

SOFT-MARGIN SVM

The linear **soft-margin** SVM is the convex quadratic program:

$$\begin{aligned} \min_{\theta, \theta_0, \zeta^{(i)}} \quad & \frac{1}{2} \|\theta\|^2 + C \sum_{i=1}^n \zeta^{(i)} \\ \text{s.t.} \quad & y^{(i)} (\langle \theta, \mathbf{x}^{(i)} \rangle + \theta_0) \geq 1 - \zeta^{(i)} \quad \forall i \in \{1, \dots, n\}, \\ \text{and} \quad & \zeta^{(i)} \geq 0 \quad \forall i \in \{1, \dots, n\}. \end{aligned}$$

This is called “soft-margin” SVM because the “hard” margin constraint is replaced with a “softened” constraint that can be violated by an amount $\zeta^{(i)}$.

SOFT-MARGIN SVM DUAL FORM

Can be derived exactly as for the hard margin case.

$$\begin{aligned} \max_{\alpha \in \mathbb{R}^n} \quad & \sum_{i=1}^n \alpha_i - \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n \alpha_i \alpha_j y^{(i)} y^{(j)} \langle \mathbf{x}^{(i)}, \mathbf{x}^{(j)} \rangle \\ \text{s.t.} \quad & 0 \leq \alpha_i \leq C, \\ & \sum_{i=1}^n \alpha_i y^{(i)} = 0, \end{aligned}$$

or, in matrix notation:

$$\begin{aligned} \max_{\alpha \in \mathbb{R}^n} \quad & \mathbf{1}^T \alpha - \frac{1}{2} \alpha^T \text{diag}(\mathbf{y}) \mathbf{K} \text{diag}(\mathbf{y}) \alpha \\ \text{s.t.} \quad & \alpha^T \mathbf{y} = 0, \\ & 0 \leq \alpha \leq C, \end{aligned}$$

with $\mathbf{K} := \mathbf{X} \mathbf{X}^T$.

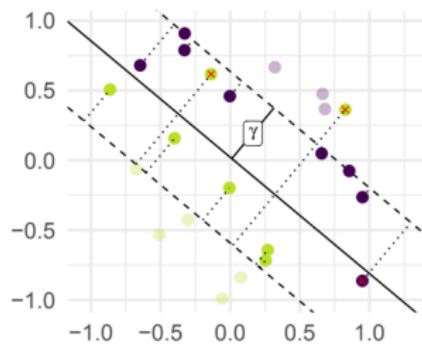
COST PARAMETER C

- The parameter C controls the trade-off between the two conflicting objectives of maximizing the size of the margin and minimizing the frequency and size of margin violations.
- It is known under different names, such as “trade-off parameter”, “regularization parameter”, and “complexity control parameter”.
- For sufficiently large C margin violations become extremely costly, and the optimal solution does not violate any margins if the data is separable. The hard-margin SVM is obtained as a special case.

SUPPORT VECTORS

There are three types of training examples:

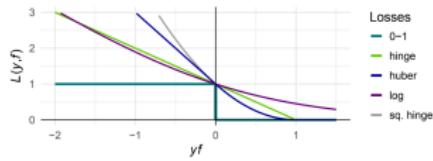
- Non-SVs have a margin > 1 and can be removed from the problem without changing the solution.
- Some SVs are located exactly on the margin and have $yf(\mathbf{x}) = 1$.
- Other SVs are margin violators, with $yf(\mathbf{x}) < 1$, and have an associated positive slack $\zeta^{(i)} > 0$. They are misclassified if $\zeta^{(i)} \geq 1$.



Introduction to Machine Learning

SVMs and Empirical Risk Minimization

Learning goals



- Know why the SVM problem can be understood as (regularized) empirical risk minimization problem
- Know that the corresponding loss is the hinge loss

REGULARIZED EMPIRICAL RISK MINIMIZATION

- We motivated SVMs from a geometrical point of view: The margin is a distance to be maximized.
- This is not really true anymore under margin violations: The slack variables are not really distances. Instead, $\gamma \cdot \zeta^{(i)}$ is the distance by which an observation violates the margin.
- This already indicates that transferring the geometric intuition from hard-margin SVMs to the soft-margin case has its limits.
- There is an alternative approach to understanding soft-margin SVMs: They are **regularized empirical risk minimizers**.

SOFT-MARGIN SVM WITH ERM AND HINGE LOSS

We derived this QP for the soft-margin SVM:

$$\begin{aligned} \min_{\theta, \theta_0, \zeta^{(i)}} \quad & \frac{1}{2} \|\theta\|^2 + C \sum_{i=1}^n \zeta^{(i)} \\ \text{s.t.} \quad & y^{(i)} (\langle \theta, \mathbf{x}^{(i)} \rangle + \theta_0) \geq 1 - \zeta^{(i)} \quad \forall i \in \{1, \dots, n\}, \\ \text{and} \quad & \zeta^{(i)} \geq 0 \quad \forall i \in \{1, \dots, n\}. \end{aligned}$$

In the optimum, the inequalities will hold with equality (as we minimize the slacks), so $\zeta^{(i)} = 1 - y^{(i)} f(\mathbf{x}^{(i)})$, but the lowest value $\zeta^{(i)}$ can take is 0 (we do not get a bonus for points beyond the margin on the correct side). So we can rewrite the above:

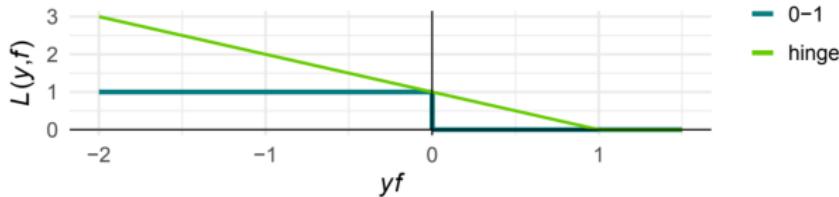
$$\frac{1}{2} \|\theta\|^2 + C \sum_{i=1}^n L(y^{(i)}, f(\mathbf{x}^{(i)})); \quad L(y, f) = \begin{cases} 1 - yf & \text{if } yf \leq 1 \\ 0 & \text{if } yf > 1 \end{cases}$$

We can also write $L(y, f) = \max(1 - yf, 0)$.

SOFT-MARGIN SVM WITH ERM AND HINGE LOSS

$$\mathcal{R}_{\text{emp}}(\theta) = \frac{1}{2} \|\theta\|^2 + C \sum_{i=1}^n L(y^{(i)}, f(\mathbf{x}^{(i)})) ; \quad L(y, f) = \max(1 - yf, 0)$$

- This now obviously L2-regularized empirical risk minimization.
- Actually, a lot of ERM theory was established when Vapnik (co-)invented the SVM in the beginning of the 90s.
- L is called hinge loss – as it looks like a door hinge.
- It is a continuous, convex, upper bound on the zero-one loss. In a certain sense it is the best upper convex relaxation of the 0-1.



SOFT-MARGIN SVM WITH ERM AND HINGE LOSS

$$\frac{1}{2} \|\theta\|^2 + C \sum_{i=1}^n L\left(y^{(i)}, f\left(\mathbf{x}^{(i)}\right)\right); \quad L(y, f) = \max(1 - yf, 0)$$

- The ERM interpretation does not require any of the terms – the loss or the regularizer – to be geometrically meaningful.
- The above form is a very compact form to define the convex optimization problem of the SVM.
- It is "well-behaved" due to convexity, every minimum is global.
- The above is convex, without constraints! We might see this as "easier to optimize" than the QP from before. But note it is non-differentiable due to the hinge. So specialized techniques (e.g. sub-gradient) would have to be used.
- Some literature claims this primal cannot be easily kernelized - which is not really true.

OTHER LOSSES

SVMs can easily be generalized by changing the loss function.

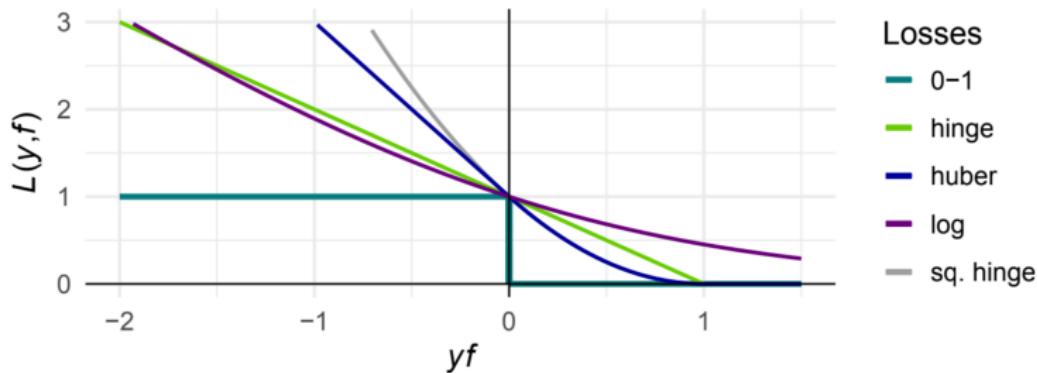
- Squared hinge loss / Least Squares SVM:

$$L(y, f) = \max(0, (1 - yf)^2)$$

- Huber loss (smoothed hinge loss)

- Bernoulli/Log loss. This is L2-regularized logistic regression!

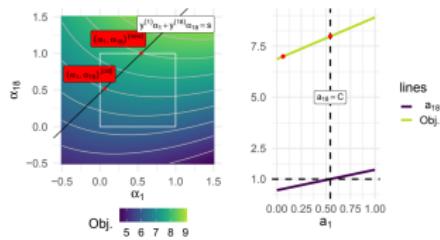
- NB: These other losses usually do not generate sparse solutions in terms of data weights and hence have no "support vectors".



Introduction to Machine Learning

Support Vector Machine Training

Learning goals



- Know that the SVM problem is not differentiable
- Know how to optimize the SVM problem in the primal via subgradient descent
- Know how to optimize SVM in the dual formulation via pairwise coordinate ascent

SUPPORT VECTOR MACHINE TRAINING

- Until now, we have ignored the issue of solving the various convex optimization problems.
- The first question is whether we should solve the **primal** or the **dual problem**.
- In the literature SVMs are usually trained in the dual.
- However, SVMs can be trained both in the primal and the dual – each approach has its advantages and disadvantages.
- It is not easy to create an efficient SVM solver, and often specialized approaches have been developed, we only cover basic ideas here.

TRAINING SVM IN THE PRIMAL

Unconstrained formulation of soft-margin SVM:

$$\min_{\theta, \theta_0} \quad \frac{\lambda}{2} \|\theta\|^2 + \sum_{i=1}^n L(y^{(i)}, f(\mathbf{x}^{(i)} | \theta))$$

where $L(y, f) = \max(0, 1 - yf)$ and $f(\mathbf{x} | \theta) = \theta^T \mathbf{x} + \theta_0$.
(We inconsequentially changed the regularization constant.)

We cannot directly use GD, as the above is not differentiable.

Solutions:

- ① Use smoothed loss (squared hinge, huber), then do GD.
NB: Will not create a sparse SVM if we do not add extra tricks.
- ② Use **subgradient** methods.
- ③ Do stochastic subgradient descent.
Pegasos: Primal Estimated sub-GrAdient SOlver for SVM.

PEGASOS: SSGD IN THE PRIMAL

Approximate the risk by a stochastic 1-sample version:

$$\frac{\lambda}{2} \|\theta\|^2 + L(y^{(i)}, f(\mathbf{x}^{(i)} | \theta))$$

With: $f(\mathbf{x} | \theta) = \theta^T \mathbf{x} + \theta_0$ and $L(y, f) = \max(0, 1 - yf)$

The subgradient for θ is $\lambda\theta - y^{(i)}\mathbf{x}^{(i)}\mathbb{I}_{yf < 1}$

Stochastic subgradient descent (without intercept θ_0)

- 1: **for** $t = 1, 2, \dots$ **do**
 - 2: Pick step size α
 - 3: Randomly pick an index i
 - 4: If $y^{(i)}f(\mathbf{x}^{(i)}) < 1$ set $\theta^{[t+1]} = (1 - \lambda\alpha)\theta^{[t]} + \alpha y^{(i)}\mathbf{x}^{(i)}$
 - 5: If $y^{(i)}f(\mathbf{x}^{(i)}) \geq 1$ set $\theta^{[t+1]} = (1 - \lambda\alpha)\theta^{[t]}$
 - 6: **end for**
-

Note the weight decay due to the L2-regularization.

TRAINING SVM IN THE DUAL

The dual problem of the soft-margin SVM is

$$\begin{aligned} \max_{\alpha} \quad & \sum_{i=1}^n \alpha_i - \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n \alpha_i \alpha_j y^{(i)} y^{(j)} \langle \mathbf{x}^{(i)}, \mathbf{x}^{(j)} \rangle \\ \text{s.t.} \quad & 0 \leq \alpha_i \leq C \quad \sum_{i=1}^n \alpha_i y^{(i)} = 0 \end{aligned}$$

We could solve this problem using coordinate ascent. That means we optimize w.r.t. α_1 , for example, while holding $\alpha_2, \dots, \alpha_n$ fixed.

But: We cannot make any progress since α_1 is determined by
 $\sum_{i=1}^n \alpha_i y^{(i)} = 0$!

TRAINING SVM IN THE DUAL

Solution: Update two variables simultaneously

$$\begin{aligned} \max_{\alpha} \quad & \sum_{i=1}^n \alpha_i - \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n \alpha_i \alpha_j y^{(i)} y^{(j)} \langle \mathbf{x}^{(i)}, \mathbf{x}^{(j)} \rangle \\ \text{s.t.} \quad & 0 \leq \alpha_i \leq C \quad \sum_{i=1}^n \alpha_i y^{(i)} = 0 \end{aligned}$$

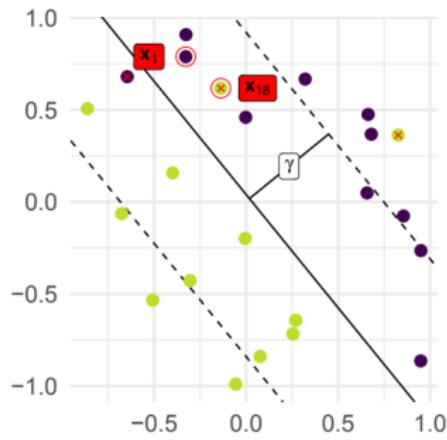
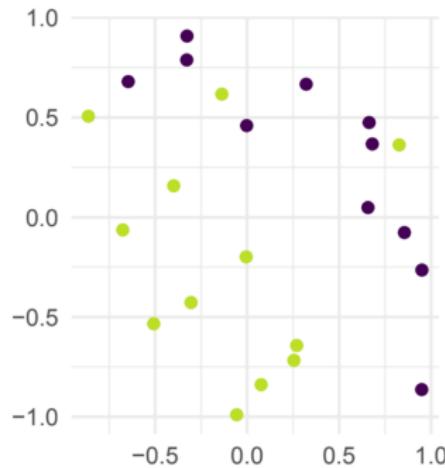
Pairwise coordinate ascent in the dual

- 1: Initialize $\alpha = 0$ (or more cleverly)
 - 2: **for** $t = 1, 2, \dots$ **do**
 - 3: Select some pair α_i, α_j to update next
 - 4: Optimize dual w.r.t. α_i, α_j , while holding α_k ($k \neq i, j$) fixed
 - 5: **end for**
-

The objective is quadratic in the pair, and $s := y^{(i)}\alpha_i + y^{(j)}\alpha_j$ must stay constant. So both α are changed by same (absolute) amount, the signs of the change depend on the labels.

TRAINING SVM IN THE DUAL

Assume we are in a valid state, $0 \leq \alpha_i \leq C$. Then we chose¹ two observations (encircled in red) for the next iteration. Note they have opposite labels so the sign of their change is equal.

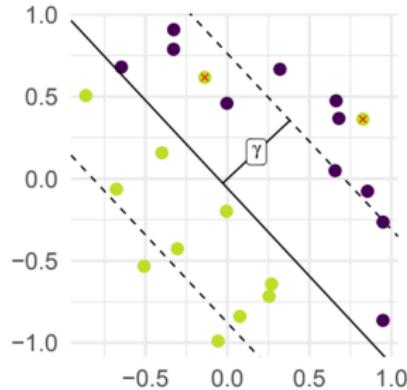
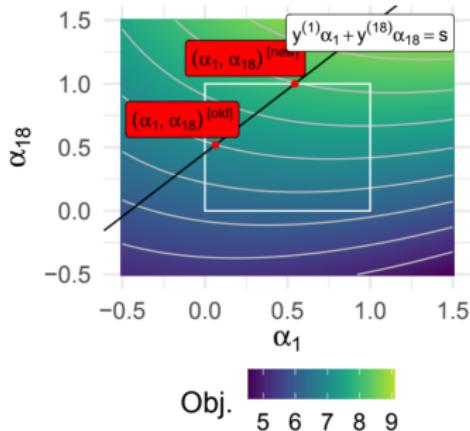


TRAINING SVM IN THE DUAL

$$\max_{\alpha} \quad \sum_{i=1}^n \alpha_i - \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n \alpha_i \alpha_j y^{(i)} y^{(j)} \langle \mathbf{x}^{(i)}, \mathbf{x}^{(j)} \rangle$$

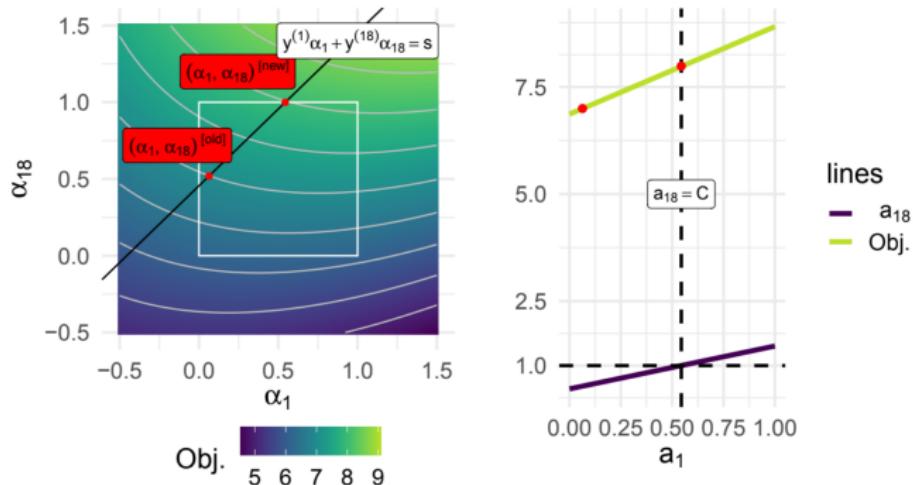
$$\text{s.t.} \quad 0 \leq \alpha_i \leq C \quad \sum_{i=1}^n \alpha_i y^{(i)} = 0$$

We move on the linear constraint until the pair-optimum or the boundary (here: $C = 1$).



TRAINING SVM IN THE DUAL

Sequential Minimal Optimization (SMO) exploits the fact that effectively we only need to solve a one-dimensional quadratic problem, over in interval, for which an analytical solution exists.



INTRODUCTION TO MACHINE LEARNING

Advanced Risk Minimization

Multiclass Classification

Information Theory

Curse of Dimensionality

Hypothesis Space

Regularization

Linear Support Vector Machine

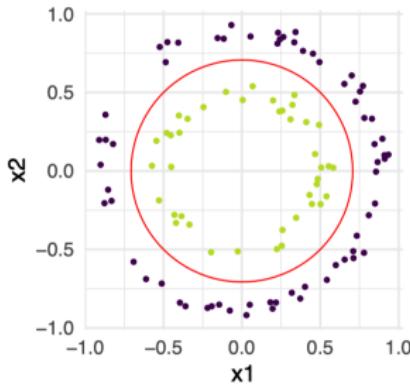
Nonlinear Support Vector Machine

Gaussian Processes

Boosting

Introduction to Machine Learning

Feature Generation for Nonlinear Separation

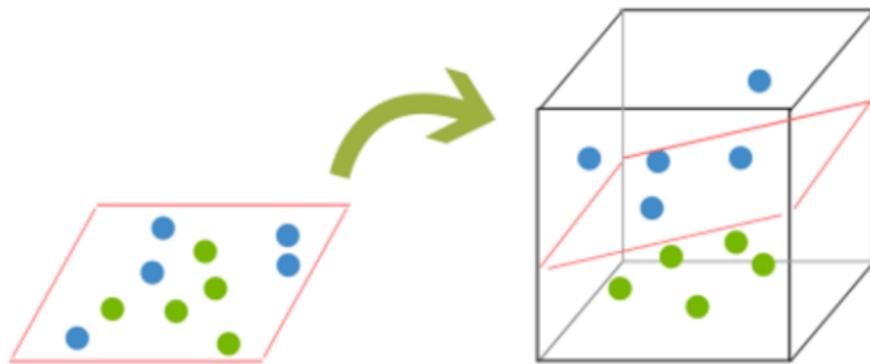


Learning goals

- Understand how nonlinearity can be introduced via feature maps in SVMs
- Know the limitation of feature maps

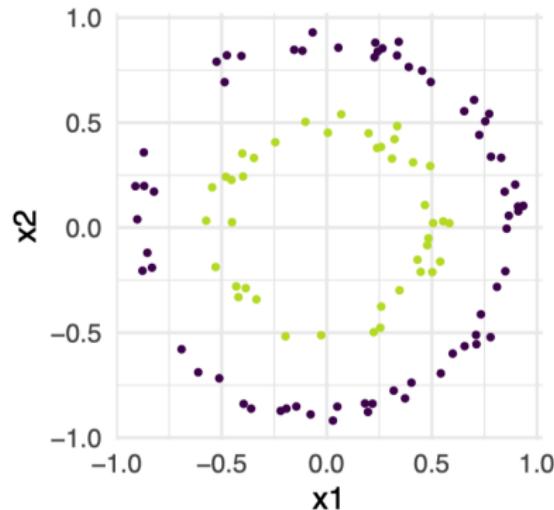
NONLINEARITY VIA FEATURE MAPS

- How to extend a linear classifier, e.g. the SVM, to nonlinear separation between classes?
- We could project the data from 2D into a richer 3D feature space!



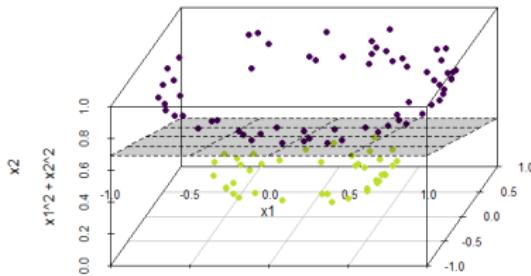
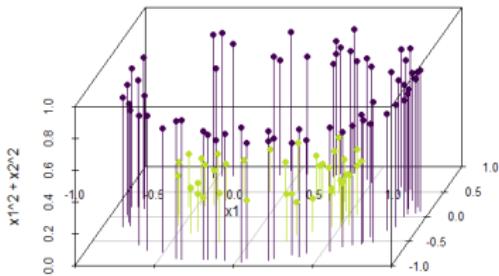
NONLINEARITY VIA FEATURE MAPS

In order to “lift” the data points into a higher dimension, we have to find a suitable **feature map** $\phi : \mathcal{X} \rightarrow \Phi$. Let us consider another example where the classes lie on two concentric circles:



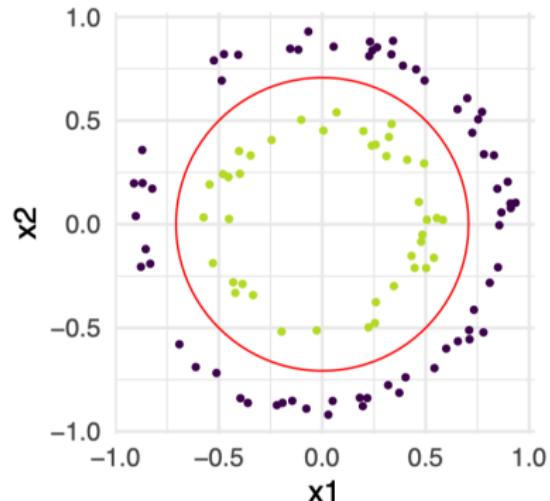
NONLINEARITY VIA FEATURE MAPS

We apply the feature map $\phi(x_1, x_2) = (x_1, x_2, x_1^2 + x_2^2)$ to map our points into a 3D space. Now our data can be separated by a hyperplane.



NONLINEARITY VIA FEATURE MAPS

The hyperplane learned in $\Phi \subset \mathbb{R}^3$ yields a nonlinear decision boundary when projected back to $\mathcal{X} = \mathbb{R}^2$.



FEATURE MAPS: COMPUTATIONAL LIMITATIONS

Let us have a look at a similar nonlinear feature map $\phi : \mathbb{R}^2 \rightarrow \mathbb{R}^5$, where we collect all monomial feature extractors up to degree 2 (pairwise interactions and quadratic effects):

$$\phi(x_1, x_2) = (x_1^2, x_2^2, x_1 x_2, x_1, x_2).$$

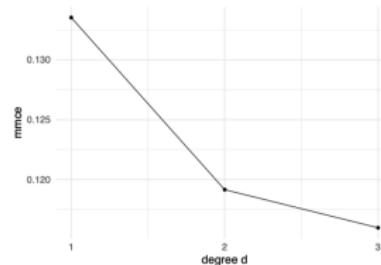
For p features vectors, there are k_1 different monomials where the degree is exactly d , and k_2 different monomials up to degree d .

$$k_1 = \binom{d + p - 1}{p} \quad k_2 = \binom{d + p}{p} - 1$$

Which is quite a lot, if p is large.

FEATURE MAPS: COMPUTATIONAL LIMITATIONS

Let us see how well we can classify the 28×28 -pixel images of the handwritten digits of the MNIST dataset (70K observations across 10 classes). We use SVM with a nonlinear feature map which projects the images to a space of all monomials up to the degree d and $C = 1$:

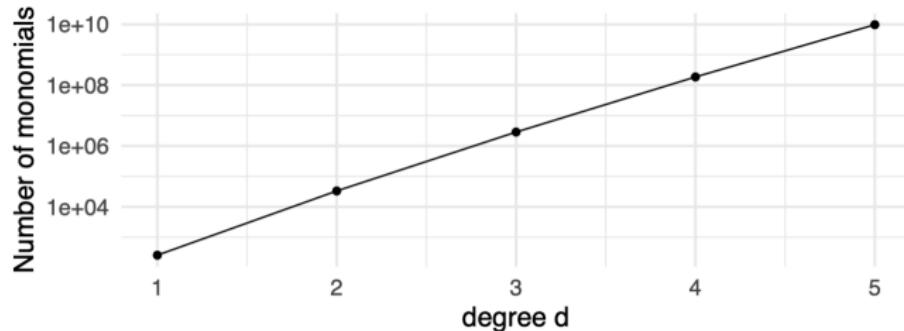


For this scenario, with increasing degree d the test mmce decreases.

NB: We handle the multiclass task with the "one-against-one" approach. We are somewhat lazy and only use 700 observations to train (rest for testing). We do not do any tuning - as we always should for the SVM!

FEATURE MAPS: COMPUTATIONAL LIMITATIONS

However, even a 16×16 -pixel input image results in infeasible dimensions for our extracted features (monomials up to degree d).



In this case, training classifiers like a linear SVM via dataset transformations will incur serious **computational and memory problems**.

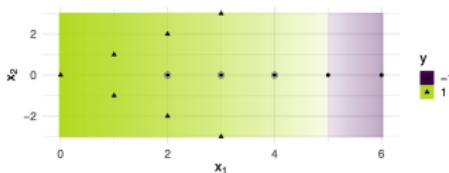
Are we at a “dead end”?

Answer: No, this is why kernels exist!

Introduction to Machine Learning

The Kernel Trick

Learning goals



- Know how to efficiently introduce non-linearity via the kernel trick
- Know common kernel functions (linear, polynomial, radial)
- Know how to compute predictions of the kernel SVM

DUAL SVM PROBLEM WITH FEATURE MAP

The dual (soft-margin) SVM is:

$$\begin{aligned} \max_{\alpha} \quad & \sum_{i=1}^n \alpha_i - \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n \alpha_i \alpha_j y^{(i)} y^{(j)} \langle \phi(\mathbf{x}^{(i)}), \phi(\mathbf{x}^{(j)}) \rangle \\ \text{s.t.} \quad & 0 \leq \alpha_i \leq C, \\ & \sum_{i=1}^n \alpha_i y^{(i)} = 0, \end{aligned}$$

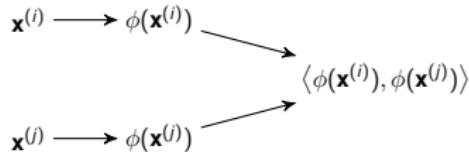
Here we replaced all features $\mathbf{x}^{(i)}$ with feature-generated, transformed versions $\phi(\mathbf{x}^{(i)})$.

We see: The optimization problem only depends on **pair-wise inner products** of the inputs.

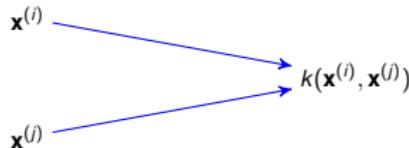
This now allows a trick to enable efficient solving.

KERNEL = FEATURE MAP + INNER PRODUCT

Instead of first mapping the features to the higher-dimensional space and calculating the inner products afterwards,



it would be nice to have an efficient “shortcut” computation:



We will see: **Kernels** give us such a “shortcut”.

MERCER KERNEL

Definition: A (**Mercer**) **kernel** on a space \mathcal{X} is a continuous function

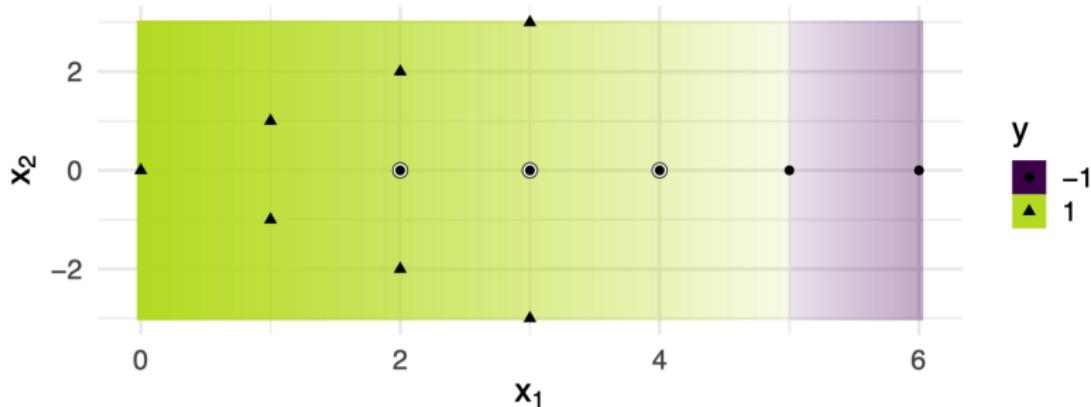
$$k : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$$

of two arguments with the properties

- Symmetry: $k(\mathbf{x}, \tilde{\mathbf{x}}) = k(\tilde{\mathbf{x}}, \mathbf{x})$ for all $\mathbf{x}, \tilde{\mathbf{x}} \in \mathcal{X}$.
- Positive definiteness: For each finite subset $\{\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(n)}\}$ the **kernel Gram matrix** $K \in \mathbb{R}^{n \times n}$ with entries $K_{ij} = k(\mathbf{x}^{(i)}, \mathbf{x}^{(j)})$ is positive semi-definite.

CONSTANT AND LINEAR KERNEL

- Every constant function taking a non-negative value is a (very boring) kernel.
- An inner product is a kernel. We call the standard inner product $k(\mathbf{x}, \tilde{\mathbf{x}}) = \mathbf{x}^\top \tilde{\mathbf{x}}$ the **linear kernel**. This is simply our usual linear SVM as discussed.



SUM AND PRODUCT KERNELS

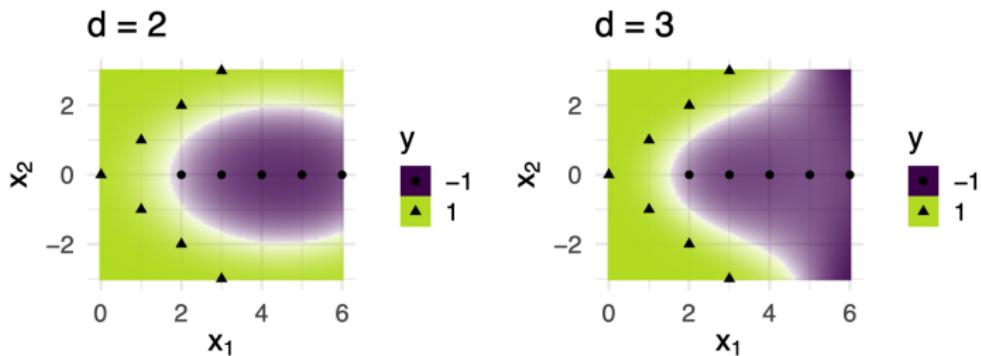
A kernel can be constructed from other kernels k_1 and k_2 :

- For $\lambda \geq 0$, $\lambda \cdot k_1$ is a kernel.
- $k_1 + k_2$ is a kernel.
- $k_1 \cdot k_2$ is a kernel (thus also k_1^n).

The proofs remain as (simple) exercises.

POLYNOMIAL KERNEL

$$k(\mathbf{x}, \tilde{\mathbf{x}}) = (\mathbf{x}^\top \tilde{\mathbf{x}} + b)^d, \text{ for } b \geq 0, d \in \mathbb{N}$$



From the sum-product rules it directly follows that this is a kernel.

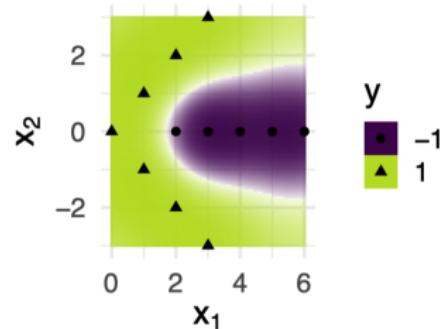
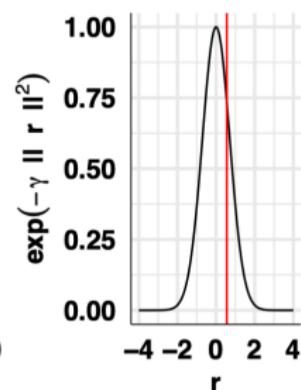
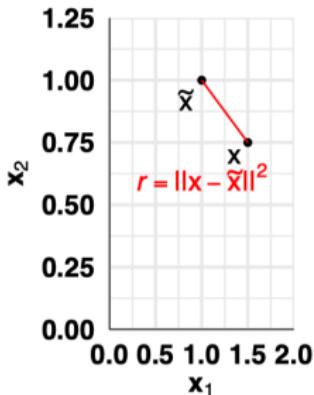
RBF KERNEL

The “radial” **Gaussian kernel** is defined as

$$k(\mathbf{x}, \tilde{\mathbf{x}}) = \exp\left(-\frac{\|\mathbf{x} - \tilde{\mathbf{x}}\|^2}{2\sigma^2}\right)$$

Or

$$k(\mathbf{x}, \tilde{\mathbf{x}}) = \exp(-\gamma \|\mathbf{x} - \tilde{\mathbf{x}}\|^2), \gamma > 0$$



KERNEL SVM

We kernelize the dual (soft-margin) SVM problem by replacing all inner products $\langle \phi(\mathbf{x}^{(i)}), \phi(\mathbf{x}^{(j)}) \rangle$ by kernels $k(\mathbf{x}^{(i)}, \mathbf{x}^{(j)})$

$$\begin{aligned} \max_{\alpha} \quad & \sum_{i=1}^n \alpha_i - \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n \alpha_i \alpha_j y^{(i)} y^{(j)} \langle \phi(\mathbf{x}^{(i)}), \phi(\mathbf{x}^{(j)}) \rangle \\ \text{s.t.} \quad & 0 \leq \alpha_i \leq C, \\ & \sum_{i=1}^n \alpha_i y^{(i)} = 0. \end{aligned}$$

This problem is still convex because \mathbf{K} is psd!

KERNEL SVM

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In more compact matrix notation with \mathbf{K} denoting the kernel matrix:

$$\begin{aligned} \max_{\alpha \in \mathbb{R}^n} \quad & \mathbf{1}^\top \alpha - \frac{1}{2} \alpha^\top \text{diag}(\mathbf{y}) \mathbf{K} \text{diag}(\mathbf{y}) \alpha \\ \text{s.t.} \quad & \alpha^\top \mathbf{y} = 0, \\ & 0 \leq \alpha \leq C. \end{aligned}$$

This problem is still convex because \mathbf{K} is psd!

KERNEL SVM: PREDICTIONS

For the linear soft-margin SVM we had:

$$f(\mathbf{x}) = \hat{\theta}^T \mathbf{x} + \theta_0 \quad \text{and} \quad \hat{\theta} = \sum_{i=1}^n \alpha_i y^{(i)} \mathbf{x}^{(i)}$$

After the feature map this becomes:

$$f(\mathbf{x}) = \langle \hat{\theta}, \phi(\mathbf{x}) \rangle + \theta_0 \quad \text{and} \quad \hat{\theta} = \sum_{i=1}^n \alpha_i y^{(i)} \phi(\mathbf{x}^{(i)})$$

Assuming that the dot-product still follows its bi-linear rules in the mapped space and using the kernel trick again:

$$\begin{aligned} \langle \hat{\theta}, \phi(\mathbf{x}) \rangle &= \left\langle \sum_{i=1}^n \alpha_i y^{(i)} \phi(\mathbf{x}^{(i)}), \phi(\mathbf{x}) \right\rangle = \sum_{i=1}^n \alpha_i y^{(i)} \langle \phi(\mathbf{x}^{(i)}), \phi(\mathbf{x}) \rangle = \\ &= \sum_{i=1}^n \alpha_i y^{(i)} k(\mathbf{x}^{(i)}, \mathbf{x}), \quad \text{so:} \quad f(\mathbf{x}) = \sum_{i=1}^n \alpha_i y^{(i)} k(\mathbf{x}^{(i)}, \mathbf{x}) + \theta_0 \end{aligned}$$

MNIST EXAMPLE

- Through this kernelization we can now conveniently perform feature generation even for higher-dimensional data. Actually, this is how we computed all previous examples, too.
- We again consider MNIST with 28×28 bitmaps of gray values.
- A polynomial kernel extracts $\binom{d+p}{d} - 1$ features and for the RBF kernel the dimensionality would be infinite.
- We train SVMs again on 700 observations of the MNIST data set and use the rest of the data for testing; and use $C=1$.

0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3
4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4
5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5
6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6
7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7
8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8
9 9 9 9 9 9 9 9 9 9 9 9 9 9 9 9

	Error
linear	0.134
poly (d = 2)	0.119
RBF (gamma = 0.001)	0.12
RBF (gamma = 1)	0.184

FINAL COMMENTS

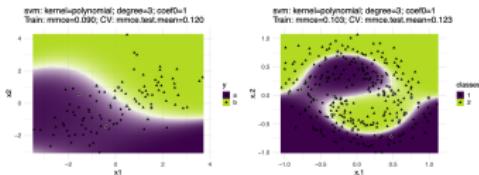
- The kernel trick allows us to make linear machines non-linear in a very efficient manner.
- Linear separation in high-dimensional spaces is **very flexible**.
- Learning takes place in the feature space, while predictions are computed in the input space.
- Both the polynomial and Gaussian kernels can be computed in linear time. Computing inner products of features is **much faster** than computing the features themselves.
- What if a good feature map ϕ is already available? Then this feature map canonically induces a kernel by defining $k(\mathbf{x}, \tilde{\mathbf{x}}) = \langle \phi(\mathbf{x}), \phi(\tilde{\mathbf{x}}) \rangle$. There is no problem with an explicit feature representation as long as it is efficiently computable.

Introduction to Machine Learning

The Polynomial Kernel

Learning goals

- Know the homogeneous and non-homogeneous polynomial kernel
- Understand the influence of the choice of the degree on the decision boundary



HOMOGENEOUS POLYNOMIAL KERNEL

$$k(\mathbf{x}, \tilde{\mathbf{x}}) = (\mathbf{x}^T \tilde{\mathbf{x}})^d, \text{ for } d \in \mathbb{N}$$

The feature map contains all monomials of exactly order d .

$$\phi(\mathbf{x}) = \left(\sqrt{\binom{d}{k_1, \dots, k_p}} x_1^{k_1} \dots x_p^{k_p} \right)_{k_i \geq 0, \sum_i k_i = d}$$

That $\langle \phi(\mathbf{x}), \phi(\tilde{\mathbf{x}}) \rangle = k(\mathbf{x}, \tilde{\mathbf{x}})$ holds can easily be checked by simple calculation and using the multinomial formula

$$(\mathbf{x}_1 + \dots + \mathbf{x}_p)^d = \sum_{k_i \geq 0, \sum_i k_i = d} \binom{d}{k_1, \dots, k_p} x_1^{k_1} \dots x_p^{k_p}$$

The map $\phi(\mathbf{x})$ has $\binom{p+d-1}{d}$ dimensions. We see that $\phi(\mathbf{x})$ contains no terms of "lesser" order, so, e.g., linear effects. As an example for $p = d = 2$: $\phi(\mathbf{x}) = (x_1^2, x_2^2, \sqrt{2}x_1 x_2)$.

NONHOMOGENEOUS POLYNOMIAL KERNEL

$$k(\mathbf{x}, \tilde{\mathbf{x}}) = (\mathbf{x}^T \tilde{\mathbf{x}} + b)^d, \text{ for } b \geq 0, d \in \mathbb{N}$$

The maths is very similar as before, we kind of add a further constant term in the original space, with

$$(\mathbf{x}^T \tilde{\mathbf{x}} + b)^d = (x_1 \tilde{x}_1 + \dots + x_p \tilde{x}_p + \sqrt{b} \sqrt{b})^d$$

The feature map contains all monomials up to order d .

$$\phi(\mathbf{x}) = \left(\sqrt{\binom{d}{k_1, \dots, k_{p+1}}} x_1^{k_1} \dots x_p^{k_p} b^{k_{p+1}/2} \right)_{k_i \geq 0, \sum_i k_i = d}$$

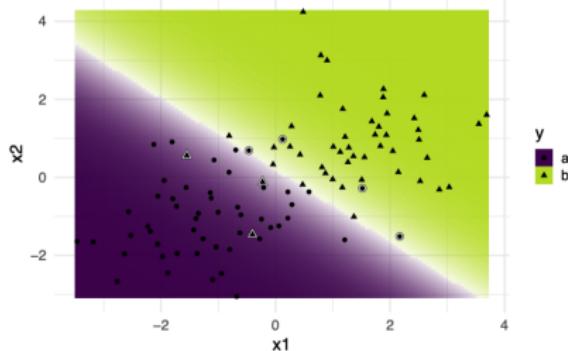
The map $\phi(\mathbf{x})$ has $\binom{p+d}{d}$ dimensions. For $p = d = 2$:

$$\phi(\mathbf{x}) = (x_1^2, x_2^2, \sqrt{2}x_1x_2, \sqrt{2b}x_1, \sqrt{2b}x_2, \sqrt{b})$$

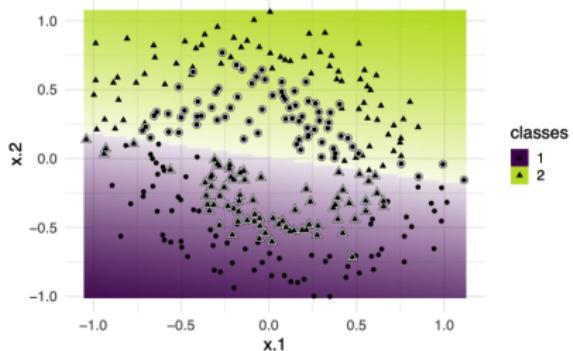
POLYNOMIAL KERNEL

Degree $d = 1$ yields a linear decision boundary.

svm: kernel=polynomial; degree=1; coef0=1
Train: mmce=0.070; CV: mmce.test.mean=0.110



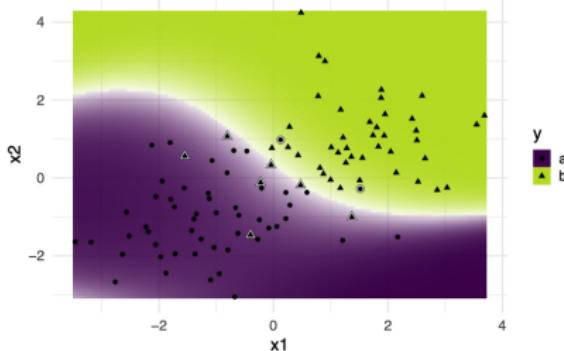
svm: kernel=polynomial; degree=1; coef0=1
Train: mmce=0.500; CV: mmce.test.mean=0.507



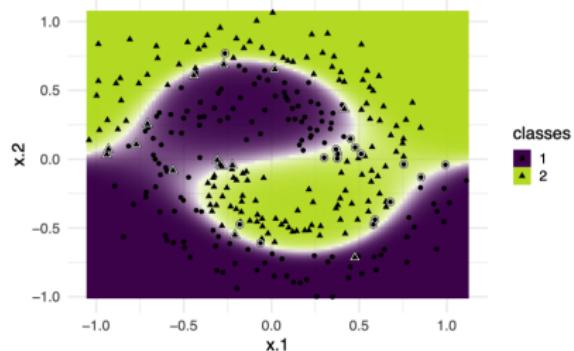
POLYNOMIAL KERNEL

The higher the degree, the more nonlinearity in the decision boundary.

svm: kernel=polynomial; degree=3; coef0=1
Train: mmce=0.090; CV: mmce.test.mean=0.120



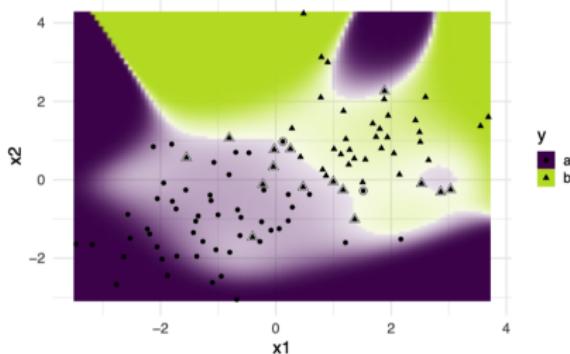
svm: kernel=polynomial; degree=3; coef0=1
Train: mmce=0.103; CV: mmce.test.mean=0.123



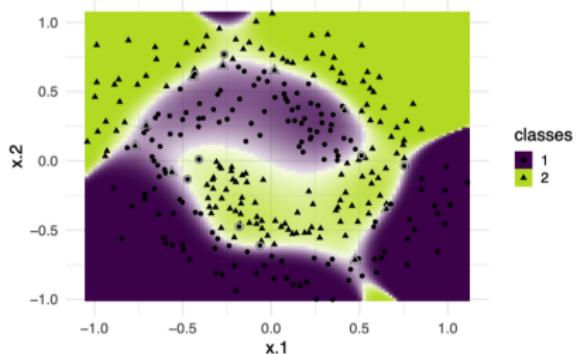
POLYNOMIAL KERNEL

The higher the degree, the more nonlinearity in the decision boundary.

svm: kernel=polynomial; degree=9; coef0=1
Train: mmce=0.170; CV: mmce.test.mean=0.250



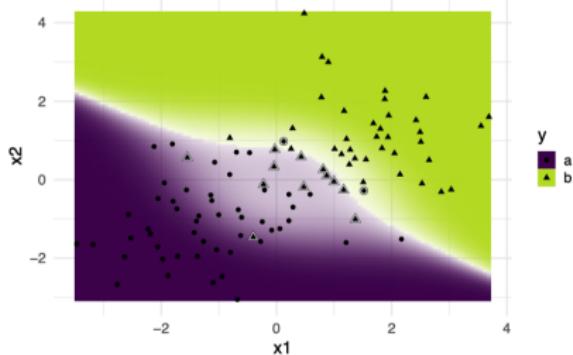
svm: kernel=polynomial; degree=9; coef0=1
Train: mmce=0.057; CV: mmce.test.mean=0.120



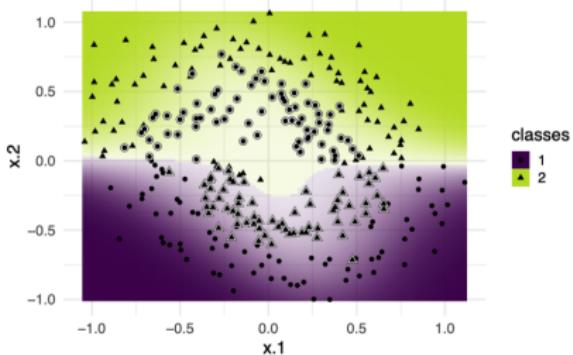
POLYNOMIAL KERNEL

For $k(\mathbf{x}, \tilde{\mathbf{x}}) = (\mathbf{x}^\top \tilde{\mathbf{x}} + 0)^d$ we get no lower order effects.

svm: kernel=polynomial; degree=3; coef0=0
Train: mmce=0.140; CV: mmce.test.mean=0.180



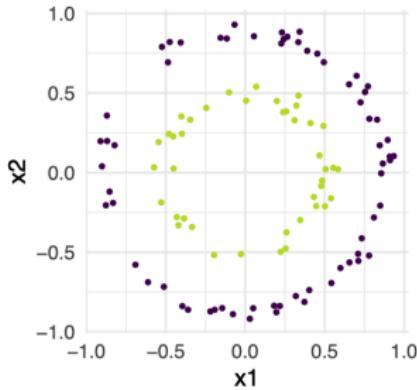
svm: kernel=polynomial; degree=3; coef0=0
Train: mmce=0.473; CV: mmce.test.mean=0.483



Introduction to Machine Learning

Reproducing Kernel Hilbert Space and Representer Theorem

Learning goals



- Know that for every kernel there is an associated feature map and space (Mercer's Theorem)
- Know that this feature map is not unique, and the reproducing kernel Hilbert space (RKHS) is a reference space
- Know the representation of the solution of a SVM is given by the

KERNELS: MERCER'S THEOREM

- Kernels are symmetric, positive definite functions $k : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$.
- A kernel can be thought of as a shortcut computation for a two-step procedure: the feature map and the inner product.

Mercer's theorem says that for every kernel there exists an associated (well-behaved) feature space where the kernel acts as a dot-product.

- There exists a Hilbert space Φ of continuous functions $\mathcal{X} \rightarrow \mathbb{R}$ (think of it as a vector space with inner product where all operations are meaningful, including taking limits of sequences; this is non-trivial in the infinite-dimensional case)
- and a continuous “feature map” $\phi : \mathcal{X} \rightarrow \Phi$,
- so that the kernel computes the inner product of the features:

$$k(\mathbf{x}, \tilde{\mathbf{x}}) = \langle \phi(\mathbf{x}), \phi(\tilde{\mathbf{x}}) \rangle .$$

REPRODUCING KERNEL HILBERT SPACE

- There are many possible Hilbert spaces and feature maps for the same kernel, but they are all “equivalent” (isomorphic).
- It is often helpful to have a reference space for a kernel $k(\cdot, \cdot)$, called the **reproducing kernel Hilbert space (RKHS)**.
- The feature map of this space is

$$\phi : \mathcal{X} \rightarrow \mathcal{C}(\mathcal{X}); \quad \mathbf{x} \mapsto k(\mathbf{x}, \cdot) ,$$

where $\mathcal{C}(\mathcal{X})$ is the space of continuous functions $\mathcal{X} \rightarrow \mathbb{R}$. The “features” of the RKHS are the kernel functions evaluated at an \mathbf{x} .

- The Hilbert space is the completion of the span of the features:

$$\Phi = \overline{\text{span}\{\phi(\mathbf{x}) \mid \mathbf{x} \in \mathcal{X}\}} \subset \mathcal{C}(\mathcal{X}) .$$

- The so-called **reproducing property** states:

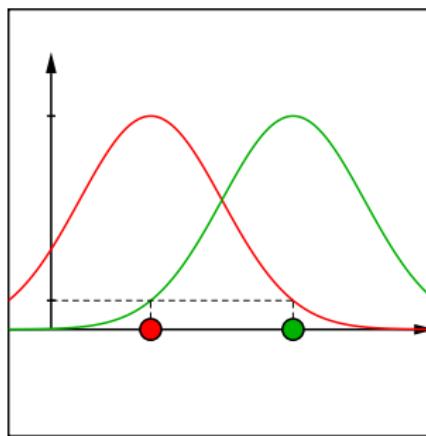
$$\langle k(\mathbf{x}, \cdot), k(\tilde{\mathbf{x}}, \cdot) \rangle = \langle \phi(\mathbf{x}), \phi(\tilde{\mathbf{x}}) \rangle = k(\mathbf{x}, \tilde{\mathbf{x}}).$$

REPRODUCING KERNEL HILBERT SPACE

- The RKHS provides us with a useful interpretation:
an input $\mathbf{x} \in \mathcal{X}$ mapped to the **basis function** $\phi(\mathbf{x}) = k(\mathbf{x}, \cdot)$.
- The kernel maps 2 points and computes the inner product:

$$\langle k(\mathbf{x}, \cdot), k(\tilde{\mathbf{x}}, \cdot) \rangle = k(\mathbf{x}, \tilde{\mathbf{x}}) .$$

- This is best illustrated with the Gaussian kernel.



REPRODUCING KERNEL HILBERT SPACE

- Caveat: Not all elements of the Hilbert space are of the form $k(\mathbf{x}, \cdot)$ for some $\mathbf{x} \in \mathcal{X}$!
- A general element in the span takes the form

$$\sum_{i=1}^n \alpha_i k(\mathbf{x}^{(i)}, \cdot) \in \Phi .$$

- A general element in the closure of the span takes the form

$$\sum_{i=1}^{\infty} \alpha_i k(\mathbf{x}^{(i)}, \cdot) \in \Phi .$$

with $\sum_{i=1}^{\infty} \alpha_i^2 < \infty$.

REPRODUCING KERNEL HILBERT SPACE

What is $\langle f, g \rangle$ for two elements

$$f = \sum_{i=1}^n \alpha_i k(\mathbf{x}^{(i)}, \cdot), \quad g = \sum_{j=1}^m \beta_j k(\mathbf{x}^{(j)}, \cdot) ?$$

We use the bilinearity of the inner product:

$$\begin{aligned} \left\langle \sum_{i=1}^n \alpha_i k(\mathbf{x}^{(i)}, \cdot), \sum_{j=1}^m \beta_j k(\mathbf{x}^{(j)}, \cdot) \right\rangle &= \sum_{i=1}^n \alpha_i \left\langle k(\mathbf{x}^{(i)}, \cdot), \sum_{j=1}^m \beta_j k(\mathbf{x}^{(j)}, \cdot) \right\rangle \\ &= \sum_{i=1}^n \sum_{j=1}^m \alpha_i \beta_j \left\langle k(\mathbf{x}^{(i)}, \cdot), k(\mathbf{x}^{(j)}, \cdot) \right\rangle \\ &= \sum_{i=1}^n \sum_{j=1}^m \alpha_i \beta_j k(\mathbf{x}^{(i)}, \mathbf{x}^{(j)}) \end{aligned}$$

The kernel defines the inner products of all elements in the span of the basis functions.

REPRESENTER THEOREM

The **representer theorem** tells us that the solution of a support vector machine problem

$$\begin{aligned} \min_{\theta, \theta_0, \zeta^{(i)}} \quad & \frac{1}{2} \theta^\top \theta + C \sum_{i=1}^n \zeta^{(i)} \\ \text{s.t.} \quad & y^{(i)} \left(\langle \theta, \phi(\mathbf{x}^{(i)}) \rangle + \theta_0 \right) \geq 1 - \zeta^{(i)} \quad \forall i \in \{1, \dots, n\}, \\ \text{and} \quad & \zeta^{(i)} \geq 0 \quad \forall i \in \{1, \dots, n\} \end{aligned}$$

can be written as

$$\theta = \sum_{j=1}^n \beta_j \phi(\mathbf{x}^{(j)})$$

for $\beta_j \in \mathbb{R}$.

REPRESENTER THEOREM

Theorem (Representer Theorem):

The solution θ, θ_0 of the support vector machine optimization problem fulfills $\theta \in V = \text{span} \{ \phi(\mathbf{x}^{(1)}), \dots, \phi(\mathbf{x}^{(n)}) \}$.

Proof: Let V^\perp denote the space orthogonal to V , so that $\Phi = V \oplus V^\perp$. The vector θ has a unique decomposition into components $v \in V$ and $v^\perp \in V^\perp$, so that $v + v^\perp = \theta$.

The regularizer becomes $\|\theta\|^2 = \|v\|^2 + \|v^\perp\|^2$. The constraints

$y^{(i)} (\langle \theta, \phi(\mathbf{x}^{(i)}) \rangle + \theta_0) \geq 1 - \zeta^{(i)}$ do not depend on v^\perp at all:

$$\langle \theta, \phi(\mathbf{x}^{(i)}) \rangle = \underbrace{\langle v, \phi(\mathbf{x}^{(i)}) \rangle}_{=0} + \underbrace{\langle v^\perp, \phi(\mathbf{x}^{(i)}) \rangle}_{\forall i \in \{1, 2, \dots, n\}}.$$

Thus, we have two independent optimization problems, namely the standard SVM problem for v and the unconstrained minimization problem of $\|v^\perp\|^2$ for v^\perp , with obvious solution $v^\perp = 0$. Thus, $\theta = v \in V$.

REPRESENTER THEOREM

- Hence, we can restrict the SVM optimization problem to the **finite-dimensional** subspace span $\{\phi(\mathbf{x}^{(1)}), \dots, \phi(\mathbf{x}^{(n)})\}$. Its dimension grows with the size of the training set.
- More explicitly, we can assume the form

$$\boldsymbol{\theta} = \sum_{j=1}^n \beta_j \cdot \phi(\mathbf{x}^{(j)})$$

for the weight vector $\boldsymbol{\theta} \in \Phi$.

- The SVM prediction on $\mathbf{x} \in \mathcal{X}$ can be computed as

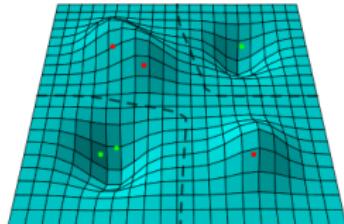
$$f(\mathbf{x}) = \sum_{j=1}^n \beta_j \left\langle \phi(\mathbf{x}^{(j)}), \phi(\mathbf{x}) \right\rangle + \theta_0 .$$

It can be shown that the sum is **sparse**: $\beta_j = 0$ for non-support vectors.

Introduction to Machine Learning

The Gaussian RBF Kernel

Learning goals

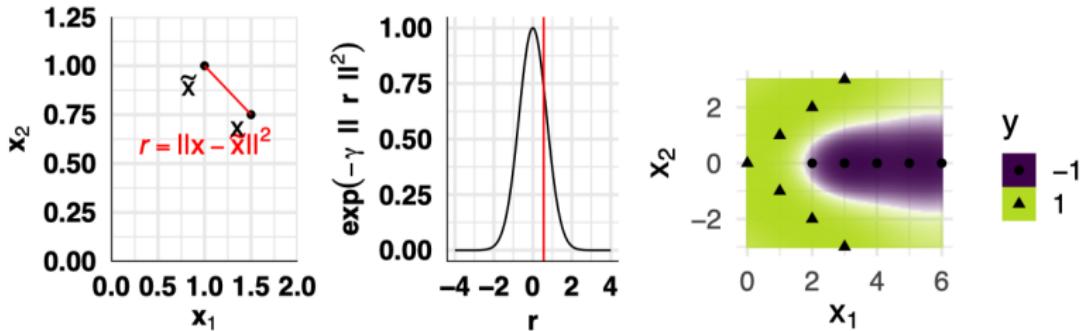


- Know the Gaussian (RBF) kernel
- Understand that all data sets are separable with this kernel
- Understand the effect of the kernel hyperparameter σ

RBF KERNEL

The “radial” **Gaussian kernel** is defined as

$$k(\mathbf{x}, \tilde{\mathbf{x}}) = \exp\left(-\frac{\|\mathbf{x} - \tilde{\mathbf{x}}\|^2}{2\sigma^2}\right) \quad \text{or} \quad k(\mathbf{x}, \tilde{\mathbf{x}}) = \exp(-\gamma \|\mathbf{x} - \tilde{\mathbf{x}}\|^2)$$



A straightforward extension is

$$k(\mathbf{x}, \tilde{\mathbf{x}}) = \exp\left(-(\mathbf{x} - \tilde{\mathbf{x}})^T C (\mathbf{x} - \tilde{\mathbf{x}})\right)$$

for a symmetric, positive definite matrix C .

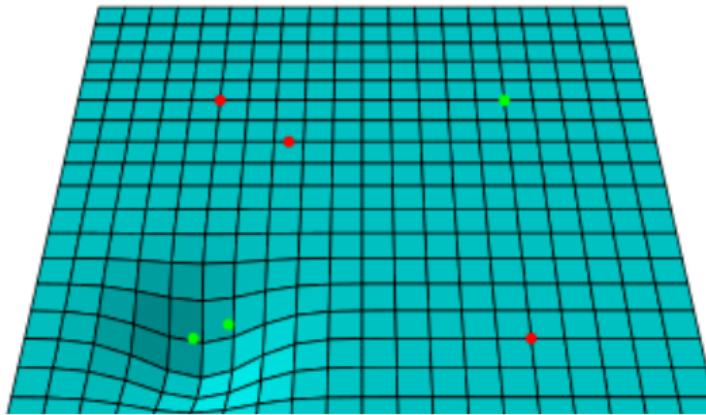
RBF KERNEL

- With a Gaussian kernel, all RKHS basis functions $\phi(\mathbf{x}) = k(\mathbf{x}, \cdot)$ are linearly independent - which we will not prove here.
- This means that all (finite) data sets are linearly separable!
- Do we then need soft-margin machines? The answer is “yes”. The roles of the nonlinear feature map and the soft-margin constraints are very different:
 - The purpose of the kernel (and its feature map) is to make learning “easy”.
 - Even in an infinite-dimensional feature space we may want some margin violators because we should not trust noisy data. A hard-margin SVM with Gaussian kernels may be able to separate any dataset but will usually overfit.

WEIGHTED MIXTURE OF GAUSSIANS

Via the RKHS / basis function intuition we can understand the effect of the RBF kernel much better as a local model.

$$f(\mathbf{x}) = \sum_{i=1}^n \alpha_i y^{(i)} k(\mathbf{x}^{(i)}, \mathbf{x}) + \theta_0$$

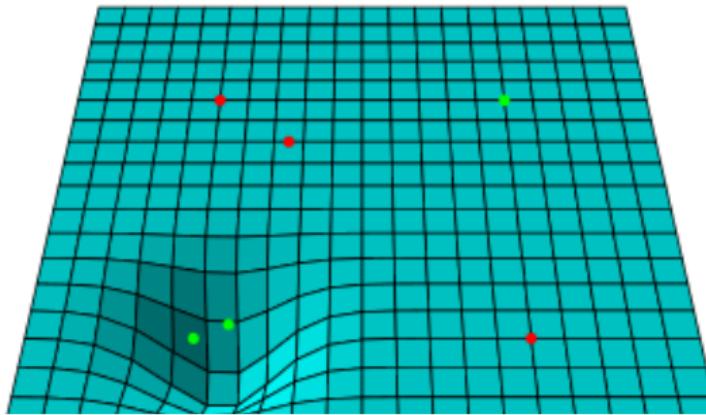


All support vectors are assigned RBF "bumps", these are weighted with the dual variables / Lagrange multipliers α_i and labels $y^{(i)}$. We then "mix" these bumps together to form the decision score function. Which becomes a bumpy surface.

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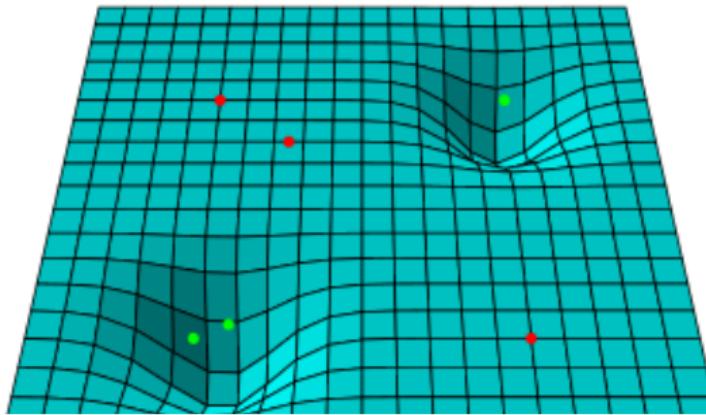


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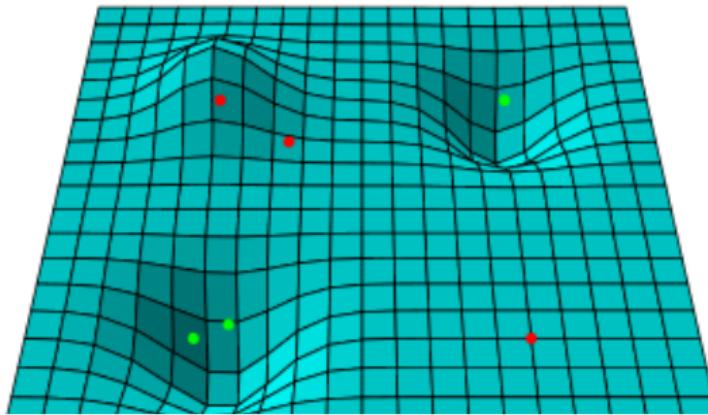


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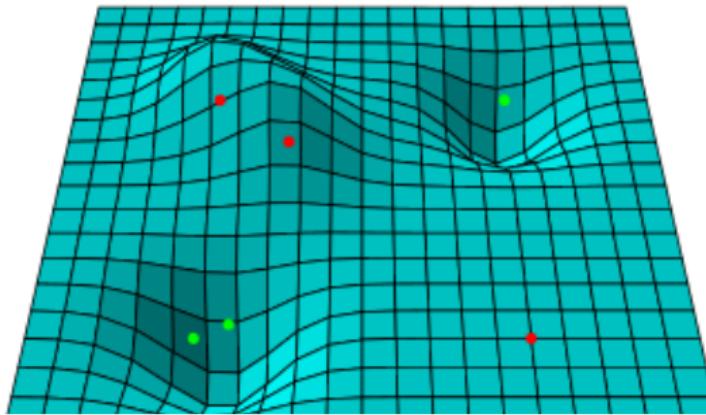


All support vectors are assigned RBF "bumps", these are weighted with the dual variables / Lagrange multipliers α_i and labels $y^{(i)}$. We then "mix" these bumps together to form the decision score function. Which becomes a bumpy surface.

WEIGHTED MIXTURE OF GAUSSIANS

Via the RKHS / basis function intuition we can understand the effect of the RBF kernel much better as a local model.

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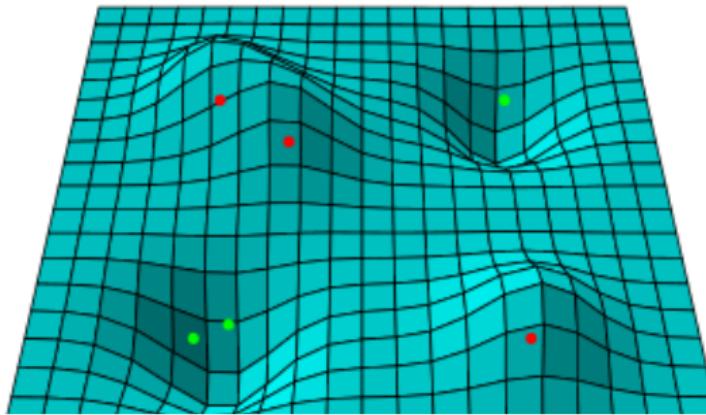


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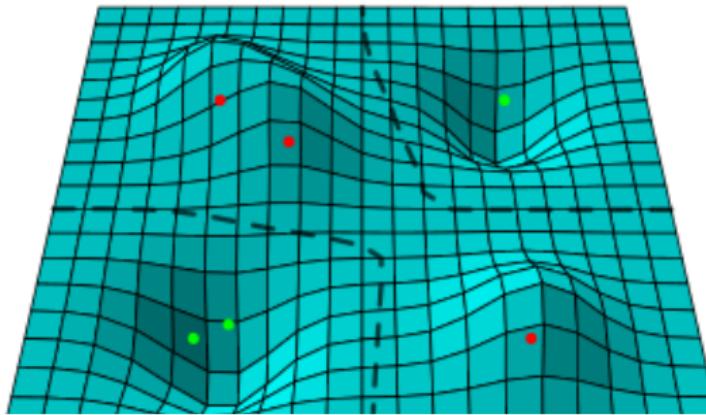


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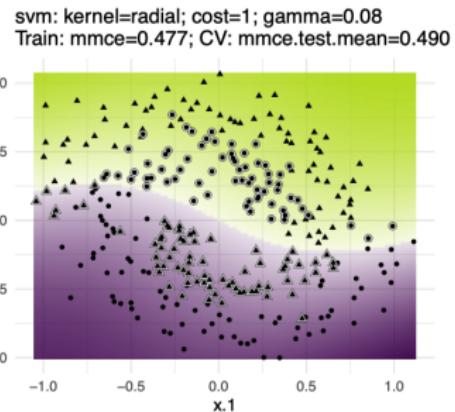
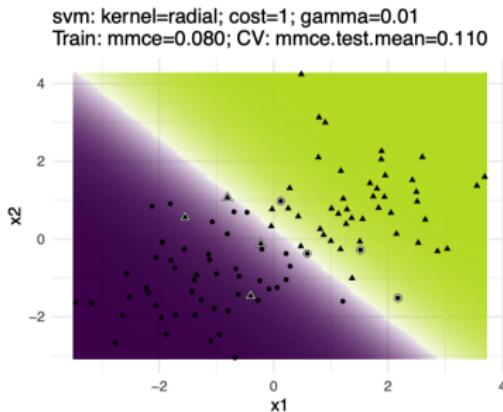
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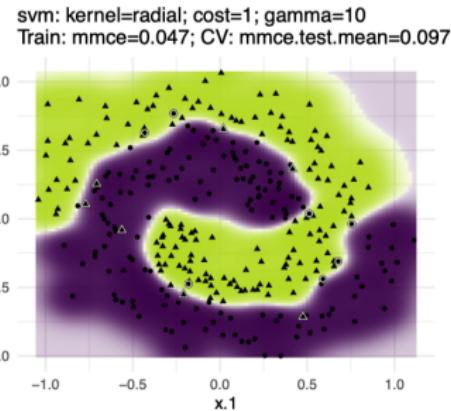
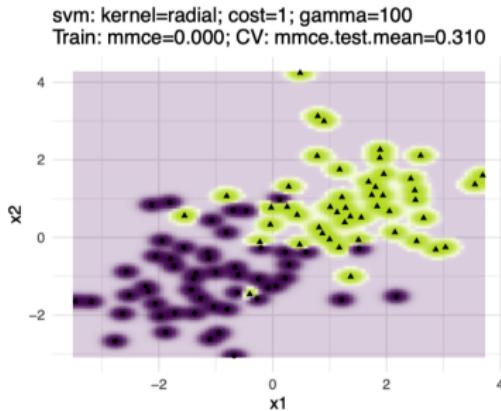
RBF KERNEL WIDTH

A large σ (or a small γ) will make the decision boundary very smooth and in the limit almost linear.



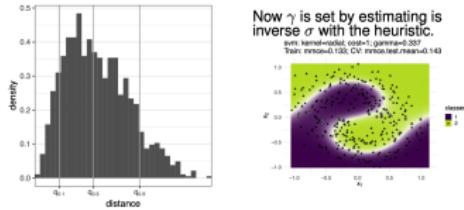
RBF KERNEL WIDTH

A small σ parameter makes the function more “wiggly”, in the limit we totally over fit the data by basically modelling each training data point - and maximal uncertainty at all other test points.



Introduction to Machine Learning

SVM Model Selection



Learning goals

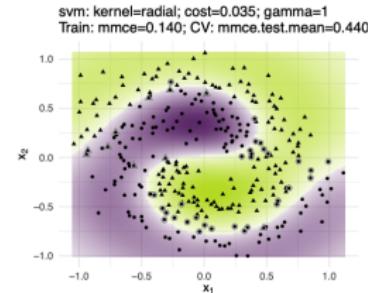
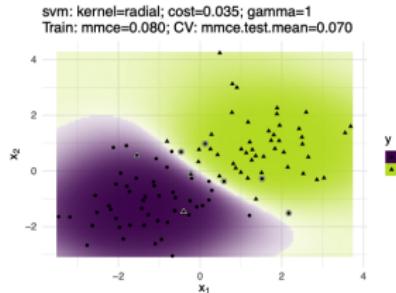
- Know that the SVM is sensitive to hyperparameter choices
- Understand the effect of different (kernel) hyperparameters

MODEL SELECTION FOR KERNEL SVMS

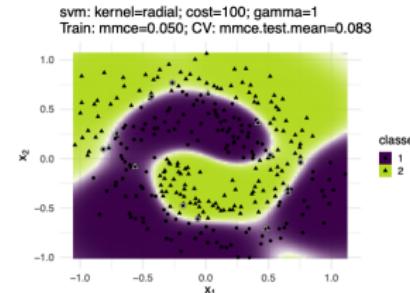
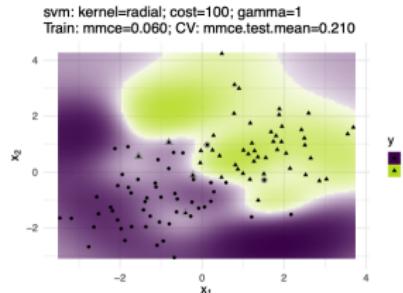
- “Kernelizing” a linear algorithm effectively turns this algorithm into a family of algorithms — one for each kernel. There are infinitely many kernels, and many efficiently computable kernels.
- However, the choice of C , the choice of the kernel, the kernel parameters are all up to the user.
- On the one hand this allows very flexible modelling, and also to incorporate prior knowledge into the learning process.
- On the other hand this puts a huge burden on the user. The machine has no mechanism for identifying a good kernel by itself.
- SVMs are somewhat sensitive to its hyperparameters and should always be tuned.
- Gaussian processes are very related kernel methods, with the big advantage that kernel parameters are directly estimated during training.

SVM HYPERPARAMETERS

Small C “allows” for margin-violating points in favor of a large margin.



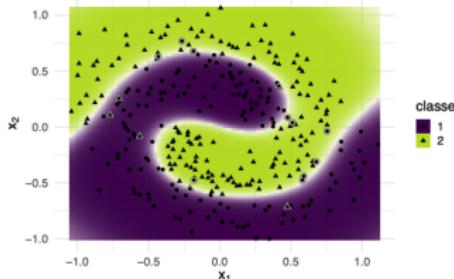
Large C penalizes margin violators, decision boundary is more “wiggly”.



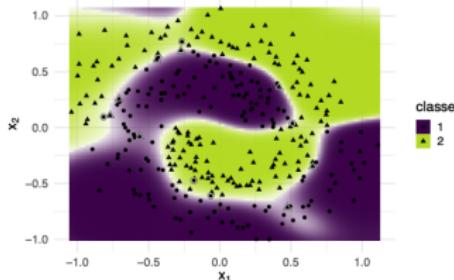
SVM HYPERPARAMETERS

Hyperparameters strongly influence the model: RBF kernel.

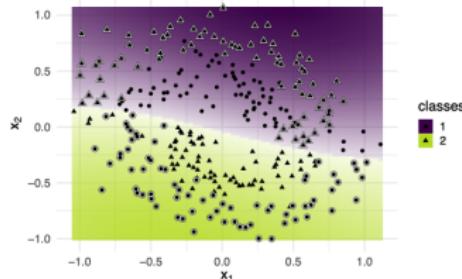
svm: kernel=radial; cost=1; gamma=1
Train: mmce=0.053; CV: mmce.test.mean=0.073



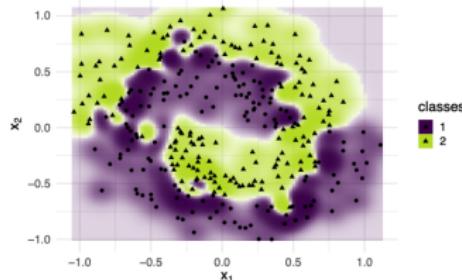
svm: kernel=radial; cost=1e+03; gamma=1
Train: mmce=0.047; CV: mmce.test.mean=0.097



svm: kernel=radial; cost=0.1; gamma=0.1
Train: mmce=0.507; CV: mmce.test.mean=0.527

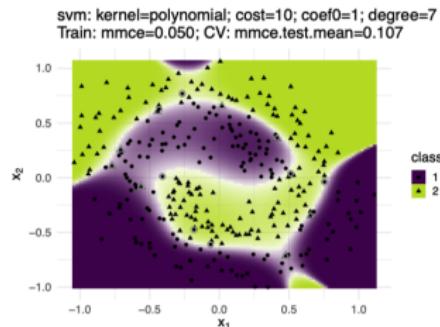
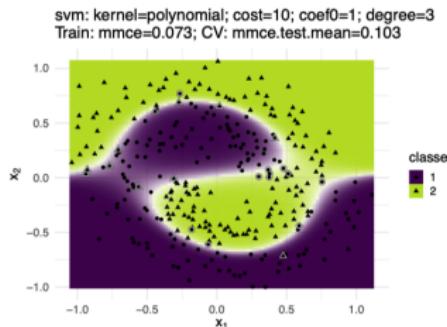
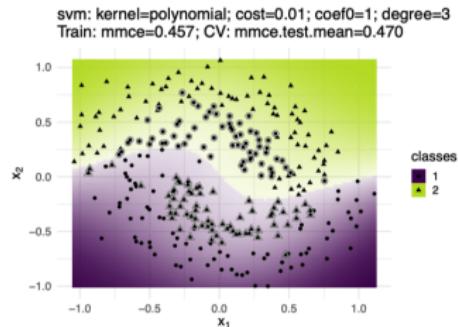
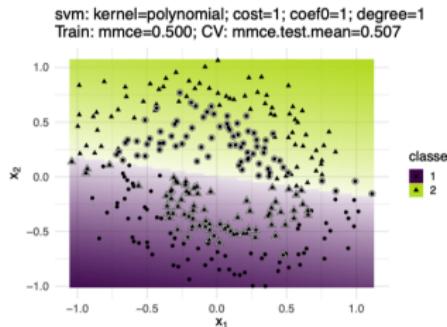


svm: kernel=radial; cost=100; gamma=20
Train: mmce=0.000; CV: mmce.test.mean=0.147



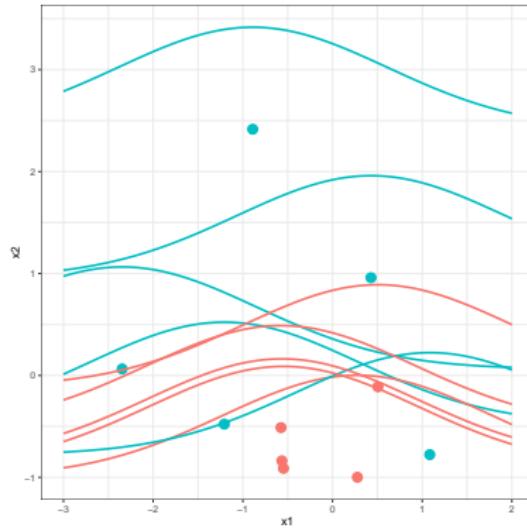
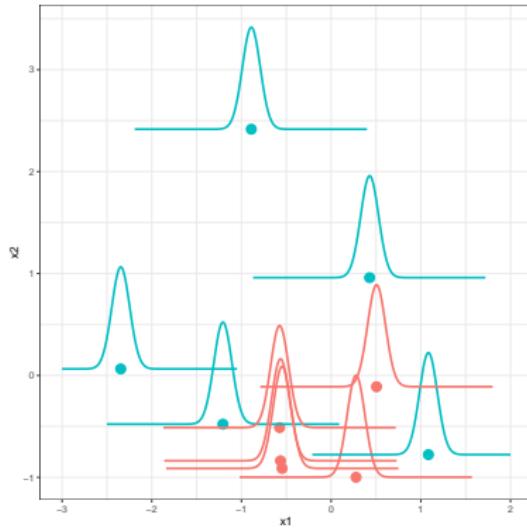
SVM HYPERPARAMETERS

Hyperparameters strongly influence the model: Polynomial kernel.



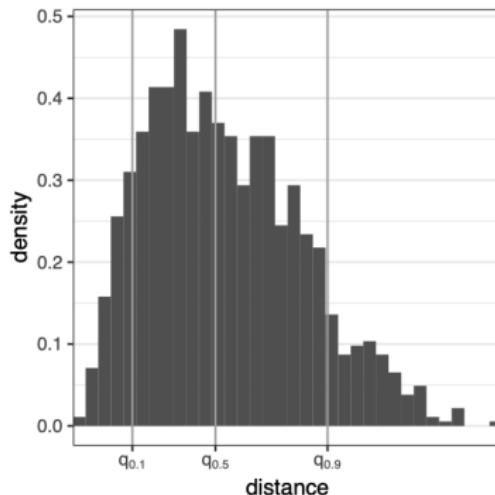
RBF SIGMA HEURISTIC

For the RBF kernel $k(\mathbf{x}, \tilde{\mathbf{x}}) = \exp\left(-\frac{\|\mathbf{x} - \tilde{\mathbf{x}}\|^2}{2\sigma^2}\right)$ a simple heuristic exists for the width hyperparameter σ^2 .



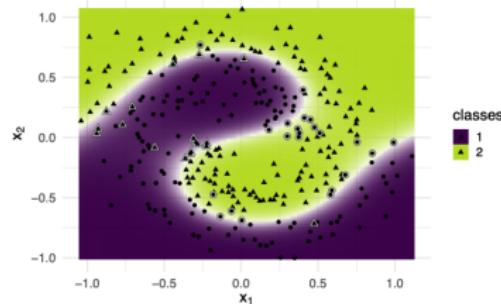
RBF SIGMA HEURISTIC

- Draw a random subset of the data.
- Compute pairwise distances $\|\mathbf{x} - \tilde{\mathbf{x}}\|$.
- Take a "central quantile" from their distribution, e.g., the median.
- This relates the kernel width to the "average distance" between points, which does make intuitive sense.



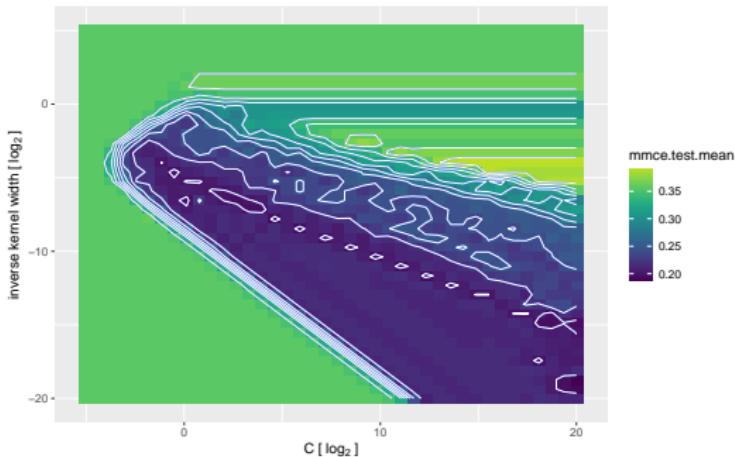
Now γ is set by estimating is inverse σ with the heuristic.

svm: kernel=radial; cost=1; gamma=0.337
Train: mmce=0.133; CV: mmce.test.mean=0.143



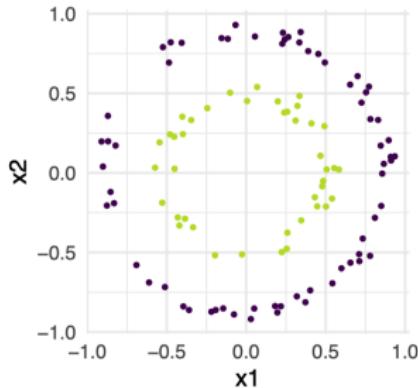
SVM HYPERPARAMETERS

- RBF-SVM parameters are often optimized on log-scale, as we want to explore large values and values close to 0.
- E.g.: $C \in [2^{-15}, 2^{15}]$, $\gamma \in [2^{-15}, 2^{15}]$
- The cross-validated performance landscape often forms a characteristics "ridge" with a larger area of equally good values.



Introduction to Machine Learning

Details on Support Vector Machines



Learning goals

- Know that SVMs are non-parameteric models
- Understand the concept of universal consistency
- Know that SVMs with an universal kernel (e.g. Gaussian kernel) are universally consistent

SVMs as Non-Parametric Models

SVMS AS NON-PARAMETRIC MODELS

- In contrast to linear models, for an SVM we do not have to decide the number of coefficients of the decision function before training.
- The number of coefficients depends on the size of the dataset, or on the number of support vectors.
- Such models are called **non-parametric**.
- The big advantage of non-parametric models is that their modeling capacity is not *a priori* restricted to a finite-dimensional subspace of a function space.
- It turns out that SVMs do even better: There exist kernels so that an SVM can model all continuous functions arbitrarily well. It is also known that the SVM learning algorithm can approximate the Bayes optimal decision function arbitrarily well in the limit of infinite data.
- This property is known as **universal consistency**.

SVMS AS NON-PARAMETRIC MODELS

Definition [Steinwart, 2002]: Let $\mathcal{X} \subset \mathbb{R}^p$ be compact. A continuous kernel $k : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ is called universal if the set of all induced functions $\sum_i \beta_i k(\mathbf{x}^{(i)}, \cdot)$ is dense in $\mathcal{C}(\mathcal{X})$; i.e., for all $g \in \mathcal{C}(\mathcal{X})$ and all $\varepsilon > 0$ there exists a function f induced by k with $\|f - g\|_\infty \leq \varepsilon$.

Example: Gaussian kernels are universal.

Theorem [simplified from Steinwart, 2002]: For compact $\mathcal{X} \subset \mathbb{R}^p$ define $C(n) = C_0 \cdot n^{q-1}$ for some $C_0 > 0$ and $0 < q < 1/p$. Fix any distribution \mathbb{P} on $\mathcal{X} \times \{\pm 1\}$ from which i.i.d. datasets \mathcal{D}_n of size n are drawn. Let h_n denote the soft-margin SVM model, trained with a universal kernel and regularization constant $C(n)$ on the data \mathcal{D}_n . Then it holds

$$\lim_{n \rightarrow \infty} \mathbb{E}[\mathcal{R}(h_n)] = \mathcal{R}^* ,$$

where \mathcal{R}^* denotes the Bayes risk.

ASYMPTOTIC PERFORMANCE

- Convergence of the risk to the Bayes risk for all distributions is called **universal consistency**.
- A universally consistent learning machine can solve all problems optimally, provided enough data.
- Parametric models are too inflexible for this property. They can model only a finite-dimensional subspace (manifold) of decision functions.
- Thus, in the limit of infinite data, they will systematically underfit.
- Universal consistency requires more than infinite-dimensional modeling power: We also need a learning rule that uses the flexibility wisely and avoids overfitting.
- The existence of universally consistent learners is one of the most exciting facts from non-parametric statistics.

ASYMPTOTIC PERFORMANCE

- Note the arbitrary positive constant C_0 in the definition of $C(n) = C_0 \cdot n^{q-1}$.
- This means that for a single fixed n , $C(n)$ can have any positive value.
- This is not a problem for the theorem since all it requires is that C changes at the right rate with n :
 - $n \cdot C(n)$ tends to infinity, which means that the relative impact of the regularizer compared to the empirical risk decays to zero, so, the risk term takes over for large n ;
 - The convergence of $n \cdot C(n)$ to infinity is slow enough to avoid overfitting (this is far from obvious, but it is in the details of the proof of the theorem).
- Importantly, since C can be arbitrary for fixed n , this theorem does not tell us which C to use for a given problem size.

Kernels on Infinite-Dimensional Vector Spaces

KERNELS ON INFINITE-DIMENSIONAL VECTOR SPACES

- Note that the input space \mathcal{X} does not need to be a finite-dimensional vector space.
- \mathcal{X} could be the set of all character strings (of unlimited length) or of graphs, or of trees.
- Such data structures are natural representations for, e.g, HTML documents.
- There are many examples of data that do not naturally come in vector form.
- Most often meaningful and cheap-to-compute kernels can be defined directly on the input data structures – they simply define a similarity measure over these data.
- SVMs (and other kernel methods) allow to learn and predict directly on these spaces.

INTRODUCTION TO MACHINE LEARNING

Advanced Risk Minimization

Multiclass Classification

Information Theory

Curse of Dimensionality

Hypothesis Space

Regularization

Linear Support Vector Machine

Nonlinear Support Vector Machine

Gaussian Processes

Boosting

Introduction to Machine Learning

The Bayesian Linear Model

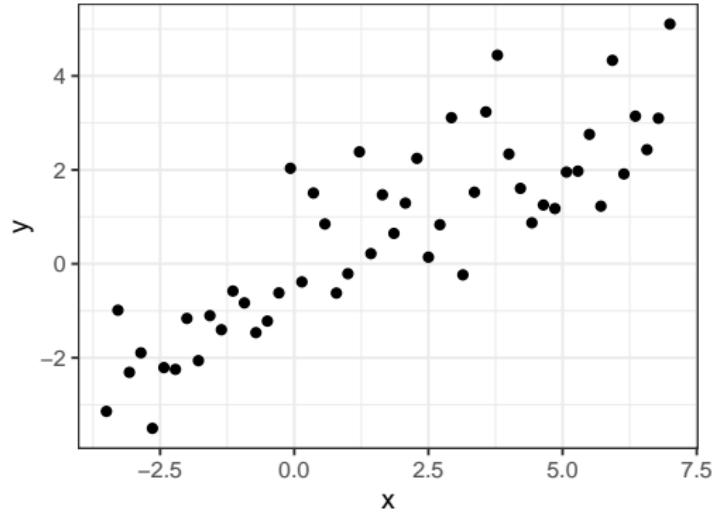


Learning goals

- XXX
- XXX

REVIEW: THE BAYESIAN LINEAR MODEL

Let $\mathcal{D} = \{(\mathbf{x}^{(1)}, y^{(1)}), \dots, (\mathbf{x}^{(n)}, y^{(n)})\}$ be a training set of i.i.d. observations from some unknown distribution.



Let $\mathbf{y} = (y^{(1)}, \dots, y^{(n)})^\top$ and $\mathbf{X} \in \mathbb{R}^{n \times p}$ be the design matrix where the i -th row contains vector $\mathbf{x}^{(i)}$.

REVIEW: THE BAYESIAN LINEAR MODEL

The linear regression model is defined as

$$y = f(\mathbf{x}) + \epsilon = \boldsymbol{\theta}^T \mathbf{x} + \epsilon$$

or on the data:

$$y^{(i)} = f(\mathbf{x}^{(i)}) + \epsilon^{(i)} = \boldsymbol{\theta}^T \mathbf{x}^{(i)} + \epsilon^{(i)}, \quad \text{for } i \in \{1, \dots, n\}$$

We now assume (from a Bayesian perspective) that also our parameter vector $\boldsymbol{\theta}$ is stochastic and follows a distribution. The observed values $y^{(i)}$ differ from the function values $f(\mathbf{x}^{(i)})$ by some additive noise, which is assumed to be i.i.d. Gaussian

$$\epsilon^{(i)} \sim \mathcal{N}(0, \sigma^2)$$

and independent of \mathbf{x} and $\boldsymbol{\theta}$.

REVIEW: THE BAYESIAN LINEAR MODEL

Let us assume we have **prior beliefs** about the parameter θ that are represented in a prior distribution $\theta \sim \mathcal{N}(\mathbf{0}, \tau^2 \mathbf{I}_p)$.

Whenever data points are observed, we update the parameters' prior distribution according to Bayes' rule

$$\underbrace{p(\theta | \mathbf{X}, \mathbf{y})}_{\text{posterior}} = \frac{\overbrace{p(\mathbf{y} | \mathbf{X}, \theta)}^{\text{likelihood}} \overbrace{q(\theta)}^{\text{prior}}}{\underbrace{p(\mathbf{y} | \mathbf{X})}_{\text{marginal}}}.$$

REVIEW: THE BAYESIAN LINEAR MODEL

The posterior distribution of the parameter θ is again normal distributed (the Gaussian family is self-conjugate):

$$\theta \mid \mathbf{X}, \mathbf{y} \sim \mathcal{N}(\sigma^{-2} \mathbf{A}^{-1} \mathbf{X}^\top \mathbf{y}, \mathbf{A}^{-1})$$

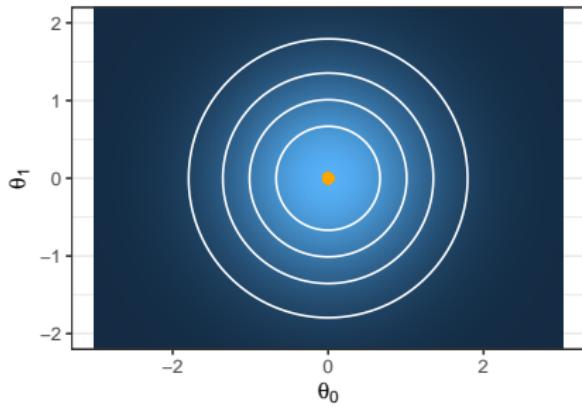
$$\text{with } \mathbf{A} := \sigma^{-2} \mathbf{X}^\top \mathbf{X} + \frac{1}{\tau^2} \mathbf{I}_p.$$

Note: If the posterior distribution $p(\theta \mid \mathbf{X}, \mathbf{y})$ are in the same probability distribution family as the prior $q(\theta)$ w.r.t. a specific likelihood function $p(\mathbf{y} \mid \mathbf{X}, \theta)$, they are called **conjugate distributions**. The prior is then called a **conjugate prior** for the likelihood.

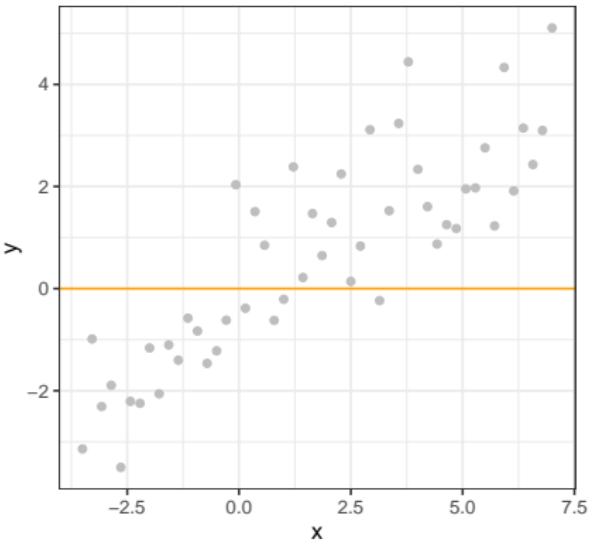
The Gaussian family is self-conjugate: Choosing a Gaussian prior for a Gaussian Likelihood ensures that the posterior is Gaussian.

REVIEW: THE BAYESIAN LINEAR MODEL

Prior $\theta \sim N(0, 1)$

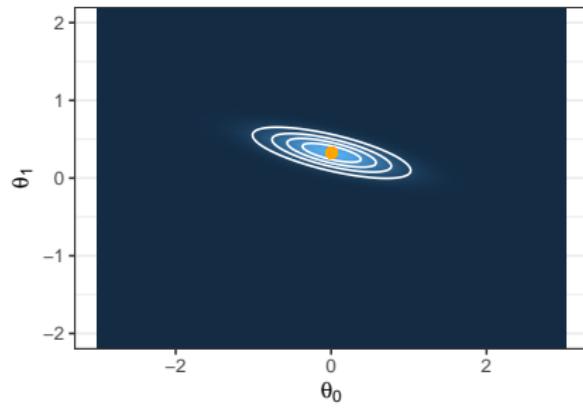


No data points observed

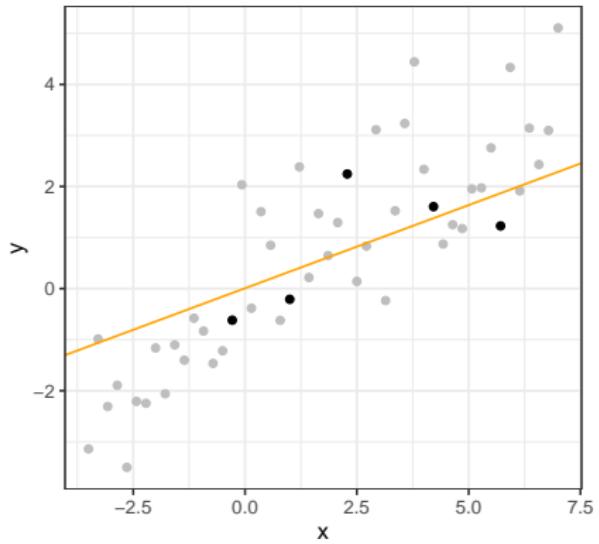


REVIEW: THE BAYESIAN LINEAR MODEL

Posterior of θ

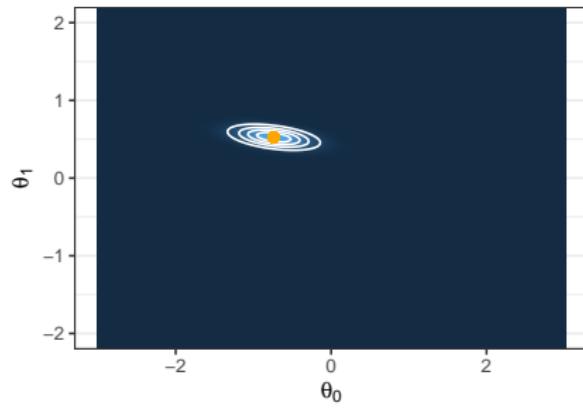


MAP after observing 5 data points

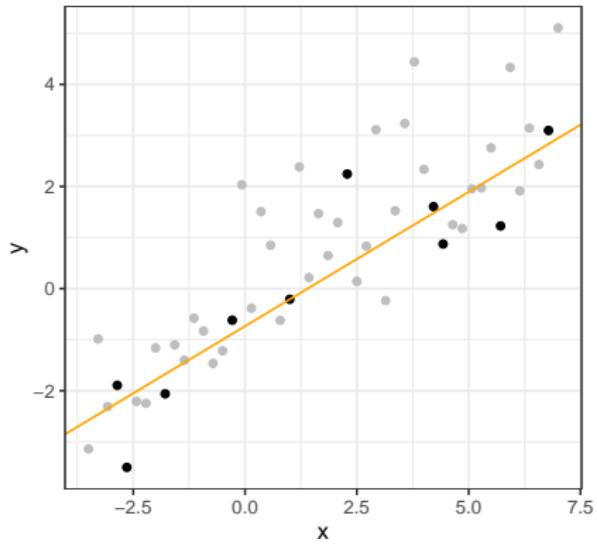


REVIEW: THE BAYESIAN LINEAR MODEL

Posterior of θ

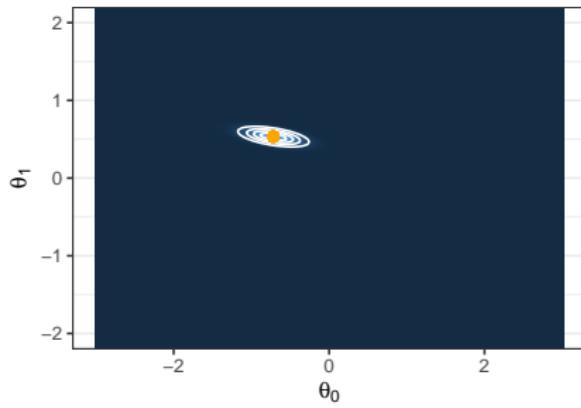


MAP after observing 10 data points

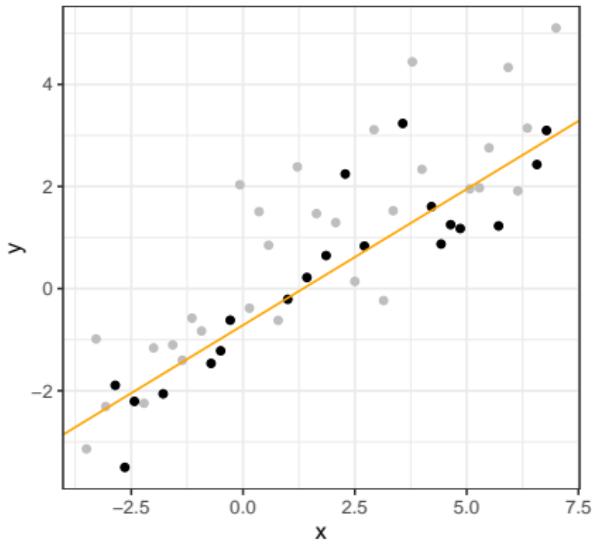


REVIEW: THE BAYESIAN LINEAR MODEL

Posterior of θ



MAP after observing 20 data points



REVIEW: THE BAYESIAN LINEAR MODEL

Proof:

We want to show that

- for a Gaussian prior on $\theta \sim \mathcal{N}(\mathbf{0}, \tau^2 \mathbf{I}_p)$
- for a Gaussian Likelihood $y | \mathbf{X}, \theta \sim \mathcal{N}(\mathbf{X}^\top \theta, \sigma^2 \mathbf{I}_n)$

the resulting posterior is Gaussian $\mathcal{N}(\sigma^{-2} \mathbf{A}^{-1} \mathbf{X}^\top \mathbf{y}, \mathbf{A}^{-1})$ with $\mathbf{A} := \sigma^{-2} \mathbf{X}^\top \mathbf{X} + \frac{1}{\tau^2} \mathbf{I}_p$.

Plugging in Bayes' rule and multiplying out yields

$$\begin{aligned} p(\theta | \mathbf{X}, \mathbf{y}) &\propto p(\mathbf{y} | \mathbf{X}, \theta) q(\theta) \propto \exp \left[-\frac{1}{2\sigma^2} (\mathbf{y} - \mathbf{X}\theta)^\top (\mathbf{y} - \mathbf{X}\theta) - \frac{1}{2\tau^2} \theta^\top \theta \right] \\ &= \exp \left[-\frac{1}{2} \left(\underbrace{\sigma^{-2} \mathbf{y}^\top \mathbf{y}}_{\text{doesn't depend on } \theta} - 2\sigma^{-2} \mathbf{y}^\top \mathbf{X}\theta + \sigma^{-2} \theta^\top \mathbf{X}^\top \mathbf{X}\theta + \tau^{-2} \theta^\top \theta \right) \right] \\ &\propto \exp \left[-\frac{1}{2} \left(\sigma^{-2} \theta^\top \mathbf{X}^\top \mathbf{X}\theta + \tau^{-2} \theta^\top \theta - 2\sigma^{-2} \mathbf{y}^\top \mathbf{X}\theta \right) \right] \\ &= \exp \left[-\frac{1}{2} \theta^\top \underbrace{\left(\sigma^{-2} \mathbf{X}^\top \mathbf{X} + \tau^{-2} \mathbf{I}_p \right)}_{:= \mathbf{A}} \theta + \cancel{\sigma^{-2} \mathbf{y}^\top \mathbf{X}\theta} \right] \end{aligned}$$

This expression resembles a normal density - except for the term in red!

REVIEW: THE BAYESIAN LINEAR MODEL

Note: We need not worry about the normalizing constant since its mere role is to convert probability functions to density functions with a total probability of one. We subtract a (not yet defined) constant c while compensating for this change by adding the respective terms (“adding 0”), emphasized in green:

$$\begin{aligned} p(\theta | \mathbf{X}, \mathbf{y}) &\propto \exp \left[-\frac{1}{2} (\theta - c)^T \mathbf{A} (\theta - c) - c^T \mathbf{A} \theta + \underbrace{\frac{1}{2} c^T \mathbf{A} c}_{\text{doesn't depend on } \theta} + \sigma^{-2} \mathbf{y}^T \mathbf{X} \theta \right] \\ &\propto \exp \left[-\frac{1}{2} (\theta - c)^T \mathbf{A} (\theta - c) - c^T \mathbf{A} \theta + \sigma^{-2} \mathbf{y}^T \mathbf{X} \theta \right] \end{aligned}$$

If we choose c such that $-c^T \mathbf{A} \theta + \sigma^{-2} \mathbf{y}^T \mathbf{X} \theta = 0$, the posterior is normal with mean c and covariance matrix \mathbf{A}^{-1} . Taking into account that \mathbf{A} is symmetric, this is if we choose

$$\begin{aligned} \sigma^{-2} \mathbf{y}^T \mathbf{X} &= c^T \mathbf{A} \\ \Leftrightarrow \sigma^{-2} \mathbf{y}^T \mathbf{X} \mathbf{A}^{-1} &= c^T \\ \Leftrightarrow c &= \sigma^{-2} \mathbf{A}^{-1} \mathbf{X}^T \mathbf{y} \end{aligned}$$

as claimed.

REVIEW: THE BAYESIAN LINEAR MODEL

Based on the posterior distribution

$$\theta | \mathbf{X}, \mathbf{y} \sim \mathcal{N}(\sigma^{-2} \mathbf{A}^{-1} \mathbf{X}^\top \mathbf{y}, \mathbf{A}^{-1})$$

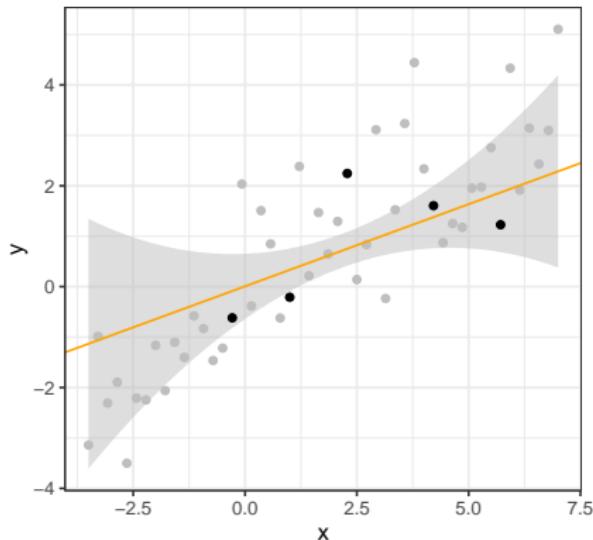
we can derive the predictive distribution for a new observations \mathbf{x}_* . The predictive distribution for the Bayesian linear model, i.e. the distribution of $\theta^\top \mathbf{x}_*$, is

$$y_* | \mathbf{X}, \mathbf{y}, \mathbf{x}_* \sim \mathcal{N}(\sigma^{-2} \mathbf{y}^\top \mathbf{X} \mathbf{A}^{-1} \mathbf{x}_*, \mathbf{x}_*^\top \mathbf{A}^{-1} \mathbf{x}_*)$$

(applying the rules for linear transformations of Gaussians).

REVIEW: THE BAYESIAN LINEAR MODEL

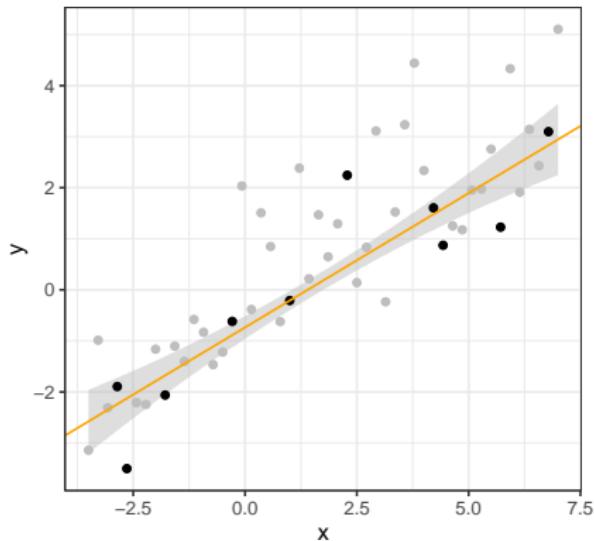
MAP after observing 5 data points



For every test input \mathbf{x}_* , we get a distribution over the prediction y_* . In particular, we get a posterior mean (orange) and a posterior variance (grey region equals \pm two times standard deviation).

REVIEW: THE BAYESIAN LINEAR MODEL

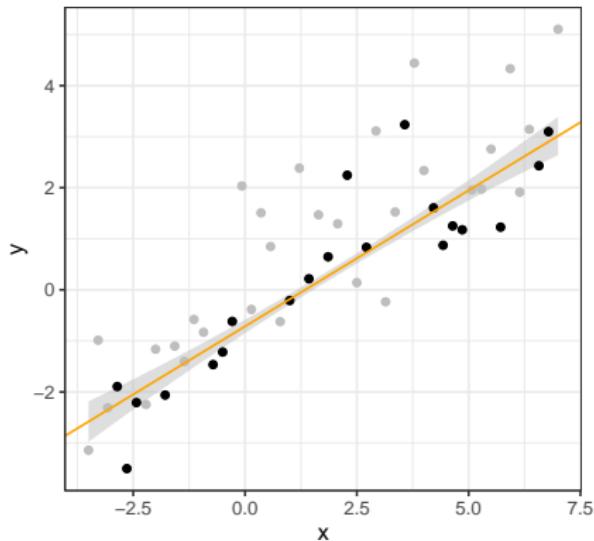
MAP after observing 10 data points



For every test input \mathbf{x}_* , we get a distribution over the prediction y_* . In particular, we get a posterior mean (orange) and a posterior variance (grey region equals \pm two times standard deviation).

REVIEW: THE BAYESIAN LINEAR MODEL

MAP after observing 20 data points



For every test input \mathbf{x}_* , we get a distribution over the prediction y_* . In particular, we get a posterior mean (orange) and a posterior variance (grey region equals \pm two times standard deviation).

SUMMARY: THE BAYESIAN LINEAR MODEL

- By switching to a Bayesian perspective, we do not only have point estimates for the parameter θ , but whole **distributions**
- From the posterior distribution of θ , we can derive a predictive distribution for $y_* = \theta^\top \mathbf{x}_*$.
- We can perform online updates: Whenever datapoints are observed, we can update the **posterior distribution** of θ

Next, we want to develop a theory for general shape functions, and not only for linear function.

Introduction to Machine Learning

Gaussian Processes

$f(x)$



$$\sim \mathcal{N}(\mu, \Sigma)$$

Learning goals

- XXX
- XXX

WEIGHT-SPACE VIEW

- Until now we considered a hypothesis space \mathcal{H} of parameterized functions $f(\mathbf{x} | \theta)$ (in particular, the space of linear functions).
- Using Bayesian inference, we derived distributions for θ after having observed data \mathcal{D} .
- Prior beliefs about the parameter are expressed via a prior distribution $q(\theta)$, which is updated according to Bayes' rule

$$\underbrace{p(\theta | \mathbf{X}, \mathbf{y})}_{\text{posterior}} = \frac{\overbrace{p(\mathbf{y} | \mathbf{X}, \theta)}^{\text{likelihood}} \overbrace{q(\theta)}^{\text{prior}}}{\underbrace{p(\mathbf{y} | \mathbf{X})}_{\text{marginal}}}.$$

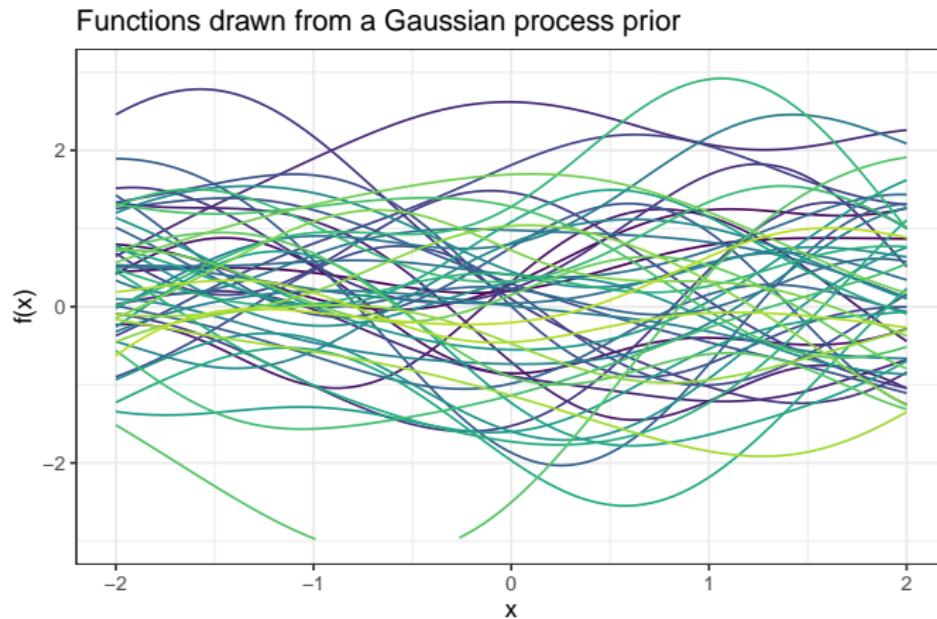
FUNCTION-SPACE VIEW

Let us change our point of view:

- Instead of “searching” for a parameter θ in the parameter space, we directly search in a space of “allowed” functions \mathcal{H} .
- We still use Bayesian inference, but instead specifying a prior distribution over a parameter, we specify a prior distribution **over functions** and update it according to the data points we have observed.

FUNCTION-SPACE VIEW

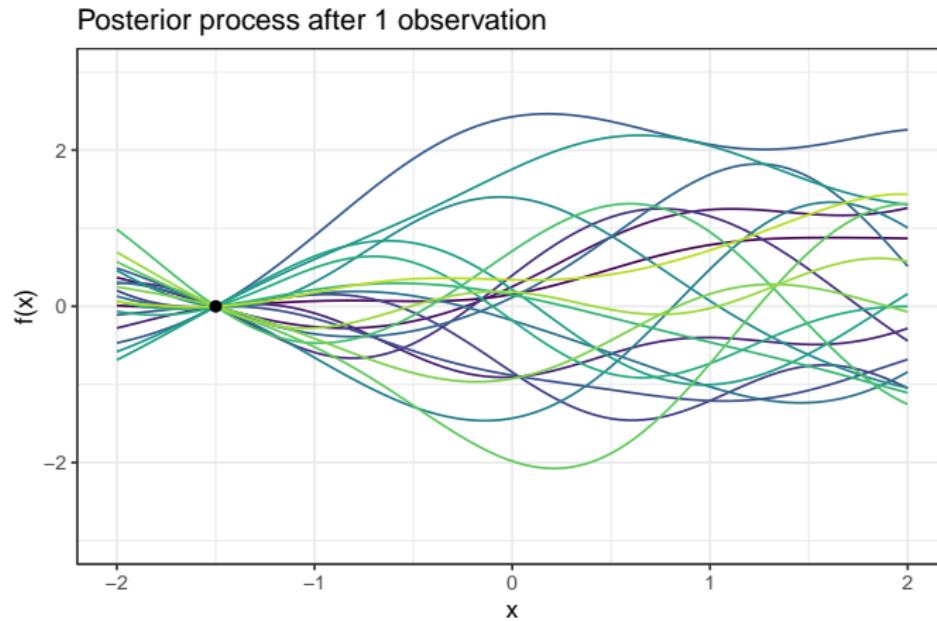
Intuitively, imagine we could draw a huge number of functions from some prior distribution over functions (*).



(*) We will see in a minute how distributions over functions can be specified.

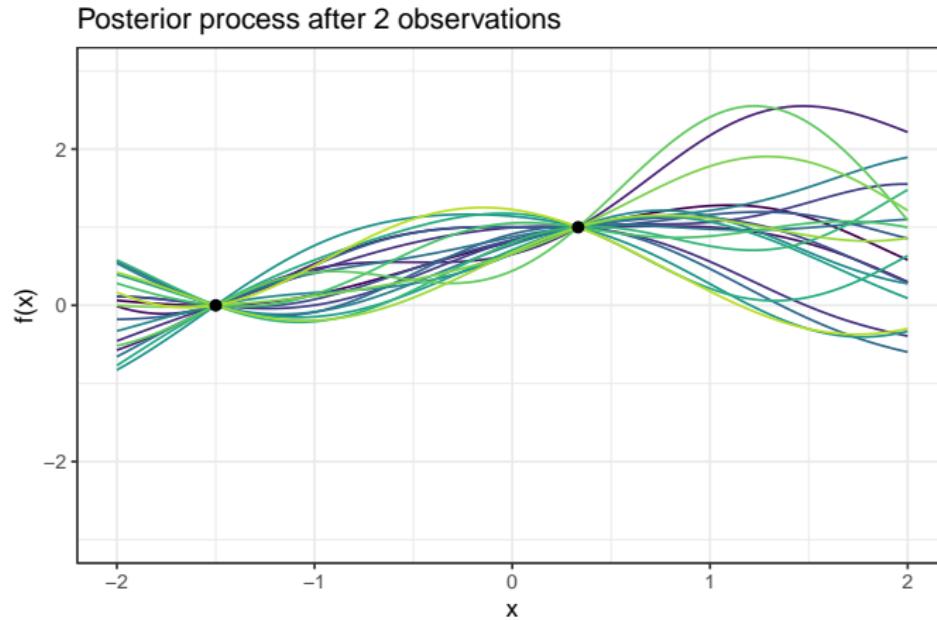
FUNCTION-SPACE VIEW

After observing some data points, we are only allowed to sample those functions, that are consistent with the data.



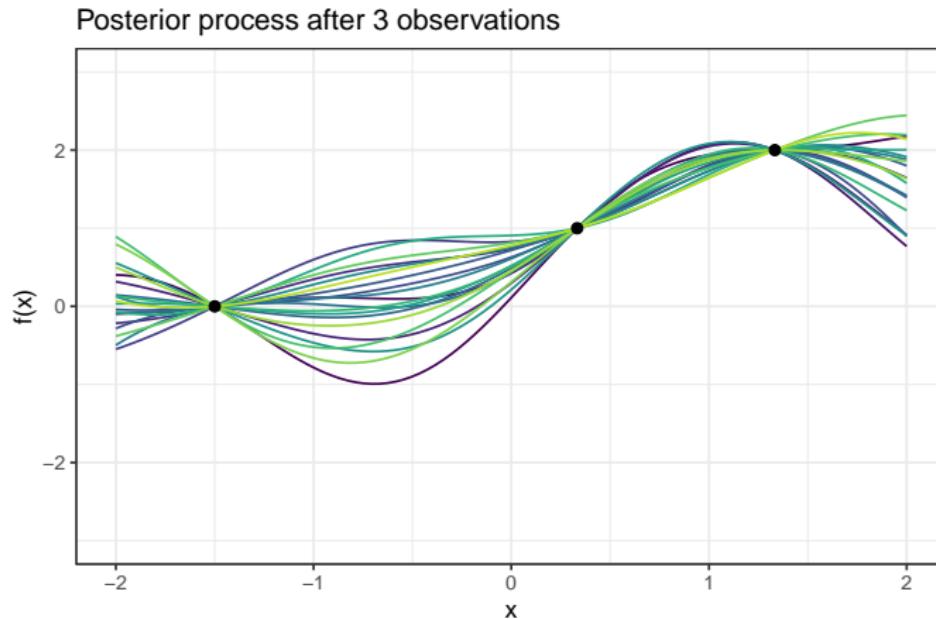
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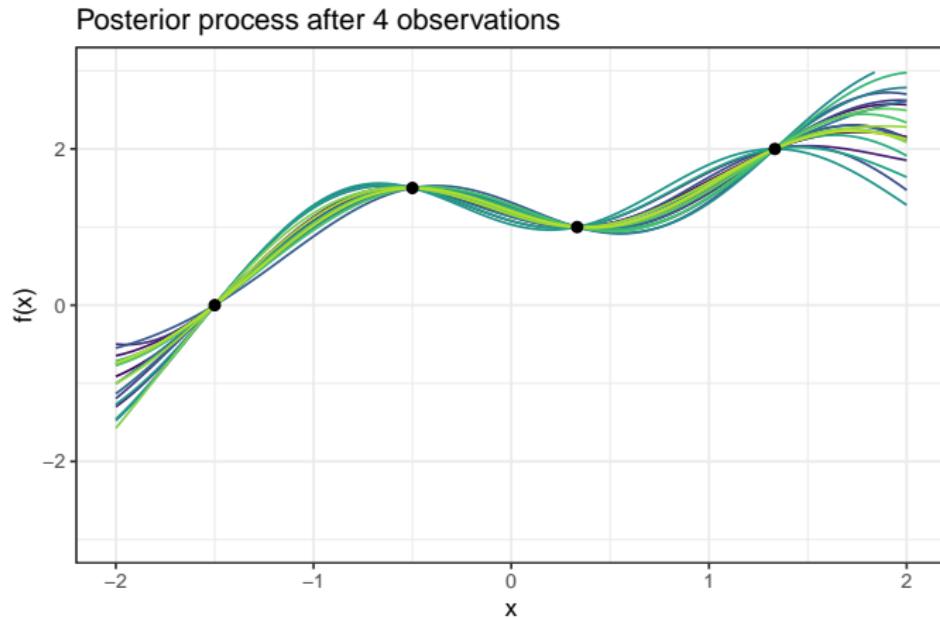
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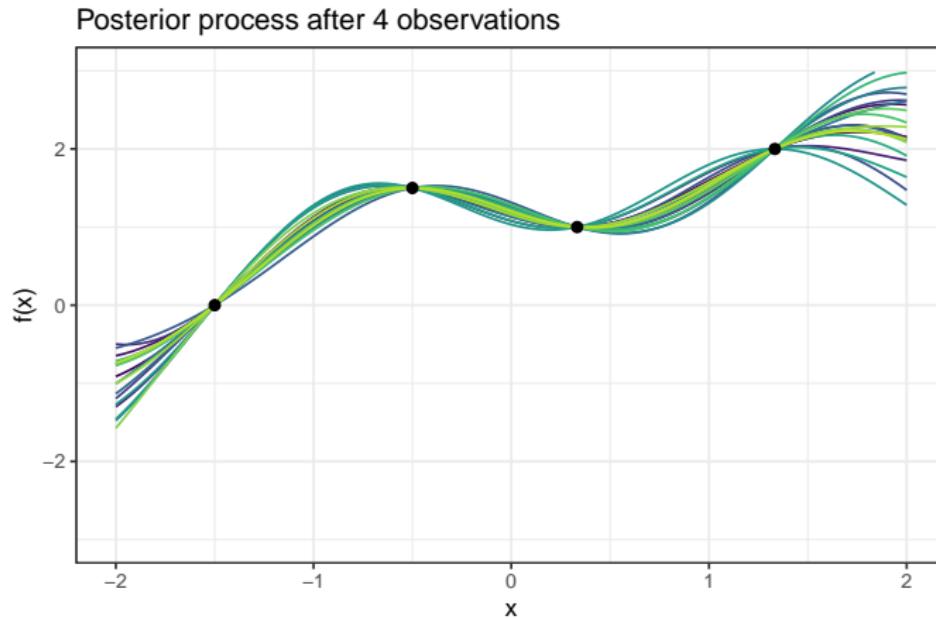
FUNCTION-SPACE VIEW

As we observe more and more data points, the variety of functions consistent with the data shrinks.



FUNCTION-SPACE VIEW

Intuitively, there is something like “mean” and a “variance” of a distribution over functions.



WEIGHT-SPACE VS. FUNCTION-SPACE VIEW

Weight-Space View

Parameterize functions

$$\text{Example: } f(\mathbf{x} \mid \boldsymbol{\theta}) = \boldsymbol{\theta}^\top \mathbf{x}$$

Define distributions on $\boldsymbol{\theta}$

Function-Space View

Define distributions on f

Inference in parameter space Θ Inference in function space \mathcal{H}

Next, we will see how we can define distributions over functions mathematically.

Distributions on Functions

DISCRETE FUNCTIONS

For simplicity, let us consider functions with finite domains first.

Let $\mathcal{X} = \{\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(n)}\}$ be a finite set of elements and \mathcal{H} the set of all functions from $\mathcal{X} \rightarrow \mathbb{R}$.

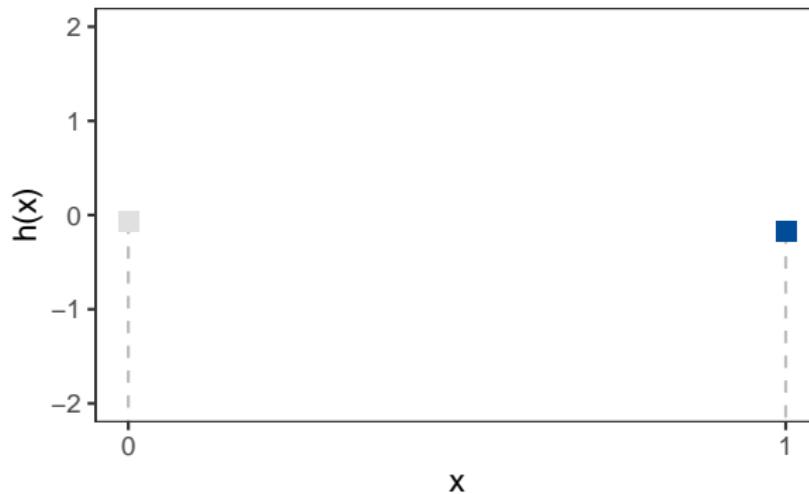
Since the domain of any $h(\cdot) \in \mathcal{H}$ has only n elements, we can represent the function $h(\cdot)$ compactly as a n -dimensional vector

$$\mathbf{h} = [h(\mathbf{x}^{(1)}), \dots, h(\mathbf{x}^{(n)})].$$

DISCRETE FUNCTIONS

Example 1: Let us consider $h : \mathcal{X} \rightarrow \mathcal{Y}$ where the input space consists of **two** points $\mathcal{X} = \{0, 1\}$.

Examples for functions that live in this space:



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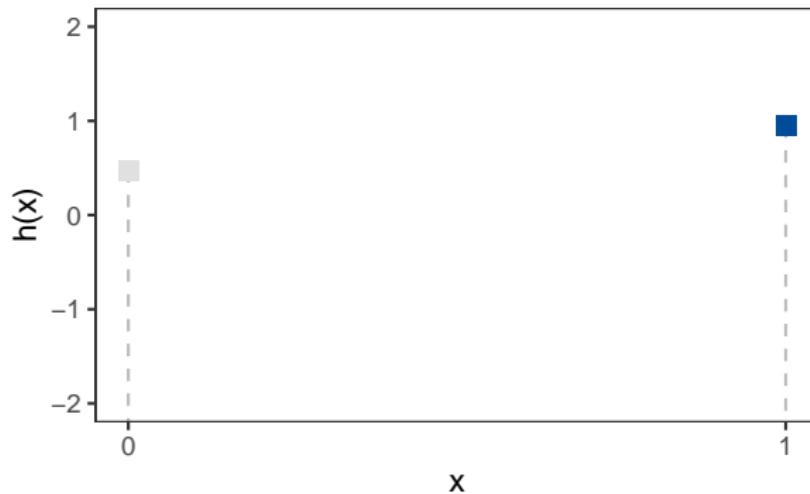
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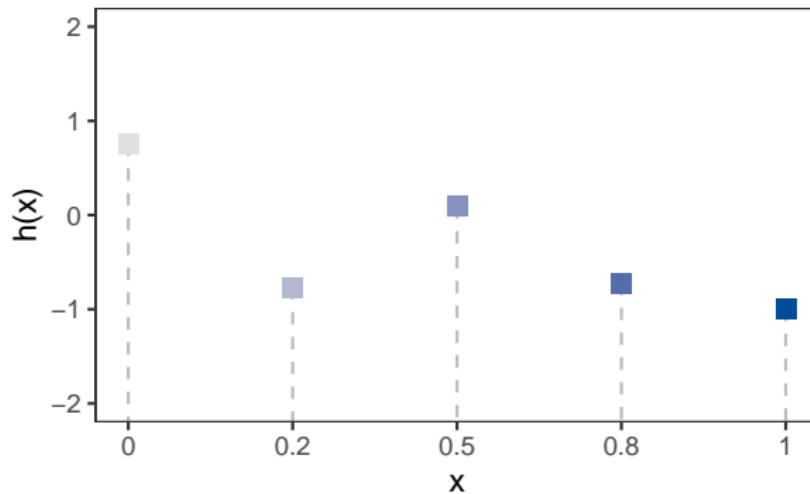
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Example 2: Let us consider $h : \mathcal{X} \rightarrow \mathcal{Y}$ where the input space consists of **five** points $\mathcal{X} = \{0, 0.25, 0.5, 0.75, 1\}$.

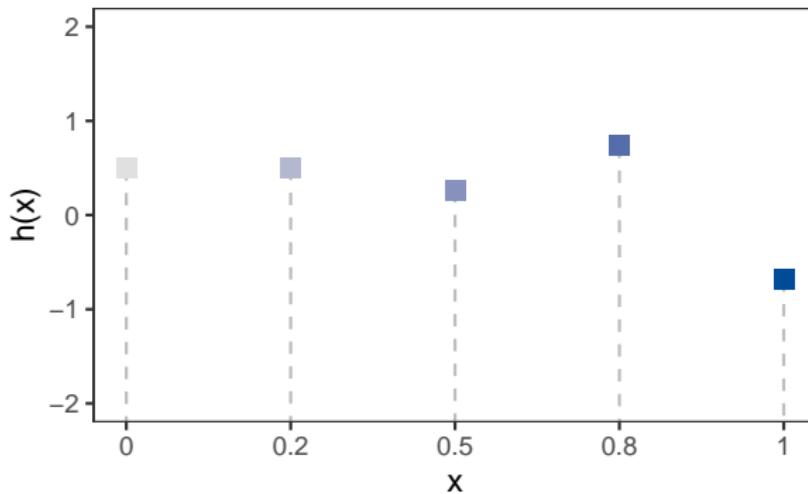
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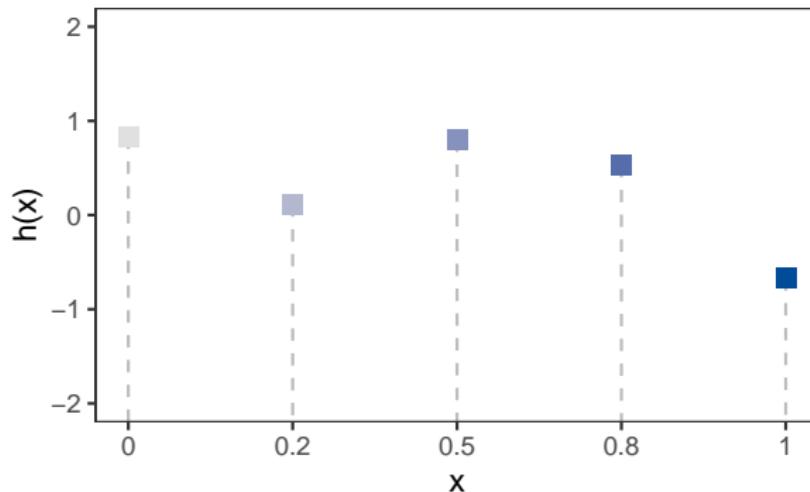
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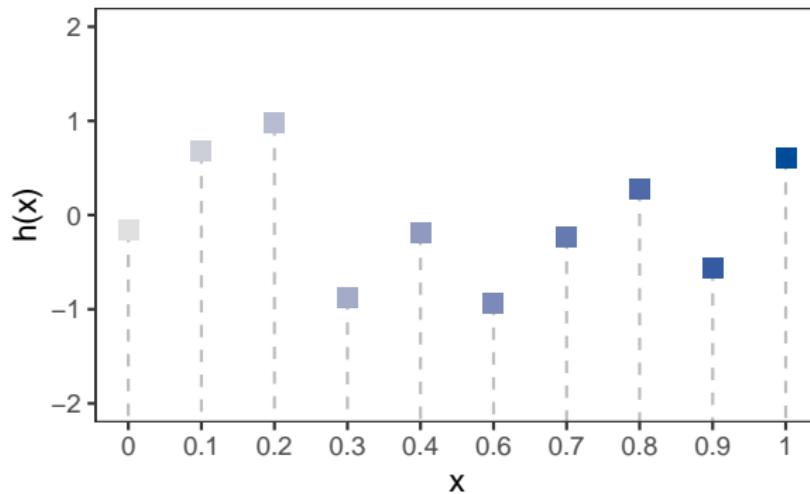
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Example 3: Let us consider $h : \mathcal{X} \rightarrow \mathcal{Y}$ where the input space consists of **ten** points.

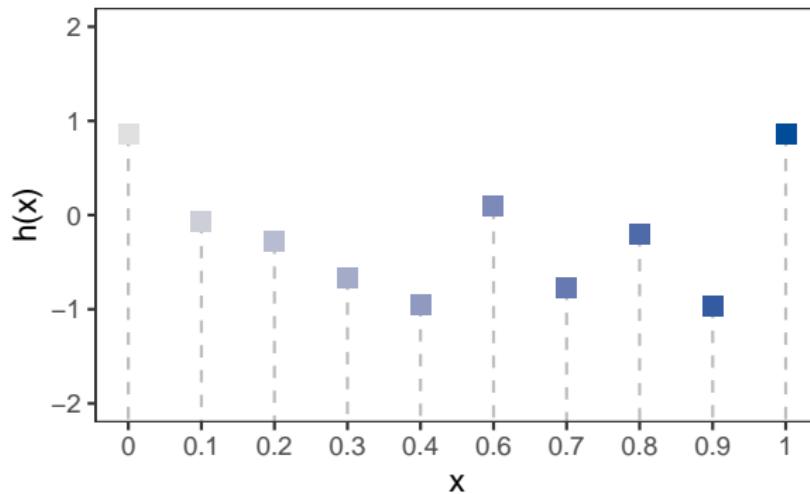
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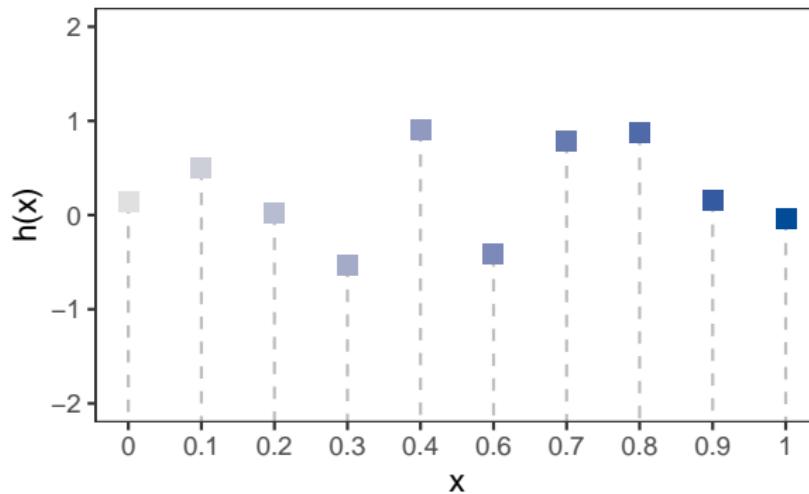
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Examples for functions that live in this space:



DISTRIBUTIONS ON DISCRETE FUNCTIONS

One natural way to specify a probability function on discrete function $h \in \mathcal{H}$ is to use the vector representation

$$\mathbf{h} = [h(\mathbf{x}^{(1)}), h(\mathbf{x}^{(2)}), \dots, h(\mathbf{x}^{(n)})]$$

of the function.

Let us see \mathbf{h} as a n -dimensional random variable. We will further assume the following normal distribution:

$$\mathbf{h} \sim \mathcal{N}(\mathbf{m}, \mathbf{K}).$$

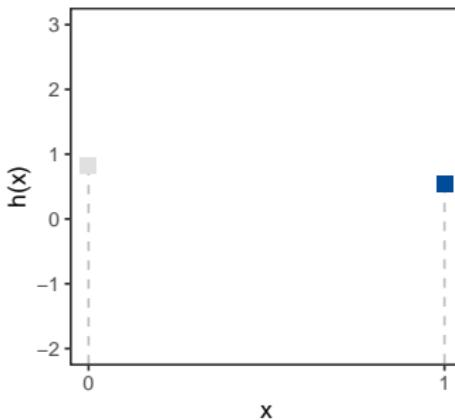
Note: For now, we set $\mathbf{m} = \mathbf{0}$ and take the covariance matrix \mathbf{K} as given. We will see later how they are chosen / estimated.

DISCRETE FUNCTIONS

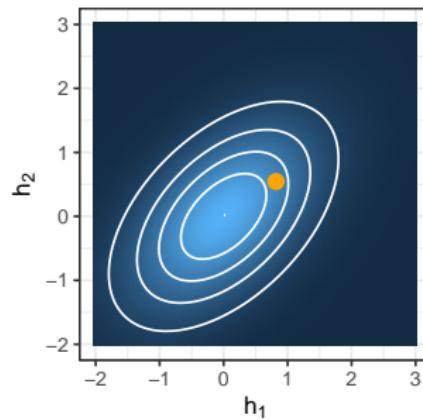
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$$\mathbf{h} = [h(1), h(2)] \sim \mathcal{N}(\mathbf{m}, \mathbf{K})$$

Sample Function 1, n = 2



Density of a 2-D Gaussian

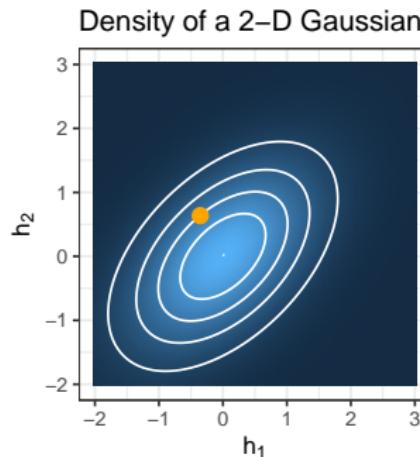
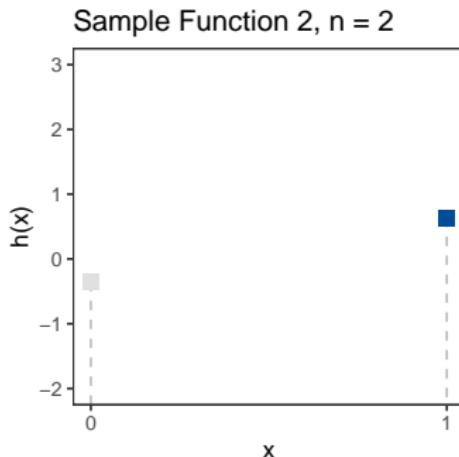


In this example, $m = (0, 0)$ and $K = \begin{pmatrix} 1 & 0.5 \\ 0.5 & 1 \end{pmatrix}$.

DISCRETE FUNCTIONS

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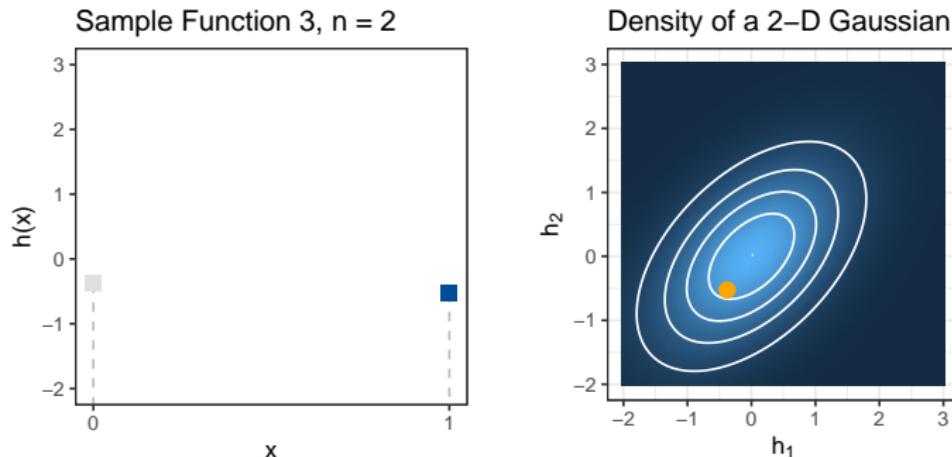


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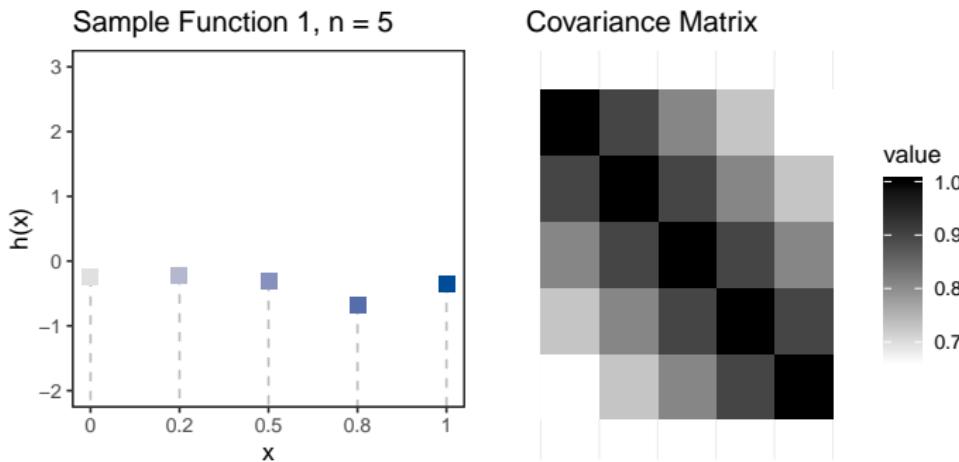


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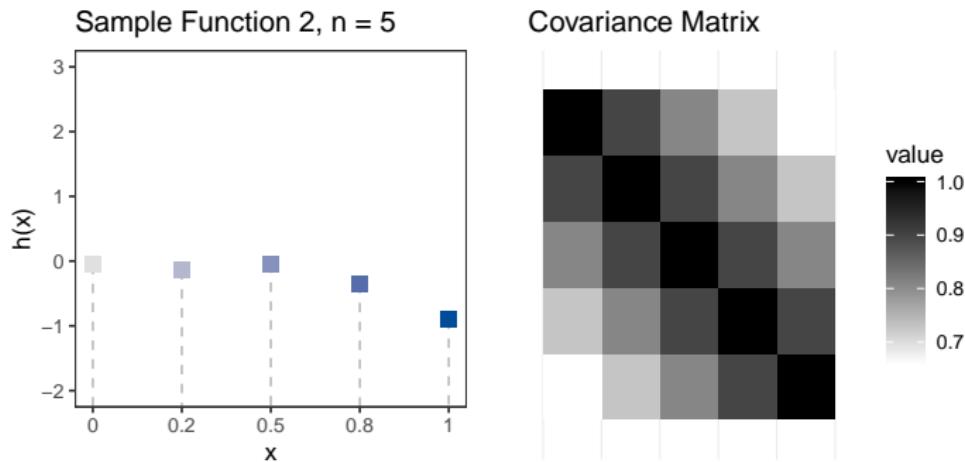
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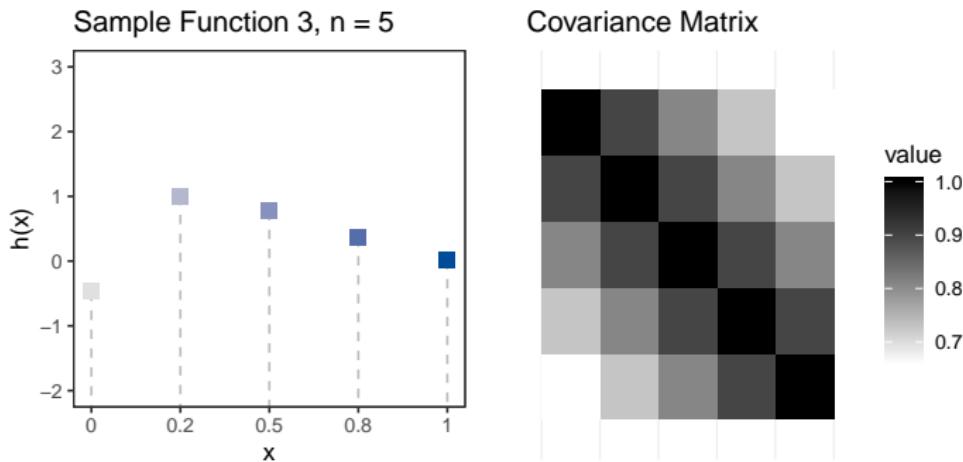
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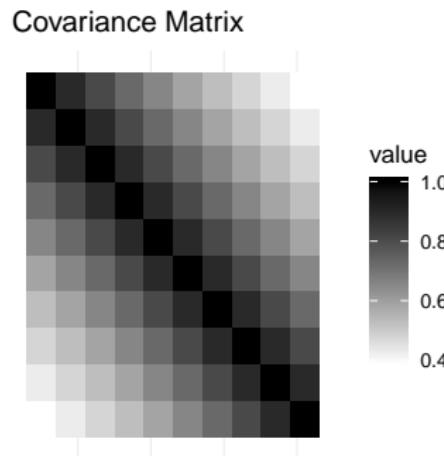
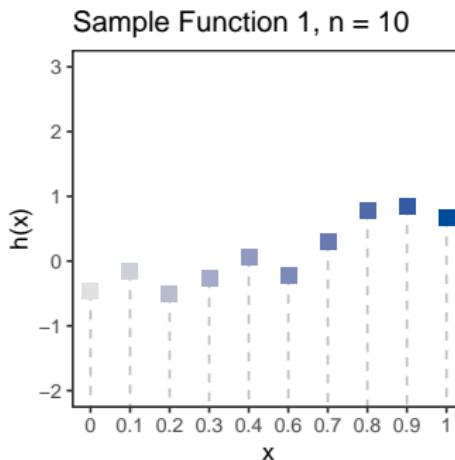
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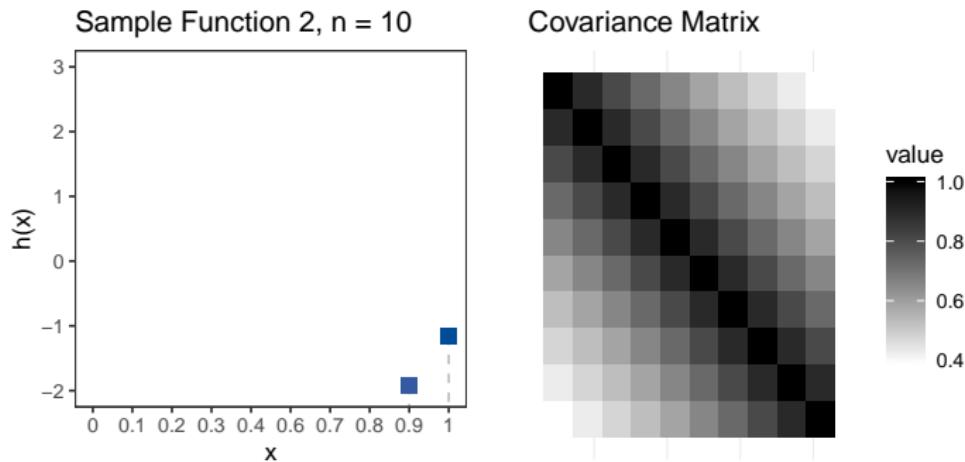
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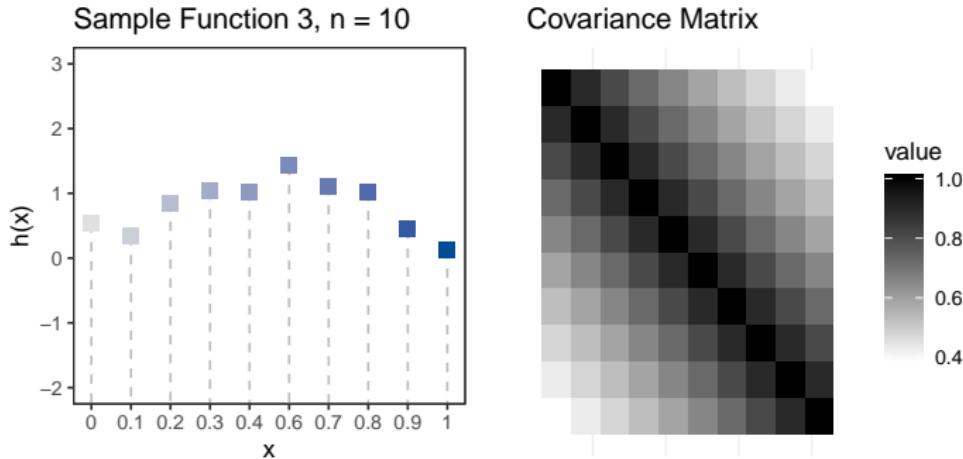
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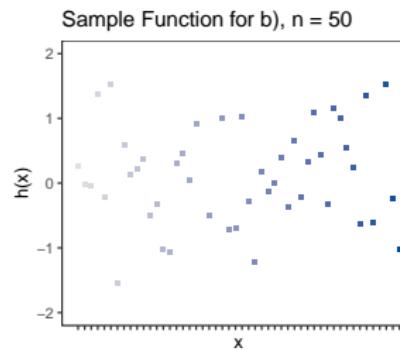
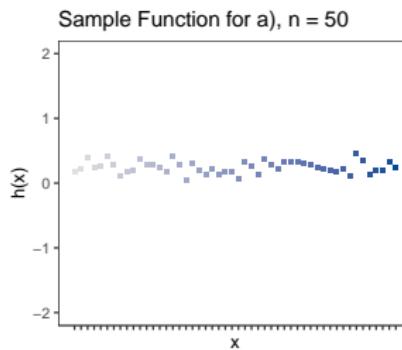


ROLE OF THE COVARIANCE FUNCTION

Note that the covariance controls the “shape” of the drawn function.

Consider two extreme cases where function values are

- a) strongly correlated: $\mathbf{K} = \begin{pmatrix} 1 & 0.99 & \dots & 0.99 \\ 0.99 & 1 & \dots & 0.99 \\ 0.99 & 0.99 & \ddots & 0.99 \\ 0.99 & \dots & 0.99 & 1 \end{pmatrix}$
- b) uncorrelated: $\mathbf{K} = \mathbf{I}$



ROLE OF THE COVARIANCE FUNCTION

- “Meaningful” functions (on a numeric space \mathcal{X}) may be characterized by a spatial property:

If two points $\mathbf{x}^{(i)}, \mathbf{x}^{(j)}$ are close in \mathcal{X} -space, their function values $f(\mathbf{x}^{(i)}), f(\mathbf{x}^{(j)})$ should be close in \mathcal{Y} -space.

In other words: If they are close in \mathcal{X} -space, their functions values should be **correlated!**

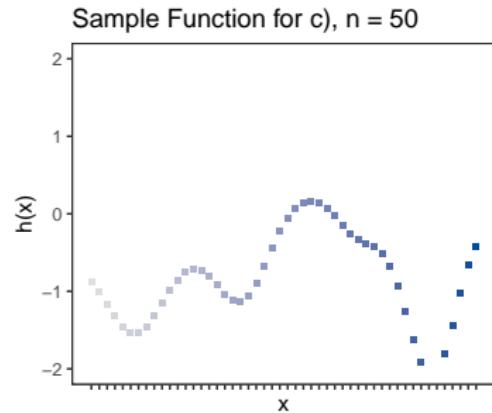
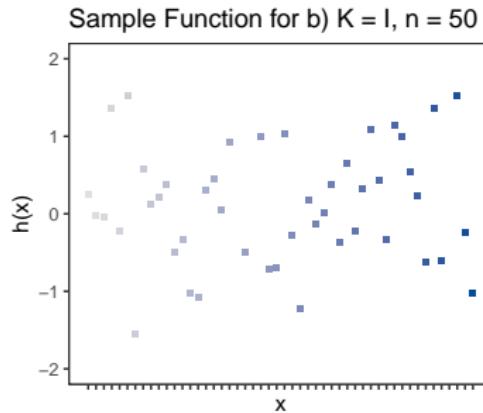
- We can enforce that by choosing a covariance function with

K_{ij} high, if $\mathbf{x}^{(i)}, \mathbf{x}^{(j)}$ close.

ROLE OF THE COVARIANCE FUNCTION

- We can compute the entries of the covariance matrix by a function that is based on the distance between $\mathbf{x}^{(i)}, \mathbf{x}^{(j)}$, for example:

c) Spatial correlation: $K_{ij} = k(\mathbf{x}^{(i)}, \mathbf{x}^{(j)}) = \exp\left(-\frac{1}{2}\left|\mathbf{x}^{(i)} - \mathbf{x}^{(j)}\right|^2\right)$



Note: $k(\cdot, \cdot)$ is known as the **covariance function** or **kernel**. It will be studied in more detail later on.

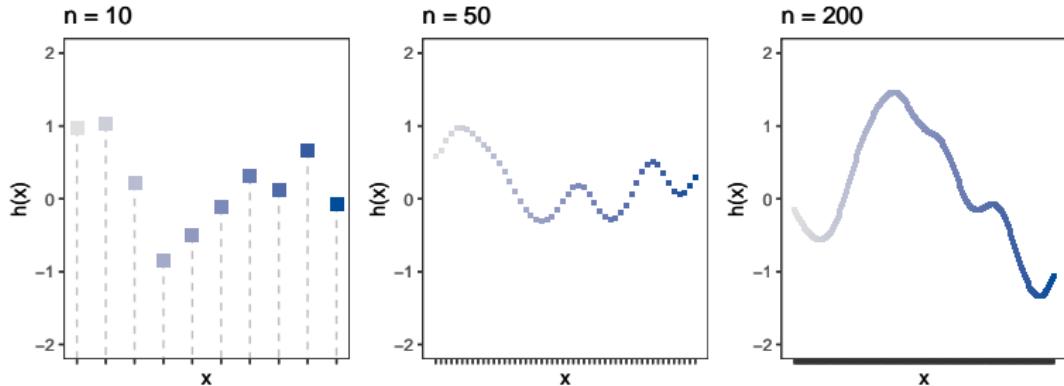
Gaussian Processes

FROM DISCRETE TO CONTINUOUS FUNCTIONS

- We defined distributions on functions with discrete domain by defining a Gaussian on the vector of the respective function values

$$\mathbf{h} = [h(\mathbf{x}^{(1)}), h(\mathbf{x}^{(2)}), \dots, h(\mathbf{x}^{(n)})] \sim \mathcal{N}(\mathbf{m}, \mathbf{K})$$

- We can do this for $n \rightarrow \infty$ (as “granular” as we want)



FROM DISCRETE TO CONTINUOUS FUNCTIONS

- No matter how large n is, we are still considering a function over a discrete domain.
- How can we extend our definition to functions with **continuous domain** $\mathcal{X} \subset \mathbb{R}$?

GAUSSIAN PROCESSES: INTUITION

- Intuitively, a function f drawn from **Gaussian process** can be understood as an “infinite” long Gaussian random vector.
- It is unclear how to handle an “infinite” long Gaussian random vector!



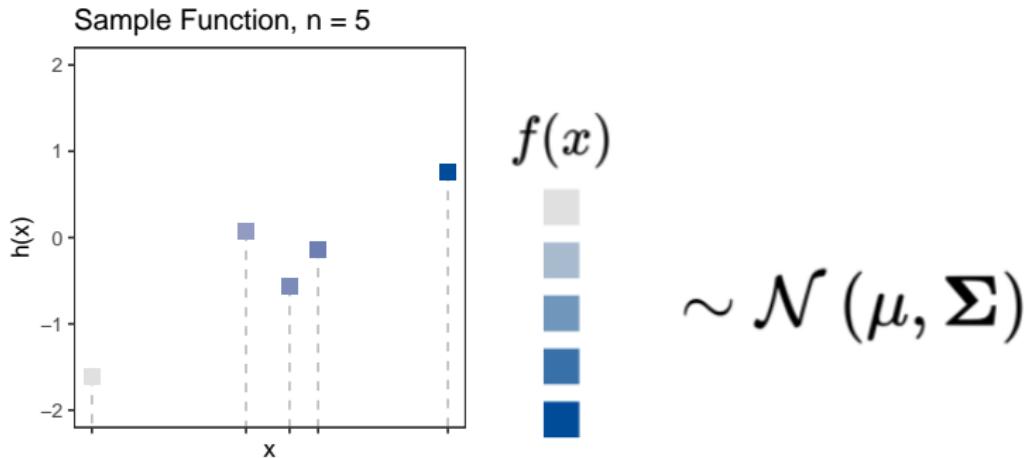
GAUSSIAN PROCESSES: INTUITION

- Thus, it is required that for **any finite set** of inputs $\{\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(n)}\} \subset \mathcal{X}$, the vector \mathbf{f} has a Gaussian distribution

$$\mathbf{f} = \left[f(\mathbf{x}^{(1)}), \dots, f(\mathbf{x}^{(n)}) \right] \sim \mathcal{N}(\mathbf{m}, \mathbf{K}),$$

with \mathbf{m} and \mathbf{K} being calculated by a mean function $m(\cdot)$ / covariance function $k(\cdot, \cdot)$.

- This property is called **Marginalization Property**.



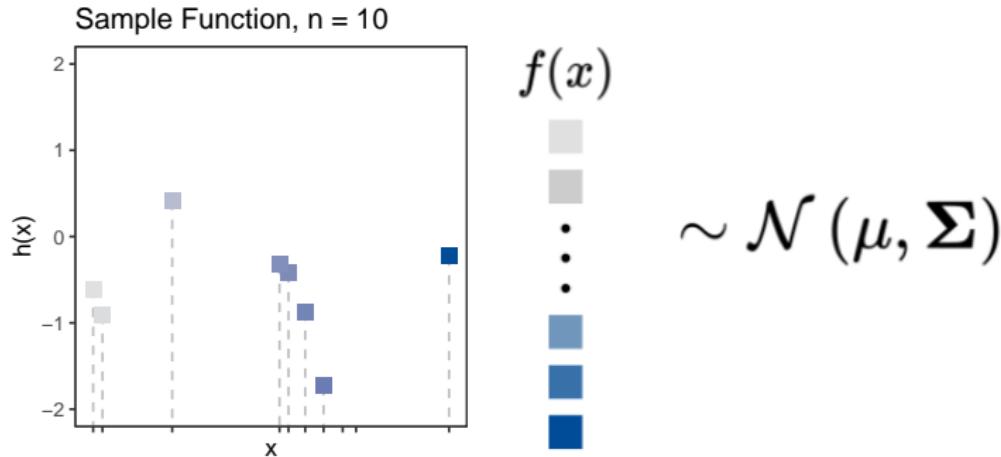
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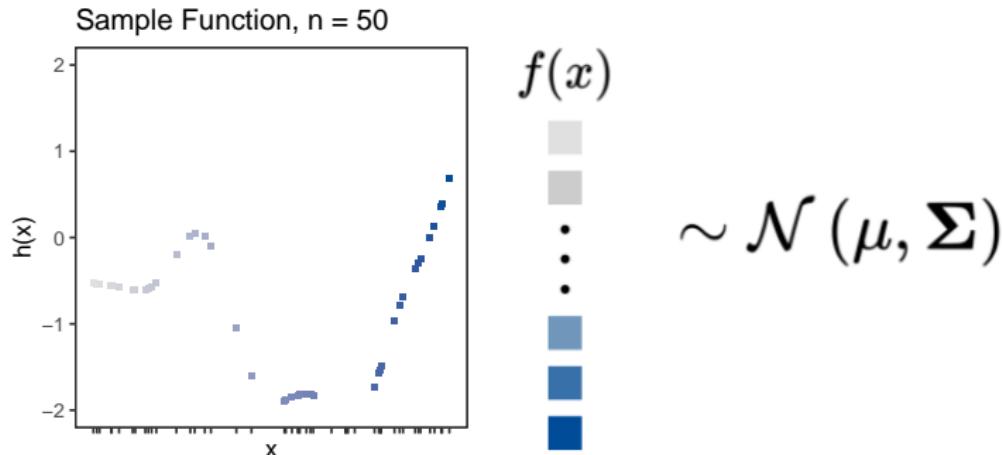
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GAUSSIAN PROCESSES

This intuitive explanation is formally defined as follows:

A function $f(\mathbf{x})$ is generated by a GP $\mathcal{GP}(m(\mathbf{x}), k(\mathbf{x}, \mathbf{x}'))$ if for **any finite** set of inputs $\{\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(n)}\}$, the associated vector of function values $\mathbf{f} = (f(\mathbf{x}^{(1)}), \dots, f(\mathbf{x}^{(n)}))$ has a Gaussian distribution

$$\mathbf{f} = \left[f\left(\mathbf{x}^{(1)}\right), \dots, f\left(\mathbf{x}^{(n)}\right) \right] \sim \mathcal{N}(\mathbf{m}, \mathbf{K}),$$

with

$$\mathbf{m} := \left(m\left(\mathbf{x}^{(i)}\right) \right)_i, \quad \mathbf{K} := \left(k\left(\mathbf{x}^{(i)}, \mathbf{x}^{(j)}\right) \right)_{i,j},$$

where $m(\mathbf{x})$ is called mean function and $k(\mathbf{x}, \mathbf{x}')$ is called covariance function.

GAUSSIAN PROCESSES

A GP is thus **completely specified** by its mean and covariance function

$$\begin{aligned} m(\mathbf{x}) &= \mathbb{E}[f(\mathbf{x})] \\ k(\mathbf{x}, \mathbf{x}') &= \mathbb{E}\left[(f(\mathbf{x}) - \mathbb{E}[f(\mathbf{x})]) (f(\mathbf{x}') - \mathbb{E}[f(\mathbf{x}')]) \right] \end{aligned}$$

Note: For now, we assume $m(\mathbf{x}) \equiv 0$. This is not necessarily a drastic limitation - thus it is common to consider GPs with a zero mean function.

SAMPLING FROM A GAUSSIAN PROCESS PRIOR

We can draw functions from a Gaussian process prior. Let us consider $f(\mathbf{x}) \sim \mathcal{GP}(0, k(\mathbf{x}, \mathbf{x}'))$ with the squared exponential covariance function (*)

$$k(\mathbf{x}, \mathbf{x}') = \exp\left(-\frac{1}{2\ell^2}\|\mathbf{x} - \mathbf{x}'\|^2\right), \quad \ell = 1.$$

This specifies the Gaussian process completely.

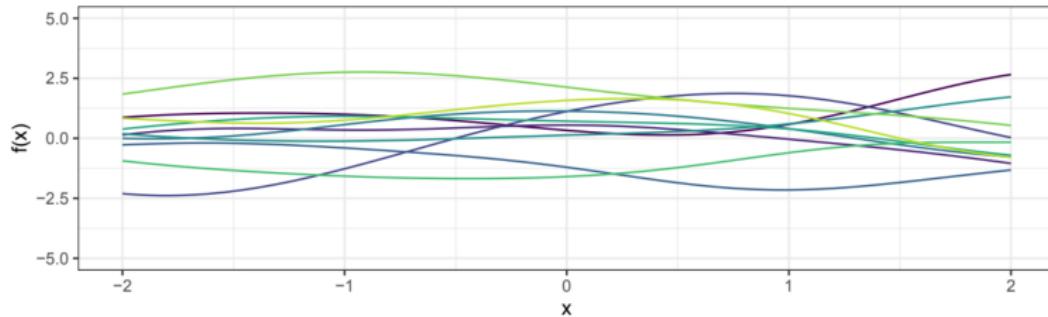
(*) We will talk later about different choices of covariance functions.

SAMPLING FROM A GAUSSIAN PROCESS PRIOR

To visualize a sample function, we

- choose a high number n (equidistant) points $\{\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(n)}\}$
- compute the corresponding covariance matrix $\mathbf{K} = (k(\mathbf{x}^{(i)}, \mathbf{x}^{(j)}))_{i,j}$ by plugging in all pairs $\mathbf{x}^{(i)}, \mathbf{x}^{(j)}$
- sample from a Gaussian $\mathbf{f} \sim \mathcal{N}(\mathbf{0}, \mathbf{K})$.

We draw 10 times from the Gaussian, to get 10 different samples.



Since we specified the mean function to be zero $m(\mathbf{x}) \equiv 0$, the drawn functions have zero mean.

Gaussian Processes as Indexed Family

GAUSSIAN PROCESSES AS AN INDEXED FAMILY

A Gaussian process is a special case of a **stochastic process** which is defined as a collection of random variables indexed by some index set (also called an **indexed family**). What does it mean?

An **indexed family** is a mathematical function (or “rule”) to map indices $t \in T$ to objects in \mathcal{S} .

Definition

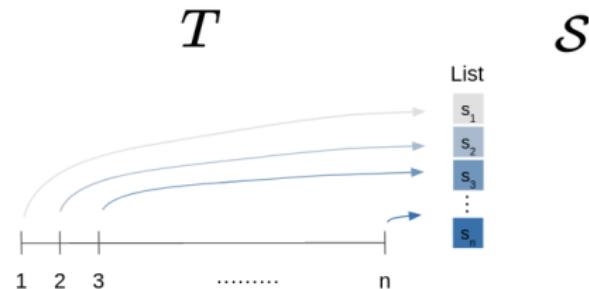
A **family of elements in \mathcal{S} indexed by T** (indexed family) is a surjective function

$$\begin{aligned} s : T &\rightarrow \mathcal{S} \\ t &\mapsto s_t = s(t) \end{aligned}$$

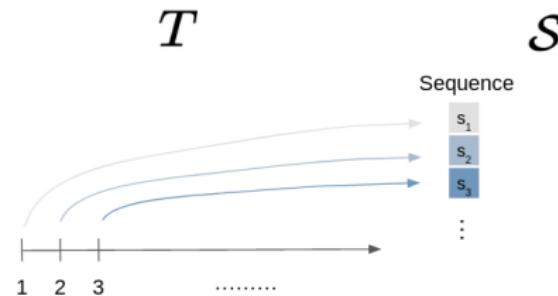
INDEXED FAMILY

Some simple examples for indexed families are:

- finite sequences (lists):
 $T = \{1, 2, \dots, n\}$ and
 $(s_t)_{t \in T} \in \mathbb{R}$



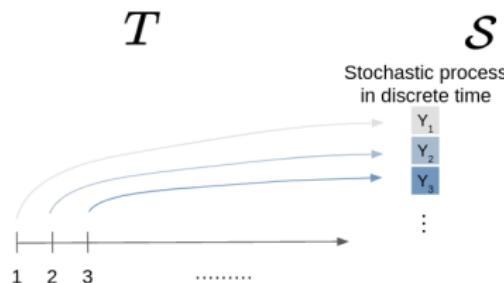
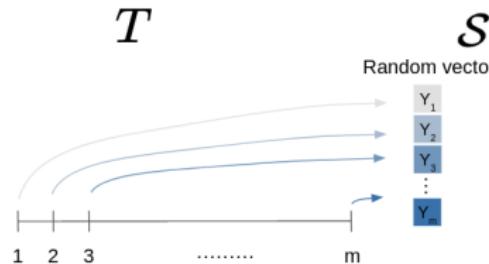
- infinite sequences:
 $T = \mathbb{N}$ and $(s_t)_{t \in T} \in \mathbb{R}$



INDEXED FAMILY

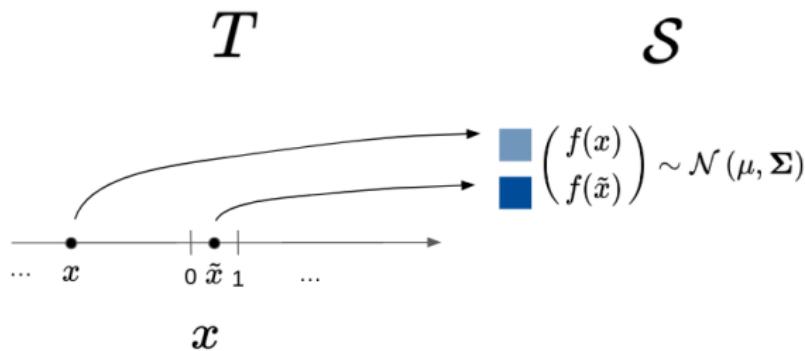
But the indexed set \mathcal{S} can be something more complicated, for example functions or **random variables** (RV):

- $T = \{1, \dots, m\}$, Y_t 's are RVs: Indexed family is a random vector.
- $T = \{1, \dots, m\}$, Y_t 's are RVs: Indexed family is a stochastic process in discrete time
- $T = \mathbb{Z}^2$, Y_t 's are RVs: Indexed family is a 2D-random walk.



INDEXED FAMILY

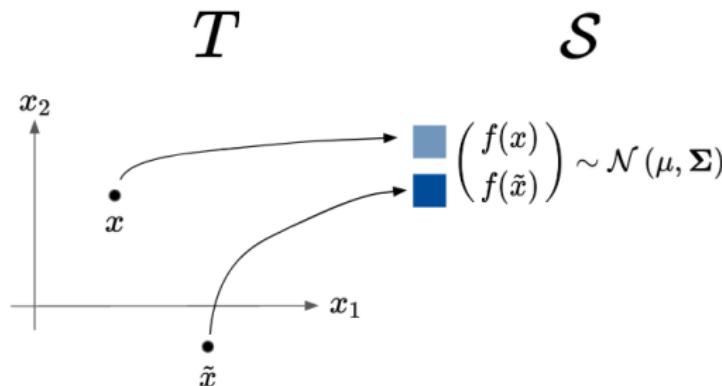
- A Gaussian process is also an indexed family, where the random variables $f(\mathbf{x})$ are indexed by the input values $\mathbf{x} \in \mathcal{X}$.
- Their special feature: Any indexed (finite) random vector has a multivariate Gaussian distribution (which comes with all the nice properties of Gaussianity!).



Visualization for a one-dimensional \mathcal{X} .

INDEXED FAMILY

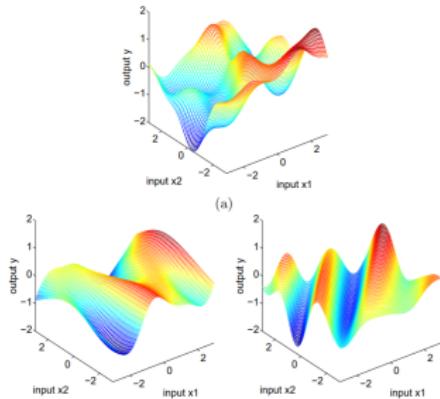
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Visualization for a two-dimensional \mathcal{X} .

Introduction to Machine Learning

Covariance Functions for GPs



Learning goals

- XXX
- XXX

COVARIANCE FUNCTION OF A GP

The marginalization property of the Gaussian process implies that for any finite set of input values, the corresponding vector of function values is Gaussian:

$$\mathbf{f} = \left[f(\mathbf{x}^{(1)}), \dots, f(\mathbf{x}^{(n)}) \right] \sim \mathcal{N}(\mathbf{m}, \mathbf{K}),$$

- The covariance matrix \mathbf{K} is constructed based on the chosen inputs $\{\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(n)}\}$.
- Entry K_{ij} is computed by $k(\mathbf{x}^{(i)}, \mathbf{x}^{(j)})$.
- Technically, for **every** choice of inputs $\{\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(n)}\}$, \mathbf{K} needs to be positive semi-definite in order to be a valid covariance matrix.
- A function $k(., .)$ satisfying this property is called **positive definite**.

COVARIANCE FUNCTION OF A GP

- Recall, the purpose of the covariance function is to control to which degree the following is fulfilled:

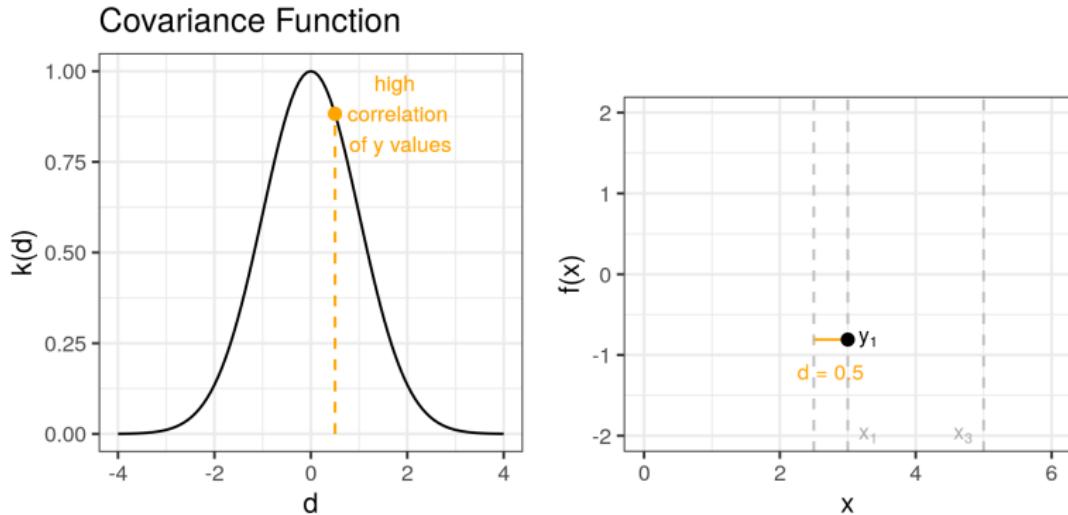
If two points $\mathbf{x}^{(i)}, \mathbf{x}^{(j)}$ are close in \mathcal{X} -space, their function values $f(\mathbf{x}^{(i)}), f(\mathbf{x}^{(j)})$ should be close (**correlated!**) in \mathcal{Y} -space.

- Closeness of two points $\mathbf{x}^{(i)}, \mathbf{x}^{(j)}$ in input space \mathcal{X} is measured in terms of $\mathbf{d} = \mathbf{x}^{(i)} - \mathbf{x}^{(j)}$:

$$k(\mathbf{x}^{(i)}, \mathbf{x}^{(j)}) = k(\mathbf{d})$$

COVARIANCE FUNCTION OF A GP: EXAMPLE

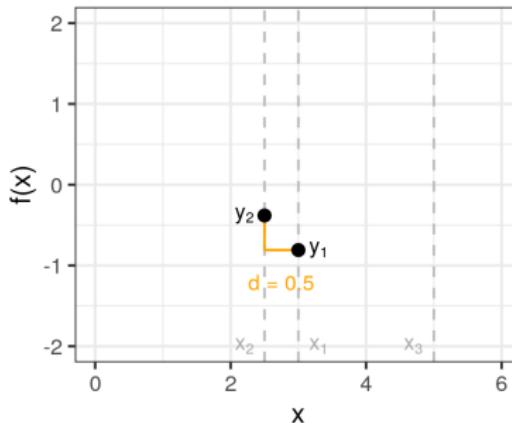
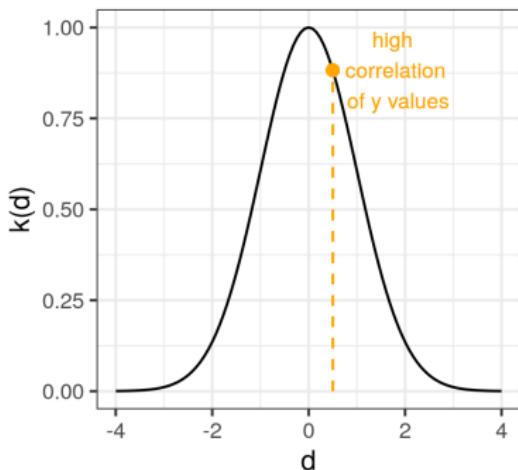
- Let $f(\mathbf{x})$ be a GP with $k(\mathbf{x}, \mathbf{x}') = \exp(-\frac{1}{2}\|\mathbf{d}\|^2)$ with $\mathbf{d} = \mathbf{x} - \mathbf{x}'$.
- Consider two points $\mathbf{x}^{(1)} = 3$ and $\mathbf{x}^{(2)} = 2.5$.
- If you want to know how correlated their function values are, compute their correlation!



COVARIANCE FUNCTION OF A GP: EXAMPLE

- Assume we observed a value $y^{(1)} = -0.8$, the value of $y^{(2)}$ should be close under the assumption of the above Gaussian process.

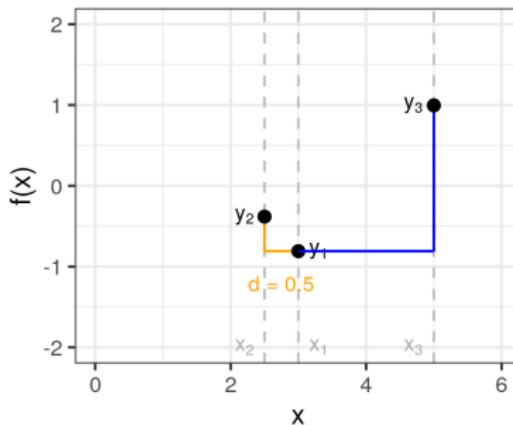
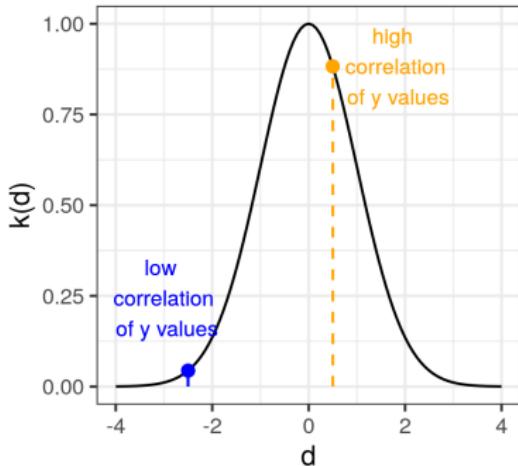
Covariance Function



COVARIANCE FUNCTION OF A GP: EXAMPLE

- Let us compare another point $\mathbf{x}^{(3)}$ to the point $\mathbf{x}^{(1)}$
- We again compute their correlation
- Their function values are not very much correlated; $y^{(1)}$ and $y^{(3)}$ might be far away from each other

Covariance Function



COVARIANCE FUNCTIONS

There are three types of commonly used covariance functions:

- $k(., .)$ is called stationary if it is as a function of $\mathbf{d} = \mathbf{x} - \mathbf{x}'$, we write $k(\mathbf{d})$.

Stationarity is invariance to translations in the input space:

$$k(\mathbf{x}, \mathbf{x} + \mathbf{d}) = k(\mathbf{0}, \mathbf{d})$$

- $k(., .)$ is called isotropic if it is a function of $r = \|\mathbf{x} - \mathbf{x}'\|$, we write $k(r)$.

Isotropy is invariance to rotations of the input space and implies stationarity.

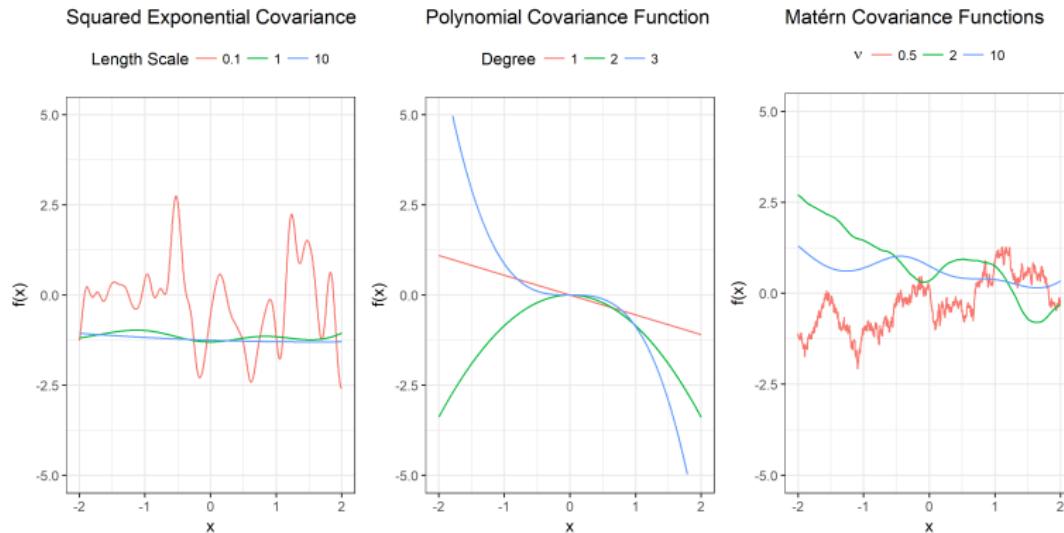
- $k(., .)$ is a dot product covariance function if k is a function of $\mathbf{x}^T \mathbf{x}'$

COMMONLY USED COVARIANCE FUNCTIONS

Name	$k(\mathbf{x}, \mathbf{x}')$
constant	σ_0^2
linear	$\sigma_0^2 + \mathbf{x}^T \mathbf{x}'$
polynomial	$(\sigma_0^2 + \mathbf{x}^T \mathbf{x}')^p$
squared exponential	$\exp(-\frac{\ \mathbf{x}-\mathbf{x}'\ ^2}{2\ell^2})$
Matérn	$\frac{1}{2^\nu \Gamma(\nu)} \left(\frac{\sqrt{2\nu}}{\ell} \ \mathbf{x} - \mathbf{x}'\ \right)^\nu K_\nu \left(\frac{\sqrt{2\nu}}{\ell} \ \mathbf{x} - \mathbf{x}'\ \right)$
exponential	$\exp \left(-\frac{\ \mathbf{x}-\mathbf{x}'\ }{\ell} \right)$

$K_\nu(\cdot)$ is the modified Bessel function of the second kind.

COMMONLY USED COVARIANCE FUNCTIONS



- Random functions drawn from Gaussian processes with a Squared Exponential Kernel (left), Polynomial Kernel (middle), and a Matérn Kernel (right, $\ell = 1$).
- The length-scale hyperparameter determines the “wiggliness” of the function.
- For Matérn, the ν parameter determines how differentiable the process is.

SQUARED EXPONENTIAL COVARIANCE FUNCTION

The squared exponential function is one of the most commonly used covariance functions.

$$k(\mathbf{x}, \mathbf{x}') = \exp\left(-\frac{\|\mathbf{x} - \mathbf{x}'\|^2}{2\ell^2}\right).$$

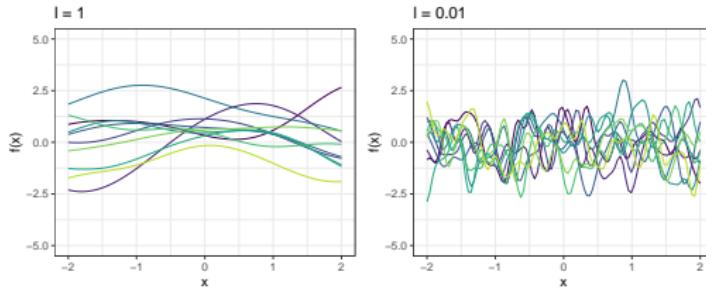
Properties:

- It depends merely on the distance $r = \|\mathbf{x} - \mathbf{x}'\| \rightarrow$ isotropic and stationary.
- Infinitely differentiable \rightarrow sometimes deemed unrealistic for modeling most of the physical processes.

CHARACTERISTIC LENGTH-SCALE

$$k(\mathbf{x}, \mathbf{x}') = \exp\left(-\frac{1}{2\ell^2} \|\mathbf{x} - \mathbf{x}'\|^2\right)$$

ℓ is called **characteristic length-scale**. Loosely speaking, the characteristic length-scale describes how far you need to move in input space for the function values to become uncorrelated. Higher ℓ induces smoother functions, lower ℓ induces more wiggly functions.



CHARACTERISTIC LENGTH-SCALE

For $p \geq 2$ dimensions, the squared exponential can be parameterized:

$$k(\mathbf{x}, \mathbf{x}') = \exp\left(-\frac{1}{2} (\mathbf{x} - \mathbf{x}')^\top \mathbf{M} (\mathbf{x} - \mathbf{x}')\right)$$

Possible choices for the matrix \mathbf{M} include

$$\mathbf{M}_1 = \ell^{-2} \mathbf{I} \quad \mathbf{M}_2 = \text{diag}(\ell)^{-2} \quad \mathbf{M}_3 = \Gamma \Gamma^\top + \text{diag}(\ell)^{-2}$$

where ℓ is a p -vector of positive values and Γ is a $p \times k$ matrix.

The 2nd (and most important) case can also be written as

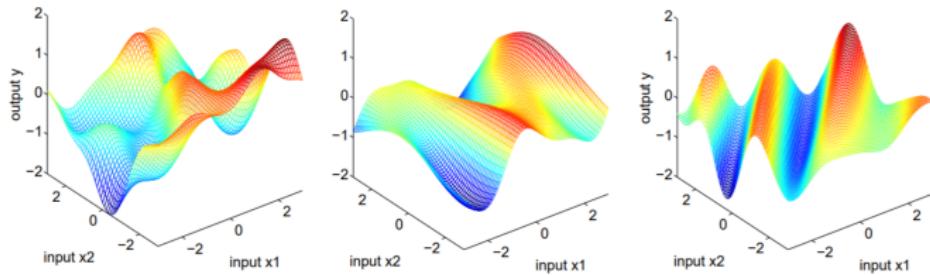
$$k(\mathbf{d}) = \exp\left(-\frac{1}{2} \sum_{j=1}^p \frac{d_j^2}{l_j^2}\right)$$

CHARACTERISTIC LENGTH-SCALE

What is the benefit of having an individual hyperparameter ℓ_i for each dimension?

- The ℓ_1, \dots, ℓ_p hyperparameters play the role of **characteristic length-scales**.
- Loosely speaking, ℓ_i describes how far you need to move along axis i in input space for the function values to be uncorrelated.
- Such a covariance function implements **automatic relevance determination** (ARD), since the inverse of the length-scale ℓ_i determines the relevancy of input feature i to the regression.
- If ℓ_i is very large, the covariance will become almost independent of that input, effectively removing it from inference.
- If the features are on different scales, the data can be automatically **rescaled** by estimating ℓ_1, \dots, ℓ_p

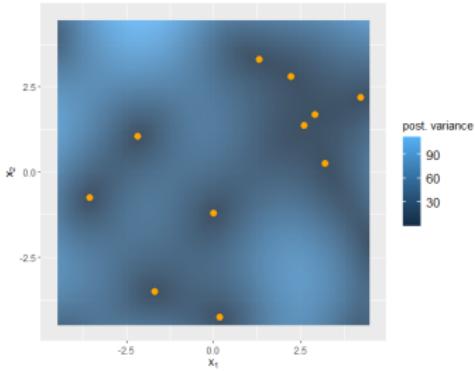
CHARACTERISTIC LENGTH-SCALE



For the first plot, we have chosen $\mathbf{M} = \mathbf{I}$: the function varies the same in all directions. The second plot is for $\mathbf{M} = \text{diag}(\ell)^{-2}$ and $\ell = (1, 3)$: The function varies less rapidly as a function of x_2 than x_1 as the length-scale for x_1 is less. In the third plot $\mathbf{M} = \Gamma\Gamma^T + \text{diag}(\ell)^{-2}$ for $\Gamma = (1, -1)^\top$ and $\ell = (6, 6)^\top$. Here Γ gives the direction of the most rapid variation. (Image from Rasmussen & Williams, 2006)

Introduction to Machine Learning

Gaussian Process Prediction



Learning goals

- XXX
- XXX

GAUSSIAN POSTERIOR PROCESS AND PREDICTION

- So far, we have learned how to **sample** from a GP prior.
- However, most of the time, we are not interested in drawing random functions from the prior. Instead, we usually like to use the knowledge provided by the training data to predict values of f at a new test point \mathbf{x}_* .
- In what follows, we will investigate how to update the Gaussian process prior (\rightarrow posterior process) and how to make predictions.

Gaussian Posterior Process and Prediction

POSTERIOR PROCESS

- Let us now distinguish between observed training inputs, also denote by a design matrix \mathbf{X} , and the corresponding observed values

$$\mathbf{f} = \left[f(\mathbf{x}^{(1)}), \dots, f(\mathbf{x}^{(n)}) \right]$$

and one single **unobserved test point** \mathbf{x}_* with $f_* = f(\mathbf{x}_*)$.

- We now want to infer the distribution of $f_* | \mathbf{x}_*, \mathbf{X}, \mathbf{f}$.

$$f_* = f(\mathbf{x}_*)$$

- Assuming a zero-mean GP prior $\mathcal{GP}(\mathbf{0}, k(\mathbf{x}, \mathbf{x}'))$ we know

$$\begin{bmatrix} \mathbf{f} \\ f_* \end{bmatrix} \sim \mathcal{N}\left(\mathbf{0}, \begin{bmatrix} \mathbf{K} & \mathbf{k}_* \\ \mathbf{k}_*^T & \mathbf{k}_{**} \end{bmatrix}\right).$$

Here, $\mathbf{K} = (k(\mathbf{x}^{(i)}, \mathbf{x}^{(j)}))_{i,j}$, $\mathbf{k}_* = [k(\mathbf{x}_*, \mathbf{x}^{(1)}), \dots, k(\mathbf{x}_*, \mathbf{x}^{(n)})]$ and $\mathbf{k}_{**} = k(\mathbf{x}_*, \mathbf{x}_*)$.

POSTERIOR PROCESS

- Given that \mathbf{f} is observed, we can apply the general rule for condition (*) of Gaussian random variables and obtain the following formula:

$$f_* \mid \mathbf{x}_*, \mathbf{X}, \mathbf{f} \sim \mathcal{N}(\mathbf{k}_*^T \mathbf{K}^{-1} \mathbf{f}, \mathbf{k}_{**} - \mathbf{k}_*^T \mathbf{K}^{-1} \mathbf{k}_*).$$

- As the posterior is a Gaussian, the maximum a-posteriori estimate, i.e. the mode of the posterior distribution, is $\mathbf{k}_*^T \mathbf{K}^{-1} \mathbf{f}$.

POSTERIOR PROCESS

(*) General rule for condition of Gaussian random variables:

If the m -dimensional Gaussian vector $\mathbf{z} \sim \mathcal{N}(\mu, \Sigma)$ can be partitioned with $\mathbf{z} = (\mathbf{z}_1, \mathbf{z}_2)$ where \mathbf{z}_1 is m_1 -dimensional and \mathbf{z}_2 is m_2 -dimensional, and:

$$(\mu_1, \mu_2), \quad \Sigma = \begin{pmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{pmatrix},$$

then the conditioned distribution of $\mathbf{z}_2 \mid \mathbf{z}_1 = \mathbf{a}$ is a multivariate normal

$$\mathcal{N}(\mu_2 + \Sigma_{21}\Sigma_{11}^{-1}(\mathbf{a} - \mu_1), \Sigma_{22} - \Sigma_{21}\Sigma_{11}^{-1}\Sigma_{12})$$

GP PREDICTION: TWO POINTS

Let us visualize this by a simple example:

- Assume we observed a single training point $\mathbf{x} = -0.5$, and want to make a prediction at a test point $\mathbf{x}_* = 0.5$.
- Under a zero-mean GP with $k(\mathbf{x}, \mathbf{x}') = \exp(-\frac{1}{2}\|\mathbf{x} - \mathbf{x}'\|^2)$, we compute the cov-matrix:

$$\begin{bmatrix} f \\ f_* \end{bmatrix} \sim \mathcal{N}\left(\mathbf{0}, \begin{bmatrix} 1 & 0.61 \\ 0.61 & 1 \end{bmatrix}\right).$$

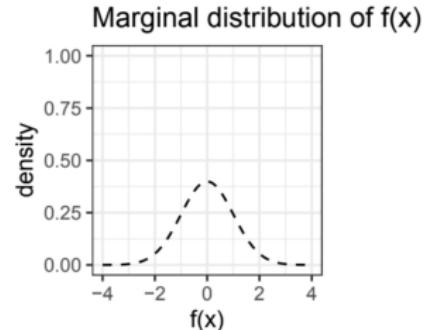
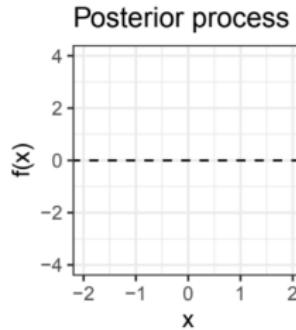
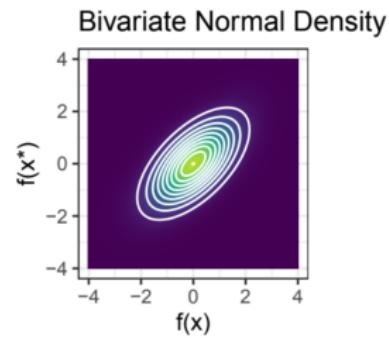
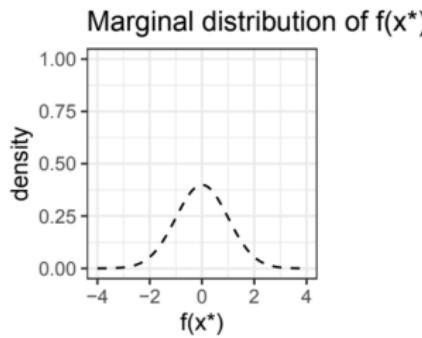
- Assume that we observe the point $f(\mathbf{x}) = 1$.
- We compute the posterior distribution:

$$\begin{aligned} f_* \mid \mathbf{x}_*, \mathbf{x}, f &\sim \mathcal{N}(\mathbf{k}_*^T \mathbf{K}^{-1} \mathbf{f}, k_{**} - \mathbf{k}_*^T \mathbf{K}^{-1} \mathbf{k}_*) \\ &\sim \mathcal{N}(0.61 \cdot 1 \cdot 1, 1 - 0.61 \cdot 1 \cdot 0.61) \\ &\sim \mathcal{N}(0.61, 0.6279) \end{aligned}$$

- The MAP-estimate for \mathbf{x}_* is $f(\mathbf{x}_*) = 0.61$, and the uncertainty estimate is 0.6279.

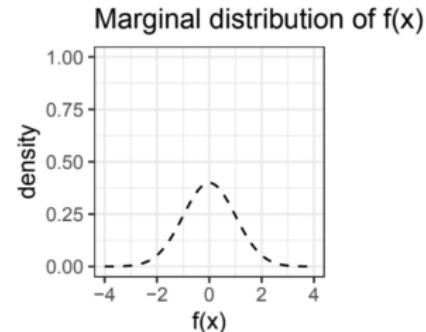
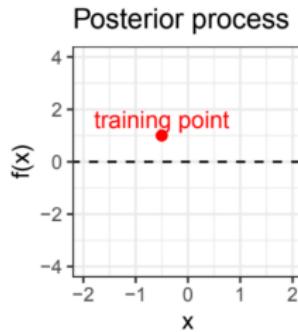
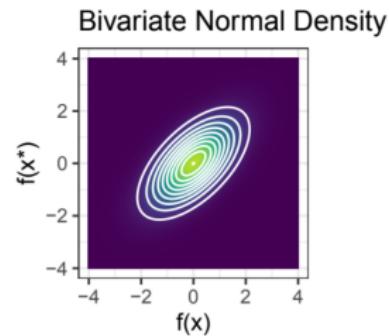
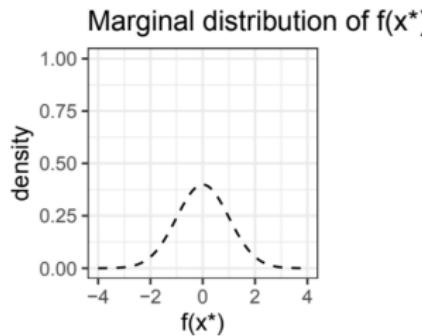
GP PREDICTION: TWO POINTS

Shown is the bivariate normal density, and the respective marginals.



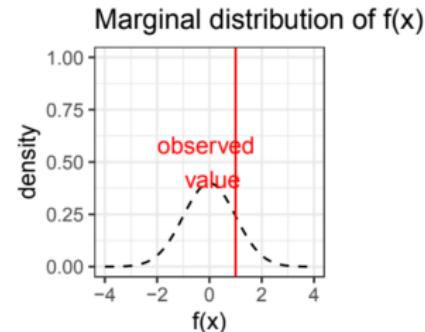
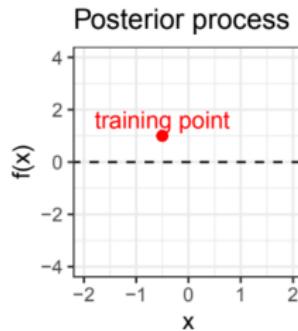
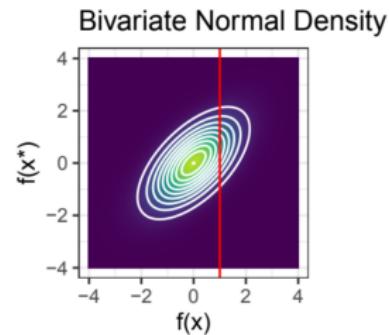
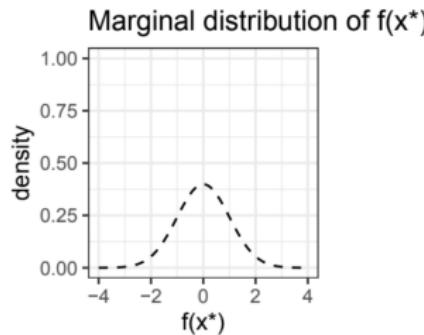
GP PREDICTION: TWO POINTS

Assume we observed $f(\mathbf{x}) = 1$ for the training point $\mathbf{x} = -0.5$.



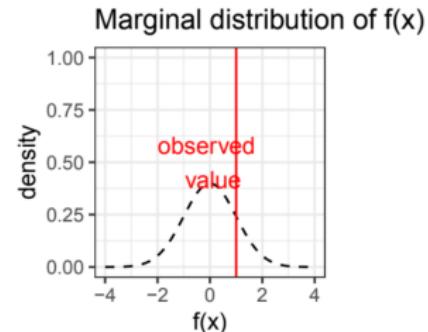
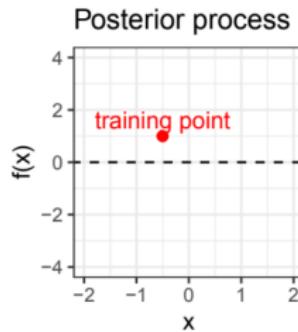
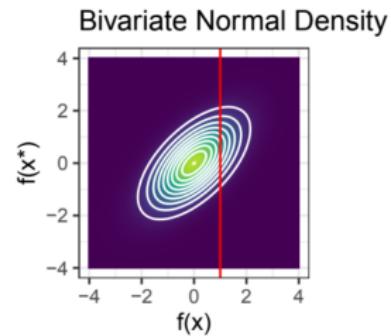
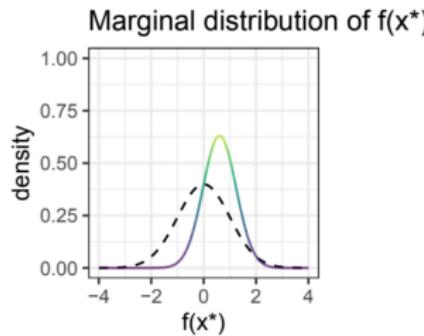
GP PREDICTION: TWO POINTS

We condition the Gaussian on $f(\mathbf{x}) = 1$.



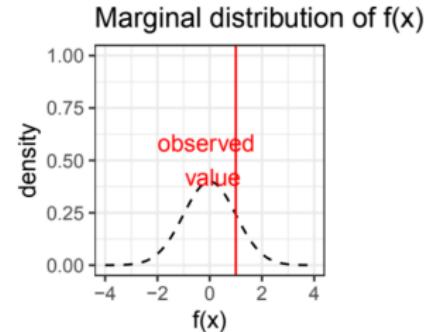
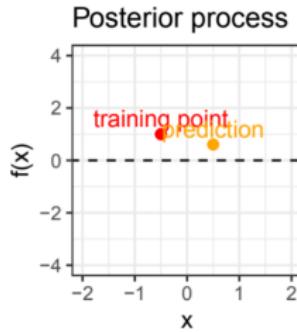
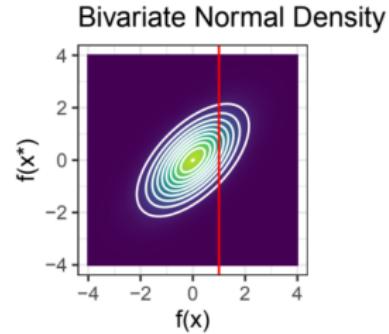
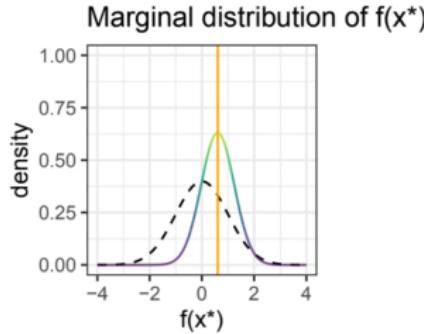
GP PREDICTION: TWO POINTS

We compute the posterior distribution of $f(\mathbf{x}_*)$ given that $f(\mathbf{x}) = 1$.



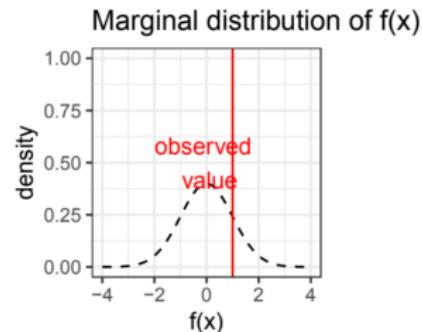
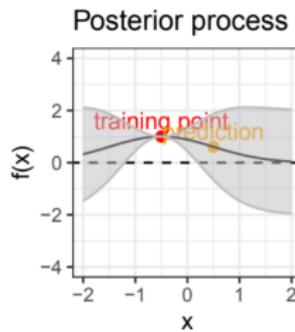
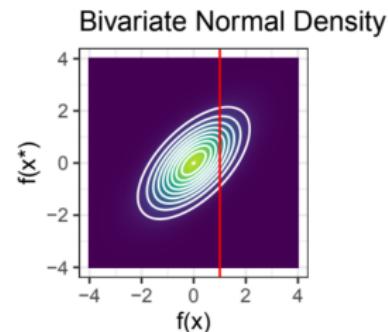
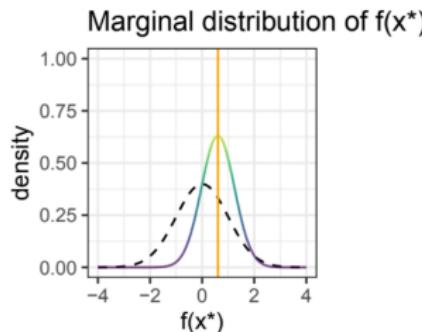
GP PREDICTION: TWO POINTS

A possible predictor for f at \mathbf{x}_* is the MAP of the posterior distribution.



GP PREDICTION: TWO POINTS

We can do this for different values x_* , and show the respective mean (grey line) and standard deviations (grey area is mean $\pm 2 \cdot$ posterior standard deviation).



POSTERIOR PROCESS

- We can generalize the formula for the posterior process for multiple unobserved test points:

$$\mathbf{f}_* = \left[f\left(\mathbf{x}_*^{(1)}\right), \dots, f\left(\mathbf{x}_*^{(m)}\right) \right].$$

- Under a zero-mean Gaussian process, we have

$$\begin{bmatrix} \mathbf{f} \\ \mathbf{f}_* \end{bmatrix} \sim \mathcal{N}\left(\mathbf{0}, \begin{bmatrix} \mathbf{K} & \mathbf{K}_* \\ \mathbf{K}_*^T & \mathbf{K}_{**} \end{bmatrix}\right),$$

with $\mathbf{K}_* = \left(k\left(\mathbf{x}^{(i)}, \mathbf{x}_*^{(j)}\right)\right)_{i,j}$, $\mathbf{K}_{**} = \left(k\left(\mathbf{x}_*^{(i)}, \mathbf{x}_*^{(j)}\right)\right)_{i,j}$.

POSTERIOR PROCESS

- Similar to the single test point situation, to get the posterior distribution, we exploit the general rule of conditioning for Gaussians:

$$\mathbf{f}_* \mid \mathbf{X}_*, \mathbf{X}, \mathbf{f} \sim \mathcal{N}(\mathbf{K}_*^T \mathbf{K}^{-1} \mathbf{f}, \mathbf{K}_{**} - \mathbf{K}_*^T \mathbf{K}^{-1} \mathbf{K}_*).$$

- This formula enables us to talk about correlations among different test points and sample functions from the posterior process.

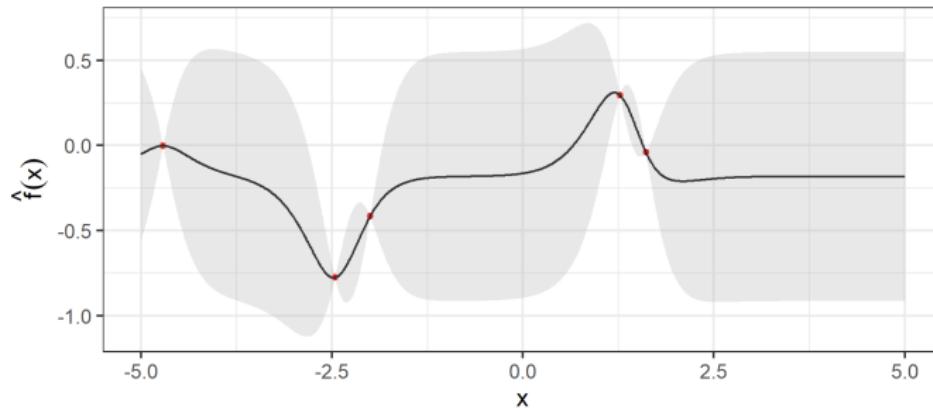
Properties of a Gaussian Process

GP AS INTERPOLATOR

The “prediction” for a training point $\mathbf{x}^{(i)}$ is the exact function value $f(\mathbf{x}^{(i)})$

$$\mathbf{f} | \mathbf{X}, \mathbf{f} \sim \mathcal{N}(\mathbf{K}\mathbf{K}^{-1}\mathbf{f}, \mathbf{K} - \mathbf{K}^T\mathbf{K}^{-1}\mathbf{K}) = \mathcal{N}(\mathbf{f}, \mathbf{0}).$$

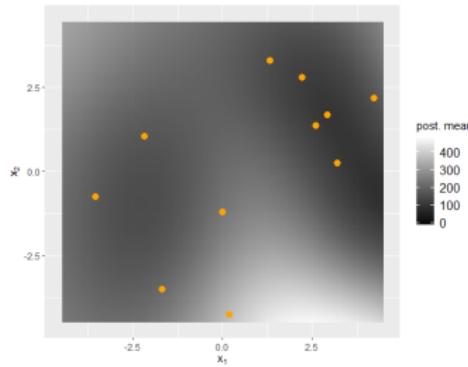
Thus, a Gaussian process is a function **interpolator**.



After observing the training points (red), the posterior process (black) interpolates the training points.
 $(k(x,x') \sim \text{Matérn}$ with $\nu = 2.5$, the default for DiceKriging::km)

GP AS A SPATIAL MODEL

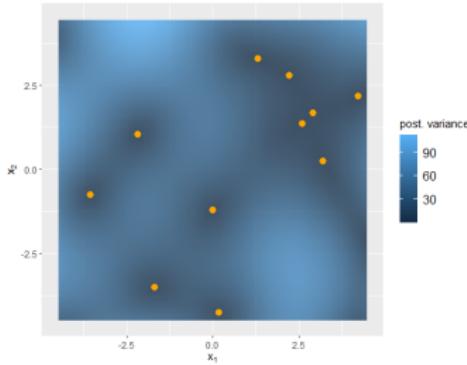
- The correlation among two outputs depends on distance of the corresponding input points \mathbf{x} and \mathbf{x}' (e.g. Gaussian covariance kernel)
$$k(\mathbf{x}, \mathbf{x}') = \exp\left(\frac{-\|\mathbf{x} - \mathbf{x}'\|^2}{2l^2}\right)$$
- Hence, close data points with high spatial similarity $k(\mathbf{x}, \mathbf{x}')$ enter into more strongly correlated predictions: $\mathbf{k}_*^\top \mathbf{K}^{-1} \mathbf{f}$ ($\mathbf{k}_* := (k(\mathbf{x}, \mathbf{x}^{(1)}), \dots, k(\mathbf{x}, \mathbf{x}^{(n)}))$).



Example: Posterior mean of a GP that was fitted with the Gaussian covariance kernel with $l = 1$.

GP AS A SPATIAL MODEL

- Posterior uncertainty increases if the new data points are far from the design points.
- The uncertainty is minimal at the design points, since the posterior variance is zero at these points.



Example (continued): Posterior variance.

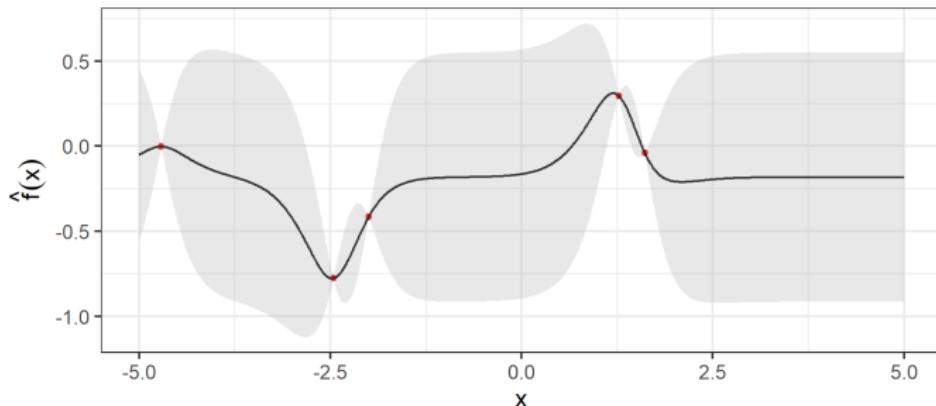
Noisy Gaussian Process

NOISY GAUSSIAN PROCESS

- So far, we implicitly assumed that we had access to the true function value $f(\mathbf{x})$.
- For the squared exponential kernel, for example, we have

$$\text{Cov}\left(f(\mathbf{x}^{(i)}), f(\mathbf{x}^{(j)})\right) = 1.$$

- As a result, the posterior Gaussian process is an interpolator:



After observing the training points (red), the posterior process (black) interpolates the training points.
($k(x, x')$ is Matérn with $\nu = 2.5$, the default for DiceKriging::km)

NOISY GAUSSIAN PROCESS

- In reality, however, this is often not the case.
- We often only have access to a noisy version of the true function value

$$y = f(\mathbf{x}) + \epsilon, \epsilon \sim \mathcal{N}(0, \sigma^2).$$

- Let us still assume that $f(\mathbf{x})$ is a Gaussian process.
- Then,

$$\begin{aligned}\text{Cov}(y^{(i)}, y^{(j)}) &= \text{Cov}\left(f\left(\mathbf{x}^{(i)}\right) + \epsilon^{(i)}, f\left(\mathbf{x}^{(j)}\right) + \epsilon^{(j)}\right) \\ &= \text{Cov}\left(f\left(\mathbf{x}^{(i)}\right), f\left(\mathbf{x}^{(j)}\right)\right) + 2 \cdot \text{Cov}\left(f\left(\mathbf{x}^{(i)}\right), \epsilon^{(j)}\right) + \text{Cov}\left(\epsilon^{(i)}, \epsilon^{(j)}\right) \\ &= k\left(\mathbf{x}^{(i)}, \mathbf{x}^{(j)}\right) + \sigma^2 \delta_{ij}.\end{aligned}$$

- σ^2 is called **nugget**.

NOISY GAUSSIAN PROCESS

- Let us now derive the predictive distribution for the case of noisy observations.
- The prior distribution of y , assuming that f is modeled by a Gaussian process is then

$$\mathbf{y} = \begin{pmatrix} y^{(1)} \\ y^{(2)} \\ \vdots \\ y^{(n)} \end{pmatrix} \sim \mathcal{N}(\mathbf{m}, \mathbf{K} + \sigma^2 \mathbf{I}_n),$$

with

$$\mathbf{m} := \left(m(\mathbf{x}^{(i)}) \right)_i, \quad \mathbf{K} := \left(k(\mathbf{x}^{(i)}, \mathbf{x}^{(j)}) \right)_{i,j}.$$

NOISY GAUSSIAN PROCESS

- We distinguish again between
 - observed training points \mathbf{X}, \mathbf{y} , and
 - unobserved test inputs \mathbf{X}_* with unobserved values \mathbf{f}_*

and get

$$\begin{bmatrix} \mathbf{y} \\ \mathbf{f}_* \end{bmatrix} \sim \mathcal{N}\left(\mathbf{0}, \begin{bmatrix} \mathbf{K} + \sigma^2 \mathbf{I}_n & \mathbf{K}_* \\ \mathbf{K}_*^T & \mathbf{K}_{**} \end{bmatrix}\right).$$

NOISY GAUSSIAN PROCESS

- Similarly to the noise-free case, we condition according to the rule of conditioning for Gaussians to get the posterior distribution for the test outputs \mathbf{f}_* at \mathbf{X}_* :

$$\mathbf{f}_* \mid \mathbf{X}_*, \mathbf{X}, \mathbf{y} \sim \mathcal{N}(\mathbf{m}_{\text{post}}, \mathbf{K}_{\text{post}}).$$

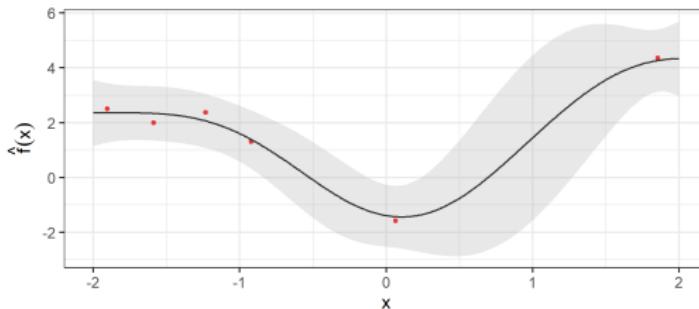
with

$$\begin{aligned}\mathbf{m}_{\text{post}} &= \mathbf{K}_*^T (\mathbf{K} + \sigma^2 \cdot \mathbf{I})^{-1} \mathbf{y} \\ \mathbf{K}_{\text{post}} &= \mathbf{K}_{**} - \mathbf{K}_*^T (\mathbf{K}^{-1} + \sigma^2 \cdot \mathbf{I}) \mathbf{K}_*,\end{aligned}$$

- This converts back to the noise-free formula if $\sigma^2 = 0$.

NOISY GAUSSIAN PROCESS

- The noisy Gaussian process is not an interpolator any more.
- A larger nugget term leads to a wider “band” around the observed training points.
- The nugget term is estimated during training.



After observing the training points (red), we have a nugget-band around the observed points.
($k(x, x')$ is the squared exponential)

Decision Theory for Gaussian Processes

RISK MINIMIZATION FOR GAUSSIAN PROCESSES

In machine learning, we learned about risk minimization. We usually choose a loss function and minimize the empirical risk

$$\mathcal{R}_{\text{emp}}(f) := \sum_{i=1}^n L(y^{(i)}, f(\mathbf{x}^{(i)}))$$

as an approximation to the theoretical risk

$$\mathcal{R}(f) := \mathbb{E}_{xy}[L(y, f(\mathbf{x}))] = \int L(y, f(\mathbf{x})) d\mathbb{P}_{xy}.$$

- How does the theory of Gaussian processes fit into this theory?
- What if we want to make a prediction which is optimal w.r.t. a certain loss function?

RISK MINIMIZATION FOR GAUSSIAN PROCESSES

- The theory of Gaussian process gives us a posterior distribution

$$p(y \mid \mathcal{D})$$

- If we now want to make a prediction at a test point \mathbf{x}_* , we approximate the theoretical risk in a different way, by using the posterior distribution:

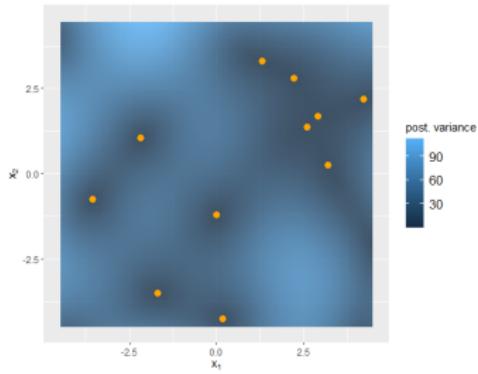
$$\mathcal{R}(y_* \mid \mathbf{x}_*) \approx \int L(\tilde{y}_*, y_*) p(\tilde{y}_* \mid \mathbf{x}_*, \mathcal{D}) d\tilde{y}_*.$$

- The optimal prediction w.r.t the loss function is then:

$$\hat{y}_* \mid \mathbf{x}_* = \arg \min_{y_*} \mathcal{R}(y_* \mid \mathbf{x}_*).$$

Introduction to Machine Learning

Gaussian Process Training



Learning goals

- XXX
- XXX

TRAINING OF A GAUSSIAN PROCESS

- To make predictions for a regression task by a Gaussian process, one simply needs to perform matrix computations.
- But for this to work out, we assume that the covariance functions is fully given, including all of its hyperparameters.
- A very nice property of GPs is that we can learn the numerical hyperparameters of a selected covariance function directly during GP training.

TRAINING A GP VIA MAXIMUM LIKELIHOOD

Let us assume

$$y = f(\mathbf{x}) + \epsilon, \quad \epsilon \sim \mathcal{N}(0, \sigma^2),$$

where $f(\mathbf{x}) \sim \mathcal{GP}(\mathbf{0}, k(\mathbf{x}, \mathbf{x}'|\theta))$.

Observing $\mathbf{y} \sim \mathcal{N}(\mathbf{0}, \mathbf{K} + \sigma^2 \mathbf{I})$, the marginal log-likelihood (or evidence) is

$$\begin{aligned}\log p(\mathbf{y} | \mathbf{X}, \theta) &= \log \left[(2\pi)^{-n/2} |\mathbf{K}_y|^{-1/2} \exp \left(-\frac{1}{2} \mathbf{y}^\top \mathbf{K}_y^{-1} \mathbf{y} \right) \right] \\ &= -\frac{1}{2} \mathbf{y}^\top \mathbf{K}_y^{-1} \mathbf{y} - \frac{1}{2} \log |\mathbf{K}_y| - \frac{n}{2} \log 2\pi.\end{aligned}$$

with $\mathbf{K}_y := \mathbf{K} + \sigma^2 \mathbf{I}$ and θ denoting the hyperparameters (the parameters of the covariance function).

TRAINING A GP VIA MAXIMUM LIKELIHOOD

The three terms of the marginal likelihood have interpretable roles, considering that the model becomes less flexible as the length-scale increases:

- the data fit $-\frac{1}{2}\mathbf{y}^T \mathbf{K}_y^{-1} \mathbf{y}$, which tends to decrease the length scale increases
- the complexity penalty $-\frac{1}{2} \log |\mathbf{K}_y|$, which depends on the covariance function only and which decreases with the length-scale, because the model gets less complex with growing length-scale
- a normalization constant $-\frac{n}{2} \log 2\pi$

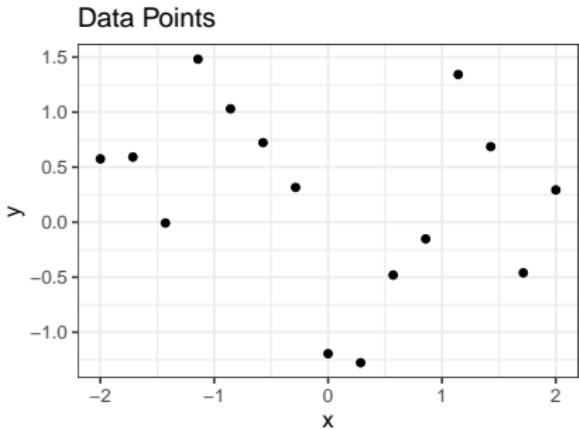
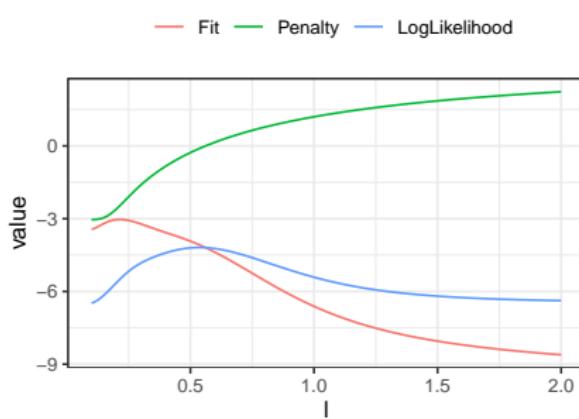
TRAINING A GP: EXAMPLE

To visualize this, we consider a zero-mean Gaussian process with squared exponential kernel

$$k(\mathbf{x}, \mathbf{x}') = \exp\left(-\frac{1}{2\ell^2}\|\mathbf{x} - \mathbf{x}'\|^2\right),$$

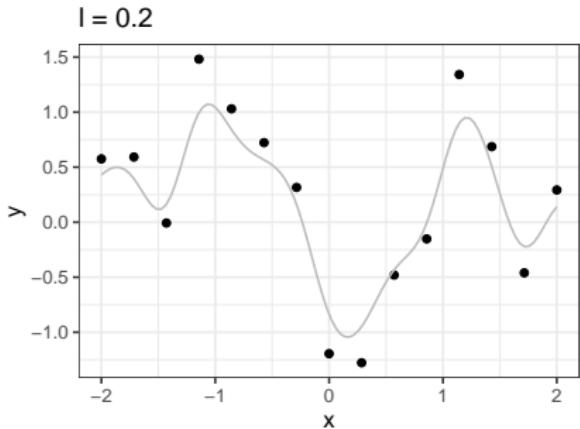
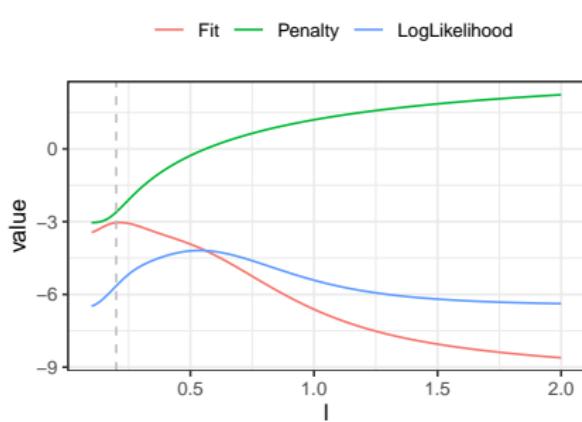
- Recall, the model is smoother and less complex for higher length-scale ℓ .
 - We show how the
 - data fit $-\frac{1}{2}\mathbf{y}^T \mathbf{K}_y^{-1} \mathbf{y}$,
 - the complexity penalty $-\frac{1}{2} \log |\mathbf{K}_y|$, and
 - the overall value of the marginal likelihood $\log p(\mathbf{y} | \mathbf{X}, \theta)$
- behave for increasing value of ℓ .

TRAINING A GP: EXAMPLE



The left plot shows how values of the data fit $-\frac{1}{2} \mathbf{y}^T \mathbf{K}_y^{-1} \mathbf{y}$, the complexity penalty $-\frac{1}{2} \log |\mathbf{K}_y|$ (high value means less penalization) and the overall marginal likelihood $\log p(\mathbf{y} | \mathbf{X}, \theta)$ behave for increasing values of ℓ .

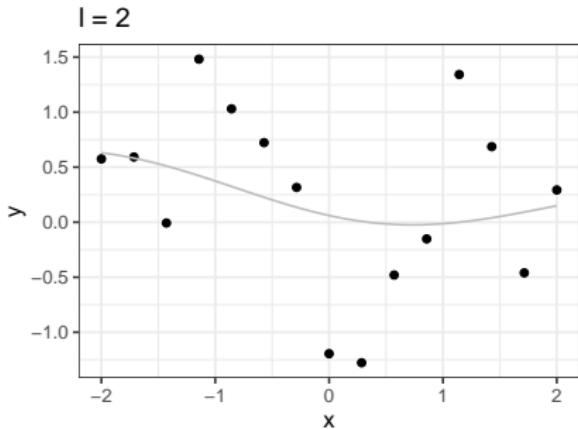
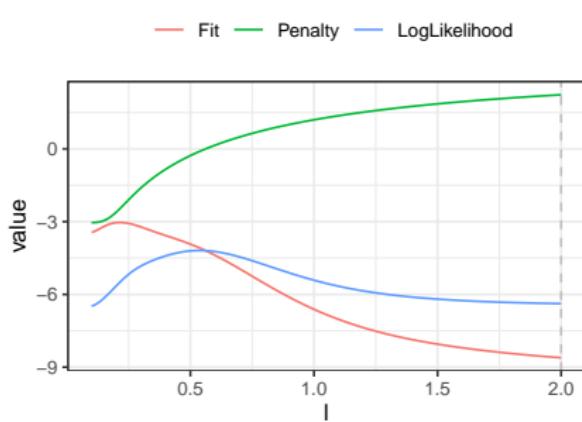
TRAINING A GP: EXAMPLE



The left plot shows how values of the data fit $-\frac{1}{2} \mathbf{y}^T \mathbf{K}_y^{-1} \mathbf{y}$, the complexity penalty $-\frac{1}{2} \log |\mathbf{K}_y|$ (high value means less penalization) and the overall marginal likelihood $\log p(\mathbf{y} | \mathbf{X}, \theta)$ behave for increasing values of ℓ .

A small ℓ results in a good fit, but a high complexity penalty (low $-\frac{1}{2} \log |\mathbf{K}_y|$).

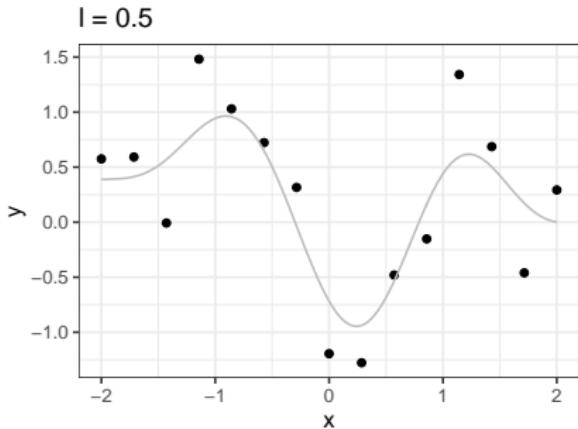
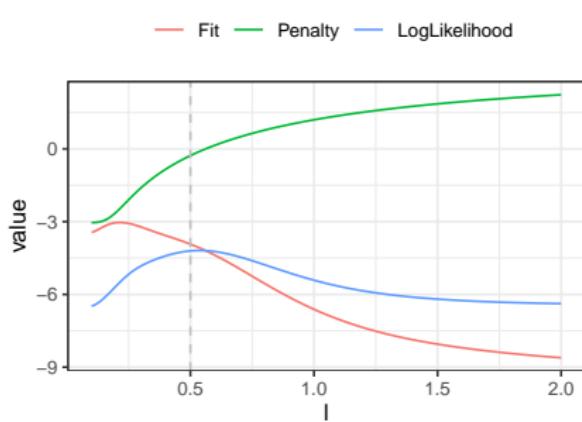
TRAINING A GP: EXAMPLE



The left plot shows how values of the data fit $-\frac{1}{2}\mathbf{y}^T \mathbf{K}_y^{-1} \mathbf{y}$, the complexity penalty $-\frac{1}{2} \log |\mathbf{K}_y|$ (high value means less penalization) and the overall marginal likelihood $\log p(\mathbf{y} | \mathbf{X}, \theta)$ behave for increasing values of ℓ .

A large ℓ results in a poor fit.

TRAINING A GP: EXAMPLE



The left plot shows how values of the data fit $-\frac{1}{2}\mathbf{y}^T \mathbf{K}_y^{-1} \mathbf{y}$, the complexity penalty $-\frac{1}{2} \log |\mathbf{K}_y|$ (high value means less penalization) and the overall marginal likelihood $\log p(\mathbf{y} | \mathbf{X}, \theta)$ behave for increasing values of ℓ .

The maximizer of the log-likelihood, $\ell = 0.5$, balances complexity and fit.

TRAINING A GP VIA MAXIMUM LIKELIHOOD

To set the hyperparameters by maximizing the marginal likelihood, we seek the partial derivatives w.r.t. the hyperparameters

$$\begin{aligned}\frac{\partial}{\partial \theta_j} \log p(\mathbf{y} | \mathbf{X}, \boldsymbol{\theta}) &= \frac{\partial}{\partial \theta_j} \left(-\frac{1}{2} \mathbf{y}^\top \mathbf{K}_y^{-1} \mathbf{y} - \frac{1}{2} \log |\mathbf{K}_y| - \frac{n}{2} \log 2\pi \right) \\ &= \frac{1}{2} \mathbf{y}^\top \mathbf{K}^{-1} \frac{\partial \mathbf{K}}{\partial \theta_j} \mathbf{K}^{-1} \mathbf{y} - \frac{1}{2} \text{tr} \left(\mathbf{K}^{-1} \frac{\partial \mathbf{K}}{\partial \theta} \right) \\ &= \frac{1}{2} \text{tr} \left((\mathbf{K}^{-1} \mathbf{y} \mathbf{y}^\top \mathbf{K}^{-1} - \mathbf{K}^{-1}) \frac{\partial \mathbf{K}}{\partial \theta_j} \right)\end{aligned}$$

using $\frac{\partial}{\partial \theta_j} \mathbf{K}^{-1} = -\mathbf{K}^{-1} \frac{\partial \mathbf{K}}{\partial \theta_j} \mathbf{K}^{-1}$ and $\frac{\partial}{\partial \theta} \log |\mathbf{K}| = \text{tr} \left(\mathbf{K}^{-1} \frac{\partial \mathbf{K}}{\partial \theta} \right)$.

TRAINING A GP VIA MAXIMUM LIKELIHOOD

- The complexity and the runtime of training a Gaussian process is dominated by the computational task of inverting \mathbf{K} - or let's rather say for decomposing it.
- Standard methods require $\mathcal{O}(n^3)$ time (!) for this.
- Once \mathbf{K}^{-1} - or rather the decomposition -is known, the computation of the partial derivatives requires only $\mathcal{O}(n^2)$ time per hyperparameter.
- Thus, the computational overhead of computing derivatives is small, so using a gradient based optimizer is advantageous.

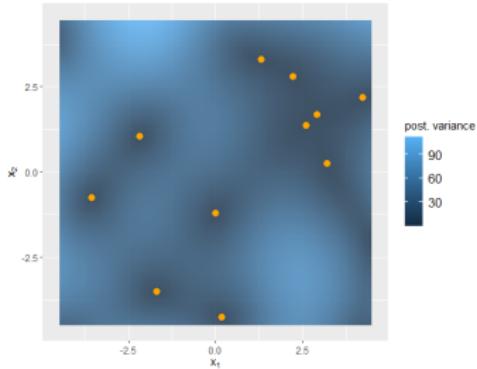
TRAINING A GP VIA MAXIMUM LIKELIHOOD

Workarounds to make GP estimation feasible for big data include:

- using kernels that yield sparse \mathbf{K} : cheaper to invert.
- subsampling the data to estimate θ : $\mathcal{O}(m^3)$ for subset of size m .
- combining estimates on different subsets of size m :
Bayesian committee, $\mathcal{O}(nm^2)$.
- using low-rank approximations of \mathbf{K} by using only a representative subset (“inducing points”) of m training data \mathbf{X}_m :
Nyström approximation $\mathbf{K} \approx \mathbf{K}_{nm}\mathbf{K}_{mm}^{-1}\mathbf{K}_{mn}$,
 $\mathcal{O}(nmk + m^3)$ for a rank-k-approximate inverse of \mathbf{K}_{mm} .
- exploiting structure in \mathbf{K} induced by the kernel: exact solutions but complicated maths, not applicable for all kernels.
... this is still an active area of research.

Introduction to Machine Learning

Mean Functions for Gaussian Processes



Learning goals

- XXX
- XXX

THE ROLE OF MEAN FUNCTIONS

- It is common but by no means necessary to consider GPs with a zero-mean function

$$m(\mathbf{x}) \equiv 0$$

- Note that this is not necessarily a drastic limitation, since the mean of the posterior process is not confined to be zero

$$\mathbf{f}_* | \mathbf{X}_*, \mathbf{X}, \mathbf{f} \sim \mathcal{N}(\mathbf{K}_*^T \mathbf{K}^{-1} \mathbf{f}, \mathbf{K}_{**} - \mathbf{K}_*^T \mathbf{K}^{-1} \mathbf{K}_*).$$

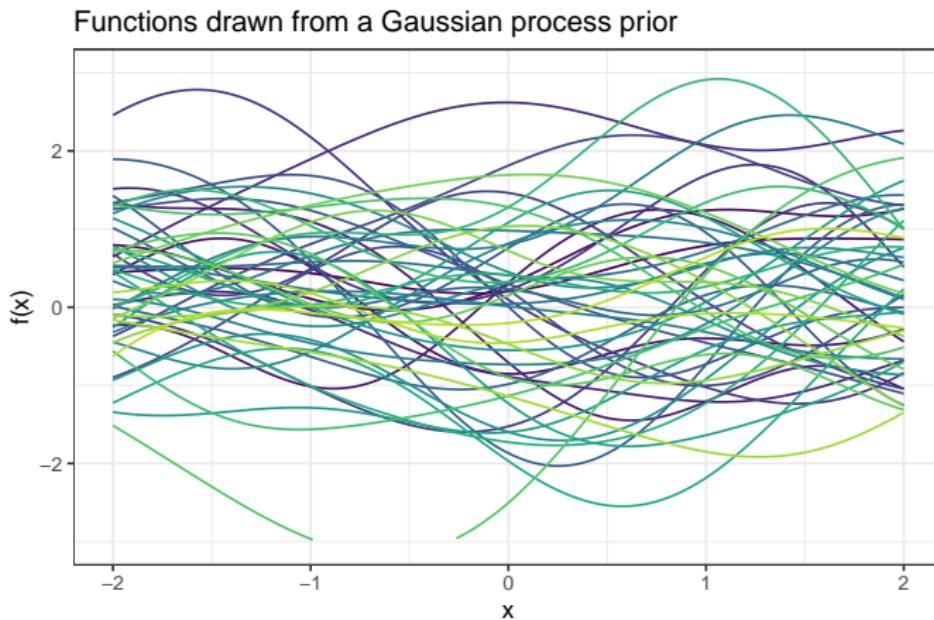
- Yet there are several reasons why one might wish to explicitly model a mean function, including interpretability, convenience of expressing prior informations, ...
- When assuming a non-zero mean GP prior $\mathcal{GP}(m(\mathbf{x}), k(\mathbf{x}, \mathbf{x}'))$ with mean $m(\mathbf{x})$, the predictive mean becomes

$$m(\mathbf{X}_*) + \mathbf{K}_* \mathbf{K}_y^{-1} (\mathbf{y} - m(\mathbf{X}))$$

while the predictive variance remains unchanged.

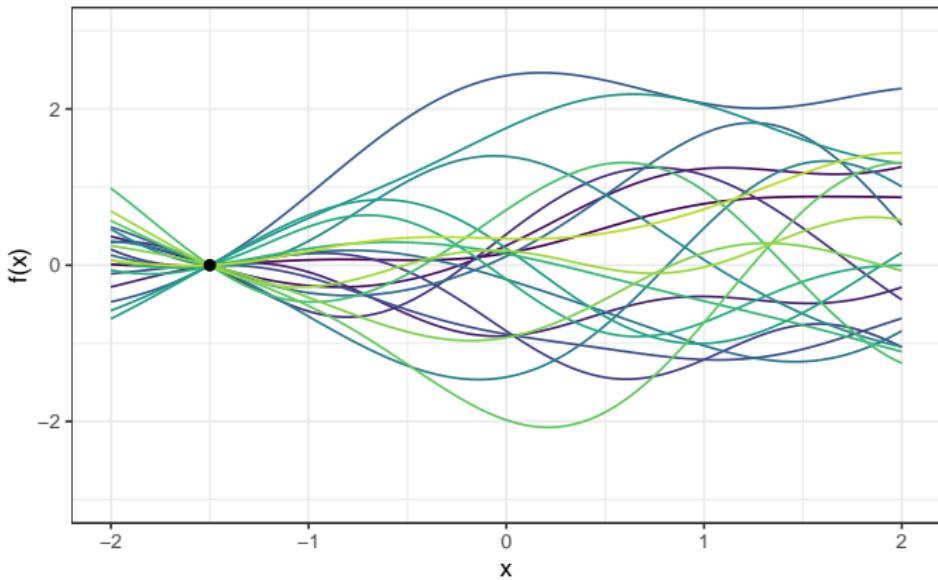
THE ROLE OF MEAN FUNCTIONS

- Gaussian processes with non-zero mean Gaussian process priors are also called Gaussian processes with trend.



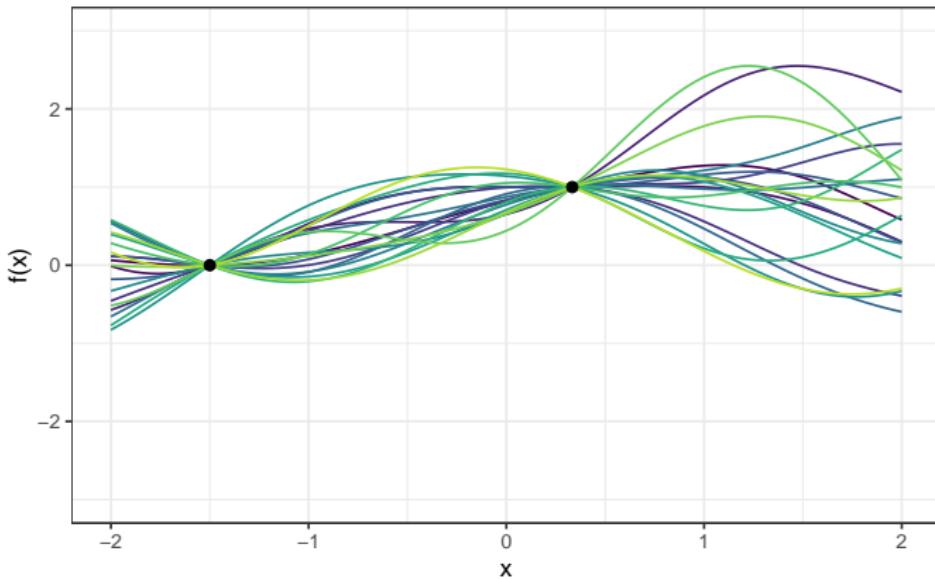
THE ROLE OF MEAN FUNCTIONS

Posterior process after 1 observation



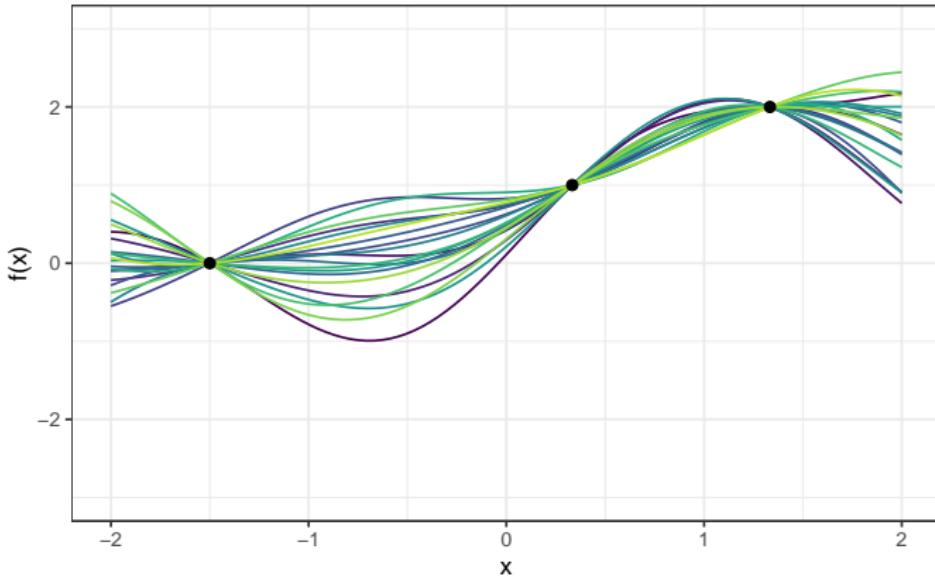
THE ROLE OF MEAN FUNCTIONS

Posterior process after 2 observations



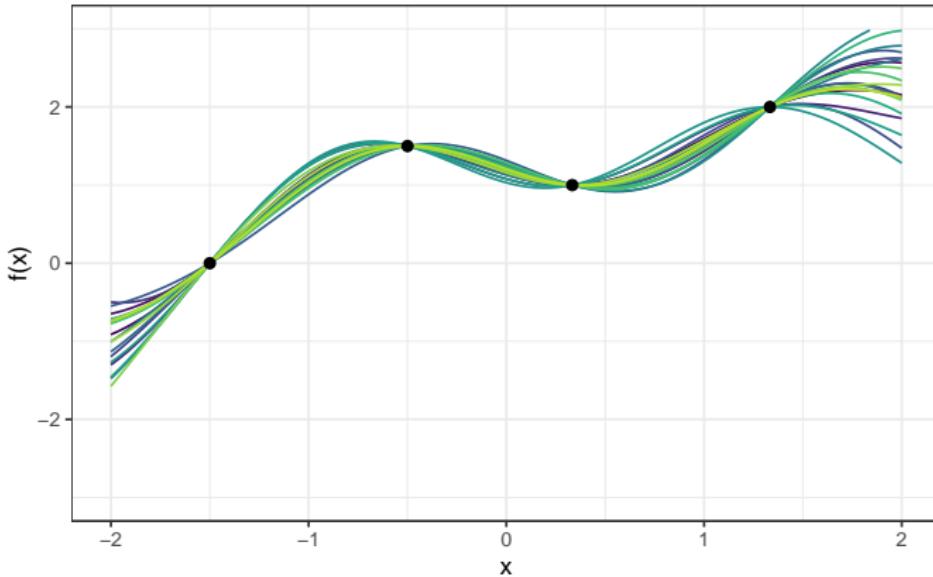
THE ROLE OF MEAN FUNCTIONS

Posterior process after 3 observations



THE ROLE OF MEAN FUNCTIONS

Posterior process after 4 observations



THE ROLE OF MEAN FUNCTIONS

- In practice it can often be difficult to specify a fixed mean function
- In many cases it may be more convenient to specify a few fixed basis functions, whose coefficients, β , are to be inferred from the data
- Consider

$$g(\mathbf{x}) = \mathbf{b}(\mathbf{x})^\top \boldsymbol{\beta} + f(\mathbf{x}), \text{ where } f(\mathbf{x}) \sim \mathcal{GP}(0, k(\mathbf{x}, \tilde{\mathbf{x}}))$$

- This formulation expresses that the data is close to a global linear model with the residuals being modelled by a GP.
- For the estimation of $g(\mathbf{x})$ please refer to *Rasmussen, Gaussian Processes for Machine Learning, 2006*

INTRODUCTION TO MACHINE LEARNING

Advanced Risk Minimization

Multiclass Classification

Information Theory

Curse of Dimensionality

Hypothesis Space

Regularization

Linear Support Vector Machine

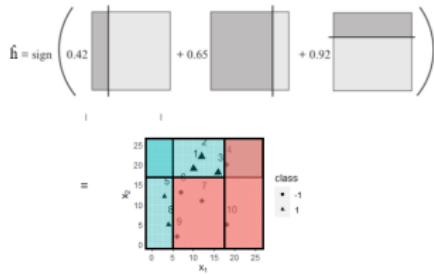
Nonlinear Support Vector Machine

Gaussian Processes

Boosting

Introduction to Machine Learning

Introduction to Boosting / AdaBoost



Learning goals

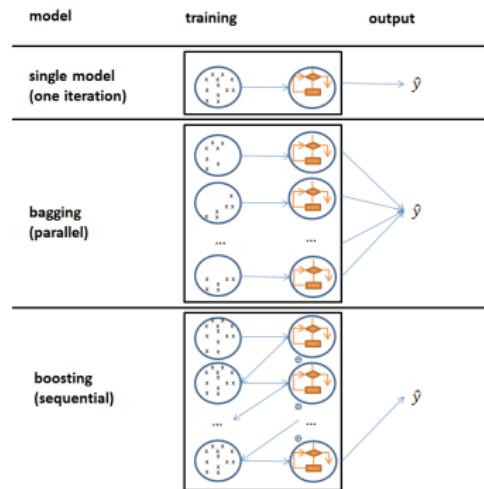
- Briefly cover the older AdaBoost and its general idea
- Understand difference between bagging and boosting

INTRODUCTION TO BOOSTING

- Boosting is one of the most powerful learning ideas since 1990.
- Originally designed for classification, (especially gradient) boosting handles regression (and many other supervised tasks) naturally nowadays.
- Homogeneous ensemble method (like bagging), but fundamentally different approach.
- **Idea:** Take a weak classifier and sequentially apply it to modified versions of the training data.
- We will begin by describing an older, simpler boosting algorithm designed for binary classification, the popular “AdaBoost”.

BOOSTING VS. BAGGING

- Homogeneous ensemble method (like bagging).
- **Idea:** Take a weak classifier and sequentially apply it to modified versions of the training data.
- Sequential not parallel model building, to minimize loss instead of variance reduction.



BOOSTING AS A THEORETICAL PROBLEM

Boosting was developed as the answer to a theoretical problem:

“Does the existence of a weak learner for a certain problem imply the existence of a strong learner?” (Kearns, 1988)

- **Weak learners** are defined as a prediction rule with a correct classification rate that is at least slightly better than random guessing (> 50% accuracy on a balanced binary problem).
- We call a learner a **strong learner** “if there exists a polynomial-time algorithm that achieves low error with high confidence for all concepts in the class” (Schapire, 1990).
- Any weak (base) learner can be iteratively boosted to become a strong learner (Schapire and Freund, 1990).
- Idea was refined into **AdaBoost** (Adaptive Boosting).

ADABOOST

- Assume binary classification with y encoded as $\{-1, +1\}$.
- We use binary classifiers as weak base learners (e.g., tree stumps) from a hypothesis space \mathcal{B} , denoted $b^{[m]}$ (or $b^{[m]}(\mathbf{x})$ or $b(\mathbf{x}, \theta^{[m]})$), which are hard labelers and output from $\{-1, +1\}$.
- Decision score of the ensemble of size M is weighted average:

$$f(\mathbf{x}) = \sum_{m=1}^M \beta^{[m]} b(\mathbf{x}, \theta^{[m]}) \in \mathbb{R}$$

- The base learner is sequentially applied to weighted training observations. After each base learner fit, currently misclassified observations receive a higher weight for the next iteration, so we focus more on instances that are harder to classify.
- BLs with higher predictive accuracy receive higher weights $\beta^{[m]}$.

ADABOOST

Algorithm AdaBoost

- 1: Initialize observation weights: $w^{[1](i)} = \frac{1}{n} \quad \forall i \in \{1, \dots, n\}$
- 2: **for** $m = 1 \rightarrow M$ **do**
- 3: Fit classifier to training data with weights $w^{[m]}$ and get $\hat{b}^{[m]}$
- 4: Calculate weighted in-sample misclassification rate

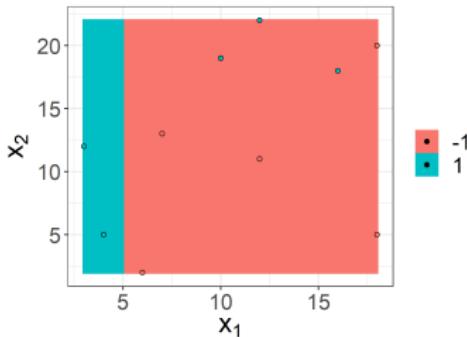
$$\text{err}^{[m]} = \sum_{i=1}^n w^{[m](i)} \cdot \mathbb{1}_{\{y^{(i)} \neq \hat{b}^{[m]}(\mathbf{x}^{(i)})\}}$$

- 5: Compute: $\hat{\beta}^{[m]} = \frac{1}{2} \log \left(\frac{1 - \text{err}^{[m]}}{\text{err}^{[m]}} \right)$
 - 6: Set: $w^{[m+1](i)} = w^{[m](i)} \cdot \exp \left(-\hat{\beta}^{[m]} \cdot y^{(i)} \cdot \hat{h}(\mathbf{x}^{(i)}) \right)$
 - 7: Normalize $w^{[m+1](i)}$ such that $\sum_{i=1}^n w^{[m+1](i)} = 1$
 - 8: **end for**
 - 9: Output: $\hat{f}(\mathbf{x}) = \sum_{m=1}^M \hat{\beta}^{[m]} \hat{b}^{[m]}(\mathbf{x})$
-

ADABOOST ILLUSTRATION

Example

- $n = 10$ observations and two features x_1 and x_2
- Tree stumps as base learners $b^{[m]}(\mathbf{x})$
- Balanced classification task with y encoded as $\{-1, +1\}$
- $M = 3$ iterations \Rightarrow initial weights $w^{[1](i)} = \frac{1}{10} \quad \forall i \in 1, \dots, 10.$



New observation weights:

- Prediction correct:
 $w^{[2](i)} = w^{[1](i)} \cdot \exp(-\hat{\beta}^{[1]} \cdot 1)$
 $\approx 0.065.$
- For 3 misclassified observations:
 $w^{[2](i)} = w^{[1](i)} \cdot \exp(-\hat{\beta}^{[1]} \cdot (-1))$
 $\approx 0.15.$

Iteration $m = 1$:

- $\text{err}^{[1]} = 0.3$
- $\hat{\beta}^{[1]} = \frac{1}{2} \log \left(\frac{1-0.3}{0.3} \right) \approx 0.42$

• After normalization:

- correctly classified: $w^{[2](i)} \approx 0.07$
- misclassified: $w^{[2](i)} \approx 0.17$

ADABOOST ILLUSTRATION

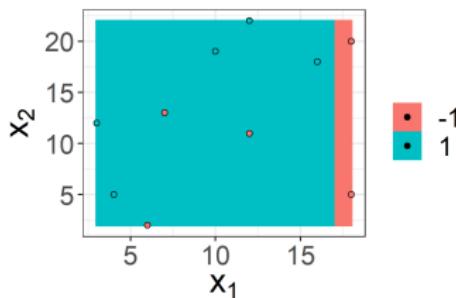


Iteration $m = 2$:

- $\text{err}^{[2]} = 3 \cdot 0.07 = 0.21$
- $\hat{\beta}^{[2]} \approx 0.65$

New observation weights:

- E.g., for 3 misclassified observations:
 $w^{[3](i)} = w^{[2](i)} \cdot \exp(-\hat{\beta}^{[1]} \cdot (-1)) \approx 0.14.$
- After normalization: $w^{[3](i)} \approx 0.17$
(misclassified)



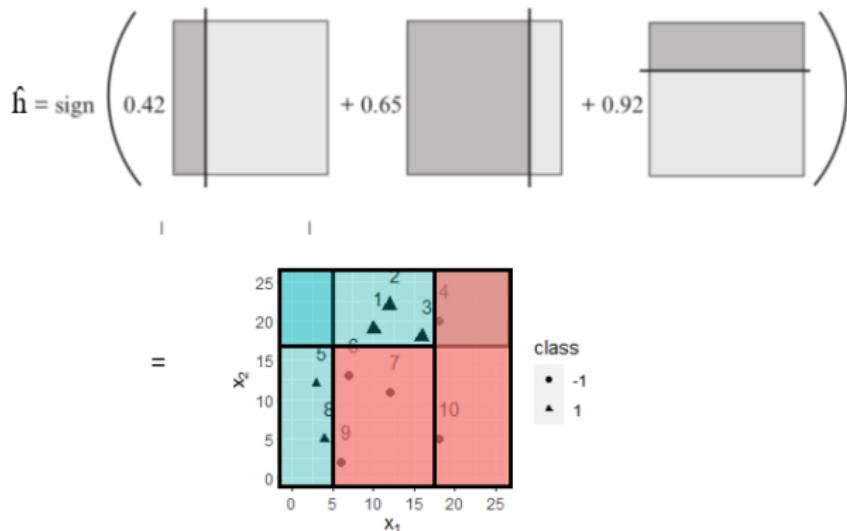
Iteration $m = 3$:

- $\text{err}^{[3]} = 3 \cdot 0.045 \approx 0.14$
- $\hat{\beta}^{[3]} \approx 0.92$

Note: the smaller the error rate of a base learner, the larger the weight, e.g., $\text{err}^{[3]} \approx 0.14 < \text{err}^{[1]} \approx 0.3$ and $\hat{\beta}^{[3]} \approx 0.92 > \hat{\beta}^{[1]} \approx 0.42$.

ADABOOST ILLUSTRATION

With $\hat{f}(\mathbf{x}) = \sum_{m=1}^M \hat{\beta}^{[m]} \hat{b}^{[m]}(\mathbf{x})$ and $h(\mathbf{x}) = \text{sign}(f(\mathbf{x})) \in \{-1, +1\}$, we get:



Hence, when all three base classifiers are combined, all samples are classified correctly.

BAGGING VS BOOSTING

Random forest

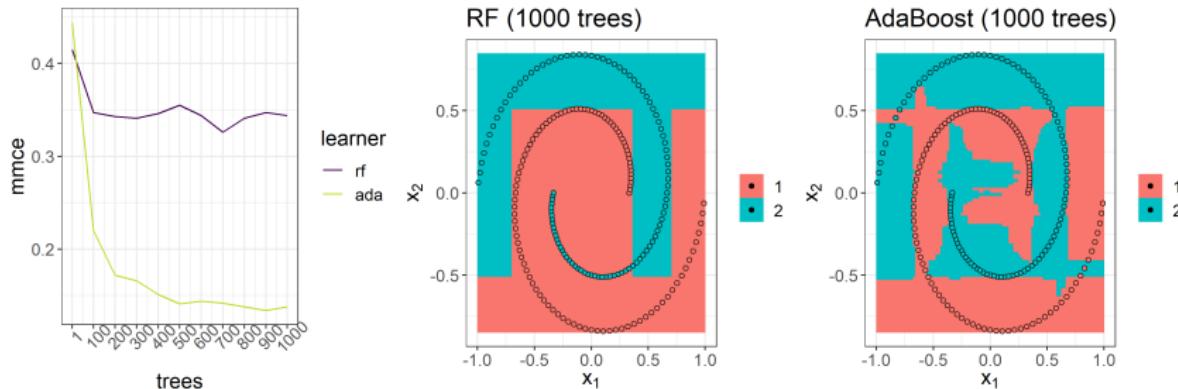
- Base learners are typically deeper decision trees (not only stumps!)
- Equal weights for BL
- BLs fitted independently
- Aim: variance reduction
- Tends **not** to overfit if ensemble size grows

AdaBoost

- BLs are weak learners, e.g., only stumps
- BL are weighted
- Sequential fitting of BLs
- Aim: loss reduction
- Tends to overfit with more iterations

BAGGING VS BOOSTING STUMPS

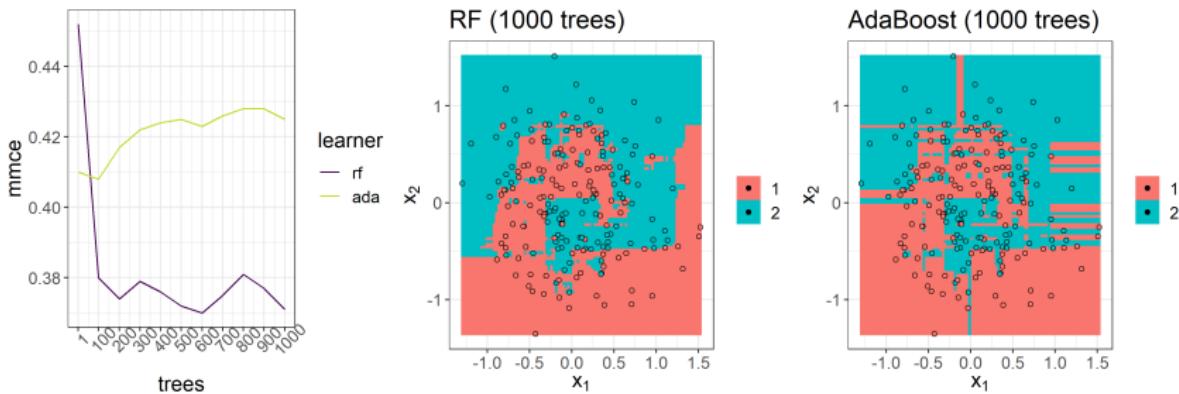
Random forest versus AdaBoost (both with stumps) on spirals data from mlbench ($n = 200$, $sd = 0$), with 5×5 repeated CV.



Weak learners do not work well with bagging as only variance, but no bias reduction happens.

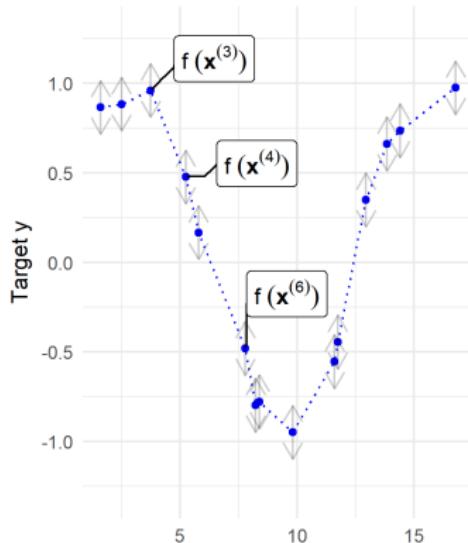
OVERFITTING BEHAVIOR

Historically, the overfitting behavior of AdaBoost was often discussed. Increasing standard deviation in spirals to $sd = 0.3$ and allowing for more flexibility in the base learners, AdaBoost overfits with increasing number of trees while the RF only saturates. The overfitting of AdaBoost here is quite typical as data is very noisy.



Introduction to Machine Learning

Gradient Boosting



Learning goals

- Understand idea of forward stagewise modelling
- Understand fitting process of gradient boosting for regression problems

FORWARD STAGEWISE ADDITIVE MODELING

Assume a regression problem for now (as this is simpler to explain); and assume a space of base learners \mathcal{B} .

We want to learn an additive model:

$$f(\mathbf{x}) = \sum_{m=1}^M \beta^{[m]} b(\mathbf{x}, \boldsymbol{\theta}^{[m]}).$$

Hence, we minimize the empirical risk:

$$\mathcal{R}_{\text{emp}}(f) = \sum_{i=1}^n L\left(y^{(i)}, f\left(\mathbf{x}^{(i)}\right)\right) = \sum_{i=1}^n L\left(y^{(i)}, \sum_{m=1}^M \beta^{[m]} b(\mathbf{x}, \boldsymbol{\theta}^{[m]})\right)$$

FORWARD STAGEWISE ADDITIVE MODELING

Why is gradient boosting a good choice for this problem?

- Because of the additive structure it is difficult to jointly minimize $\mathcal{R}_{\text{emp}}(f)$ w.r.t. $((\beta^{[1]}, \theta^{[1]}), \dots, (\beta^{[M]}, \theta^{[M]}))$, which is a very high-dimensional parameter space (though this is less of a problem nowadays, especially in the case of numeric parameter spaces).
- Considering trees as base learners is worse as we would have to grow M trees in parallel so they work optimally together as an ensemble.
- Stagewise additive modeling has nice properties, which we want to make use of, e.g. for regularization, early stopping, ...

FORWARD STAGewise ADDITIVE MODELING

Hence, we add additive components in a greedy fashion by sequentially minimizing the risk only w.r.t. the next additive component:

$$\min_{\beta, \theta} \sum_{i=1}^n L \left(y^{(i)}, \hat{f}^{[m-1]} \left(\mathbf{x}^{(i)} \right) + \beta b \left(\mathbf{x}^{(i)}, \theta \right) \right)$$

Doing this iteratively is called **forward stagewise additive modeling**.

Algorithm Forward Stagewise Additive Modeling.

- 1: Initialize $\hat{f}^{[0]}(\mathbf{x})$ with loss optimal constant model
 - 2: **for** $m = 1 \rightarrow M$ **do**
 - 3: $(\hat{\beta}^{[m]}, \hat{\theta}^{[m]}) = \arg \min_{\beta, \theta} \sum_{i=1}^n L \left(y^{(i)}, \hat{f}^{[m-1]} \left(\mathbf{x}^{(i)} \right) + \beta b \left(\mathbf{x}^{(i)}, \theta \right) \right)$
 - 4: Update $\hat{f}^{[m]}(\mathbf{x}) \leftarrow \hat{f}^{[m-1]}(\mathbf{x}) + \hat{\beta}^{[m]} b \left(\mathbf{x}, \hat{\theta}^{[m]} \right)$
 - 5: **end for**
-

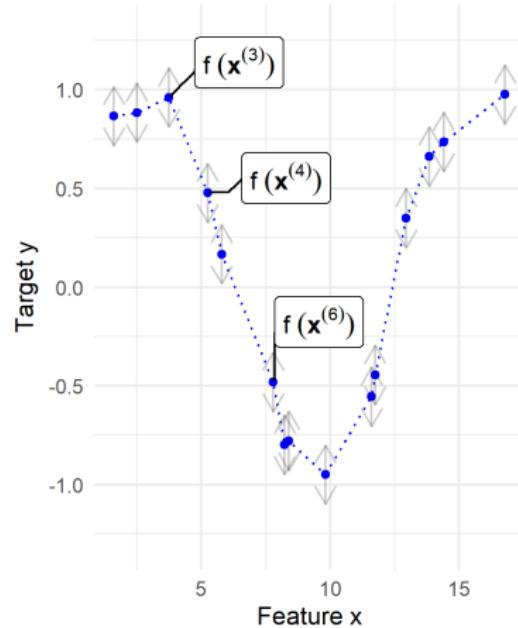
GRADIENT BOOSTING

This is not really an algorithm, but an abstract principle. To find $b(\mathbf{x}, \theta^{[m]})$ and $\beta^{[m]}$, we use gradient descent, but in function space!

Consider a model f whose predictions we can arbitrarily define for each training $\mathbf{x}^{(i)}$, i.e., f is a finite vector

$$\left(f\left(\mathbf{x}^{(1)}\right), \dots, f\left(\mathbf{x}^{(n)}\right) \right)^\top$$

This implies n parameters $f(\mathbf{x}^{(i)})$ (and the model would provide no generalization...). Also, we let's assume L to be differentiable.

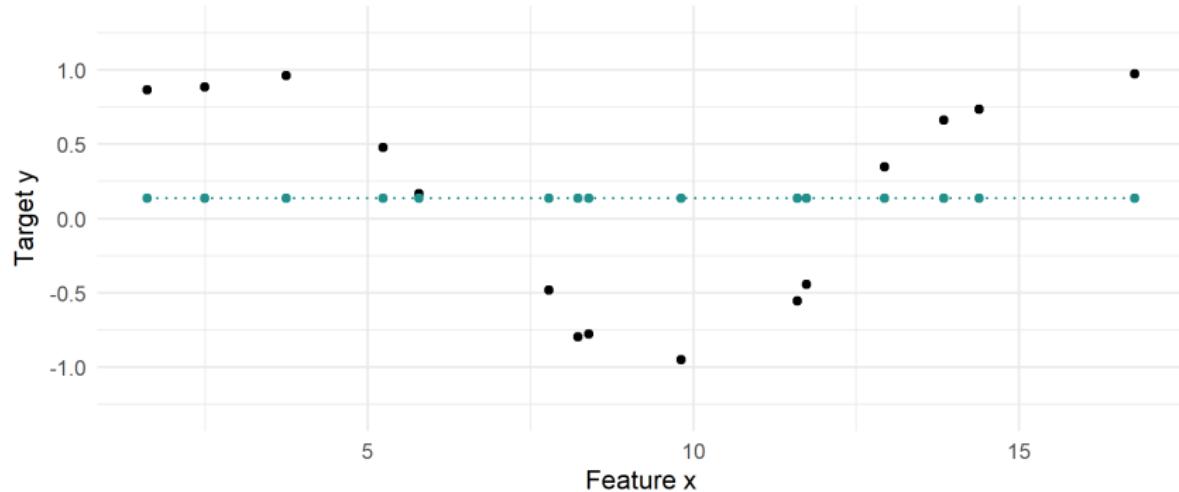


GRADIENT BOOSTING

Aim: Define a movement in function space so we can push our current function towards the data points.

Given: Regression problem with one feature x and target variable y .

Initialization: Set all parameters to the optimal constant value (e.g., the mean of y for $L2$).



PSEUDO RESIDUALS

How do we distort our f to move it towards the labels and reduce risk?
Let's minimize risk with GD.

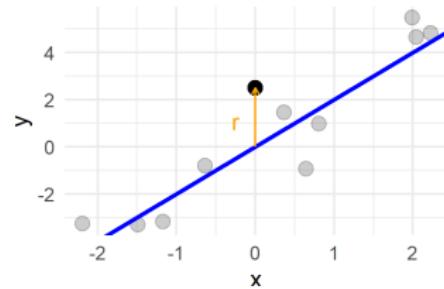
So, we calculate the (negative) gradient of the risk for each parameter, which (weirdly) here are the outputs $f(\mathbf{x}^{(i)})$ (0 if $i \neq j$):

$$\tilde{r}^{(i)} = -\frac{\partial \mathcal{R}_{\text{emp}}}{\partial f(\mathbf{x}^{(i)})} = -\frac{\partial \sum_j L(y^{(j)}, f(\mathbf{x}^{(j)}))}{\partial f(\mathbf{x}^{(i)})} = -\frac{\partial L(y^{(i)}, f(\mathbf{x}^{(i)}))}{\partial f(\mathbf{x}^{(i)})}.$$

At each point, we would like to change the output via: $\tilde{r}(f) = -\frac{\partial L(y, f)}{\partial f}$.

L2 Example: The PRs match
the usual residuals:

$$\tilde{r}(f) = -\frac{\partial 0.5(y - f)^2}{\partial f} = y - f$$



BOOSTING AS GRADIENT DESCENT

Combining this with “forward stagewise modeling”, we are at $f^{[m-1]}$ during minimization. Here, we calculate the direction of the negative gradient or vector of PRs:

$$\tilde{r}^{[m](i)} = - \left[\frac{\partial L(y^{(i)}, f(\mathbf{x}^{(i)}))}{\partial f(\mathbf{x}^{(i)})} \right]_{f=f^{[m-1]}}$$

The gradient descent update for each vector component of f is:

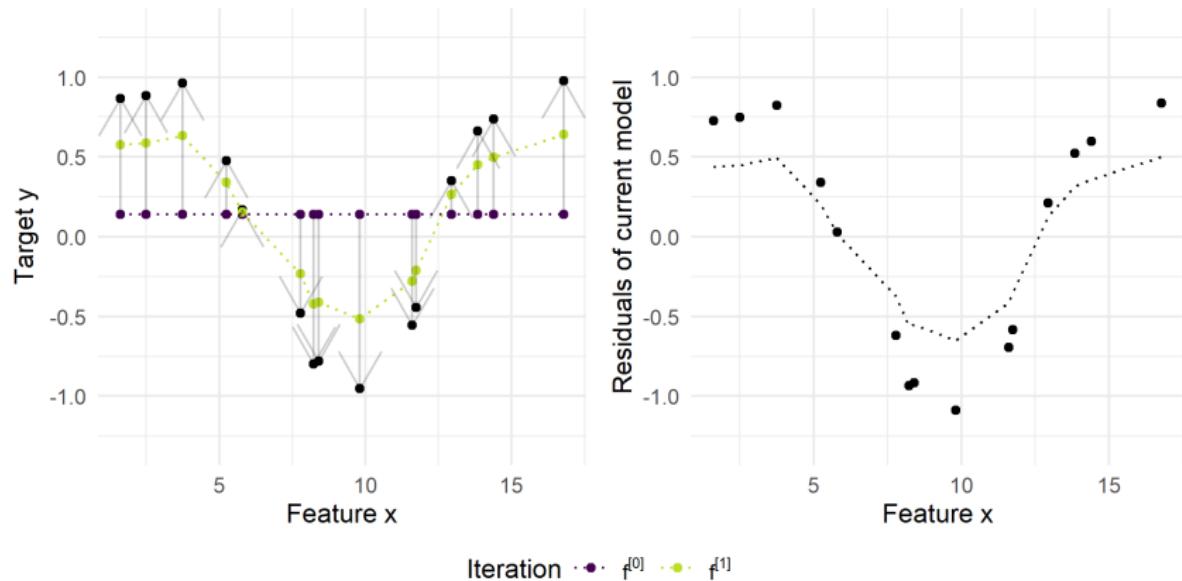
$$f^{[m]}(\mathbf{x}^{(i)}) = f^{[m-1]}(\mathbf{x}^{(i)}) + \beta \tilde{r}^{[m](i)}.$$

Like this, we should “nudge” f in the direction best risk reduction.

GRADIENT BOOSTING

Iteration 1:

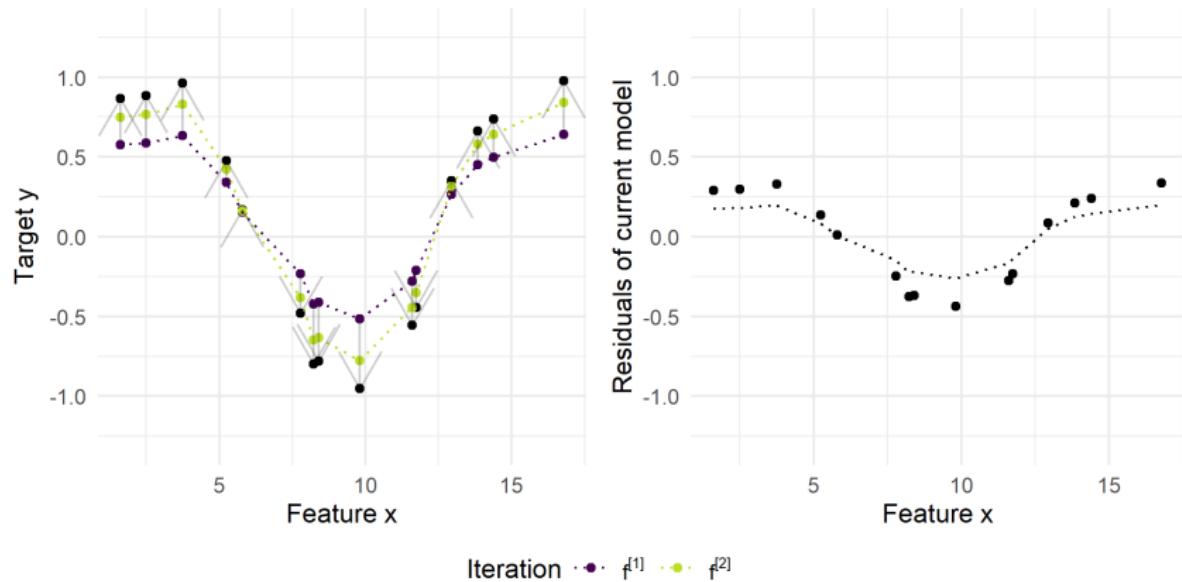
Let's move our function $f(\mathbf{x}^{(i)})$ a fraction towards the pseudo-residuals with a learning rate of $\beta = 0.6$.



GRADIENT BOOSTING

Iteration 2:

Let's move our function $f(\mathbf{x}^{(i)})$ a fraction towards the pseudo-residuals with a learning rate of $\beta = 0.6$.



GRADIENT BOOSTING

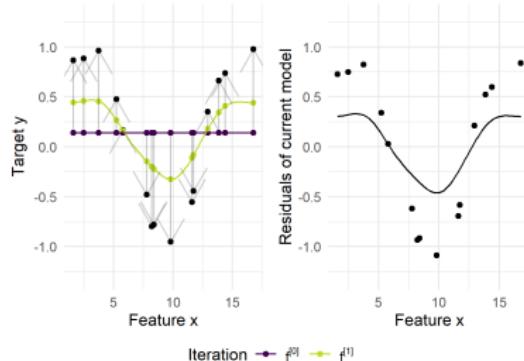
As said, such a model parameterization is pointless.

So, we restrict our additive components to $b(\mathbf{x}, \theta^{[m]}) \in \mathcal{B}$.

The pseudo-residuals are calculated exactly as stated above, then we fit a simple model $b(\mathbf{x}, \theta^{[m]})$ to them:

$$\hat{\theta}^{[m]} = \arg \min_{\theta} \sum_{i=1}^n \left(\tilde{r}^{[m](i)} - b(\mathbf{x}^{(i)}, \theta) \right)^2.$$

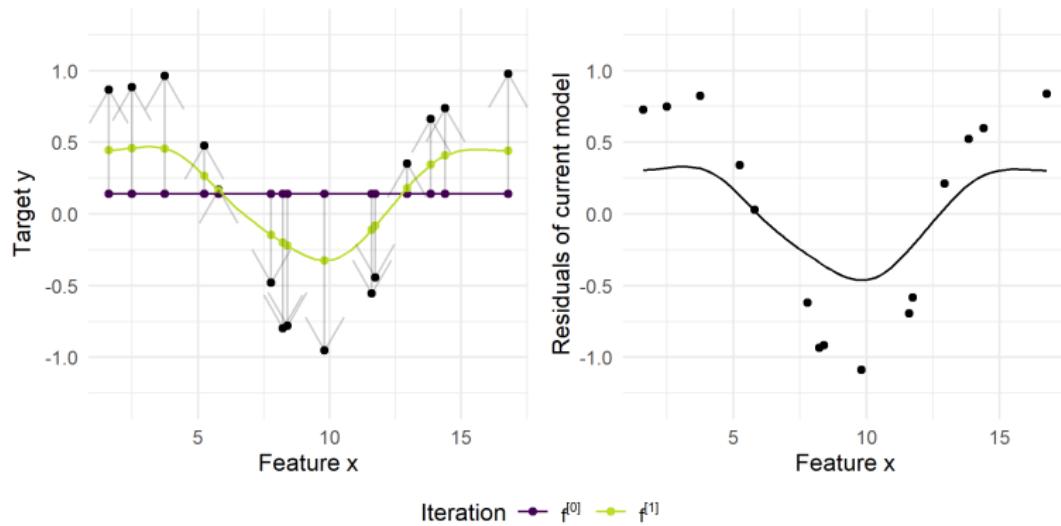
So, evaluated on the training data, $b(\mathbf{x}, \theta^{[m]})$ corresponds as closely as possible to the negative risk gradient and generalizes over \mathcal{X} .



GRADIENT BOOSTING

In a nutshell: One boosting iteration is exactly one approximated gradient descent step in function space, which minimizes the empirical risk as much as possible.

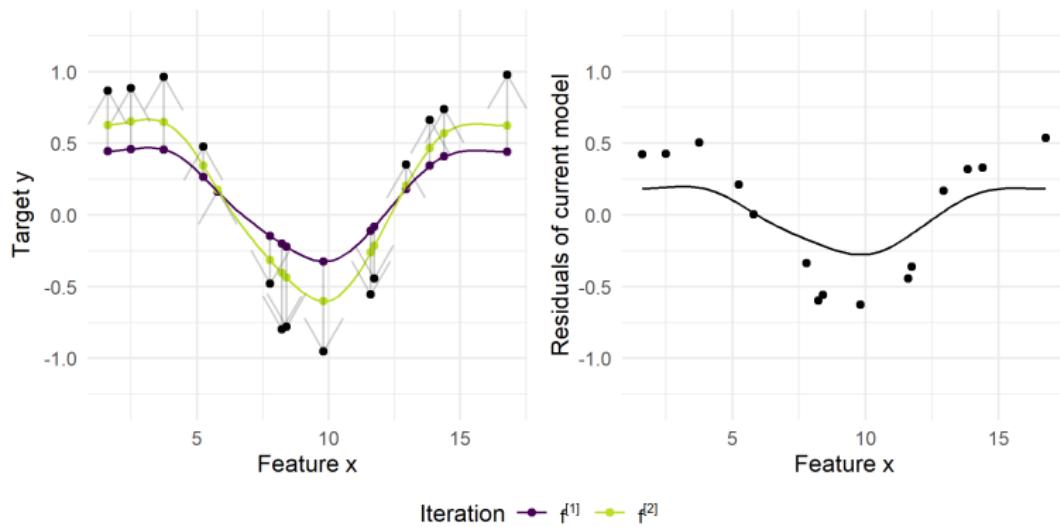
Iteration 1:



GRADIENT BOOSTING

Instead of moving the function values for each observation by a fraction closer to the observed data, we fit a regression base learner to the pseudo-residuals (right plot).

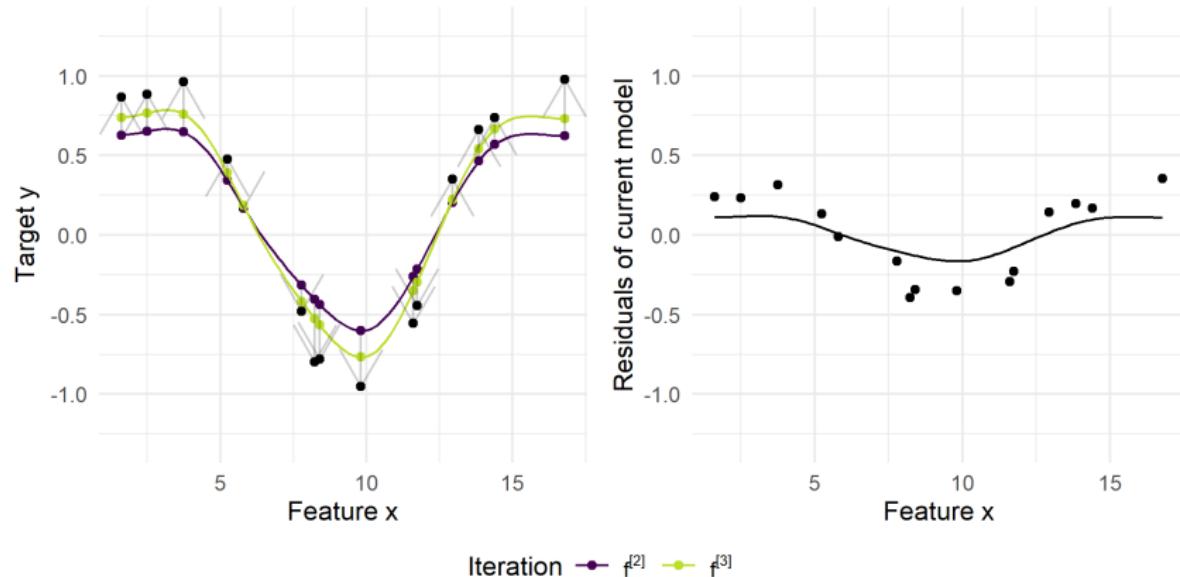
Iteration 2:



GRADIENT BOOSTING

This BL is added to the of the ensemble, weighted by a learning rate (here: $\beta = 0.4$). Then we iterate.

Iteration 3:



GRADIENT BOOSTING ALGORITHM

Algorithm Gradient Boosting Algorithm.

- 1: Initialize $\hat{f}^{[0]}(\mathbf{x}) = \arg \min_{\theta} \sum_{i=1}^n L(y^{(i)}, b(\mathbf{x}^{(i)}, \theta))$
 - 2: **for** $m = 1 \rightarrow M$ **do**
 - 3: For all i : $\tilde{r}^{[m](i)} = - \left[\frac{\partial L(y^{(i)}, f(\mathbf{x}^{(i)}))}{\partial f(\mathbf{x}^{(i)})} \right]_{f=\hat{f}^{[m-1]}}$
 - 4: Fit a regression base learner to the pseudo-residuals $\tilde{r}^{[m](i)}$:
 - 5: $\hat{\theta}^{[m]} = \arg \min_{\theta} \sum_{i=1}^n (\tilde{r}^{[m](i)} - b(\mathbf{x}^{(i)}, \theta))^2$
 - 6: Set $\beta^{[m]}$ to β being a small constant value or via line search
 - 7: Update $\hat{f}^{[m]}(\mathbf{x}) = \hat{f}^{[m-1]}(\mathbf{x}) + \beta^{[m]} b(\mathbf{x}, \hat{\theta}^{[m]})$
 - 8: **end for**
 - 9: Output $\hat{f}(\mathbf{x}) = \hat{f}^{[M]}(\mathbf{x})$
-

Note that we also initialize the model in a loss-optimal manner.

LINE SEARCH

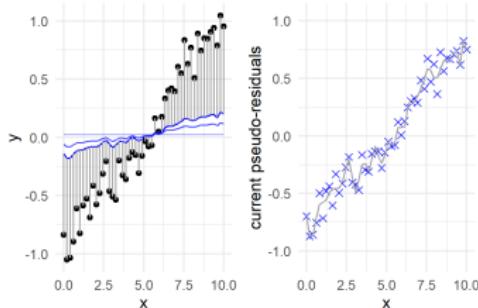
The learning rate, as always, influences how we converge. Although a small constant LR is commonly used, we can also run line search,

$$\hat{\beta}^{[m]} = \arg \min_{\beta} \sum_{i=1}^n L(y^{(i)}, f^{[m-1]}(\mathbf{x}) + \beta b(\mathbf{x}, \hat{\theta}^{[m]}))$$

Alternatively, an (inexact) backtracking line search can be used to find the $\beta^{[m]}$ that minimizes the above equation.

Introduction to Machine Learning

Gradient Boosting - Illustration



Learning goals

- Understand impact of different loss functions and
- Understand impact of different base learners for regression

GRADIENT BOOSTING ILLUSTRATION - GAM

We now compare different loss functions and base learners. We start with a GAM as base learner and compare the $L2$ loss with the $L1$ loss.

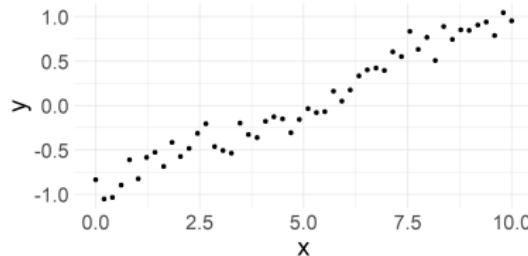
Reminder: Pseudo-residuals

- $L2$: $\tilde{r}(f) = r(f) = y - f(\mathbf{x})$
- $L1$: $\tilde{r}(f) = \text{sign}(y - f(\mathbf{x}))$

We consider a regression task with a single feature x and target y , with the following true underlying relationship:

$$y^{(i)} = -1 + 0.2 \cdot x^{(i)} + 0.1 \cdot \sin(x^{(i)}) + \epsilon^{(i)}$$

with $n = 50$ and $\epsilon^{(i)} \sim \mathcal{N}(0, 0.1)$ $\forall i \in \{1, \dots, n\}$

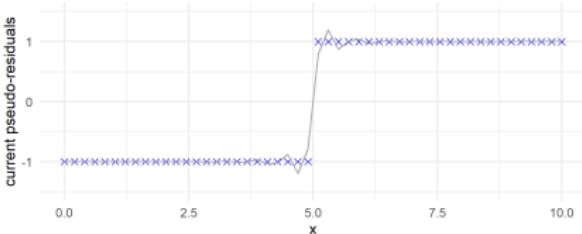
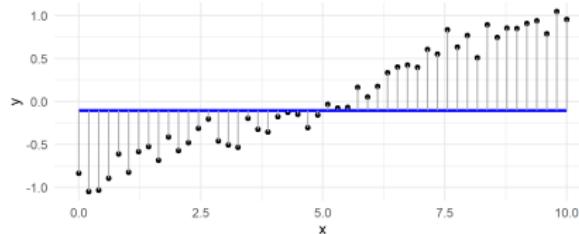
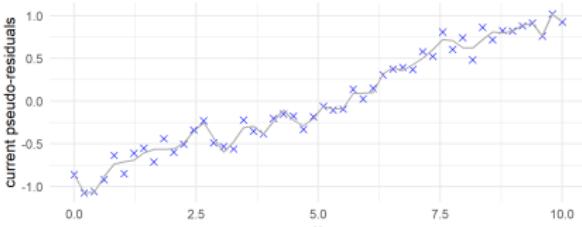
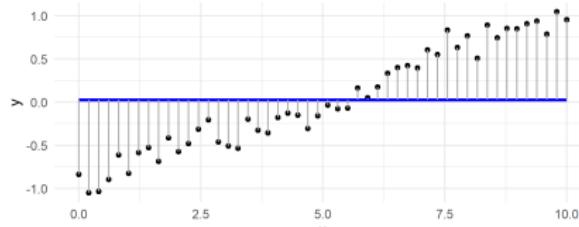


GRADIENT BOOSTING ILLUSTRATION - GAM

- ① We start with the simplest model, the optimal constant – mean of the target variable in the case of $L2$ loss and median in the case of $L1$ loss.
- ② We improve the model by calculating the pointwise pseudo-residuals on the training data, and fit a GAM on the residuals.
 - ① The GAM base learners model the conditional mean via cubic B -splines with 40 knots.
 - ② In each step, the GAM fitted on the current pseudo-residuals is multiplied by a constant learning rate of 0.2 and added to the previous model.
 - ③ This procedure is repeated multiple times.

GAM WITH $L2$ VS $L1$ LOSS

Top: $L2$ loss, bottom: $L1$ loss

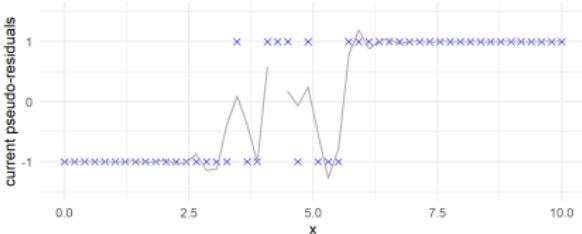
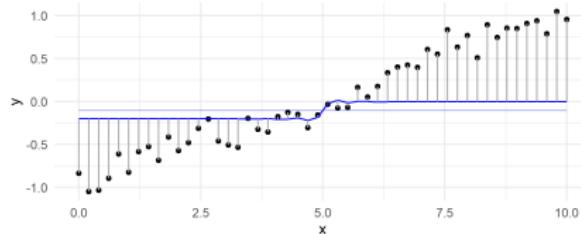
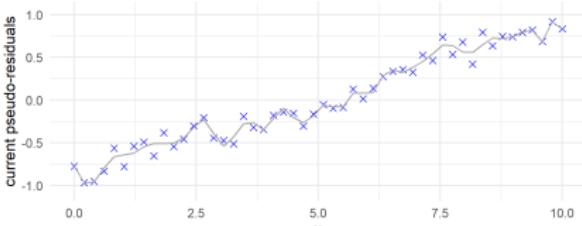
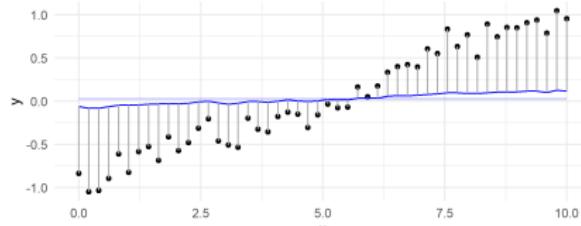


Iteration 1

The nature of the pseudo-residuals affects gradual model fit: as $L1$ only considers residuals' sign, the corresponding base learners are less affected by very large or small values compared to $L2$ and hence lead to more moderate changes.

GAM WITH $L2$ VS $L1$ LOSS

Top: $L2$ loss, bottom: $L1$ loss

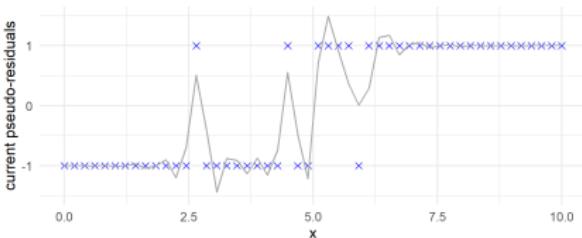
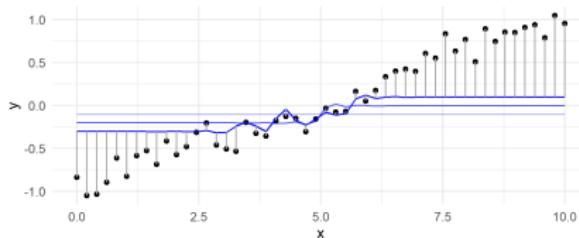
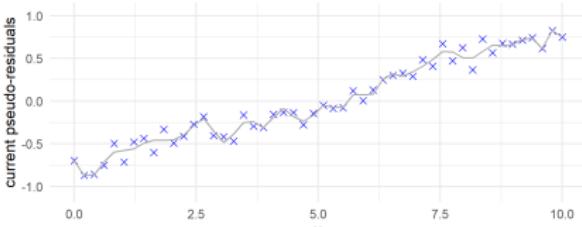
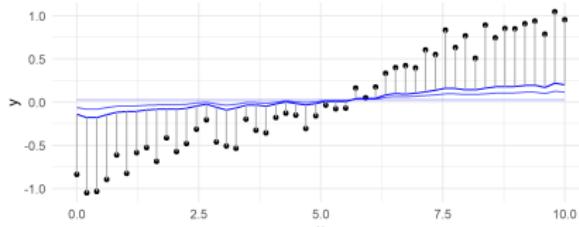


Iteration 2

The nature of the pseudo-residuals affects gradual model fit: as $L1$ only considers residuals' sign, the corresponding base learners are less affected by very large or small values compared to $L2$ and hence lead to more moderate changes.

GAM WITH $L2$ VS $L1$ LOSS

Top: $L2$ loss, bottom: $L1$ loss

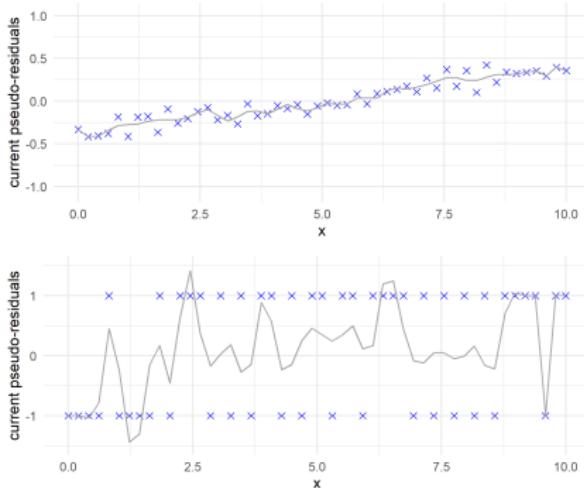
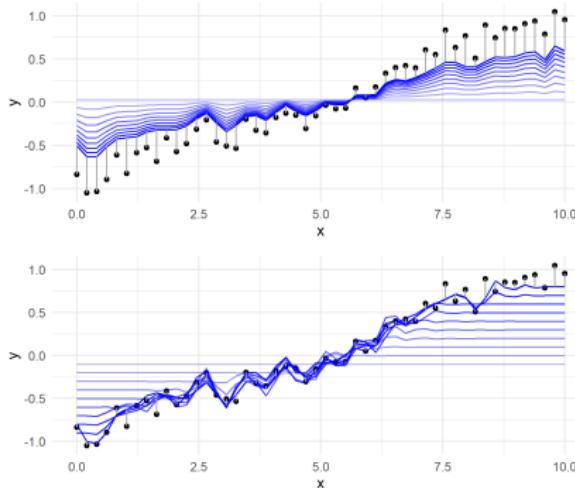


Iteration 3

The nature of the pseudo-residuals affects gradual model fit: as $L1$ only considers residuals' sign, the corresponding base learners are less affected by very large or small values compared to $L2$ and hence lead to more moderate changes.

GAM WITH L_2 VS L_1 LOSS

Top: L_2 loss, bottom: L_1 loss

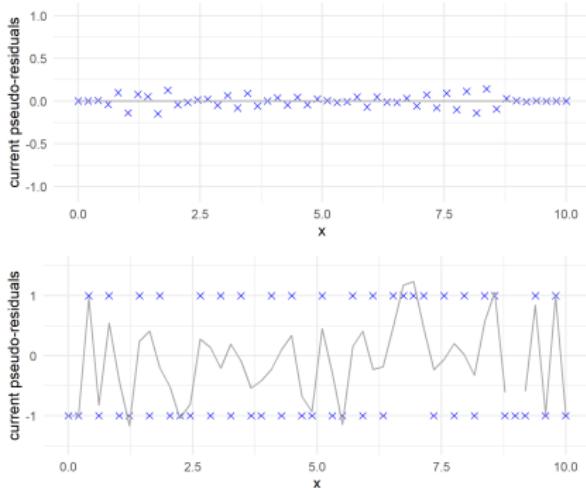
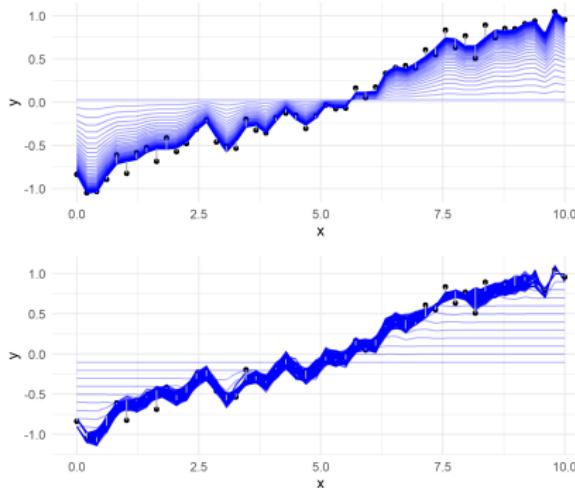


Iteration 10

The nature of the pseudo-residuals affects gradual model fit: as L_1 only considers residuals' sign, the corresponding base learners are less affected by very large or small values compared to L_2 and hence lead to more moderate changes.

GAM WITH $L2$ VS $L1$ LOSS

Top: $L2$ loss, bottom: $L1$ loss

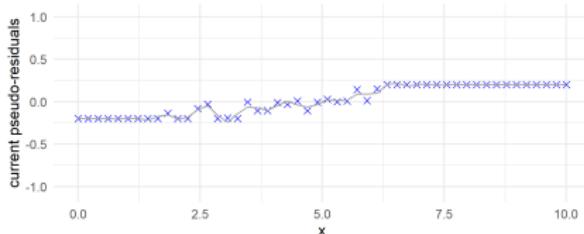
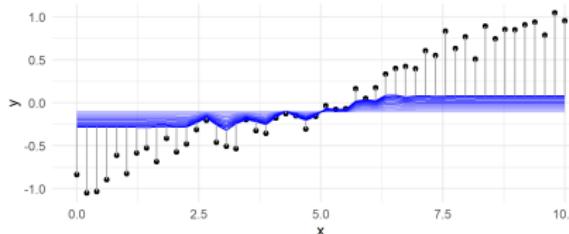
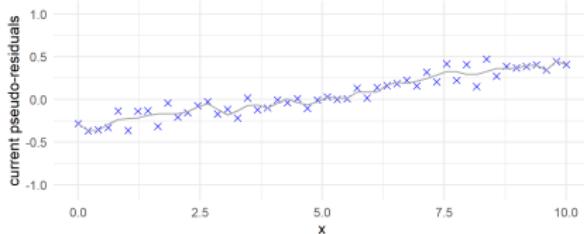
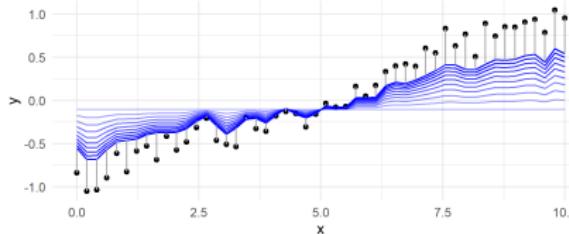


Iteration 100

The nature of the pseudo-residuals affects gradual model fit: as $L1$ only considers residuals' sign, the corresponding base learners are less affected by very large or small values compared to $L2$ and hence lead to more moderate changes.

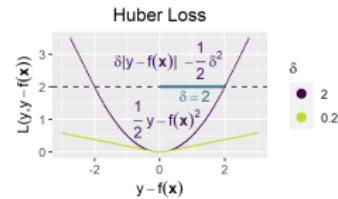
GAM WITH HUBER LOSS

We can also use Huber loss, which is closer to L_2 for large δ values and closer to L_1 for smaller δ values. Top: $\delta = 2$, bottom: $\delta = 0.2$.



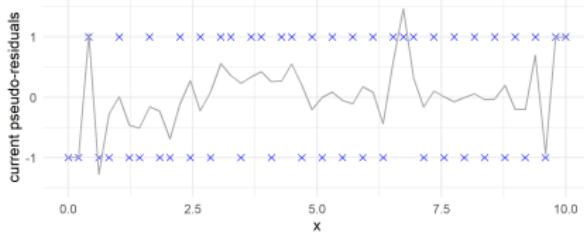
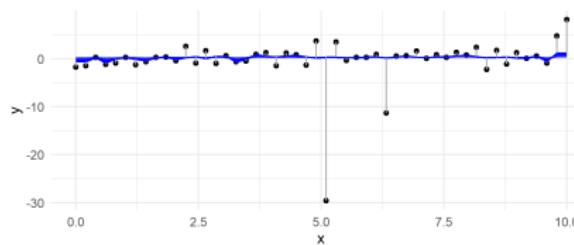
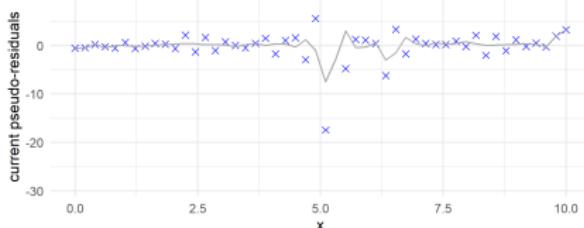
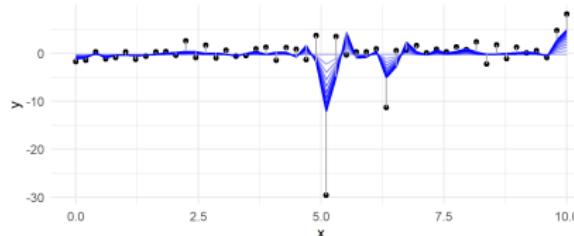
Iteration 10

We see how for smaller δ (bottom) pseudo-residuals are often effectively bounded, resulting in L_1 -like behavior, while the upper plot more closely resembles L_2 loss.



GAM WITH OUTLIERS

Instead of normally distributed noise we can assume a t -distribution, leading to outliers in the observed target values. Top: L_2 , bottom: L_1 .

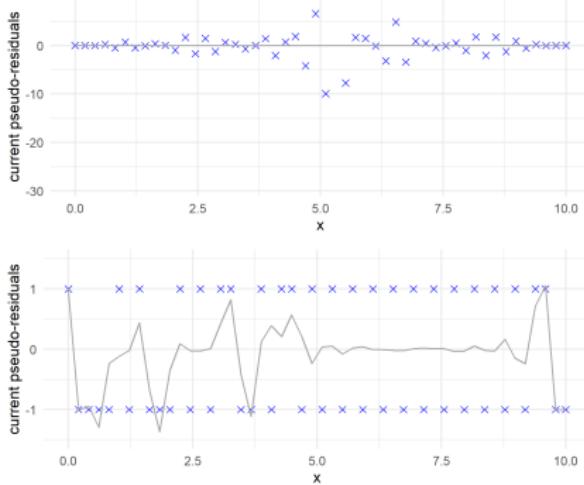
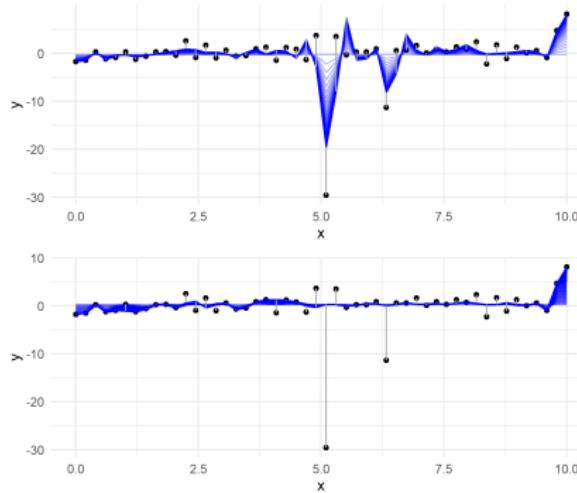


Iteration 10

L_2 loss is affected by outliers rather strongly, whereas L_1 solely considers residuals' sign and not their magnitude, resulting in a more robust model.

GAM WITH OUTLIERS

Instead of normally distributed noise we can assume a t -distribution, leading to outliers in the observed target values. Top: L_2 , bottom: L_1 .

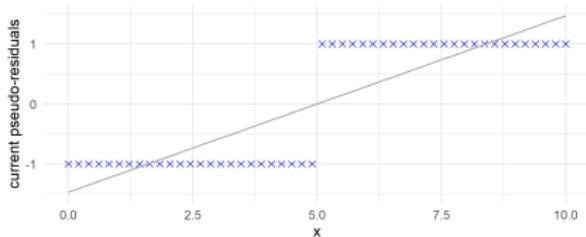
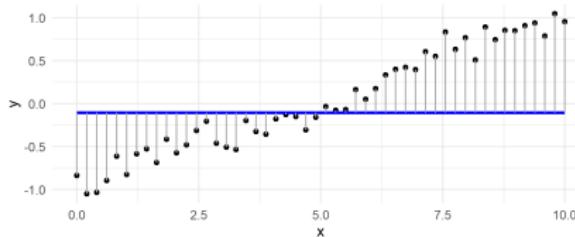
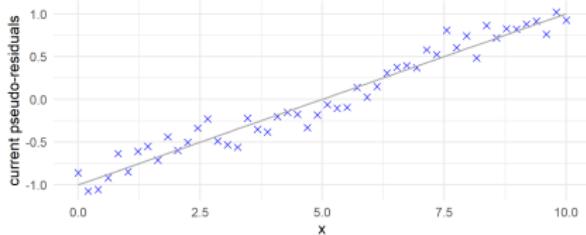
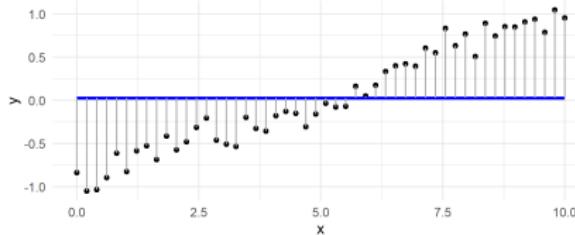


Iteration 100

L_2 loss is affected by outliers rather strongly, whereas L_1 solely considers residuals' sign and not their magnitude, resulting in a more robust model.

LM WITH $L2$ VS $L1$ LOSS

Instead of using a GAM as base learner we now use a simple linear model. Top: $L2$, bottom: $L1$.

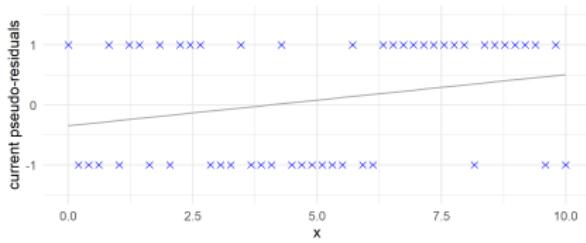
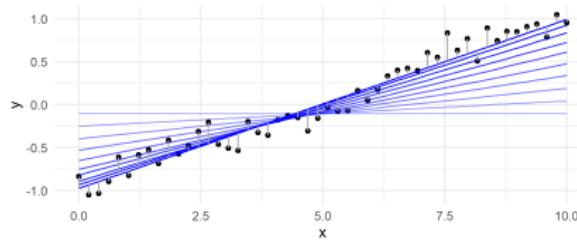
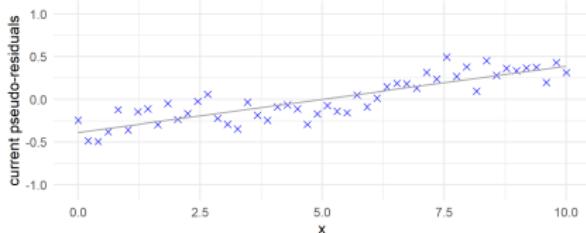
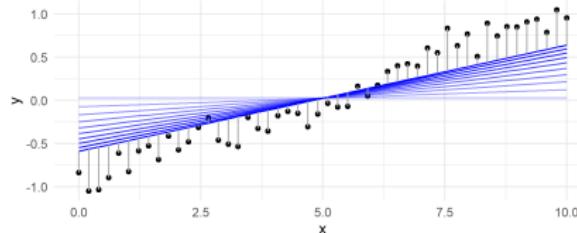


Iteration 1

For $L2$, as $\tilde{r}(f) = r(f)$, we find the optimal model in the very first iteration; only the multiplicative learning rate slows down optimization. In the $L1$ case the base learner LMs fit pseudo-residuals that differ from model residuals, leading to a less monotonic optimization path.

LM WITH $L2$ VS $L1$ LOSS

Instead of using a GAM as base learner we now use a simple linear model. Top: $L2$, bottom: $L1$.

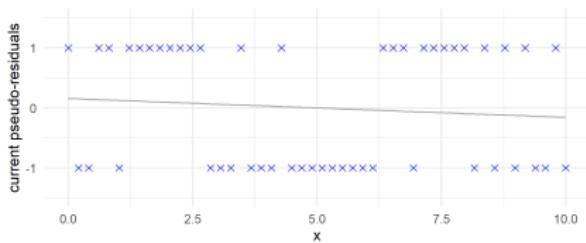
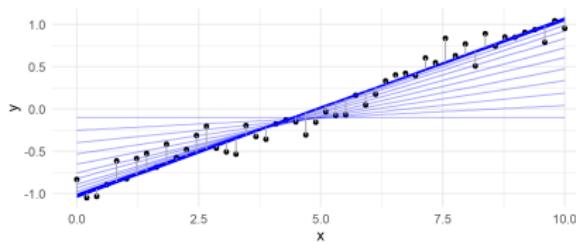
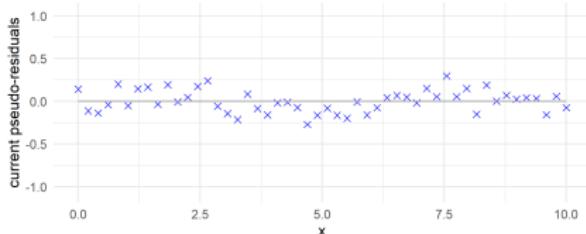
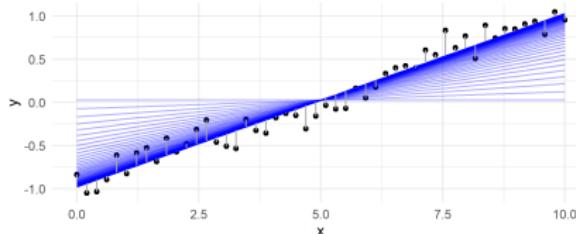


Iteration 10

For $L2$, as $\tilde{r}(f) = r(f)$, we find the optimal model in the very first iteration; only the multiplicative learning rate slows down optimization. In the $L1$ case the base learner LMs fit pseudo-residuals that differ from model residuals, leading to a less monotonic optimization path.

LM WITH $L2$ VS $L1$ LOSS

Instead of using a GAM as base learner we now use a simple linear model. Top: $L2$, bottom: $L1$.



Iteration 100

For $L2$, as $\tilde{r}(f) = r(f)$, we find the optimal model in the very first iteration; only the multiplicative learning rate slows down optimization. In the $L1$ case the base learner LMs fit pseudo-residuals that differ from model residuals, leading to a less monotonic optimization path.

LM: GB VS GD

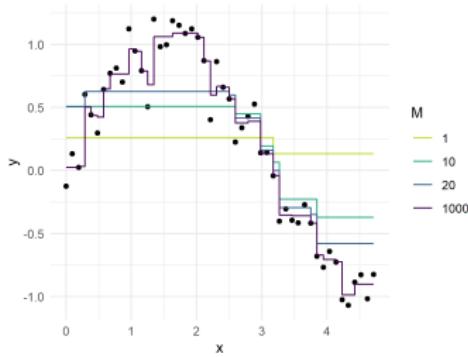
- As we have seen, boosting with LMs and $L2$ loss simply approaches the closed-form OLS solution with a speed determined by the learning rate β .
- This is perfectly equivalent to fitting an LM via **gradient descent**, as a gradient step in parameter space is a gradient step in function space for this specific case.
- Recall the parameter update for GD with learning rate β :
$$\theta^{[m+1]} \leftarrow \theta^{[m]} - \beta \cdot \nabla_{\theta^{[m]}} \mathcal{R}_{\text{emp}}(\theta^{[m]}) = \theta^{[m]} + \beta(-\mathbf{X}^T \mathbf{y} + \mathbf{X}^T \mathbf{X} \theta^{[m]}).$$
- Now compute the update for a boosted LM with current model $\mathbf{X}\theta^{[m]}$ (note that adding a linear base learner to an LM is equivalent to summing parameters):

$$\begin{aligned}\frac{\partial}{\partial \theta^{[m+1]}} \left\| (\mathbf{y} - \mathbf{X}\theta^{[m]}) - \mathbf{X}\theta^{[m+1]} \right\|_2^2 &= 0 \\ -2\mathbf{X}^T(\mathbf{y} - \mathbf{X}\theta^{[m]}) + 2\mathbf{X}^T\mathbf{X}\theta^{[m+1]} &= 0 \\ \theta^{[m+1]} &= (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T (\mathbf{y} - \mathbf{X}\theta^{[m]}) \\ \theta^{[m+1]} &= (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y} - (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{X} \theta^{[m]} \\ \theta^{[m+1]} &= (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y} - \theta^{[m]} \\ \theta^{[m+1]} &= -\mathbf{X}^T \mathbf{y} + \mathbf{X}^T \mathbf{X} \theta^{[m]}.\end{aligned}$$

$$\Rightarrow \hat{f}^{[m+1]} = \mathbf{X}\tilde{\theta}^{[m+1]} = \mathbf{X} \left(\theta^{[m]} + \beta(-\mathbf{X}^T \mathbf{y} + \mathbf{X}^T \mathbf{X} \theta^{[m]}) \right).$$

Introduction to Machine Learning

Gradient Boosting: Regularization



Learning goals

- Learn about three main regularization options: number of iterations, tree depth and shrinkage
- Understand how regularization influences model fit

REGULARIZATION AND SHRINKAGE

If GB runs for a large number of iterations, it can overfit due to its aggressive loss minimization.

Options for regularization:

- Limit the number of boosting iterations M (“early stopping”), i.e., limit the number of additive components.
- Limit the depth of the trees. This can also be interpreted as choosing the order of interaction.
- Shorten the learning rate $\beta^{[m]}$ of each iteration.

Note: If $\beta^{[m]}$ is found via line search, we multiply the next base learner by an additional constant **shrinkage parameter** $\nu \in (0, 1]$ to shorten the step length. In the case of a (commonly used) constant learning rate β , ν can be neglected by choosing a smaller value for β . Hence, on the following slides, we call β the shrinkage parameter or learning rate.

REGULARIZATION AND SHRINKAGE

Obviously, the optimal values for M and β strongly depend on each other: by increasing M one can use a smaller value for β and vice versa.

In practice, a common recommendation to find a good first model without tuning both parameters is thus to choose β quite small and determine M by cross-validation.

It is probably best to tune all three parameters (M and β as well as the tree depths) jointly based on the training data via cross-validation or a related method.

STOCHASTIC GRADIENT BOOSTING

Stochastic gradient boosting is a minor modification to boosting to incorporate the advantages of bagging into the method. The idea was formulated quite early by Breiman.

Instead of fitting on all the data points, a random subsample is drawn in each iteration.

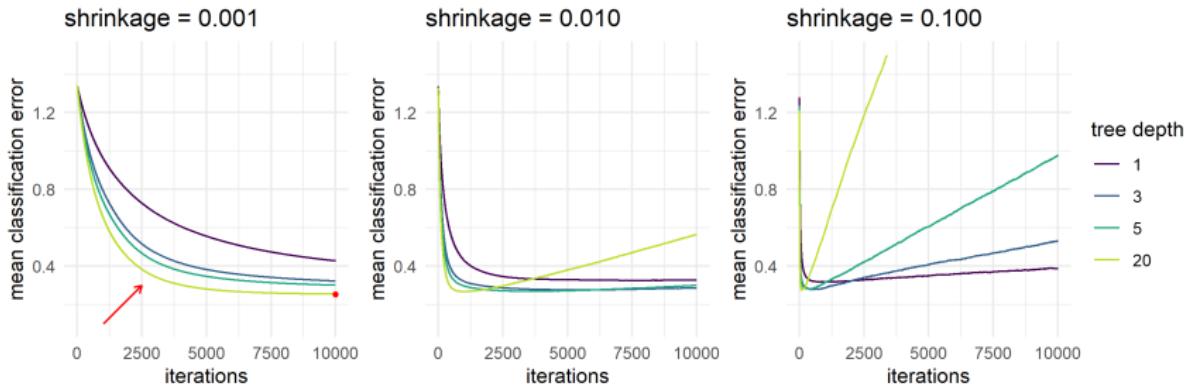
Especially for small training sets, this simple modification often leads to substantial empirical improvements. How large the improvements are depends on data structure, size of the dataset, base learner and size of the subsamples (so this is another tuning parameter).

EXAMPLE: SPAM DETECTION

We fit a gradient boosting model for different parameter values:

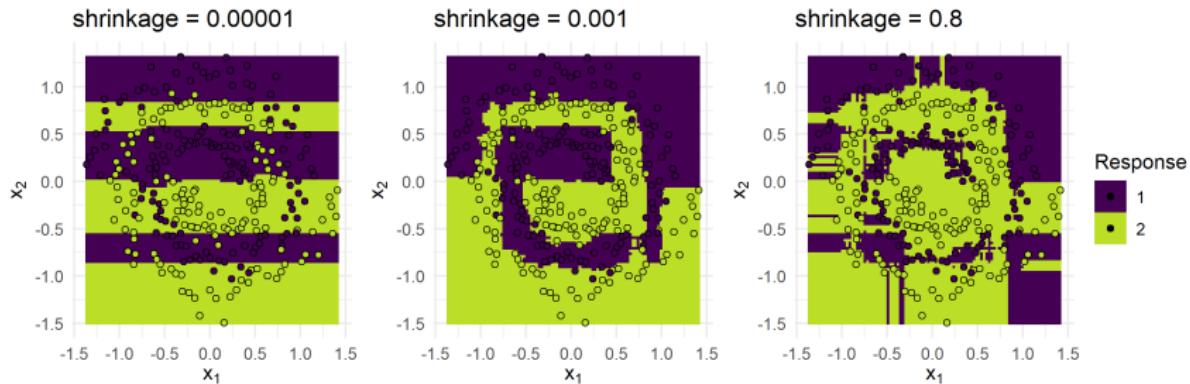
Parameter name	Values
Loss	Bernoulli (for classification)
Number of trees M	$\{0, 1, \dots, 10000\}$
Shrinkage β	$\{0.001, 0.01, 0.1\}$
Max. tree depth	$\{1, 3, 5, 20\}$

We consider the 3-CV test error to find the optimal parameters (red):



EXAMPLE: SPIRALS DATA

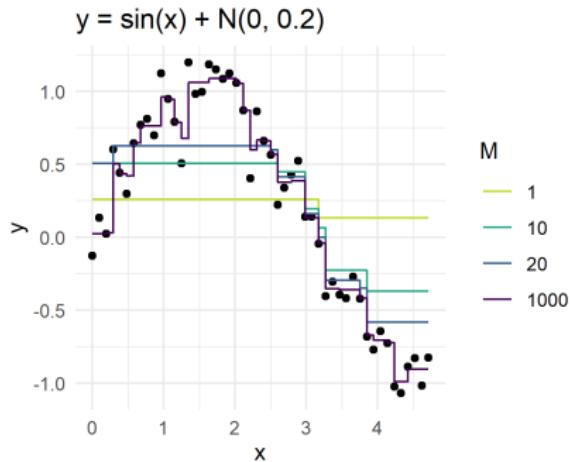
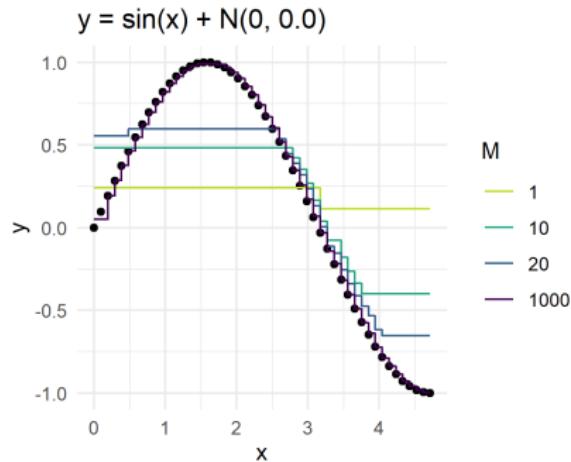
Consider the spirals data set with $sd = 0.1$ and $n = 300$. We examine the effect of the shrinkage parameter, holding the number of trees fixed at 10k and choosing a tree depth of 10:



We observe an oversmoothing effect in the left scenario with strong regularization (i.e., very small learning rate) and overfitting when regularization is too weak (right). $\beta = 0.001$ yields a pretty good fit.

EXAMPLE: SINUSOIDAL DATA

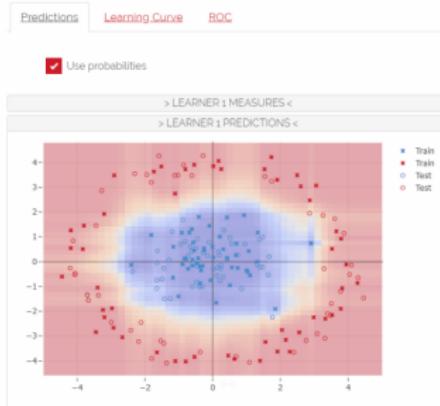
Here we choose a tree-stump base learner to model univariate data with sinusoidal behavior.



- Iterating this very simple base learner achieves a rather nice approximation of a smooth model in the end.
- Again, the model overfits the noisy case with less regularization.

Introduction to Machine Learning

Gradient Boosting for Classification



Learning goals

- Transferring gradient boosting for regression to binary classification problems
- Introducing gradient boosting for multiclass problems

BINARY CLASSIFICATION

For $\mathcal{Y} = \{0, 1\}$, we simply have to select an appropriate loss function, so let us use Bernoulli loss as in logistic regression:

$$L(y, f(\mathbf{x})) = -y \cdot f(\mathbf{x}) + \log(1 + \exp(f(\mathbf{x}))).$$

Then,

$$\begin{aligned}\tilde{r}(f) &= -\frac{\partial L(y, f(\mathbf{x}))}{\partial f(\mathbf{x})} \\ &= y - \frac{\exp(f(\mathbf{x}))}{1 + \exp(f(\mathbf{x}))} \\ &= y - \frac{1}{1 + \exp(-f(\mathbf{x}))} = y - s(f(\mathbf{x})).\end{aligned}$$

Here, $s(f(\mathbf{x}))$ is the logistic function, applied to a scoring model. Hence, effectively, the pseudo-residuals are $y - \pi(\mathbf{x})$.

Through $\pi(\mathbf{x}) = s(f(\mathbf{x}))$ we can also estimate posterior probabilities.

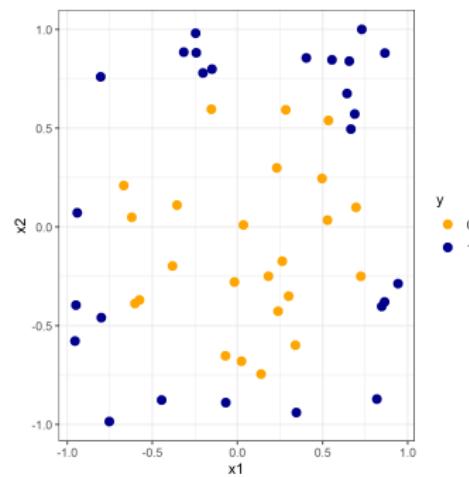
BINARY CLASSIFICATION

- Using this loss function, we can simply run GB as for regression.
NB: Also here, we fit regression base learners against our numerical vector of pseudo-residuals with L_2 loss.
- We could also have used the exponential loss for classification with GB. It can be shown that the resulting GB algorithm is basically equivalent to AdaBoost. In practice there is no big difference, although Bernoulli loss makes a bit more sense from a theoretical (maximum likelihood) perspective.
- It follows that GB is a generalization of AdaBoost which can also use other loss functions and be used for different ML scenarios.

EXAMPLE

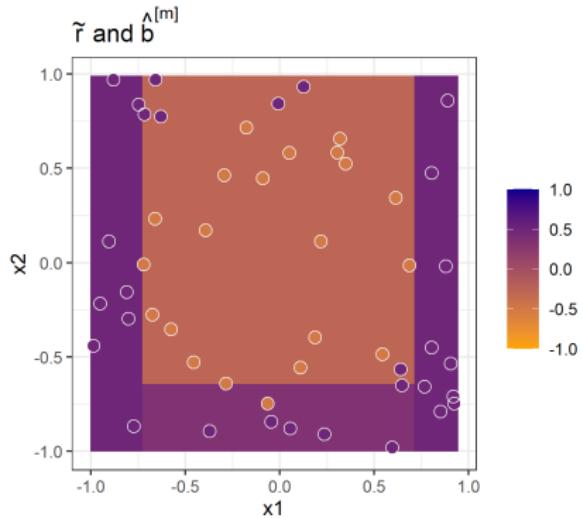
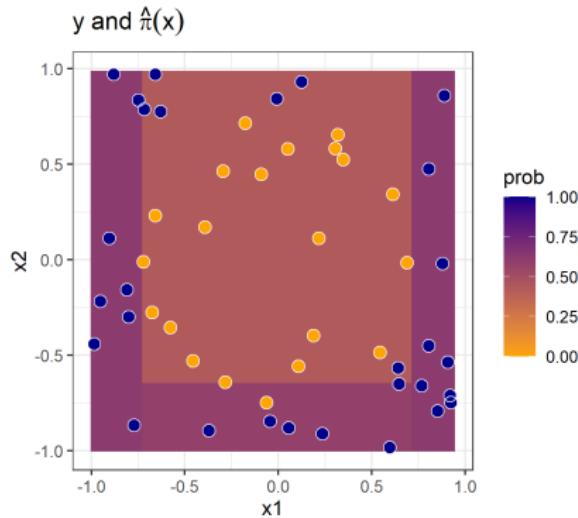
We now illustrate the boosting iterations for a classification example in a similar manner as we did for regression. However, we will now look at a simulation example with 2 instead of 1 influential features and one binary target variable.

- We used the mlbench dataset circle with $n = 50$ observations.
- We used the Bernoulli loss to calculate pseudo-residuals and fitted in each iteration a base learner (regression tree with max. depth of 3) on them.
- We initialized with $f^{[0]} = \log(1) = 0$.



EXAMPLE

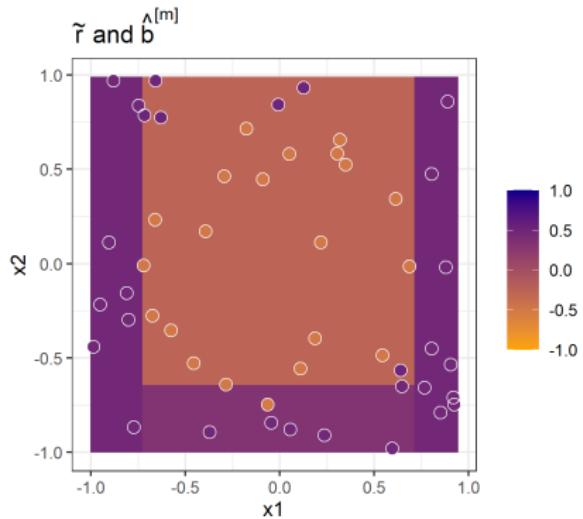
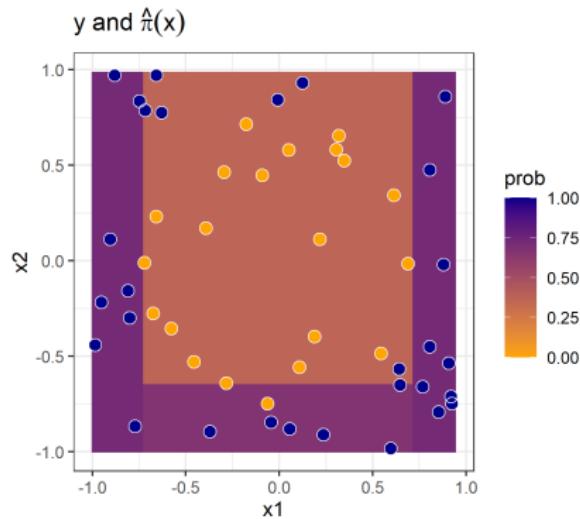
Left: Background color refers to prediction probabilities $\hat{\pi}^{[m]}$ and points to y (probabilities); Right: Background color refers to predictions of base learner $\hat{b}^{[m]}$ and points to \tilde{r} .



Iteration 1

EXAMPLE

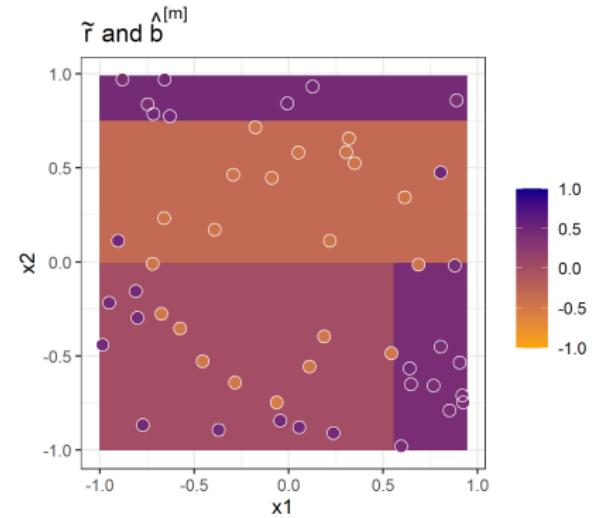
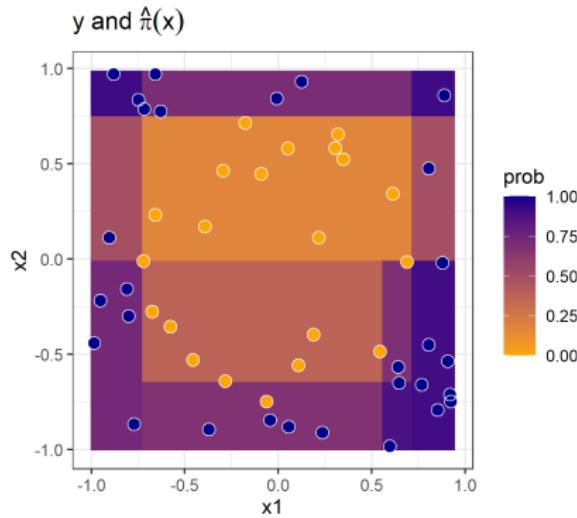
Left: Background color refers to prediction probabilities $\hat{\pi}^{[m]}$ and points to y (probabilities); Right: Background color refers to predictions of base learner $\hat{b}^{[m]}$ and points to \tilde{r} .



Iteration 2

EXAMPLE

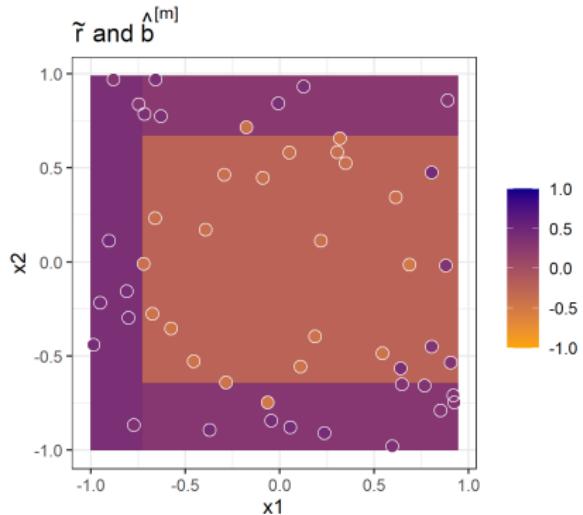
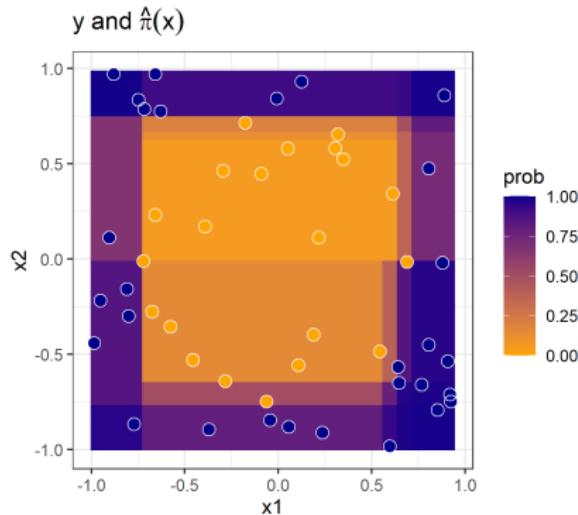
Left: Background color refers to prediction probabilities $\hat{\pi}^{[m]}$ and points to y (probabilities); Right: Background color refers to predictions of base learner $\hat{b}^{[m]}$ and points to \tilde{r} .



Iteration 5

EXAMPLE

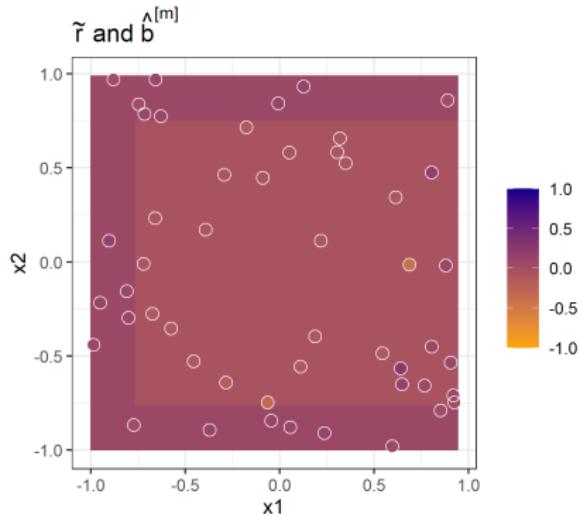
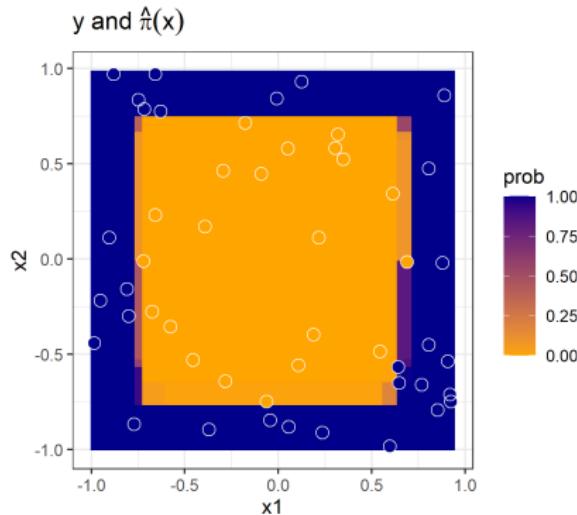
Left: Background color refers to prediction probabilities $\hat{\pi}^{[m]}$ and points to y (probabilities); Right: Background color refers to predictions of base learner $\hat{b}^{[m]}$ and points to \tilde{r} .



Iteration 10

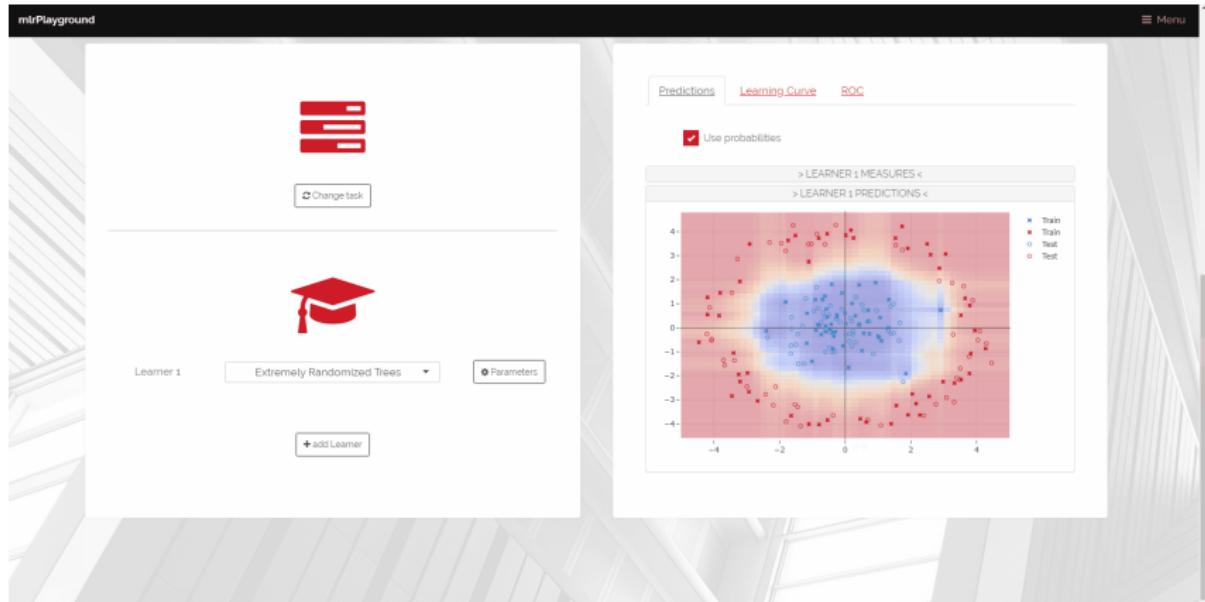
EXAMPLE

Left: Background color refers to prediction probabilities $\hat{\pi}^{[m]}$ and points to y (probabilities); Right: Background color refers to predictions of base learner $\hat{b}^{[m]}$ and points to \tilde{r} .



Iteration 100

MLRPLAYGROUND



▶ Open in browser.

MULTICLASS PROBLEMS

We proceed as in softmax regression and model a categorical distribution with multinomial / log loss. For $\mathcal{Y} = \{1, \dots, g\}$, we create g discriminant functions $f_k(x)$, one for each class and each one being an **additive** model of base learners.

We define the $\pi_k(\mathbf{x})$ through the softmax function:

$$\pi_k(\mathbf{x}) = s_k(f_1(\mathbf{x}), \dots, f_g(\mathbf{x})) = \exp(f_k(\mathbf{x})) / \sum_{j=1}^g \exp(f_j(\mathbf{x})).$$

Multinomial loss L :

$$L(y, f_1(\mathbf{x}), \dots, f_g(\mathbf{x})) = - \sum_{k=1}^g \mathbb{1}_{\{y=k\}} \ln \pi_k(\mathbf{x}).$$

Pseudo-residuals:

$$-\frac{\partial L(y, f_1(\mathbf{x}), \dots, f_g(\mathbf{x}))}{\partial f_k(\mathbf{x})} = \mathbb{1}_{\{y=k\}} - \pi_k(\mathbf{x}).$$

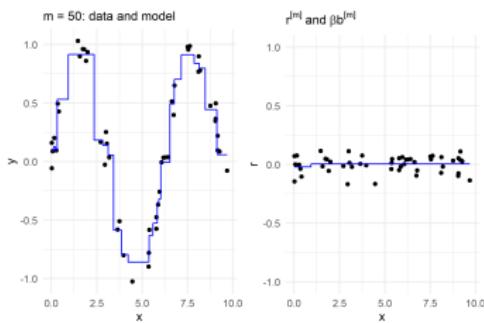
MULTICLASS PROBLEMS

Algorithm GB for Multiclass

```
1: Initialize  $f_k^{[0]}(\mathbf{x}) = 0$ ,  $k = 1, \dots, g$ 
2: for  $m = 1 \rightarrow M$  do
3:   Set  $\pi_k^{[m]}(\mathbf{x}) = \frac{\exp(f_k^{[m]}(\mathbf{x}))}{\sum_j \exp(f_j^{[m]}(\mathbf{x}))}$ ,  $k = 1, \dots, g$ 
4:   for  $k = 1 \rightarrow g$  do
5:     For all  $i$ : Compute  $\tilde{r}_k^{[m](i)} = \mathbb{1}_{\{y^{(i)}=k\}} - \pi_k^{[m]}(\mathbf{x}^{(i)})$ 
6:     Fit a regression base learner  $\hat{b}_k^{[m]}$  to the pseudo-residuals  $\tilde{r}_k^{[m](i)}$ .
7:     Obtain  $\hat{\beta}_k^{[m]}$  by constant learning rate or line-search.
8:     Update  $\hat{f}_k^{[m]} = \hat{f}_k^{[m-1]} + \hat{\beta}_k^{[m]} \hat{b}_k^{[m]}$ 
9:   end for
10: end for
11: Output  $\hat{f}_1^{[M]}, \dots, \hat{f}_g^{[M]}$ 
```

Introduction to Machine Learning

Gradient Boosting with Trees



Learning goals

- See how gradient boosting process is adapted for trees
- Understand relationship between model structure and interaction depth
- Understand multiclass extension for gradient boosting with trees

GRADIENT BOOSTING WITH TREES

Trees are mainly used as base learners for gradient boosting in ML. A great deal of research has been done on this combination so far, and it often provides the best results.

Reminder: advantages of trees

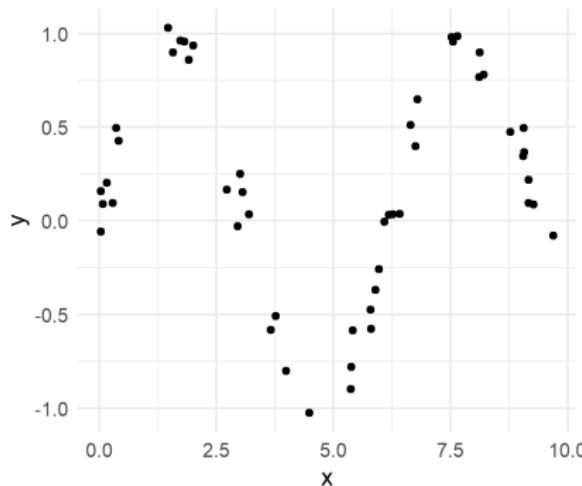
- No problems with categorical features.
- No problems with outliers in feature values.
- No problems with missing values.
- No problems with monotone transformations of features.
- Trees (and stumps!) can be fitted quickly, even for large n .
- Trees have a simple, built-in type of variable selection.

The gradient-boosted trees method retains all of them, and strongly improves the trees' predictive power. Furthermore, it is possible to adapt gradient boosting to tree learners in a targeted manner.

EXAMPLE 1

Simulation setting:

- Given: one feature x and one numeric target variable y of 50 observations.
- x is uniformly distributed between 0 and 10.
- y depends on x as follows: $y^{(i)} = \sin(x^{(i)}) + \epsilon^{(i)}$ with $\epsilon^{(i)} \sim \mathcal{N}(0, 0.01)$,
 $\forall i \in \{1, \dots, 50\}$.



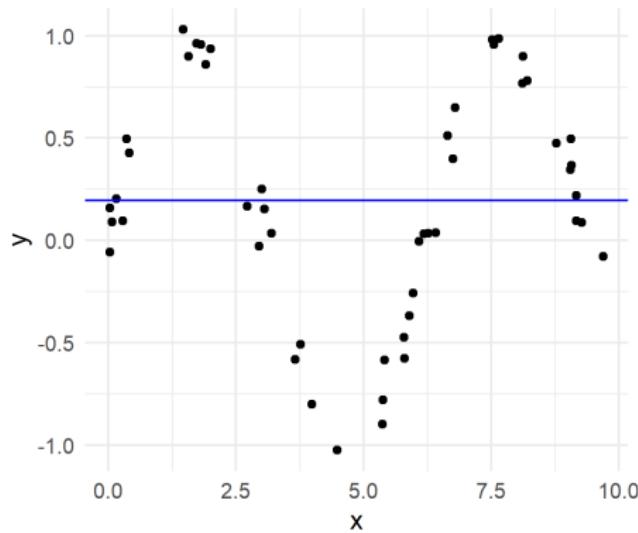
Aim: we want to fit a gradient boosting model to the data by using stumps as base learners.

Since we are facing a regression problem, we use $L2$ loss.

EXAMPLE 1

Iteration 0: initialization by optimal constant (mean) prediction $\hat{f}^{[0]}(x) = \bar{y} \approx 0.2$.

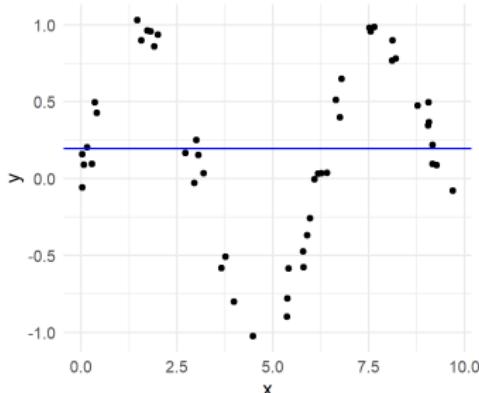
i	$x^{(i)}$	$y^{(i)}$	$\hat{f}^{[0]}$
1	0.03	0.16	0.20
2	0.03	-0.06	0.20
3	0.07	0.09	0.20
\vdots	\vdots	\vdots	\vdots
50	9.69	-0.08	0.20



EXAMPLE 1

Iteration 1: (1) Calculate pseudo-residuals $\tilde{r}^{[m](i)}$ and (2) fit a regression stump $b^{[m]}$.

i	$x^{(i)}$	$y^{(i)}$	$\hat{f}^{[0]}$	$\tilde{r}^{[1](i)}$	$\hat{b}^{[1](i)}$
1	0.03	0.16	0.20	-0.04	-0.17
2	0.03	-0.06	0.20	-0.25	-0.17
3	0.07	0.09	0.20	-0.11	-0.17
:	:	:	:	:	:
50	9.69	-0.08	0.20	-0.27	0.33

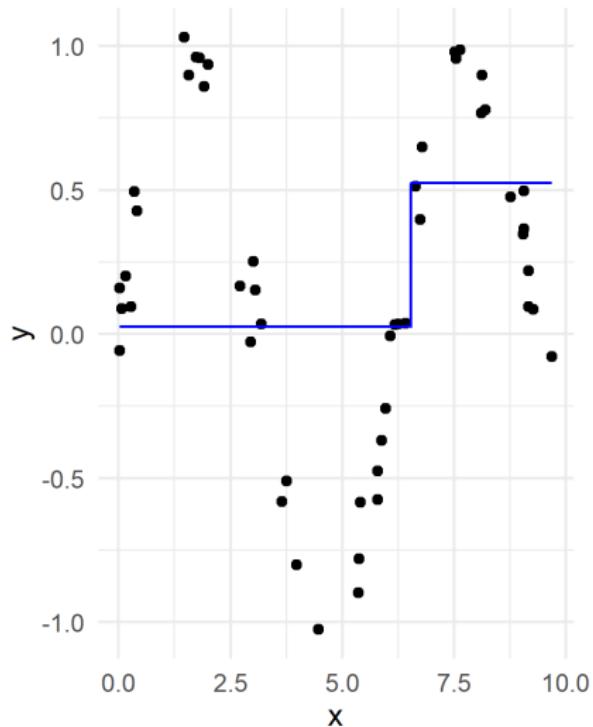


(3) Update model by $\hat{f}^{[1]}(x) = \hat{f}^{[0]}(x) + \hat{b}^{[1]}$.

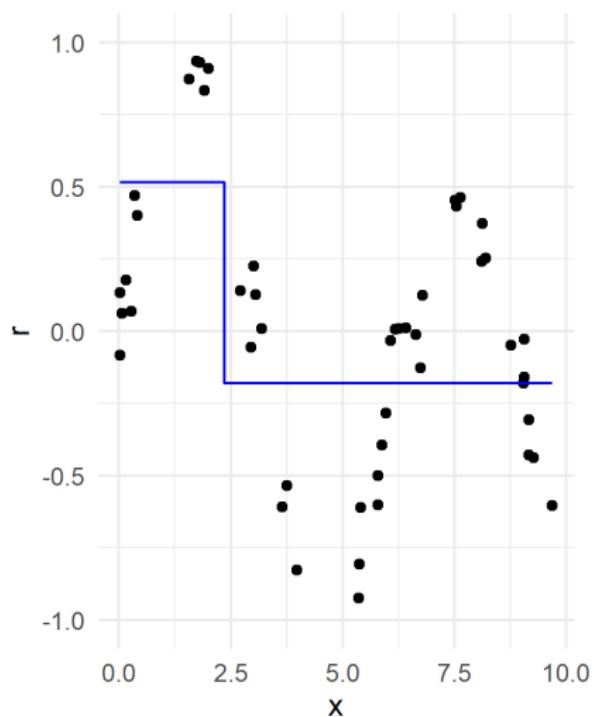
EXAMPLE 1

Repeat step (1) to (3):

$m = 1$: data and model



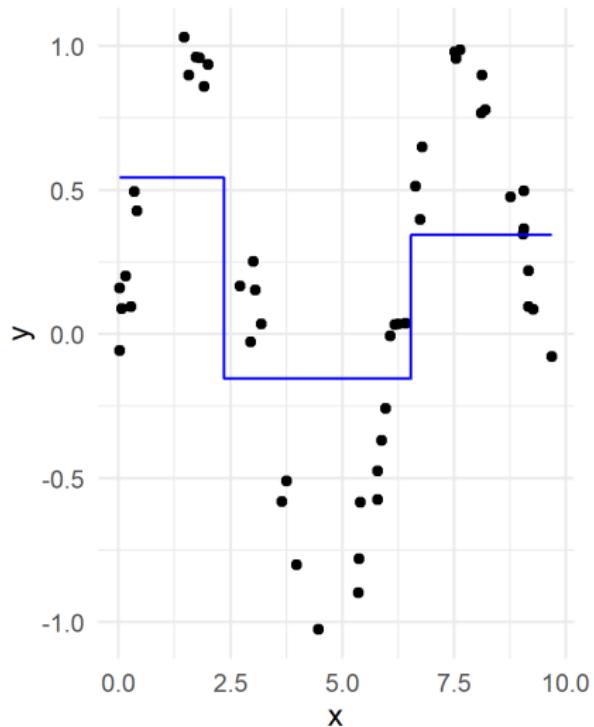
$r^{[m]}$ and $\beta b^{[m]}$



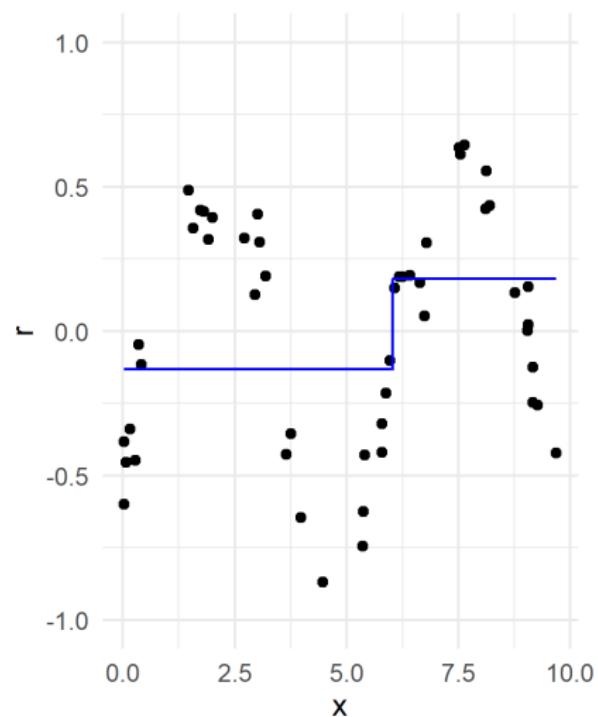
EXAMPLE 1

Repeat step (1) to (3):

$m = 2$: data and model



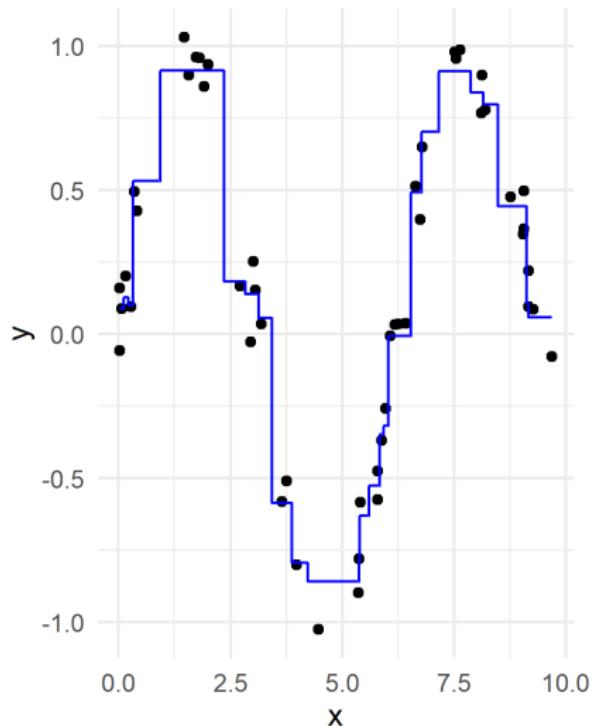
$r^{[m]}$ and $\beta b^{[m]}$



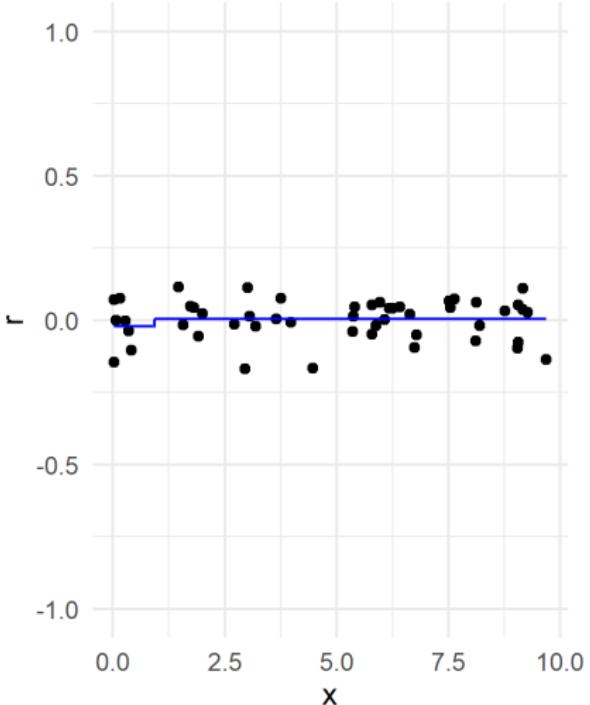
EXAMPLE 1

Repeat step (1) to (3):

$m = 50$: data and model

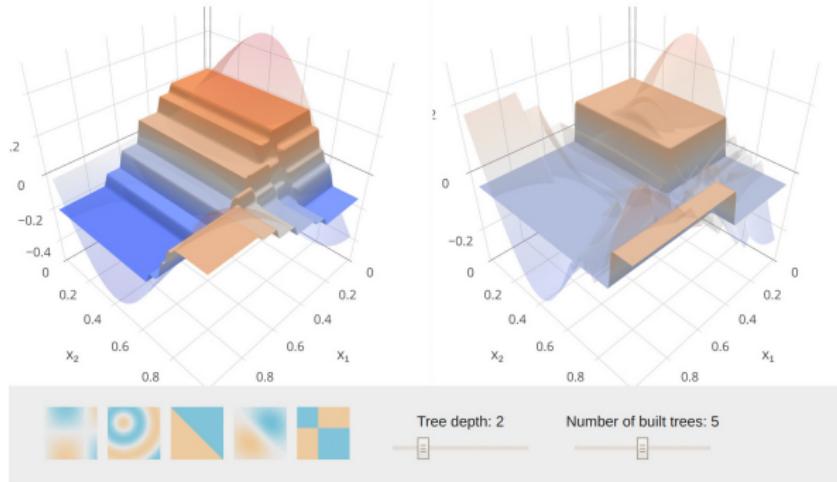


$r^{[m]}$ and $\beta b^{[m]}$



EXAMPLE 2

This [website](#) shows on various 3D examples how tree depth and number of iterations influence the model fit of a GBM with trees.



MODEL STRUCTURE AND INTERACTION DEPTH

The model structure of a gradient boosting model with trees is influenced by the chosen tree / interaction depth of $b^{[m]}(\mathbf{x})$.

$$f(\mathbf{x}) = \sum_{m=1}^M \beta^{[m]} b^{[m]}(\mathbf{x})$$

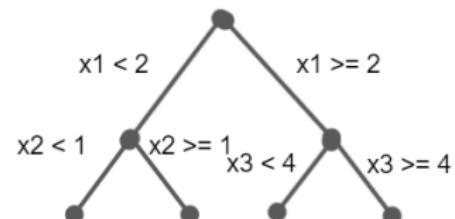
When using stumps (depth = 1), the resulting model is an additive model (GAM) without any interactions:

$$f(\mathbf{x}) = f_0 + \sum_{j=1}^p f_j(x_j)$$

When also including trees with a depth of 2, 2-way interactions are included and we get:

$$f(\mathbf{x}) = f_0 + \sum_{j=1}^p f_j(x_j) + \sum_{j \neq k} f_{j,k}(x_j, x_k)$$

with f_0 being a constant intercept.

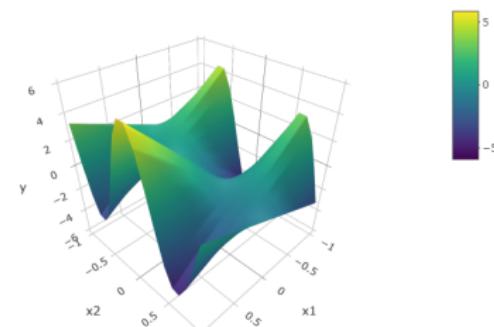


MODEL STRUCTURE AND INTERACTION DEPTH

Simulation setting:

- Given: two features x_1 and x_2 and one numeric target variable y of 500 observations.
- x_1 and x_2 are uniformly distributed between -1 and 1.
- Target function: $y^{(i)} = x_1^{(i)} - x_2^{(i)} + 5 \cos(5x_2^{(i)}) \cdot x_1^{(i)} + \epsilon^{(i)}$ with $\epsilon^{(i)} \sim \mathcal{N}(0, 1)$, $\forall i \in \{1, \dots, 500\}$.

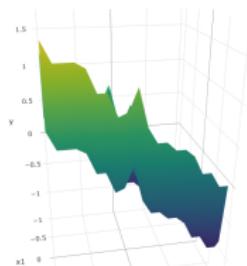
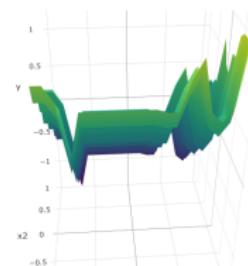
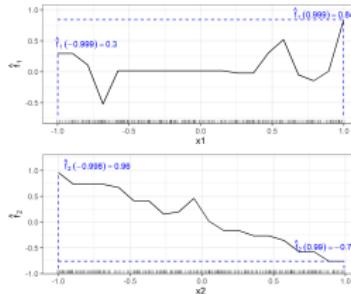
We fit two tree-based GBMs, one with an interaction depth (ID) of 1 (GAM) and one with an interaction depth of 2 (all possible interactions included).



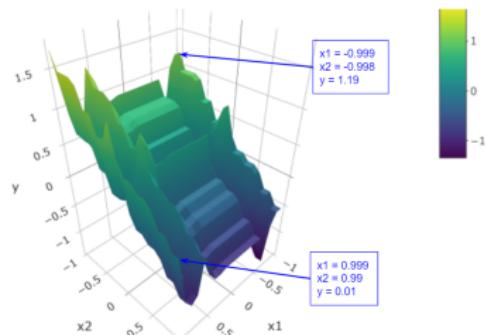
MODEL STRUCTURE AND INTERACTION DEPTH

GBM with interaction depth of 1 (GAM)

No interactions are modelled: Marginal effects of x_1 and x_2 add up to joint effect (plus the constant intercept $\hat{f}_0 = -0.07$).



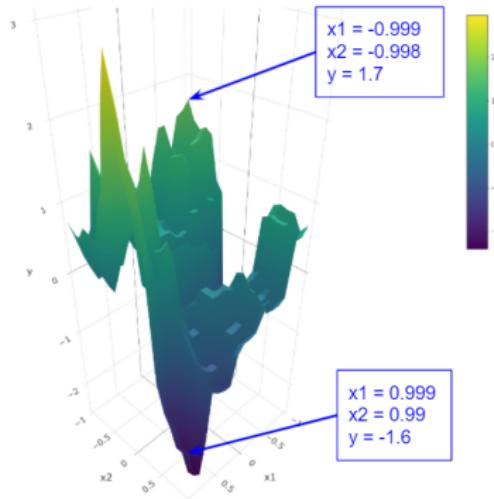
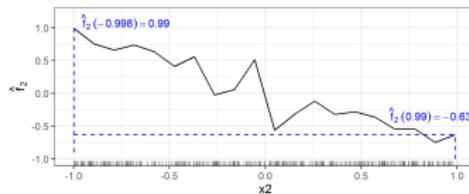
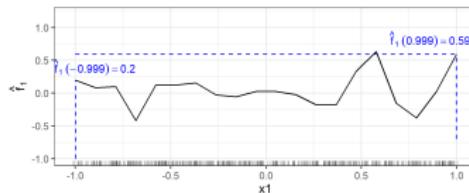
$$\begin{aligned}\hat{f}(-0.999, -0.998) &= \hat{f}_0 + \hat{f}_1(-0.999) + \hat{f}_2(-0.998) \\ &= -0.07 + 0.3 + 0.96 = 1.19\end{aligned}$$



MODEL STRUCTURE AND INTERACTION DEPTH

GBM with interaction depth of 2

Interactions between x_1 and x_2 are modelled: Marginal effects of x_1 and x_2 do NOT add up to joint effect due to interaction effects.



THEORETICAL BACKGROUND

One can write a tree as: $b(\mathbf{x}) = \sum_{t=1}^T c_t \mathbb{1}_{\{\mathbf{x} \in R_t\}}$, where R_t are the terminal regions and c_t the corresponding constant parameters.

For a fitted tree with regions R_t , the special additive structure can be exploited in boosting:

$$\begin{aligned} f^{[m]}(\mathbf{x}) &= f^{[m-1]}(\mathbf{x}) + \beta^{[m]} b^{[m]}(\mathbf{x}) \\ &= f^{[m-1]}(\mathbf{x}) + \beta^{[m]} \sum_{t=1}^{T^{[m]}} c_t^{[m]} \mathbb{1}_{\{\mathbf{x} \in R_t^{[m]}\}} \\ &= f^{[m-1]}(\mathbf{x}) + \sum_{t=1}^{T^{[m]}} \tilde{c}_t^{[m]} \mathbb{1}_{\{\mathbf{x} \in R_t^{[m]}\}}. \end{aligned}$$

With $\tilde{c}_t^{[m]} = \beta^{[m]} \cdot c_t^{[m]}$ in the case that $\beta^{[m]}$ is a constant learning rate

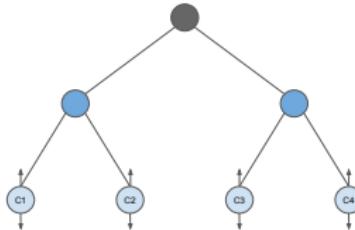
THEORETICAL BACKGROUND

We do the same steps as before: (1) calculate the pseudo-residuals, (2) fit a tree against pseudo-residuals, **but now** we keep only the structure of the tree and optimize the c parameter in a (further) post-hoc step.

$$f^{[m]}(\mathbf{x}) = f^{[m-1]}(\mathbf{x}) + \sum_{t=1}^{T^{[m]}} \tilde{c}_t^{[m]} \mathbb{1}_{\{\mathbf{x} \in R_t^{[m]}\}}.$$

We can determine/change all $\tilde{c}_t^{[m]}$ individually and directly L -optimally:

$$\tilde{c}_t^{[m]} = \arg \min_c \sum_{\mathbf{x}^{(i)} \in R_t^{[m]}} L(y^{(i)}, f^{[m-1]}(\mathbf{x}^{(i)}) + c).$$



THEORETICAL BACKGROUND

An alternative approach is to directly fit a loss-optimal tree. The risk function is then defined by:

$$\mathcal{R}(\mathcal{N}') = \sum_{i \in \mathcal{N}'} L(y^{(i)}, f^{[m-1]}(\mathbf{x}^{(i)}) + c)$$

with \mathcal{N}' being the index set of a specific (left or right) node after splitting and c being a constant value added to the current model for this node. Thus, instead of having a two-step approach of first fitting a tree to the pseudo-residuals of the current model and then finding the optimal value for c , we now directly build a tree that finds c loss-optimally. Since c is unknown, it needs to be determined, which can either be done by a line search or by taking the derivative:

$$\frac{\partial \mathcal{R}(\mathcal{N}')}{\partial c} = \sum_{i \in \mathcal{N}'} \frac{\partial L(y^{(i)}, f^{[m-1]}(\mathbf{x}^{(i)}) + c)}{\partial f|_{f=f^{[m-1]}+c}} = 0$$

THEORETICAL BACKGROUND

Algorithm Tree Algorithm for Gradient Boosting.

```
1: Input: All observations  $\mathcal{N}$  and risk function  $\mathcal{R}$ 
2: Output:  $\mathcal{N}_l^{j^*, s^*}$  and  $\mathcal{N}_r^{j^*, s^*}$ 
3: for  $j = x_1 \dots x_p$  do
4:   for every split  $s$  on feature  $j$  do
5:      $\mathcal{N}_l^{j, s} = \{i \in \mathcal{N}\}_{j^{(i)} \leq s}$ 
6:      $\mathcal{N}_r^{j, s} = \{i \in \mathcal{N}\}_{j^{(i)} > s}$ 
7:     Find  $c$  which minimizes  $\mathcal{R}$  for each node
8:      $\mathcal{I}(j, s) = \mathcal{R}(\mathcal{N}_l^{j, s}) + \mathcal{R}(\mathcal{N}_r^{j, s})$ 
9:   end for
10: end for
11:  $(j^*, s^*) \in \arg \min_{j, s} \mathcal{I}(j, s)$ 
```

The tree algorithm based on the CART algorithm of Breiman shows one partitioning step based on the risk function we introduced before.

GB MULTICLASS WITH TREES

- From Friedman, J. H. - Greedy Function Approximation: A Gradient Boosting Machine (1999)
- Determining the tree structure for each $\hat{b}_k^{[m]}$ by $L2$ loss works just like before in the 2-class problem.
- In the estimation of the c values, i.e., the heights of the terminal regions, however, all models depend on each other because of the definition of L . Optimizing this is more difficult, so we will skip some details and present the main idea and results.

GB MULTICLASS WITH TREES

- The post-hoc, loss-optimal heights of the terminals $\hat{c}_{tk}^{[m]}$ are:

$$\hat{c}_{tk}^{[m]} = - \arg \min_{c_{tk}^{[m]}} \sum_{i=1}^n \sum_{k=1}^g \mathbb{1}_{\{y=k\}} \ln \pi_k^{[m]}(\mathbf{x}^{(i)}).$$

- Softmax trafo: $\pi_k^{[m]}(\mathbf{x}) = \frac{\exp(f_k^{[m]}(\mathbf{x}))}{\sum_j \exp(f_j^{[m]}(\mathbf{x}))}$, with
- The k -th model: $\hat{f}_k^{[m]}(\mathbf{x}^{(i)}) = \hat{f}_k^{[m-1]}(\mathbf{x}^{(i)}) + \sum_{t=1}^{T_k^{[m]}} \hat{c}_{tk}^{[m]} \mathbb{1}_{\{\mathbf{x}^{(i)} \in R_{tk}^{[m]}\}}.$

GB MULTICLASS WITH TREES

- There is no closed-form solution for finding the optimal $\hat{c}_{tk}^{[m]}$ values. Additionally, the regions corresponding to the different class trees overlap, so that the solution does not reduce to a separate calculation within each region of each tree.
- Hence, we approximate the solution with a single Newton-Raphson step, using a diagonal approximation to the Hessian (we leave out the details here).
- This decomposes the problem into a separate calculation for each terminal node of each tree.
- The result is

$$\hat{c}_{tk}^{[m]} = \frac{g-1}{g} \frac{\sum_{\mathbf{x}^{(i)} \in R_{tk}^{[m]}} \tilde{r}_k^{[m](i)}}{\sum_{\mathbf{x}^{(i)} \in R_{tk}^{[m]}} \left| \tilde{r}_k^{[m](i)} \right| \left(1 - \left| \tilde{r}_k^{[m](i)} \right| \right)}.$$

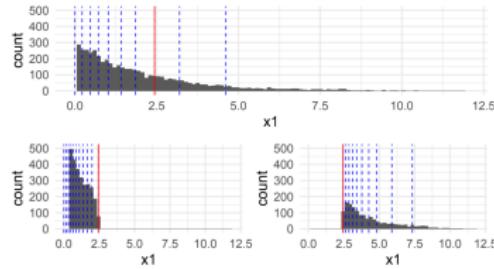
GB MULTICLASS WITH TREES

Algorithm Gradient Boosting for g -class Classification.

- 1: Initialize $f_k^{[0]}(\mathbf{x}) = 0$, $k = 1, \dots, g$
 - 2: **for** $m = 1 \rightarrow M$ **do**
 - 3: Set $\pi_k(\mathbf{x}) = \frac{\exp(f_k^{[m]}(\mathbf{x}))}{\sum_j \exp(f_j^{[m]}(\mathbf{x}))}$, $k = 1, \dots, g$
 - 4: **for** $k = 1 \rightarrow g$ **do**
 - 5: For all i : Compute $\tilde{r}_k^{[m](i)} = \mathbb{1}_{\{y^{(i)}=k\}} - \pi_k(\mathbf{x}^{(i)})$
 - 6: Fit regr. tree to the $\tilde{r}_k^{[m](i)}$ giving terminal regions $R_{tk}^{[m]}$
 - 7: Compute
$$\hat{c}_{tk}^{[m]} = \frac{g-1}{g} \frac{\sum_{\mathbf{x}^{(i)} \in R_{tk}^{[m]}} \tilde{r}_k^{[m](i)}}{\sum_{\mathbf{x}^{(i)} \in R_{tk}^{[m]}} |\tilde{r}_k^{[m](i)}| \left(1 - |\tilde{r}_k^{[m](i)}|\right)}$$
 - 9: Update $\hat{f}_k^{[m]}(\mathbf{x}) = \hat{f}_k^{[m-1]}(\mathbf{x}) + \sum_t \hat{c}_{tk}^{[m]} \mathbb{1}_{\{\mathbf{x} \in R_{tk}^{[m]}\}}$
 - 10: **end for**
 - 11: **end for**
 - 12: Output $\hat{f}_1^{[M]}, \dots, \hat{f}_g^{[M]}$
-

Introduction to Machine Learning

XGBoost



Learning goals

- XXX
- XXX

MOTIVATION

Chen and Guestrin (2016):

XGBoost (short for eXtreme Gradient Boosting) is an open-source software library with R/Python/Julia/Spark interface.

A scalable regularized tree boosting system:

- Efficient implementation in *C++*.
- Parallel (approximate) split finding.
- Handling of *sparse data*.
- Support of cluster-computing frameworks.

State-of-the-art machine learning method:

- Many winning solutions at Kaggle use XGBoost.
- KDDCup 2015 Top 10 used XGBoost.

LOSS MINIMIZATION

XGBoost uses a risk function with 3 regularization terms:

$$\begin{aligned}\mathcal{R}_{\text{reg}}^{[m]} = & \sum_{i=1}^n L\left(y^{(i)}, f^{[m-1]}(\mathbf{x}^{(i)}) + b^{[m]}(\mathbf{x}^{(i)})\right) \\ & + \lambda_1 J_1(b^{[m]}) + \lambda_2 J_2(b^{[m]}) + \lambda_3 J_3(b^{[m]}),\end{aligned}$$

with $J_1(b^{[m]}) = T^{[m]}$ to regularize tree depth, where $T^{[m]}$ is the number of leaves in the tree.

$J_2(b^{[m]}) = \|\mathbf{c}^{[m]}\|_2^2$ and $J_3(b^{[m]}) = \|\mathbf{c}^{[m]}\|_1$ are $L2$ and $L1$ regularizers of the terminal region scores $c_t^{[m]}, t = 1, \dots, T^{[m]}$.

Note: In the following we define

$J(b^{[m]}) := \lambda_1 J_1(b^{[m]}) + \lambda_2 J_2(b^{[m]}) + \lambda_3 J_3(b^{[m]})$ to simplify the notation.

LOSS MINIMIZATION

To approximate the loss in iteration m , use a second-order Taylor expansion around $f^{[m-1]}(\mathbf{x})$:

$$L(y, f^{[m-1]}(\mathbf{x}) + b^{[m]}(\mathbf{x})) \approx L(y, f^{[m-1]}(\mathbf{x})) + g^{[m]}(\mathbf{x})b^{[m]}(\mathbf{x}) + \frac{1}{2}h^{[m]}(\mathbf{x})b^{[m]}(\mathbf{x})^2,$$

with gradient

$$g^{[m]}(\mathbf{x}) = \frac{\partial L(y, f^{[m-1]}(\mathbf{x}))}{\partial f^{[m-1]}(\mathbf{x})}$$

and Hessian

$$h^{[m]}(\mathbf{x}) = \frac{\partial^2 L(y, f^{[m-1]}(\mathbf{x}))}{\partial f^{[m-1]}(\mathbf{x})^2}.$$

Note: $g^{[m]}(\mathbf{x})$ are the negative pseudo-residuals $-\tilde{r}^{[m]}$ we use in standard gradient boosting to determine the direction of the update.

LOSS MINIMIZATION

Since $L(y, f^{[m-1]}(\mathbf{x}))$ is a constant, the optimization criterion simplifies to

$$\begin{aligned}\mathcal{R}_{\text{reg}}^{[m]} &\approx \sum_{i=1}^n g^{[m]}(\mathbf{x}^{(i)}) b^{[m]}(\mathbf{x}^{(i)}) + \frac{1}{2} h^{[m]}(\mathbf{x}^{(i)}) b^{[m]}(\mathbf{x}^{(i)})^2 + J(b^{[m]}) + \text{const} \\ &\propto \sum_{t=1}^{T^{[m]}} \sum_{\mathbf{x}^{(i)} \in R_t^{[m]}} g^{[m]}(\mathbf{x}^{(i)}) c_t^{[m]} + \frac{1}{2} h^{[m]}(\mathbf{x}^{(i)}) (c_t^{[m]})^2 + J(b^{[m]}).\end{aligned}$$

Defining $G_t^{[m]}$ and $H_t^{[m]}$ as the sum of the gradients and Hessians, respectively, in terminal node t yields

$$= \sum_{t=1}^{T^{[m]}} G_t^{[m]} c_t^{[m]} + \frac{1}{2} H_t^{[m]} (c_t^{[m]})^2 + J(b^{[m]}).$$

LOSS MINIMIZATION

Expanding $J(b^{[m]})$, we get

$$\begin{aligned}\mathcal{R}_{\text{reg}}^{[m]} &= \sum_{t=1}^{T^{[m]}} \left(G_t^{[m]} c_t^{[m]} + \frac{1}{2} H_t^{[m]} (c_t^{[m]})^2 + \frac{1}{2} \lambda_2 (c_t^{[m]})^2 + \lambda_3 |c_t^{[m]}| \right) + \lambda_1 T^{[m]} \\ &= \sum_{t=1}^{T^{[m]}} \left(G_t^{[m]} c_t^{[m]} + \frac{1}{2} (H_t^{[m]} + \lambda_2) (c_t^{[m]})^2 + \lambda_3 |c_t^{[m]}| \right) + \lambda_1 T^{[m]}.\end{aligned}$$

Note: The factor $\frac{1}{2}$ is added to the *L2* regularization to simplify the notation as shown in the second step. This does not impact estimation since we can just define $\lambda_2 = 2\tilde{\lambda}_2$.

LOSS MINIMIZATION

Since

$$\frac{\partial \mathcal{R}_{\text{reg}}^{[m]}}{\partial c_t^{[m]}} = \begin{cases} (G_t^{[m]} - \lambda_3) + (H_t^{[m]} + \lambda_2)c_t^m & \text{for } c_t^m < 0 \\ (G_t^{[m]} + \lambda_3) + (H_t^{[m]} + \lambda_2)c_t^m & \text{for } c_t^m > 0, \end{cases}$$

the optimal weights $\tilde{c}_1^{[m]}, \dots, \tilde{c}_{T^{[m]}}^{[m]}$ can then be calculated as

$$\tilde{c}_t^{[m]} = -\frac{t_{\lambda_3}\left(G_t^{[m]}\right)}{H_t^{[m]} + \lambda_2}, \quad t = 1, \dots, T^{[m]},$$

with

$$t_{\lambda_3}(x) = \begin{cases} x - \lambda_3 & \text{for } x > \lambda_3 \\ x + \lambda_3 & \text{for } x < -\lambda_3 \\ 0 & \text{for } |x| \leq \lambda_3. \end{cases}$$

LOSS MINIMIZATION - SPLIT FINDING

To evaluate the performance of a candidate split that divides the instances in region $R_t^{[m]}$ into a left and right node we use the **risk reduction** achieved by that split:

$$\tilde{S}_{LR} = \frac{1}{2} \left[\frac{t_{\lambda_3} (G_{tL}^{[m]})^2}{H_{tL}^{[m]} + \lambda_2} + \frac{t_{\lambda_3} (G_{tR}^{[m]})^2}{H_{tR}^{[m]} + \lambda_2} - \frac{t_{\lambda_3} (G_t^{[m]})^2}{H_t^{[m]} + \lambda_2} \right] - \lambda_1,$$

where the subscripts L and R denote the left and right leaves after the split.

LOSS MINIMIZATION - SPLIT FINDING

Algorithm (Exact) Algorithm for split finding

```
1: Input  $I$ : instance set of current node
2: Input  $p$ : dimension of feature space
3:  $gain \leftarrow 0$ 
4:  $G \leftarrow \sum_{i \in I} g(\mathbf{x}^{(i)})$ ,  $H \leftarrow \sum_{i \in I} h(\mathbf{x}^{(i)})$ 
5: for  $j = 1 \rightarrow p$  do
6:    $G_L \leftarrow 0$ ,  $H_L \leftarrow 0$ 
7:   for  $i$  in sorted( $I$ , by  $x_j$ ) do
8:      $G_L \leftarrow G_L + g(\mathbf{x}^{(i)})$ ,  $H_L \leftarrow H_L + h(\mathbf{x}^{(i)})$ 
9:      $G_R \leftarrow G - G_L$ ,  $H_R \leftarrow H - H_L$ 
10:    compute  $\tilde{S}_{LR}$ 
11:   end for
12: end for
13: Output Split with maximal  $\tilde{S}_{LR}$ 
```

APPROXIMATE SPLIT-FINDING ALGORITHMS

Three different algorithms to search for these splits are implemented in XGBoost.

The **exact greedy algorithm** iterates over all possible splits of all features.

The **global approximate algorithm** iterates over percentiles of the empirical distribution of each feature.

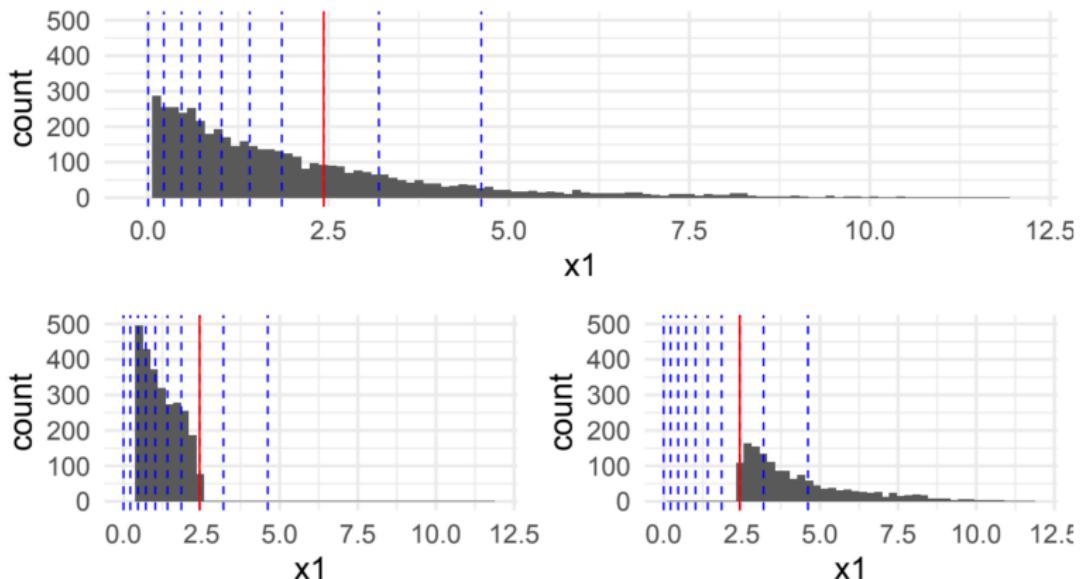
The **local approximate algorithm** does the same as the global, but recalculates the percentiles after each split.

APPROXIMATE SPLIT-FINDING ALGORITHMS

Algorithm Approximate algorithm for split finding

- 1: **for** $j = 1 \rightarrow p$ **do**
 - 2: Define possible split proposals $S_j = \{s_j^{(1)}, s_j^{(2)}, \dots, s_j^{(l)}\}$ by percentiles on feature j .
 - 3: Proposal can be done once per tree (global), or in each node (local).
 - 4: **end for**
 - 5: **for** $j = 1 \rightarrow p$ **do**
 - 6: $G_{kv} \leftarrow \sum_{i \in \{i | s_j^{(v)} \geq x_j^{(i)} > s_k^{(v-1)}\}} g(\mathbf{x}^{(i)})$
 - 7: $H_{kv} \leftarrow \sum_{i \in \{i | s_j^{(v)} \geq x_j^{(i)} > s_k^{(v-1)}\}} h(\mathbf{x}^{(i)})$
 - 8: **end for**
 - 9: Follow same steps as exact algorithm to find max score only among proposed splits.
-

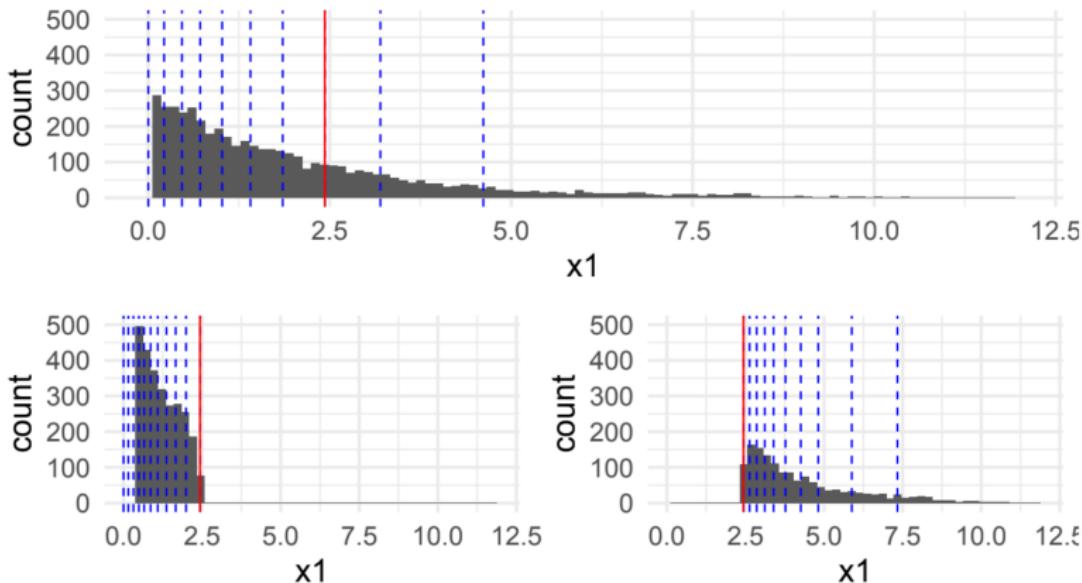
APPROXIMATE SPLIT-FINDING ALGORITHMS



Approximate **global** split finding.

Blue lines indicate percentiles, red line is the chosen split. Proposals are not recomputed, allowing the right node only two possibilities.

APPROXIMATE SPLIT-FINDING ALGORITHMS



Approximate **local** split finding.

Blue lines indicate percentiles, red line is the chosen split. Percentiles are recalculated after each split.

APPROXIMATE SPLIT-FINDING ALGORITHMS

Both approximate splitting algorithms are useful for large datasets as iteration over all splits becomes very expensive.

XGBoost also allows for sparsity-aware split finding, which means that for a large number of zero (or missing) values, a default direction in each node is introduced.

The calculation of the percentiles in the feature distributions can be parallelized, allowing parallel split finding for the approximate algorithms.

EVEN MORE REGULARIZATION

Besides the regularization terms discussed above, XGBoost also incorporates a step length ν for the updates.

Furthermore, it uses **feature subsampling** similar to the random forest. Only a random subset of all features is considered for each split.

Stochastic gradient boosting, as introduced before, is utilized as well, which means that in each iteration only a subset of the observations is used.

A final possibility for regularization is DART (Dropout Additive Regression Trees). For each iteration only a fraction of previously fitted trees is considered. After an update the joint contribution of the dropped tree and the tree new to the ensemble are scaled to avoid overshooting.

STORAGE AND OUT-OF-MEMORY CALCULATION

The data is stored in **blocks**. Each of these blocks is stored in a compressed column format.

Depending on the split finding algorithm, these blocks contain the complete (sorted) data, or subsets of rows.

These blocks can be stored out-of-memory (on disk) to save memory and distributed across multiple machines for parallel computations.

For more details on this see *Chen and Guestrin (2016)*.

SUMMARY

XGBoost is an extremely powerful method, but also hard to configure correctly. Overall, eight hyperparameters have to be set, which is difficult to do in practice and almost always requires tuning.

Different split finding algorithms can be selected, which allows XGBoost to be efficient even on very large datasets.

A large number of different regularization strategies is included to prevent overfitting.

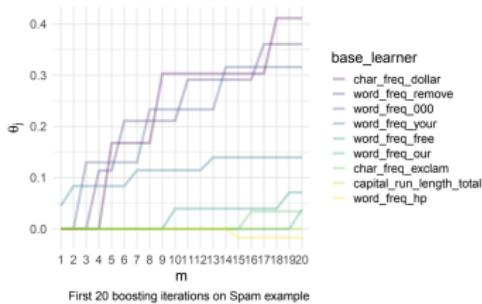
COMPARISON OF MAJOR BOOSTING SYSTEMS

System	Exact algo.	Approx. algo.	Sparsity-aware	Variable importance	Parallel	Language
ada	yes	no	no	no	no	R
GBM	yes	no	partially	yes	no	R
mboost	yes	no	no	no	no	R
compboost	yes	no	yes	yes	yes	R
H2O	no	yes	partially	yes	yes	R (Java)
XGBoost	yes	yes	yes	yes	yes	R + Python
lightGBM	no	yes	yes	yes	yes	R + Python
catboost	no	yes	no	yes	yes	R + Python
scikit-learn	yes	no	no	yes	no	Python
pGBRT	no	no	no	no	yes	Python
Spark MLLib	no	yes	partially	yes	yes	R, Python, Java, Scala

Note: H2O is a commercial software written in Java with a solid R interface. In the free version only two CPUs can be used.

Introduction to Machine Learning

Componentwise Gradient Boosting



Learning goals

- Learn the concept of componentwise boosting and its relation to GLM
- Understand the built-in feature selection process
- Understand the problem of fair base learner selection

COMPONENTWISE GRADIENT BOOSTING

Gradient boosting, especially when using trees, has strong predictive performance but is difficult to interpret unless the base learners are stumps.

The aim of componentwise gradient boosting is to find a model that:

- has strong predictive performance,
- has components that are still interpretable,
- does automatic selection of components,
- is sparser than a model fitted with maximum-likelihood estimation.

This is achieved by using “nice” base learners which yield familiar statistical models in the end.

Because of this, componentwise gradient boosting is also often referred to as **model-based boosting**.

BASE LEARNERS

In classical gradient boosting only one kind of base learner is used, e.g., regression trees.

For componentwise gradient boosting we generalize this to multiple base learners

$$\{b_j^{[m]}(\mathbf{x}, \boldsymbol{\theta}^{[m]}) : j = 1, 2, \dots, J\},$$

where j indexes the type of base learner.

Again, in each iteration, only the best base learner $b_{j^*}^{[m]}(\mathbf{x}, \boldsymbol{\theta}^{[m]})$ is selected and updated.

BASE LEARNERS

We restrict these base learners to additive models, i.e.,

$$b_j^{[m]}(\mathbf{x}, \boldsymbol{\theta}^{[m]}) + b_j^{[m']}(\mathbf{x}, \boldsymbol{\theta}^{[m']}) = b_j(\mathbf{x}, \boldsymbol{\theta}^{[m]} + \boldsymbol{\theta}^{[m']}).$$

Often base learners are not defined on the entire feature vector \mathbf{x} but on a single feature x_j :

$$b_j^{[m]}(x_j, \boldsymbol{\theta}^{[m]}) \quad \text{for } j = 1, 2, \dots, p.$$

This directly incorporates a variable selection mechanism into the fitting process, since in each iteration only the best base learner is selected in combination with the associated feature, and each base learner can be (substantially) more complex than a stump (e.g., univariate linear effects or splines).

COMPONENTWISE BOOSTING ALGORITHM

Algorithm Componentwise Gradient Boosting.

```
1: Initialize  $f^{[0]}(\mathbf{x}) = \arg \min_{\theta} \sum_{i=1}^n L(y^{(i)}, \theta)$ 
2: for  $m = 1 \rightarrow M$  do
3:   For all  $i$ :  $\tilde{r}^{[m](i)} = - \left[ \frac{\partial L(y^{(i)}, f(\mathbf{x}^{(i)}))}{\partial f(\mathbf{x}^{(i)})} \right]_{f=f^{[m-1]}}$ 
4:   for  $j = 1 \rightarrow J$  do
5:     Fit regression base learner  $b_j$  to the pseudo-residuals  $\tilde{r}^{[m](i)}$ :
6:      $\hat{\theta}_j^{[m]} = \arg \min_{\theta_j} \sum_{i=1}^n (\tilde{r}^{[m](i)} - b_j(\mathbf{x}^{(i)}, \theta_j))^2$ 
7:   end for
8:    $j^* = \arg \min_j \sum_{i=1}^n (\tilde{r}^{[m](i)} - b_j(\mathbf{x}^{(i)}, \hat{\theta}_j^{[m]}))^2$ 
9:   Update  $f^{[m]}(\mathbf{x}) = f^{[m-1]}(\mathbf{x}) + \nu b_{j^*}(\mathbf{x}, \hat{\theta}_{j^*}^{[m]})$ 
10: end for
11: Output  $\hat{f}(\mathbf{x}) = f^{[M]}(\mathbf{x})$ 
```

RELATION TO GLM

In the simplest case we use linear models (without intercept) on single features as base learners:

$$b(x_j, \theta^{[m]}) = x_j \theta^{[m]} \quad \text{for } j = 1, 2, \dots, p.$$

This definition will result in an ordinary **linear regression** model (note that linear base learners without intercept only make sense for covariates that have been centered before).

- If we let the boosting algorithm converge, i.e., let it run for a really long time, the parameters estimated by the boosting model will converge to the **same solution** as the ML estimate.
- This means that, by specifying a loss function according to the negative likelihood of a distribution from an exponential family and defining a link function accordingly, this kind of boosting is equivalent to a (regularized) **generalized linear model (GLM)**.

RELATION TO GLM

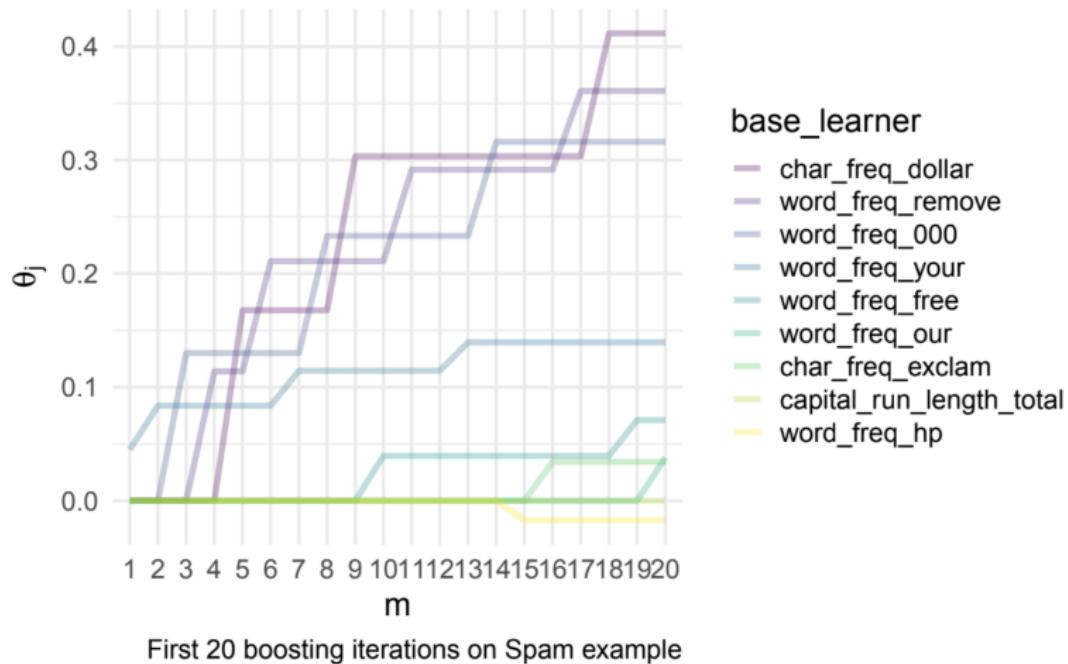
But: We do not *need* an exponential family and thus are able to fit models to all kinds of other distributions and losses, as long as we can calculate (or approximate) a derivative of the loss.

Usually we do not let the boosting model converge fully, but **stop early** for the sake of regularization and feature selection.

Even though the resulting model looks like a GLM, we do not have valid standard errors for our coefficients, so cannot provide confidence or prediction intervals or perform tests etc. → post-selection inference.

FEATURE SELECTION

We can visualize the updates of the θ_j together with the number of iterations to see which base learner was selected when.



FEATURE SELECTION

- We can further exploit the additive structure of the boosted ensemble to compute measures of **variable importance**.
- To this end, we simply sum for each feature x_j the improvements in empirical risk achieved over all iterations until $1 < m_{\text{stop}} \leq M$:

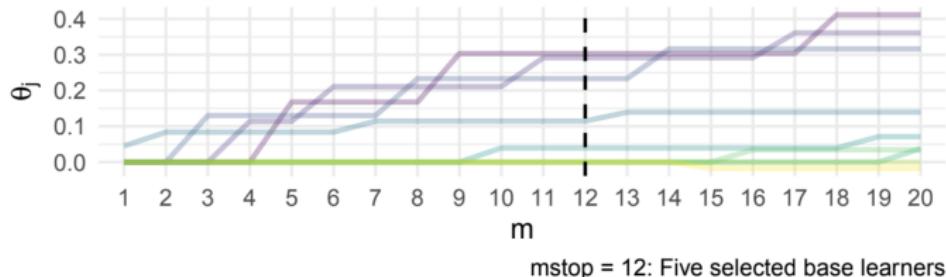
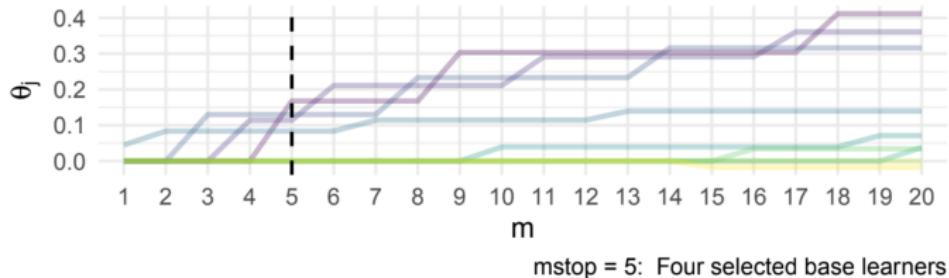
$$VI_j = \sum_{m=1}^{m_{\text{stop}}} \left(\mathcal{R}_{\text{emp}} \left(f^{[m-1]}(\mathbf{x}) \right) - \mathcal{R}_{\text{emp}} \left(f^{[m]}(\mathbf{x}) \right) \right) \cdot \mathbb{I}_{[j \in \text{sel}(m)]},$$

where $\text{sel}(m)$ denotes the index set of features selected in the m -th iteration.

FEATURE SELECTION

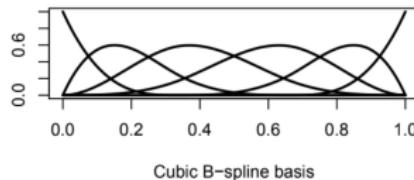
The number of features effectively included in the final model depends on the value of M .

→ A sparse logistic regression is fitted.

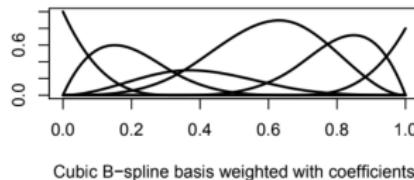


NONLINEAR BASE LEARNERS

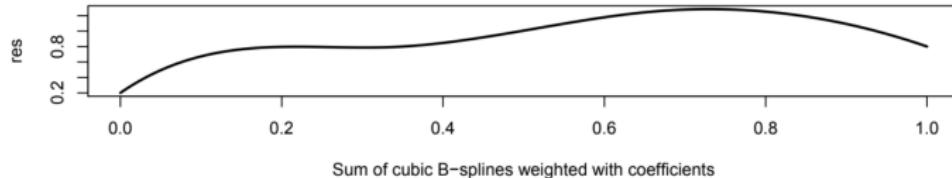
Nonlinear base learners like P - or B -splines make the model equivalent to a **generalized additive model (GAM)**, as long as the base learners keep their additive structure (which is the case for splines).



Cubic B-spline basis



Cubic B-spline basis weighted with coefficients



Sum of cubic B-splines weighted with coefficients

NONLINEAR BASE LEARNERS

Even when allowing for more complexity we typically want to keep solutions as simple as possible.

Kneib et al. (2009) proposed a decomposition of each base learner into a constant, a linear and a nonlinear part. The boosting algorithm will automatically decide which feature to include – linear, nonlinear, or none at all:

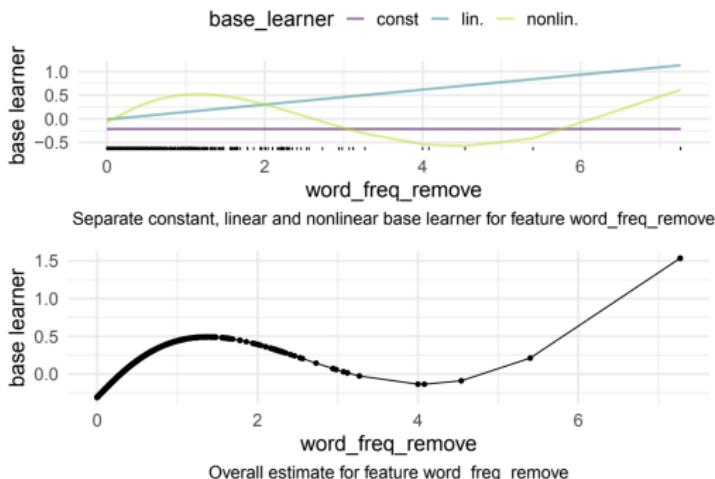
$$\begin{aligned} b_j(x_j, \theta^{[m]}) &= b_{j,\text{const}}(x_j, \theta^{[m]}) + b_{j,\text{lin}}(x_j, \theta^{[m]}) + b_{j,\text{nonlin}}(x_j, \theta^{[m]}) \\ &= \theta_{\text{const}}^{[m]} + x_j \cdot \theta_{j,\text{lin}}^{[m]} + s_j(x_j, \theta_{j,\text{nonlin}}^{[m]}), \end{aligned}$$

where

- θ_{const} is a constant term over all base learners,
- $x_j \cdot \theta_{j,\text{lin}}^{[m]}$ is a feature-specific linear base learner, and
- $s_j(x_j, \theta_{j,\text{nonlin}}^{[m]})$ is a (centered) nonlinear base learner capturing deviation from the linear effect.

SPAM EXAMPLE: CONTINUED

- This time we fit a componentwise gradient boosting model to the spam dataset using the R package mboost with $M = 100$.
- We specify a linear and nonlinear (P -spline) base learner for each feature and let the boosting model decide which to select.
- The model selects 17 different base learners (out of 114):



FAIR BASE LEARNER SELECTION

- Using splines and linear base learners in componentwise boosting will favor the more complex spline base learner over the linear base learner.
- This makes it harder to achieve the desired behavior of the base learner decomposition as explained previously.
- To conduct a fair base learner selection we set the degrees of freedom of all base learners equal.
- The idea is to set the regularization/penalty term of a single learner in a manner that their complexity is treated equally.

FAIR BASE LEARNER SELECTION

Especially for linear models and GAMs it is possible to transform the degrees of freedom into a corresponding penalty term.

- Parameters of the base learners are estimated via:

$$\boldsymbol{\theta}_j^{[m]} = (\mathbf{Z}_j^T \mathbf{Z}_j + \lambda_j \mathbf{K}_j)^{-1} \mathbf{Z}_j^T \tilde{r}^{[m]},$$

with \mathbf{Z}_j the design matrix of the j -th base learner, λ_j the penalty term, and \mathbf{K}_j the penalty matrix.

- Having that kind of model, we use the hat matrix

$$\mathbf{S}_j = \mathbf{Z}_j \left(\mathbf{Z}_j^T \mathbf{Z}_j + \lambda_j \mathbf{K}_j \right)^{-1} \mathbf{Z}_j^T$$
 to define the degrees of freedom:

$$df(\lambda_j) = \text{tr} (2\mathbf{S}_j - \mathbf{S}_j^T \mathbf{S}_j).$$

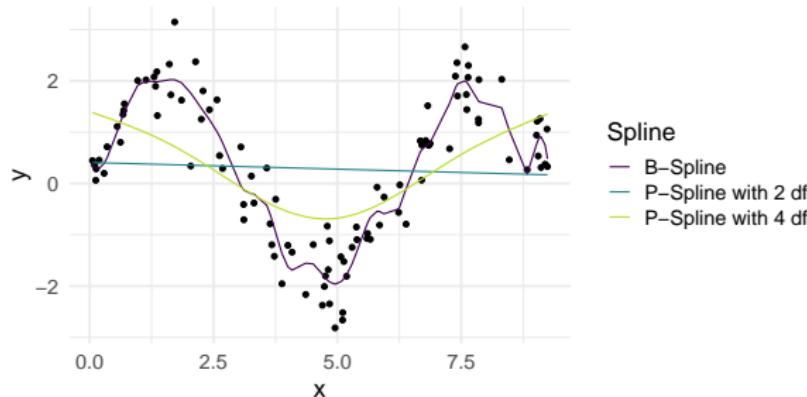
Note: With $\lambda_j = 0$, \mathbf{S}_j is the projection matrix into the target space with $\text{tr}(\mathbf{S}_j) = \text{rank}(\mathbf{X})$, which corresponds to the number of parameters in the model.

FAIR BASE LEARNER SELECTION

It is possible to calculate λ_j by applying the Demmler-Reinsch orthogonalization (see Hofer et al. (2011)).

Consider the following example of a GAM using splines with 24 parameters:

- Setting $df = 24$ gives B -splines with $\lambda_j = 0$.
- Setting $df = 4$ gives P -splines with $\lambda_j = 418$.
- Setting $df = 2$ gives P -splines with $\lambda_j = 42751174892$.



AVAILABLE BASE LEARNERS

There is a large amount of possible base learners, e.g.:

- Linear effects and interactions (with or without intercept)
- Uni- or multivariate splines and tensor product splines
- Trees
- Random effects and Markov random fields
- Effects of functional covariates
- ...

In combination with the flexible choice of loss functions, this allows boosting to fit a huge number of different statistical models with the same algorithm. Recent extensions include GAMLSS-models, where multiple additive predictors are boosted to model different distribution parameters (e.g., conditional mean and variance for a Gaussian model).

TAKE-HOME MESSAGE

- Componentwise gradient boosting is the statistical re-interpretation of gradient boosting.
- We can fit a large number of statistical models, even in high dimensions ($p \gg n$).
- A drawback compared to statistical models is that we do not get valid inference for coefficients → post-selection inference.
- In most cases, gradient boosting with tree will dominate componentwise boosting in terms of performance due to its inherent ability to include higher-order interaction terms.