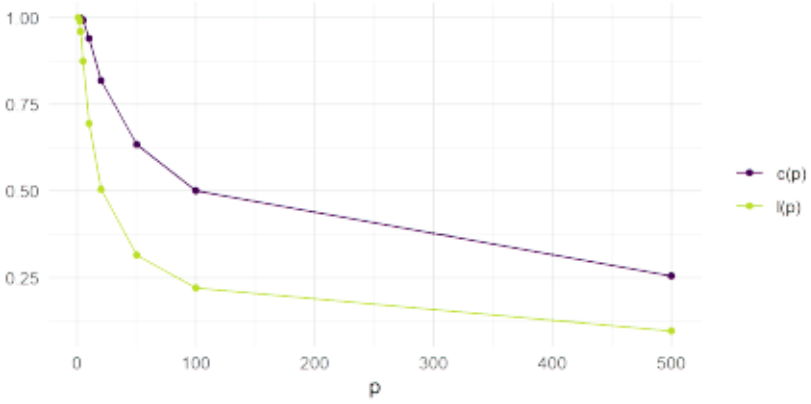
EXAMPLE: K-NN / 2

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

p	$\min d(\mathbf{x}, \tilde{\mathbf{x}})$	$\overline{d(\mathbf{x}, \tilde{\mathbf{x}})}$	$\max d(\mathbf{x}, \tilde{\mathbf{x}})$	$\overline{d_{NN1}(\mathbf{x})}$	$\max d_{NN1}(\mathbf{x})$
1	1.2e-08	0.33	1	5e-05	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 / 3

We see a decrease of relative contrast[1] $c := \frac{\max(d(\mathbf{x},\tilde{\mathbf{x}})) - \min(d(\mathbf{x},\tilde{\mathbf{x}}))}{\max(d(\mathbf{x},\tilde{\mathbf{x}}))}$ and "locality"[2] $l := \frac{\overline{d(\mathbf{x},\tilde{\mathbf{x}})} - \overline{d_{NN1}(\mathbf{x})}}{d(\mathbf{x},\tilde{\mathbf{x}})}$ with increasing number of dimensions p:



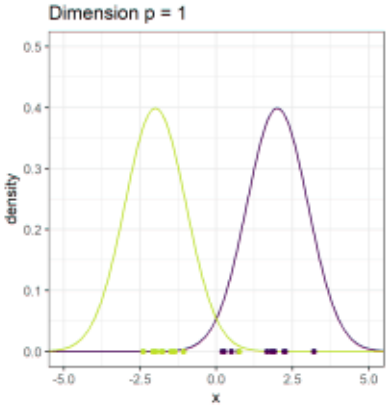
[1] [Aggarwal et al., 2001]
[2] our non-standard definition

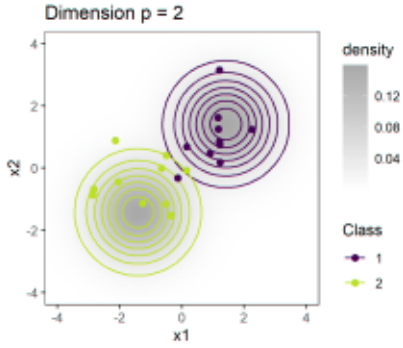
EXAMPLE: K-NN / 2

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

EXAMPLE: K-NN / 3





EXAMPLE: K-NN / 4

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

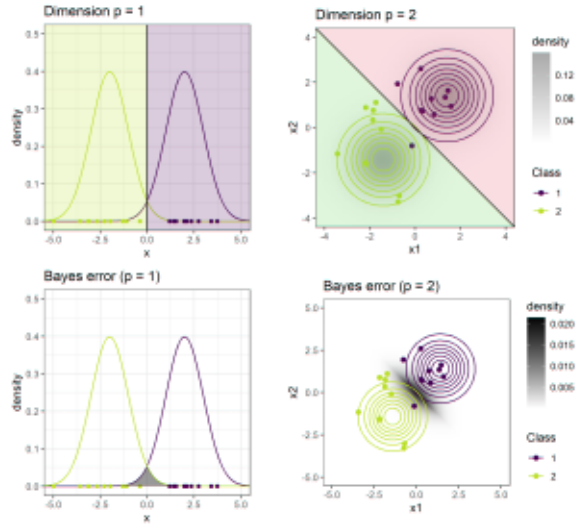
$$\begin{aligned}
\mathbb{P}(y = 1 \mid \mathbf{x}) &= \frac{p(\mathbf{x} \mid y = 1)\mathbb{P}(y = 1)}{p(\mathbf{x})} = \frac{1}{2} \cdot \frac{p(\mathbf{x} \mid y = 1)}{p(\mathbf{x})} \\
&\geq \frac{1}{2} \cdot \frac{p(\mathbf{x} \mid y = 2)}{p(\mathbf{x})} \\
&= \frac{p(\mathbf{x} \mid y = 2)\mathbb{P}(y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

This is equivalent to

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

EXAMPLE: K-NN / 5

Optimal Bayes classifier and Bayes error (shaded area):



EXAMPLE: K-NN / 6

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

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

$\sum_{i=1}^{p} \mathbf{x}_i \mid y = 1 \sim \mathcal{N}(p \cdot a,\ p)$, 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 $\mathcal{N}(\boldsymbol{\mu}, \boldsymbol{I})$ distribution with $\boldsymbol{\mu} = (a, ..., a)$).

EXAMPLE: K-NN / 7

We get for the Bayes error:

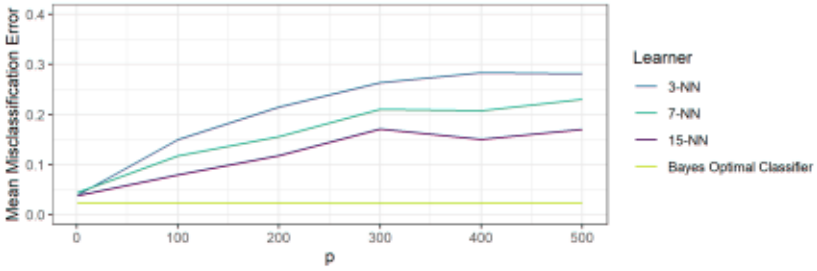
$$
\begin{aligned}
&= p\left(\frac{\sum_{i=1}^{p} \mathbf{x}_i - p \cdot a}{\sqrt{p}} \leq \frac{-p \cdot a}{\sqrt{p}} \mid y = 1\right) \\
&= \Phi(-\sqrt{p}a) \overset{a=\frac{2}{\sqrt{p}}}{=} \Phi(-2) \approx 0.0228,
\end{aligned}
$$

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 / 8

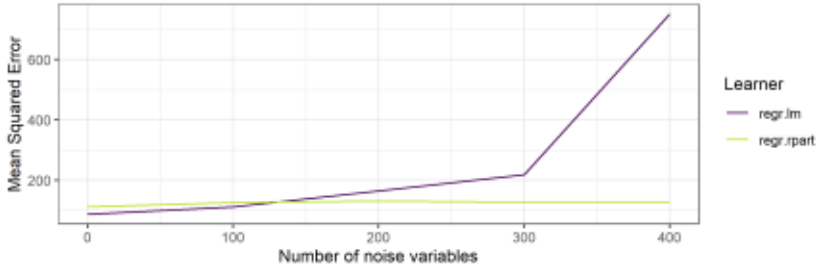
We also train a k-NN classifier for $k = 3, 7, 15$ for increasing dimensions and monitor its performance (evaluated by 10 times repeated 10-fold CV).



→ k-NN deteriorates quickly with increasing dimension

EXAMPLE: LINEAR MODEL / 2

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



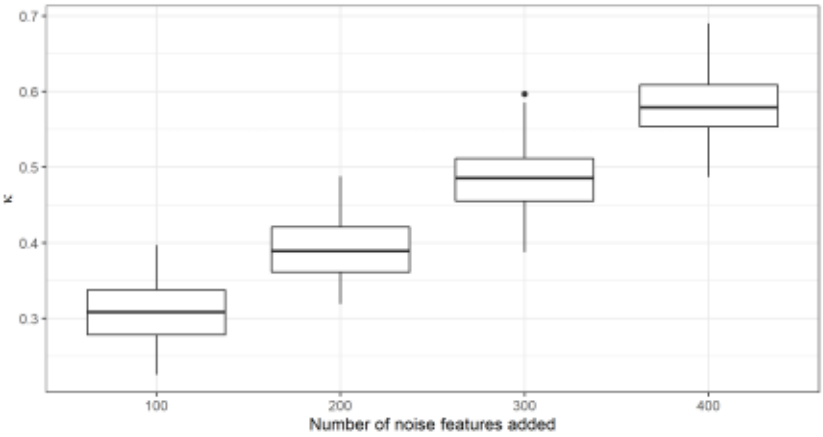
→ The unregularized LM struggles with the added noise features, while our tree seems to nicely filter them out.

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 / 3

- 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 observation.
  Therefore we decompose the response $\hat{y}^{(i)}$ of each iterations' test set into $\hat{y}^{(i)}_{\text{true}}$ (predicted with noise features set to 0) and $\hat{y}^{(i)}_{\text{noise}}$ (predicted with true features set to 0), s.t.
  $\hat{y}^{(i)} = \hat{y}^{(i)}_{\text{true}} + \hat{y}^{(i)}_{\text{noise}} + \text{intercept}$.
  With this, we can define the "average proportional influence of the noise features" $\kappa := \overline{\left(\frac{|\hat{y}^{(i)}_{\text{noise}}|}{|\hat{y}^{(i)}_{\text{true}}| + |\hat{y}^{(i)}_{\text{noise}}|} \right)}$.

EXAMPLE: LINEAR MODEL / 4



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.