Knowledge Discovery in Databases
SS 2016

Chapter 7: Numerical Prediction

Lecture: Prof. Dr. Thomas Seidl

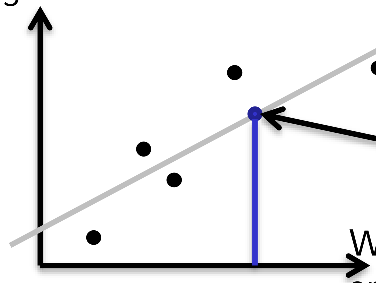
Tutorials: Julian Busch, Evgeniy Faerman, Florian Richter, Klaus Schmid

Chapter 7: Numerical Prediction

1) Introduction
   – Numerical Prediction problem, linear and nonlinear regression, evaluation measures
2) Piecewise Linear Numerical Prediction Models
   – Regression Trees, axis parallel splits, oblique splits
   – Hinging Hyperplane Models
3) Bias-Variance Problem
   – Regularization , Ensemble methods

Numerical Prediction

- Related problem to classification: numerical prediction
  - Determine the numerical value of an object
  - Method: e.g., regression analysis
  - Example: prediction of flight delays



- Numerical prediction is *different* from classification
  - Classification refers to predict categorical class label
  - Numerical prediction models continuous-valued functions
- Numerical prediction is *similar* to classification
  - First, construct a model
  - Second, use model to predict unknown value
    - Major method for numerical prediction is regression
      - Linear and multiple regression
      - Non-linear regression

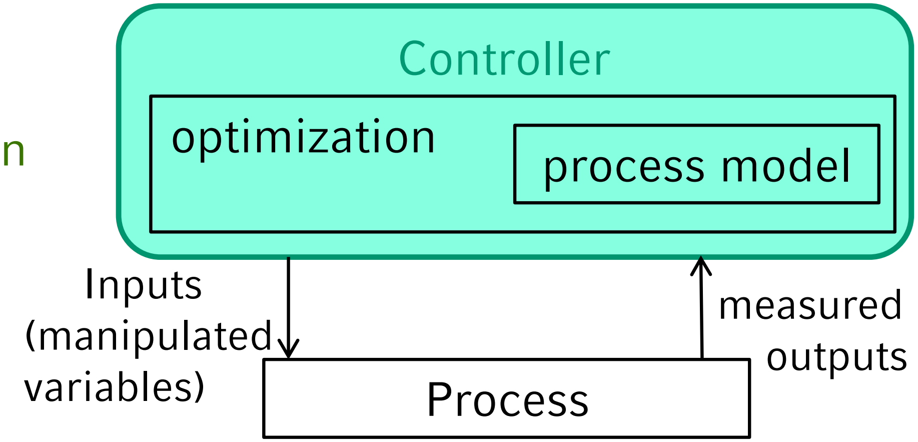
Examples

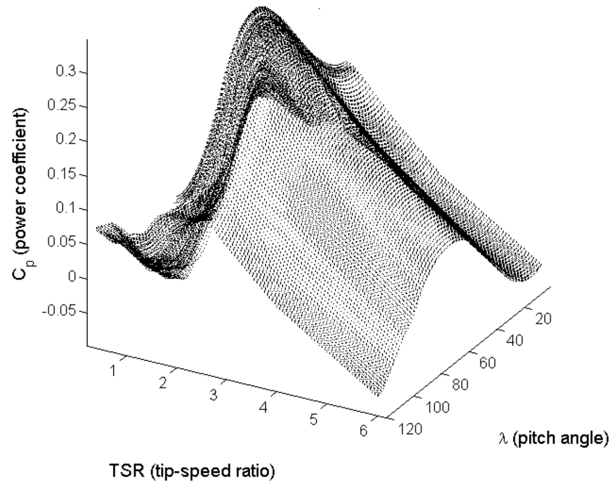
- Housing values in suburbs of Boston
- Inputs
  - number of rooms
  - Median value of houses in the neighborhood
  - Weighted distance to five Boston employment centers
  - Nitric oxides concentration
  - Crime rate per capita
  - ...

- Goal: compute a model of the housing values, which can be used to predict the price for a house in that area

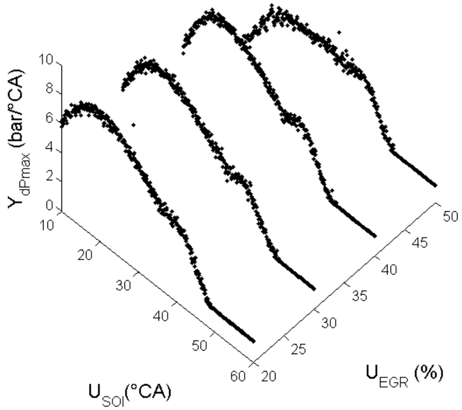
Examples

- Control engineering:
  - Control the inputs of a system in order to lead the outputs to a given reference value
  - Required: a model of the process





Wind turbine

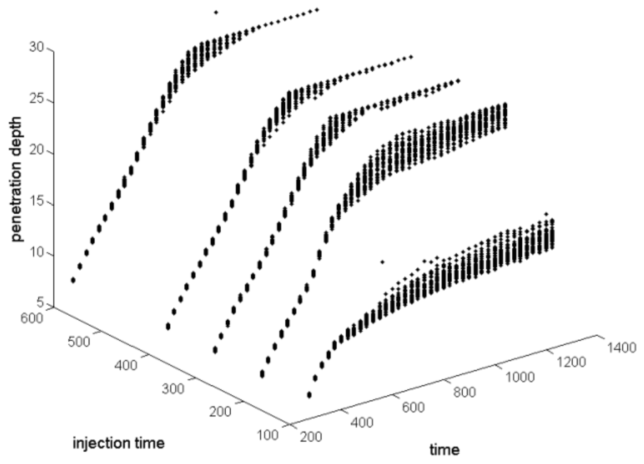


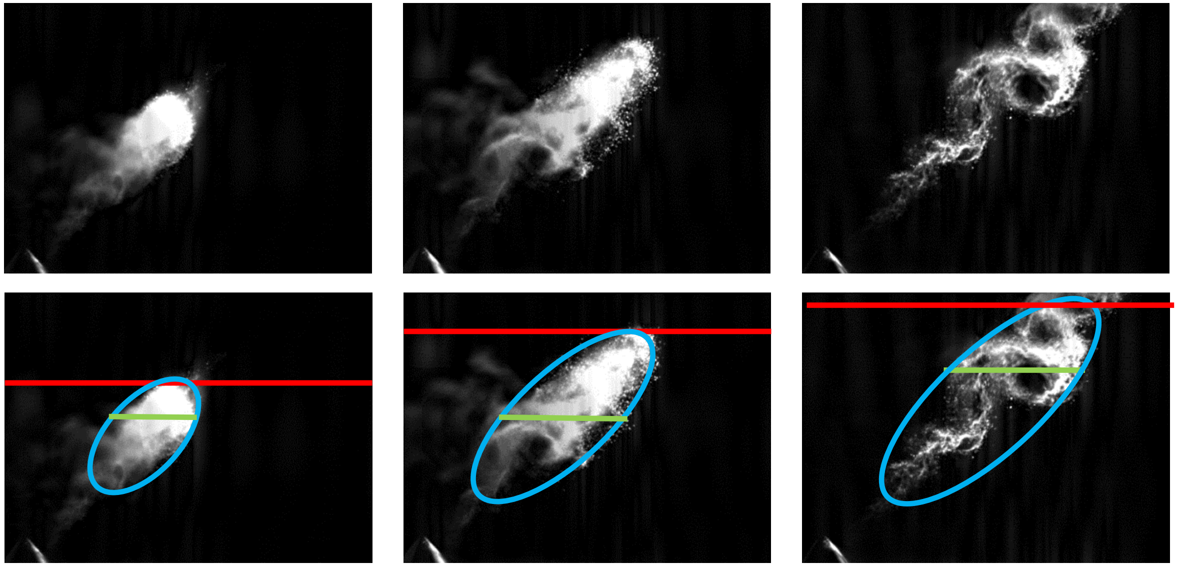
Diesel engine

Examples

- Fuel injection process:
  - database of spray images
  - Inputs: settings in the pressure chamber
  - Outputs: spray features, e.g., penetration depth, spray width, spray area

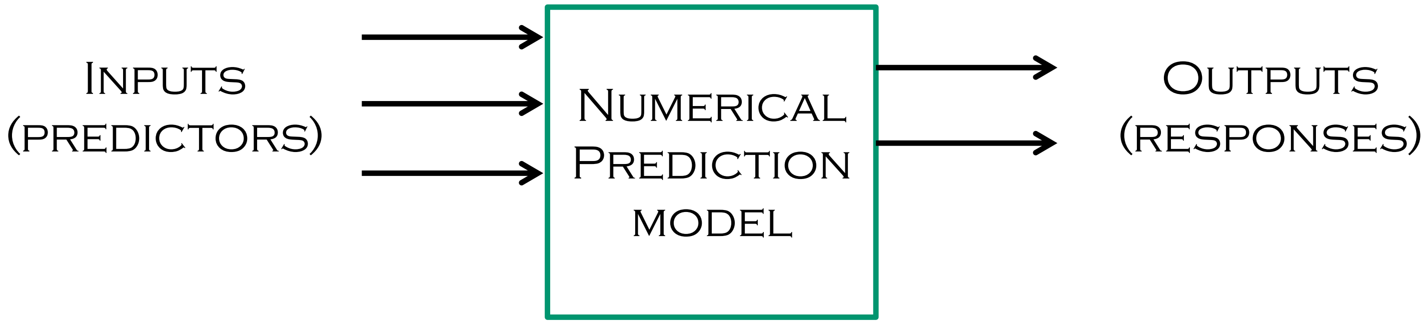
} compute a model which predicts the spray features, for input settings which have not been measured





Numerical Prediction

- Given: a set of observations
- Compute: a generalized model of the data which enables the prediction of the output as a continuous value



- Quality measures:
  - Accuracy of the model
  - Compactness of the model
  - Interpretability of the model
  - Runtime efficiency (training, prediction)

Linear Regression

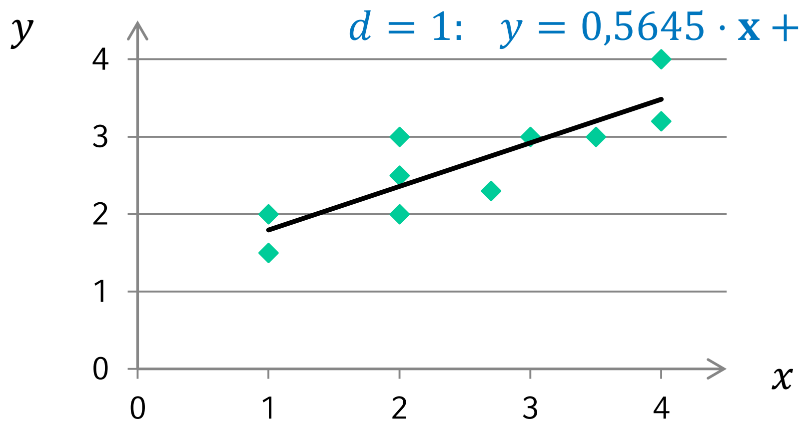
- Given a set of N observations with inputs of the form $\mathbf{x} = [x_1, \dots, x_d]$ and outputs $y \in \mathbb{R}$
- Approach: minimize the **Sum of Squared Errors (SSE)**
- Numerical Prediction: describe the outputs y as a linear equation of the inputs

$$\hat{y} = f(\mathbf{x}) = \beta_0 + \beta_1 \cdot x_1 + \dots + \beta_d \cdot x_d = [1\ \ x_1\ \ \dots\ \ x_d] \cdot \begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_d \end{bmatrix} = [1\ \ x_1\ \ \dots x_d] \cdot \boldsymbol{\beta}$$

- Train the parameters $\boldsymbol{\beta} = [\beta_0\ \beta_1\ \dots \beta_d]$:

$$\sum_{i=1}^{N} \left(y_i - f(\mathbf{x}_i)\right)^2 \rightarrow min$$

$d = 1$: $y = 0{,}5645 \cdot \mathbf{x} + 1{,}2274$



Linear Regression

- Matrix notation: let $X \in \mathbb{R}^{N\times(d+1)}$ be the matrix containing the inputs, $Y \in \mathbb{R}^N$ the outputs, and β the resulting coefficients:

$$\mathrm{X} = \begin{bmatrix} 1 & x_{11} & \dots & x_{1d} \\ \vdots & \ddots & \vdots & \vdots \\ 1 & x_{N1} & \dots & x_{Nd} \end{bmatrix}, \qquad Y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{bmatrix} \quad \Rightarrow \quad \beta = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_d \end{bmatrix}$$

- Goal: find the coefficients β, which minimize the SSE:

$$\min_{\beta} g(\beta) = \min_{\beta} \|X\beta - Y\|_2^2 = \min_{\beta} (X\beta - Y)^T (X\beta - Y)$$

$$= \min_{\beta} (\beta^T X^T X\beta - 2Y^T X\beta + Y^T Y)$$

Linear Regression

- Set the first derivative of $g(\beta) = \beta^T X^T X\beta - 2Y^T X\beta + Y^T Y$ to zero:

$$X^T X\beta = X^T Y$$

- If $X^T X$ is non-singular then:

$$\beta = (X^T X)^{-1} \cdot X^T Y$$

- For $d = 1$, the regression coefficients β_0 and β_1 can be computed as:

$$\beta_1 = \frac{Cov(\mathbf{x}, y)}{Var(\mathbf{x})} = \frac{\tilde{\mathbf{x}}^T \cdot \tilde{y}}{\tilde{\mathbf{x}}^T \cdot \tilde{\mathbf{x}}} \quad \text{and} \quad \beta_0 = \bar{y} - \beta_1 \cdot \bar{\mathbf{x}}$$

$$\tilde{\mathbf{x}} = \mathbf{x} - \bar{\mathbf{x}}$$
$$\tilde{y} = y - \bar{y}$$

Note that if $\bar{\mathbf{x}} = 0 \Rightarrow \beta_1 = \frac{\mathbf{x}^T y}{\mathbf{x}^T \mathbf{x}}$ and $\beta_0 = 0$

Polynomial Regression

- Second order polynomial for $d = 1$:

$$\hat{y} = \beta_0 + \beta_1 \cdot x_1 + \beta_2 \cdot x_1^2 = x_d = [1 \;\; x_1 \;\; x_1^2] \cdot \begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \end{bmatrix}$$

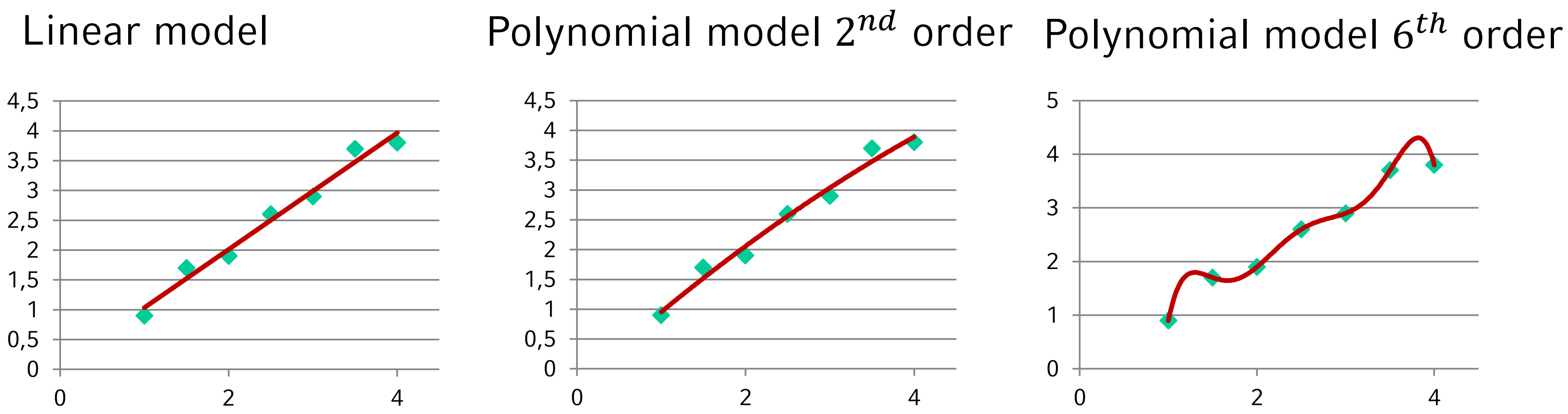
with $\mathrm{X} = \begin{bmatrix} 1 & x_{11} & x_{11}^2 \\ \vdots & \vdots & \vdots \\ 1 & x_{N1} & x_{N1}^2 \end{bmatrix}$ and $\beta = (X^T \cdot X)^{-1} \cdot X^T \cdot Y$

- Second order polynomial for $d = 2$:

$$\hat{y} = \beta_0 + \beta_1 \cdot x_1 + \beta_2 \cdot x_2 + \beta_3 \cdot x_1^2 + \beta_4 \cdot x_2^2 + \beta_5 \cdot x_1 \cdot x_2$$

Polynomial Regression

- The number of coefficients increases exponentially with k and d
- Model building strategies: forward selection, backward elimination
- The order of the polynomial should be as low as possible, high order polynomials tend to overfit the data



Nonlinear Regression

- Different nonlinear functions can be approximated
- Transform the data to a linear domain

$$\hat{y} = \boldsymbol{\alpha} \cdot e^{\boldsymbol{\gamma} x} \Rightarrow \ln(\hat{y}) = \ln(\alpha) + \gamma x$$

$$\Rightarrow \hat{y}' = \beta_0 + \beta x$$

(for $\hat{y}' = \ln(\hat{y})$, $\beta_0 = \ln(\alpha)$, and $\beta_1 = \gamma$)

- The parameters β_0 and β are estimated with LS
- The parameters $\boldsymbol{\alpha}$ and $\boldsymbol{\gamma}$ are obtained, describing an exponential curve which passes through the original observations
- Problem: LS determines normally distributed errors in the transformed space ⇒ skewed error distribution in the original space

Nonlinear Regression

- Different nonlinear functions can be approximated
- Outputs are estimated by a function with nonlinear parameters, e.g., exponential, trigonometric
- Example type of function:

$$\hat{y} = \beta_0 + \beta_1 e^{\beta_2 x} + \sin(\beta_3 x)$$

- Approach: the type of nonlinear function is chosen and the corresponding parameters are computed
- No closed form solution exists ⇒ numerical approximations:
  - Gauss Newton, Gradient descent, Levenberg-Marquardt

Linear and Nonlinear Regression

- Problems:
  - Linear regression – most of the real world data has a nonlinear behavior
  - Polynomial regression – limited, cannot describe arbitrary nonlinear behavior
  - General nonlinear regression – the type of nonlinear function must be specified in advance

Piecewise Linear Regression

- Piecewise linear functions:

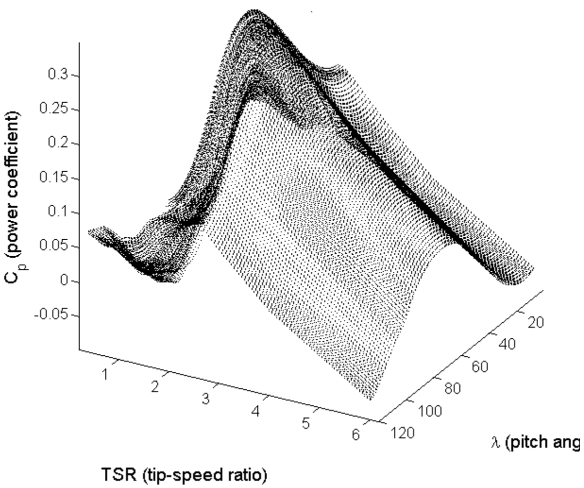
$$f(\mathbf{x}) = \begin{cases} \beta_{00} + \beta_{01} \cdot x_1 + \ldots + \beta_{0d} \cdot x_d, & \mathbf{x} \in \wp_1 \\ \vdots & \\ \beta k_0 + \beta_{k1} \cdot x_1 + \ldots + \beta_{kd} \cdot x_d, & \mathbf{x} \in \wp_k \end{cases}$$

$\wp_1, \ldots, \wp_k$ are partitions in the input space

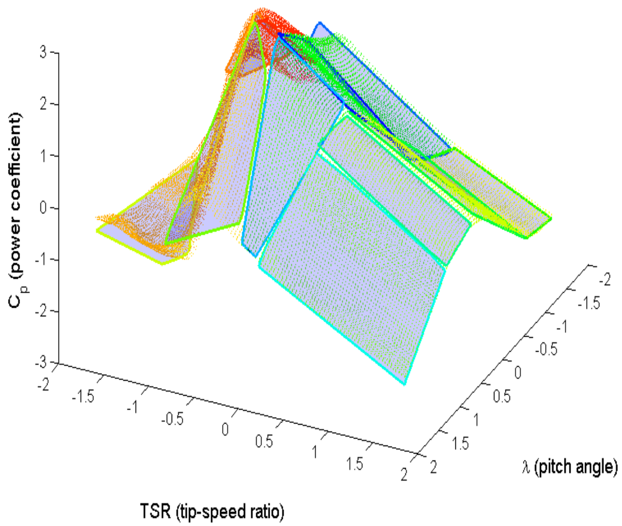
- Simple approach
- Able to describe arbitrary functions
- The **accuracy** is increasing with an increasing number of partitions/linear models
- The **compactness & interpretability** is increasing with a decreasing number of partitions/ linear models
- Challenge: find an appropriate partitioning in the input space (number and shapes)

Goals

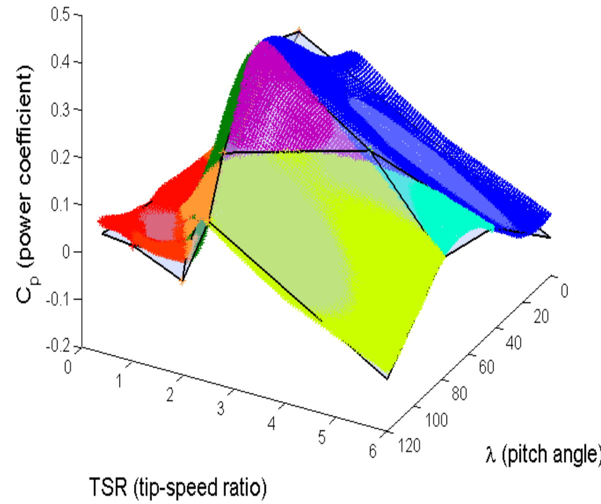
1. Introduction of different learning techniques for piecewise linear models



Training set



Piecewise linear model with regression trees



Continuous piecewise linear model with HH-models

2. Discussion of the bias-variance problem, regression and *ensemble techniques*

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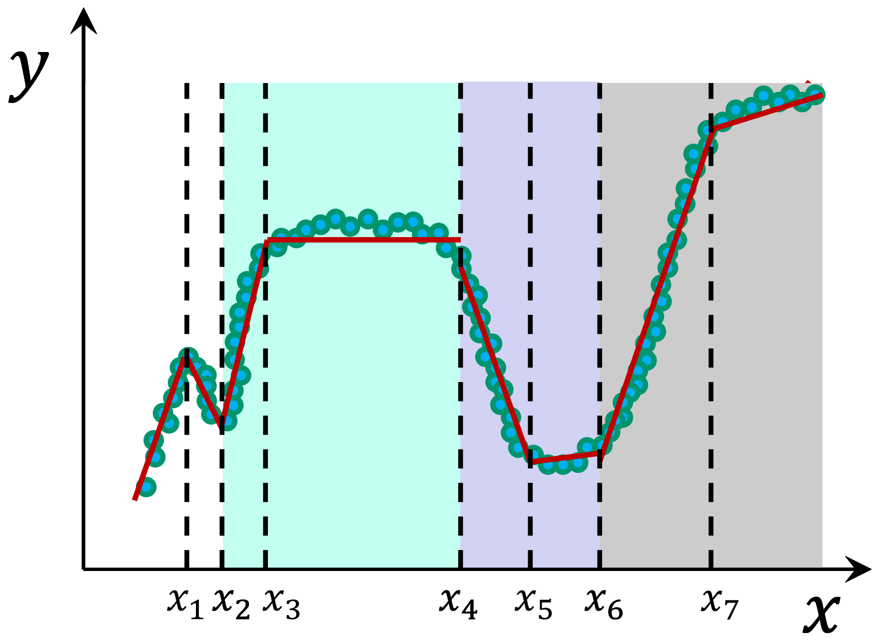
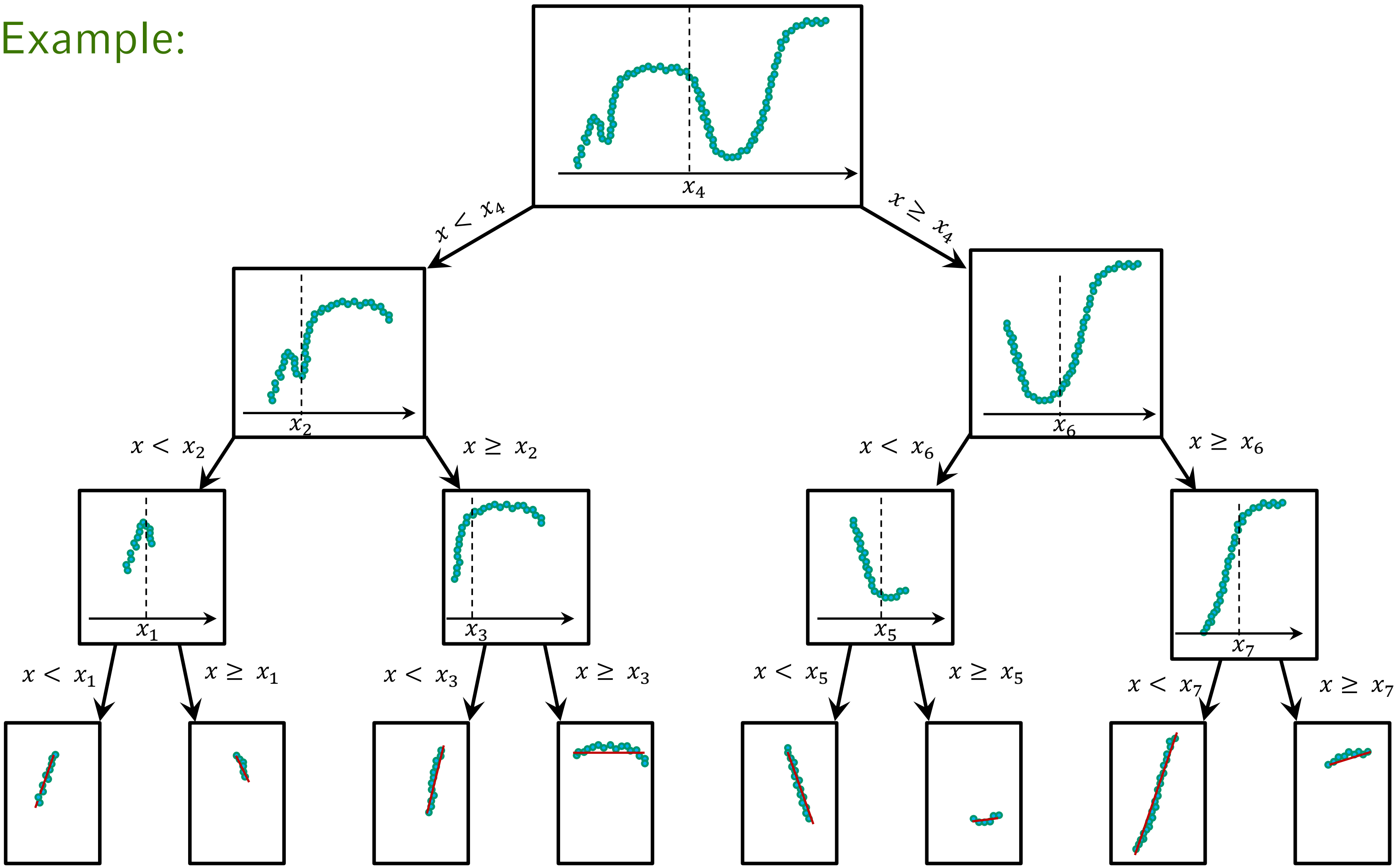
Regression Trees

- Greedy divide and conquer: recursive partitioning of the input space
- Example with input x and output y :



Regression Trees

- Example:

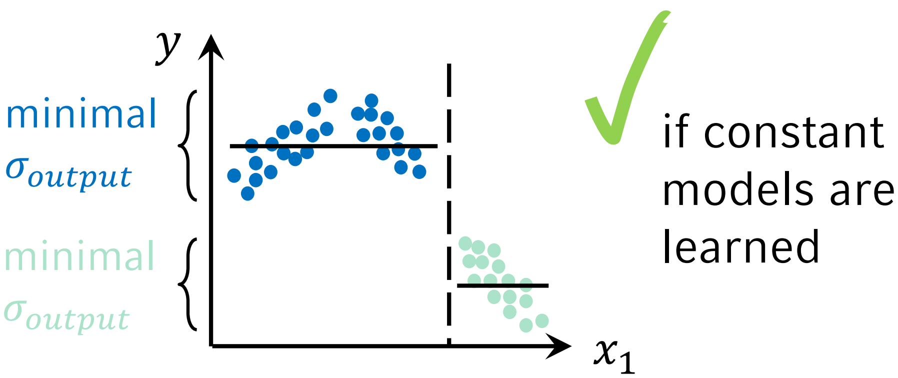


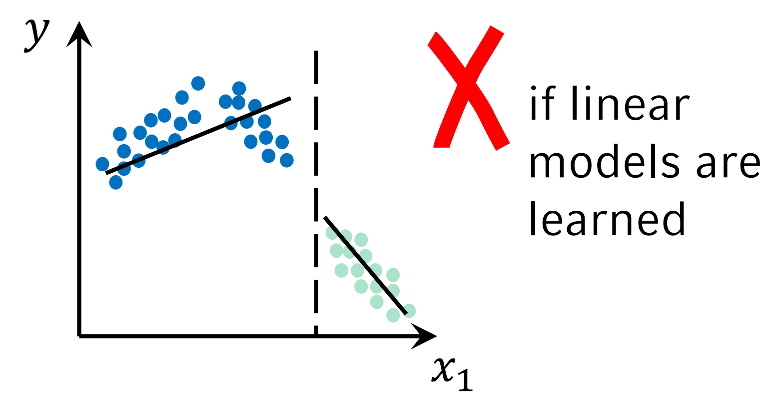
Regression Trees

- General approach of learning a regression tree:
  - Given: set of observations T
  - Find a split of T in T_1 and T_2 with minimal summed impurity
    $$\text{imp}(T_1) + \text{imp}(T_2)$$
  - If the stopping criterion is not reached: repeat for T_1 and T_2
  - If the stopping criterion is reached: undo the split
- Internal node denotes a test in the input space
- Branch represents an outcome of the test
- Leaf nodes contain a linear function, used to predict the output

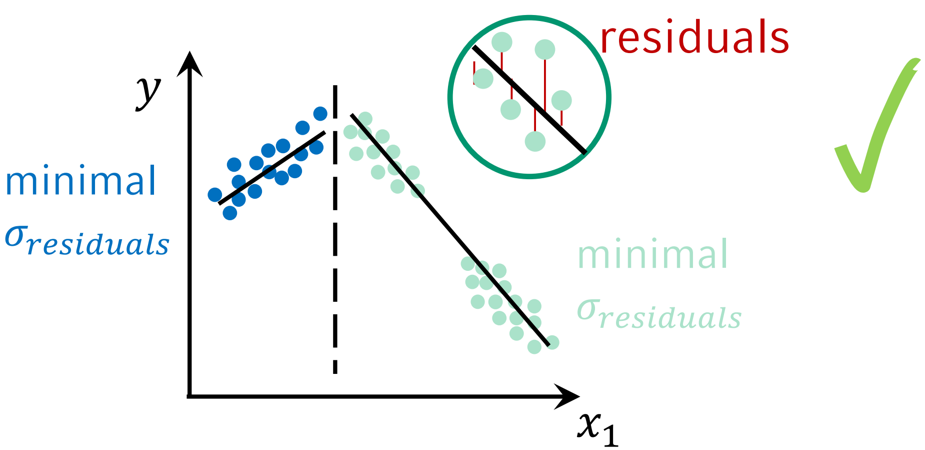
Impurity Measure

- Variance of the output: $imp(T) = \frac{1}{|T|}\sum_{(\mathbf{x},y)\in T}(y - \bar{y})^2$





- Better: variance of the residuals:



$$imp(T) = \frac{1}{|T|}\sum_{(\mathbf{x},y)\in T}(y - f(\mathbf{x}))^2$$

Stopping Criterion: Impurity Ratio

- The recursive splitting is stopped if:
  a) The sample size of a node is below a specified threshold
  b) The split is not significant:
     - If the relative impurity ratio induced by a split is higher than a given threshold, then the split is not significant

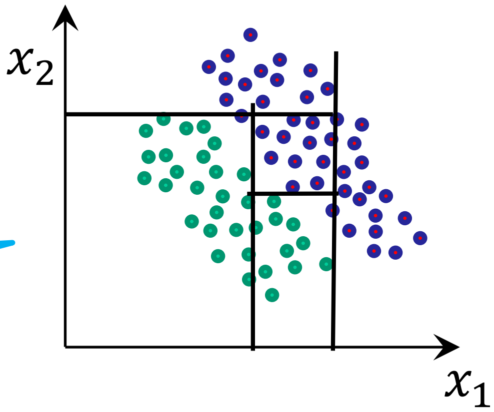
$$\tau = \frac{imp(T_1) + imp(T_2)}{imp(T)} > \tau_0$$

     - As the tree grows the resulting piecewise linear model gets more accurate. τ increases, becoming higher than τ_0
- Choosing the parameter τ_0 ⇔ trading accuracy with overfitting
- stopping too soon ⇒ model is not accurate enough
- stopping too late ⇒ model overfits the observations

Split Strategy

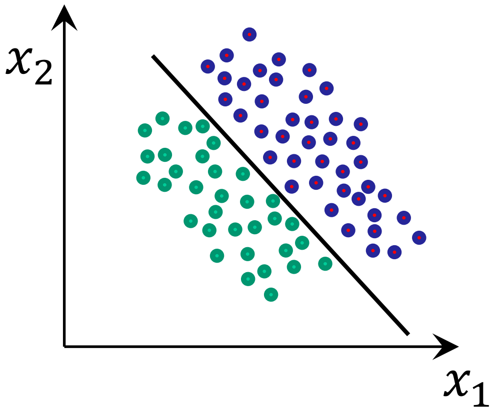
- The split strategy determines how the training samples are partitioned, whether the split is actually performed is decided by the stopping criterion
- The most common splits are axis parallel:
  - Split = a value in one input dimension
  - Compute the impurity of all possible splits in all input dimensions and choose at the end the split with the lowest impurity
  - For each possible split compute the two corresponding models and their impurity ⇒ expensive to compute

4 axis parallel splits in the 2D input space, in order to separate the red from the blue samples



Strategy for Oblique Splits

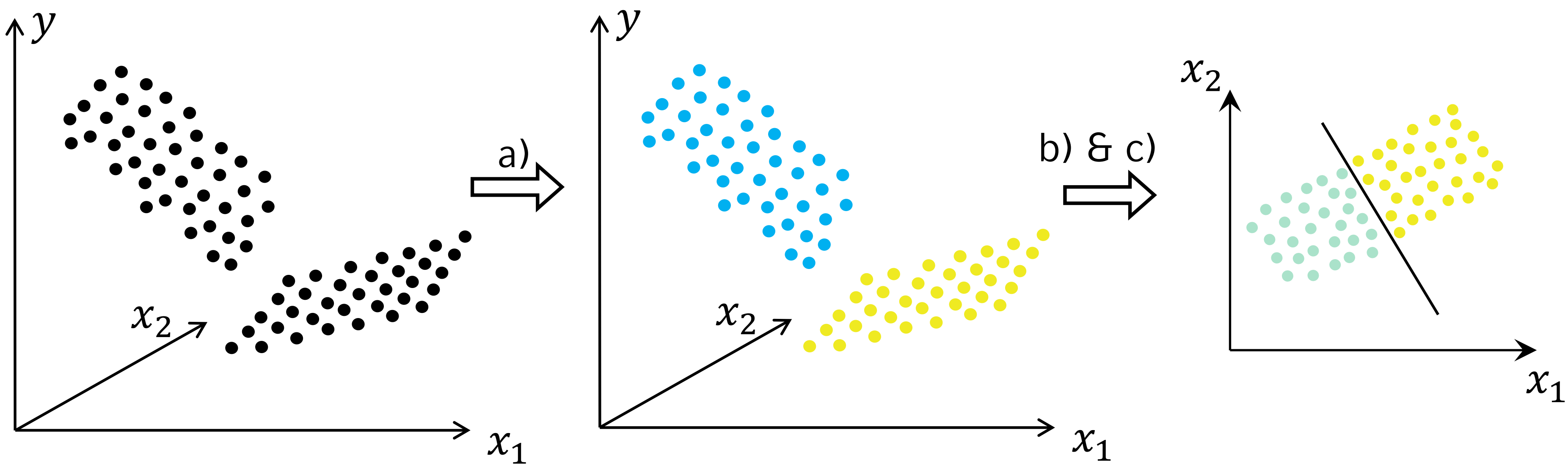
- More intuitive to use oblique splits
- An oblique split is a linear separator in the input space instead of a split value in an input dimension
- The optimal split (with minimal impurity measure) cannot be efficiently computed
- Heuristic approach required



1 oblique split in the 2D input space, in order to separate the red from the blue samples

Strategy for Oblique Splits

- Heuristic approach:
  a) Compute a clustering in the full (input + output) space, such that the samples are as well as possible described by linear equations
  b) Project the clusters onto the input space
  c) Use the clusters to train a linear classifier in the input space. Split = separating hyperplane in input space



Strategy for Oblique Splits

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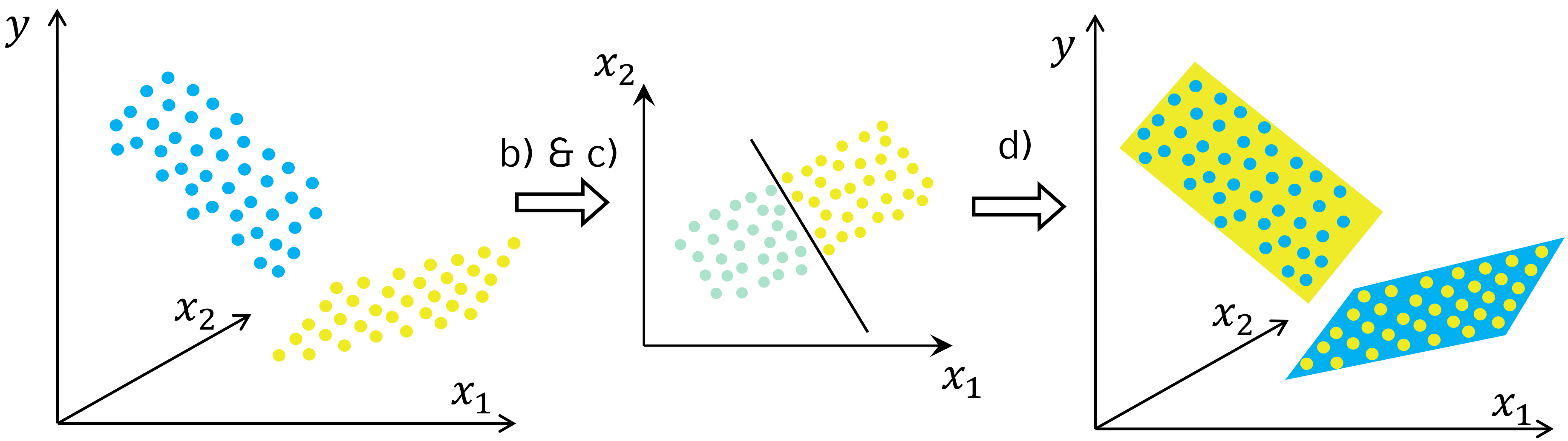
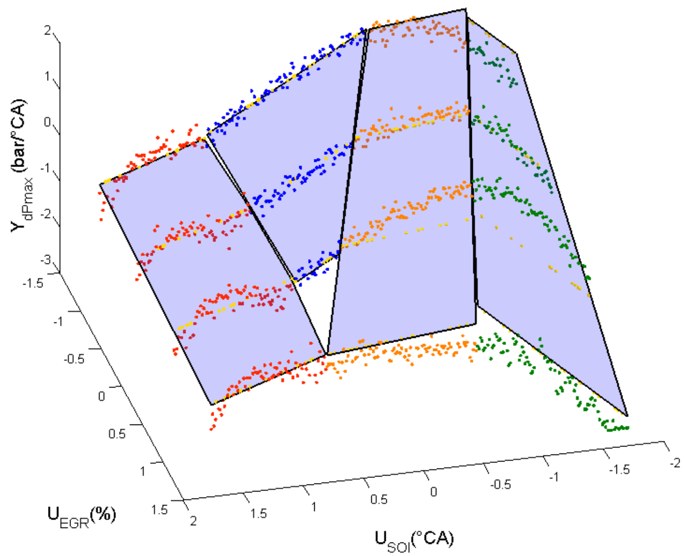
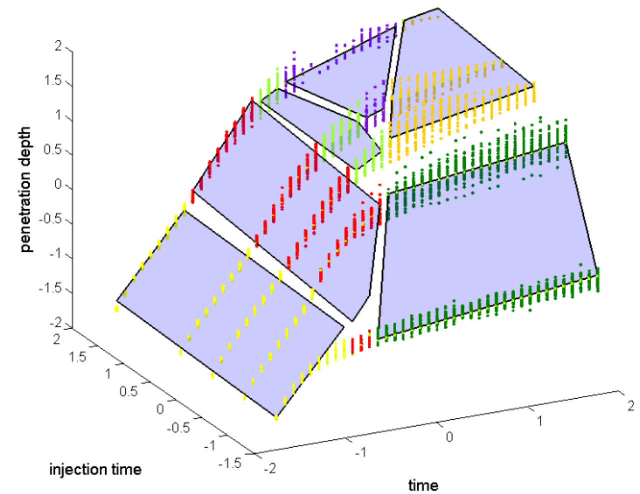
  b) Project the clusters onto the input space
  c) Use the clusters to train a linear classifier in the input space. Split = separating hyperplane in input space
  d) Compute linear models for the two linearly separated clusters

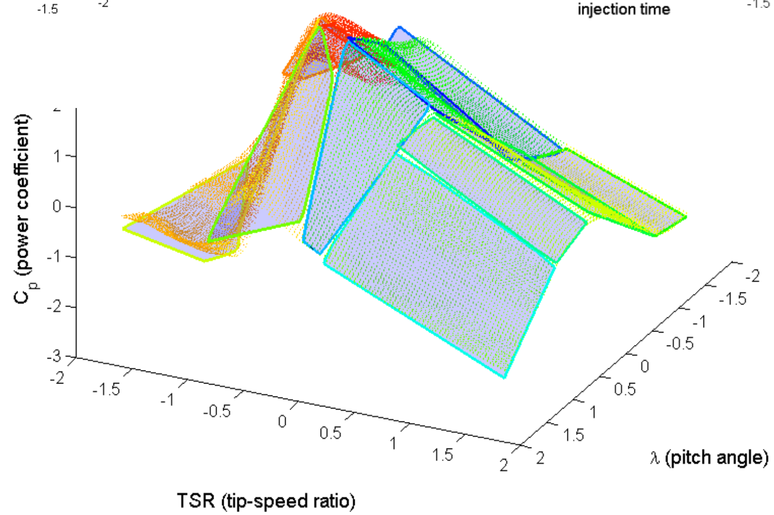


Example Models

- Example piecewise linear models (with oblique splits in the input space):







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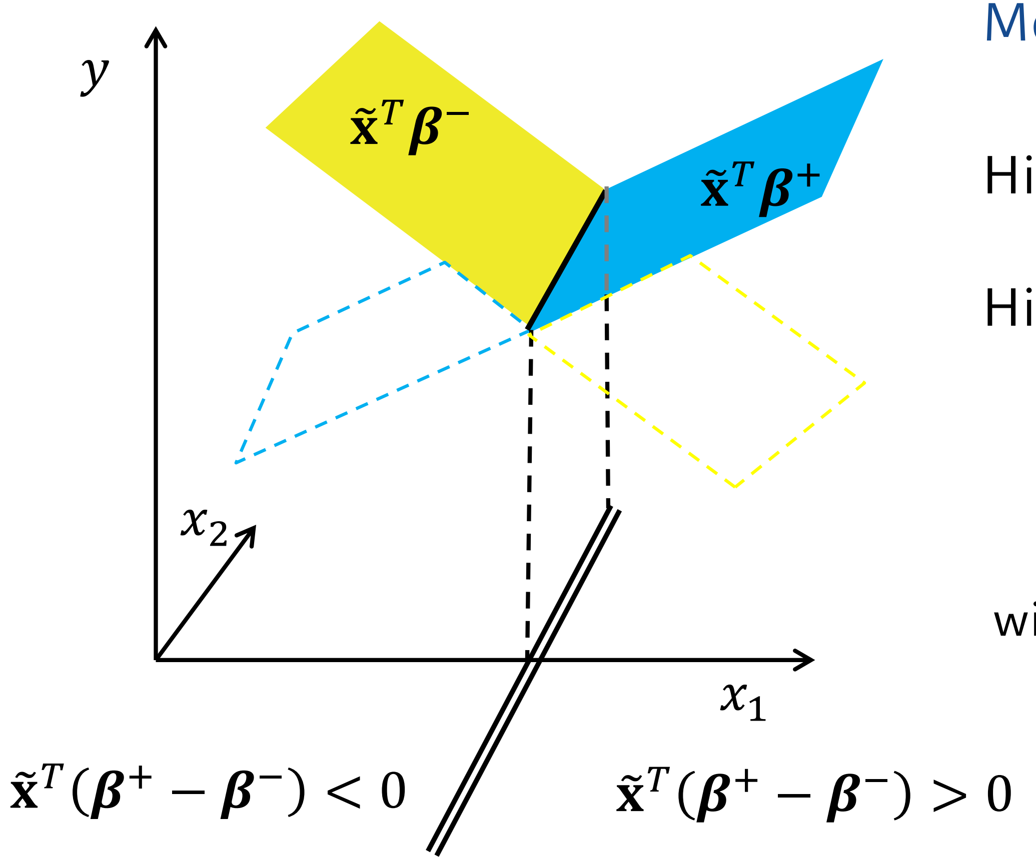
Hinging Hyperplane Models

- Hinging Hyperplane Model (HH-model) for continuous models



Model: $\boldsymbol{f}(\mathbf{x}) = \sum_{i=1}^{K} \boldsymbol{h}_i(\mathbf{x})$

Hinge: $\boldsymbol{\Delta} = \boldsymbol{\beta}^+ - \boldsymbol{\beta}^-$

Hinge function:

$$h(\mathbf{x}) = \begin{cases} \tilde{\mathbf{x}}^T \boldsymbol{\beta}^+, & \tilde{\mathbf{x}}^{\mathbf{T}} \cdot \boldsymbol{\Delta} > 0 \\ \tilde{\mathbf{x}}^T \boldsymbol{\beta}^-, & \tilde{\mathbf{x}}^{\mathbf{T}} \cdot \boldsymbol{\Delta} \leq 0 \end{cases}$$

with $\tilde{\mathbf{x}}^T = (1, \mathrm{x}_1, \ldots, \mathrm{x}_n)$.

[L. Breiman (1993)]

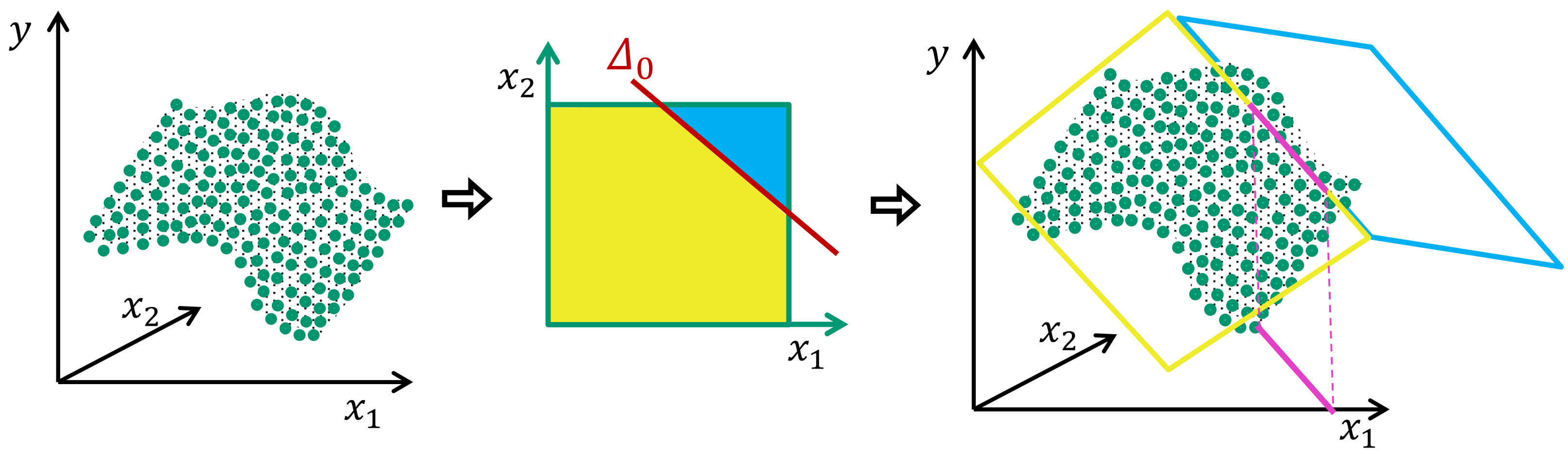
Hinging Hyperplane Models

- **Hinge Finding Algorithm (HFA)**

1) Start with a random partitioning of the input space: $\boldsymbol{\Delta}_j \;\; (j = 0)$
2) Determine the two corresponding partitions:

– $S_j^- = \{\, \mathbf{x} \mid \tilde{\mathbf{x}}^T \boldsymbol{\Delta}_j \leq 0\}$ and $S_j^+ = \{\, \mathbf{x} \mid \tilde{\mathbf{x}}^T \boldsymbol{\Delta}_j > 0\}$

3) Compute the regression hyperplanes for S_j^+ and S_j^-



Hinging Hyperplane Models

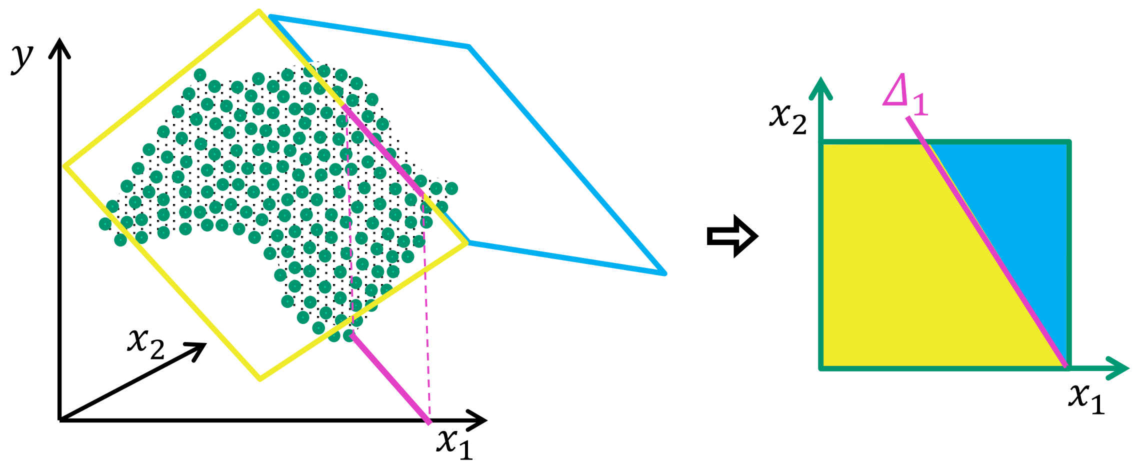
- **Hinge Finding Algorithm (HFA)**

3) Compute the regression hyperplanes for S_j^+ and S_j^-

4) Compute the hinge $\boldsymbol{\Delta}_{j+1}$ from the regression coefficients $\boldsymbol{\beta}_j^-$ and $\boldsymbol{\beta}_j^+$

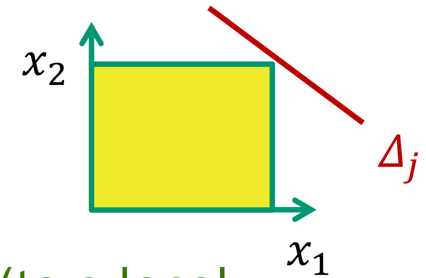
5) Determine the new partitions S_{j+1}^+ and S_{j+1}^- determined by $\boldsymbol{\Delta}_{j+1}$

6) If $S_{j+1}^+ = S_j^+$ or $S_{j+1}^+ = S_j^-$, then stop, else return to step 3).

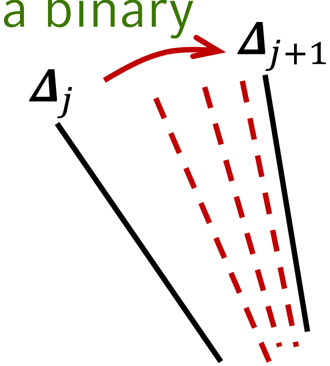


Line Search for the Hinge Finding Algorithm

- The Hinge Finding Algorithm (HFA) might not converge – a hinge might induce a partitioning outside the defined input space



- *Line search*: binary search to guarantee convergence (to a local minimum)
- Instead of updating the hinge directly $\boldsymbol{\Delta}_j \longrightarrow \boldsymbol{\Delta}_{j+1}$, first check the accuracy improvement brought by $\boldsymbol{\Delta}_{j+1}$
- If $\boldsymbol{\Delta}_{j+1}$ does not improve the model impurity, then perform a binary search after the linear combination of $\boldsymbol{\Delta}_j$ and $\boldsymbol{\Delta}_{j+1}$ yielding the lowest impurity



$$\boldsymbol{\Delta}'_{j+1} = \boldsymbol{\Delta}_i + \lambda(\boldsymbol{\Delta}_{j+1} - \boldsymbol{\Delta}_j), \quad \lambda \in \left\{\frac{1}{2}, \frac{1}{4}, \frac{1}{8}, \frac{1}{16}\right\}$$

Fit Multiple Hinges

- Goal: Describe the target function y as a sum of N hinge functions

$$y = \sum_{i=1}^{N} h_i(x)$$

- Each hinge function h_i can be seen as fitted to the residual function

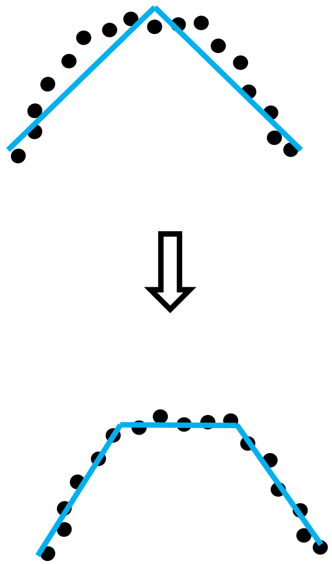
$$y_{[i]} = y - \sum_{j \neq i} h_j(x),$$

since then $h_i(x) = y - \sum_{j \neq i} h_j(x)$.

- Fit multiple hinges iteratively in N steps:
  - Start with $h_1(x) = \cdots = h_N(x) = 0$
  - Step n: Fit the n-th hinge h_n to $y_{[n]} = y - \left(h_1(x) + \cdots + h_{n-1}(x)\right)$.
    Then repeatedly refit h_1 to $y_{[1]}$, … , and h_{n-1} to $y_{[n-1]}$
    until the hinges do not change anymore.

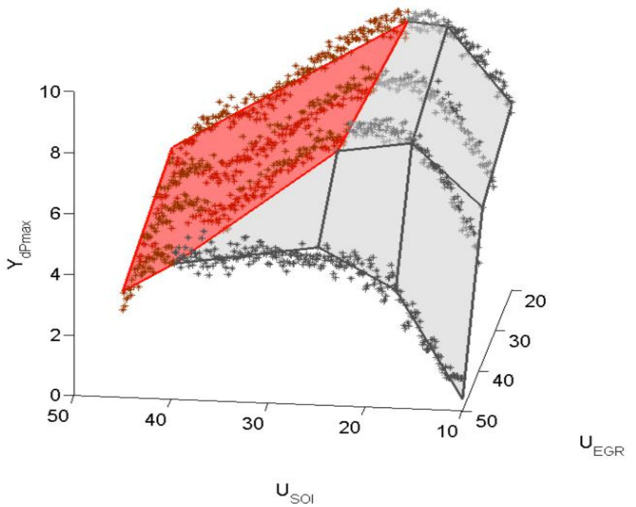
Fit Multiple Hinges

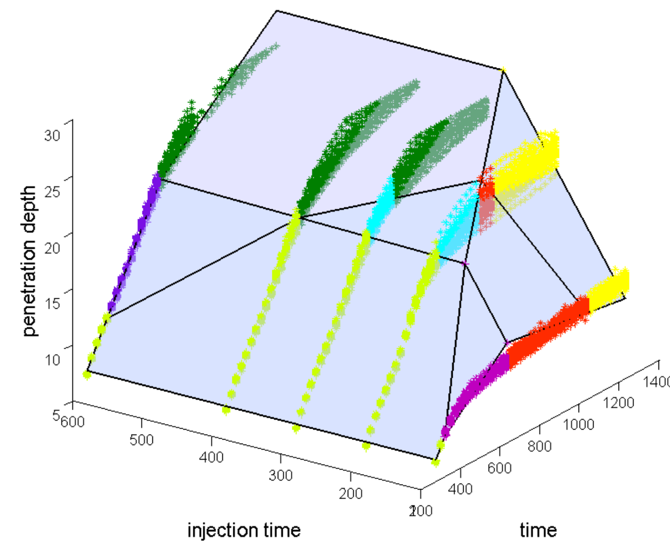
- Example:
  - Step 1: Fit the first hinge function h_1 to $y_{[1]} = y - 0$.
  - Step 2: Compute the residual outputs
    $$y_{[2]} = y - h_1(x).$$
    Fit the second hinge function h_2 to $y_{[2]}$.
    Then refit the first hinge to $y_{[1]} = y - h_2(x)$.
  - Step 3: Compute the residual outputs
    $$y_{[3]} = y - h_1(x) - h_2(x).$$
    Fit the third hinge function h_3 to $y_{[3]}$.
    Then repeatedly refit
    $$h_1 \text{ to } y_{[1]} = y - h_2(x) - h_3(x) \text{ and}$$
    $$h_2 \text{ on } y_{[2]} = y - h_1(x) - h_3(x).$$
    until no more changes occur.

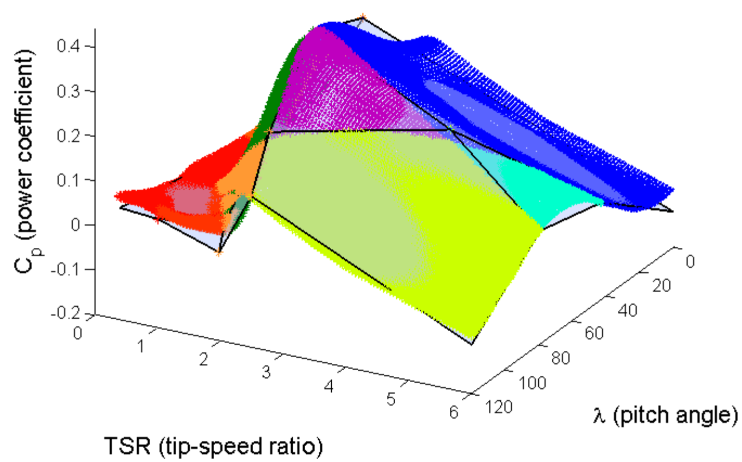


Example Models

- Example piecewise linear models (with oblique splits in the input space):







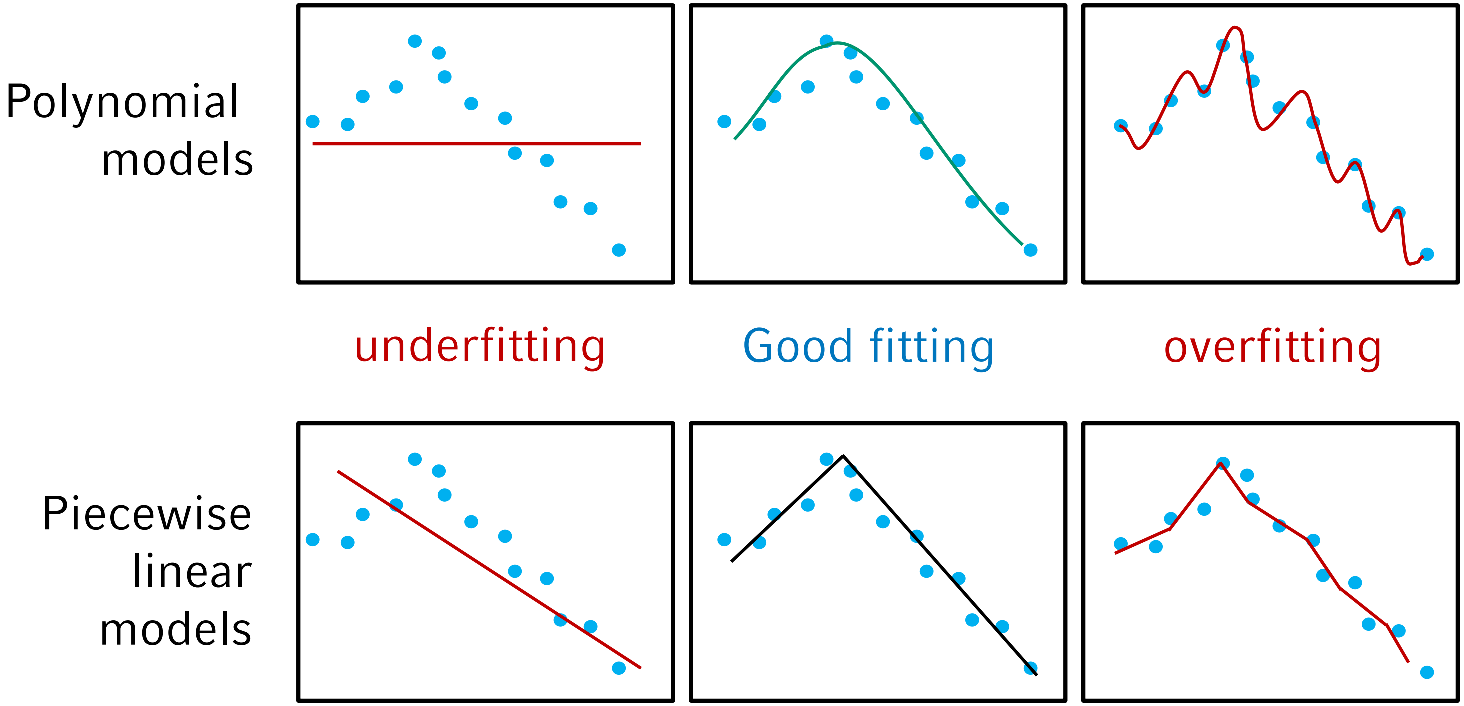
x_1

Chapter 7: Numerical Prediction

1) Introduction
   – Numerical Prediction problem, linear and nonlinear regression, evaluation measures
2) Piecewise Linear Numerical Prediction Models
   – Regression Trees, axis parallel splits, oblique splits
   – Hinging Hyperplane Models
3) Bias-Variance Problem
   – Regularization , Ensemble methods

Underfitting vs. Overfitting

- Underfitting = a learned model is not flexible enough to capture the underlying trend
- Overfitting = a learned model is too flexible, allowing to capture illusory trends in the data, which appear due to noise



Bias and Variance

- Assuming that the data generation process can be repeated (with a certain amount of randomness) ⇒ obtain several datasets D_i & for each D_i a model f_i is learned
- Bias = the difference between the average prediction of these models and the correct value
- Variance = the variability of the predictions of the different models

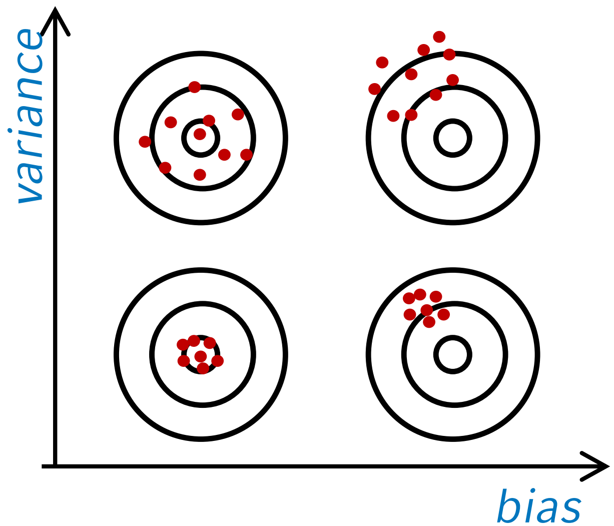


Image after *http://scott.fortmann-roe.com/docs/BiasVariance.html*

Bias-Variance Tradeoff

- Underfitting = low variance, high bias (e.g. use mean output as estimator)
- *High bias* = a model does not approximate the underlying function well
- Overfitting = high variance, low bias
- When a model is too complex, small changes in the data cause the predicted value to change a lot ⇒ *high variance*
- **Search for the best tradeoff between bias and variance**
- Regression: control the bias-variance tradeoff by means of the polynomial order/number of coefficients
- Regression trees: control the bias-variance tradeoff by means of the tree size/number of submodels

Bias and Variance

$(\star)$: $E[z^2] = E[(z - E[z])^2] + E[z]^2$

- Consider the expected prediction error of a learned model:

$$Err(\mathbf{x}) = E[(f(\mathbf{x}) - y)^2]$$

$$Err(\mathbf{x}) = E[f(\mathbf{x})^2 - 2f(\mathbf{x})y + y^2]$$

$$Err(\mathbf{x}) = E[f(\mathbf{x})^2] - 2E[f(\mathbf{x})]E[y] + E[y^2]$$

$$Err(\mathbf{x}) \overset{(\star)}{=} E\left[(f(\mathbf{x}) - \overline{f(\mathbf{x})})^2\right] + \overline{f(\mathbf{x})}^2 - 2\overline{f(\mathbf{x})}E[y] + E[(y - E[y])^2] + E[y]^2$$

$$Err(\mathbf{x}) = \underbrace{E\left[(f(\mathbf{x}) - \overline{f(\mathbf{x})})^2\right]}_{\text{error due to the variance of } f} + \underbrace{\left(\overline{f(\mathbf{x})} - E[y]\right)^2}_{\text{error due to the bias of } f \text{ (systematic error)}} + \underbrace{E[(y - E[y])^2]}_{\text{irreducible error}}$$

Bias and Variance

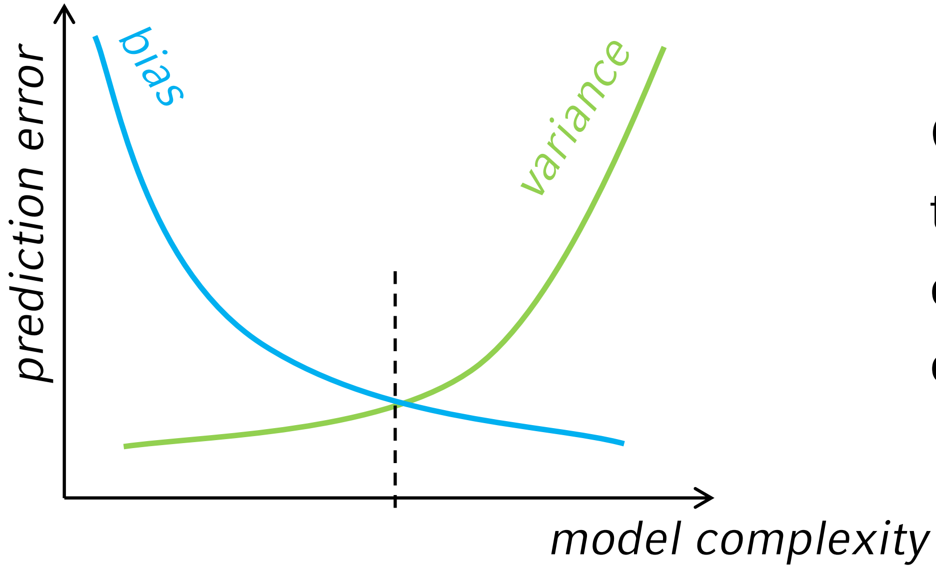
- Consider the expected prediction error of a learned model:

$$Err(\mathbf{x}) = \underbrace{E\left[\left(f(\mathbf{x}) - \overline{f(\mathbf{x})}\right)^2\right]}_{\text{error due to the variance of } f} + \underbrace{\left(\overline{f(\mathbf{x})} - E[y]\right)^2}_{\text{error due to the bias of } f \text{ (systematic error)}} + \underbrace{E\left[(y - E[y])^2\right]}_{\text{irreducible error}}$$

error due to the variance of f

error due to the bias of f (systematic error)

irreducible error



Carefully balance between these two types of error, in order to minimize the total expected prediction error

Regularization

- Minimizing the sum of squared errors

$$\sum_{(x,y)\in T} (f(x) - y)^2 \longrightarrow min$$

computes an unbiased linear model with very high variance

- Idea: give up the unbiasedness and obtain a variance decrease by penalizing the model complexity
- Regularization: simultaneously minimize the sum of squared errors and the norm of the coefficient vector
- Linear regularization (*ridge regression*):

$$\sum_{(x,y)\in T} (f(x) - y)^2 + \lambda \|\beta\|_2^2 \longrightarrow min$$

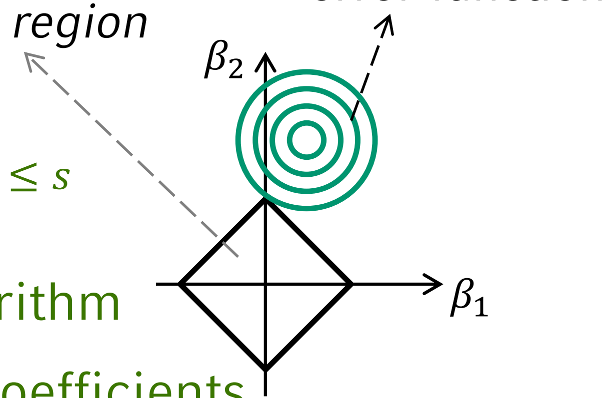
Regularization

- Lasso regularization:

$$\underset{\beta}{\operatorname{argmin}} \sum_{(x,y)\in T} (f(x)-y)^2, \qquad s.t. \|\beta\|_1 \leq s$$

  – solvable with a quadratic programming algorithm

  – With an increasing penalty more and more coefficients are shrunk towards zero, generating more sparse models

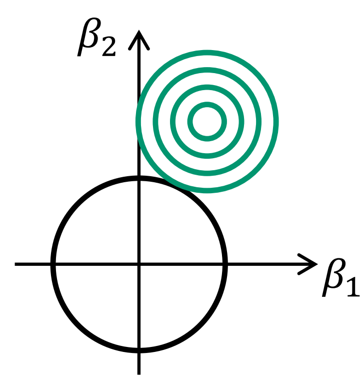


- Linear regularization (*ridge regression*):

$$\underset{\beta}{\operatorname{argmin}} \sum_{(x,y)\in T} (f(x)-y)^2, \qquad s.t. \|\beta\|_2^2 \leq s$$

  – solvable similar to SSE: $\beta = (X^T X + \lambda I)^{-1} \cdot X^T Y$

  – Reduces all coefficients simultaneously



Bagging

- When discussing the bias-variance tradeoff, we assumed infinitely many replications of our data set, but in practice we have only one training set T
- Simulate multiple training sets $T_1, T_2, \ldots T_k$ by constructing bootstrap replicates of the original training set T, by randomly drawing samples from T (with replacement) such that $|T_j| = |T|, j \in \{1, \ldots k\}$
- Learn a model f_j for each replicate T_j (use as test set $T_{Sj} = T \setminus T_j$)
- For each input $\mathbf{x}$, we have several predictions $y_1, \ldots, y_k$ ⇒ compute the average prediction
- $f(\mathbf{x}) \approx \overline{f(\mathbf{x})} \Rightarrow (f(\mathbf{x}) - \overline{f(\mathbf{x})})^2 \approx 0 \Rightarrow$ the variance is removed/reduced
- Bias: $\left(\overline{f(\mathbf{x})} - E[y]\right)^2$ is the same as before

Ensemble Methods

- Bagging:
  - use it for models with a low bias
  - If the bias is low, bagging reduces the variance, while bias remains the same
  - use it for complex models, which tend to overfit the training data
  - in practice it might happen that the bagging approach slightly increases the bias
- Boosting:
  - Can be adapted for regression models
  - Reduces the bias in the first iterations
  - Reduces the variance in later iterations