Machine Learning

Lecture 1 - Introduction to ML, k-NN and Decision Trees

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Course overview

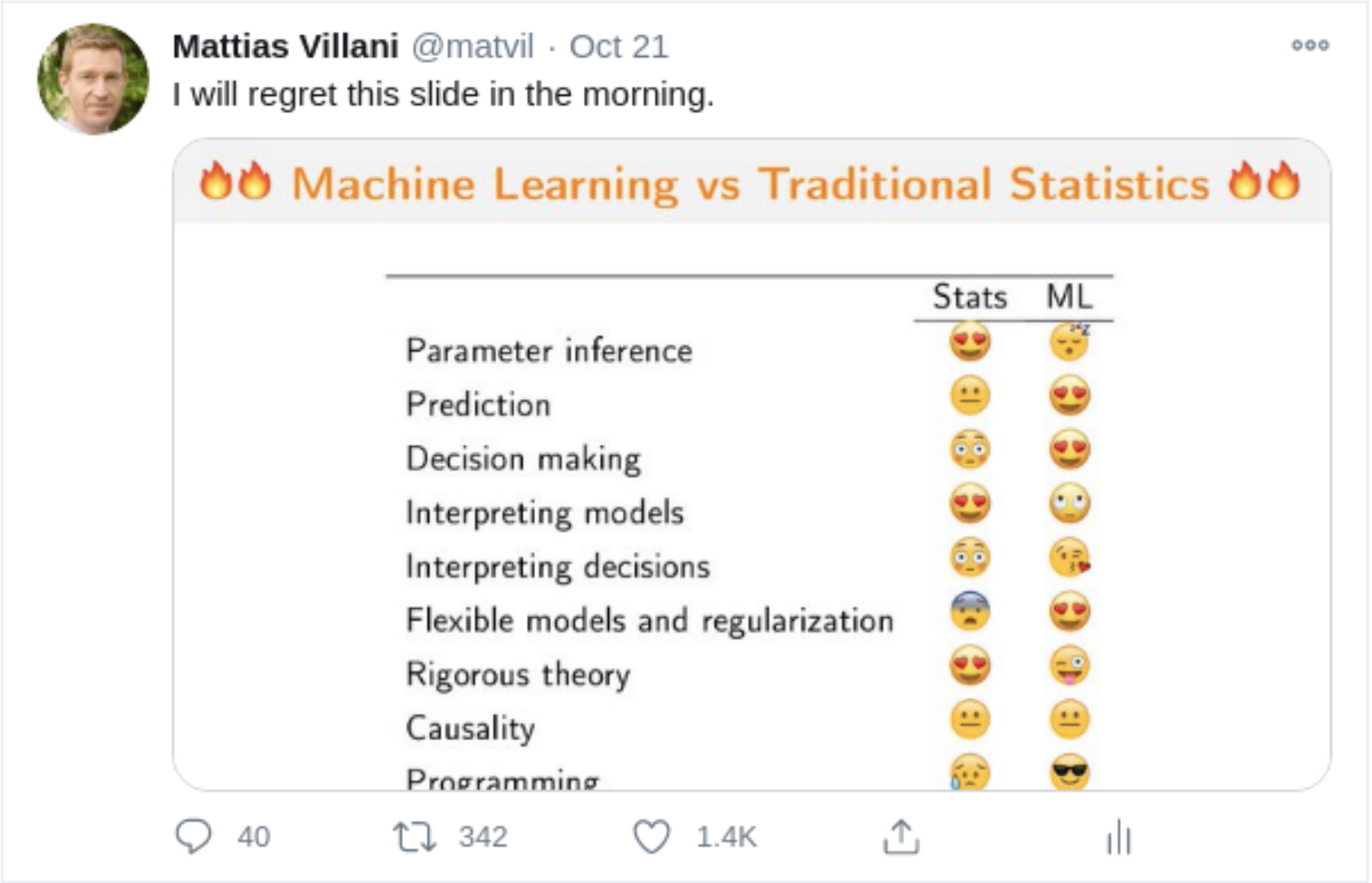
- Course webpage. Course syllabus.
- Modes of teaching:
  - Lectures 1-10 (Mattias Villani)
  - Lectures 11-12 (Frank Miller)
  - Computer labs 1-3 (Karl Sigfrid)
- **Modules**:
  - **Supervised learning** with **regularized regression** and **classification.**
  - **Neural networks and deep learning**
  - **Unsupervised**, **semisupervised** and **active learning**.
- **Examination**
  - Three computer lab reports, 3 credits (in pairs of students)
  - Exam (5+1 hours computer-based exam. Take home this semester), 4.5 credits

What is Machine Learning?

Wikipedia (Nov 2, 2019)

- **Machine learning** is the scientific study of algorithms and statistical models that computer systems use to perform a specific task without using explicit instructions, relying on patterns and inference instead.
- It is seen as a subfield of **artificial intelligence**. Machine learning algorithms build a mathematical model based on sample data to make **predictions** or **decisions**.
- Machine learning is closely related to **computational statistics**.
- **Data mining** is a field of study within machine learning, and focuses mainly on exploratory data analysis through unsupervised learning.
- Machine learning for business applications: **predictive analytics**.
- **Data science**. Data science is an interdisciplinary field that uses scientific methods, processes, algorithms and systems to extract knowledge and insights from structured and unstructured data.

How to become viral on Twitter

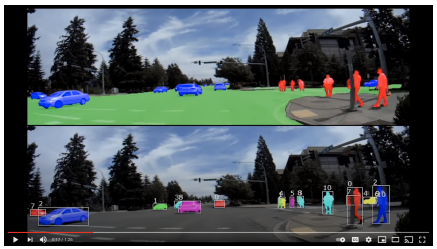


🔥🔥 Machine Learning vs Traditional Statistics 🔥🔥

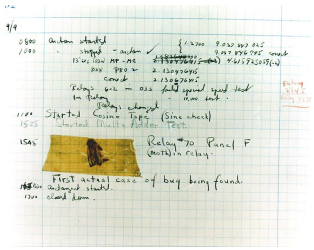
	Stats	ML
Parameter inference	😍	😴
Prediction	😐	😍
Decision making	😳	😍
Interpreting models	😍	🙄
Interpreting decisions	😳	😘
Checking model assumptions	😎	🤫
Flexible models and regularization	😨	😍
Rigorous theory	😍	😜
Causality	😐	😐
Programming	😥	😎
Scalability, big data	😱	😎
Real-time/Online	🤫	🤠
Data collection and experimental design	😎	🤫

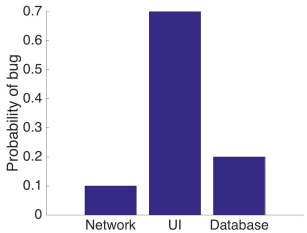
ML applications

- Finding and tracking objects in traffic (image data).

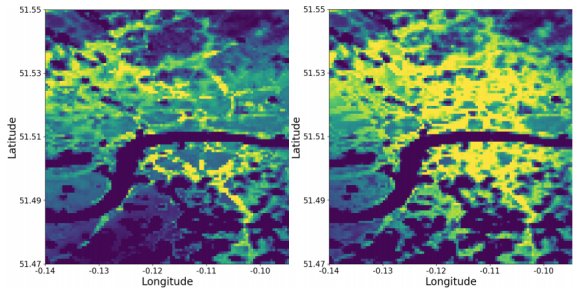


- Finding bugs in computer code from bug reports (text data).





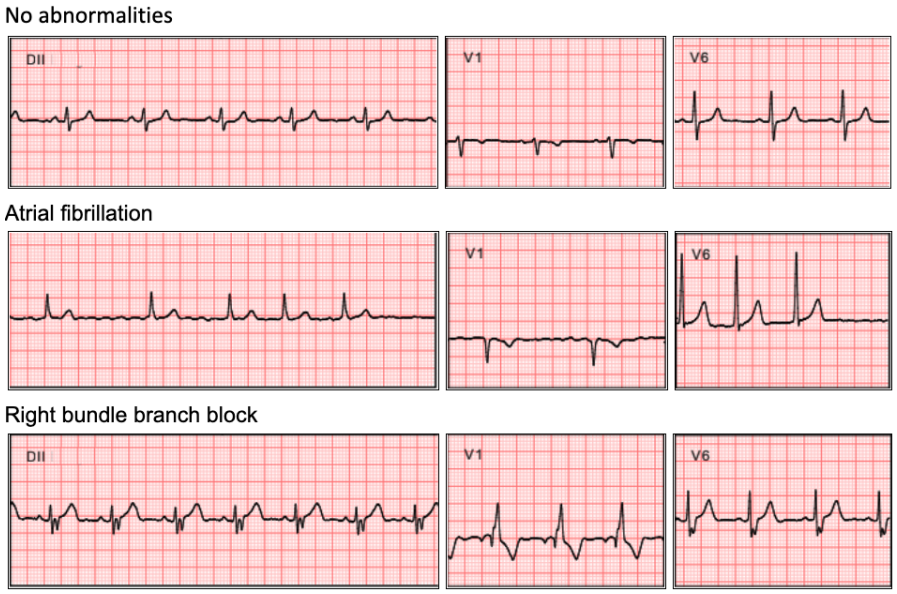
- Predicting pollution (spatiotemporal sensor data).



- Predicting defaults on bank loans (standard tabular data).

ML applications

Training data



Test data

Figures from Lindholm et al (2021).

Supervised machine learning workflow

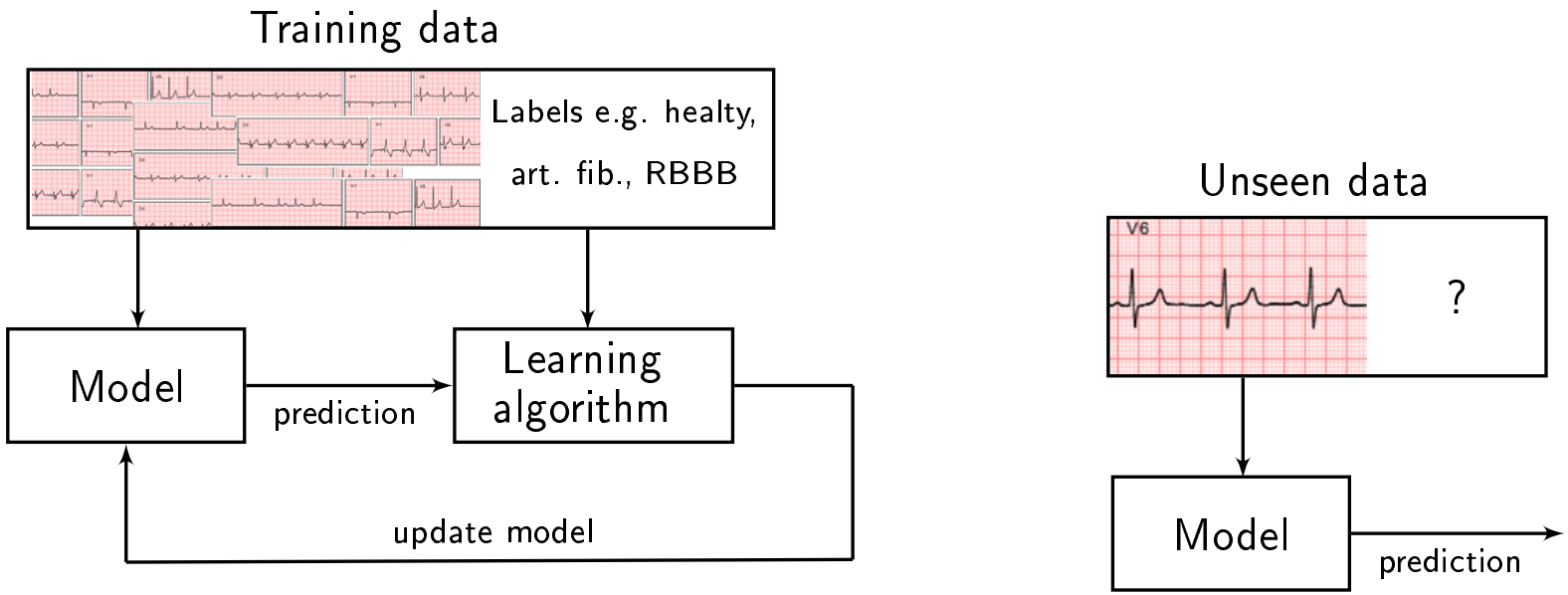
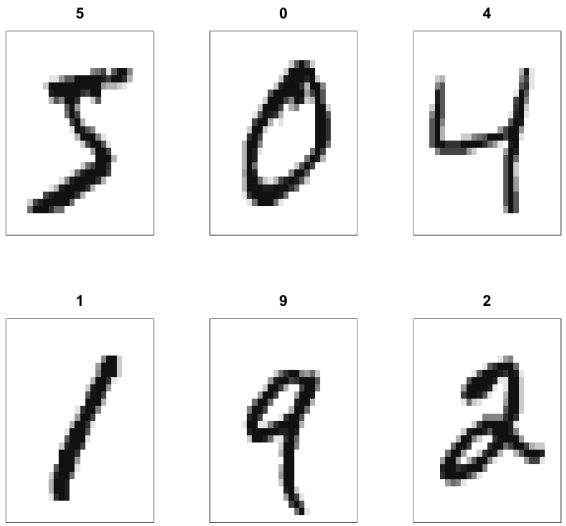
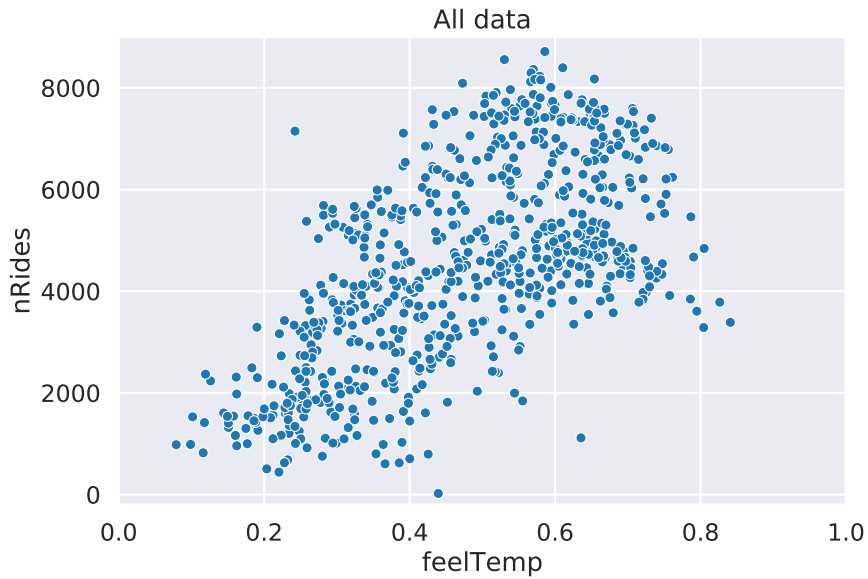


Figure from Lindholm et al (2021).

Labeling distinctions

- Availability of labels
  - **Supervised learning**: labeled training data.
  - **Unsupervised learning**: unlabeled training data.
  - **Semi-supervised learning**: labels for a subset of training data
  - **Reinforcement learning**: sequential learning with incremental rewards for good behavior.
- Types of labels
  - **Regression** - labels are real numbers
  - **Classification** - labels are discrete





Data distinctions

- **Regression** data
  - Real valued
  - Counts
  - Proportions
- **Categorical** data (binary, multi-class)
- **Structured non-tabular data** common in ML applications:
  - **Images**
  - **Text**
  - **Sound**
- Other **dependence structures**:
  - **Time series** (sensor data over time)
  - **Longitudinal data** (one short time series for many objects)
  - **Spatial data** (sensors at different locations, images)
  - **Survival data** (lifetime of hard drives)

Why Statistics in ML?

- Probability models and statistical inference is a **framework**.
- Principled **way to think** about any problem in ML.
- Can be **evaluated** and critiqued.
- **Quantify uncertainties**. Crucial for **Decision making**.

> *As robotics is now moving into the open world, the issue of **uncertainty** has become a major stumbling block for the design of capable robot systems. Managing uncertainty is possibly the most important step towards robust real-world robot systems.*
>
> *from the book Probabilistic Robotics by Thrun et al.*

Linear/Nonlinear - Parametric/Nonparametric

- **Regression**:
  - Labels are continuous.
  - Linear regression: $y = \mathrm{x}^\top \beta + \varepsilon,\ \varepsilon \sim N(0, \sigma^2)$.
- **Classification**:
  - Labels are binary or categorical.
  - Logistic regression: $\Pr(y = 1|\mathrm{x}) = \frac{\exp(\mathrm{x}^\top \beta)}{1+\exp(\mathrm{x}^\top \beta)}$.
- Linear regression and logistic regression are:
  - **Parametric**
  - **Linear** (log-odds and decision boundaries given by $\mathrm{x}^\top \beta$)
- ML
  - **Flexible**, richly parametrized models
  - **Non-linear** models
  - **Non-parametric** models

k-nearest neighbor models

- **Nonparametric** model for regression and classification.
- Aim: predict $y_\star$ for new $\mathrm{x}_\star$.
- **k-NN regression**: predict by **average of k nearest neighbors** to $\mathrm{x}_\star$

$$\hat{y}(\mathrm{x}_\star) = \frac{1}{k} \sum_{i \in \mathcal{N}_\star} y_i = \text{Average}\{y_i : i \in \mathcal{N}_\star\}$$

  where $\mathcal{N}_\star$ is the set of k observations with smallest $\|\mathrm{x}_i - \mathrm{x}_\star\|_2$.
- **k-NN classification**: **majority vote** of k nearest neighbors.
- Any distance measure can be used instead of $\|\mathrm{x}_i - \mathrm{x}_\star\|_2$.
- **Input data** (x) should be **normalized** (zero mean, unit variance, or scaled so $x \in [-1, 1]$).
- **Hyperparameter** k selected from predictive performance.

k-nearest neighbor classification

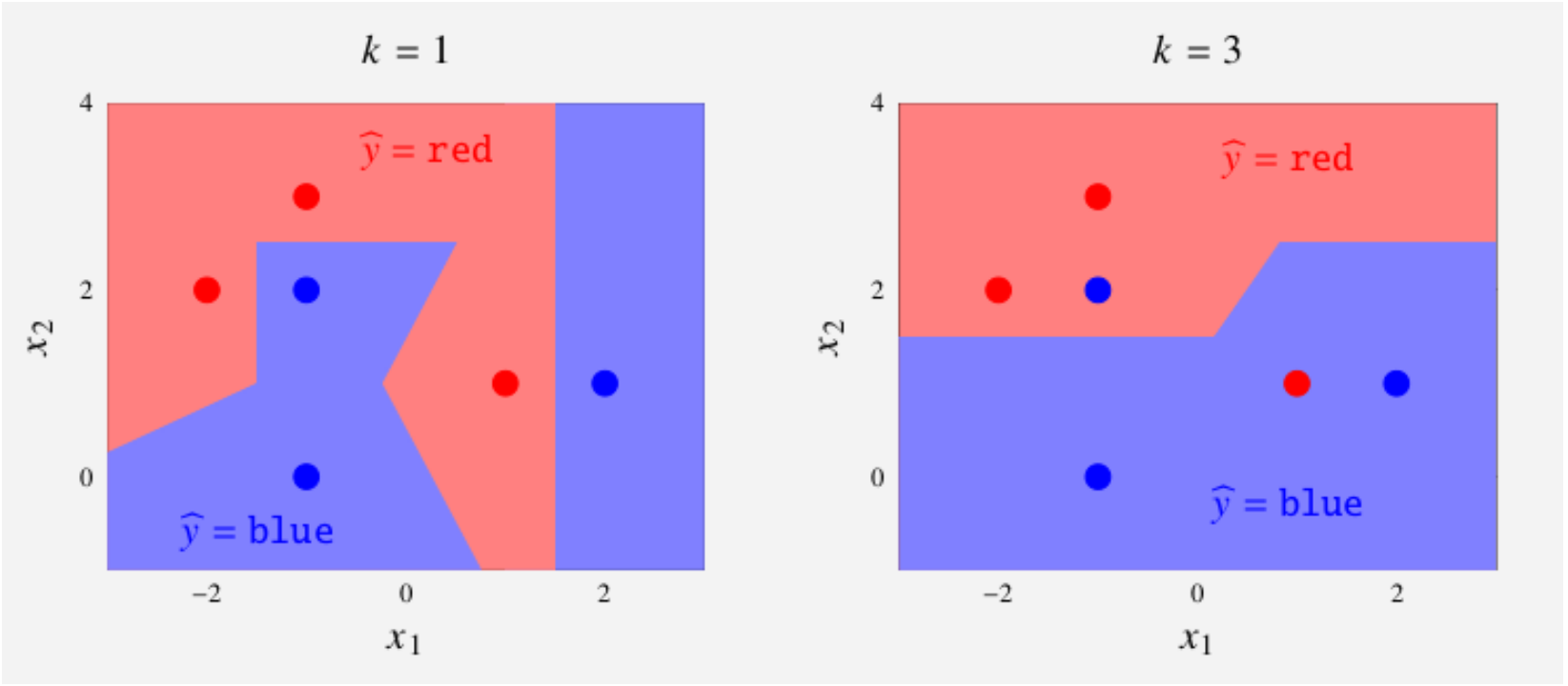


Figure from Lindholm et al (2021).

Song classification

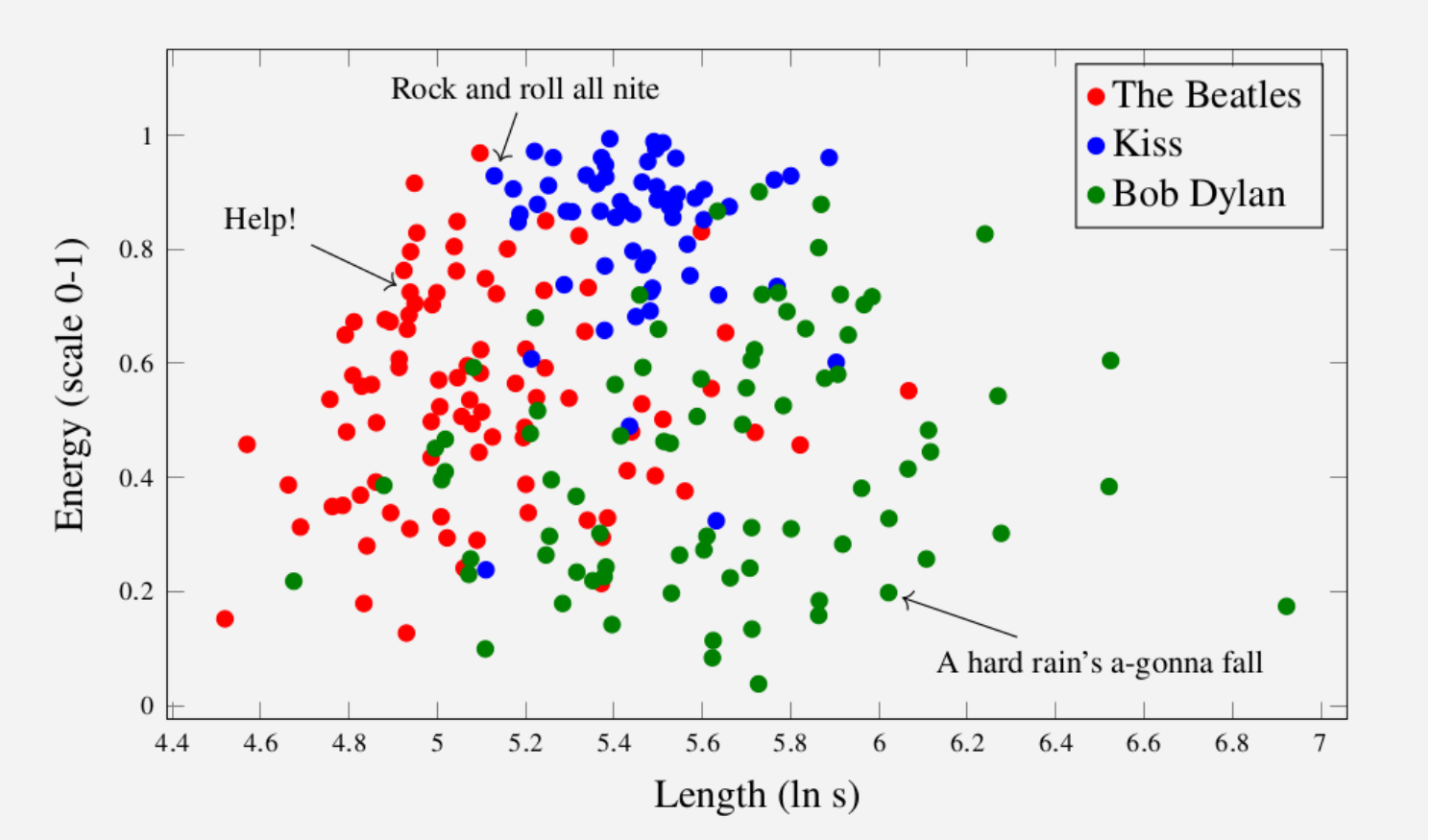


Figure from Lindholm et al (2021).

Song classification with k-NN

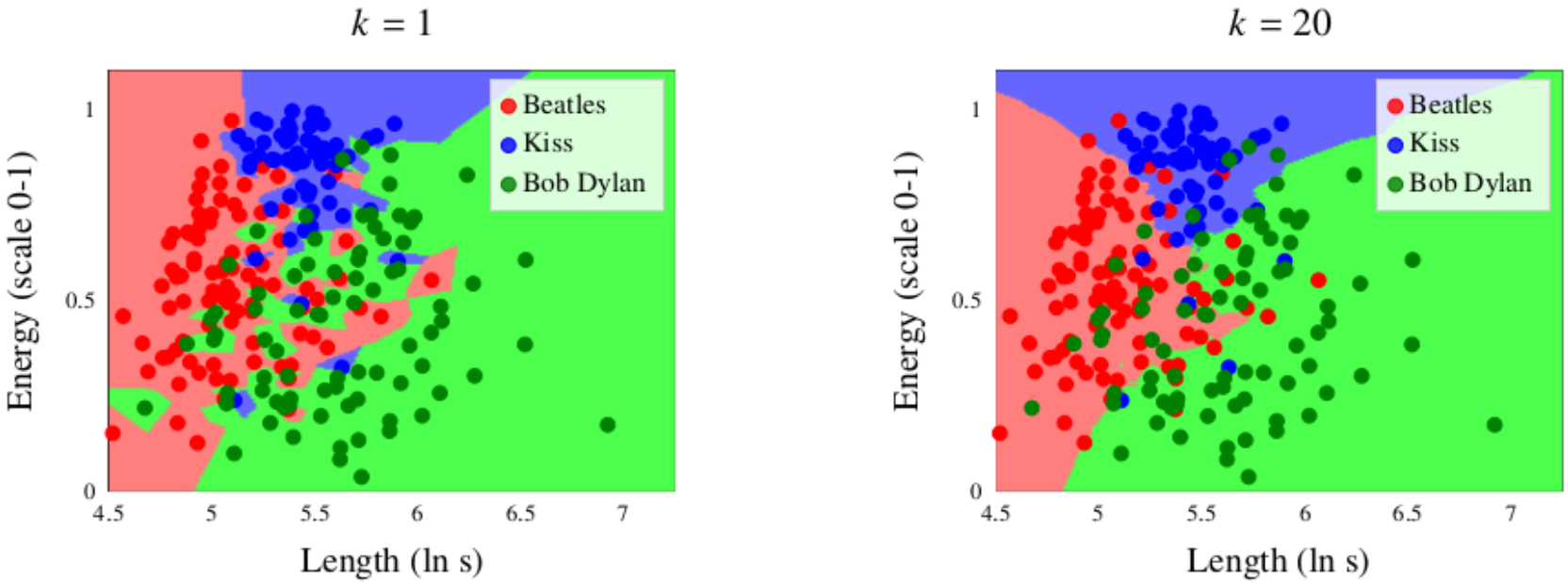
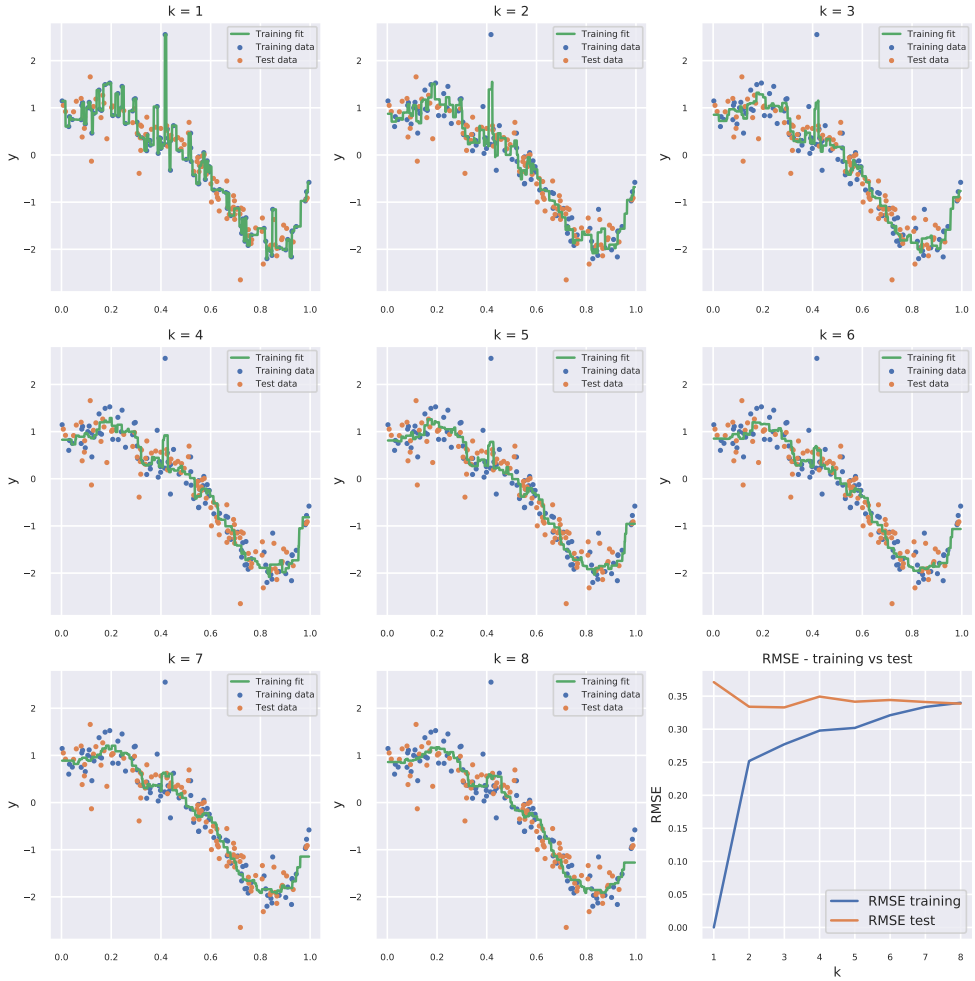


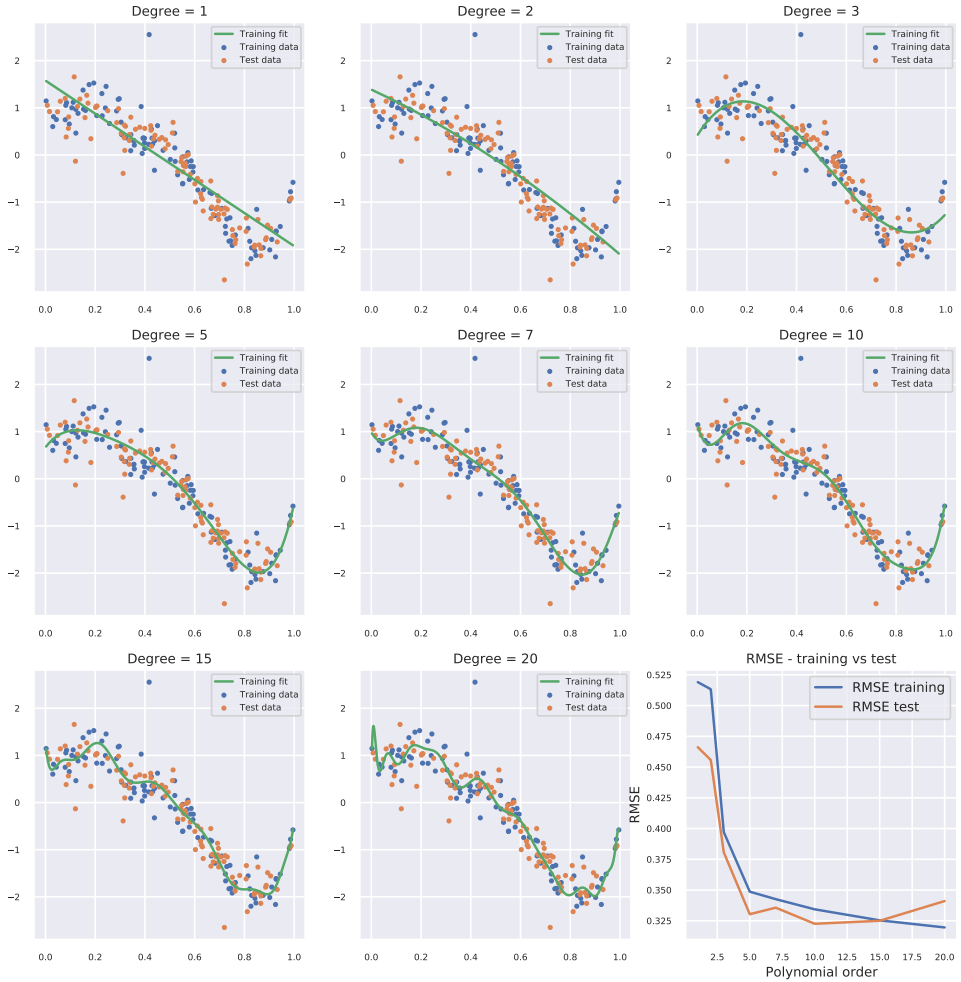
Figure from Lindholm et al (2021).

k-nearest neighbor regression

k-nearest neighbor regression



Polynomial regression



Regression trees

- **Partition the feature space** into L **rectangles**, $R_1, ..., R_L$.
- Predict with a model which is constant in each R_ℓ:

$$\hat{y}(\mathrm{x}_\star) = \sum_{\ell=1}^{L} w_\ell \mathbb{I}\{\mathrm{x}_\star \in R_\ell\}$$

  - **Rectangle indicator functions**:

$$\mathbb{I}\{\mathrm{x} \in R_\ell\} = \begin{cases} 1 & \text{if } \mathrm{x} \in R_\ell \\ 0 & \text{if } \mathrm{x} \notin R_\ell \end{cases}$$

  - **Level** in rectangle R_ℓ is w_ℓ which can be estimated by

$$\hat{w}_\ell = \hat{y}_\ell = \text{Average}\left\{y_i : \mathrm{x}_i \in R_\ell\right\}.$$

- **Regression trees** use **binary splits**, one feature at the time.
- Computationally efficient and nice interpretation.

Regression trees

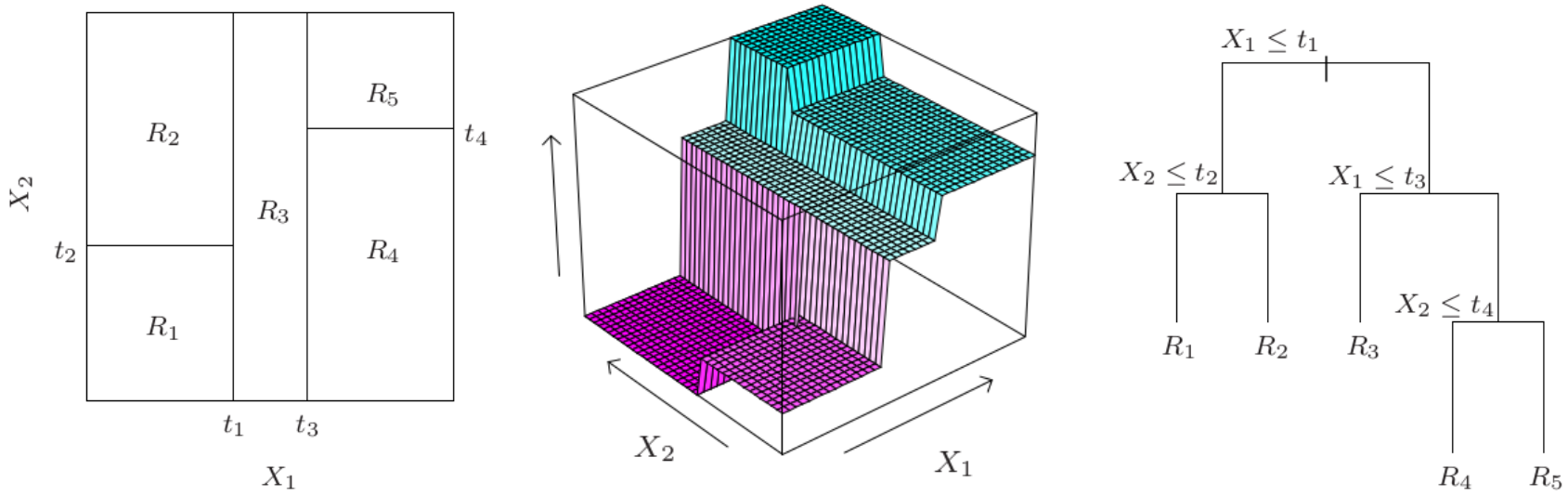


Figure from Hastie et al (2009).

Fitting regression trees

- **Parameters**:
  - **split variable** at each stage: $j_1, j_2, \ldots$
  - **splitting point** at each stage: $s_1, s_2, \ldots$
  - **level constants** $c_1, c_2, \ldots$
- A given split (j, s) defines two half-planes in x-space:

$$R_L(j,s) = \{\mathrm{x} | x_j \leq s\} \text{ and } R_H(j,s) = \{\mathrm{x} | x_j > s\}$$

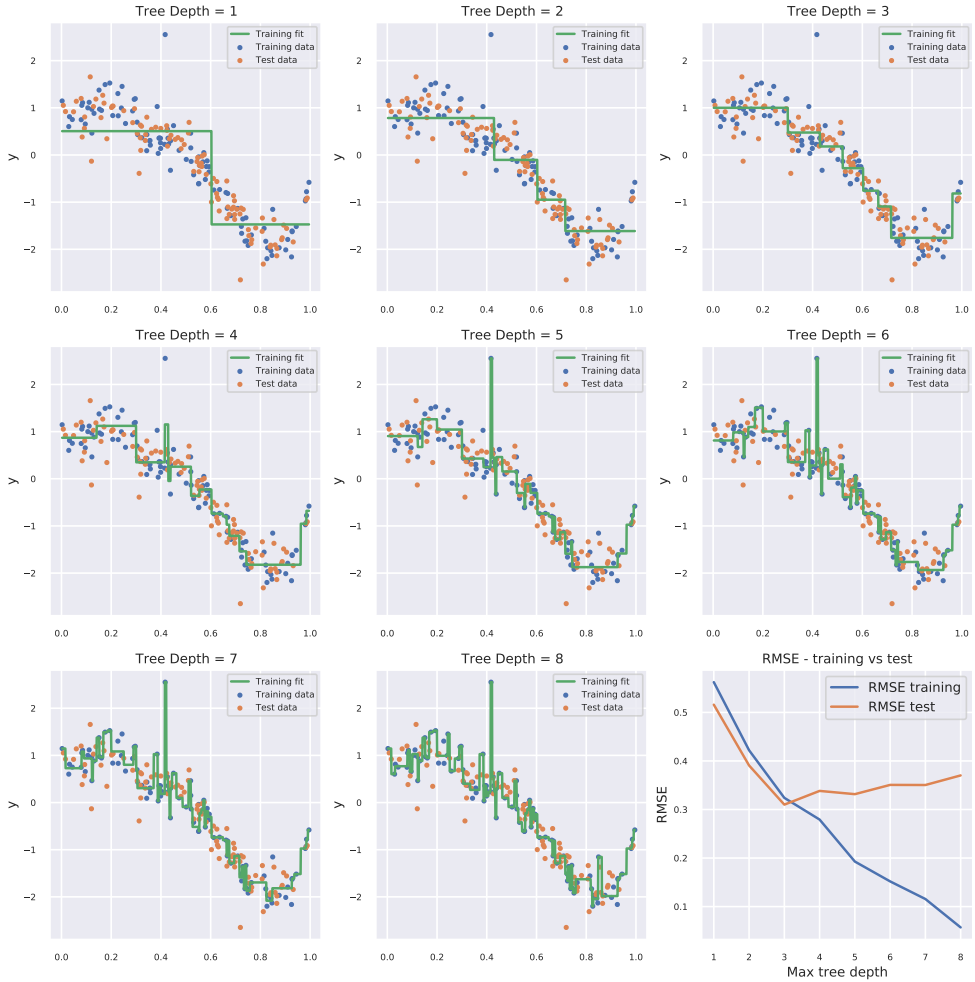
- **Level constants**. For a given split (j, s), estimate

$$\hat{y}_L(j,s) = \text{Average}\{y_i : \mathrm{x}_i \in R_L(j,s)\}$$
$$\hat{y}_H(j,s) = \text{Average}\{y_i : \mathrm{x}_i \in R_H(j,s)\}$$

- Greedy for **split variable** j and **splitting point** s

$$\min_{j,s}\left[\min_{\hat{y}_L}\sum_{i:\mathrm{x}_i \in R_L(j,s)}(y_i - \hat{y}_L(j,s))^2 + \min_{\hat{y}_H}\sum_{i:\mathrm{x}_i \in R_H(j,s)}(y_i - \hat{y}_H(j,s))^2\right].$$

Regression tree



Cost-complexity pruning

- **How big** tree?
- **Bias** (small tree) vs **Variance** (large tree)
- **Cost-complexity pruning**:
  - grow a large tree (few observation at each leave)
  - **prune** the tree by collapsing non-terminal nodes to minimize

$$\frac{1}{n}\sum_{i=1}^{n} L\left(\hat{y}(\mathrm{x}_i), y_i\right) + \eta\,|T| + \lambda\,\|\mathrm{w}\|_2^2$$

    - $L\left(\hat{y}(\mathrm{x}_i), y_i\right)$ is a **loss function** (e.g. squared error)
    - $|T|$ is the **number of leaves** in the subtree T.
    - $\lambda\,\|\mathrm{w}\|_2^2$ is am L2-regularization term (more later!)
  - Hyperparameters η and λ can be set with cross-validation.
- **Variable importance** for x_j: summing the improvement in fit at each node that is split by x_j.