Introduction to Learning from Data
1. Overview

Fall 2015

Machine Learning

- Era of "BIG" data deluge:
  - Almost 1 trillion websites
  - 1 hour of video uploaded to YouTube every second
  - Walmart handles 1 million transactions per hour
  - Genomes of 1000s people sequenced, each 3.8 billion base pairs long…

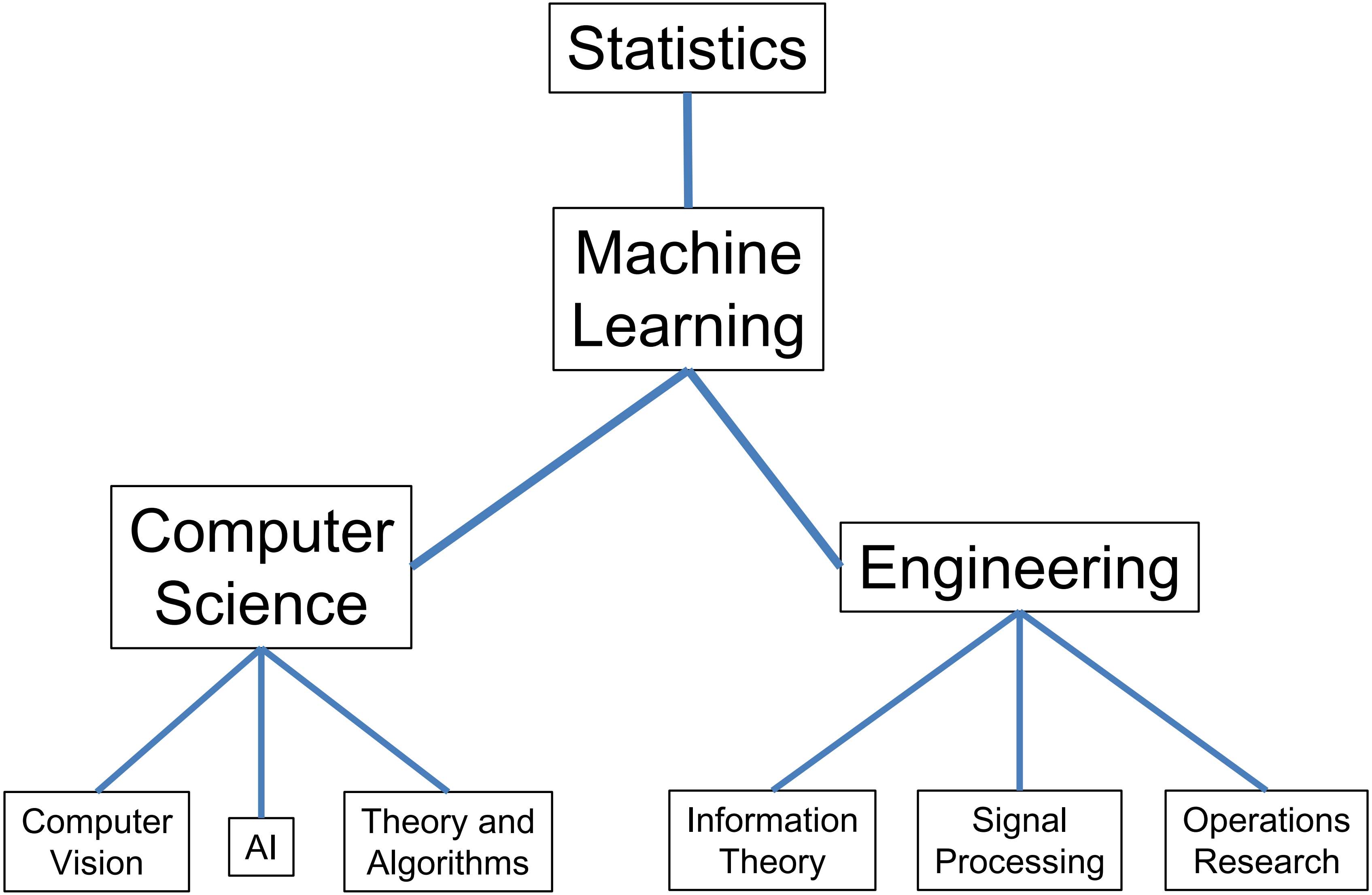
- ➔Need automated methods of data analysis

- Machine Learning = set of methods that can:
  - automatically learn regularities in observed data and
  - use them to make accurate decisions about unobserved data

Applications

- Detection: spam, fraud (credit card), network intrusion, faces (in images), motion (in video),…
- Recognition: characters, speech, faces, actions,…
- Prediction: weather conditions, stock prices, target position, drug-response, missing values,…
- Clustering: image segmentation (medicine/astronomy), gene families, communities in social networks,…

Connections

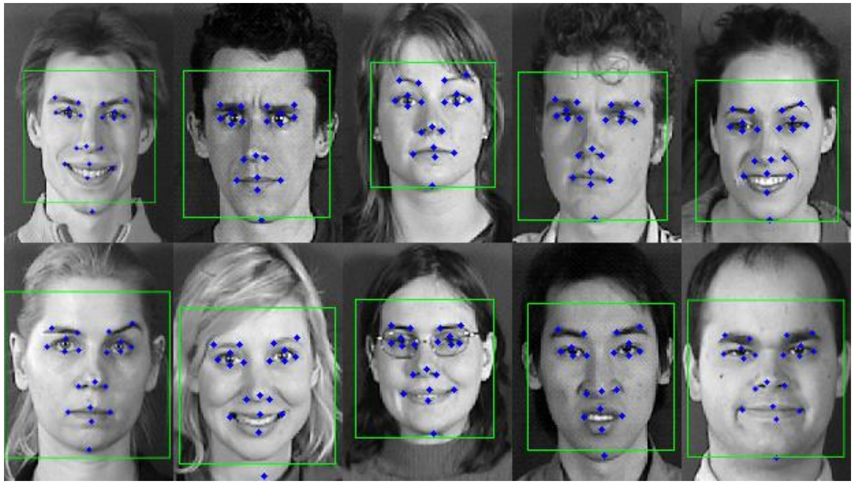


Skill Set

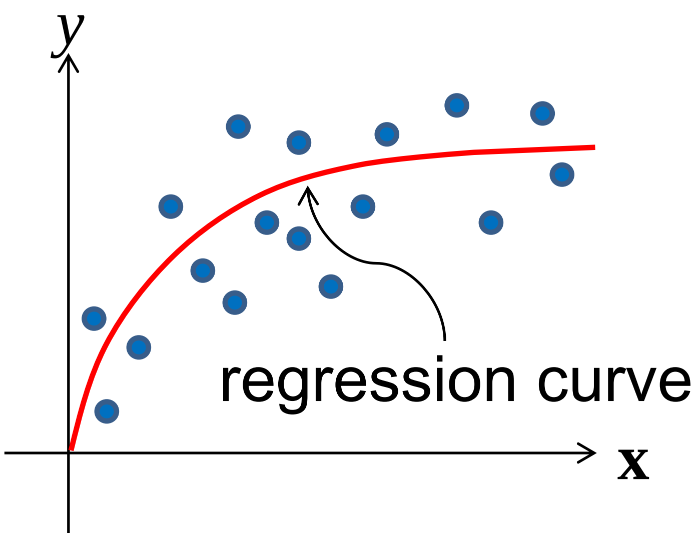
- Probability
- Optimization
  - Linear Algebra
  - Multivariate Calculus
- Algorithms
- Software

Main classes of learning problems

- Supervised (preditive) learning: given examples with labels, predict labels for all unseen examples
  - Classification: label = category
  - Regression: label = quantity (real value)
  - Ranking: label = order (relative position)

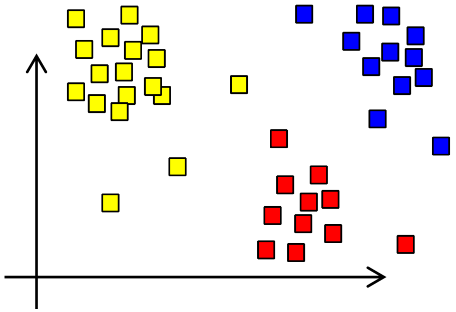


$\mathbf{x}$ = facial geometry features
y = gender label

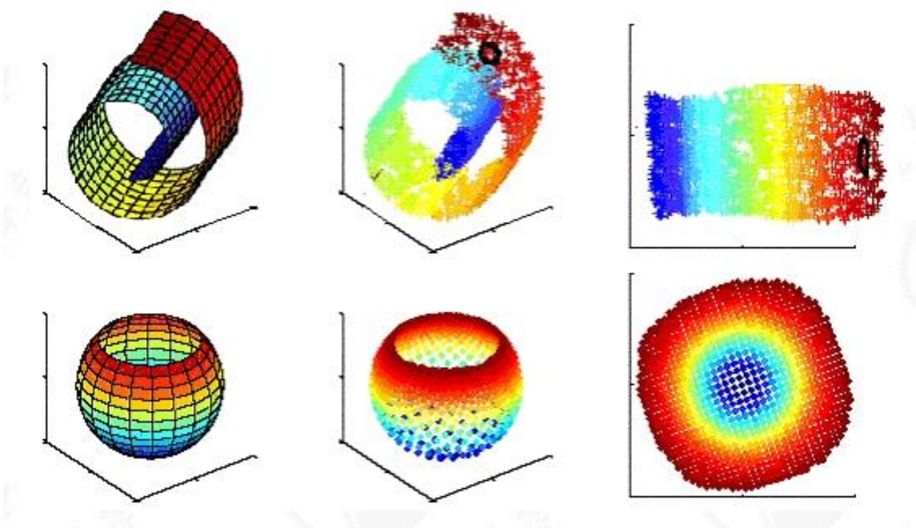


Main classes of learning problems

- Unsupervised (descriptive) learning: given un-labeled examples, find hidden structure
  - (Probability) Density Estimation
  - Clustering: partition examples into groups that are intrinsically similar and extrinsically dissimilar



  - Dimensionality Reduction: decrease the number of variables used to represent examples while preserving some properties of the original representation



Other learning scenarios

- Semi-supervised learning: given both labeled and unlabeled examples, predict labels for all unseen examples

- Transductive inference: similar to semi-supervised, but only need to predict labels for seen unlabeled examples, not all unseen examples

- Active learning: sequentially choose unlabeled examples for labeling to accurately and quickly predict labels for all unseen examples

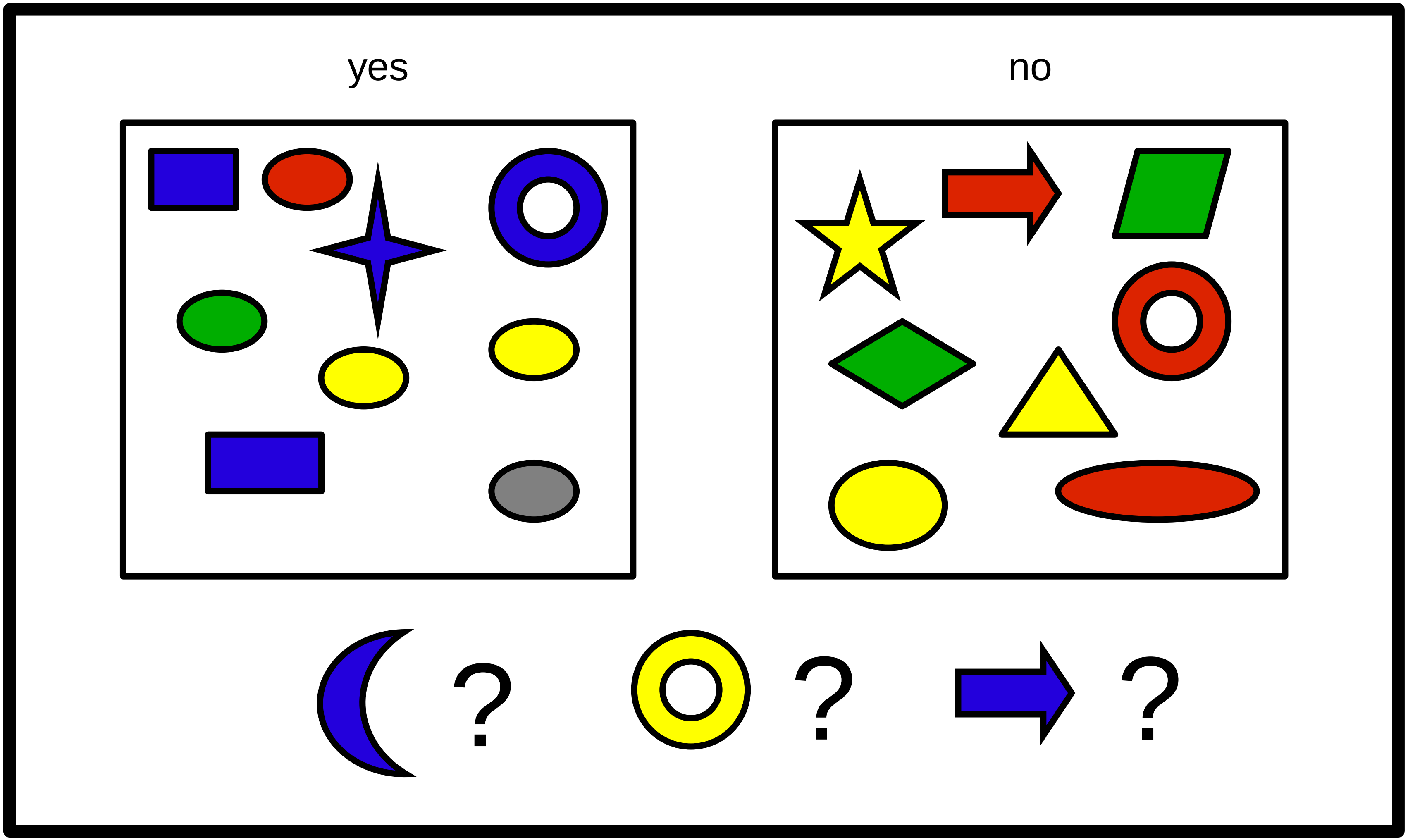
Other learning scenarios

- Online learning: multiple rounds of learning and decision making: receive unlabeled example ➔ predict label ➔ receive true label ➔ incur loss ➔ receive unlabeled example ➔…
  Goal: minimize cumulative loss

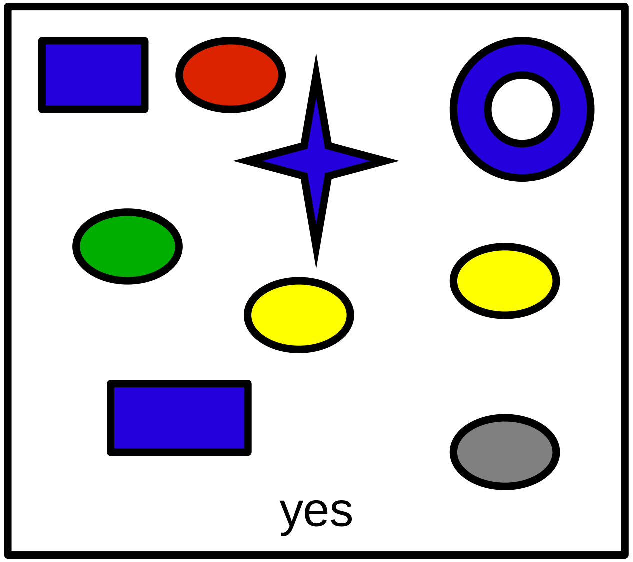
- Reinforcement learning: multi-round learning like online, but:
  - no long-term reward (only immediate reward)
  - decisions can change environment
  - e.g., search a terrain or the internet and learn as much new information as possible: explore vs exploit tradeoff

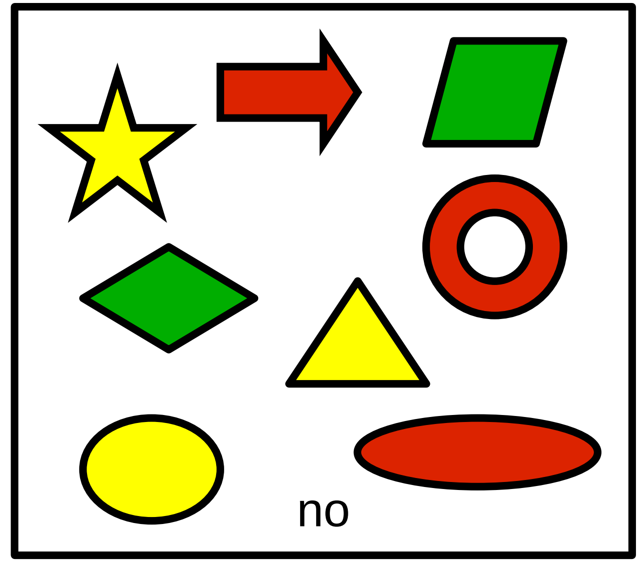
Supervised Learning

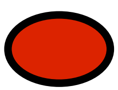
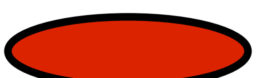
- Toy binary classification example



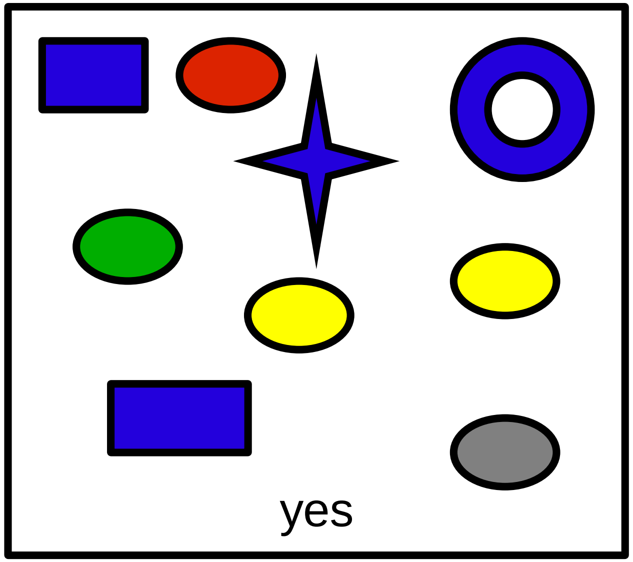
Supervised Learning

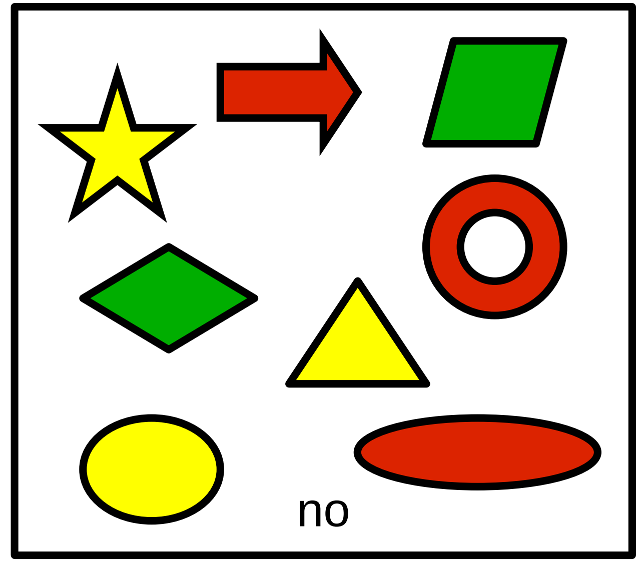


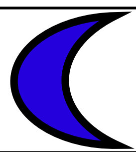
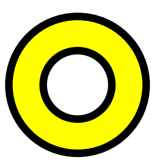
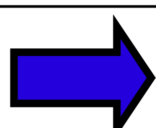


Training sample	Feature vector: $\mathbf{x}_i$ = (color, shape, size)^T	Label (Yes→1,No→0)
	$\mathbf{x}_1$ = (blue, rectangle, 10)^T	$y_1 = 1$
	$\mathbf{x}_2$ = (red, ellipse, 2.4)^T	$y_2 = 1$
	$\mathbf{x}_3$ = (red, ellipse, 20.7)^T	$y_3 = 0$
…	…	…

Supervised Learning

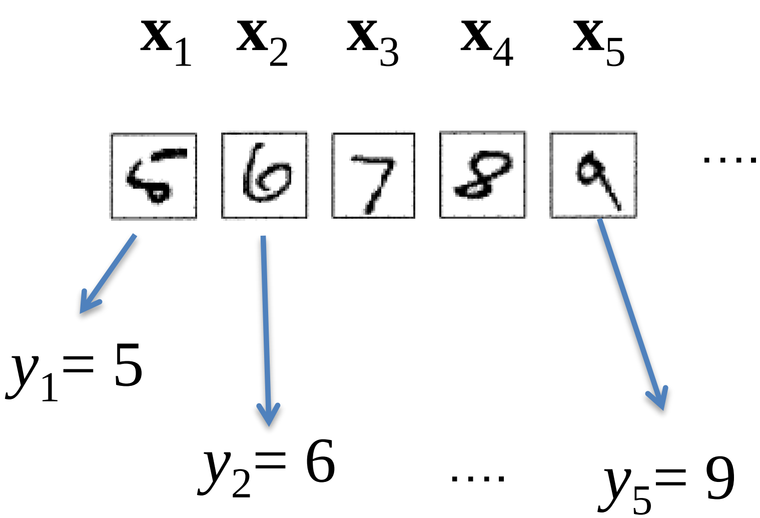




Test sample	Feature vector: $\mathbf{x}$ = (color, shape, size)^T	Label (Yes→1,No→0)
	$\mathbf{x}$ = (blue, crescent, 17)^T	$y = 1$
	$\mathbf{x}$ = (yellow, ring, 8)^T	$y = ?$
	$\mathbf{x}$ = (blue, arrow, 11)^T	$y = ?$

Supervised Learning

- Real-world example: character recognition
  - MNIST dataset: document image preprocessed to isolate and center individual handwritten characters into 28 x 28 grayscale images (grayscale value = integer in 0-255)
  - 60,000 training and 10,000 test images of digits 0-9 with ground-truth labels



Supervised Learning

- More real-world examples
  - Medicine:
    - $\mathbf{x}$ = symptoms, y = disease-type
    - $\mathbf{x}$ = EEG signal, y = seizure / no-seizure
  - Social Networks:
    - $\mathbf{x}$ = profile-pair, y = friend / not friend
  - Image/Video Analysis, Computer Vision:
    - $\mathbf{x}$ = image/video snippet, y = object-category, activity, etc.

Need for Probability

- Inductive reasoning:
  - going from particular instances to broader generalizations, e.g., 1➔2, 2➔4, 3➔?
  - inherently uncertain: allows for the possibility of the conclusion to be false even if all premises are true
- Randomness (variability/complexity/uncertainty) inherent in most real-world data, e.g.,

- Examples, features, and labels ➔random variables

Definitions, Terminology, Notation

- Examples
- Features: $\mathbf{x} \in \mathcal{X}$ (feature/input space)
- Labels: $\mathbf{y} \in \mathcal{Y}$ (label/output space)
- Training-samples: $\mathcal{D} = \{\mathbf{z}_1, \ldots, \mathbf{z}_n\}, \quad \mathbf{z}_i = (\mathbf{x}_i, y_i)$
- Validation-samples
- Test-samples
- Hypothesis set: $\mathcal{H} = \{h : \mathcal{X} \rightarrow \mathcal{Y}\}$
- Loss function: $\ell(\mathbf{x}, y, h) : \mathcal{X} \times \mathcal{Y} \times \mathcal{H} \rightarrow \mathbb{R}_+ = [0, \infty)$

Definitions, Terminology, Notation

- Examples:
  - data used for training or evaluation
  - e.g., email messages in Spam Detection

- Features:
  - set of attributes, represented as vector $\mathbf{x} \in \mathcal{X}$ (in some feature/input space, e.g., $\mathbb{R}^d$), associated to example
  - e.g., message length, name of sender, presence of keywords in subject/body, etc., in Spam Detection

Definitions, Terminology, Notation

- Features:
  - 3 types:
    - Categorical/Nominal: no intrinsic value or ordering, just a listing, e.g., gender, blood-type, shape, etc.
    - Quantitative: has intrinsic numerical value, e.g., physical measurements (space, time, mass, charge, etc.); can be discrete (counts) or continuous; represented by real numbers
    - Ordinal: has intrinsic ordering, but no numeric value, e.g., economic-bracket: $\in$ {poor, middle-class, rich}
  - Euclidean-space embedding: convert categorical/ ordinal variable into a real-valued vector.
    - Categorical: e.g., for blood-type $\in$ {A,B,AB,O} , A→$(1,0,0,0)^T$, B→$(0,1,0,0)^T$, AB→$(0,0,1,0)^T$, O→$(0,0,0,1)^T$
    - Ordinal: e.g., {low→⅓, medium→⅔, high→1}

Definitions, Terminology, Notation

- Labels: categories, values, or ordering in output/ label space assigned to examples
  - Classification: label $\mathbf{y} \in \mathcal{Y} = \{1, \ldots, m\}$, m = number of classes
  - Regression: label $\mathbf{y} \in \mathcal{Y} = \mathbb{R}$, a real value
- Training-samples: $\mathcal{D} = \{\mathbf{z}_1, \ldots, \mathbf{z}_n\}, \quad \mathbf{z}_j = (\mathbf{x}_j, y_j)$
  - examples (features + labels) used to train a learning algorithm
- Validation-samples:
  - examples used to tune parameters of learning algorithm, e.g., polynomial degree in regression (as opposed to the polynomial coefficients which are learned during training)

Definitions, Terminology, Notation

- Test-samples:
  - examples (features + labels) used to evaluate performance of learning algorithm
  - must be kept separate from training and validation samples and not made available in the learning stage
  - predictions on test-sample features compared against test-sample labels to measure performance
- Hypothesis set: $\mathcal{H} = \{h : \mathcal{X} \to \mathcal{Y}\}$
  - set of functions or decision rules mapping feature vectors to labels
  - e.g., if $\mathcal{X} = \mathbb{R}^d, \mathcal{Y} = \{-1, +1\}$ (binary classification), a hyperplane classifier is described by: $h(\mathbf{x}) = \mathrm{sign}(\mathbf{w}^\top \mathbf{x} + b)$
  - may have additional tuning parameters α, e.g. poly deg.

Definitions, Terminology, Notation

- Loss function: $\ell(\mathbf{x}, y, h) : \mathcal{X} \times \mathcal{Y} \times \mathcal{H} \rightarrow \mathbb{R}_+ = [0, \infty)$
  - function that quantifies the degree of disagreement between the predicted and true label
  - 0-1 loss (classification): $\ell(\mathbf{x}, y, h) = 1(h(\mathbf{x}) \neq y)$
  - squared loss (regression): $\ell(\mathbf{x}, y, h) = (h(\mathbf{x}) - y)^2$

Main stages of any learning problem

- Data-partitioning → Training, validation, testing sets
- Pre-processing and Feature Selection → Black Art
- Training
- Validation
- Testing

Main stages of any learning problem

- Data-partitioning ➔ Training, validation, testing sets
  - available data randomly partitioned into training, validation, and testing sets
  - # validation samples ➔ # parameters to be tuned
  - # training samples > # testing samples when total number of labeled samples is small
  - must ensure that all 3 have similar composition, e.g., similar proportion of all classes in a classification problem
- Pre-processing and Feature Selection
  - leverages prior domain knowledge/beliefs
  - often “messy”, heuristic
  - critical step: can dramatically effect performance, positively or negatively

Main stages of any learning problem

- Pre-processing
  - **Missing data:** either discard or “fill-in” with most frequently seen values from similar samples
  - **Imbalanced data:** replicate/re-sample/increase weight of under-represented populations or discard/down-sample/decrease weight over-represented ones
  - **Outliers:** detect samples most inconsistent with bulk of samples. Either remove them or design a robust loss function that is insensitive to outliers.
  - **Prefiltering:** reduce effects of noise, aliasing, quantization, misalignments
  - **Normalization:** compensate for unequal dynamic ranges of variables, e.g., mean-variance equalization, known nonlinearities in sensors
  - **Data augmentation:** make dataset richer by incorporating desirable invariances, e.g., color, position, orientation of objects in images.
- Feature selection
  - Identify most relevant subsets or functions of input variables
  - Unsupervised learning, specifically, clustering and dimensionality reduction play important roles

Main stages of any learning problem

- Training
  - Given training set: $\mathcal{D} = \{\mathbf{z}_1, \ldots, \mathbf{z}_n\}, \quad \mathbf{z}_j = (\mathbf{x}_j, y_j)$
  - fix tuning parameters α and select best decision rule
  - Structural Risk Minimization (SRM) Principle:

$$\mathcal{L}_{\text{train}}(h, \alpha, \lambda) = \left[\underbrace{\frac{1}{n} \sum_{j=1}^{n} \ell(\mathbf{x}_j, y_j, h)}_{\substack{\text{Empirical Risk} \\ \text{(data term)}}} + \lambda \underbrace{\text{complexity}(h, n)}_{\substack{\text{Structure Penalty} \\ \text{(prior beliefs)}}} \right]$$

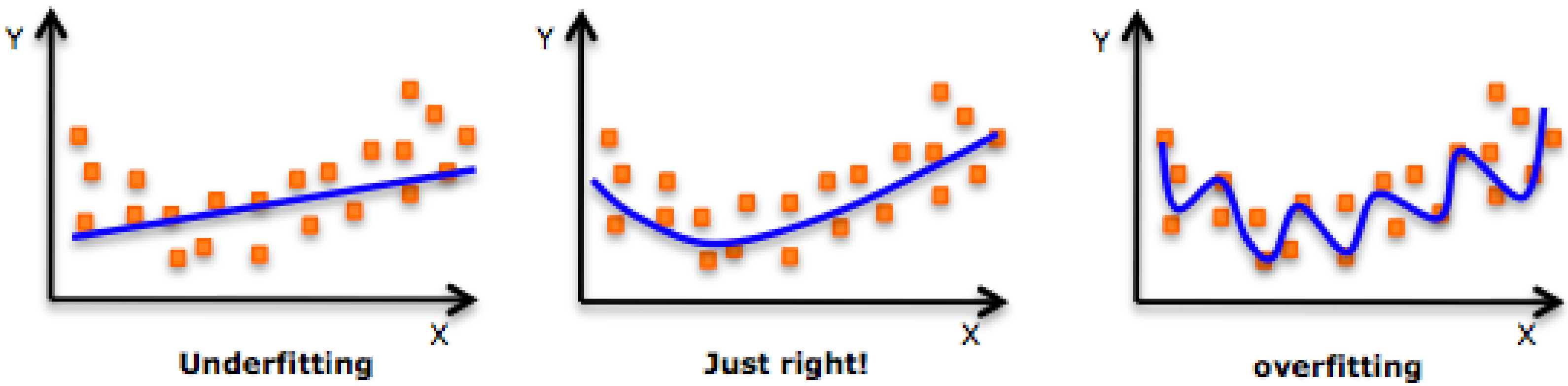
$$h^{SRM}(\alpha, \lambda) = \arg\min_{h \in \mathcal{H}} \mathcal{L}_{\text{train}}(h, \alpha, \lambda)$$

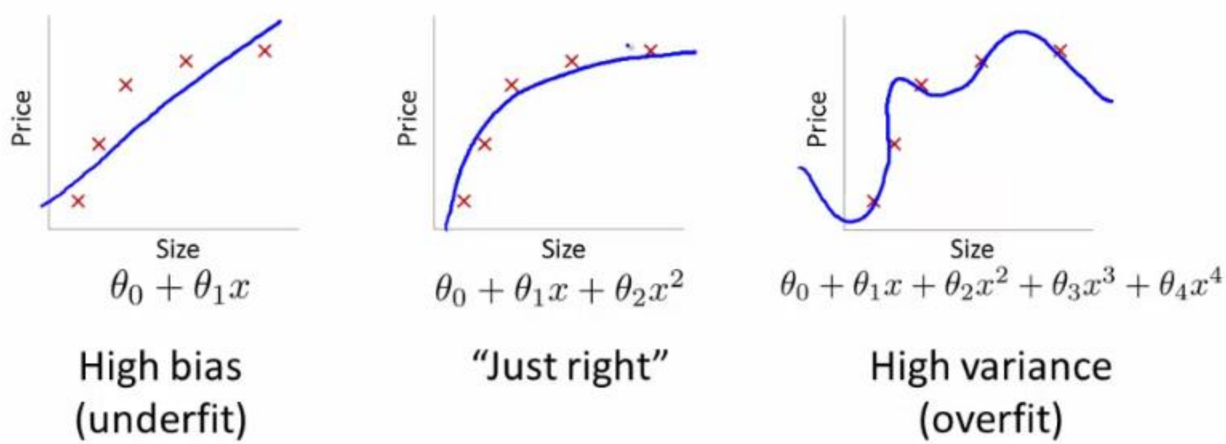
Main stages of any learning problem

- Training
  - Empirical Risk Minimization (ERM): special case of SRM with $\lambda=0$. Corresponds to minimizing only 1st term of $\mathcal{L}_{\text{train}}(h,\alpha,\lambda)$.
  - Overfitting: if n << # free parameters in h, α (complex model), solution based on ERM will be too noisy (will have high variance)→model starts "memorizing" training data instead of learning to generalize from trend
  - Complexity regularization (2nd term of $\mathcal{L}_{\text{train}}(h,\alpha,\lambda)$): mitigates overfitting by biasing solutions to be faithful to prior beliefs
  - 2nd term typically → 0 as n → infinity (prior beliefs can be ignored when there is overwhelming data)

Bias-Variance tradeoff

- $\lambda = 0$: Prior beliefs completely ignored. Complex solutions have low bias, but high variance
- $\lambda >> 1$: Prior beliefs dominate. Solutions have low variance, but high bias





Main stages of any learning problem

- Validation
  - Learn best values of α, λ using validation samples
  - Best α_*, λ_* minimizes the validation error:

$$\mathcal{L}_{\text{valid}}(\alpha, \lambda) = \frac{1}{|\text{validation set}|} \sum_{(\mathbf{x},y) \in \substack{\text{validation} \\ \text{set}}} \ell(\mathbf{x}, y, h^{SRM}(\alpha, \lambda))$$

$$(\alpha_*, \lambda_*) = \arg\min_{\alpha,\lambda} \mathcal{L}_{\text{valid}}(\alpha, \lambda)$$

- Testing
  - Evaluate performance using test samples
  - Test error:

$$\mathcal{L}_{\text{test}}(\alpha_*, \lambda_*) = \frac{1}{|\text{test set}|} \sum_{(\mathbf{x},y) \in \substack{\text{test} \\ \text{set}}} \ell(\mathbf{x}, y, h^{SRM}(\alpha_*, \lambda_*))$$

Main stages of any learning problem

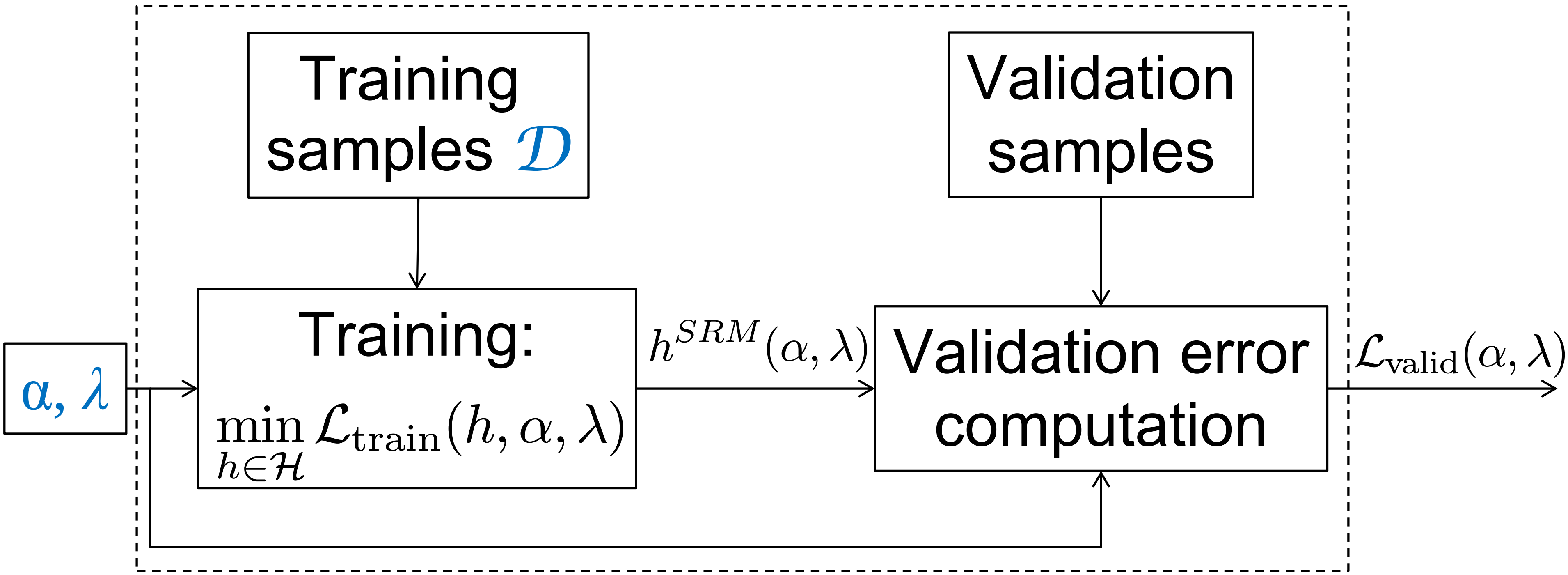
- Testing
  - Performance metrics other than the loss function used for training and validation may be used for evaluation:
    - Correct Classification Rate (CCR)
    - Confusion Matrix
    - Prob. of False Alarm, Missed Detection, Precision, Recall, Sensitivity, Specificity, F-score, Area Under the ROC Curve, etc.
    - Mean Square Error (MSE), Mean Absolute Error (MAE),
    - Predictive log-probability

- Small training error $\nRightarrow$ Small validation or test error
  - Memorization vs Generalization (Overfitting)

Training-Validation-Testing summary

- **Training:** given $\alpha, \lambda, \mathcal{D}$ find best $h^{SRM}(\alpha, \lambda)$ in $\mathcal{H}$ by minimizing structural risk
- **Validation:** given validation samples, find best α_*, λ_* by minimizing validation error of $h^{SRM}(\alpha, \lambda)$ over choices of α, λ
  - In practice, the search for the best α, λ is typically done via a greedy coarse-to-fine grid search
- **Testing:** use α_*, λ_* , $h^{SRM}(\alpha_*, \lambda_*)$ to evaluate performance on test samples

Training-Validation-Testing summary



- **Validation:** given validation samples, find best α_*, λ_* by minimizing validation error of $h^{SRM}(\alpha, \lambda)$ over choices of α, λ

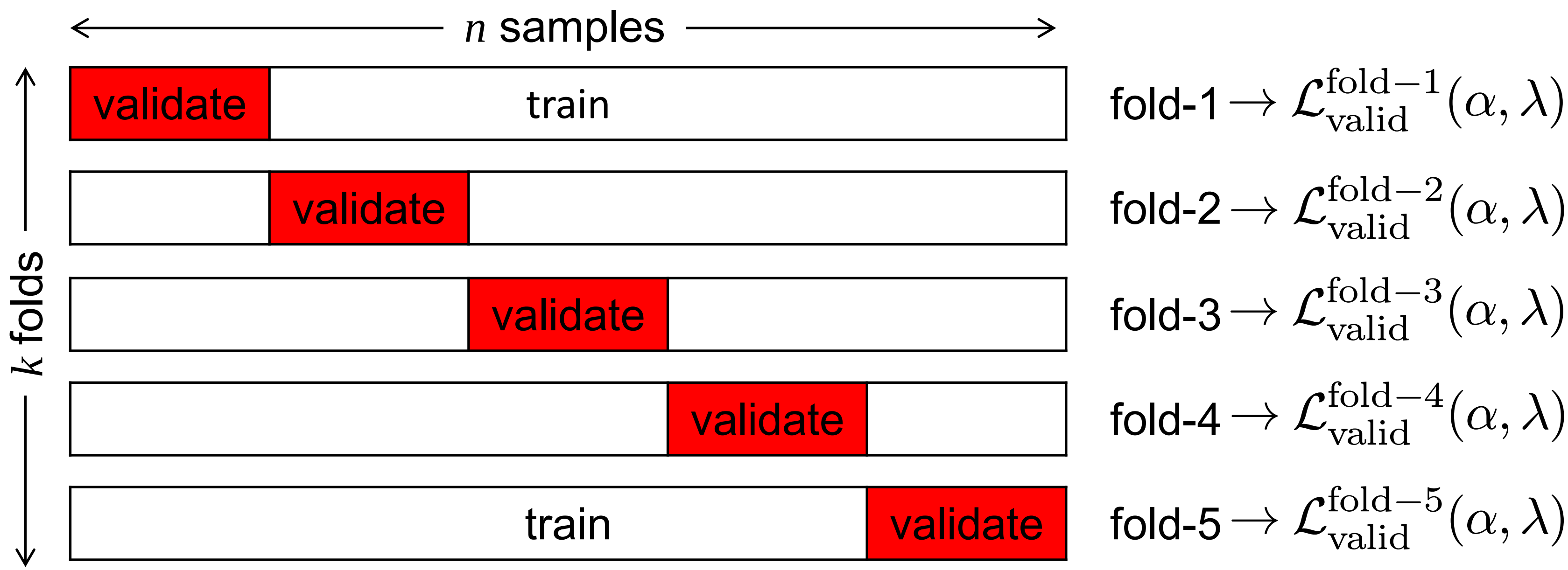
- **Testing:** use α_*, λ_* , $h^{SRM}(\alpha_*, \lambda_*)$ to evaluate performance on test samples

Example: polynomial regression

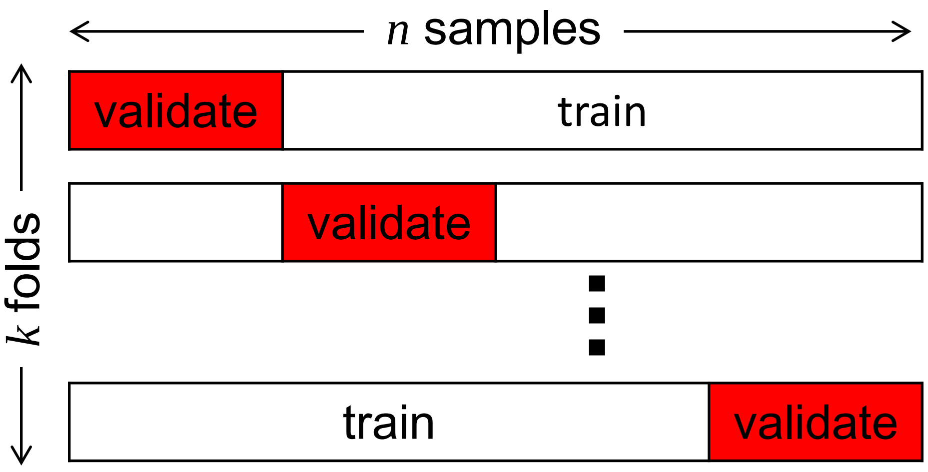
- $\mathcal{X} = \mathcal{Y} = \mathbb{R}$,
- $\mathcal{H} = \{h(x) = \sum_{k=0}^{\alpha} h_k x^k\}$,
- $\ell(x, y, h) = (y - h(x))^2$
- $\mathcal{L}_{\text{train}}(h, \alpha, \lambda) = \dfrac{1}{n} \displaystyle\sum_{i=1}^{n} \left(y_i - \sum_{k=0}^{\alpha} h_k x_i^k \right)^2 + \lambda \sum_{k=0}^{\alpha} |h_k|$
- $(h_0^{SRM}(\alpha, \lambda), \ldots, h_\alpha^{SRM}(\alpha, \lambda)) = \arg\min_{h_0, \ldots, h_\alpha} \mathcal{L}_{\text{train}}(h_0, \ldots, h_\alpha, \alpha, \lambda)$
- $\mathcal{L}_{\text{valid}}(\alpha, \lambda) = \dfrac{1}{|\text{validation set}|} \displaystyle\sum_{(x,y) \in \substack{\text{validation} \\ \text{set}}} \left(y - \sum_{k=0}^{\alpha} h_k^{SRM}(\alpha, \lambda) x^k \right)^2$
- $(\alpha_*, \lambda_*) = \arg\min\limits_{\alpha, \lambda} \mathcal{L}_{\text{valid}}(\alpha, \lambda)$
- $\mathcal{L}_{\text{test}}(\alpha_*, \lambda_*) = \dfrac{1}{|\text{test set}|} \sum_{(x,y) \in \substack{\text{test} \\ \text{set}}} \left(y - \sum_{k=0}^{\alpha_*} h_k^{SRM}(\alpha_*, \lambda_*) x^k \right)^2$

Cross-Validation

- Not enough labeled data for creating separate validation samples
- Idea: cycle samples through training and validation
- Can also do this for testing (if needed)
- How? Many approaches: bootstrap, exhaustive methods,…focus on *k*-fold cross-validaton



Cross-Validation



$$\mathcal{L}_{\mathrm{CV}}(\alpha,\lambda) = \frac{1}{k}\sum_{j=1}^{k} \mathcal{L}_{\mathrm{valid}}^{\mathrm{fold}-j}(\alpha,\lambda)$$

$$(\alpha_*,\lambda_*) = \arg\min_{\alpha,\lambda} \mathcal{L}_{\mathrm{CV}}(\alpha,\lambda)$$

- Then train on all n samples with α_*, λ_* to obtain $h^{SRM}(\alpha_*, \lambda_*)$
- Then evaluate performance on test samples
- Holdout cross-validation: $k = 2$
- Leave-one-out-cross-validation (LOOCV): $k = n$
- Typical choices for number of folds: $k = 5, 10$