INSTITUTE FOR MACHINE LEARNING AND ANALYTICS

Linear Machine Learning

Janis Keuper

Introduction to ML

Basic Types of Machine Learning Algorithms

Supervised Learning

Unsupervised Learning

Reinforcement Learning

- Labeled data
- Direct and quantitative evaluation

- Learn model from „ground truth“ examples
- Predict unseen examples

Recall Classification

Supervised Learning: Annotated Training Data

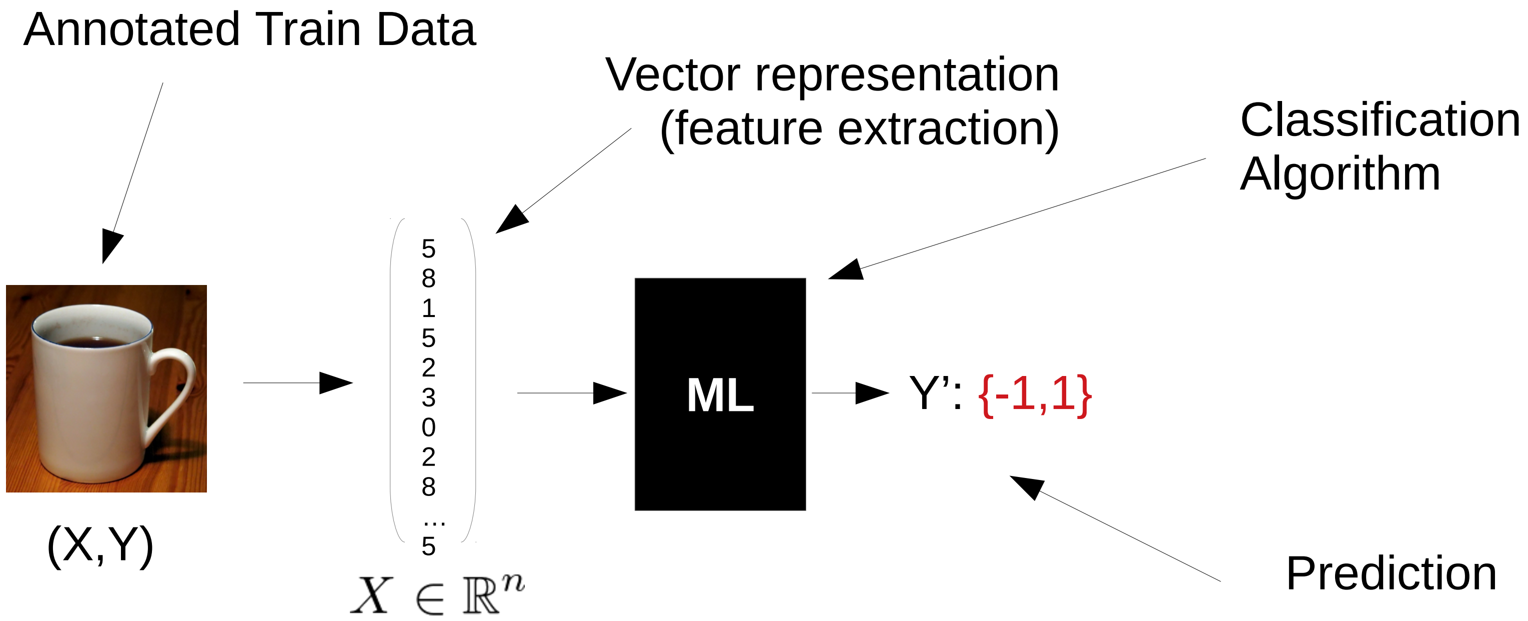
(X,Y)

$$\begin{pmatrix} 5 \\ 8 \\ 1 \\ 5 \\ 2 \\ 3 \\ 0 \\ 2 \\ 8 \\ \dots \\ 5 \end{pmatrix} \rightarrow \boxed{\textbf{ML}} \rightarrow Y': \{-1,1\}$$

$$X \in \mathbb{R}^n$$

Recall Classification

Supervised Learning: Annotated Training Data



Recall Classification

LEARNING: is a optimization problem → Finding the best function separating

$$min(\|f(X,Y),Y'\|)$$

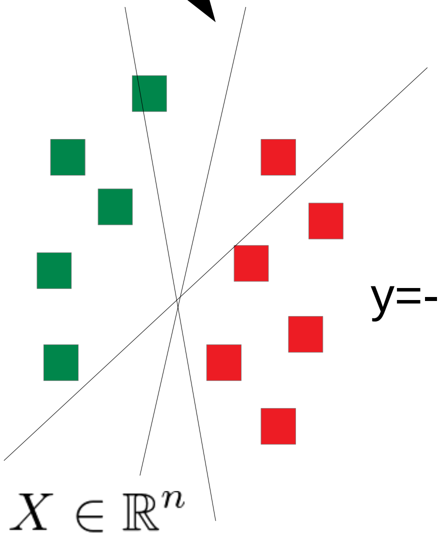
(X,Y)

$$\begin{pmatrix} 5 \\ 8 \\ 1 \\ 5 \\ 2 \\ 3 \\ 0 \\ 2 \\ 8 \\ \dots \\ 5 \end{pmatrix}$$

$X \in \mathbb{R}^n$

→ **ML** → Y’: {-1,1}

y=1



y=-1

$X \in \mathbb{R}^n$

Example: MNIST

The MNIST hand written digits classification Problem

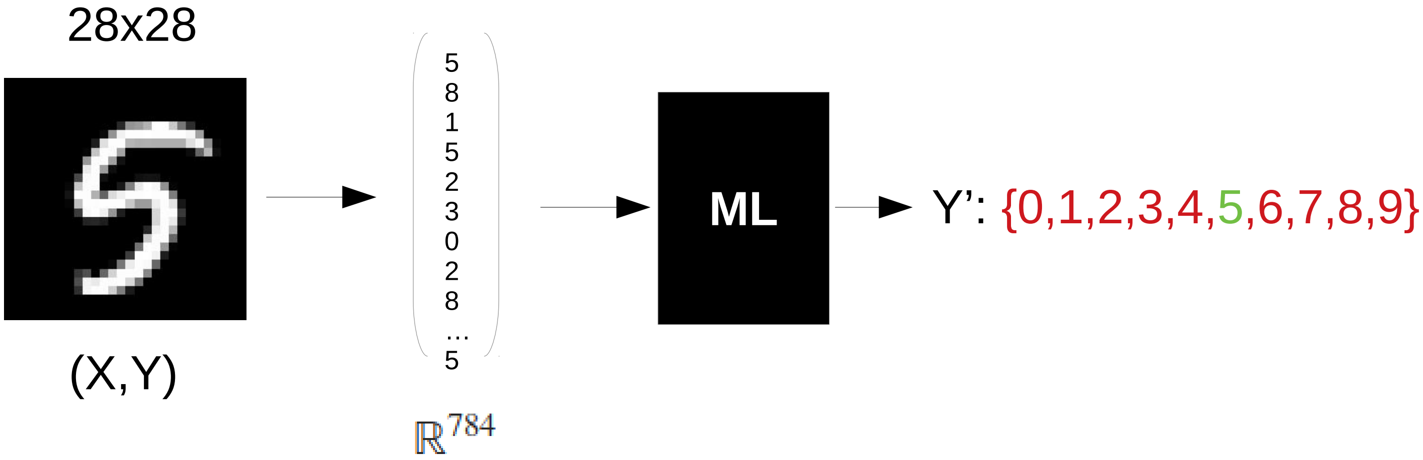
The MNIST database (Modified National Institute of Standards and Technology database) is a large database of handwritten digits that is commonly used for training various image processing systems.

Data specs:

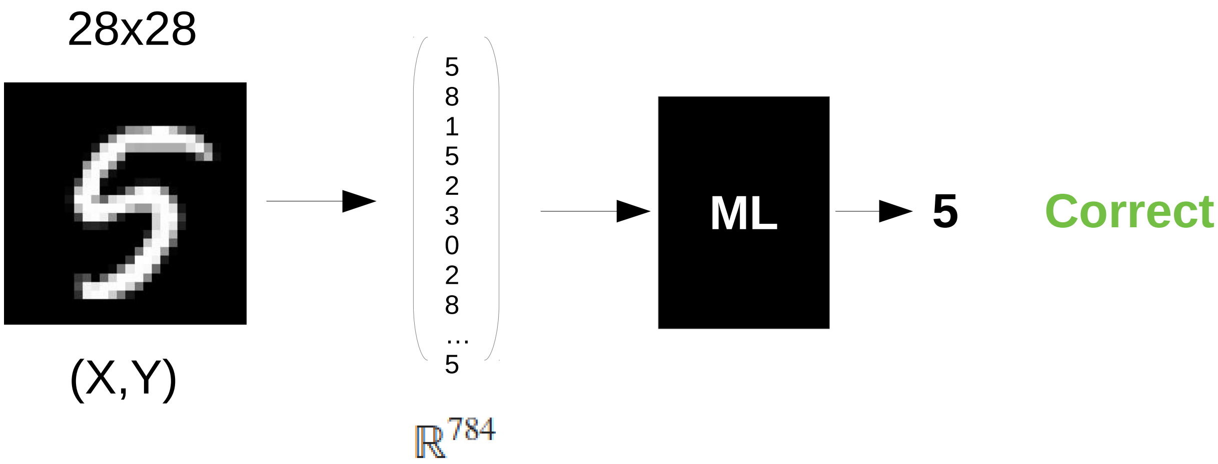
- 10 Classes (digest 0-9)
- 28x28 gray scale images
- 60000 train samples
- 10000 test samples

Example: MNIST

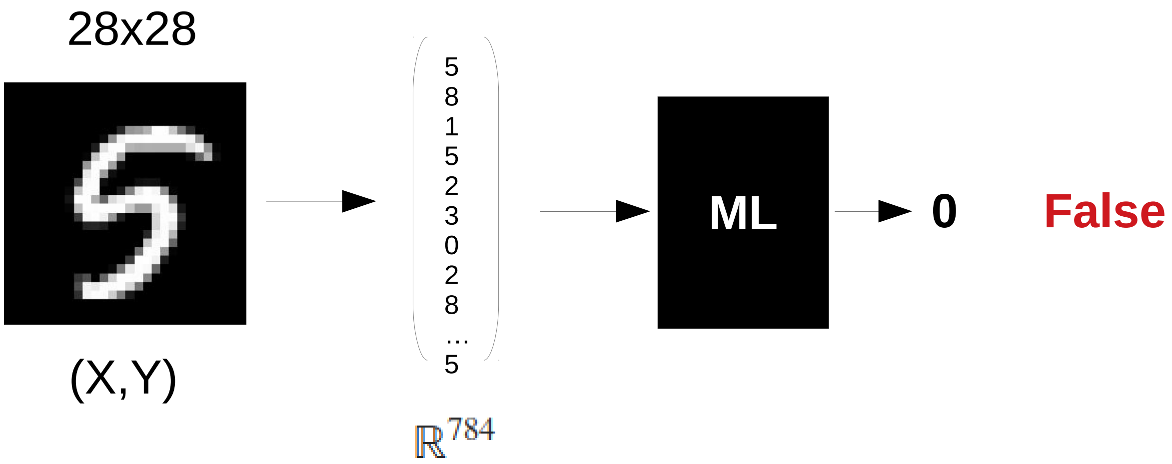
The MNIST hand written digits classification Problem



Evaluation



Evaluation



Recall: Evaluation

Basic evaluation of a model:

Train error: measure of how well the model predicts the given labels

$$Err_{train} := \frac{1}{|X_{train}|} \sum_{x_i \in X_{train}} |f(x_i) - y_i|$$

low train error is the necessary condition for a "good" model

Test error: **same as train error: low test error is the sufficient condition**

$$Err_{test} := \frac{1}{|X_{test}|} \sum_{x_i \in X_{test}} |f(x_i) - y_i|$$

Evaluation

Confusion Matrix and True and False Positives/Negatives

Predicted Label \ True label	0	1	2	3	4	5	6	7	8	9
0	.93			.03			.03			
1		.97						.03		
2		.03	.90		.03			.03		
3				.83		.03			.13	
4					.67		.03		.03	.27
5				.30		.57	.03		.10	
6		.03					.97			
7		.07			.13			.73		.07
8			.13				.03		.80	.03
9				.03	.13			.10	.07	.67

Evaluation

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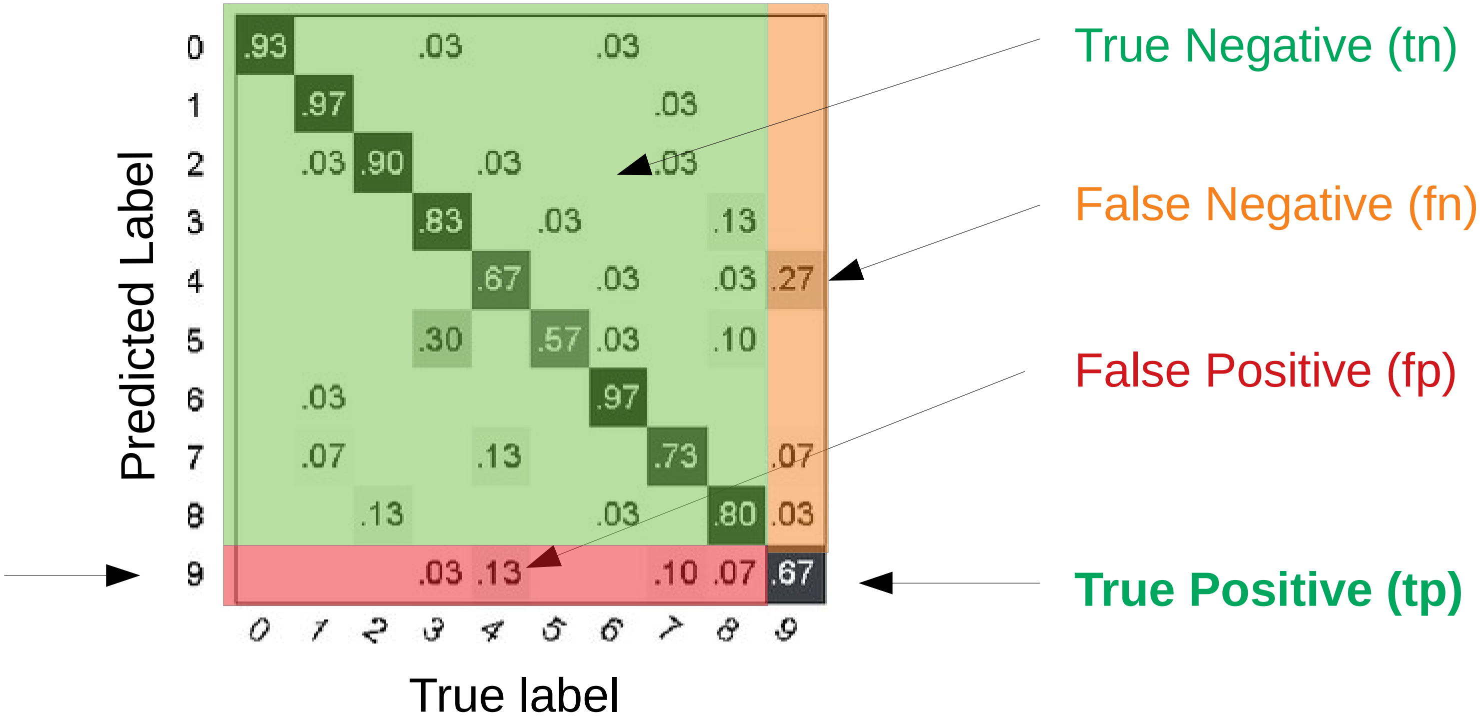
Confusion Matrix and True and False Positives/Negatives

Example for true digit “9”



Evaluation

Accuracy:

Most commonly used error metric:

Correct samples

$$\text{Accuracy} = \frac{tp + tn}{tp + tn + fp + fn}$$

All samples

Evaluation

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Problems with Accuracy Unbalanced classes:

If the prior probability of one class is much higher than others, *fp* will have little impact.

$$\text{Accuracy} = \frac{tp + tn}{tp + tn + fp + fn}$$

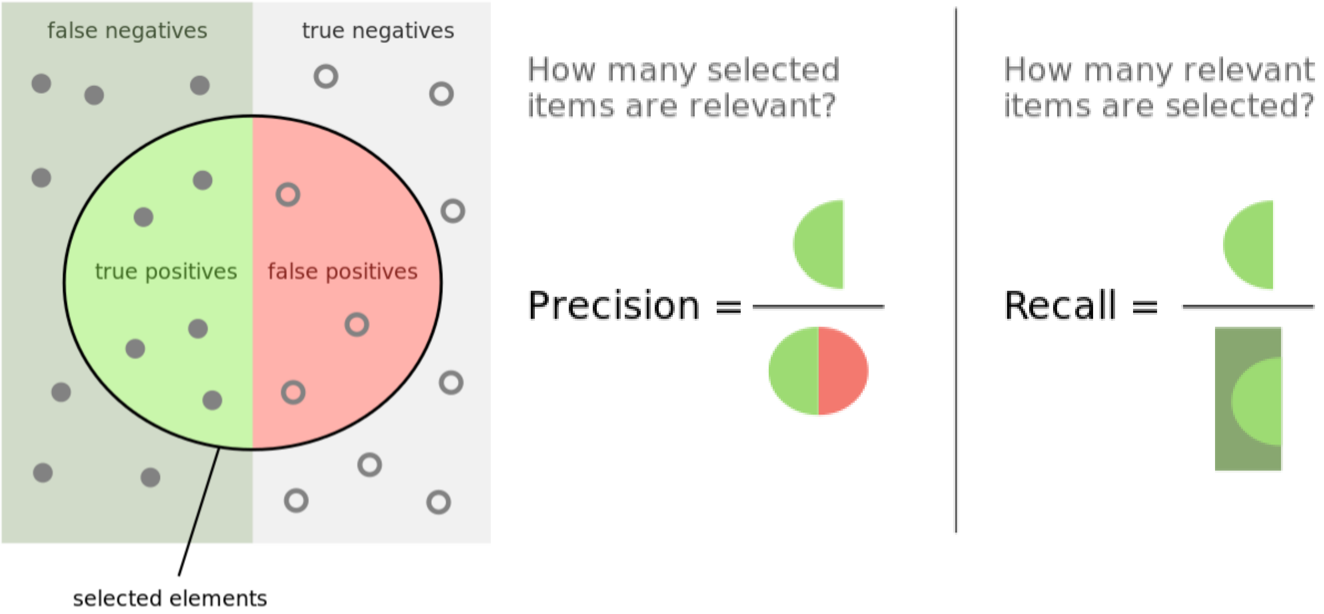
Extreme example: if 90% of the digits are “1”, classifying every digit to “1” will will have 90% accuracy!

Evaluation

Precision and Recall

$$\text{Precision} = \frac{tp}{tp + fp}$$

$$\text{Recall} = \frac{tp}{tp + fn}$$



[image by wikipedia]

Evaluation

F-Measure or balanced F-score is the harmonic mean of precision and recall:

$$F = 2 \cdot \frac{\text{precision} \cdot \text{recall}}{\text{precision} + \text{recall}}$$

Evaluation

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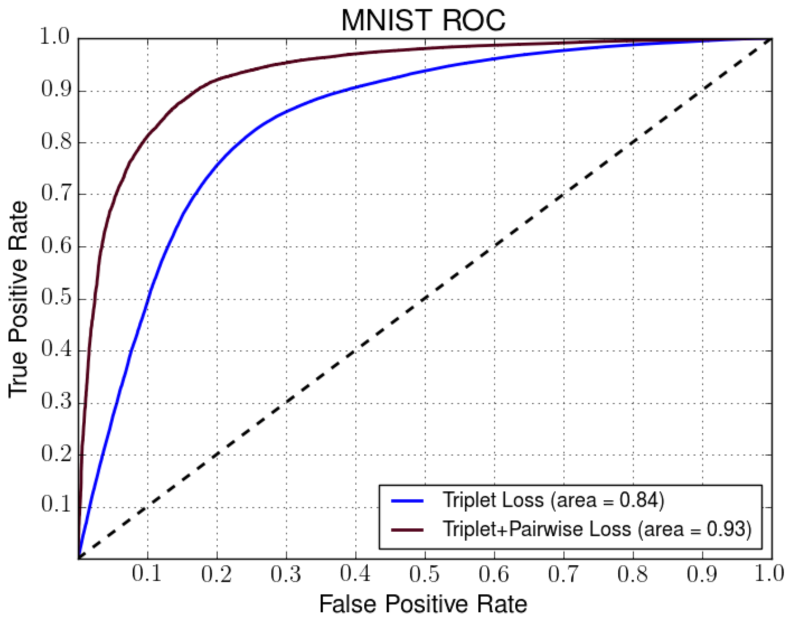
Receiver Operating Characteristic Curve

A receiver operating characteristic curve, or ROC curve, is a graphical plot that illustrates the diagnostic ability of a **binary classifier** system as its discrimination threshold is varied.

Example: comparing two different models



Linear Classifier

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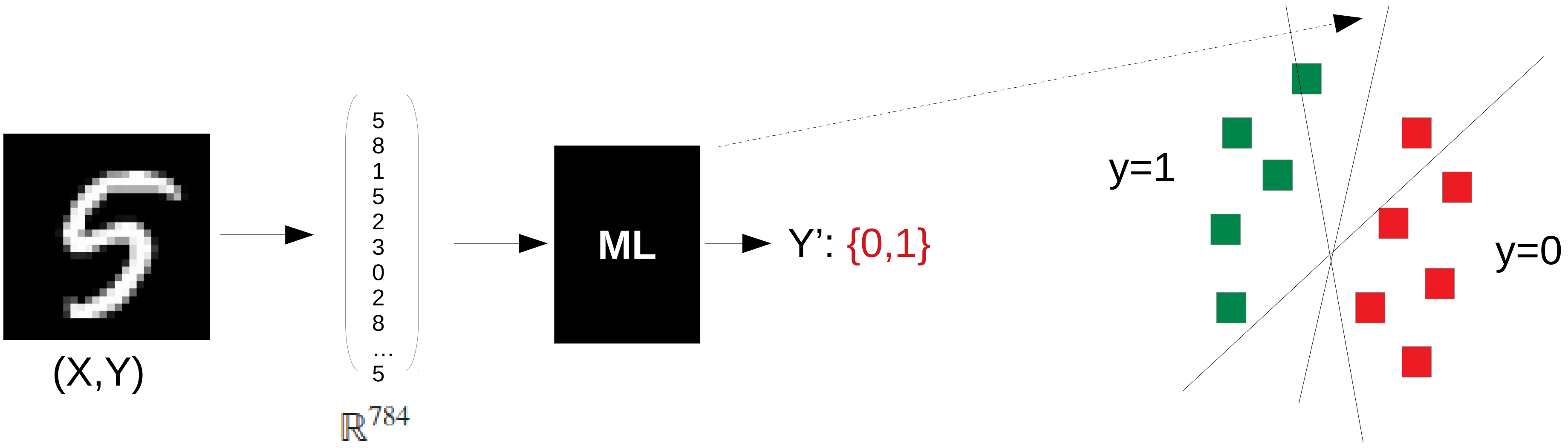
A Simple Linear Model: binary classification

Example: “5” vs “other digit”

Model: hyper plane



Linear Classifier

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A Simple Linear Model: binary classification

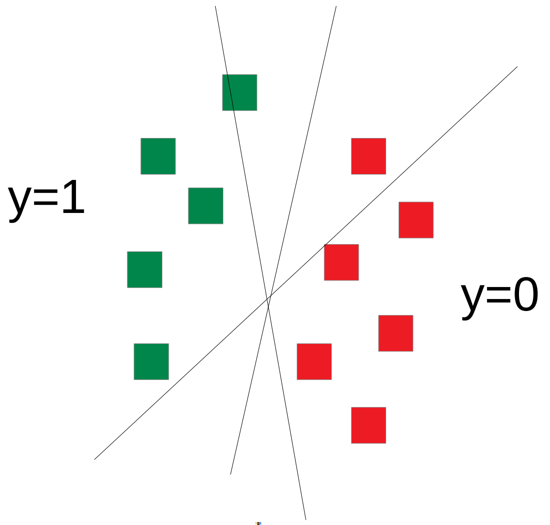
Parameterization of prediction function f with d-dimensional data as:

$$f(x) = y' = w^T x = \sum_{j=0}^{d} w_j x_j$$

With data samples $x \in \mathbb{R}^d$

Model parameters $w \in \mathbb{R}^d$

Model: hyper plane



$x \in \mathbb{R}^d$

Linear Classifier

A Simple Linear Model: binary classification

Parameterization of prediction function f with d-dimensional data as:

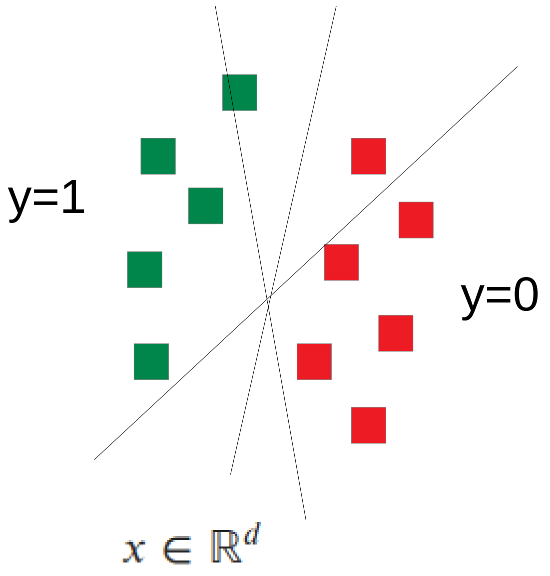
$$f(x) = y' = w^T x = \sum_{j=0}^{d} w_j x_j$$

With data samples $x \in \mathbb{R}^d$

Model parameters $w \in \mathbb{R}^d$

How to find the parameters?

Model: hyper plane



Linear Classifier

Optimization problem to find parameters

$$\arg\min_{w} \sum_{i=0}^{N} L(y_i, w^T x_i)$$

With a differential *Loss* function like

$$L(y=1, y') := \frac{1}{1+e^{-y'}}$$

$$L(y=0, y') := 1 - L(y=1, y')$$

Linear Classifier

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Optimization problem to find parameters

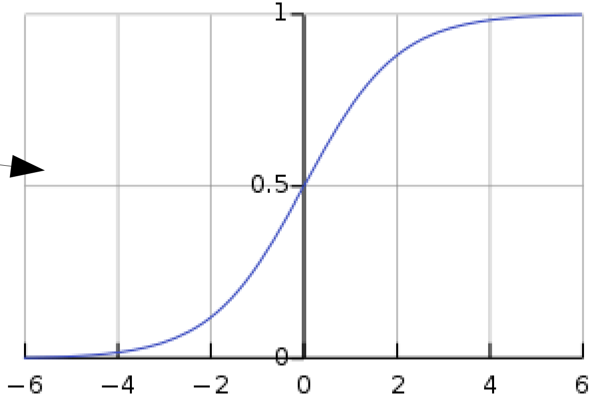
$$\arg\min_{w} \sum_{i=0}^{N} L(y_i, w^T x_i)$$

Only one of many possible Loss functions, but common choice

With a differential *Loss* function like: **logistic function**

$$L(y=1, y') := \frac{1}{1+e^{-y'}}$$

$$L(y=0, y') := 1 - L(y=1, y')$$



- **pseudo probability:** Out put always between 0 and 1
- Apply **threshold** function on probability that class label =1

Gradient Descent Optimization

Goal: find w to minimize $\arg\min_{w} \sum_{i=0}^{N} L(y_i, w^T x_i)$

Gradient Descent Optimization

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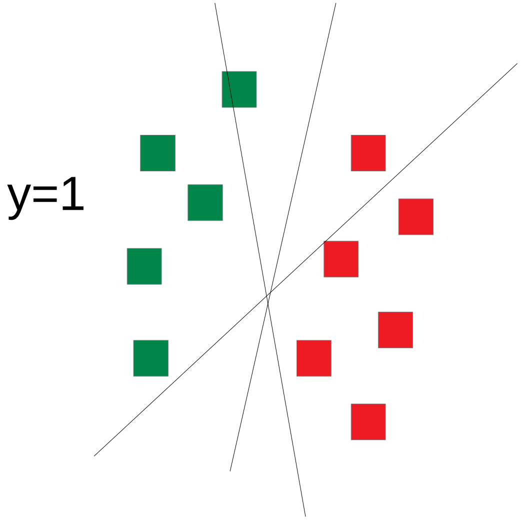
2D Example:



$x \in \mathbb{R}^2$

Feature Space

Gradient Descent Optimization

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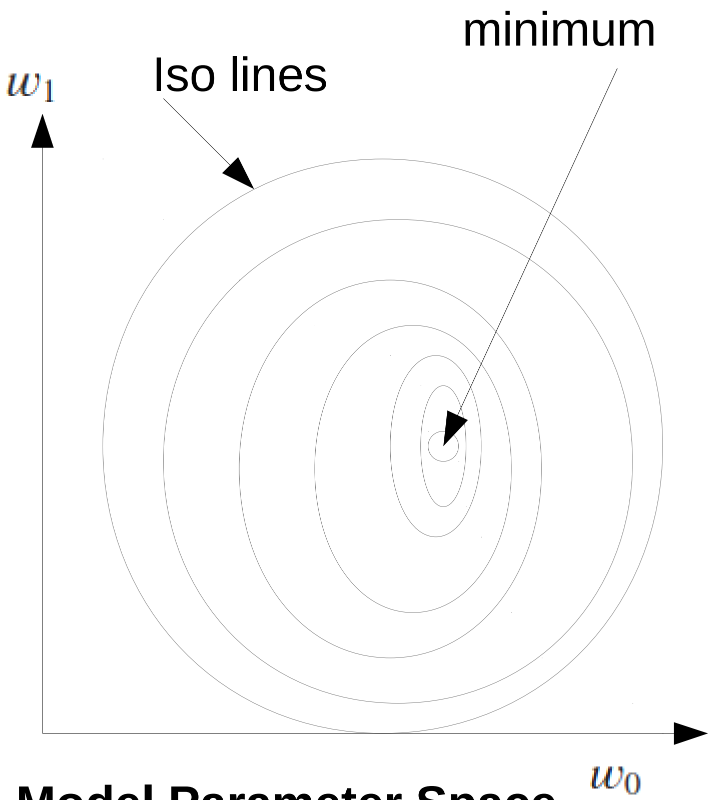
Goal: find w to minimize $\arg\min_{w} \sum_{i=0}^{N} L(y_i, w^T x_i)$

2D Example:

- How many (and which) parameters do we have to find?
- *L* spans a (loss) surface in the d-dimensional space of the data X **(parameter space)**
- We can evaluate *L* at each point *w*
- We can compute the gradient at each point *w* in *L* *(assuming L to be Lipschitz)*



Model Parameter Space

Gradient Descent Optimization

Goal: find w to minimize $\arg\min_{w} \sum_{i=0}^{N} L(y_i, w^T x_i)$

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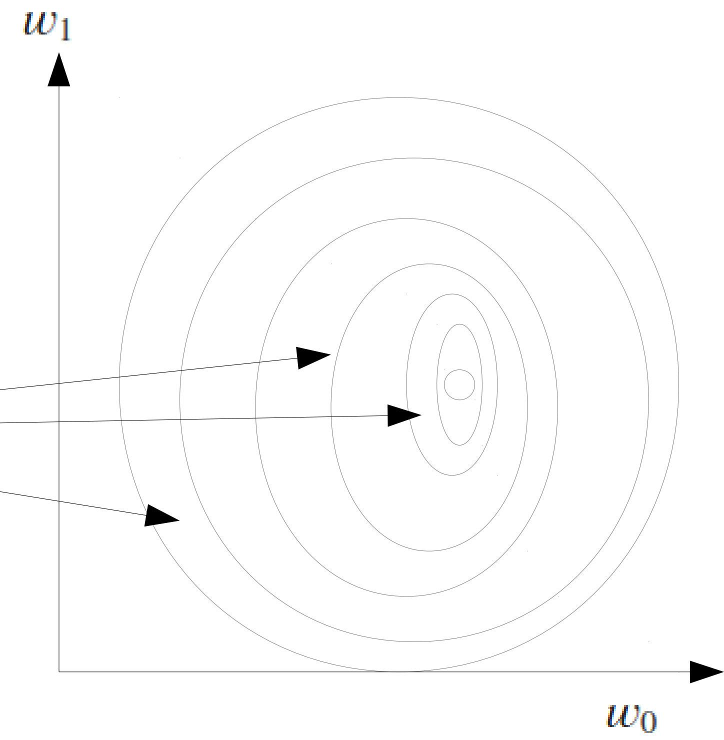

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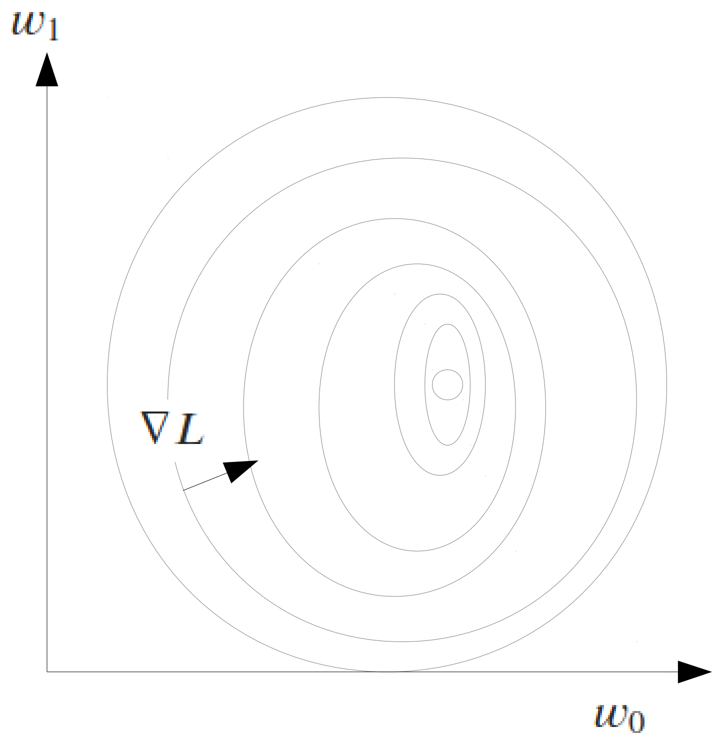
$$\nabla L = \frac{dL}{dw}$$



Gradient Descent Optimization

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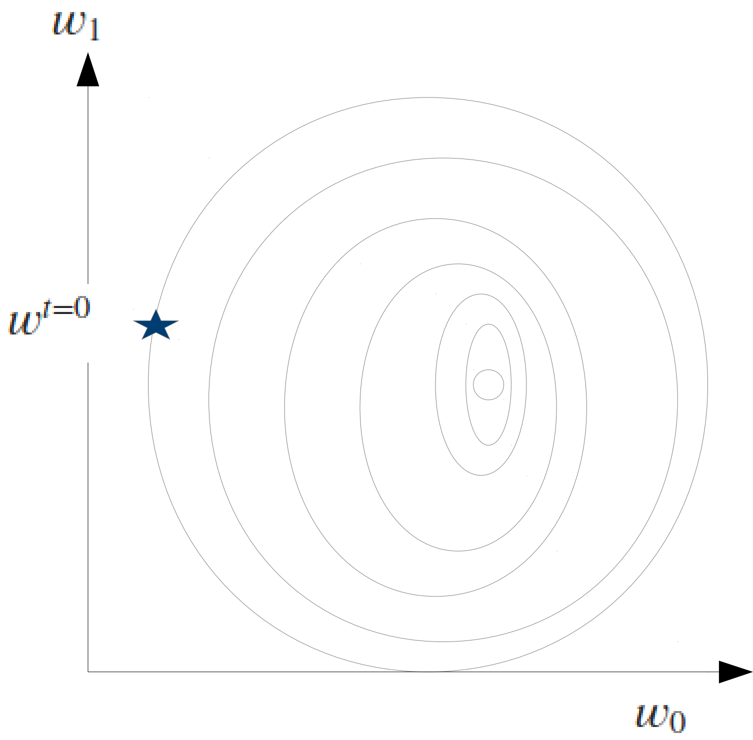
Goal: find w to minimize $\arg\min_{w} \sum_{i=0}^{N} L(y_i, w^T x_i)$

Gradient Descent Algorithm:

I. Start with random $w^{t=0}$



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Gradient Descent Algorithm:

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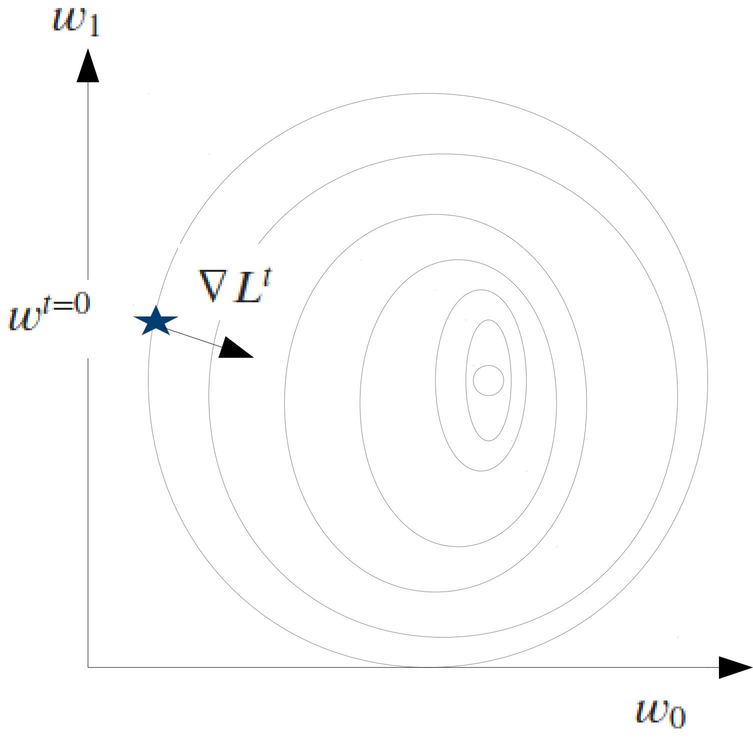
II. Compute gradient for all training samples

$$\nabla L^t = \sum_{i=0}^{|(X,y)|} \frac{dL(y_i, w^t x_i)}{dw^t}$$



Gradient Descent Optimization

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Goal: find w to minimize $\arg\min_{w} \sum_{i=0}^{N} L(y_i, w^T x_i)$

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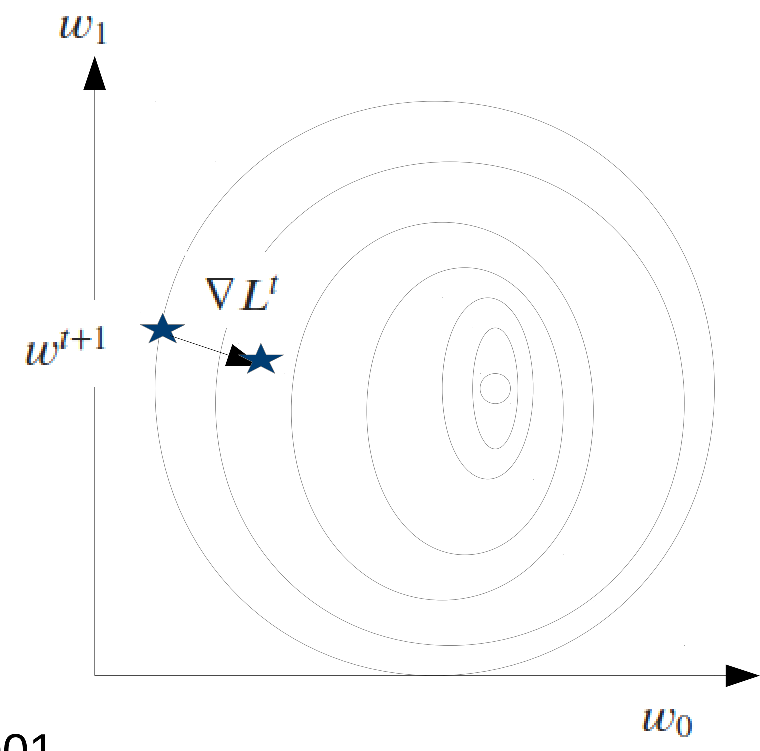
II. Compute gradient for all training samples

$$\nabla L^t = \sum_{i=0}^{|(X,y)|} \frac{dL(y_i, w^t x_i)}{dw^t}$$

III. Update parameters

$$w^{t+1} = w^t + \lambda \nabla L^t$$

Step size or Learning rate
Usually quite small scalar like 0.001



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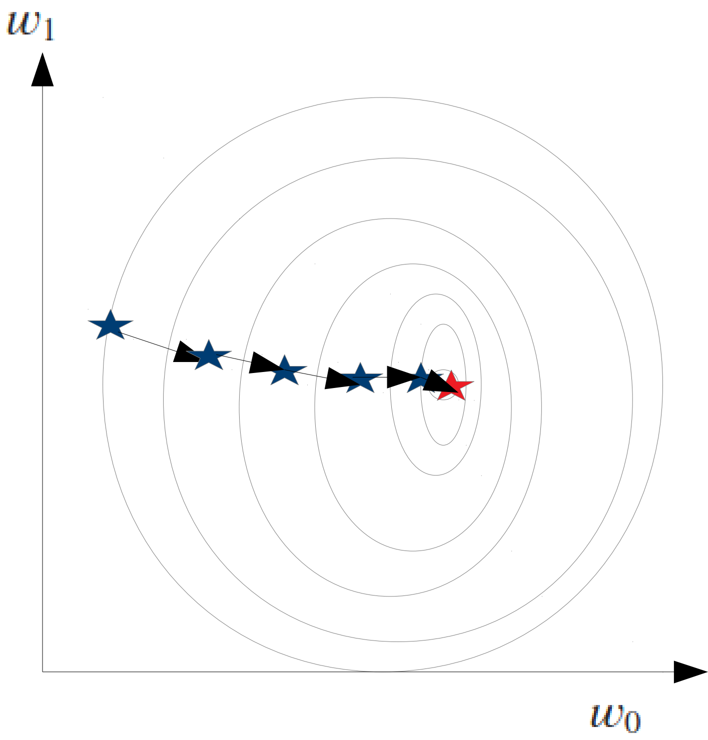
III. Update parameters

$$w^{t+1} = w^t + \lambda \nabla L^t$$

IV. Repeat II-III till convergence



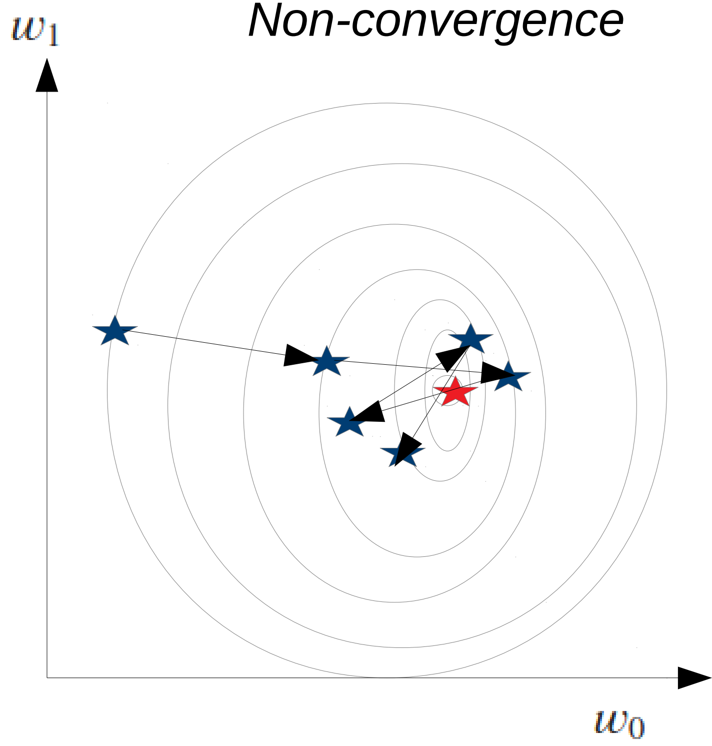
Gradient Descent Optimization

Goal: find w to minimize $\arg\min_{w} \sum_{i=0}^{N} L(y_i, w^T x_i)$

Convergence

I. Theory: need to decrease λ to guarantee convergence to minimum

Simplification: Non-convergence



Gradient Descent Optimization

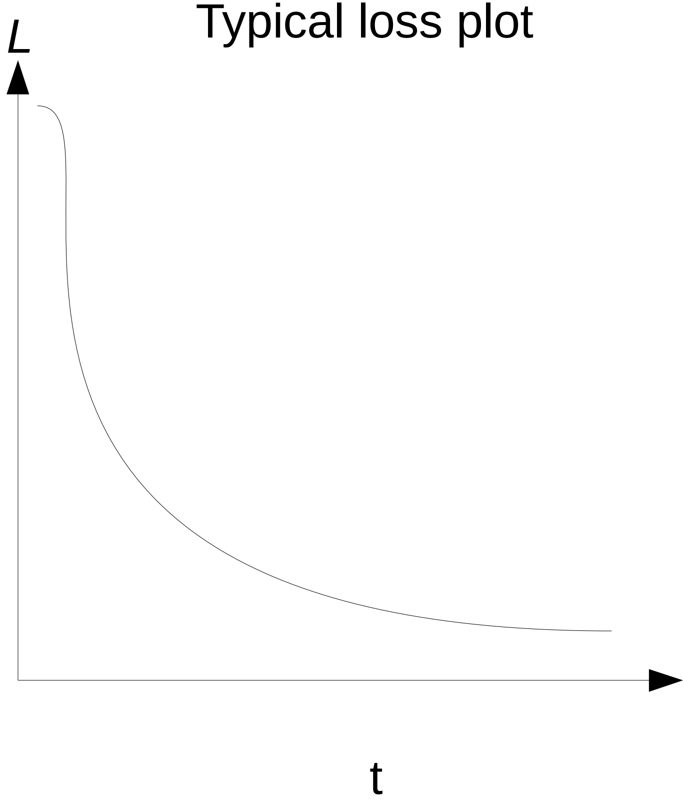
Goal: find w to minimize $\underset{w}{\arg\min} \sum_{i=0}^{N} L(y_i, w^T x_i)$

Convergence

I. Theory: need to decrease λ to guarantee convergence to minimum

II. How to know when to stop?
   I. Pre set number of iterations
   II. Loss limit
   III. Loss not changing

Typical loss plot



Multi Class Problems

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What if we have more than two classes? → simple extension of our model

$$f(x) = y' = argmax(Wx)$$

Replace parameter vector by Matrix
→ One vector per class
→ Matrix vector Multiplication
→ returns vector with class-wise response
→ argmax selects maximum class label

Multi Class Problems

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What if we have more than two classes? → simple extension of our model

$$f(x) = y' = argmax(Wx)$$

Optimization problem is almost the same

$$\arg\min_{w} \sum_{i=0}^{N} L(y_i, Wx_i)$$

Change *Loss* to *SOFTMAX* function to normalize sum aver all probabilities to one

$$L(y^i, y^{i\prime}) := \frac{e^{y^{i\prime}}}{\sum_j^k e^{y^{j\prime}}}$$

Use "one-hot" coding of y

Multi Class Problems

What if we have more than two classes? → simple extension of our model

$$f(x) = y' = argmax(Wx)$$

Optimization problem is almost the same

$$\arg\min_{w} \sum_{i=0}^{N} L(y_i, Wx_i)$$

Change *Loss* to *SOFTMAX* function to normalize sum aver all probabilities to one

$$L(y^i, {y^i}') := \frac{e^{{y^i}'}}{\sum_j^k e^{{y^j}'}}$$

Use “one-hot” coding of y

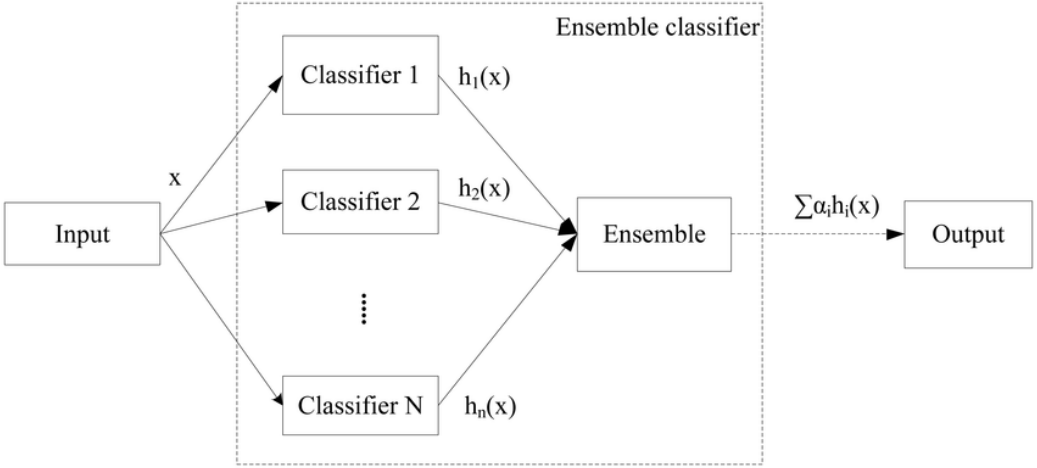
Y is now a vector with k (number of classes) entries and y^i is the kth class label

Discussion

Random Forests

Ensemble Learning

- Very popular method based on ensemble learning
  → many weak models decide together (by voting)
- Simple but powerful method
- Easy to implement and to parallelize
- Does not tend to overfit
- Build in Feature-Selection
  (next Lecture)



Random Forests

Ensemble Learning

- Very popular method based on ensemble learning
  → many weak models decide together (by voting)

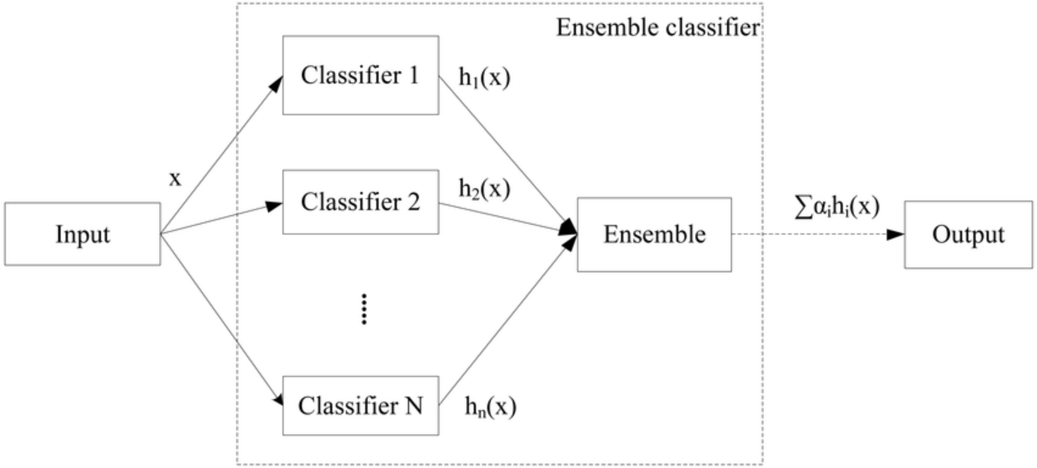
- Simple but powerful method

- Approximating non-linear decision function by combination of piecewise linear functions

- Easy to implement and to parallelize

- Build in Feature-Selection (next Lecture)

Statistics: Bagging and Boosting

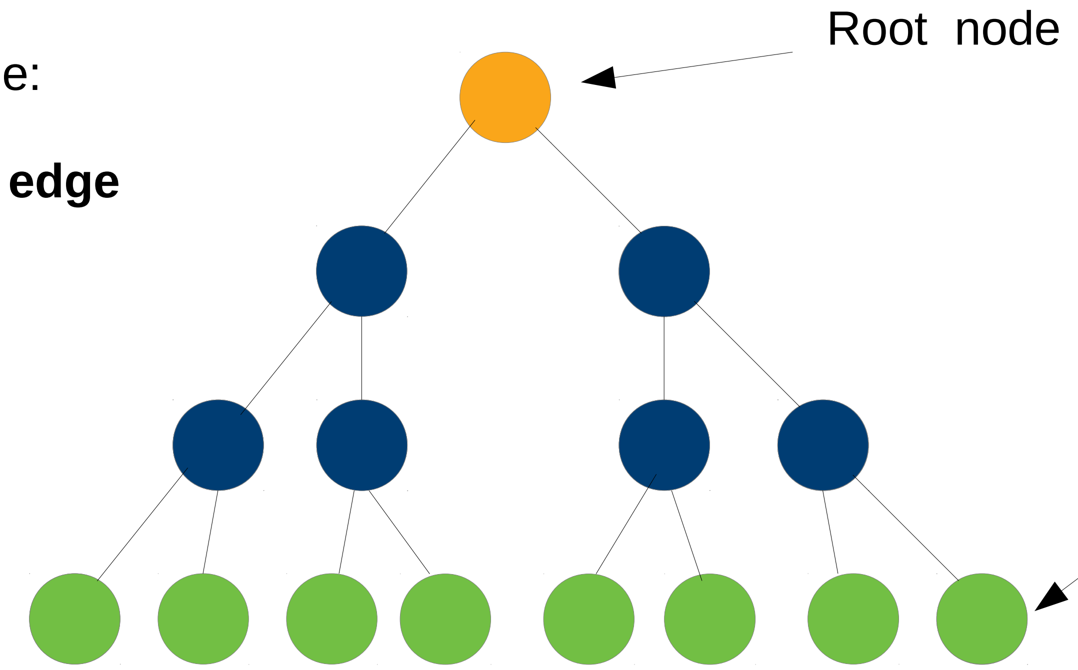


Random Forests

Decision Trees: the base classifier for Random Forests

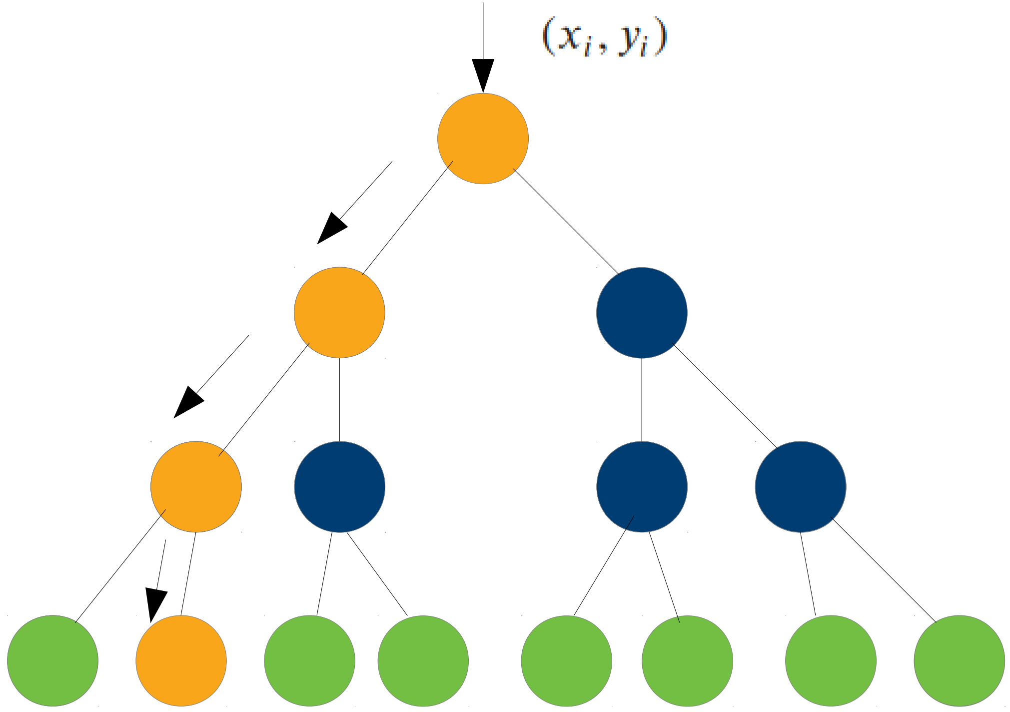
Typically Binary Tree:

Vertex (Node) and edge



Random Forests

Goal: divide training data samples X at each node such that leafs have (mostly) Pure class labels

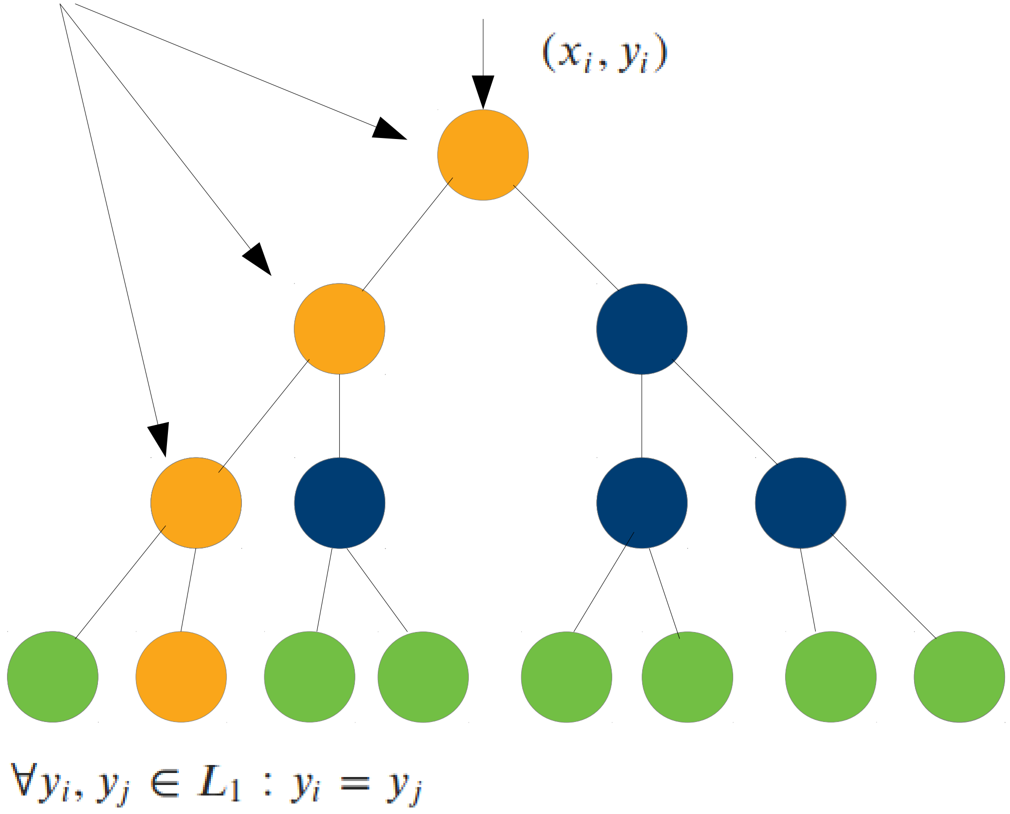


Classification: label y' is the label of the leaf node

$\forall y_i, y_j \in L_1 : y_i = y_j$

Random Forests

All we need is a splitting function that will produce (almost) pure class labels



Random Forests

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Top Down Training:

Assume ***k*** classes and data of dimension ***d***

- Fill tree with ALL training samples from the root down
- In each node: compute probability for all class labels in node *n*

$$p_i := p(y = i) = \frac{|(x,i)| \in X_n}{|X_n|}$$

- Compute **node purity** based on class probabilities
- Split node along one dimension such that purity of children is increasing $\leftarrow$ **optimization**

Random Forests

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All we need is a splitting function that will produce (almost) pure class labels.

Entropy (a way to measure impurity):

$$Entropy = -\sum_j p_j \log_2 p_j$$

Gini index:

$$Gini = 1 - \sum_j p_j^2$$

Random Forests

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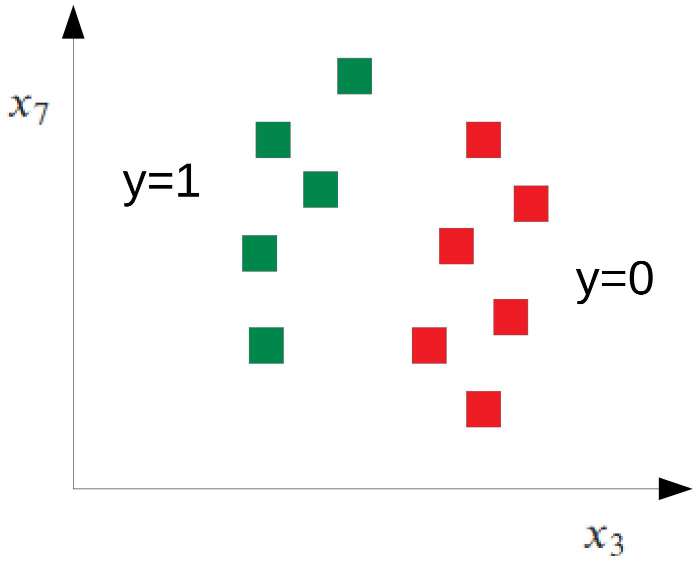
Split optimization is a simple line search (Example):

I. Select a random subset of variables (feature dimensions) from the data X
e.g. x_7 x_3



Random Forests

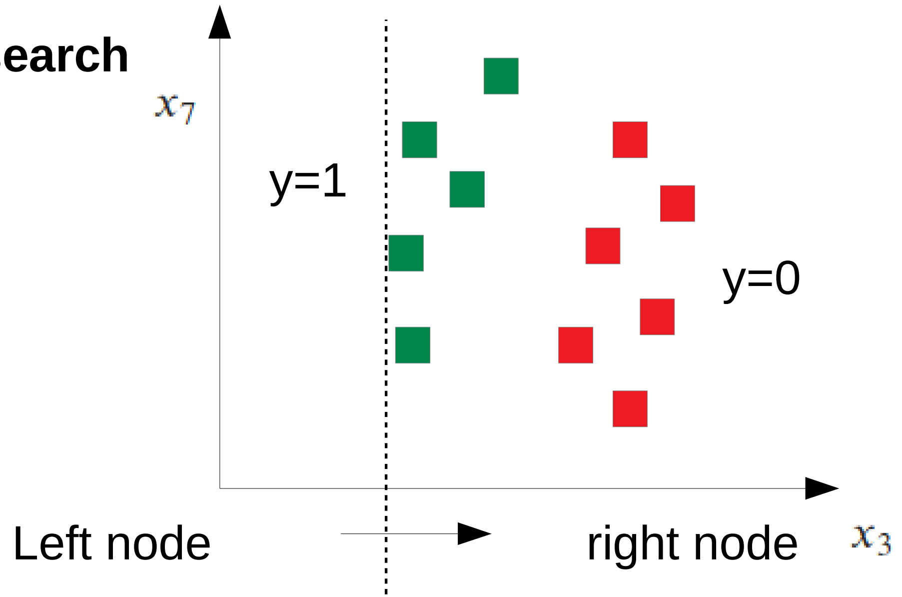
Split optimization is a simple line search (Example):

I. Select a random subset of variables (feature dimensions) from the data X
e.g. x_7 x_3

II. For each variable: find best split via line search
e.g. for x_3

Left: Undefined (div by zero)

Right: $p_1 = \frac{4}{11} = 0.36, p_0 = \frac{6}{11} = 0.54$



Random Forests

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I. Select a random subset of variables (feature dimensions) from the data X
e.g. x_7 x_3

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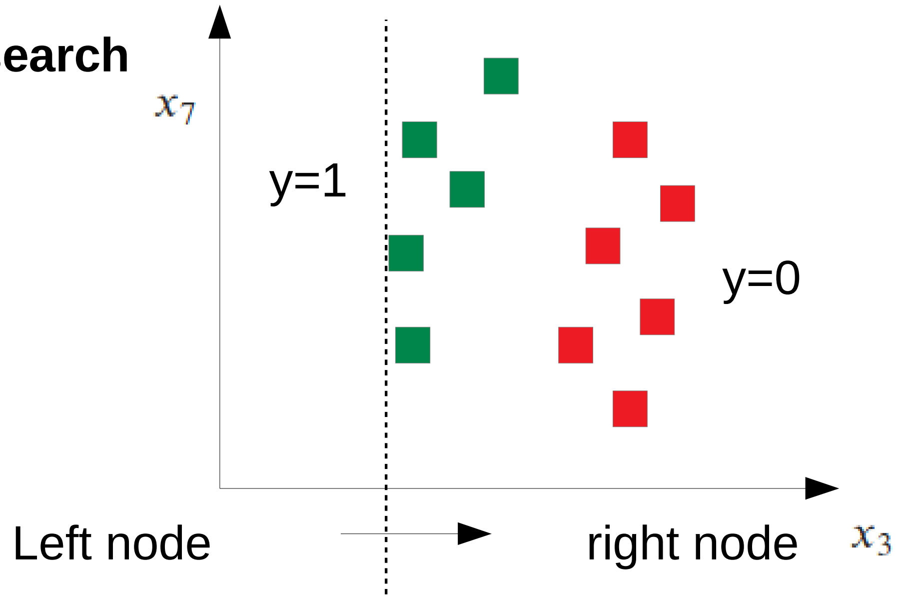
e.g. for x_3

Left: $gini = 1 - (0^2 + 0^2) = 1$

Right: $gini = 1 - (0.36^2 + 0.54^2) = 0.57$



Random Forests

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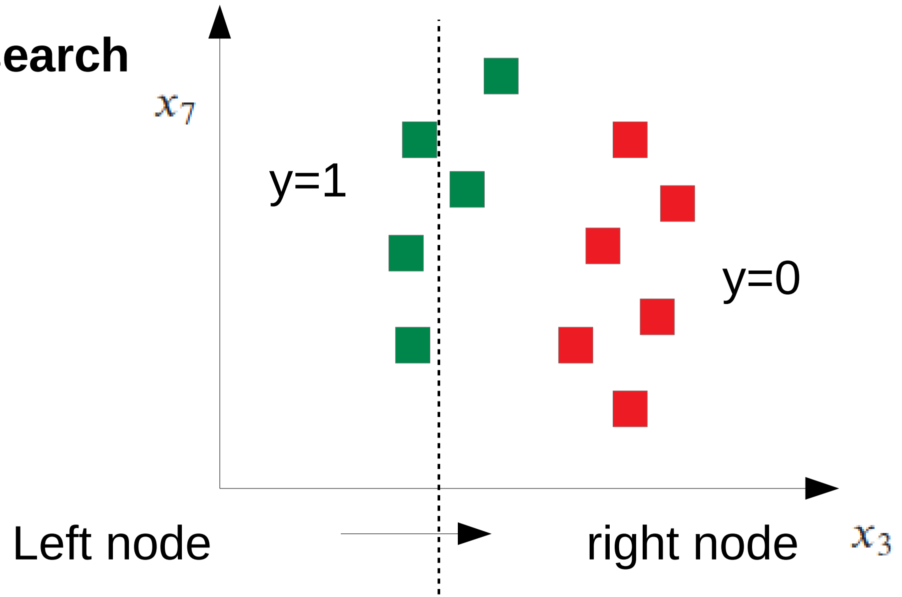
I. Select a random subset of variables (feature dimensions) from the data X
e.g. x_7 x_3

II. For each variable: find best split via line search
e.g. for x_3

Left: $p_1 = \frac{3}{3} = 1, p_0 = \frac{0}{3} = 0$

Right: $p_1 = \frac{2}{8} = 0.25, p_0 = \frac{6}{8} = 0.75$



Random Forests

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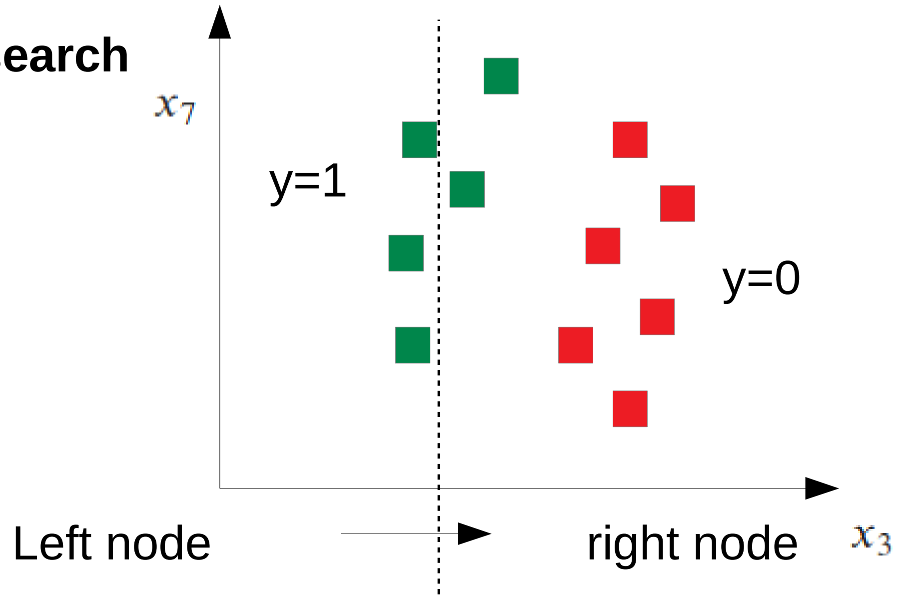
Split optimization is a simple line search (Example):

I. Select a random subset of variables (feature dimensions) from the data X
e.g. x_7 x_3

II. For each variable: find best split via line search
e.g. for x_3

Left: $gini = 1 - (1^2 + 0^2) = 0$

Right: $gini = 1 - (0.25^2 + 0.75^2) = 0.375$



Random Forests

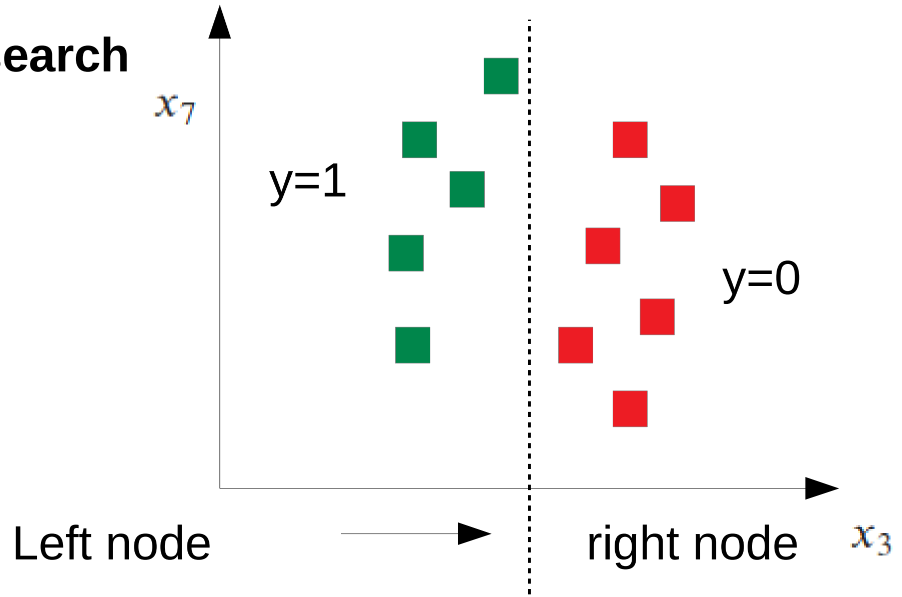
Split optimization is a simple line search (Example):

I. Select a random subset of variables (feature dimensions) from the data X
e.g. x_7 x_3

II. For each variable: find best split via line search
e.g. for x_3

Left: $p_1 = \frac{5}{5} = 1, p_0 = \frac{0}{5} = 0$

Right: $p_1 = \frac{0}{6} = 0, p_0 = \frac{6}{6} = 1$



Random Forests

Split optimization is a simple line search (Example):

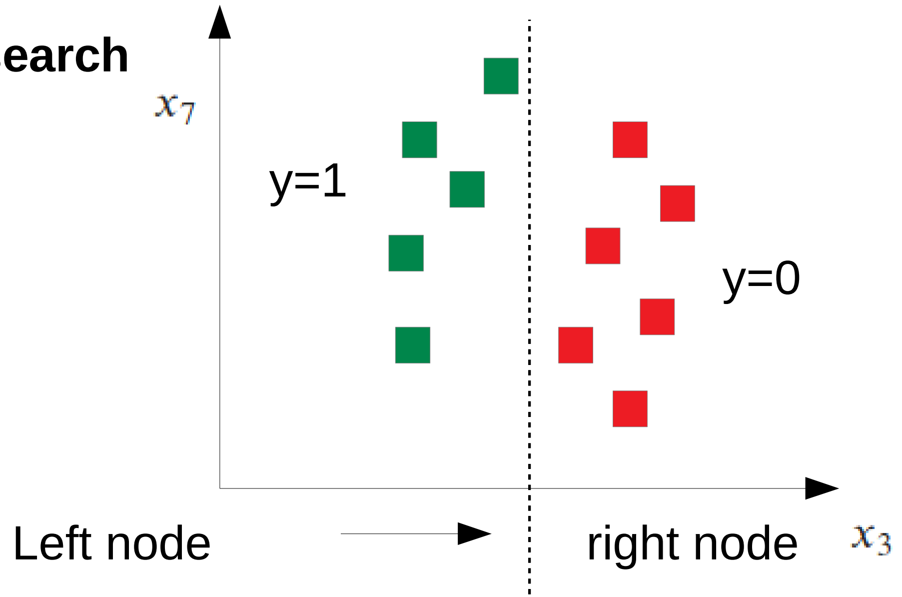
I. Select a random subset of variables (feature dimensions) from the data X
e.g. $x_7 \quad x_3$

II. For each variable: find best split via line search
e.g. for x_3

Left: $gini = 1 - (1^2 + 0^2) = 0$

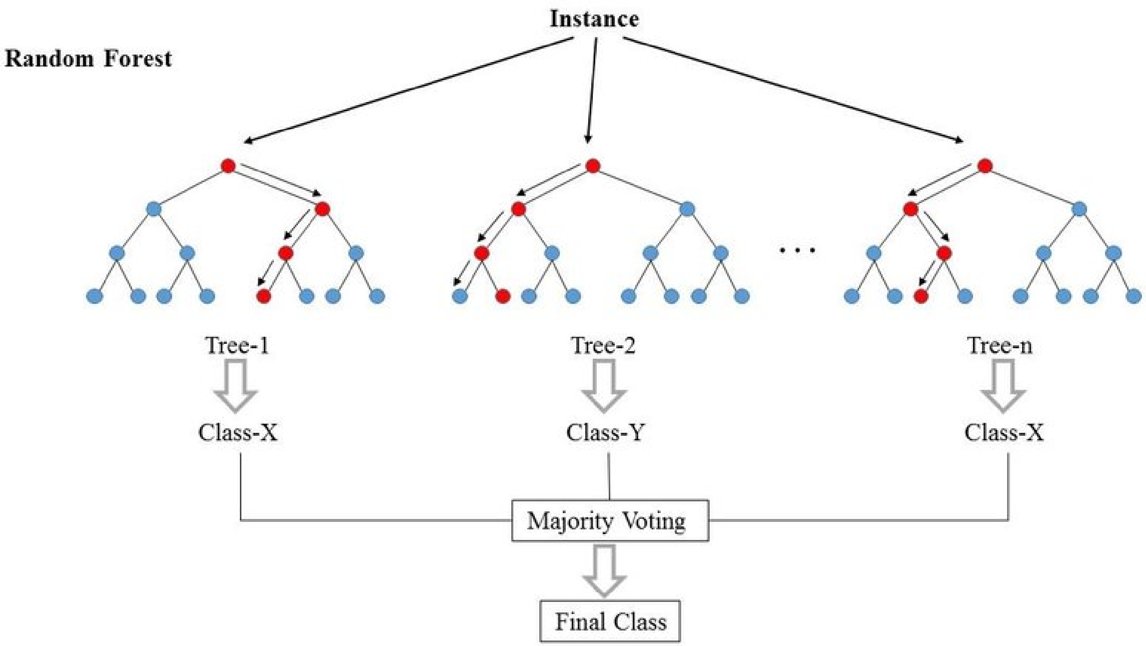
Right: $gini = 1 - (0^2 + 1^2) = 0$

Perfect split!



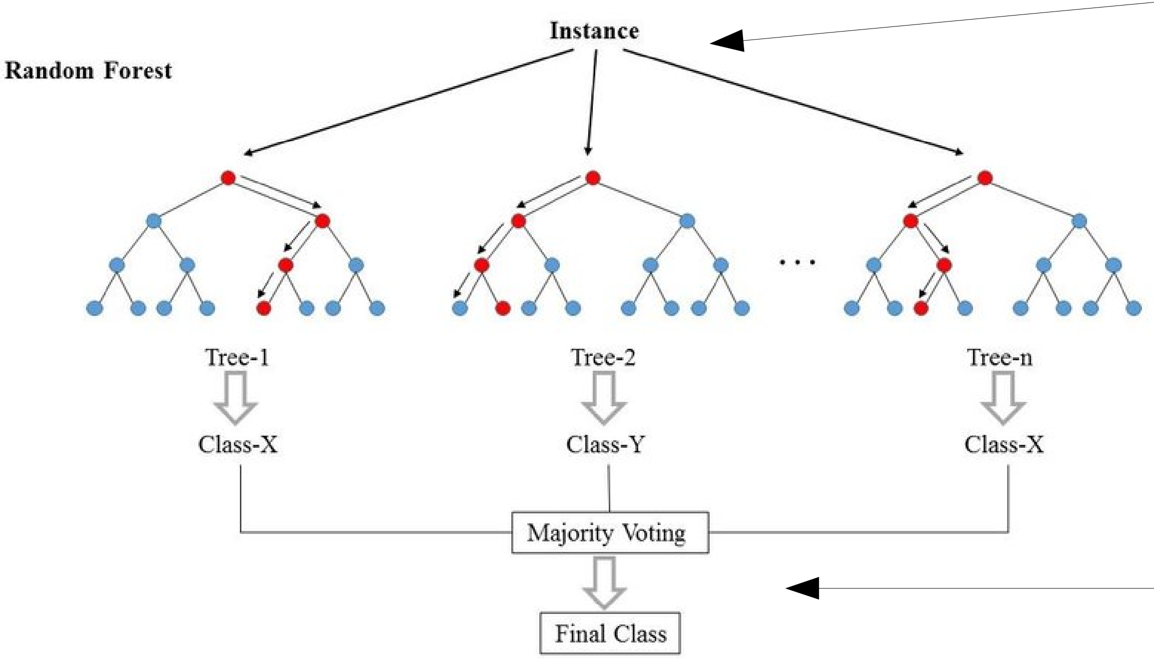
Random Forests

Ensemble Learning: A Forest of Trees



Random Forests

Ensemble Learning: A Forest of Trees

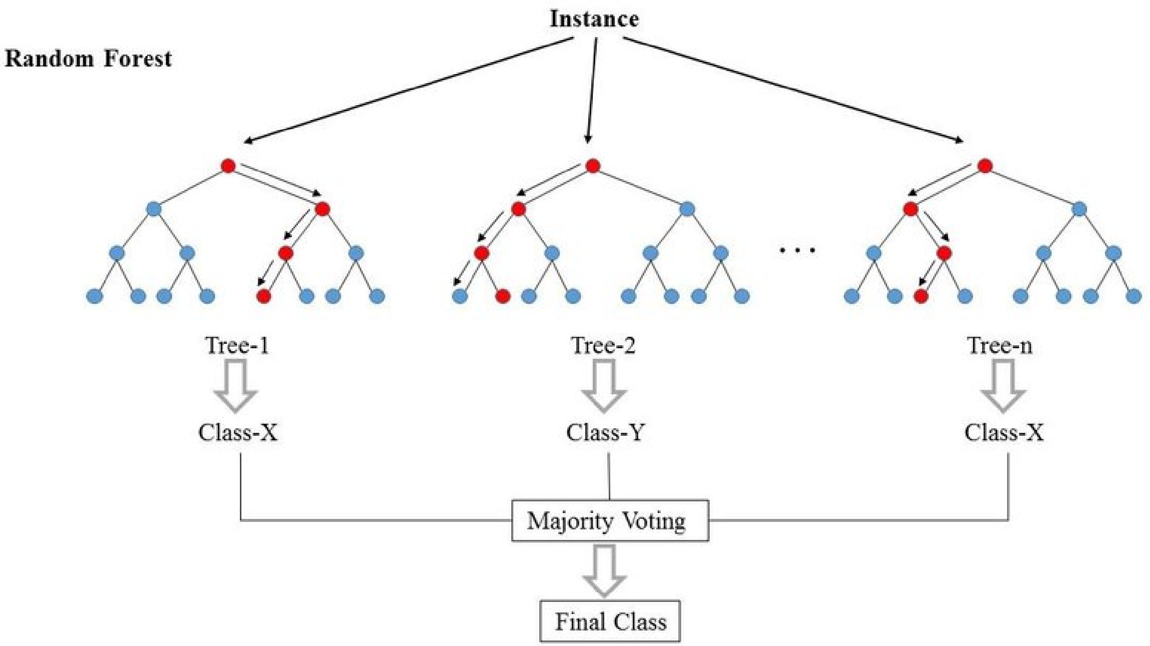


Split Training data into random subsets
→ Bootstrap

Combine Models
→ Bagging

Random Forests

Ensemble Learning: A Forest of Trees



Parameters:

- #trees
- Portion of data per tree
- #vars per split
- Stopping
  - max depth
  - min samples per node

Random Forests

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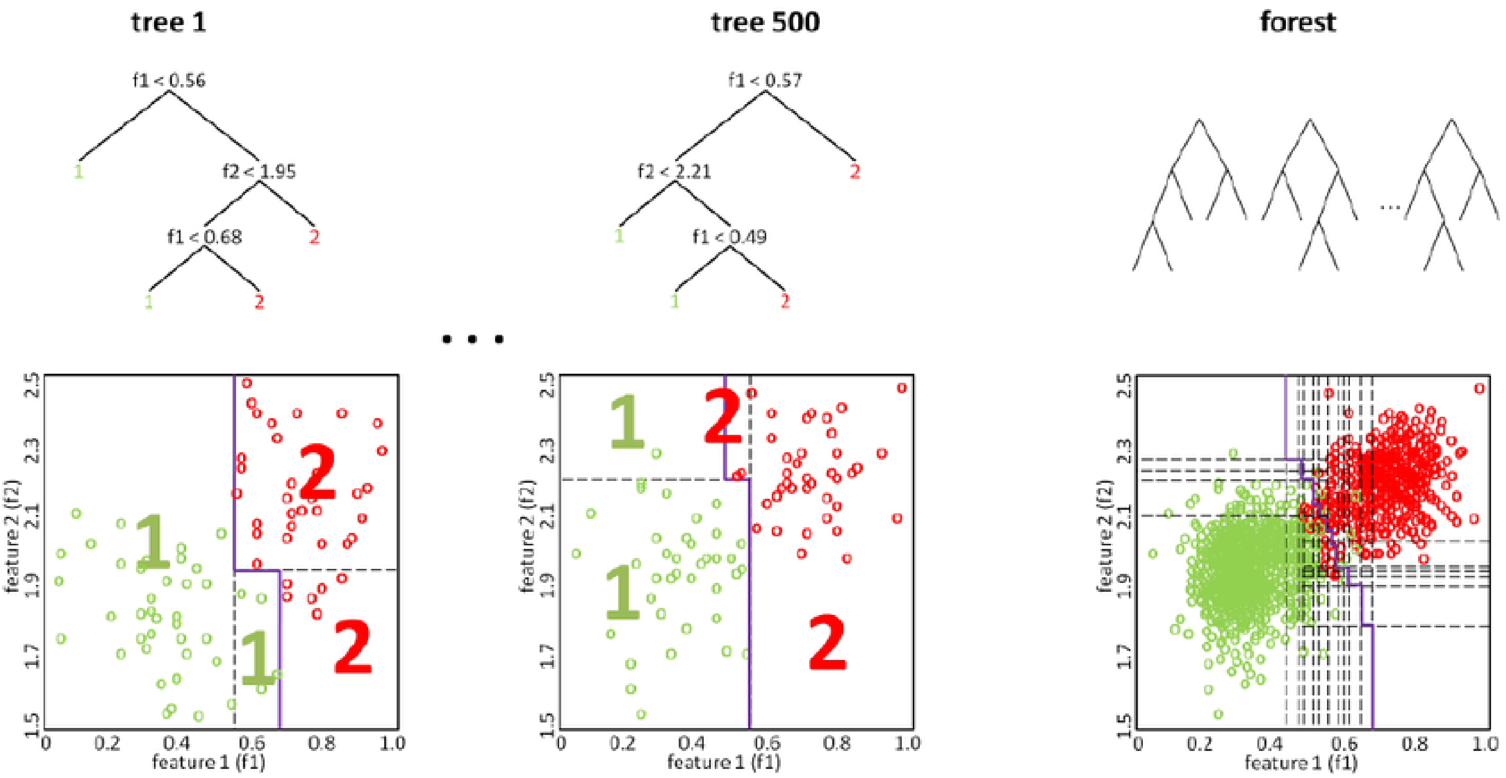
Classification example



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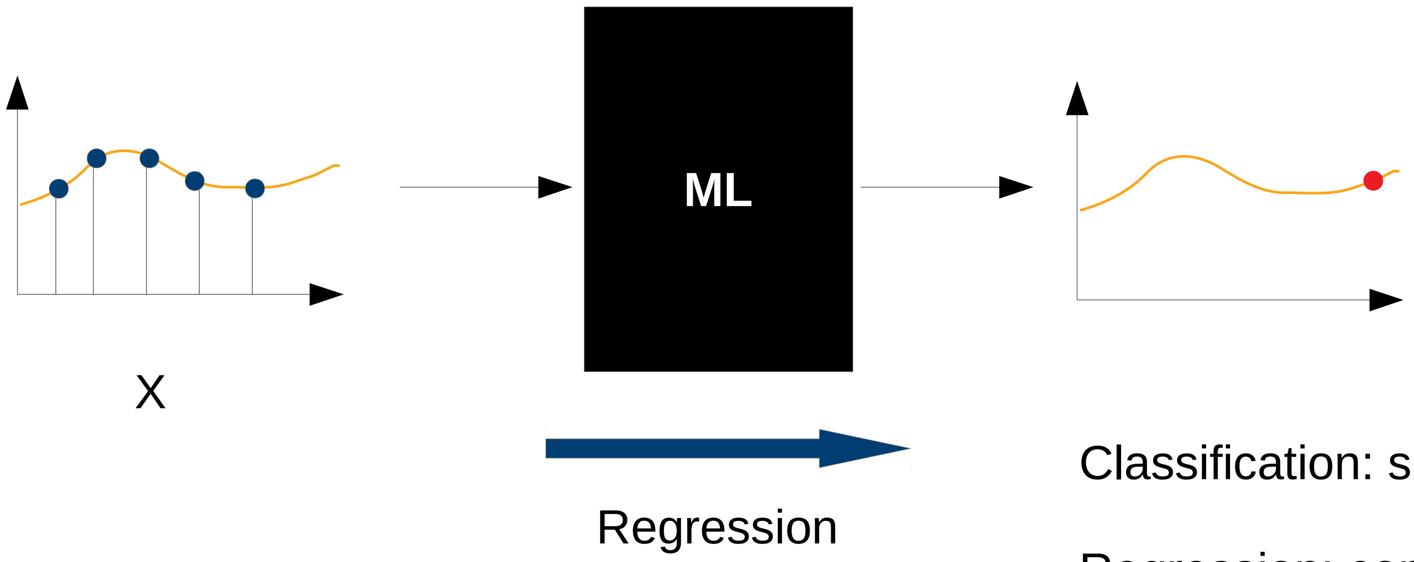
Discussion

Regression

Recall:



Y is **continuous**

Classification: separation function

Regression: continuous mapping
→ harder problem

Linear Regression

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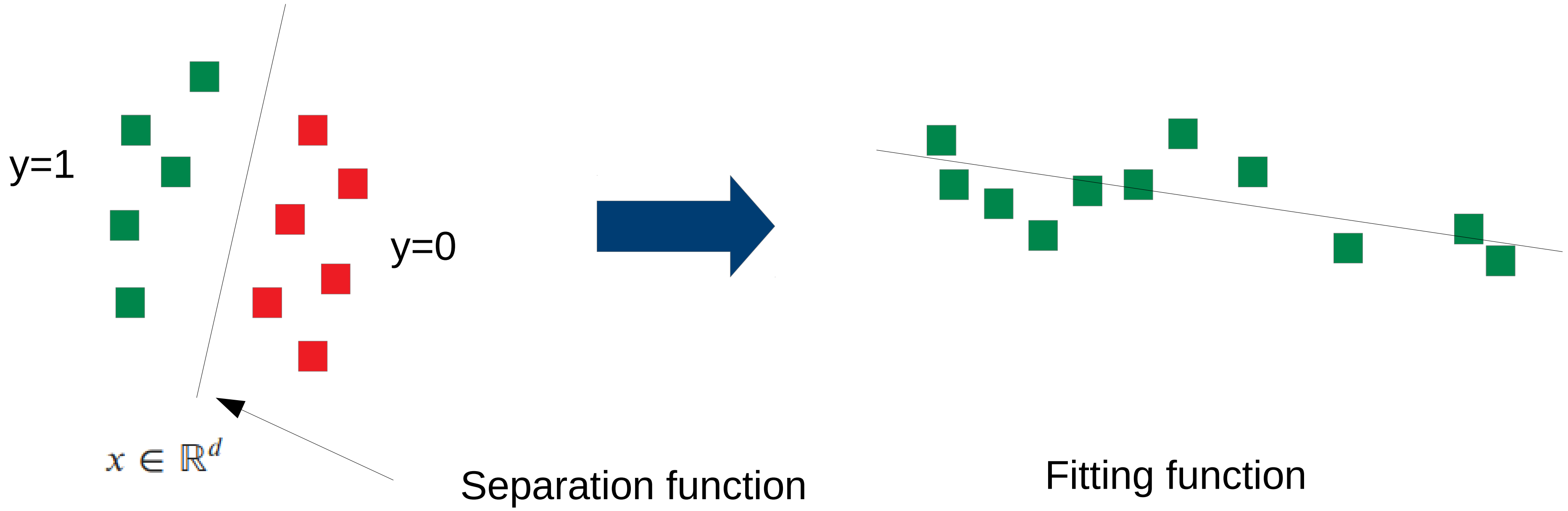
How do we have to change out linear classifier to predict continuous values?



Linear Regression

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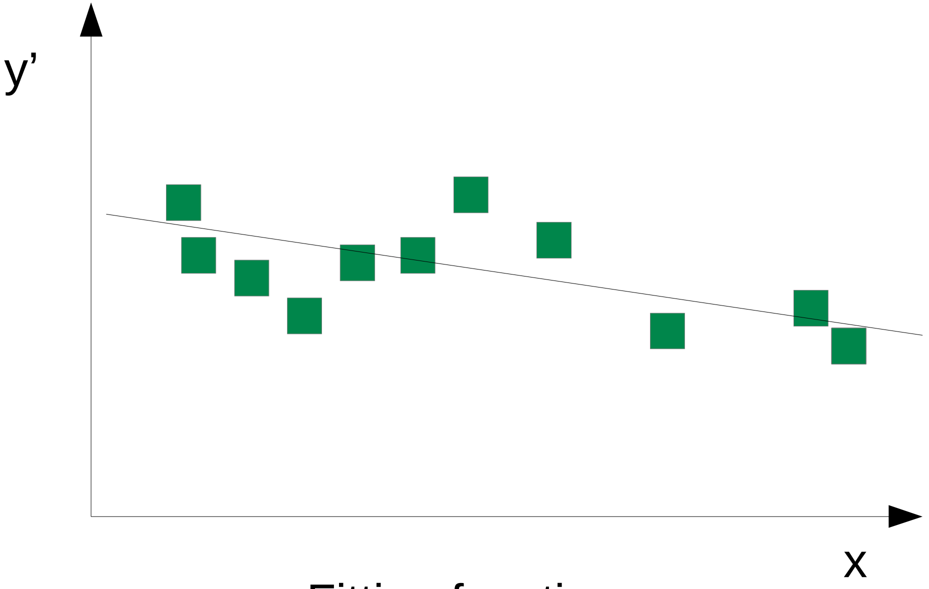
How do we have to change out linear classifier to predict continuous values?

Still can use the same framework

$$f(x) = y' = w^T x = \sum_{j=0}^{d} w_j x_j$$



Fitting function

Linear Regression

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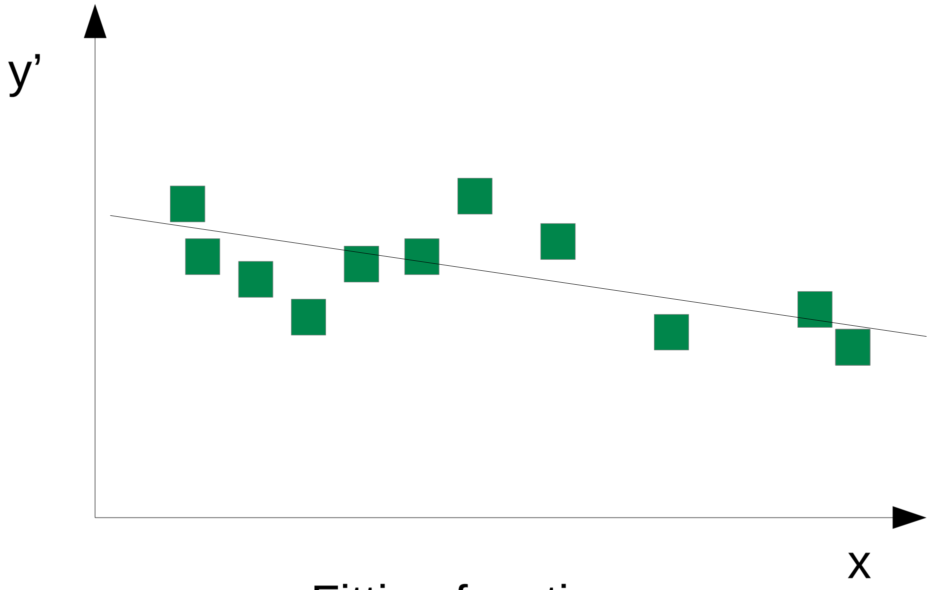
How do we have to change out linear classifier to predict continuous values?

Still can use the same framework

$$f(x) = y' = w^T x = \sum_{j=0}^{d} w_j x_j$$

Simply need new loss function in the optimization

$$\arg\min_{w} \sum_{i=0}^{N} L(y_i, w^T x_i)$$



Fitting function

Linear Regression

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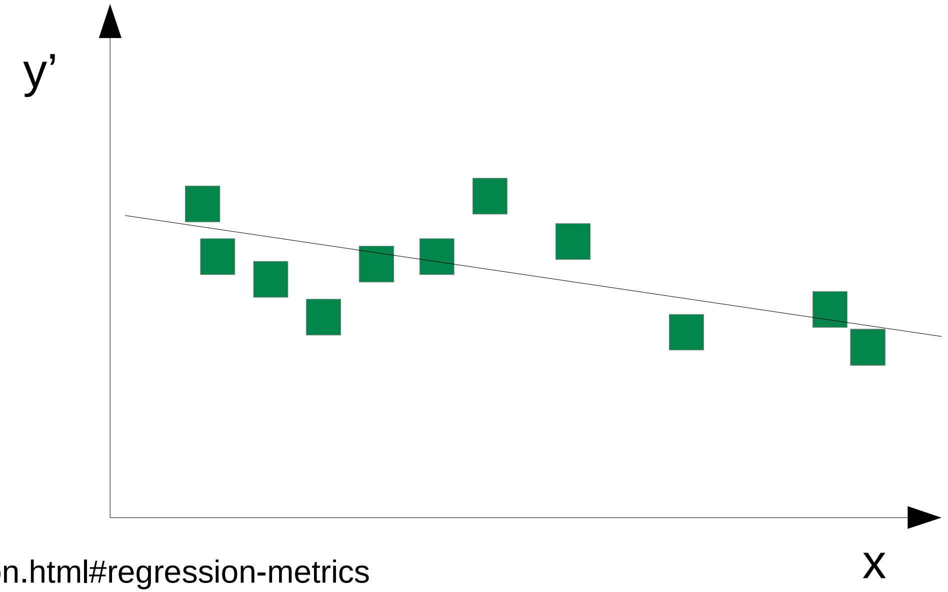
Loss functions for regression:

$$\arg\min_{w} \sum_{i=0}^{N} L(y_i, w^T x_i)$$

As simple as least squares error

$$L_{LSE}(y, y') := \|y - y'\|^2$$



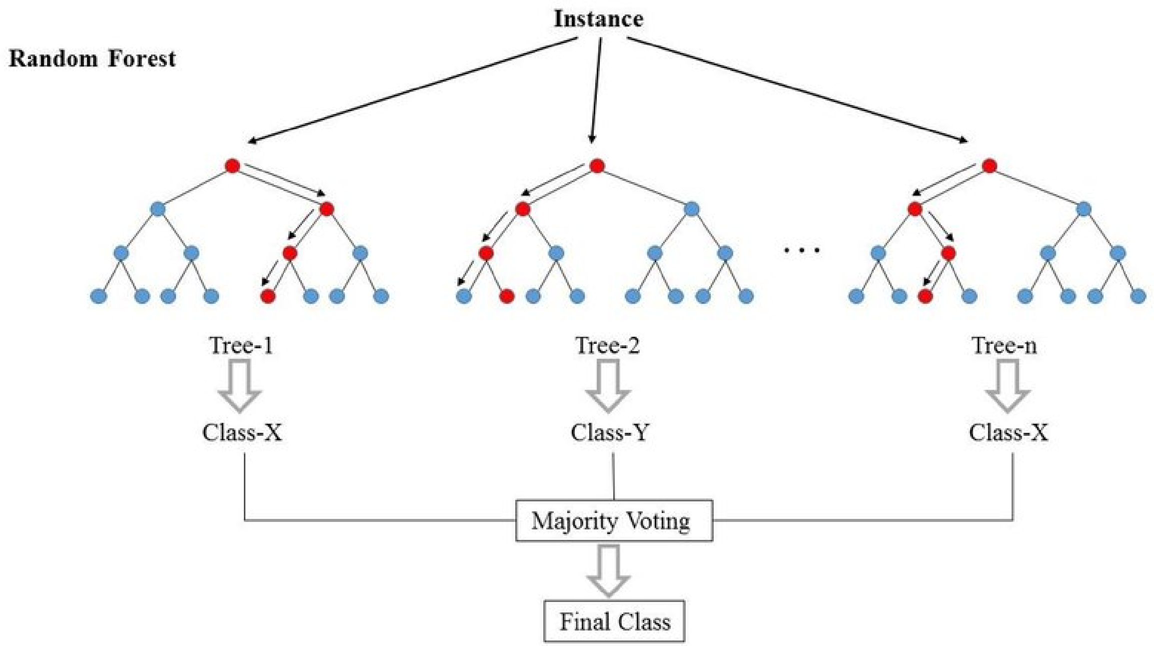
Many other error measures possible

- L1 (Histogram intersection)
- …

→ see https://scikit-learn.org/stable/modules/model_evaluation.html#regression-metrics

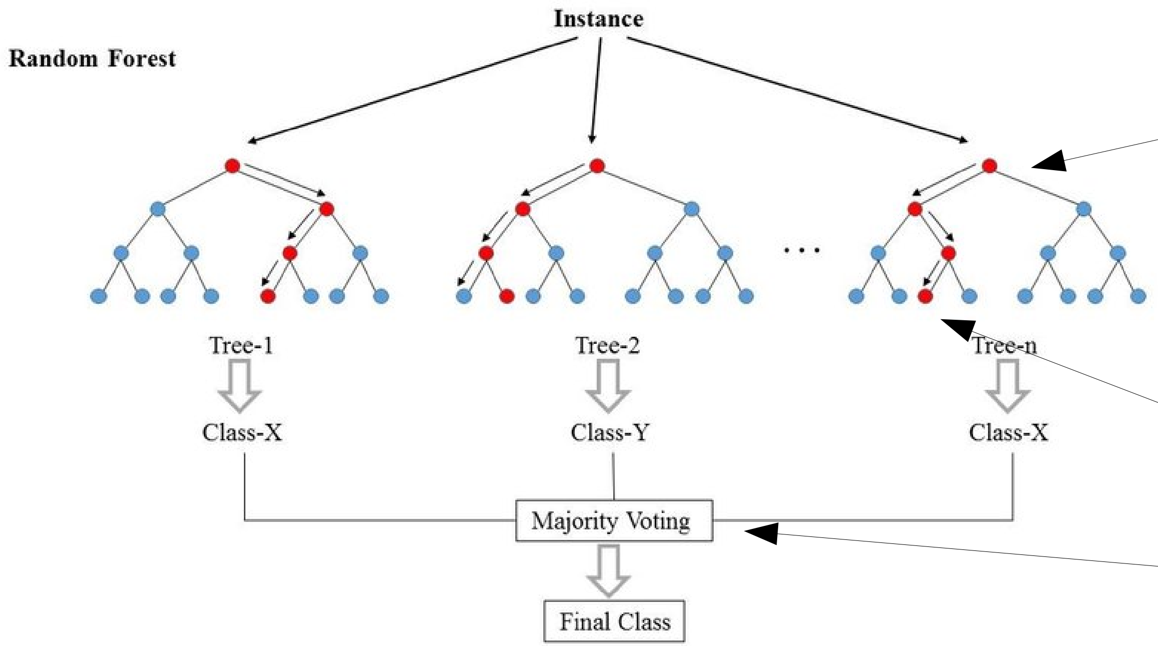
Regression with Random Forests

Recall:



Regression with Random Forests

Recall:



New splitting function

Replace majority vote by average

Regression with Random Forests

Splitting functions for regression:

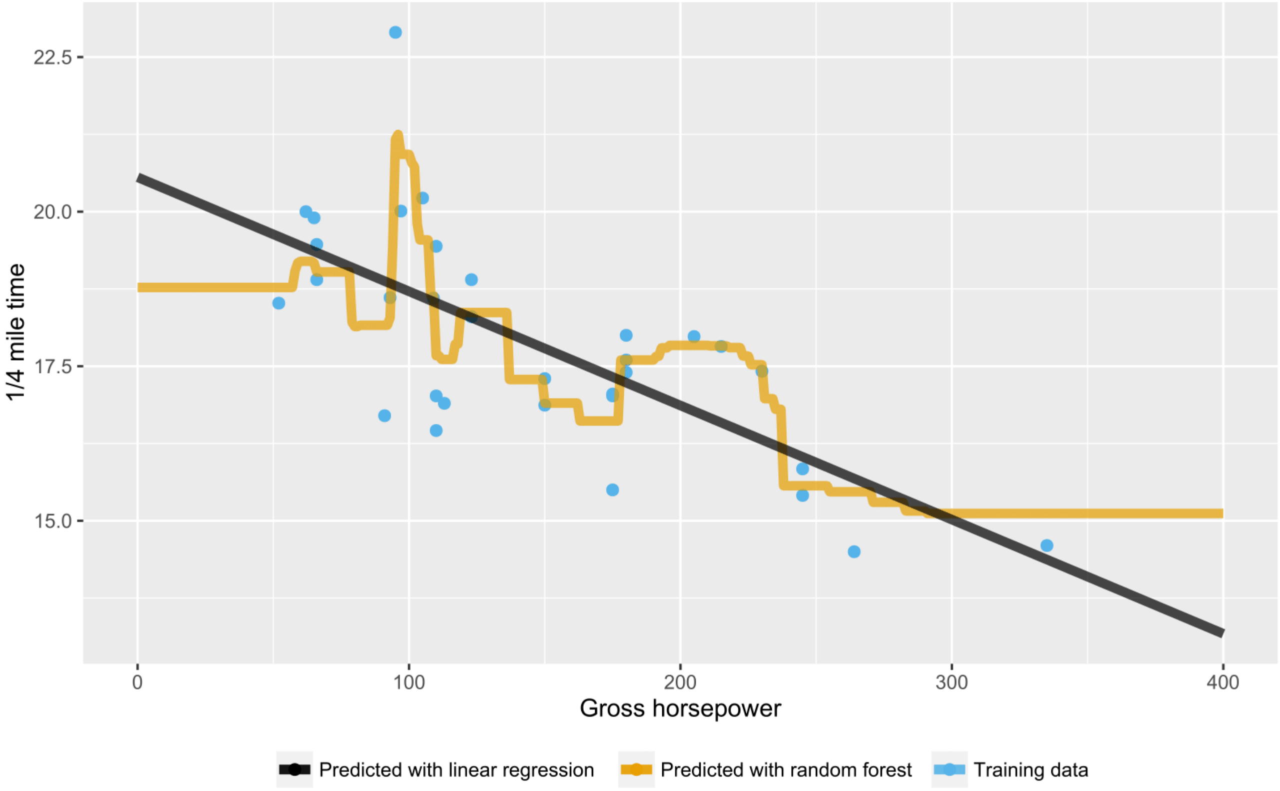
Goal: reduce “data spread” in node

→ **use simple statistical measure like “mean square error”**

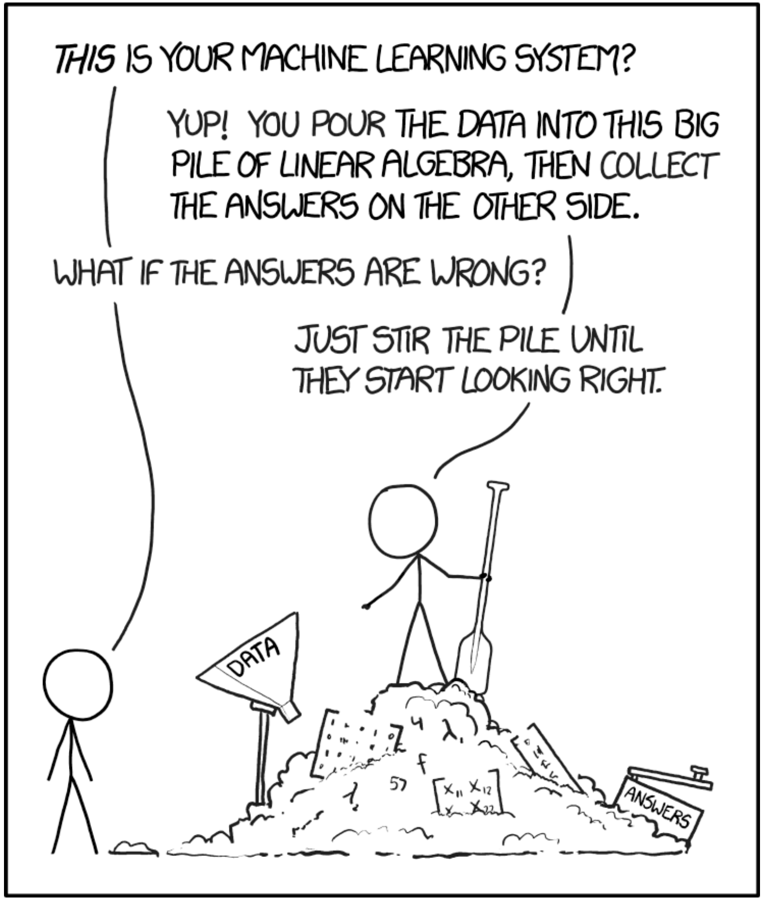
$$MSE: \sum_{(x_i,y_i)\in X_n} ||\mu_y - y_i||^2$$

Regression with Random Forests

Example



Discussion



https://xkcd.com/1838/