16-11-2020

CosmoML 2020/21- 3rd meeting

- Recap
- Evaluation metrics
- Decision Trees, Random Forests, Support Vector Machines, k Nearest Neighbors
- Hyperparameter tuning+pipelines in sklearn

Michele Mancarella

Recap & classification metrics

Supervised ML workflow

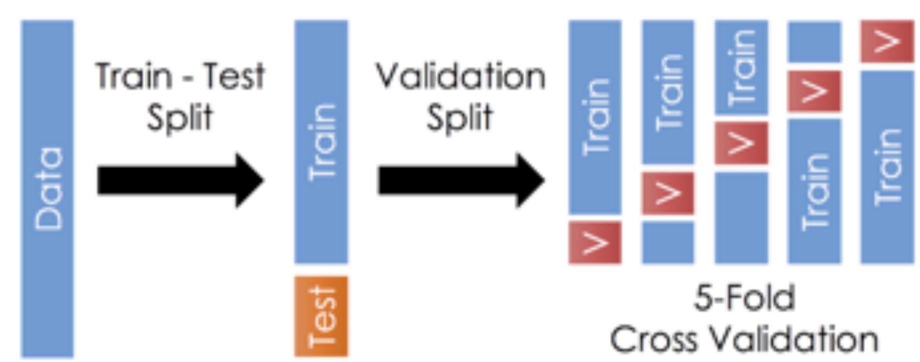
Data $\mathcal{D} = \{(\mathbf{X}, y)_i\}_{i=1}^{N}$

Model $f(\mathbf{X}; \mathbf{w})$ + cost $\mathcal{C}\Big(y, f(\mathbf{X}; \mathbf{w})\Big)$ Must be differentiable wrt weights!

Train $\hat{\mathbf{w}} = \arg\min_{\mathbf{w}} \mathcal{C}\Big(y, f(\mathbf{X}; \mathbf{w})\Big)$ by gradient descent

Split dataset

Hyperparameter tuning

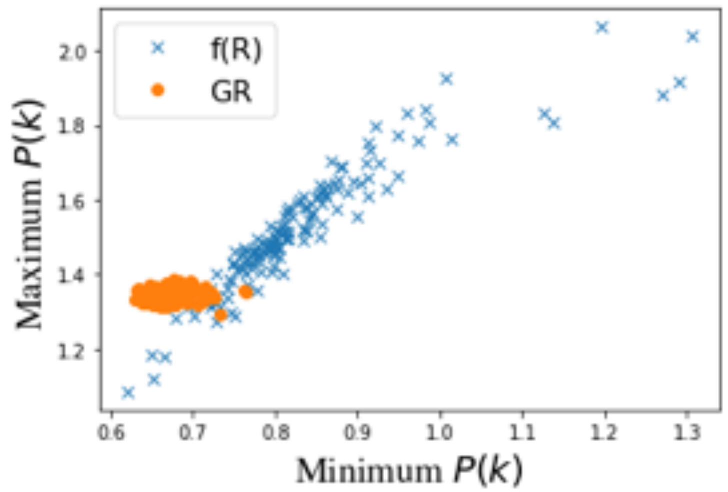


Test - Evaluation metric

In general evaluation metric != cost, not differentiable wrt weights

Classification problems

Data



$$\mathcal{D} = \{(\mathbf{X}, y)_i\}_{i=1}^N$$

y = fR, GR

X = (minP, maxP) (+ powers...)

Model $f(\mathbf{X}; \mathbf{w})$

$$\sigma(\mathbf{w}^T\mathbf{X}), \ \sigma(t) = \frac{1}{1+e^{-t}}$$

Cost $\mathcal{C}\Big(y, f(\mathbf{X}; \mathbf{w})\Big)$

binomial likelihood/ binary cross-entropy loss.

$$\mathcal{C} = -\log \mathcal{L}(\mathcal{D}; \mathbf{w}) = -\sum_i y_i \log f(\mathbf{w}^T\mathbf{x}_i) - (1-y_i)\log[1 - f(\mathbf{w}^T\mathbf{x}_i)]$$

Train

Test /validation

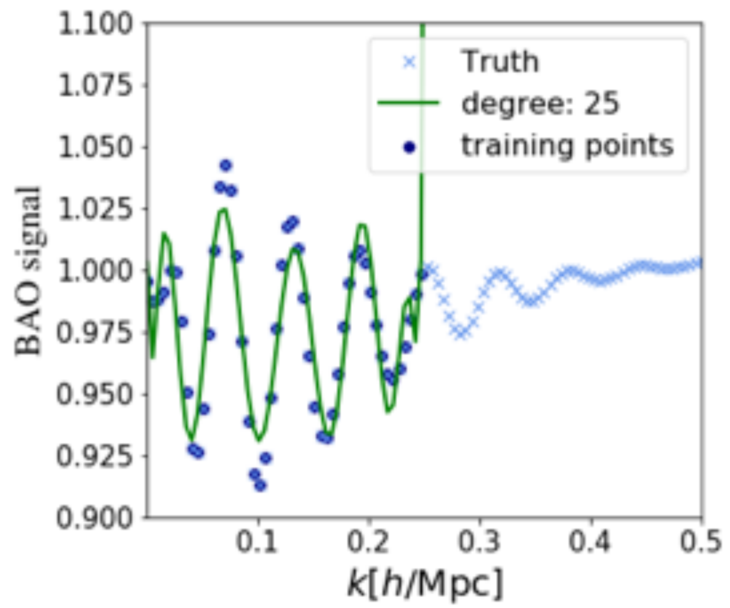
Set threshold prob.

Get sigmoid output & assign label depending on threshold

Evaluation metric = accuracy

Regression problems

Data



y = BAO signal
X = k (+ powers...)

Model $f(\mathbf{X};\mathbf{w})$

$$f(k;\mathbf{w}) = w_o + w_1 k + w_2 k^2 + \ldots$$

Cost $\mathcal{C}\Big(y, f(\mathbf{X};\mathbf{w})\Big)$

MSE / gaussian likelihood

$$\mathcal{C} = -\log \mathcal{L}(\mathcal{D};\mathbf{w}) \propto -\sum_i (y-f)^2$$

Train

Test /validation

Evaluation metric = cost

Metrics for classification

Classification problems: Confusion matrix (not a "metric", but check it...)

		Actual	
		1	0
Predicted	1	True positive	False positive
	0	False negative	True negative

LCDM=0
fR=1 (or: has covid-19)

ACCURACY= % of correctly predicted.

!! Careful with unbalanced datasets/type of problem. E.g. if I want to be sure to catch an fR in a dataset with 99 LCDM and 1 fR, a classifier that always predicts LCDM would have a 99% accuracy!
(or fraud/spam detection, covid-19 tests...)

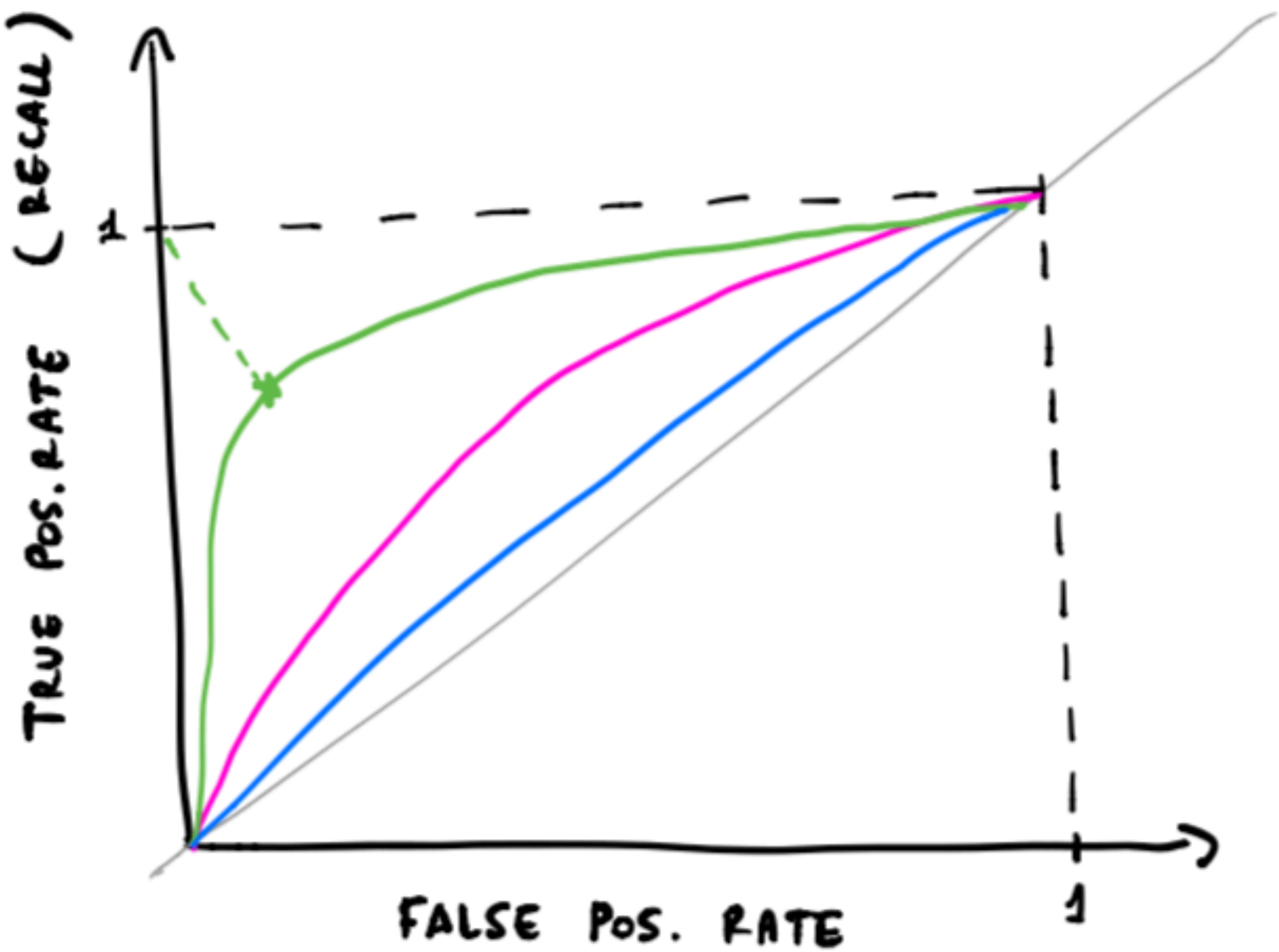
RECALL = fraction of samples from a class which are correctly predicted
(e.g. precision on fR: TP/(TP+FN)
how many that actually have covid are caught?)

"Well then let's predict all positive all the time!"

PRECISION = fraction of samples predicted in a class which are actually in that class
(e.g. precision on fR: TP/(TP+FP)
how many that are predictive positive are actually positive?)

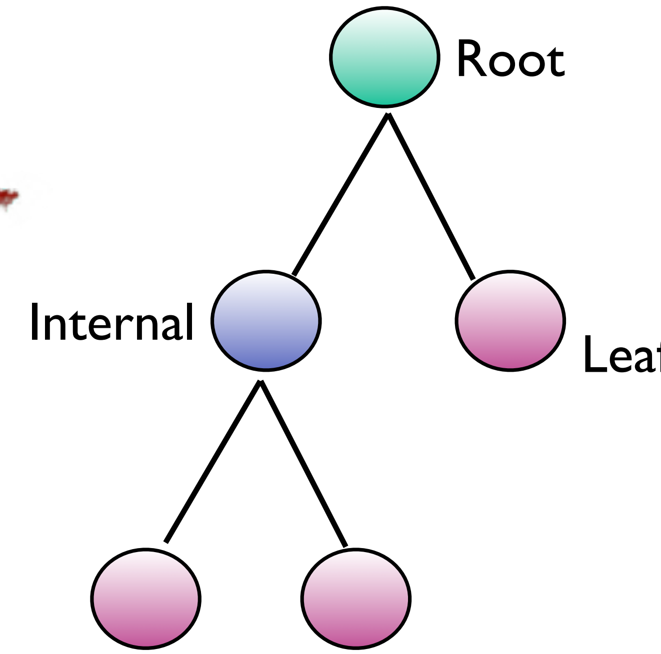
Metrics

ROC CURVE



ML Algorithms

Decision trees



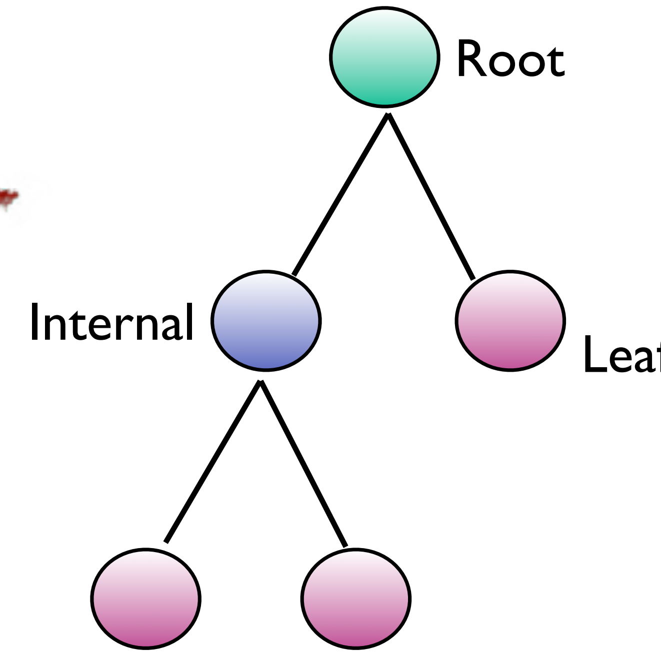
Tree = Oriented graph w. any two nodes connected by 1 edge

Algorithm 1 Decision Tree

Start at root node
repeat
  $\forall$ partition $S(\theta)$, $\theta = (j, t_j)$ consisting of feature j and threshold t_j of data at node k:
  Compute *impurity* $I(S,\theta) = \frac{n_{\text{left}}}{N_k} H(S_{\text{left}}) + \frac{n_{\text{right}}}{N_k} H(S_{\text{right}})$
  Choose the partition corresponding to $\hat{\theta} = \arg\min_\theta I(S,\theta)$
until Max depth is reached or $N_k = N_{min}$

$S_{\text{left}} =$ partition of data w. feature $j < t_j$, $\quad S_{\text{right}} = S \backslash S_{\text{left}}$

Decision trees



Gini $$H(x_k) = \sum_{i=1}^{N_{classes}} p_{ik}(1 - p_{ik})$$

$$p_{ik} = \text{fraction of points in node k in class i}$$

Entropy $$H(x_k) = -\sum_{i=1}^{N_{classes}} p_{ik} \log p_{ik}$$

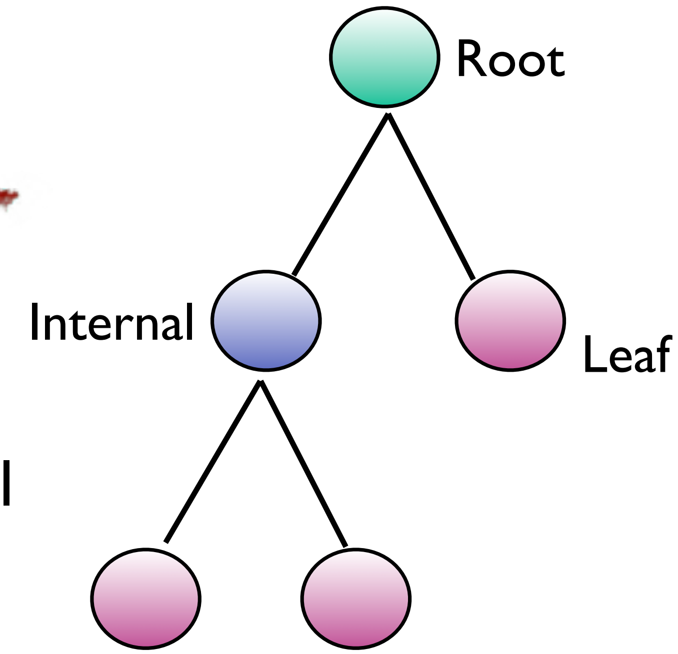
(For regression problems: MSE)

`sklearn.tree`.DecisionTreeClassifier

class `sklearn.tree.`**`DecisionTreeClassifier`**(*criterion='gini', splitter='best', max_depth=None, min_samples_split=2, min_samples_leaf=1, min_weight_fraction_leaf=0.0, max_features=None, random_state=None, max_leaf_nodes=None, min_impurity_decrease=0.0, min_impurity_split=None, class_weight=None, presort='deprecated', ccp_alpha=0.0*) [source]

A decision tree classifier.

Decision trees



Advantages:

✦ No feature preparation - also w. mixed numerical&categorical
✦ "**White box**" ! (Visualizable, interpretable, simple). Feature importance:

$$\frac{n_k}{N}\left(I(S) - \frac{n_{\text{left}}}{N_k} I(S_{\text{left}}) - \frac{n_{\text{right}}}{N_k} I(S_{\text{right}})\right)$$

$$FI_{f_i} = \frac{\sum_{\text{j s.t. node j splits on i-th feature}} GI_j}{\sum_j GI_j}$$

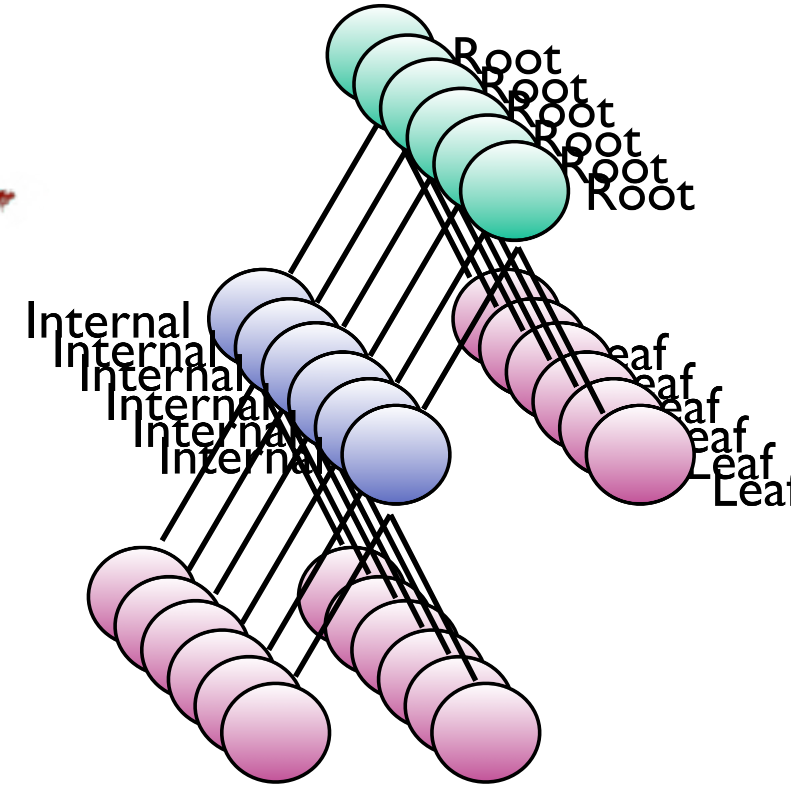
Disadvantages:

✦ Easily overfit ⟵ REGULARIZATION: max depth, max n. of leafs, min. sample split
✦ Handling of unbalanced classes
✦ Unstable to variations in training data
✦ Greedy ! (local minima)

Ensemble methods

✤ Random Forests - grow different trees w. bootstrap
✤ AdaBoost - re-weight error to reinforce points where classifier performs poorly (i.e. concentrate on difficult examples)
✤ Gradient Boosted Trees/XGBoost

Random Forests



Add randomness to prevent overfit (everywhere in ML, cfr dropout in NN)

(1) Grow different trees on bootstrap sample
(2) When splitting each node, partition using a random subset of features

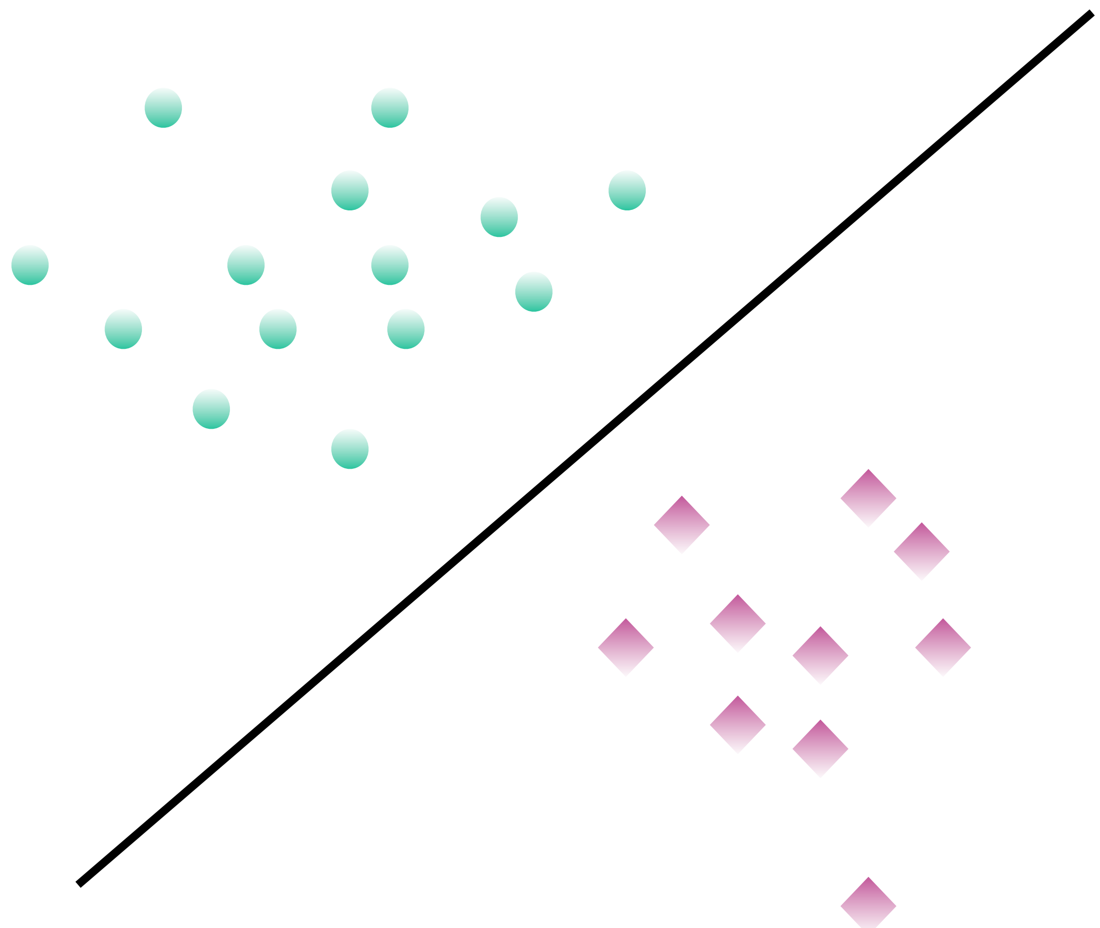
3.2.4.3.1. `sklearn.ensemble`.RandomForestClassifier

class `sklearn.ensemble.`**`RandomForestClassifier`**(*n_estimators=100, criterion='gini', max_depth=None, min_samples_split=2, min_samples_leaf=1, min_weight_fraction_leaf=0.0, max_features='auto', max_leaf_nodes=None, min_impurity_decrease=0.0, min_impurity_split=None, bootstrap=True, oob_score=False, n_jobs=None, random_state=None, verbose=0, warm_start=False, class_weight=None, ccp_alpha=0.0, max_samples=None*) [source]

A random forest classifier.

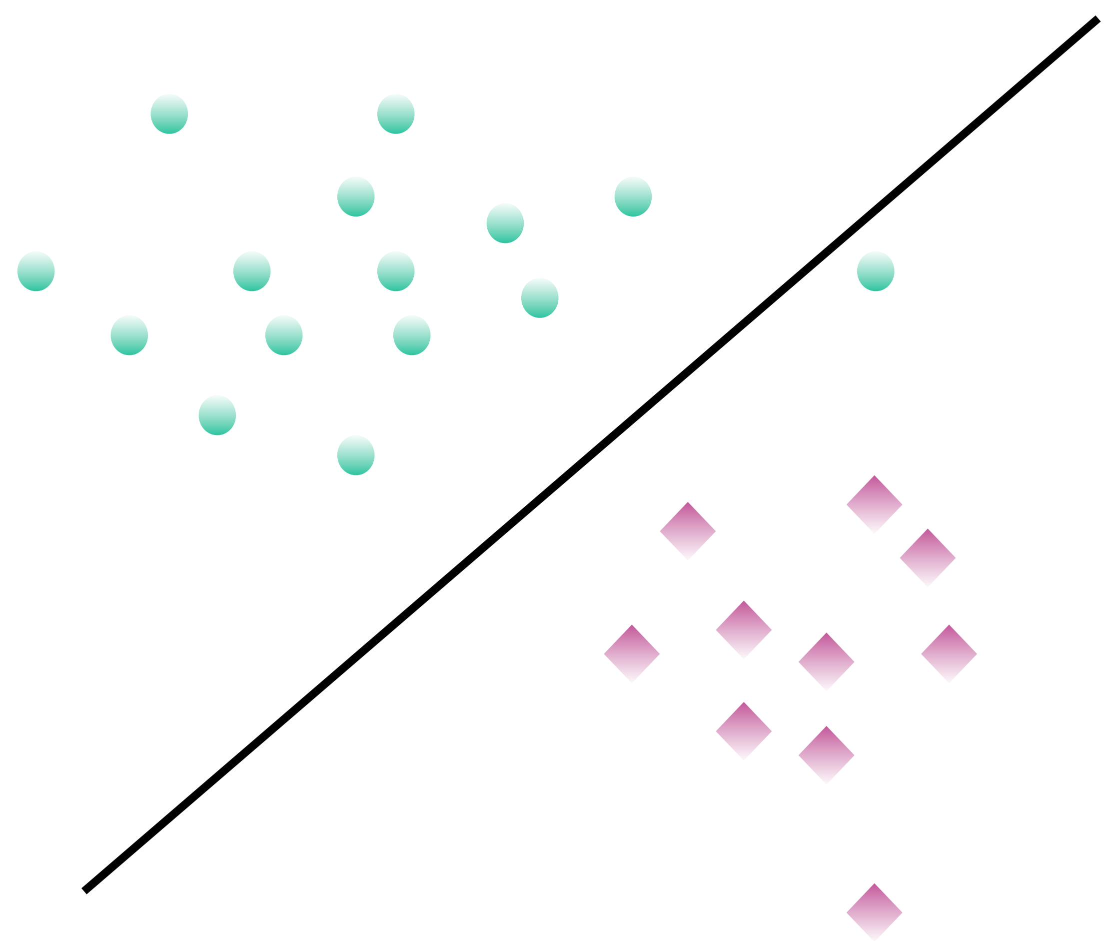
Support Vector Machines

Basic idea: find optimal separating hyperplane (then generalize to non-linear boundaries)



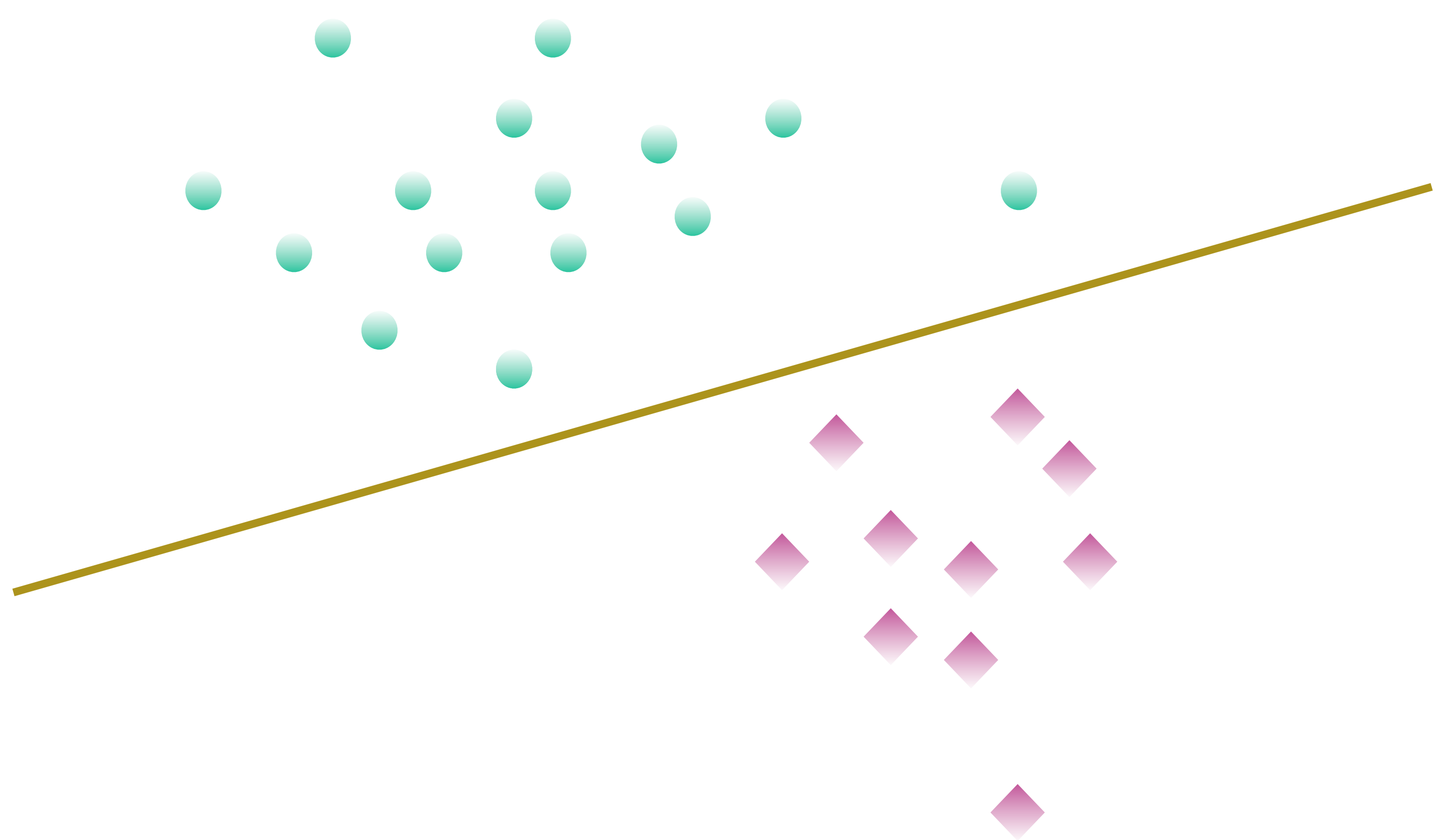
Support Vector Machines

Basic idea: find optimal separating hyperplane (then generalize to non-linear boundaries)



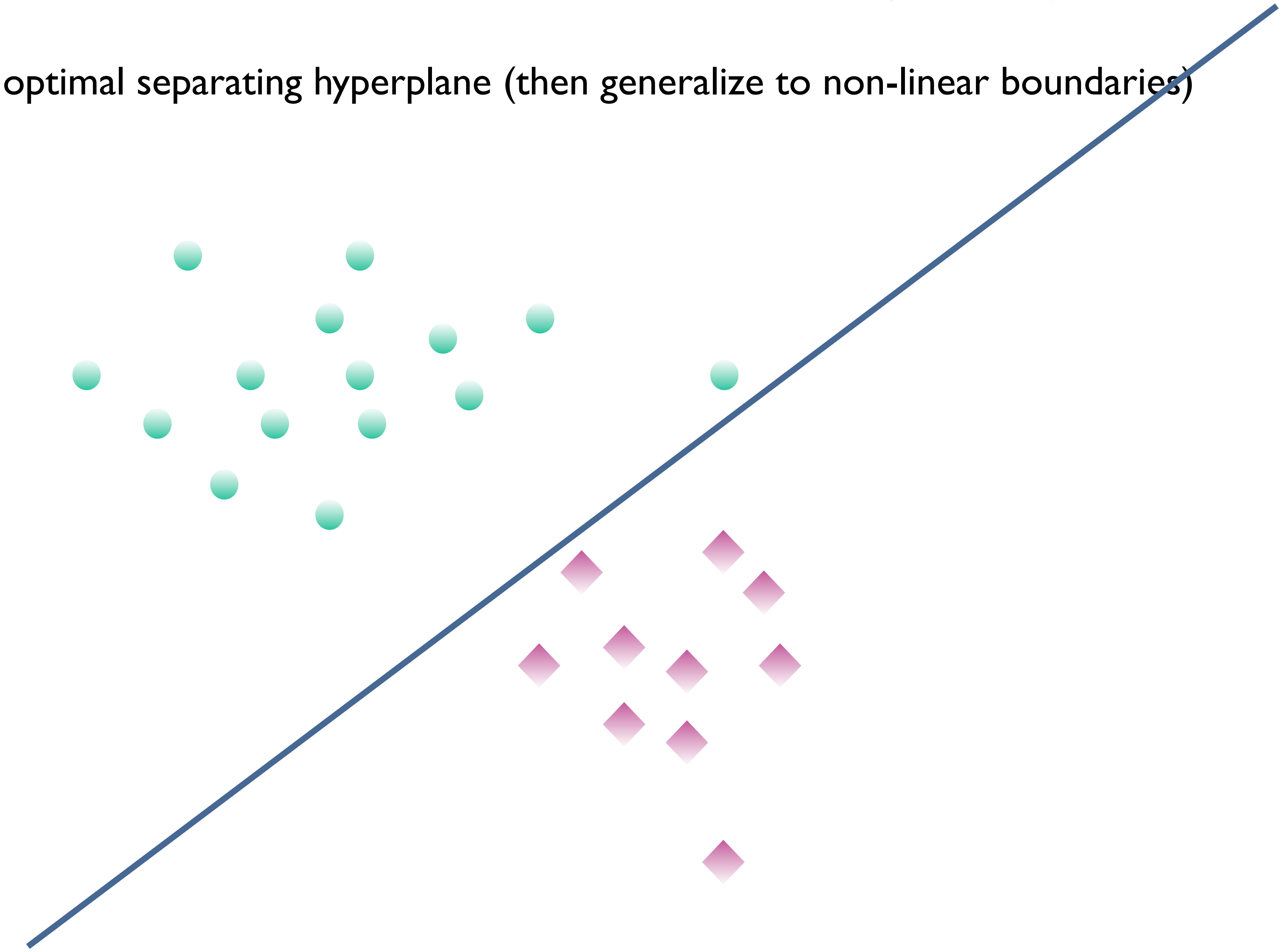
Support Vector Machines

Basic idea: find optimal separating hyperplane (then generalize to non-linear boundaries)



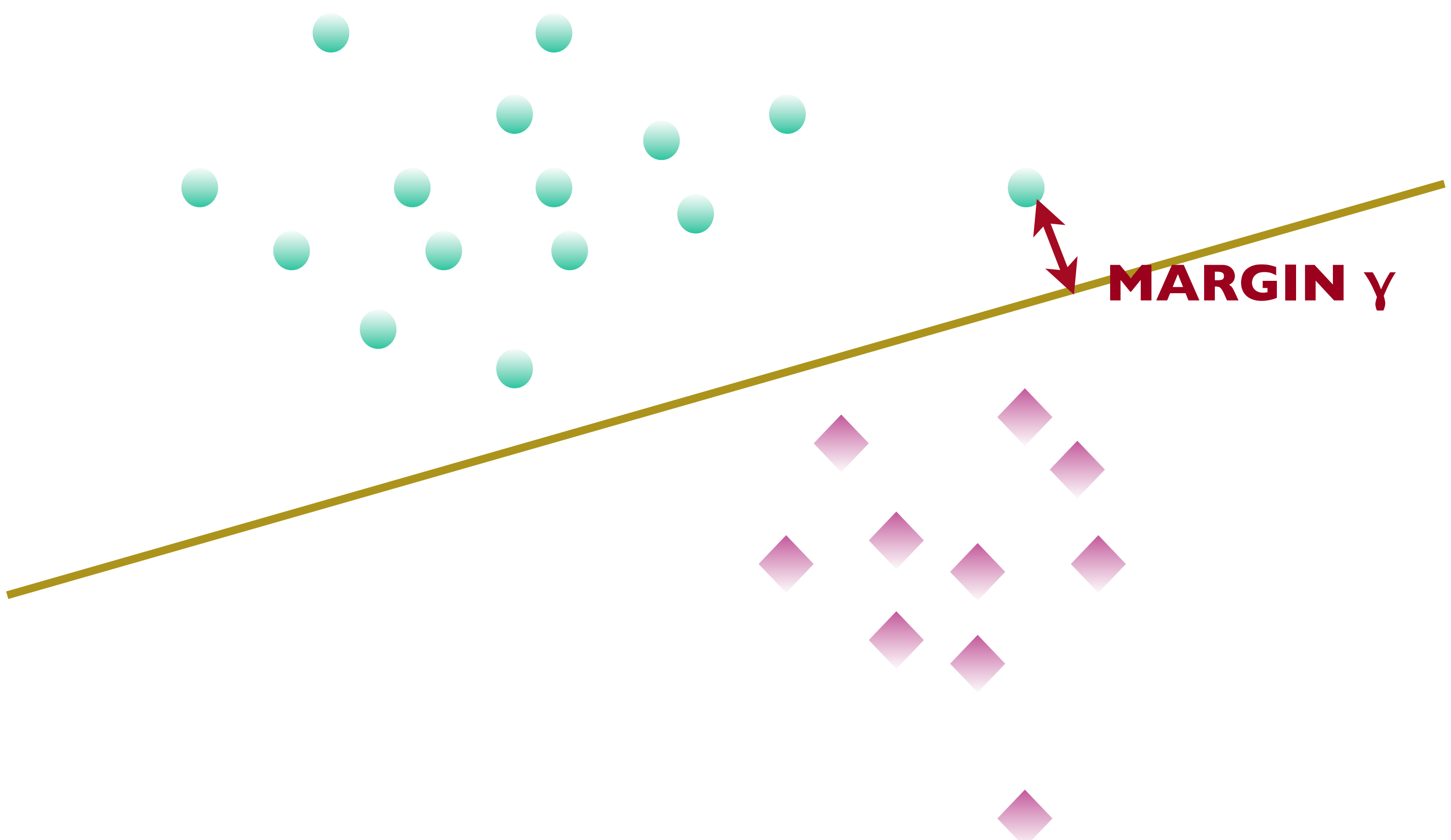
Support Vector Machines

Basic idea: find optimal separating hyperplane (then generalize to non-linear boundaries)



Support Vector Machines

Basic idea: find optimal separating hyperplane (then generalize to non-linear boundaries)



$$\gamma = \min_{i=1,\ldots,m} \gamma^{(i)}$$

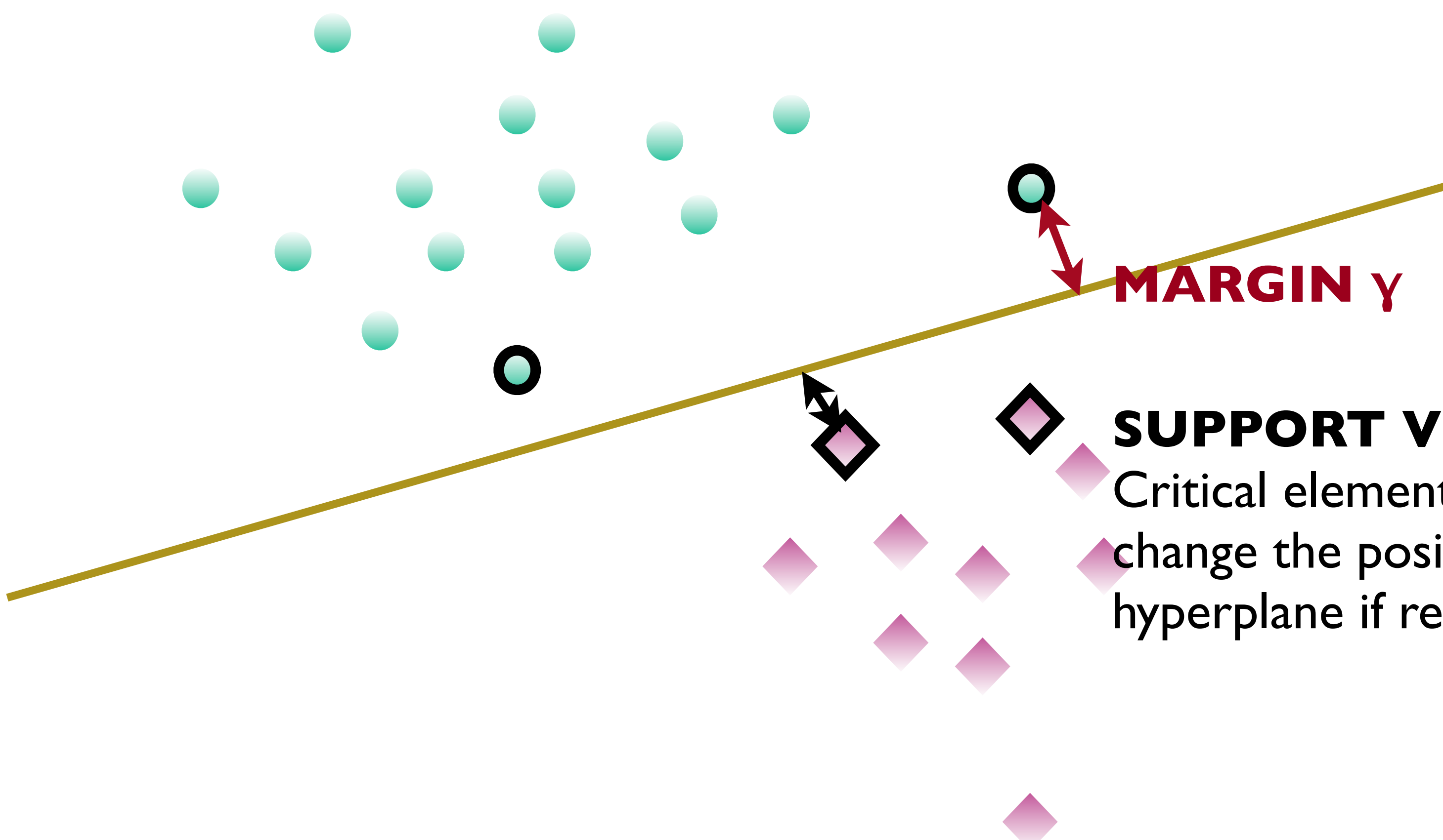
Intuitive formulation:

$$\begin{aligned} \max_{\gamma,w,b} \quad & \gamma \\ \text{s.t.} \quad & y^{(i)}(w^T x^{(i)} + b) \geq \gamma, \quad i = 1, \ldots, m \\ & ||w|| = 1. \end{aligned}$$

- Tough constraint to solve
- Far away points should not count

Support Vector Machines

Basic idea: find optimal separating hyperplane (then generalize to non-linear boundaries)



$$\gamma = \min_{i=1,\ldots,m} \gamma^{(i)}$$

SUPPORT VECTORS
Critical elements of the set, those that would change the position of the separating hyperplane if removed

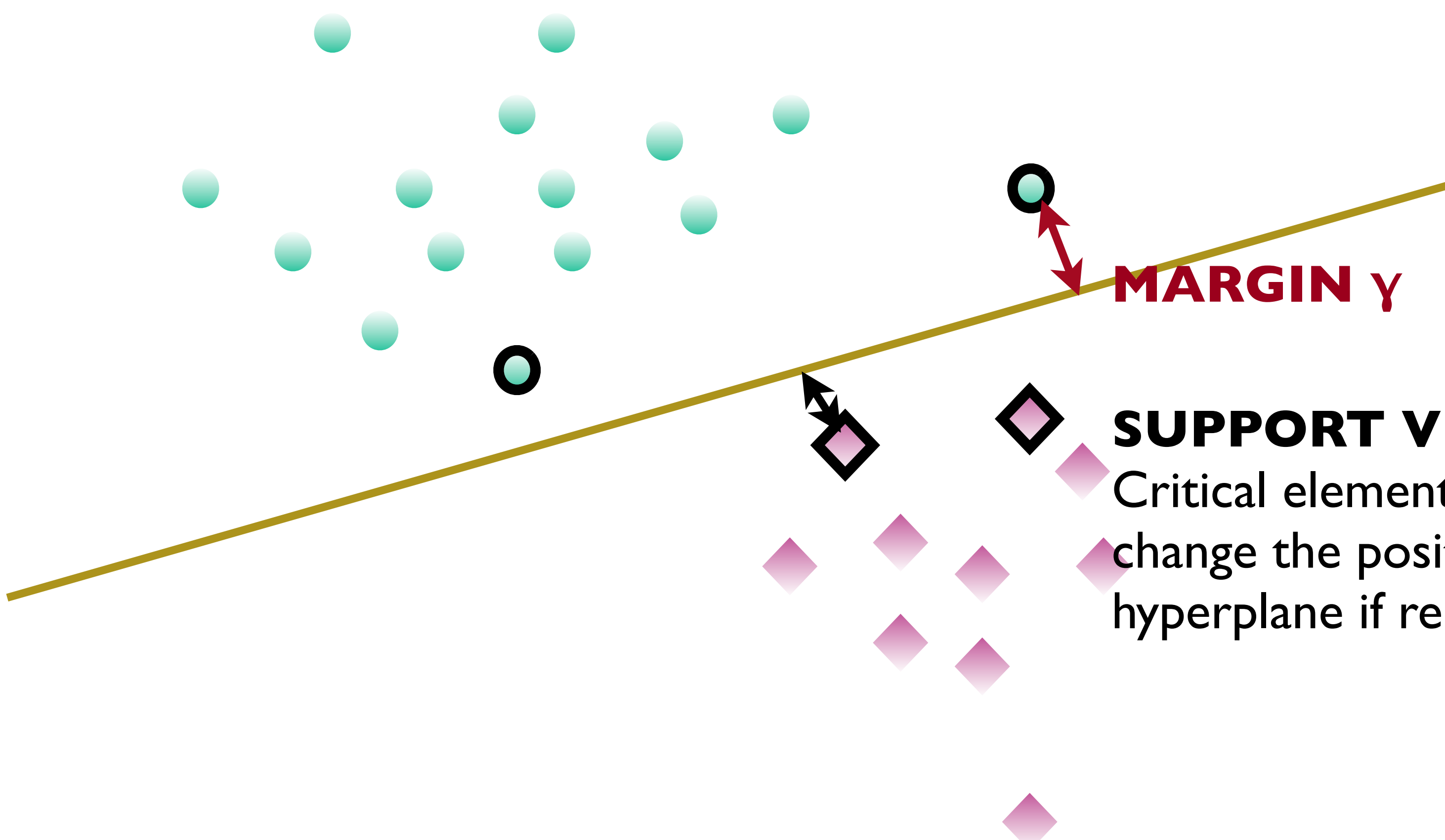
Less intuitive but optimal formulation:

$$\begin{aligned} \max_\alpha \quad & W(\alpha) = \sum_{i=1}^{m} \alpha_i - \frac{1}{2}\sum_{i,j=1}^{m} y^{(i)} y^{(j)} \alpha_i \alpha_j \langle x^{(i)}, x^{(j)} \rangle. \\ \text{s.t.} \quad & \alpha_i \geq 0, \quad i = 1, \ldots, m \\ & \sum_{i=1}^{m} \alpha_i y^{(i)} = 0, \end{aligned}$$

- Use Lagrange multipliers α
- Solve the **dual** problem, i.e. maximize over α subject to relations implied by the constraints for **w** and **b** instead of maximizing over **w** and **b** subject to the constraint involving α

Support Vector Machines

Basic idea: find optimal separating hyperplane (then generalize to non-linear boundaries)



MARGIN γ $\gamma = \min_{i=1,\ldots,m} \gamma^{(i)}$

SUPPORT VECTORS
Critical elements of the set, those that would change the position of the separating hyperplane if removed

Less intuitive but optimal formulation:

scalar product

$$\max_\alpha \quad W(\alpha) = \sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{m} y^{(i)} y^{(j)} \alpha_i \alpha_j \langle x^{(i)}, x^{(j)} \rangle.$$

$$\text{s.t.} \quad \alpha_i \geq 0, \quad i = 1, \ldots, m$$

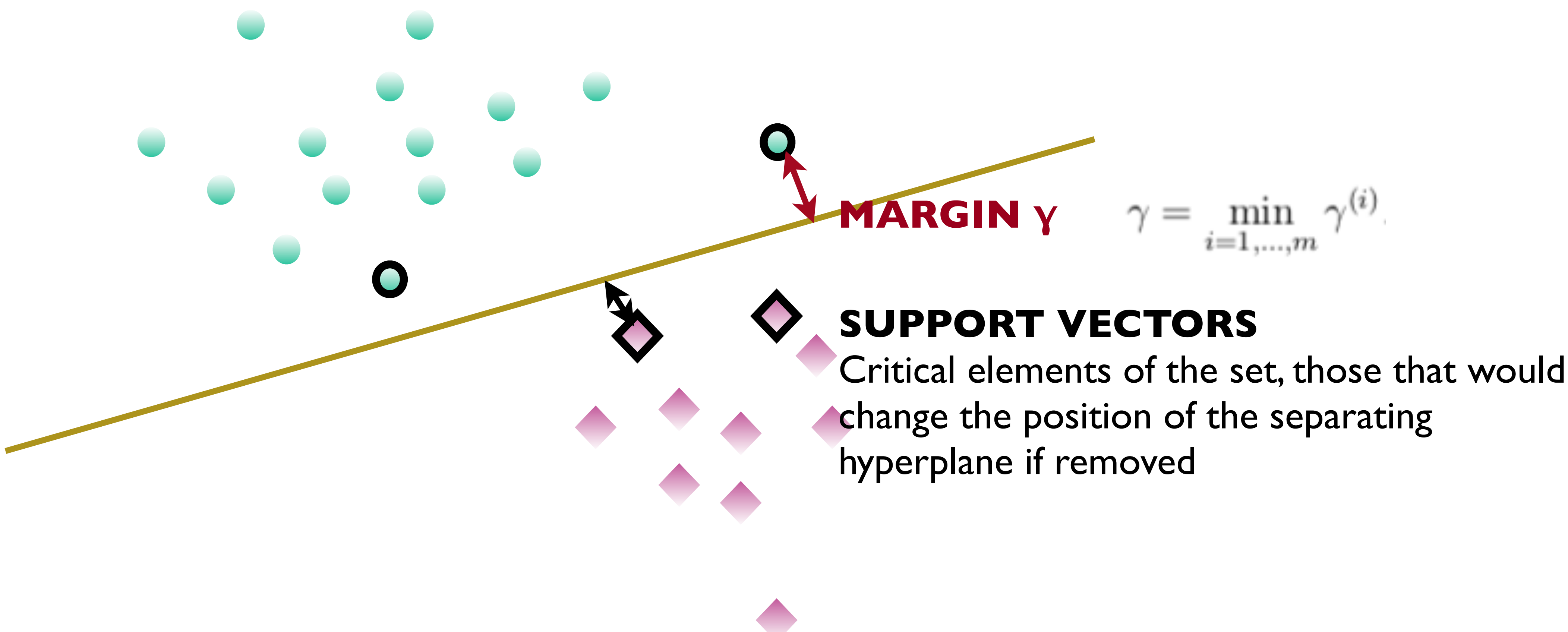
$$\sum_{i=1}^{m} \alpha_i y^{(i)} = 0,$$

Only true for SV !!

- Use Lagrange multipliers α
- Solve the **dual** problem, i.e. maximize over α subject to relations implied by the constraints for **w** and **b** instead of maximizing over **w** and **b** subject to the constraint involving α

Support Vector Machines

Basic idea: find optimal separating hyperplane (then generalize to non-linear boundaries)



Less intuitive but optimal formulation:

scalar product

$$\max_\alpha \quad W(\alpha) = \sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{m} y^{(i)} y^{(j)} \alpha_i \alpha_j \langle x^{(i)}, x^{(j)} \rangle.$$

$$\text{s.t.} \quad \alpha_i \geq 0, \quad i = 1, \dots, m$$

$$\sum_{i=1}^{m} \alpha_i y^{(i)} = 0,$$

Only true for SV !!

Non-linear boundaries

- Replace scalar product w. $\langle \phi(x), \phi(z) \rangle$ for any non-linear mapping
- Or directly define a KERNEL $K(x, z) = \phi(x)^T \phi(z)$

Support Vector Machines

Regularization:

$$\begin{aligned} \max_\alpha \quad & W(\alpha) = \sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{m} y^{(i)} y^{(j)} \alpha_i \alpha_j \langle x^{(i)}, x^{(j)} \rangle \\ \text{s.t.} \quad & 0 \le \alpha_i \le C, \quad i = 1, \ldots, m \\ & \sum_{i=1}^{m} \alpha_i y^{(i)} = 0, \end{aligned}$$

Advantages:

- ✦ Nicely generalizes to non-linear boundaries, versatile
- ✦ Good for higher-dimensional problems
- ✦ Quadratic optimization problem

Disadvantages:

- ✦ No probability estimates!
- ✦ Don’t forget normalization !

k-Nearest Neighbors

Basic idea: assign as label the most frequent label among the closest k point (k nearest neighbors) in the feature space

✦ Not a minimization problem/nonparametric : simply stores instances of training data
✦ Can tune k and distance

Algorithm 1 kNN

---

for $i = 1, .., N_{new}$ **do** Compute distance $d(X_i, x_{new})$
end for
Find set S of points with k smallest distances $d(X_i, x_{new})$, $i \in S$
return Majority label in S

Advantages:

✦ Simple but effective
✦ Can handle complex boundaries

Disadvantages:

✦ No probability estimates!
✦ Don't forget normalization !
✦ O(N^2) if you don't use smart algorithms