COMP 432 Machine Learning

Multiclass Classification

Computer Science & Software Engineering
Concordia University, Fall 2021

Multiclass Classification

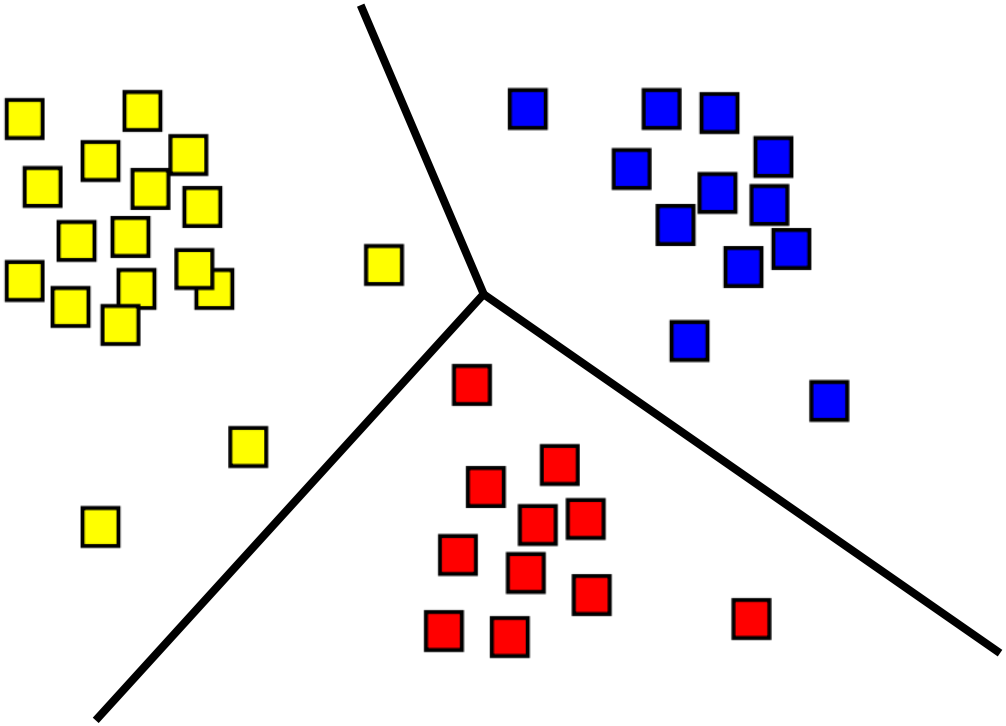
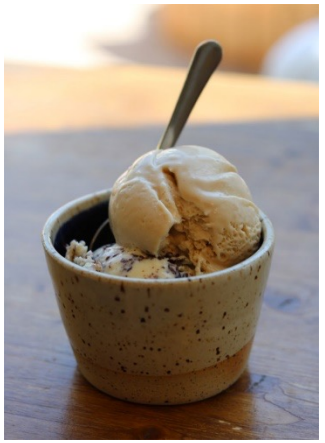


Image source: Wikipedia

Multiclass vs Multilabel vs Tagging

- **Multi-class** *classification:* given $\mathbf{x}$ predict one unique class (one "class label") out of *K* classes
- **Multilabel** classification: given $\mathbf{x}$ predict the subset of *K* labels that should be associated
  - Essentially multiple-output binary classification
  - Terminology ambiguous with "labeling problems" which are essentially classification (assign one "label" to $\mathbf{x}$)
- **Tagging**: multi-*label* classification, usually of images:



tags:
"ice cream"
"dessert"
"bowl"
"table"
"cold"
...

Multiclass SVM strategies

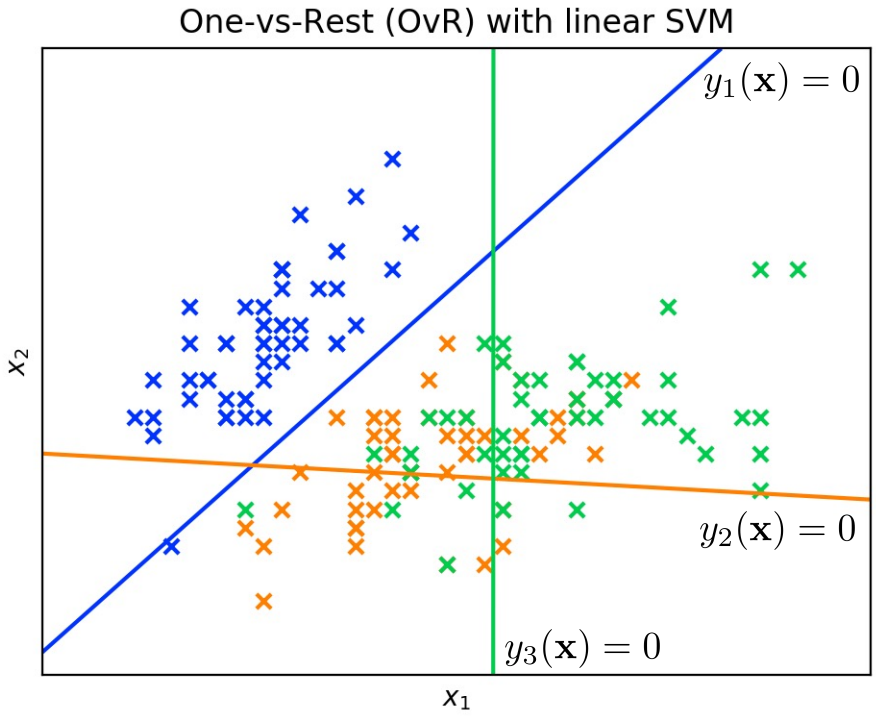
- For binary classification, the *maximum margin* principle is elegant to formulate and to solve.
- For multiclass classification, the notion of "*maximum margin*" is harder to formulate.
- Can we reuse nice 2-class formulations for *K*-class?
  - **One-vs-Rest:** for each class *k*, train an SVM that is an expert at classifying *k* (one) versus non-*k (the rest).*
  - **One-vs-One:** for each pair of classes (*k, k')*, train an SVM that is an expert at classifying *k* versus *k'.*
  - In either case, make multiclass prediction by combining individual binary predictions.

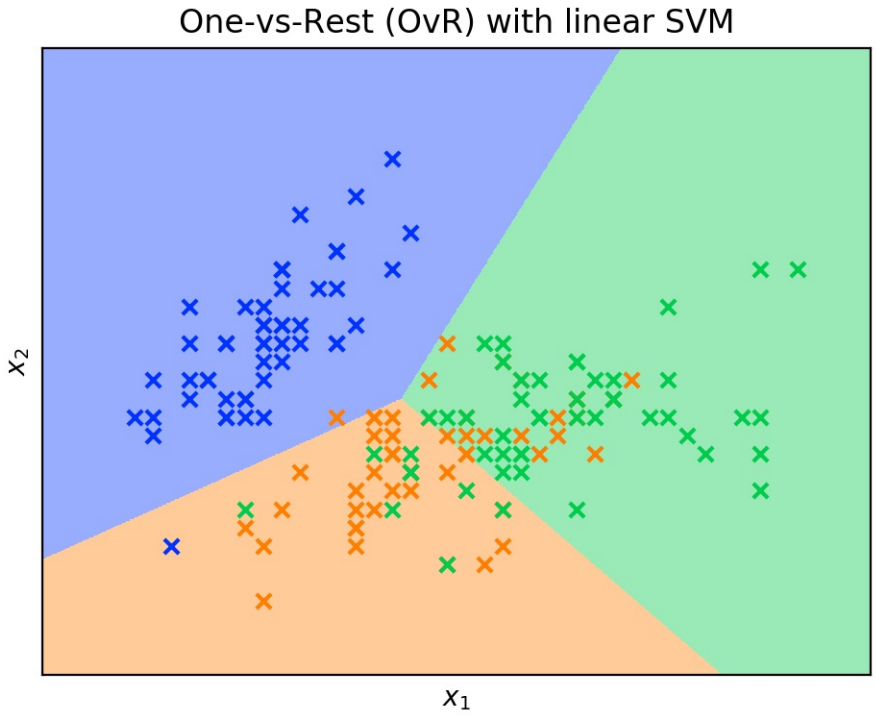
quadratic program!

One-vs-Rest (OvR)

- For each class *k*, train an SVM that is an expert at classifying *k* (one) versus non-*k (the rest).*
- Predict class of $\mathbf{x}$ by choosing class *k* with highest decision function value $k^* = \underset{k=1,\ldots,K}{\arg\max}\ y_k(\mathbf{x})$

decision function of k^{th} binary SVM





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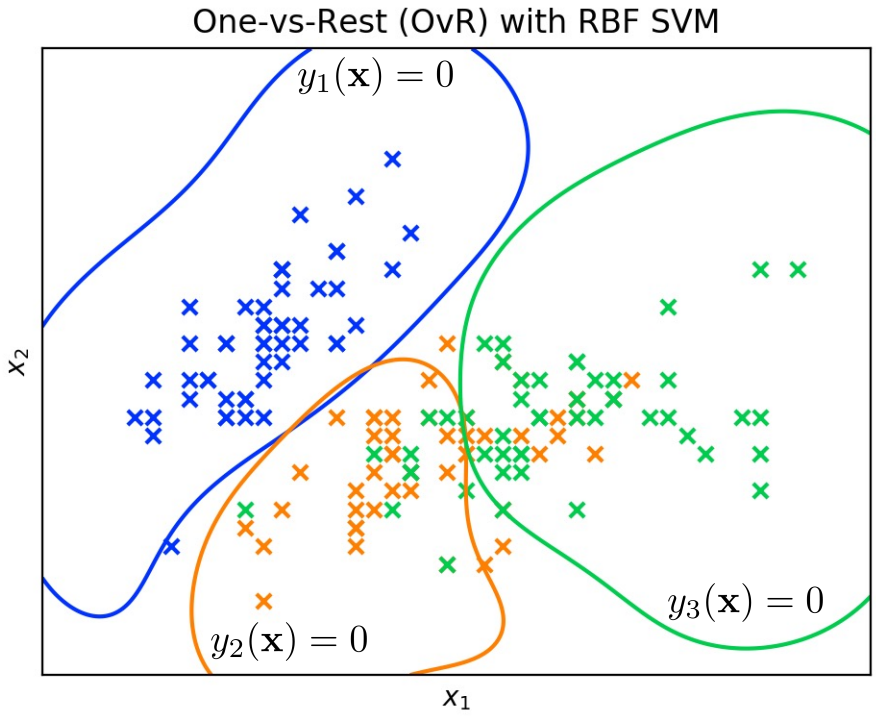
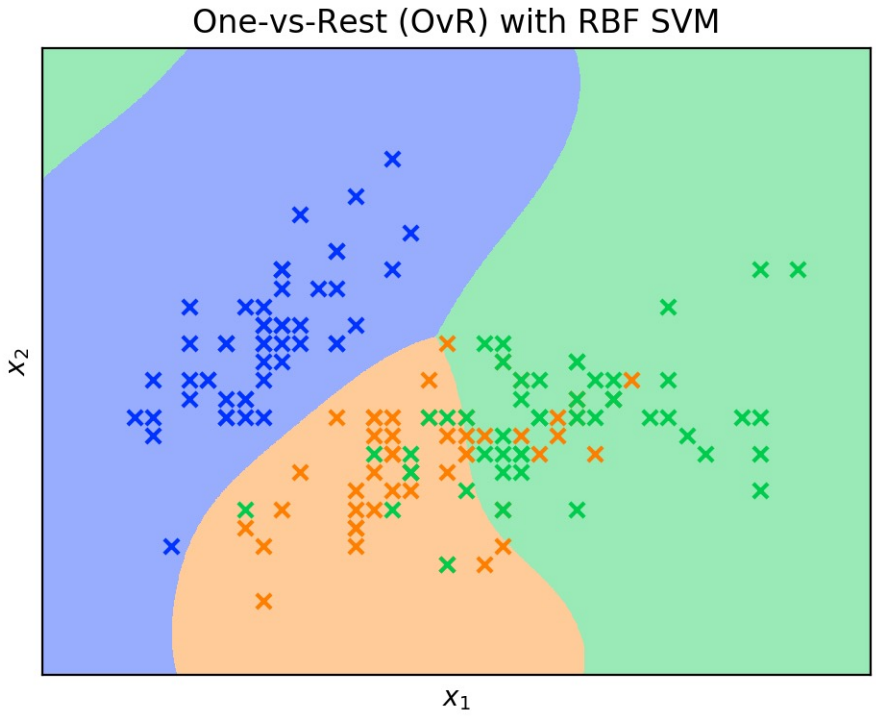
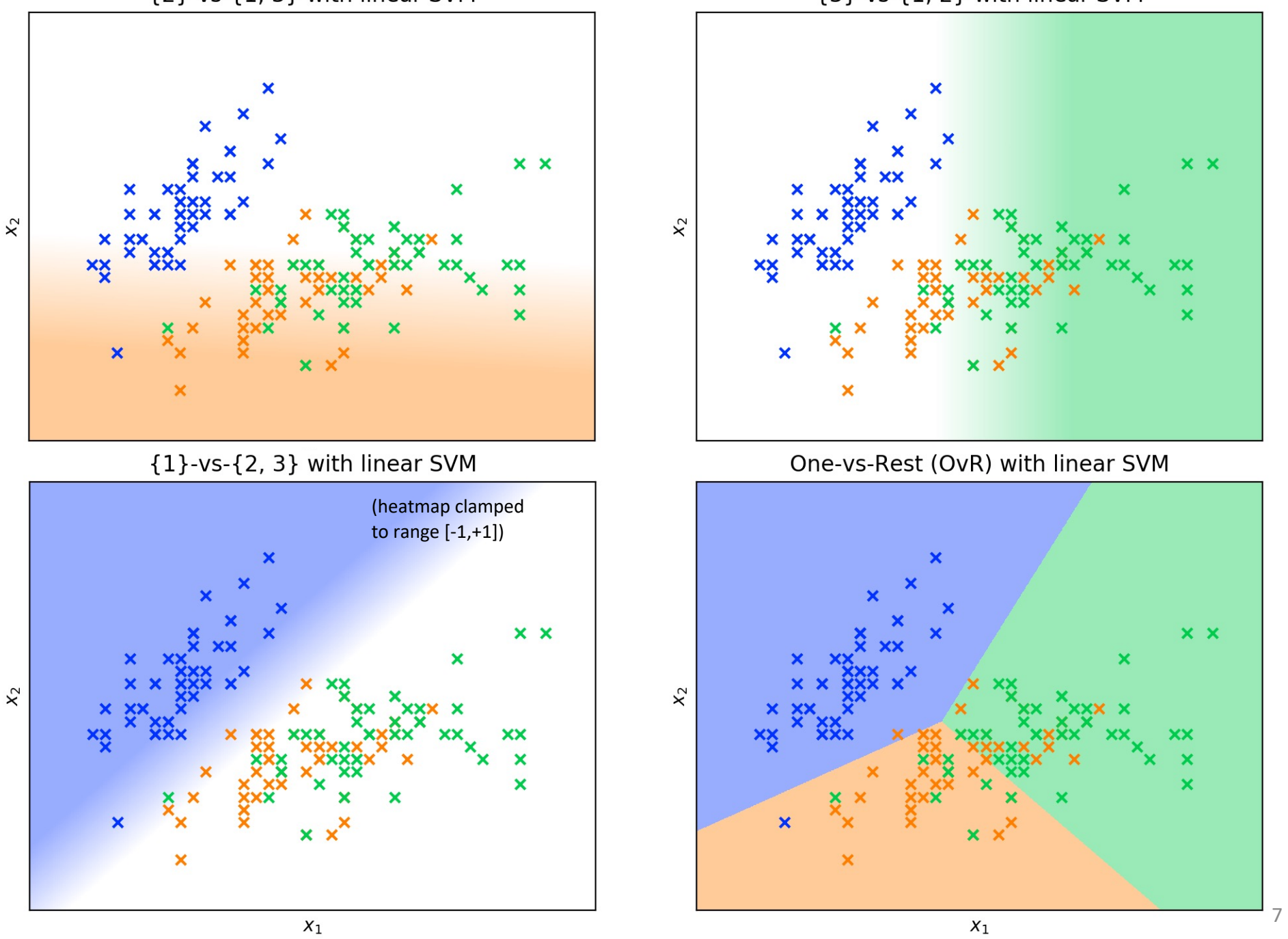
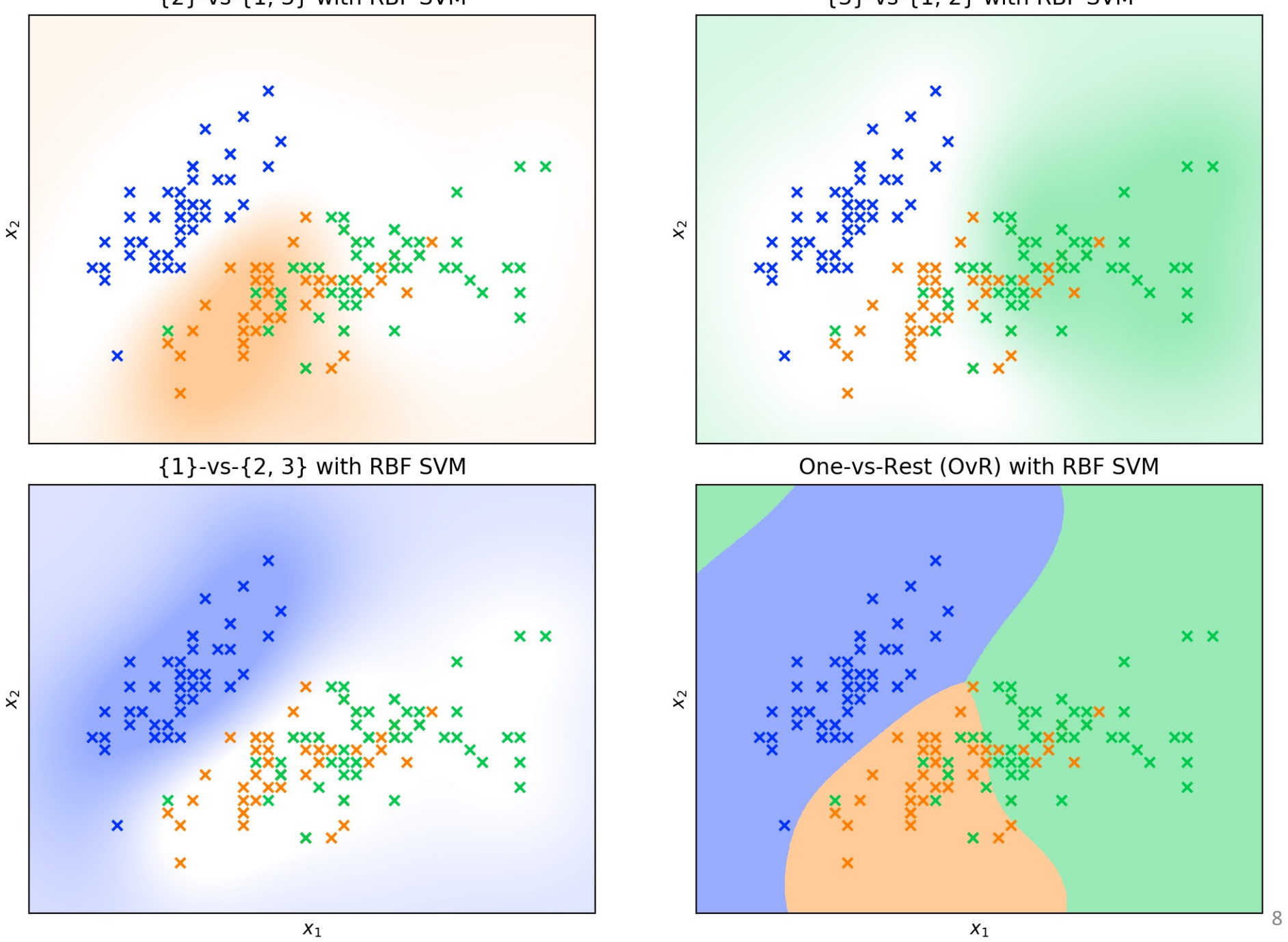


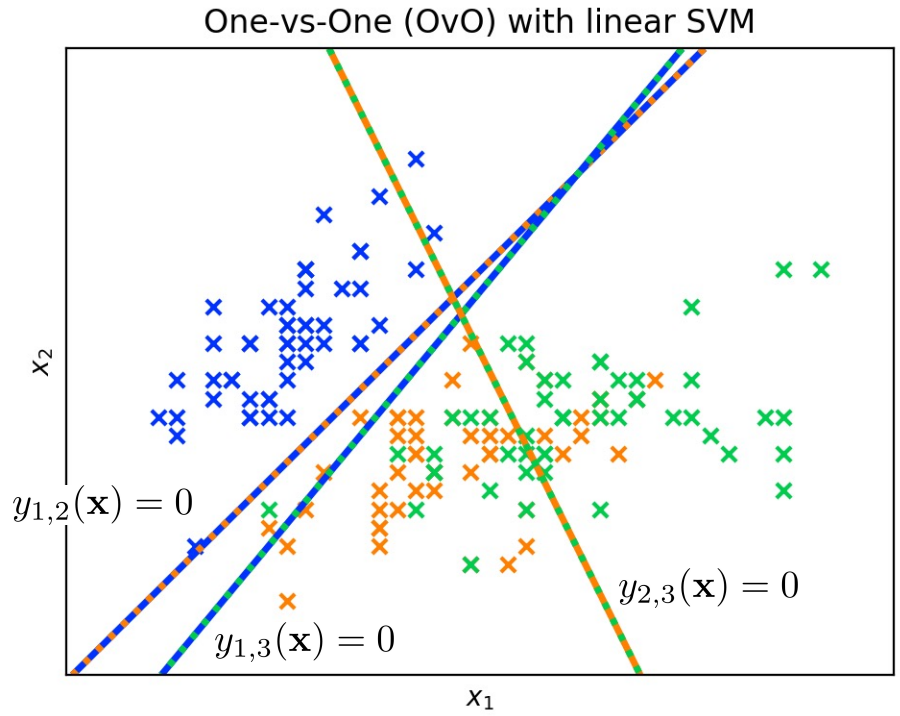


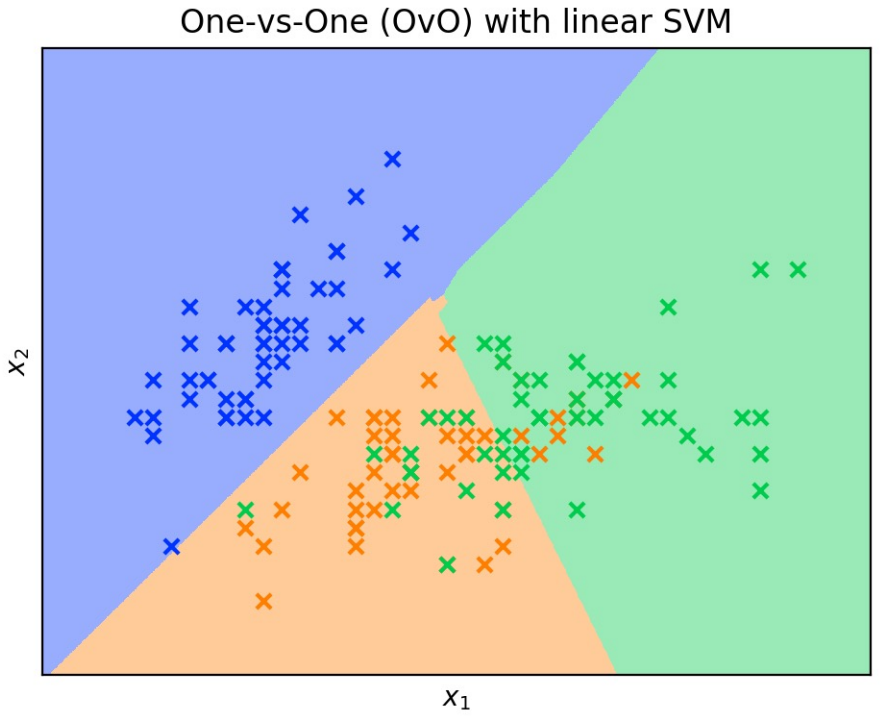

{2}-vs-{1, 3} with linear SVM
{3}-vs-{1, 2} with linear SVM
{1}-vs-{2, 3} with linear SVM
(heatmap clamped
to range [-1,+1])
One-vs-Rest (OvR) with linear SVM
x_1
x_2


{2}-vs-{1, 3} with RBF SVM
{3}-vs-{1, 2} with RBF SVM
{1}-vs-{2, 3} with RBF SVM
One-vs-Rest (OvR) with RBF SVM
x_1
x_2

One-vs-One (OvO)

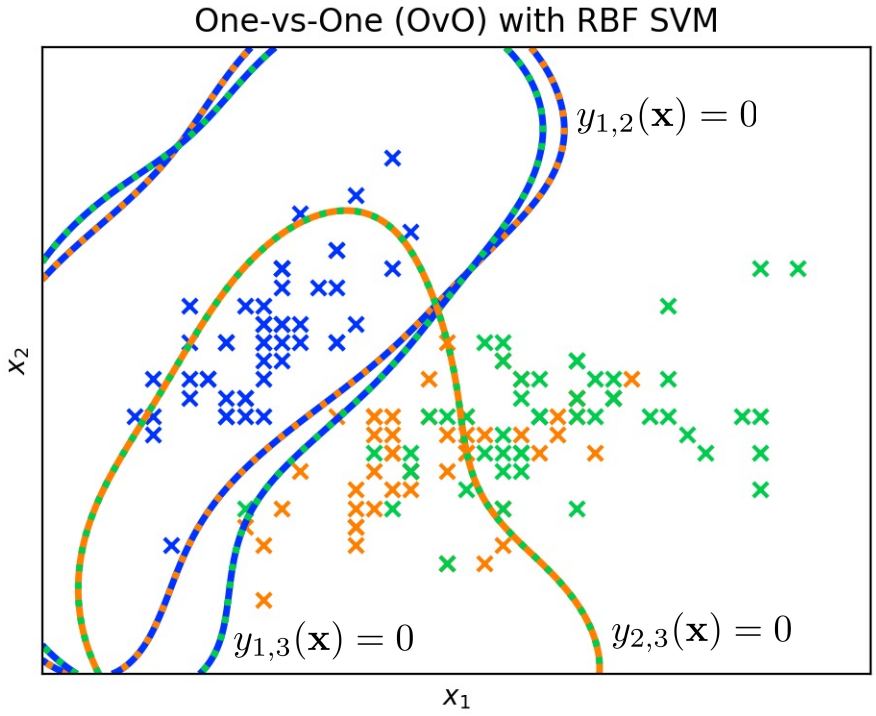
- For each pair of classes (*k, k'*), train an SVM that is classifies *k* versus *k'*. A total of $K(K-1)/2$ classifiers.
- Predict class of $\mathbf{x}$ by choosing *k* with highest number of "votes" where $y_{k,k'}(\mathbf{x}) > 0$ over all *k' != k*.

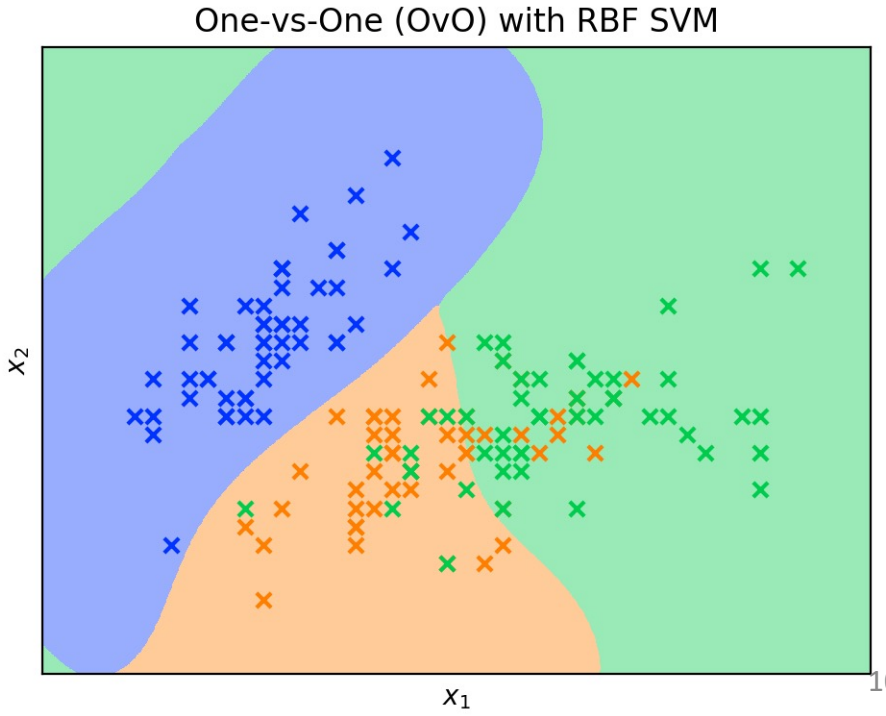


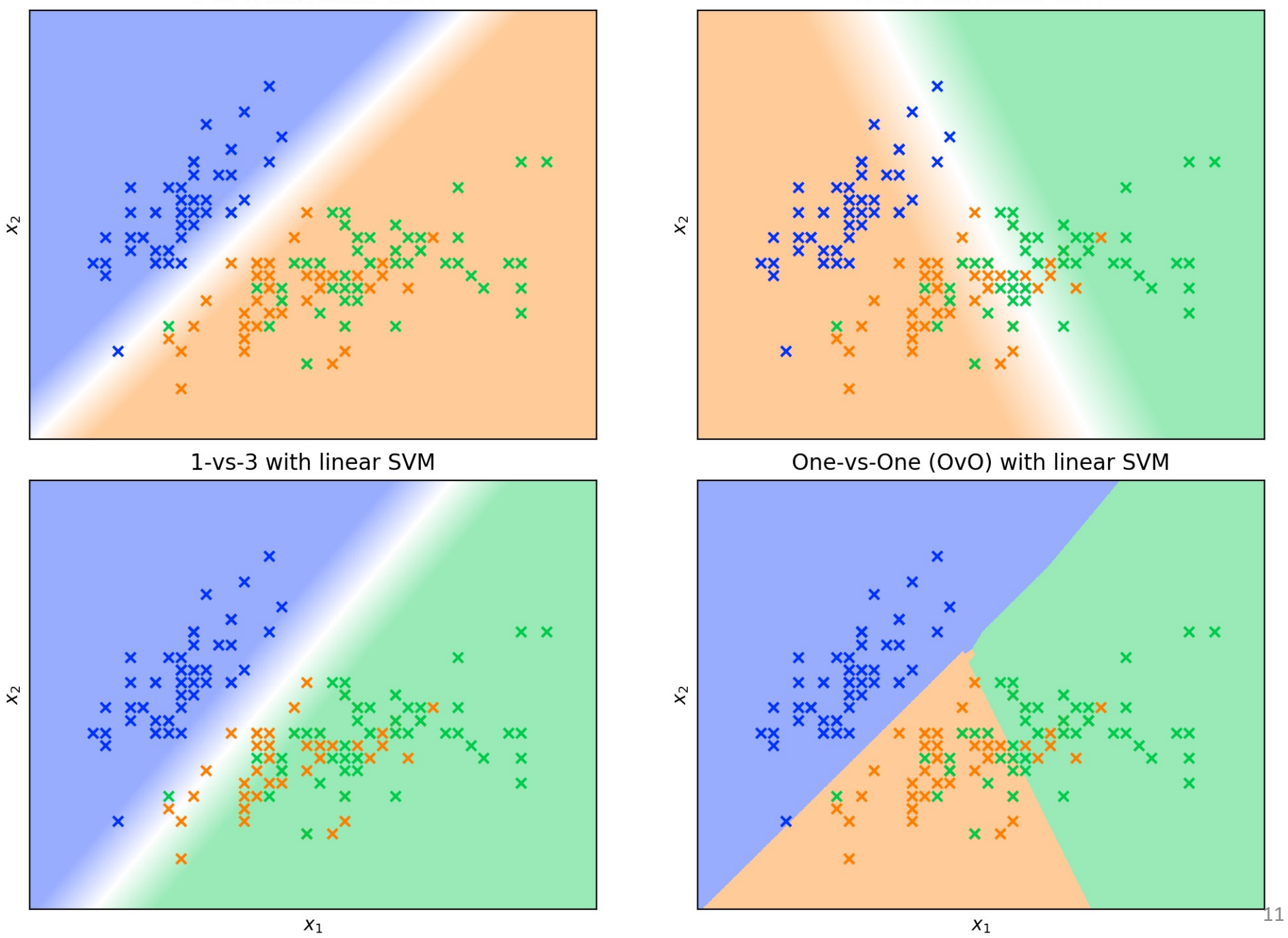


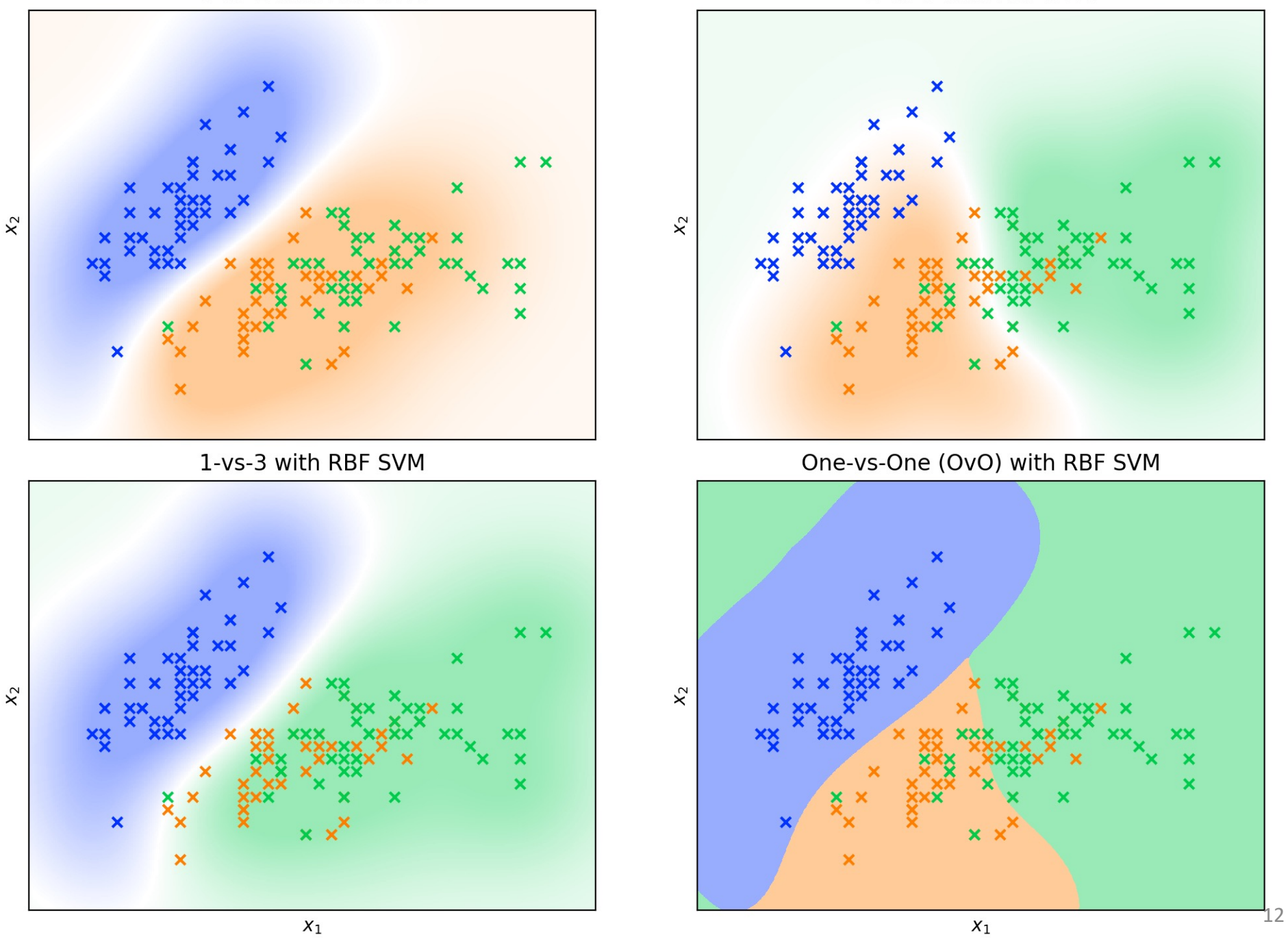
One-vs-One (OvO)

- For each pair of classes (*k, k'*), train an SVM that is classifies *k* versus *k'*. A total of $K(K-1)/2$ classifiers.
- Predict class of $\mathbf{x}$ by choosing *k* with highest number of "votes" where $y_{k,k'}(\mathbf{x}) > 0$ over all *k'*.






1-vs-2 with linear SVM
2-vs-3 with linear SVM
1-vs-3 with linear SVM
One-vs-One (OvO) with linear SVM
x_1
x_2


1-vs-2 with RBF SVM
2-vs-3 with RBF SVM
1-vs-3 with RBF SVM
One-vs-One (OvO) with RBF SVM
x_1
x_2

1.12. Multiclass and multilabel algorithms

Warning: All classifiers in scikit-learn do multiclass classification out-of-the-box. You don't need to use the `sklearn.multiclass` module unless you want to experiment with different multiclass strategies.

1.12.2.1. Multiclass learning

Below is an example of multiclass learning using OvR:

```
>>> from sklearn import datasets
>>> from sklearn.multiclass import OneVsRestClassifier
>>> from sklearn.svm import LinearSVC
>>> iris = datasets.load_iris()
>>> X, y = iris.data, iris.target
>>> OneVsRestClassifier(LinearSVC(random_state=0)).fit(X, y).predict(X)
array([0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
       0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
       0, 0, 0, 0, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1,
       1, 2, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 2, 2, 1, 1, 1, 1, 1,
       1, 1, 1, 1, 1, 1, 1, 1, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2,
       2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 1, 2, 2, 2, 1, 2, 2,
       2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2])
```

https://scikit-learn.org/stable/modules/multiclass.html#one-vs-the-rest

Problems with these approaches

- Scale of SVM decision function $y(\mathbf{x})$ is arbitrary
  - Strictly speaking they are *not comparable* values
  - But we compare anyway *as a heuristic*; often works
- Can be slow to train
  - One-vs-Rest trains *K* SVMs, each on *full* dataset
  - One-vs-One trains $O(K^2)$ SVMs, each on *fraction* of data
- One-vs-Rest SVMs trained on imbalanced data
  - Data for the "rest" is all *K*-1 classes; more data than class *k.*

Other approaches to multiclass?

What about Logistic Regression?

- Logistic regression has similar decision function $y(\mathbf{x})$, but different training principle
  - *maximum likelihood* not "maximum margin"
- Logistic regression's decision function can also be thresholded (e.g. at zero) to give binary classifier
  - So, could try using OvR and OvO to logistic regression
- **However, logistic regression turns out to have a *natural multiclass maximum-likelihood formulation*!** 
- We'll build to multiclass logistic regression in 3 steps:
  1. Extend linear regression to multiple outputs
  2. Extend logistic regression to multiple outputs (trivial)
  3. Normalize those outputs with **softmax** function

Multi-output Linear Regression

Given supervised training set with multiple outputs $\mathcal{D} = \{(\mathbf{x}_1, \mathbf{y}_1), \ldots, (\mathbf{x}_N, \mathbf{y}_N)\}$ where data has form

$$\mathbf{x} = \begin{bmatrix} 1 & x_1 & x_2 & \cdots & x_D \end{bmatrix}^T \quad (D+1)\text{-dimensional inputs}$$

$$\mathbf{y} = \begin{bmatrix} y_1 & y_2 & \cdots & y_K \end{bmatrix}^T \quad K\text{-dimensional outputs}$$

We can define a multivariate model as $\hat{\mathbf{y}}(\mathbf{x}, \mathbf{W}) = \mathbf{W}\mathbf{x}$ where

$$\underset{K \times (D+1)}{\mathbf{W}} = \begin{bmatrix} w_{1,0} & w_{1,1} & \cdots & w_{1,D} \\ w_{2,0} & w_{2,1} & \cdots & w_{2,D} \\ \vdots & \vdots & \ddots & \vdots \\ w_{K,0} & w_{K,1} & \cdots & w_{K,D} \end{bmatrix}$$

Row k is a parameter vector $\mathbf{w}_k = \begin{bmatrix} w_{k,0} & w_{k,1} & \cdots & w_{k,D} \end{bmatrix}^T$ of a single independent linear model, where row i determines output y_i

$$\hat{y}_{ik} \equiv \hat{y}_k(\mathbf{x}_i, \mathbf{w}_k)$$

And can of course define a loss $\ell(\mathbf{W}) = \frac{1}{2} \sum_{i=1}^{N} \sum_{k=1}^{K} (y_{ik} - \hat{y}_{ik})^2$

Multi-output Logistic Regression

Just slap an element-wise sigmoid onto the output!

$$\hat{\mathbf{y}}(\mathbf{x}, \mathbf{W}) = \sigma\left(\mathbf{W}\mathbf{x}\right)$$

Since this is just regressing multiple standard logistic models, one per output, can define multivariate logistic regression loss in terms of NLL as before:

$$\ell(\mathbf{W}) = -\ln p(\mathbf{Y} \mid \mathbf{X}, \mathbf{W})$$ (negative log likelihood)

$$\hat{y}_{ik} \equiv \hat{y}_k(\mathbf{x}_i, \mathbf{w}_k)$$

$$= -\sum_{i=1}^{N}\sum_{k=1}^{K} y_{ik} \ln \hat{y}_{ik} + (1 - y_{ik}) \ln(1 - \hat{y}_{ik})$$

thereby maximizing the likelihood of all training targets $\mathbf{Y} = \begin{bmatrix} \mathbf{y}_1^T \\ \mathbf{y}_2^T \\ \vdots \\ \mathbf{y}_N^T \end{bmatrix}$

Using $\hat{y}_{ik}$ for multi*label* is trivial, but is this multi*class*?

Toward regression for multiclass

A regression formulation for multi*class* must involve *competition* between class labels, *i.e.* one class must ultimately "win out" among all the possible labels.

Example: $\mathbf{y} = \begin{bmatrix} \texttt{car} & \texttt{dog} & \texttt{cat} & \texttt{bike} \\ 1.0 & 0.0 & 0.0 & 0.0 \end{bmatrix}^T$ (training target, 1-of-*K*)

$\hat{\mathbf{y}} = \begin{bmatrix} 0.9 & 0.0 & 0.3 & 0.8 \end{bmatrix}^T$ (*K* independent predictions)

How to predict one class from *K* independent class probabilities?

Just select the class label with maximum probability?

$$\hat{\mathbf{y}}(\mathbf{x}, \mathbf{W}) = \text{hardmax}\left(\sigma(\mathbf{W}\mathbf{x})\right)$$

where $\text{hardmax}\left(\begin{bmatrix} 0.9 \\ 0.0 \\ 0.3 \\ 0.8 \end{bmatrix}\right) = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}$

Works "OK," but not quite ideal:

1. Forces other classes to predict "zero" despite already "losing"
2. Not differentiable, so problematic for gradient-based training

Toward regression for multiclass

Key: For classification, the actual probabilities of $\mathbf{x}$ belonging each class *cannot* be predicted independently. Must satisfy:

$$\sum_{k=1}^{K} p(y_k = 1 \mid \mathbf{x}, \mathbf{W}) = 1$$

If our confidence in $p(y_k = 1 \mid \mathbf{x}, \mathbf{W})$ goes up, then our confidence in $p(y_{k'} = 1 \mid \mathbf{x}, \mathbf{W})$ should automatically go down for one or more $k' \neq k$.

Idea: Rather than predict K independent binary class probabilities $\hat{y}_k = p(y_k = 1 \mid \mathbf{x}, \mathbf{w}_k)$, predict a **joint** probability $\hat{\mathbf{y}} = p(\mathbf{y} \mid \mathbf{x}, \mathbf{W})$ over class membership, where the model itself ensures $\hat{y}_k \geq 0$, $\sum_{k=1}^{K} \hat{y}_k = 1$.

Multinomial Logistic Regression

Multi-output logistic regression (labeling) outputs the probabilities of *K* independent ***binomial*** variables (flip of a 2-sided coin) so model each $p(y = 1 \mid \mathbf{x}, \mathbf{w}_k)$ using a separate logistic model $\mathbf{w}_k$.

We *want* a model that outputs the probability of a single 1-of-*K* outcome (roll of "*K*-sided dice"), which corresponds to ***multinomial*** random variable over values *K* possible outcomes, so model $p(y = k \mid \mathbf{x}, \mathbf{W})$ using a single model with normalized output. We output a vector $\hat{\mathbf{y}}$ of probabilities $\hat{y}_k = p(y = k \mid \mathbf{x}, \mathbf{W})$

Softmax function

Inputs called 'activations' (have *nothing* to do with SVM dual variables $\boldsymbol{\alpha}$)

$$\text{softmax}(\mathbf{a}) = \frac{\exp(\mathbf{a})}{\sum_{j=1}^{K} \exp(a_j)}$$

Intuition: Amplify the largest value(s) in vector $\mathbf{a}$, then normalize to ensure $\sum_{k=1}^{K} \text{softmax}(\mathbf{a})_k = 1$

$$\lim_{\gamma \to \infty} \text{softmax}(\gamma \mathbf{a}) = \text{hardmax}(\mathbf{a})$$

Example:

$$\text{softmax}\left(\begin{bmatrix} -2 \\ 2 \end{bmatrix}\right) = \begin{bmatrix} 0.018 \\ 0.982 \end{bmatrix}$$

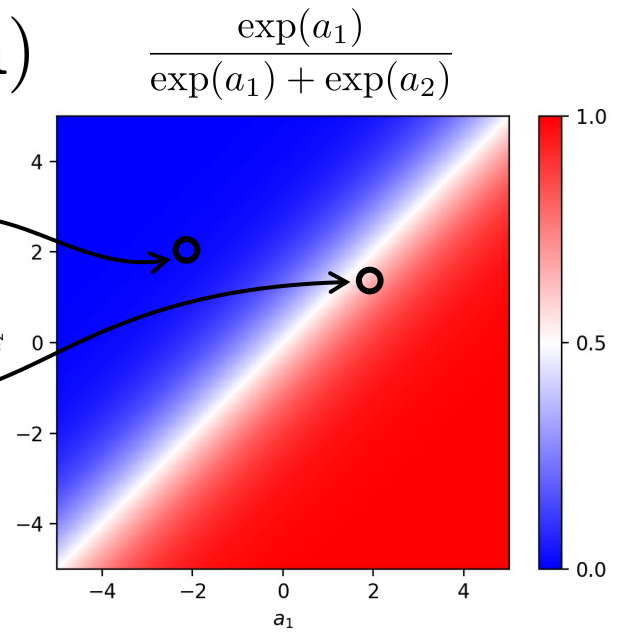
$$\text{softmax}\left(\begin{bmatrix} 2 \\ \frac{3}{2} \end{bmatrix}\right) = \begin{bmatrix} 0.622 \\ 0.378 \end{bmatrix}$$

$$\text{softmax}\left(\begin{bmatrix} 20 \\ 15 \end{bmatrix}\right) = \begin{bmatrix} 0.993 \\ 0.007 \end{bmatrix}$$

Notice connection to logistic sigmoid...

$$\sigma(2 - \tfrac{3}{2}) = 0.622$$

$$\sigma(20 - 15) = 0.993$$



Softmax vs Logistic Sigmoid

Consider 2-class softmax of linear function

$$\begin{bmatrix}\hat{y}_1\\ \hat{y}_2\end{bmatrix} = \text{softmax}\left(\begin{bmatrix}a_1\\ a_2\end{bmatrix}\right) = \frac{1}{e^{a_1}+e^{a_2}}\begin{bmatrix}e^{a_1}\\ e^{a_2}\end{bmatrix}$$

Focus on just $\hat{y}_1$: $\hat{y}_1 = \dfrac{e^{a_1}}{e^{a_1}+e^{a_2}} = \dfrac{1}{1+e^{a_2-a_1}}$

Assume softmax inputs are linear function $\mathbf{a} = \mathbf{W}\mathbf{x}$ $\mathbf{W} = \begin{bmatrix}\mathbf{w}_1^T\\ \mathbf{w}_2^T\end{bmatrix}$

$$\hat{y}_1 = \frac{1}{1+e^{(\mathbf{w}_2^T-\mathbf{w}_1^T)\mathbf{x}}} = \sigma(\mathbf{w}^T\mathbf{x}) \text{ where we let } \mathbf{w} = \mathbf{w}_1 - \mathbf{w}_2$$

Similarly $\hat{y}_2 = 1 - \hat{y}_1$, so 2-class softmax regression is just over-parameterized logistic regression!

(this is "Softmax regression")

Multinomial Logistic Regression

Prediction: $\hat{\mathbf{y}}(\mathbf{x}, \mathbf{W}) = \mathrm{softmax}(\mathbf{W}\mathbf{x})$ $\quad \mathbf{W} = \begin{bmatrix} \mathbf{w}_1^T \\ \vdots \\ \mathbf{w}_K^T \end{bmatrix}$

In other words, each component $\hat{y}_k$ of the output (the predicted class probabilities) depends on *all K* linear decision functions fed into the softmax.

Directly models *class probabilities* $\hat{y}_k = p(y = k \mid \mathbf{x}, \mathbf{W})$

Likelihood: $p(\mathbf{Y} \mid \mathbf{X}, \mathbf{W}) = \prod_{i=1}^{N} \prod_{k=1}^{K} \hat{y}_{ik}^{y_{ik}}$ $\quad \mathbf{Y} = \begin{bmatrix} \mathbf{y}_1^T \\ \vdots \\ \mathbf{y}_N^T \end{bmatrix}$

"Only the one $\hat{y}_{ik}$ for which $y_{ik} = 1$ matters in this product.
Maximizing likelihood means increase the $\hat{y}_{ik}$ of the 'correct' class.

$\hat{y}_{ik} \equiv \hat{y}_k(\mathbf{x}_i, \mathbf{W})$

("Softmax regression")

Multinomial Logistic Regression

Negative log likelihood for multinomial LR:

$$\ell(\mathbf{W}) = -\ln p(\mathbf{Y} \mid \mathbf{X}, \mathbf{W}) = -\sum_{i=1}^{N}\sum_{k=1}^{K} y_{ik} \ln \hat{y}_{ik}$$

`sklearn.linear_model`.LogisticRegression

multi_class : *{'auto', 'ovr', 'multinomial'}, default='auto'*

If the option chosen is 'ovr', then a binary problem is fit for each label. For 'multinomial' the loss minimised is the multinomial loss fit across the entire probability distribution, *even when the data is binary*. 'multinomial' is

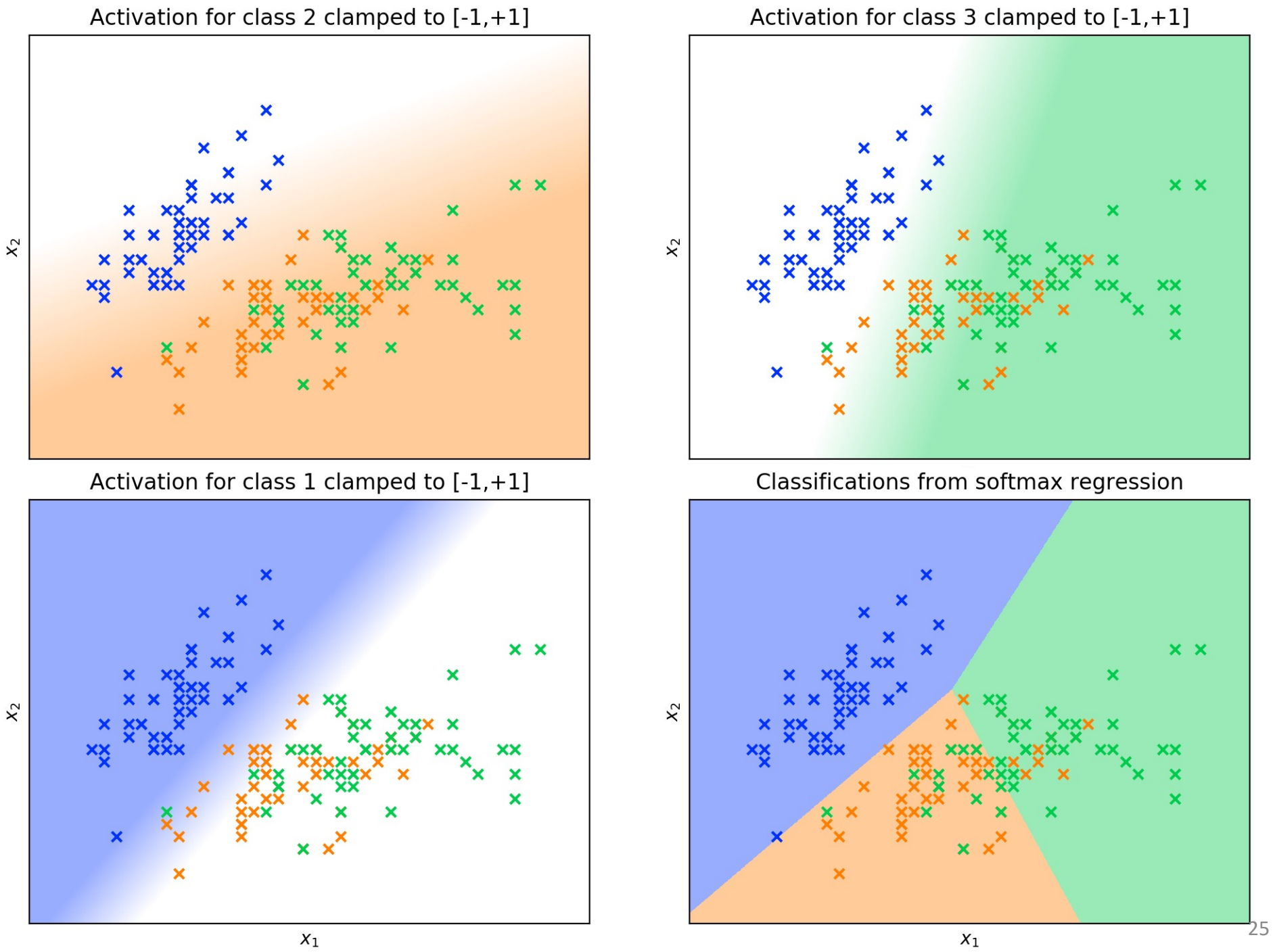
Contrast with NLL of *2-class* logistic regression:

$$-\sum_{i=1}^{N} y_i \ln \hat{y}_i + (1 - y_i) \ln(1 - \hat{y}_i)$$

2-class NLL took the same form as the version! Logistic regression implicitly sums over *K*=2 classes, so the subscript for *k* is omitted.

$$= \sum_{i=1}^{N} y_{i1} \ln \hat{y}_{i1} + y_{i2} \ln \hat{y}_{i2}$$

$$\text{with } \hat{y}_2 = 1 - \hat{y}_1$$


Activation for class 2 clamped to [-1,+1]
Activation for class 3 clamped to [-1,+1]
Activation for class 1 clamped to [-1,+1]
Classifications from softmax regression
x_1
x_2

k-Nearest Neighbours

- Softmax regression (multinomial logistic regression) is a parametric model.
- SVM dual is non-parametric model. Are there other *non-parametric* multiclass classification methods?
- Suppose given training set $\mathcal{D} = \{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_N, y_N)\}$ where each $y_i \in \{1, \ldots, C\}$ is a class label.
- **Idea:** given a new sample $\mathbf{x}$, predict its class label to be the same as the y_i of the "most similar" $\mathbf{x}_i$
  - The 1-nearest neighbour (1-NN) classification algorithm!

k-Nearest Neighbours

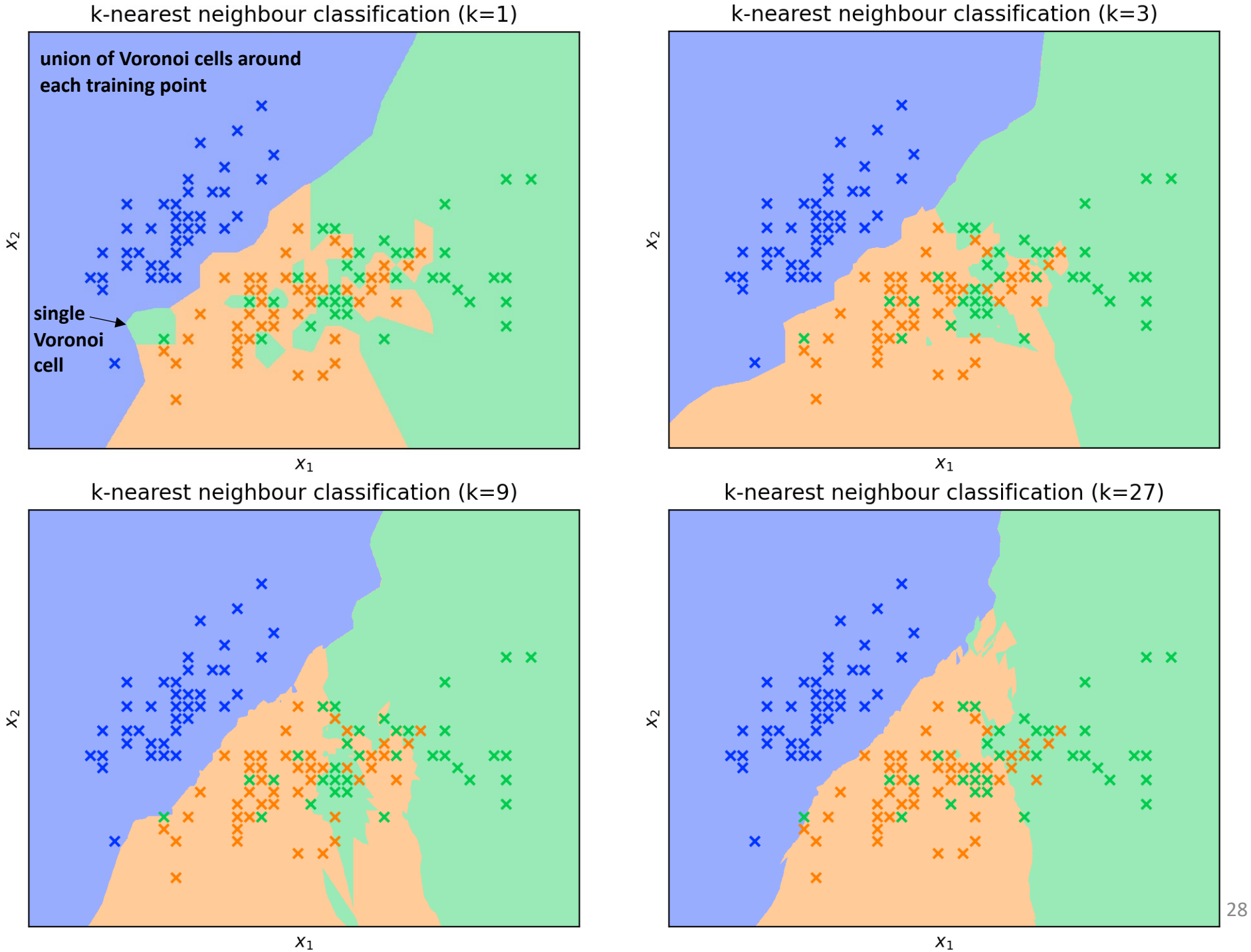
This *k* has nothing to do with the number *K* of classes!

Idea: Given query $\mathbf{x}$ and hyperparameter *k*, we...

1. Find the *k* "nearest neighbours" of $\mathbf{x}$, i.e. the *k* training instances $\mathbf{x}_i$ that are closest to $\mathbf{x}$ by some metric (e.g. $\|\mathbf{x} - \mathbf{x}_i\|^2$) .
2. Predict the class of $\mathbf{x}$ to be the class that wins the majority vote of the y_i corresponding to the nearest neighbours.

Non-parametric since the data *is* the model.

Like kernel density, prediction can be slow, so often build efficient *D*-dimensional search tree structure over the training data.


k-nearest neighbour classification (k=1)
union of Voronoi cells around each training point
single Voronoi cell
x_2
x_1
k-nearest neighbour classification (k=3)
x_2
x_1
k-nearest neighbour classification (k=9)
x_2
x_1
k-nearest neighbour classification (k=27)
x_2
x_1

sklearn.neighbors.KNeighborsClassifier

class sklearn.neighbors. **KNeighborsClassifier**(*n_neighbors=5, weights='uniform', algorithm='auto', leaf_size=30, p=2, metric='minkowski', metric_params=None, n_jobs=None, **kwargs*) [source]

Classifier implementing the k-nearest neighbors vote.

Read more in the User Guide.

Parameters:

n_neighbors : *int, optional (default = 5)*

Number of neighbors to use by default for `kneighbors` queries.

weights : *str or callable, optional (default = 'uniform')*

weight function used in prediction. Possible values:

- 'uniform' : uniform weights. All points in each neighborhood are weighted equally.
- 'distance' : weight points by the inverse of their distance. in this case, closer neighbors of a query point will have a greater influence than neighbors which are further away.
- [callable] : a user-defined function which accepts an array of distances, and returns an array of the same shape containing the weights.

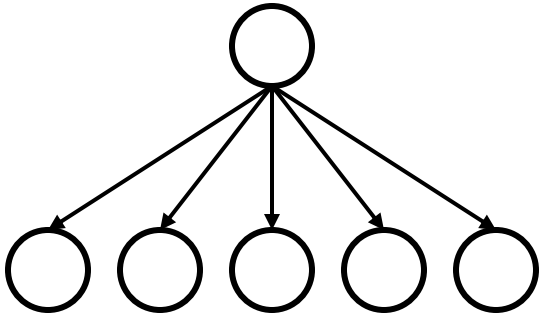
algorithm : *{'auto', 'ball_tree', 'kd_tree', 'brute'}, optional*

Algorithm used to compute the nearest neighbors:

- 'ball_tree' will use `BallTree` OK
- 'kd_tree' will use `KDTree` OK
- 'brute' will use a brute-force search. super slow
- 'auto' will attempt to decide the most appropriate algorithm based on the values passed to `fit` method.

Naïve Bayes is also an important multiclass classifier...

Naive Bayes



However, instead of introducing this now, we'll introduce it in the context of "generative versus discriminative models" later on in the course!

PRML Readings

§2.5.2 Nearest-neighbour methods

§4.1.2 Multiple classes

§4.3.4 Multiclass logistic regression

- See also equation 4.6.2 in section §4.2.0