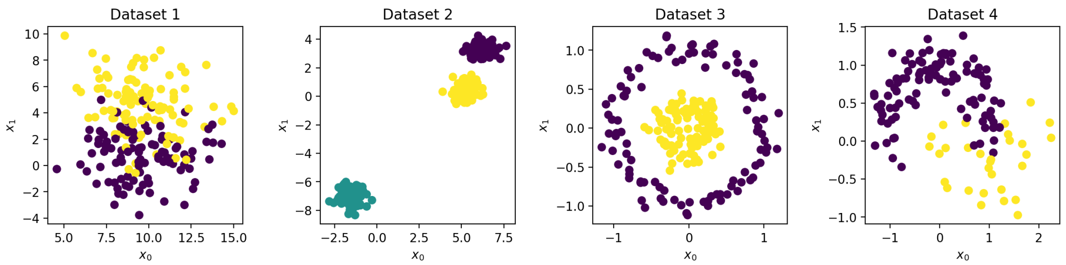
Classification - Assignment 6

Data and Package Import

In [1]:
```
%matplotlib inline
import numpy as np
import pandas as pd
import pylab as plt
```

In [2]:
```
from sklearn.datasets import make_blobs, make_moons, make_circles
np.random.seed(4)

noisiness = 1

X_blob, y_blob = make_blobs(n_samples = 200, centers = 2, cluster_std = 2 * noisiness, n_feat

X_mc, y_mc = make_blobs(n_samples = 200, centers = 3, cluster_std = 0.5 * noisiness, n_featu

X_circles, y_circles = make_circles(n_samples = 200, factor = 0.3, noise = 0.1 * noisiness)

X_moons, y_moons = make_moons(n_samples = 200, noise = 0.25 * noisiness)

N_include = 30
idxs = []
Ni = 0
for i, yi in enumerate(y_moons):
    if yi == 1 and Ni < N_include:
        idxs.append(i)
        Ni += 1
    elif yi == 0:
        idxs.append(i)

y_moons = y_moons[idxs]
X_moons = X_moons[idxs]

fig, axes = plt.subplots(1, 4, figsize = (15, 3), dpi = 200)

all_datasets = [[X_blob, y_blob], [X_mc, y_mc], [X_circles, y_circles], [X_moons, y_moons]]

labels = ['Dataset 1', 'Dataset 2', 'Dataset 3', 'Dataset 4']
for i, Xy_i in enumerate(all_datasets):
    Xi, yi = Xy_i
    axes[i].scatter(Xi[:, 0], Xi[:, 1], c = yi)
    axes[i].set_title(labels[i])
    axes[i].set_xlabel('$x_0$')
    axes[i].set_ylabel('$x_1$')

fig.subplots_adjust(wspace = 0.4);
```



1. Discrimination Lines

Derive the equation for the line that discriminates between the two classes.

Consider a model of the form:

$\bar{\bar{X}}\vec{w} > 0$ if $y_i = 1$ (class 1)

$\bar{\bar{X}}\vec{w} < 0$ if $y_i = -1$ (class 2)

where $\bar{\bar{X}} = [\vec{x_0}, \vec{x_1}, \vec{1}]$ and $\vec{w} = [w_0, w_1, w_2]$.

The equation should be in the form of $x_1 = f(x_0)$. Show your work, and/or explain the process you used to arrive at the answer.

The discrimination line will be drawn where $\bar{\bar{X}}\vec{w}$=0.

$\bar{\bar{X}}\vec{w}$ = w_0x_0 + w_1x_1 + w_2=0

$\therefore x_1 = -\frac{w_0}{w_1}x_0 - \frac{w_2}{w_1}$

Derive the discrimination line for a related non-linear model

In this case, consider a model defined by:

$y_i = w_0x_0 + w_1x_1 + w_2(x_0^2 + x_1^2)$

where the model predicts class 1 if $y_i > 0$ and predicts class 2 if $y_i \leq 0$.

The equation should be in the form of $x_1 = f(x_0)$. Show your work, and/or explain the process you used to arrive at the answer.

Discrimination line: $w_0x_0 + w_1x_1 + w_2(x_0^2 + x_1^2)$ = 0

$w_2x_1^2 + w_1x_1 + w_2x_0^2 + w_0x_0$ = 0

$x_1^2 + \frac{w_1}{w_2}x_1 = -x_0^2 - \frac{w_0}{w_2}x_0$

$\left(x_1 + \frac{w_1}{2w_2}\right)^2 = -x_0\left(x_0 + \frac{w_0}{w_2}\right) + \frac{w_1^2}{4w_2^2}$

$\therefore x_1 = \pm\sqrt{-x_0\left(x_0 + \frac{w_0}{w_2}\right) + \frac{w_1^2}{4w_2^2}} - \frac{w_1}{2w_2}$

Briefly describe the nature of this boundary.

What is the shape of the boundary? Is it linear or non-linear?

1-1. Shape of the boundary: straight line and linear

2. Assessing Loss Functions

In [3]:
```
def add_intercept(X):
    intercept = np.ones((X.shape[0], 1))
    X_intercept = np.append(intercept, X, 1)
    return X_intercept
```

In [4]:
```
def linear_classifier(X, w):
    X_intercept = add_intercept(X)
    p = np.dot(X_intercept, w)
    return p > 0
```

Write a function that computes the loss function for the perceptron model.

The function should take the followings as arguments:

- weight vector w
- the feature matrix $\bar{\bar{X}}$
- the output vector $\vec{y}$

You may want to use functions above.

In [5]:
```
def perceptron(w, X, y):
    X_intercept = add_intercept(X)
    Xb = np.dot(X_intercept, w)
    loss = sum(np.maximum(0, -y*Xb))

    return loss
```

Write a function that computes the loss function for the logistic regression model.

The function should take the followings as arguments:

- weight vector w
- the feature matrix $\bar{\bar{X}}$
- the output vector $\vec{y}$

You may want to use functions above.

In [6]:
```
def log_reg(w, X, y):
    X_intercept = add_intercept(X)
    Xb = np.dot(X_intercept, w)
    exp_yXb = np.exp(-y * Xb)
    loss = sum(np.log(1 + exp_yXb))

    return loss
```

Minimize the both loss functions using the Dataset 3 above.

In [7]:
```
from scipy.optimize import minimize

w = [-10, -4, -10]

result_perceptron = minimize(perceptron, w, args = (X_circles, 2 * y_circles - 1))
result_log_reg = minimize(log_reg, w, args = (X_circles, 2 * y_circles - 1))
```

What is the value of the loss function for the perceptron model after optimization?

In [8]:
```
w_perceptron = result_perceptron.x
loss_perceptron = perceptron(w_perceptron, X_circles, 2 * y_circles - 1)
print(loss_perceptron)
```

```
1.723441663333635e-07
```

What is the value of the loss function for the logistic regression model after optimization?

In [9]:
```
w_log_reg = result_log_reg.x
loss_log_reg = log_reg(w_log_reg, X_circles, 2 * y_circles - 1)
print(loss_log_reg)
```

```
138.60070170523946
```

What are the two main challenges of the perceptron loss function?

- non-differentiable at w = $\vec{0}$
- trivial solution at w = $\vec{0}$

3. Support Vector Machine

Write a function that computes the loss function of the support vector machine model.

This functions should take the followings as arguments:

- weight vector w
- the feature matrix $\bar{\bar{X}}$
- the output vector $\vec{y}$
- regularization strength α

You may want to use `add_intercept` and `linear_classifier` functions from the Problem 2.

In [10]:
```
def svm(w, X, y, alpha):
    X_intercept = add_intercept(X)
    Xb = np.dot(X_intercept, w)
    loss = sum(np.maximum(0, 1 - y*Xb))
    loss += alpha * np.linalg.norm(w[1:], 2)

    return loss
```

Evaluate the effect of regularization strength.

Optimize the SVM model for **Dataset 1**.

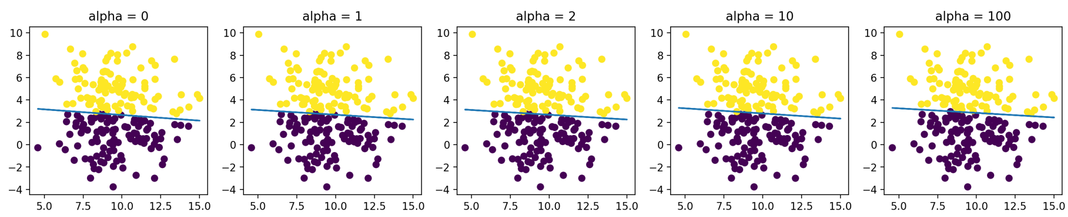
Search over α = [0, 1, 2, 10, 100] and assess the loss function of the SVM model.

In [11]:
```
alphas = [0, 1, 2, 10, 100]

for alpha in alphas:
    result_svm = minimize(svm, w, args = (X_blob, 2 * y_blob - 1, alpha))
    w_svm = result_svm.x

    loss_svm = svm(w_svm, X_blob, 2 * y_blob - 1, alpha)
    print('Value of loss function with alpha = {}: {}'.format(alpha, loss_svm))
```

```
Value of loss function with alpha = 0: 74.19151063967898
Value of loss function with alpha = 1: 74.9684059609181
Value of loss function with alpha = 2: 75.7625348368162
Value of loss function with alpha = 10: 81.69977723457326
Value of loss function with alpha = 100: 127.00264726004937
```

Plot the discrimination lines for α = [0, 1, 2, 10, 100].

In [12]:
```
fig, axes = plt.subplots(1, 5, figsize = (18, 3), dpi = 200)

for i, alpha in enumerate(alphas):
    result_svm = minimize(svm, w, args = (X_blob, 2 * y_blob - 1, alpha))
    w_svm = result_svm.x

    prediction = linear_classifier(X_blob, w_svm)

    m = -w_svm[1] / w_svm[2]
    b = -w_svm[0] / w_svm[2]

    axes[i].scatter(X_blob[:, 0], X_blob[:, 1], c = prediction)
    axes[i].plot(X_blob[:, 0], m * X_blob[:, 0] + b, '-')

    axes[i].set_title('alpha = {}'.format(alpha))
```



Find the optimal set of hyperparameters for an SVM model with Dataset 1.

Use `GridSearchCV` and find the optimal value of α and γ.

In [13]:
```
from sklearn.svm import SVC
from sklearn.model_selection import GridSearchCV

svc = SVC(kernel = 'rbf')

# Note that candidates of gamma are not provided so please be aware of this when you do y
# Focus on the process how your classmates approached this problem, not on the final resul

# I will set a simple list of sigmas and transform it to a list of gammas
sigmas = np.linspace(5, 50, 10)
gammas = 1. / sigmas

Cs = 1. / np.array(alphas[1:])

param_grid = {'gamma': gammas, 'C': Cs}

# You can do train/test split before GridSearchCV
# In this solution, I won't
# Make sure that you have to shuffle the data before GridSearchCV unless you do train/test

from sklearn.utils import shuffle

X_shuffle, y_shuffle = shuffle(X_blob, y_blob)

svm_search = GridSearchCV(svc, param_grid, cv = 3)
svm_search.fit(X_shuffle, y_shuffle)

opt_C = svm_search.best_estimator_.C
opt_gamma = svm_search.best_estimator_.gamma

print('Optimal C: {}'.format(opt_C))
print('Optimal gamma: {}'.format(opt_gamma))
```

```
Optimal C: 1.0
Optimal gamma: 0.2
```

Calculate the accruacy, precision, and recall for the best model.

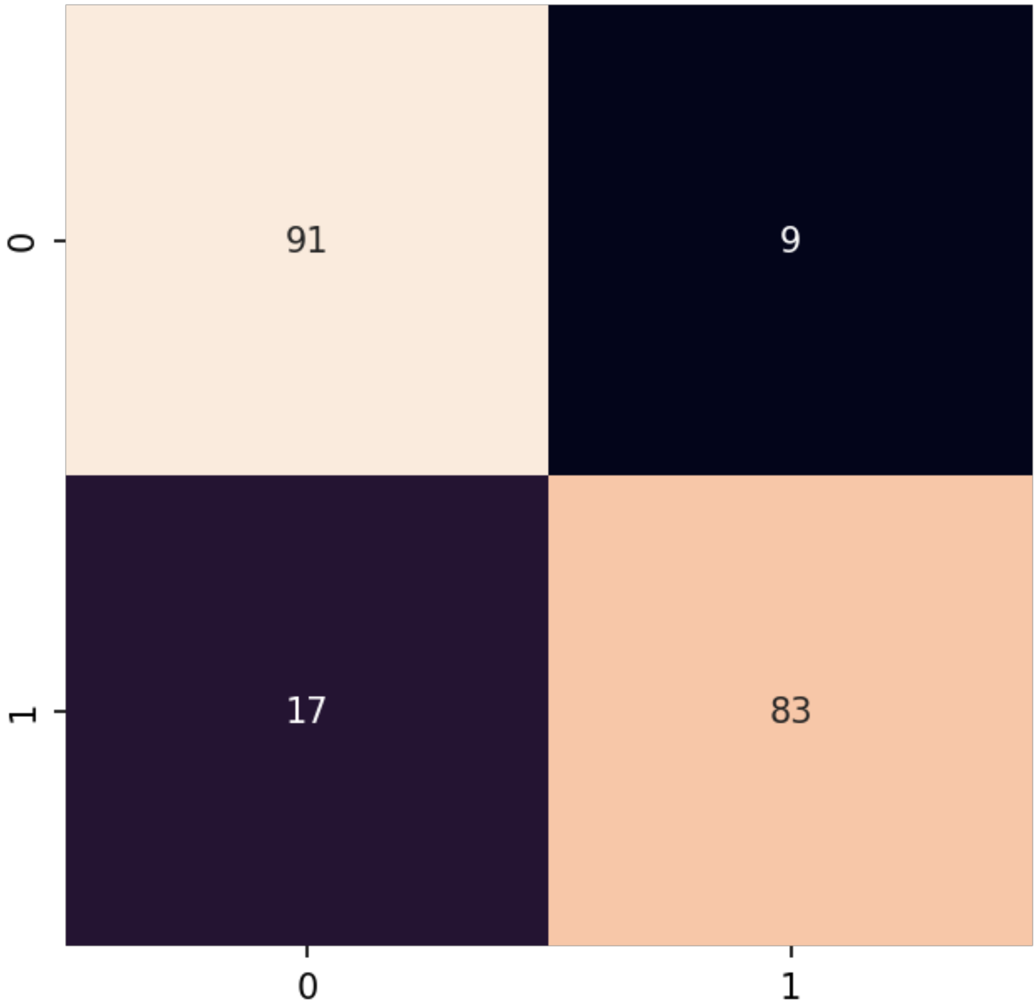
You can write your own function that calculates the metrics or you may use built-in functions.

In [14]:
```
from sklearn.metrics import accuracy_score, recall_score, precision_score

print('Accuracy: {}'.format(accuracy_score(y_blob, svm_search.best_estimator_.predict(X_blob
print('Precision: {}'.format(precision_score(y_blob, svm_search.best_estimator_.predict(X_blob
print('Recall: {}'.format(recall_score(y_blob, svm_search.best_estimator_.predict(X_blob))))
```

```
Accuracy: 0.87
Precision: 0.9021739130434783
Recall: 0.83
```

Plot the confusion matrix.

In [15]:
```
from sklearn.metrics import confusion_matrix
import seaborn as sns

cm = confusion_matrix(y_blob, svm_search.best_estimator_.predict(X_blob))

fig, ax = plt.subplots(figsize = (5, 5), dpi = 150)
sns.heatmap(cm, annot = True, ax = ax, cbar = False);
```



What happens to the decision boundary as α goes to ∞?

> The weights will be over-regularized such that the boundary will be a straight line.

What happens to the decision boundary as γ goes to 0?

If γ goes to 0, each element in RBF kernel will be just 1. This means that data points become indistinguishable even though they are far from each other. As a result, the boundary will enclose all the data

4. 6745 Only: Analytical Derivation

Derive an analytical expression for the gradient of the softmax function with respect to $\vec{w}$.

The **softmax** loss function is defined as:

$$g(\vec{w}) = \sum_i log(1 + \exp(-y_i \vec{x}_i^T \vec{w}))$$

where $\vec{x}_i$ is the i-th row of the input matrix $\bar{\bar{X}}$.

Hint 1: The function $g(\vec{w})$ can be expressed as $f(r(s(\vec{w})))$ where r and s are arbitrary functions and the chain rule can be applied.

Hint 2: You may want to review Ch. 4 of "Machine Learning Refined, 1st Ed."

$log\left\{1 + exp(-y_i \overrightarrow{x_i}^T \vec{w})\right\} = f(r(s(\vec{w})))$ where $f(r) = log\{r\}$,
$r(s) = 1 + e^{-s}$, $s(\vec{w}) = y_i \overrightarrow{x_i}^T \vec{w}$

Using the chain rule,

$$\frac{\partial}{\partial \vec{w}} f(r(s(\vec{w}))) = \frac{df}{dr} \cdot \frac{dr}{ds} \cdot \frac{\partial}{\partial \vec{w}} s(\vec{w}) = \frac{1}{r} \cdot (-e^{-s}) \cdot y_i \overrightarrow{x_i} = \frac{1}{1+e^{-y_i \overrightarrow{x_i}^T \vec{w}}} \cdot (-e^-$$

$$\therefore \frac{\partial g(\vec{w})}{\partial \vec{w}} = \sum_i \frac{1}{1+e^{-y_i \overrightarrow{x_i}^T \vec{w}}} \cdot (-e^{-y_i \overrightarrow{x_i}^T \vec{w}}) \cdot y_i \overrightarrow{x_i}$$

Optional: Logistic regression from the regression perspective

An alternate interpretation of classification is that we are performing non-linear regression to fit a **step function** to our data (because the output is whether 0 or 1). Since step functions are not differentiable at the step, a smooth approximation with non-zero derivatives must be used. One such approximation is the *tanh* function:

$$\tanh(x) = \frac{2}{1+\exp(-x)} - 1$$

This leads to a reformulation of the classification problem as:

$$\vec{y} = \tanh(\bar{\bar{X}}\vec{w})$$

Show that this is mathematically equivalent to **logistic regression**, or minimization of the **softmax** cost function.

$y_i \approx 1$ if $\bar{\bar{X}}\vec{w} > 0$

$y_i \approx -1$ if $\bar{\bar{X}}\vec{w} < 0$

$y_i \bar{\bar{X}}\vec{w}$ will always be positive.

$$y_i \bar{\bar{X}}\vec{w} > 0 \rightarrow tanh(y_i \bar{\bar{X}}\vec{w}) \approx 1$$

$$tanh(y_i \bar{\bar{X}}\vec{w}) = \frac{2}{1+\exp{(y_i \bar{\bar{X}}\vec{w})}} - 1 \approx 1$$

$$1 + \exp{(y_i \bar{\bar{X}}\vec{w})} \approx 1$$

Therefore,

$$log\left\{1 + exp(-y_i \bar{\bar{X}}\vec{w})\right\} \approx 0$$

$$\therefore g_{softmax}(\vec{w}) = \sum_i log\left\{1 + exp(-y_i \bar{\bar{X}}\vec{w})\right\} \approx 0$$