In [2]:
```
# import basic libraries and autograd wrapped numpy
import autograd.numpy as np
from datetime import datetime
import copy
import math
import sys
sys.path.append('../')
nonlinear_datapath = '../mlrefined_datasets/nonlinear_superlearn_datasets/'
datapath = '../mlrefined_datasets/nonlinear_superlearn_datasets/'

# imports from custom library
from mlrefined_libraries import math_optimization_library as optlib
from mlrefined_libraries import nonlinear_superlearn_library as nonlib
from mlrefined_libraries import basics_library

# demos for this notebook
regress_plotter = nonlib.nonlinear_regression_demos
classif_plotter = nonlib.nonlinear_classification_visualizer_multiple_panels
static_plotter = optlib.static_plotter.Visualizer()
basic_runner = nonlib.basic_runner
classif_plotter_crossval = nonlib.crossval_classification_visualizer

# this is needed to compensate for %matplotlib notebook's tendancy to blow up ima
ges when plotted inline
%matplotlib notebook
from matplotlib import rcParams
rcParams['figure.autolayout'] = True
```

Exercise 12.1. Complex Fourier representation

$$
\begin{aligned}
& w_0 + \sum_{m=1}^{M} \cos\left(2\pi m x\right) w_{2m-1} + \sin\left(2\pi m x\right) w_{2m} \\
&= w_0 + \sum_{m=1}^{M} \frac{1}{2}\left(e^{2\pi i m x} + e^{-2\pi i m x}\right) w_{2m-1} + \frac{1}{2i}\left(e^{2\pi i m x} - e^{-2\pi i m x}\right) w_{2m} \\
&= w_0 + \sum_{m=1}^{M} \frac{1}{2}\left(w_{2m-1} - i w_{2m}\right) e^{2\pi i m x} + \frac{1}{2}\left(w_{2m-1} + i w_{2m}\right) e^{-2\pi i m x} \\
&= w_0 + \sum_{m=1}^{M} \frac{1}{2}\left(w_{2m-1} - i w_{2m}\right) e^{2\pi i m x} + \sum_{m=1}^{M} \frac{1}{2}\left(w_{2m-1} + i w_{2m}\right) e^{-2\pi i m x} \\
&= w_0 + \sum_{m=1}^{M} \frac{1}{2}\left(w_{2m-1} - i w_{2m}\right) e^{2\pi i m x} + \sum_{m=-1}^{-M} \frac{1}{2}\left(w_{1-2m} + i w_{-2m}\right) e^{2\pi i m x} \\
&= v_0 e^{2\pi i 0} + \sum_{m=1}^{M} v_m e^{2\pi i m x} + \sum_{m=-1}^{-M} v_m e^{2\pi i m x} = \sum_{m=-M}^{M} v_m e^{2\pi i m x}.
\end{aligned}
$$

Exercise 12.2. Combinatorial explosion in monomials

A polynomial unit of degree-D with N-dimensional input takes the form

$$f(x_1, x_2, \ldots, x_N) = x_1^{j_1} x_2^{j_2} \cdots x_N^{j_N}$$

where j_1 through j_N are nonnegative integers and

$$j_1 + j_2 + \cdots + j_N \leq D.$$

Defining $i_n = j_n + 1$ for all $1 \leq n \leq N$, we want to find the number of tuples $(i_1, i_2, \ldots, i_N)$ satisfying

$$i_1 + i_2 + \cdots + i_N \leq N + D$$

where i_1 through i_N are all positive integers. Note that the number of such tuples is equal to the number of tuples satisfying the equality

$$i_1 + i_2 + \cdots + i_N = k$$

summed over all values of $N \leq k \leq N + D$.

To find the number of all positive integer solutions to the equality above, consider a sequence of k ones as shown below

$$1\ 1\ 1\ \cdots 1\ 1$$

.

Notice, of all the $k-1$ spaces between the consecutive ones, we need to choose $N-1$ of them to place addition signs, and each such configuration then becomes a unique solution to the equation above, giving a total of $\binom{k-1}{N-1}$ solutions.

Finally, summing over all valid values of k and using the Hockey-stick identity (https://en.wikipedia.org/wiki/Hockey-stick_identity) we have

$$\sum_{k=N}^{N+D} \binom{k-1}{N-1} = \binom{N+D}{N}.$$

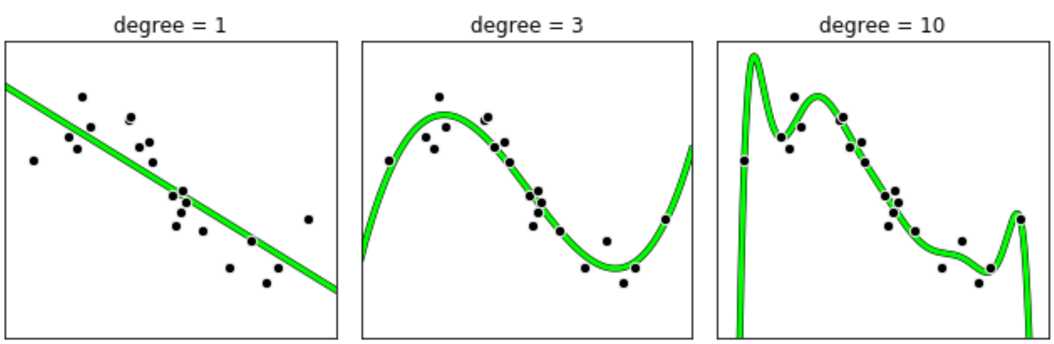
This number includes the solution $(j_1, j_2, \ldots, j_N) = (0, 0, \ldots, 0)$. Therefore, the number of non-constant polynomial units of degree-D can be written simply as

$$\binom{N+D}{N} - 1.$$

Exercise 12.3. Polynomial kernel regression

In [3]:
```
# This code cell will not be shown in the HTML version of this notebook
# import data
csvname = datapath + 'noisy_sin_sample.csv'
data = np.loadtxt(csvname,delimiter = ',')
x = copy.deepcopy(data[:-1,:])
y = copy.deepcopy(data[-1:,:])

# range of degrees
degrees = [1,3,10]
betas = [10**(-4),10**(-3),10**(-2)]

# loop over degrees and fit
runs = []
for d in degrees:
    # initialize with input/output data
    mylib1 = nonlib.kernel_lib.classic_superlearn_setup.Setup(x,y)

    # perform preprocessing step(s) - especially input normalization
    mylib1.choose_normalizer(name = 'standard')

    # split into training and validation sets
    mylib1.make_train_valid_split(train_portion = 1)

    # choose cost
    mylib1.choose_cost(name = 'least_squares')

    # choose dimensions of fully connected multilayer perceptron layers
    mylib1.choose_kernel(name = 'polys',degree = d,scale = 0)

    # fit an optimization
    mylib1.fit(name = 'newtons_method',max_its = 1,verbose = False,epsilon = 1
0**(-10))

    # store
    runs.append(copy.deepcopy(mylib1))
```

In [4]:
```
demo = nonlib.kernel_visualizer.Visualizer(csvname)
labels = ['degree = ' + str(d) for d in degrees]
demo.show_regression_runs(runs,labels = labels)
```



Exercise 12.4. Kernelize the L2 regularized Least Squares cost

The ℓ_2 regularized Least Squares cost is given as

$$g(b, \mathbf{w}) = \frac{1}{P}\sum_{p=1}^{P}\left(b + \mathbf{f}_p^T\mathbf{w} - y_p\right)^2 + \lambda\|\mathbf{w}\|_2^2$$

Applying the fundamental theorem of linear algebra we may then write $\mathbf{w}$ as $\mathbf{w} = \mathbf{F}\mathbf{z} + \mathbf{r}$ where $\mathbf{F}^T\mathbf{r} = \mathbf{0}$. Substituting into the cost and noting that

$$\mathbf{w}^T\mathbf{w} = (\mathbf{F}\mathbf{z} + \mathbf{r})^T\,(\mathbf{F}\mathbf{z} + \mathbf{r}) = \mathbf{z}^T\mathbf{F}^T\mathbf{F}\mathbf{z} + \mathbf{r}^T\mathbf{r} = \mathbf{z}^T\mathbf{H}\mathbf{z} + \|\mathbf{r}\|_2^2,$$

denoting $\mathbf{H} = \mathbf{F}^T\mathbf{F}$ as the kernel matrix we may rewrite the above equivalently as

$$g(b, \mathbf{z}, \mathbf{r}) = \frac{1}{P}\sum_{p=1}^{P}\left(b + \mathbf{h}_p^T\mathbf{z} - y_p\right)^2 + \lambda\,\mathbf{z}^T\mathbf{H}\mathbf{z} + \lambda\|\mathbf{r}\|_2^2.$$

Note that since we are aiming to minimize the quantity above over $(b, \mathbf{z}, \mathbf{r})$, and since the only term with $\mathbf{r}$ remaining is $\|\mathbf{r}\|_2^2$, the optimal value of $\mathbf{r}$ is zero, for otherwise the value of the cost function would be larger than necessary. Therefore we can ignore $\mathbf{r}$ and write the cost function above in kernelized form as

$$g(b, \mathbf{z}) = \frac{1}{P}\sum_{p=1}^{P}\left(b + \mathbf{h}_p^T\mathbf{z} - y_p\right)^2 + \lambda\,\mathbf{z}^T\mathbf{H}\mathbf{z}.$$

Exercise 12.5. Kernelize the multi-class Softmax cost

The multi-class Softmax cost is given as

$$g(b_0, \ldots, b_{C-1}, \mathbf{w}_0, \ldots, \mathbf{w}_{C-1}) = \frac{1}{P}\sum_{p=1}^{P}\log\left(1 + \sum_{\substack{j=0\\ j\neq y_p}}^{C-1} e^{\left(b_j - b_{y_p}\right) + \mathbf{f}_p^T\left(\mathbf{w}_j - \mathbf{w}_{y_p}\right)}\right).$$

Rewriting each $\mathbf{w}_j$ as $\mathbf{w}_j = \mathbf{F}\mathbf{z}_j + \mathbf{r}_j$, where $\mathbf{F}^T\mathbf{r}_j = \mathbf{0}$ for all j, we can rewrite each $\mathbf{f}_p^T\left(\mathbf{w}_j - \mathbf{w}_{y_p}\right)$ term as

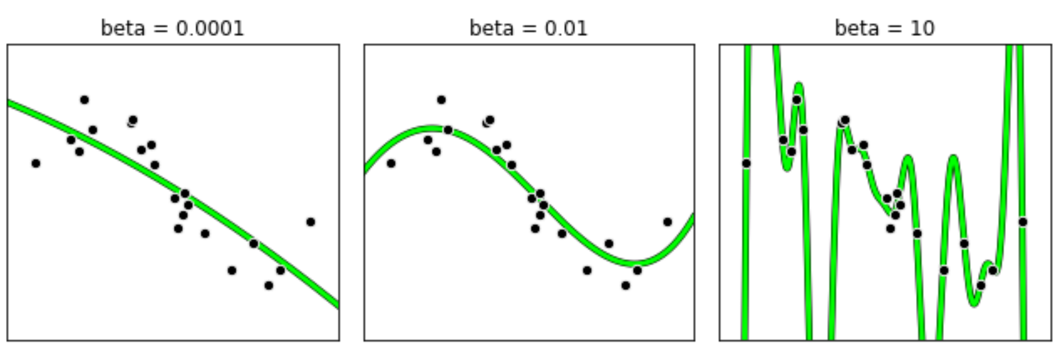
$$\mathbf{f}_p^T\left(\mathbf{w}_j - \mathbf{w}_{y_p}\right) = \mathbf{f}_p^T\left(\mathbf{F}\left(\mathbf{z}_j - \mathbf{z}_{y_p}\right) + \left(\mathbf{r}_j - \mathbf{r}_{y_p}\right)\right) = \mathbf{f}_p^T\mathbf{F}\left(\mathbf{z}_j - \mathbf{z}_{y_p}\right).$$

And denoting $\mathbf{H} = \mathbf{F}^T\mathbf{F}$, we have that $\mathbf{f}_p^T\left(\mathbf{w}_j - \mathbf{w}_{y_p}\right) = \mathbf{h}_p^T\left(\mathbf{z}_j - \mathbf{z}_{y_p}\right)$ and so the cost may be written equivalently as

$$g(b_0, \ldots, b_{C-1}, \mathbf{z}_0, \ldots, \mathbf{z}_{C-1}) = \frac{1}{P}\sum_{p=1}^{P}\log\left(1 + \sum_{\substack{j=0\\ j\neq y_p}}^{C-1} e^{\left(b_j - b_{y_p}\right) + \mathbf{h}_p^T\left(\mathbf{z}_j - \mathbf{z}_{y_p}\right)}\right).$$

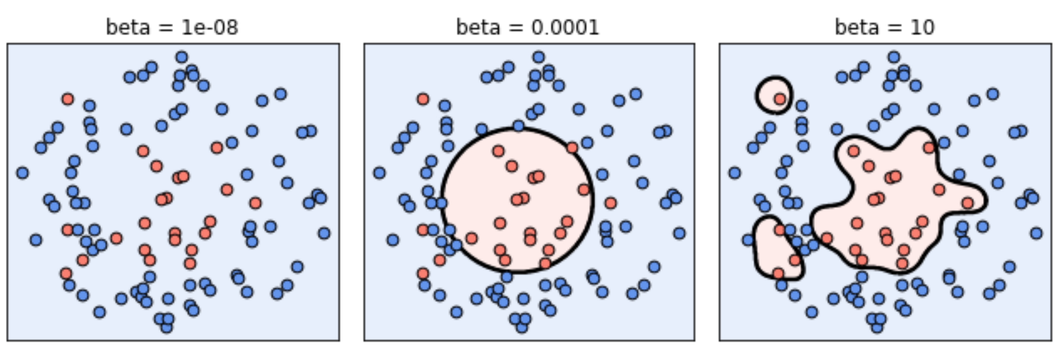
Exercise 12.6. Regression with the RBF kernel

In [6]:
```
# This code cell will not be shown in the HTML version of this notebook
#### regression example ####
# import data
csvname = datapath + 'noisy_sin_sample.csv'
data = np.loadtxt(csvname,delimiter = ',')
x = copy.deepcopy(data[:-1,:])
y = copy.deepcopy(data[-1:,:])

# range of degrees
betas = [10**(-4),10**(-2),10**(1)]

# loop over degrees and fit
runs = []
for d in betas:
    # initialize with input/output data
    mylib1 = nonlib.kernel_lib.classic_superlearn_setup.Setup(x,y)

    # perform preprocessing step(s) - especially input normalization
    mylib1.choose_normalizer(name = 'standard')

    # split into training and validation sets
    mylib1.make_train_valid_split(train_portion = 1)

    # choose cost
    mylib1.choose_cost(name = 'least_squares')

    # choose dimensions of fully connected multilayer perceptron layers
    mylib1.choose_kernel(name = 'gaussian',beta = d,scale = 0)

    # fit an optimization
    mylib1.fit(name = 'newtons_method',max_its = 1,verbose = False,epsilon = 1
0**(-10))

    # store
    runs.append(copy.deepcopy(mylib1))

# plot
demo = nonlib.kernel_visualizer.Visualizer(csvname)
labels = ['beta = ' + str(d) for d in betas]
demo.show_regression_runs(runs,labels = labels)
```



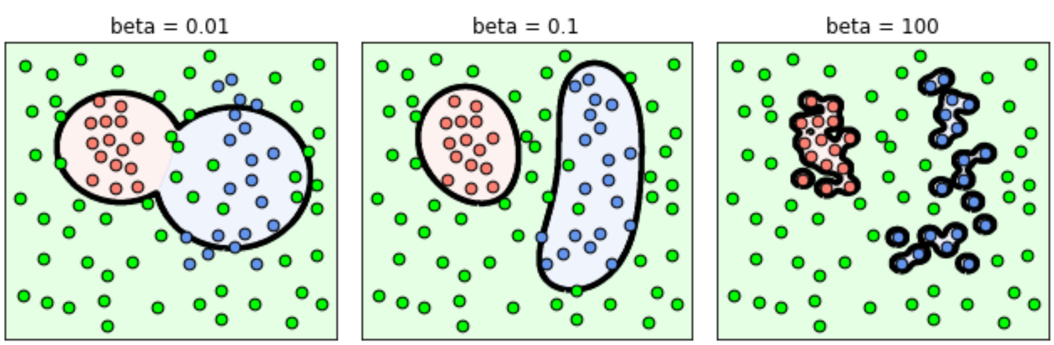
Exercise 12.7. Two-class classification with the RBF kernel

In [7]:
```
#### two-class classification example ####
# import data
csvname = datapath + 'new_circle_data.csv'

data = np.loadtxt(csvname,delimiter = ',')
x = copy.deepcopy(data[:-1,:])
y = copy.deepcopy(data[-1:,:])

# range of degrees
betas = [10**(-8),10**(-4),10**(1)]

# loop over degrees and fit
runs = []
for d in betas:
    # initialize with input/output data
    mylib1 = nonlib.kernel_lib.classic_superlearn_setup.Setup(x,y)

    # perform preprocessing step(s) - especially input normalization
    mylib1.choose_normalizer(name = 'standard')

    # choose cost
    mylib1.choose_cost(name = 'softmax')

    # choose dimensions of fully connected multilayer perceptron layers
    mylib1.choose_kernel(name = 'gaussian',beta = d,scale = 0)

    # fit an optimization
    mylib1.fit(name = 'newtons_method',max_its = 5,verbose = False,epsilon = 1
0**(-10))

    # store
    runs.append(copy.deepcopy(mylib1))

# plot results
demo = nonlib.kernel_visualizer.Visualizer(csvname)
labels = ['beta = ' + str(d) for d in betas]
demo.show_twoclass_runs(runs,labels = labels)
```



Exercise 12.8. Multi-class classification with the RBF kernel

In [11]:
```
### multi-class classification ###
# import data
csvname = datapath + '2eggs_multiclass.csv'
data = np.loadtxt(csvname,delimiter = ',')
x = copy.deepcopy(data[:-1,:])
y = copy.deepcopy(data[-1:,:])

# range of degrees
betas = [10**(-2),10**(-1),10**(2)]

# loop over degrees and fit
runs = []
for d in betas:
    # initialize with input/output data
    mylib1 = nonlib.kernel_lib.classic_superlearn_setup.Setup(x,y)

    # perform preprocessing step(s) - especially input normalization
    mylib1.choose_normalizer(name = 'standard')

    # choose cost
    mylib1.choose_cost(name = 'multiclass_softmax')

    # choose dimensions of fully connected multilayer perceptron layers
    mylib1.choose_kernel(name = 'gaussian',beta = d,scale = 0)

    # fit an optimization
    mylib1.fit(name = 'newtons_method',max_its = 5,verbose = False,epsilon = 1
0**(-5))

    # store
    runs.append(copy.deepcopy(mylib1))

# plot results
demo = nonlib.kernel_visualizer.Visualizer(csvname)
labels = ['beta = ' + str(d) for d in betas]
demo.show_multiclass_runs(runs,labels = labels)
```



Exercise 12.9. Polynomial kernels for arbitrary degree and input dimension

In [ ]:

Exercise 12.10. An infinite-dimensional feature transformation

$$h_{i,j} = f_1(x_i)f_1(x_j) + f_2(x_i)f_2(x_j) + f_3(x_i)f_3(x_j) + \cdots$$
$$= \left(e^{-\beta x_i^2}\sqrt{\frac{(2\beta)^0}{(0)!}}x_i^0\, e^{-\beta x_j^2}\sqrt{\frac{(2\beta)^0}{(0)!}}x_j^0\right) + \left(e^{-\beta x_i^2}\sqrt{\frac{(2\beta)^1}{(1)!}}x_i^1\, e^{-\beta x_j^2}\sqrt{\frac{(2\beta)^1}{(1)!}}x_j^1\right) + \left(e^{-\beta x_i^2}\sqrt{\frac{(2\beta)^2}{(2)!}}x_i^2\, e^{-\beta x_j^2}\sqrt{\frac{(2\beta)^2}{(2)!}}x_j^2\right.$$
$$= e^{-\beta x_i^2}e^{-\beta x_j^2}\left(\frac{(2\beta)^0}{(0)!}x_i^0x_j^0 + \frac{(2\beta)^1}{(1)!}x_i^1x_j^1 + \frac{(2\beta)^2}{(2)!}x_i^2x_j^2 + \cdots\right)$$
$$= e^{-\beta x_i^2}e^{-\beta x_j^2}e^{\,2\beta x_i x_j} = e^{\,-\beta\left(x_i^2+x_j^2-2x_ix_j\right)} = e^{\,-\beta\left(x_i-x_j\right)^2}$$

Exercise 12.11. Fourier kernel for vector-valued input

Like the multidimensional polynomial basis element with the complex exponential notation for a general N dimensional input each Fourier basis element takes the form $f_{\mathbf{m}}\left(\mathbf{x}\right) = e^{2\pi i m_1 x_1}e^{2\pi i m_2 x_2}\cdots e^{2\pi i m_N x_N} = e^{2\pi i \mathbf{m}^T\mathbf{x}}$ where $\mathbf{m} = \begin{bmatrix} m_1 & m_2 & \cdots & m_N\end{bmatrix}^T$, a product of one dimensional basis elements. Further a 'degree D' sum contains all such basis elements where $-D \leq m_1,\ m_2,\ \cdots,\ m_N \leq D$, and one may deduce that there are $M = (2D+1)^N - 1$ non constant basis elements in this sum.

The the corresponding (i,j)th entry of the kernel matrix in this instance takes the form

$$\mathbf{H}_{ij} = \mathbf{f}_i^T\overline{\mathbf{f}_j} = \left(\sum_{-D\leq m_1,\, m_2,\, \cdots,\, m_N\leq D} e^{2\pi i \mathbf{m}^T\left(\mathbf{x}_i-\mathbf{x}_j\right)}\right) - 1.$$

Since $e^{a+b} = e^a e^b$ we may write each summand above as $e^{2\pi i \mathbf{m}^T\left(\mathbf{x}_i-\mathbf{x}_j\right)} = \prod_{n=1}^N e^{2\pi i m_n\left(x_{in}-x_{jn}\right)}$, and the entire summation as \noindent

$$\sum_{-D\leq m_1,\, m_2,\, \cdots,\, m_N\leq D}\ \prod_{n=1}^N e^{2\pi i m_n\left(x_{in}-x_{jn}\right)}.$$

Finally one can show that the above can be written simply as \noindent

$$\sum_{-D\leq m_1,\, m_2,\, \cdots,\, m_N\leq D}\ \prod_{n=1}^N e^{2\pi i m_n\left(x_{in}-x_{jn}\right)} = \prod_{n=1}^N\left(\sum_{m=-D}^{D} e^{2\pi i m\left(x_{in}-x_{jn}\right)}\right).$$

Since we already have that $\sum_{m=-D}^{D} e^{2\pi i m\left(x_{in}-x_{jn}\right)} = \frac{\sin\left((2D+1)\pi\left(x_{in}-x_{jn}\right)\right)}{\sin\left(\pi\left(x_{in}-x_{jn}\right)\right)}$, the (i,j)th entry of the kernel matrix can easily be calculated as \noindent

$$\mathbf{H}_{ij} = \prod_{n=1}^N \frac{\sin\left(\left(2D+1\right)\pi\left(x_{in}-x_{jn}\right)\right)}{\sin\left(\pi\left(x_{in}-x_{jn}\right)\right)} - 1.$$

Exercise 12.12. Kernels and a cancer dataset

Below - via a backend package organized into coherent modules - we perform regularization based cross validation using a Gaussian kernel, ranging over the hyperparameter β.

In [17]:
```
# load in data
datapath = '../mlrefined_datasets/superlearn_datasets/'
data = np.loadtxt(datapath + 'breast_cancer_data.csv',delimiter = ',')
x = copy.deepcopy(data[:-1,:])
y = copy.deepcopy(data[-1:,:])

# initialize with input/output data
mylib1 = nonlib.kernel_lib_regularized.classic_superlearn_setup.Setup(x,y)

# split into training and testing sets
mylib1.make_train_valid_split(train_portion = 0.8)

# perform preprocessing step(s) - especially input normalization
mylib1.choose_normalizer(name = 'standard')
mylib1.choose_kernel(name = 'gaussian',beta = 2,scale = 0.1)
mylib1.choose_cost(name = 'softmax',lam=0)
mylib1.w_init = mylib1.initializer()

# run
w_init = mylib1.initializer()
betas = np.linspace(0.01,1,50)
j=0
for beta in betas:
    # choose dimensions of fully connected multilayer perceptron layers
    mylib1.choose_kernel(name = 'gaussian',beta = beta,scale = 0.1)

    # choose cost
    mylib1.choose_cost(name = 'softmax',lam=0)

    # fit an optimization
    mylib1.fit(name = 'newtons_method',max_its = 1,verbose = False,epsilon = 1
0**(-10),w_init=w_init)
```

In [18]:
```
import matplotlib.pyplot as plt
from matplotlib import gridspec

def show_history(run):
    # initialize figure
    fig = plt.figure(figsize = (10,4))

    # create subplot with 1 panel
    gs = gridspec.GridSpec(1, 1)
    ax = plt.subplot(gs[0]);

    # colors
    colors = [[0,0.7,1],[1,0.8,0.5]]

    # plot test cost function history
    train_history = run.train_count_histories
    ax.plot(betas,train_history,linewidth = 3*(0.8)**(0),color = colors[0],label
= 'training')

    val_history = run.valid_count_histories
    ax.plot(betas,val_history,linewidth = 3*(0.8)**(0),color = colors[1],label =
'validation')

    # clean up panel / axes labels
    xlabel = r'$\beta$ value'
    ylabel = 'misclassifications'
    ax.set_xlabel(xlabel,fontsize = 14)
    ax.set_ylabel(ylabel,fontsize = 14,rotation = 90,labelpad = 25)
    title = 'misclassification history'
    ax.set_title(title,fontsize = 18)

    plt.show()
```

In [19]:
```
show_history(mylib1)
```