# About the presentation

- We are in 370 during each session. Be there on time! We have pizzas. :)
- Check piazza for the rubric and sign up. There are still some empty slots.
- **Imagine what it is like for your audience!**
- Don't write too much text on the slides - noone reads it. Write short bullet points.
- Figures must have x and y labels, the characters must be readable from a distance, the objects of the graph must be visible.
- EDA figures:
  - three different visualization types!
  - e.g., one bar pot, one scatter plot, one heatmap.
  - if you only show bar plots, those are all of the same type and points will be subtracted.

# Mud card

- **Pls give more exercises on coordinates and p-criti**
  - in HW5 :)
- **What does accuracy refer to? the accuracy of the model?**
  - accuracy as the classification metric (TP + TN) / (TP + TN + FP + FN)
  - accuracy as the predictive power of the model ("the model is accurate" meaning that it gives good predictions)

- **Is there a reason why you would change the value for epsilon in log loss?**
  - 1e-15 is used because python's float contains 16 significant digits (double precision)
    - 1e-15 has at least one significant digit
  - if you represent your numbers with a different precision level, you might want to adjust epsilon accordingly
    - e.g., single precision (8 significant digits), eps = 1e-7
- **It would be great if you could clarify logloss once again in the next class**
- **What is y_true in log loss**
- **Can you explain extreme cases in logloss?**

# The logloss metric

$$logloss = -\frac{1}{N}\sum(y_{true}\ln(p_{pred}) + (1-y_{true})(1-\ln(1-p_{pred})))$$

- $p_{pred}$ is the predicted probability of the **positive class**
- the predicted probabilities are not converted into predicted classes
- two scenarios:
  - y_true = 0 - left term disappears
  - y_true = 1 - right term disappears
- log(0) is undefined
  - $p_{pred}$ is replaced with $\max(\min(p, 1-10^{-15}), 10^{-15})$ to avoid this issue

## The extreme cases

- the classifier is confidently wrong
  - $p_{pred} = 10^{-15}$ for points in class 1
  - $p_{pred} = 1-10^{-15}$ for points in class 0

$$logloss = -\frac{1}{N}\sum\ln(10^{-15}) = -\ln(10^{-15})$$
$$logloss \sim 34.5$$

- the classifier is correct
  - $p_{pred} = 10^{-15}$ for points in class 0
  - $p_{pred} = 1-10^{-15}$ for points in class 1

$$logloss = -\frac{1}{N}\sum(1-0)(1-\ln(1-10^{-15})) = 10^{-15} \text{ for class 0}$$
$$logloss = -\frac{1}{N}\sum 1 * \ln(1-10^{-15}) = 10^{-15} \text{ for class 1}$$
$$logloss \sim 0$$

In [1]:
```
from sklearn.metrics import log_loss
import pandas as pd
import numpy as np
df = pd.read_csv('data/true_labels_pred_probs.csv')

y_true = df['y_true']
pred_prob_class1 = df['pred_prob_class1']

print(log_loss(y_true,pred_prob_class1))
help(log_loss)
```

```
0.35015190545328556
Help on function log_loss in module sklearn.metrics.classification:

log_loss(y_true, y_pred, eps=1e-15, normalize=True, sample_weight=None,
labels=None)
    Log loss, aka logistic loss or cross-entropy loss.

    This is the loss function used in (multinomial) logistic regression
    and extensions of it such as neural networks, defined as the negati
ve
    log-likelihood of the true labels given a probabilistic classifie
r's
    predictions. The log loss is only defined for two or more labels.
    For a single sample with true label yt in {0,1} and
    estimated probability yp that yt = 1, the log loss is

        -log P(yt|yp) = -(yt log(yp) + (1 - yt) log(1 - yp))

    Read more in the :ref:`User Guide <log_loss>`.

    Parameters
    ----------
    y_true : array-like or label indicator matrix
        Ground truth (correct) labels for n_samples samples.

    y_pred : array-like of float, shape = (n_samples, n_classes) or (n_
samples,)
        Predicted probabilities, as returned by a classifier's
        predict_proba method. If ``y_pred.shape = (n_samples,)``
        the probabilities provided are assumed to be that of the
        positive class. The labels in ``y_pred`` are assumed to be
        ordered alphabetically, as done by
        :class:`preprocessing.LabelBinarizer`.

    eps : float
        Log loss is undefined for p=0 or p=1, so probabilities are
        clipped to max(eps, min(1 - eps, p)).

    normalize : bool, optional (default=True)
        If true, return the mean loss per sample.
        Otherwise, return the sum of the per-sample losses.

    sample_weight : array-like of shape = [n_samples], optional
        Sample weights.

    labels : array-like, optional (default=None)
        If not provided, labels will be inferred from y_true. If ``labe
ls``
        is ``None`` and ``y_pred`` has shape (n_samples,) the labels ar
e
        assumed to be binary and are inferred from ``y_true``.
        .. versionadded:: 0.18

    Returns
    -------
    loss : float
```

```
        Examples
        --------
        >>> from sklearn.metrics import log_loss
        >>> log_loss(["spam", "ham", "ham", "spam"],  # doctest: +ELLIPSIS
        ...          [[.1, .9], [.9, .1], [.8, .2], [.35, .65]])
        0.21616...

        References
        ----------
        C.M. Bishop (2006). Pattern Recognition and Machine Learning. Sprin
    ger,
        p. 209.

        Notes
        -----
        The logarithm used is the natural logarithm (base-e).
```

# Evaluation metrics in regression and gradient descent

By the end of this lecture, you will be able to

- Describe the most commonly used regression metrics
- Describe what the cost function is
- Explain how a simple gradient descent algorithm works

# Evaluation metrics in regression and gradient descent

By the end of this lecture, you will be able to

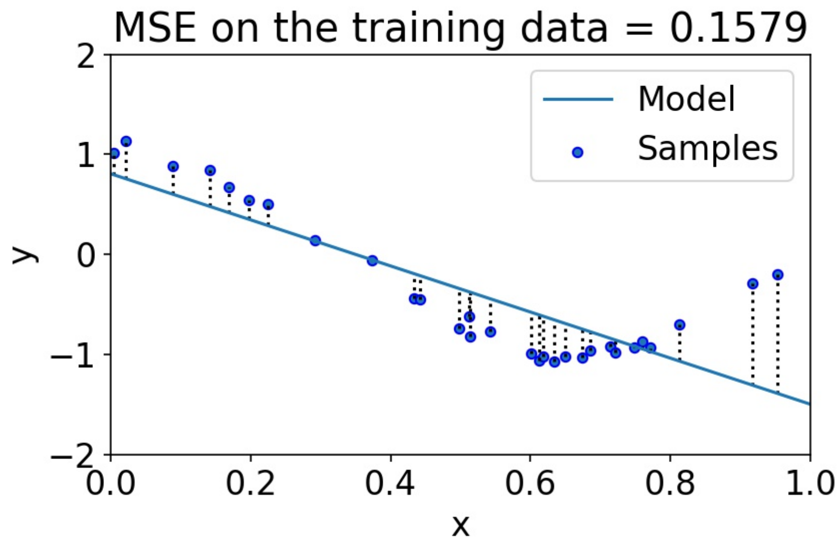
- **Describe the most commonly used regression metrics**
- Describe what the cost function is
- Explain how a simple gradient descent algorithm works

# Regression metrics

- the target variable is continuous
- the predicted values are also continuous
- regression metrics measure some type of difference between y (true values) and y' (predicted values)
- three types of metrics:
  - unit of metric is different than the unit of targe variable
  - same units
  - dimensionless

## Mean Squared Error

$$MSE(y, y') = \frac{1}{n} \sum_{i=1}^{n} (y_i - y'_i)^2$$




## Root Mean Square Error

$$RMSE(y, y') = \sqrt{\frac{1}{n} \sum_{i=1}^{n} (y_i - y'_i)^2}$$

## Mean Absolute Error

$$MAE(y, y') = \frac{1}{n} \sum_{i=1}^{n} |y_i - y'_i|$$

**Both RMSE and MAE have the same unit as the target variable.**

# R2 score - coefficient of determination

$$R^2(y, y') = 1 - \frac{\sum_{i=1}^{n}(y_i - y_i')^2}{\sum_{i=1}^{n}(y_i - \bar{y})^2},$$

where $\bar{y}$ is the mean of $y$.

- R2 = 1 is the perfect regression model ($y == y'$)
- R2 = 0 is as good as a constant model that always predicts the expected value of y, $\bar{y}$
- R2 < 0 is a bad regression model

**R2 is dimensionless.**

In [2]:
```
from sklearn.metrics import mean_squared_error
from sklearn.metrics import mean_absolute_error
from sklearn.metrics import r2_score
```

- RMSE is not implemented in sklearn, but you can calculate it as `np.sqrt(mean_squared_error(y_true,y_pred))`
- you can find more on regression metrics [here (https://scikit-learn.org/stable/modules/model_evaluation.html#regression-metrics)](https://scikit-learn.org/stable/modules/model_evaluation.html#regression-metrics)

# Exercise 1

Read in `data/reg_preds.csv` . It contains two columns:

- y_true: value of owner-occupied homes in $1000's in Boston
- y_pred: predictions of a regression model

What's the ratio between the MSE and the variance of the home values? How does this ratio relate to the R2 score?

In [ ]:
```

```

# Evaluation metrics in regression and gradient descent

By the end of this lecture, you will be able to

- Describe the most commonly used regression metrics
- **Describe what the cost function is**
- Explain how a simple gradient descent algorithm works

## Supervised ML algorithms

- What mathematical model is used to represent the data? What are the parameters of the model?
- How do we compare different parameter values of the same model?
  - this is done with the cost function
  - WARNING!
    - the evaluation metric is used to compare different models!
    - the cost function compares different parameter values of the same model!
- What algorithm do we use to find the best model parameter values?
  - e.g., brute force, gradient descent, backpropagation

## Today

- The mathematical model is linear regression: ###
$$y_i' = \theta_0 + x_{i1}\theta_1 + x_{i2}\theta_2 + ... = \theta_0 + \sum_{j=1}^{m} \theta_j x_{ij}$$
where $y_i'$ is the prediction of the linear regression model and $\theta$ are parameters.
- The cost function is MSE
- We will find the best parameter values by brute force first, then simple gradient descent.

## Let's generate some data

In [6]:
```
# load packages and generate data
import numpy as np
import matplotlib.pyplot as plt
import pandas as pd
import matplotlib
matplotlib.rcParams.update({'font.size': 16})

# the true function to generate y (gaussian noise is added later)
def true_fun(X):
    return np.cos(1.5 * np.pi * X)

# fix the seed so code is reproducable
np.random.seed(10)

# generate n_samples points
n_samples = 30

# generate data
X = np.random.rand(n_samples)
y = true_fun(X) + np.random.randn(n_samples) * 0.1 # noise added here
```

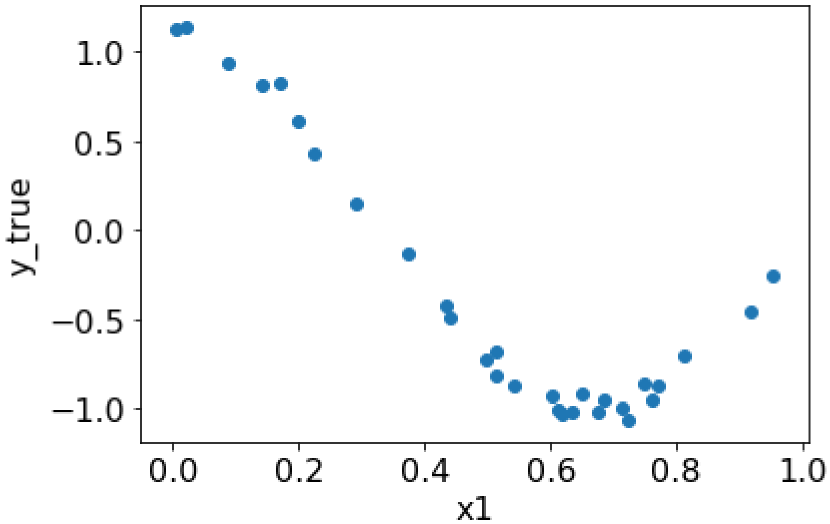
In [7]:
```
df = pd.DataFrame()
for i in range(10):
    df['x'+str(i+1)] = X**(i+1)
df['y'] = y
print(df.head())
df.to_csv('data/regression_example.csv',index=False)
```

```
         x1        x2        x3            x4            x5            
x6  \
0  0.771321  0.594936  0.458886  3.539483e-01  2.730076e-01  2.105764e-
01
1  0.020752  0.000431  0.000009  1.854537e-07  3.848527e-09  7.986443e-
11
2  0.633648  0.401510  0.254416  1.612103e-01  1.021507e-01  6.472758e-
02
3  0.748804  0.560707  0.419860  3.143926e-01  2.354184e-01  1.762822e-
01
4  0.498507  0.248509  0.123884  6.175684e-02  3.078622e-02  1.534715e-
02

             x7            x8            x9           x10         y
0  1.624219e-01  1.252794e-01  9.663058e-02  7.453316e-02 -0.870922
1  1.657343e-12  3.439309e-14  7.137237e-16  1.481116e-17  1.135022
2  4.101452e-02  2.598878e-02  1.646774e-02  1.043476e-02 -1.015044
3  1.320008e-01  9.884272e-02  7.401381e-02  5.542183e-02 -0.864701
4  7.650660e-03  3.813908e-03  1.901260e-03  9.477913e-04 -0.728846
```

In [8]:
```
def predict(X,theta):
    if len(np.shape(theta)) != 2:
        theta = np.array(theta)[np.newaxis,:] # just a numpy trick to ma
ke the dot product work
    y_pred = theta[0,0] + X.dot(theta[0,1:]) # intercept + theta_i*x_i
    return y_pred

def cost_function(X,y_true,theta):
    """
    Take in a numpy array X,y_true, theta and generate the cost function
    of using theta as parameter in a linear regression model
    """
    m = len(y)
    theta = np.array(theta)[np.newaxis,:] # just a numpy trick to make t
he dot product work in predict
    y_pred = predict(X,theta)
    cost = (1/m) * np.sum(np.square(y_true-y_pred)) # this is MSE
    return cost
```

## For simplicity, let's focus on x1 and y only!

In [9]:
```
plt.scatter(df['x1'],df['y'])
plt.xlabel('x1')
plt.ylabel('y_true')
plt.savefig('figures/data.png',dpi=300)
plt.show()
```



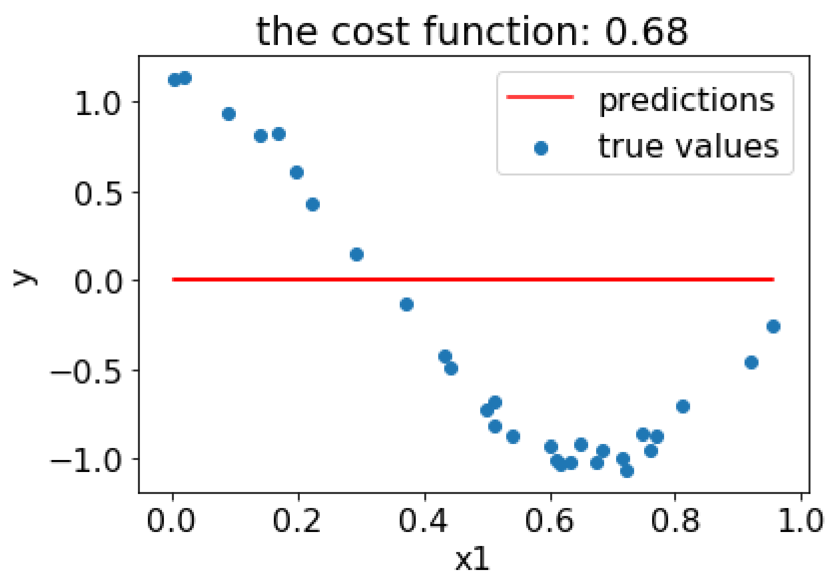

$$y_i' = \theta_0 + x_{i1}\theta_1$$

- $\theta_0$ is the intercept
- $\theta_1$ is the slope

**We are looking for the best fit line!**

For a given $\theta$ vector, the cost function returns the MSE.

In [11]:
```
theta = [0,0] # intercept is theta[0], the slope is theta[1]

plt.scatter(df['x1'],df['y'],label='true values')
plt.plot(df['x1'],predict(df['x1'].values[:,np.newaxis],theta),label='pr
edictions',color='r')
plt.title('the cost function: '+str(np.around(cost_function(df['x1'].val
ues[:,np.newaxis],df['y'],theta),2)))
plt.xlabel('x1')
plt.ylabel('y')
plt.legend()
plt.savefig('figures/line_fit.png',dpi=300)
plt.show()
```




## What we want:

- Find the theta vector that minimizes the cost function!
    - that's our best fit model

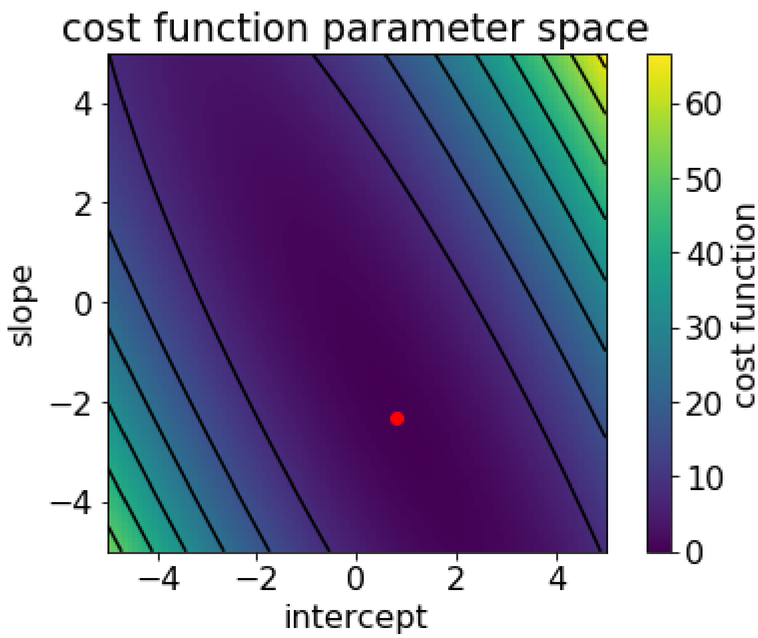
## How we do it:

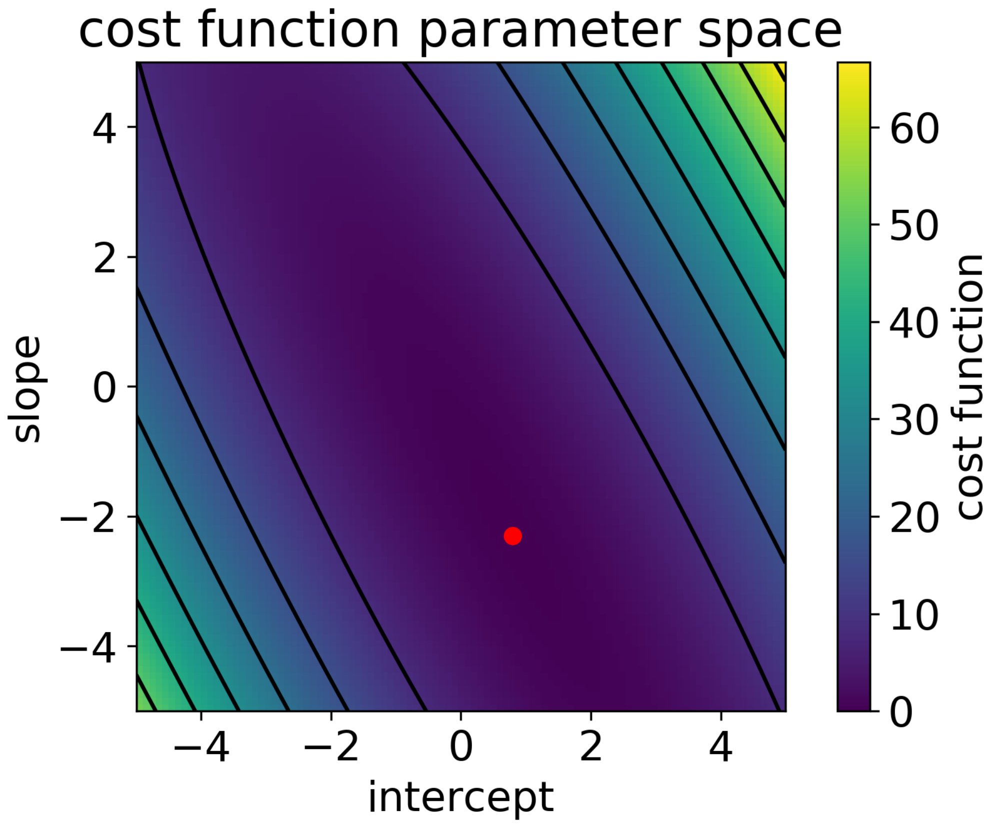
- brute force
    - create a grid of theta[0] and theta[1] values
    - loop through all theta vectors on the grid
    - find the theta vector that comes with the smallest cost

In [12]:
```
n_vals = 101

theta0 = np.linspace(-5,5,n_vals) # the intercept values to explore
theta1 = np.linspace(-5,5,n_vals) # the slope values to explore

cost = np.zeros([len(theta0),len(theta1)]) # the cost function's value f
or each theta

# loop through all intercept-slope combinations and calculate the cost f
unction
for i in range(n_vals):
    for j in range(n_vals):
        theta = [theta0[i],theta1[j]]
        cost[i,j] = cost_function(df['x1'].values[:,np.newaxis],df['y'],
theta)

print('min(cost):',np.min(cost))
min_coords = np.unravel_index(cost.argmin(),np.shape(cost))
print('best intercept:',theta0[min_coords[0]])
print('best slope:',theta1[min_coords[1]])
```

```
min(cost): 0.14851645747269254
best intercept: 0.8000000000000007
best slope: -2.3
```

In [13]:
```
plt.figure(figsize=(6.4,4.8))
ax = plt.gca()
extent = (np.min(theta0),np.max(theta0),np.min(theta1),np.max(theta1))
fig = ax.imshow(cost.T,origin='lower',extent=extent,vmin=0)
plt.colorbar(fig,label='cost function')
ax.contour(theta0,theta1,cost.T,levels=10,colors='black')
plt.scatter(theta0[min_coords[0]],theta1[min_coords[1]],c='r')
ax.xaxis.set_ticks_position("bottom")
plt.xlabel('intercept')
plt.ylabel('slope')
plt.title('cost function parameter space')
plt.tight_layout()
plt.savefig('figures/cost_function.png',dpi=300)
plt.show()
```




cost function parameter space
slope
intercept
cost function
4
2
0
−2
−4
−4
−2
0
2
4
60
50
40
30
20
10
0

### The brute force approach works but...

- the number of theta vectors to loop through explodes with the number of features we have
  - with n features, we would need to loop through ~ $100^n$ theta vectors.
  - no guarantee that the best theta vector is within our grid.
- We need to use a smarter numerical method to find the best theta!
  - gradient descent to the rescue!

## Evaluation metrics in regression and gradient descent

By the end of this lecture, you will be able to

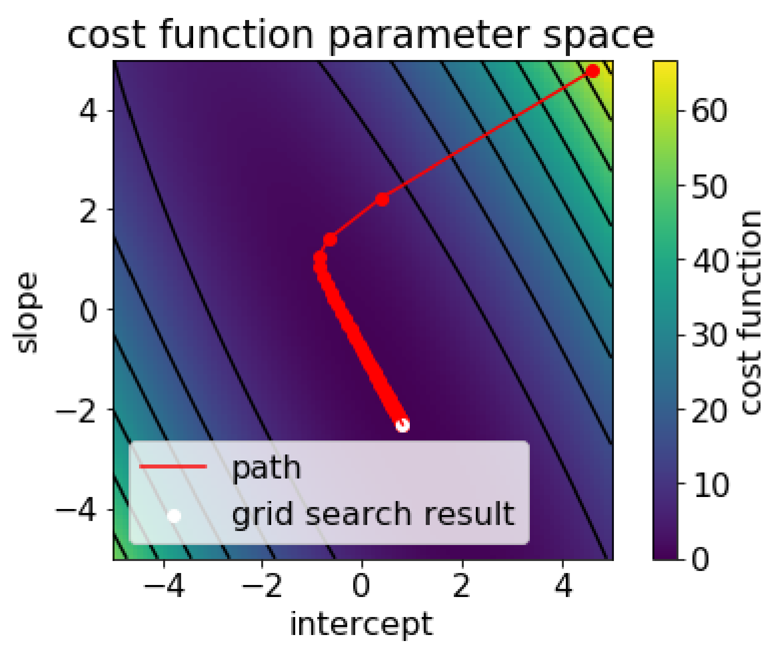
- Describe the most commonly used regression metrics
- Describe what the cost function is
- **Explain how a simple gradient descent algorithm works**

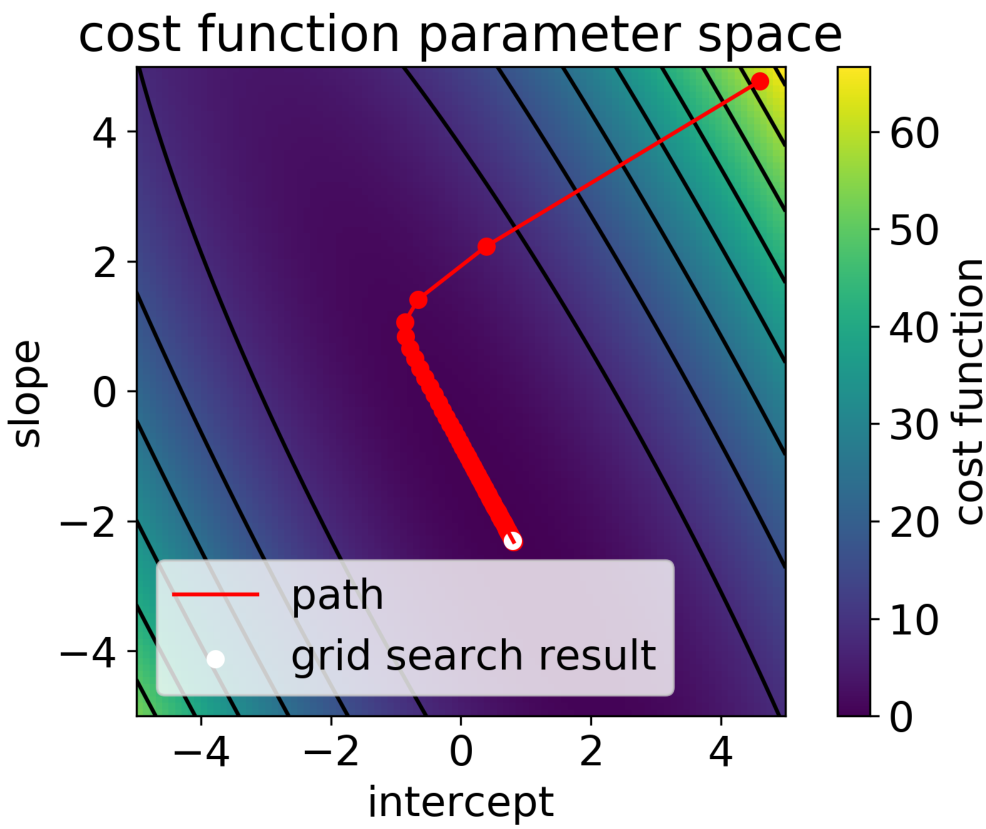
In [14]:
```
def gradient_descent(X,y_true,theta,learning_rate=0.01,iterations=100):
    '''
    X     = Matrix of X with added bias units
    y     = Vector of Y
    theta=Vector of thetas np.random.randn(j,1)
    learning_rate
    iterations = no of iterations

    Returns the final theta vector and array of cost history over no of
 iterations
    '''
    m = len(y_true)
    theta = np.array(theta)[np.newaxis,:]

    cost_history = np.zeros(iterations)
    theta_history = np.zeros([iterations,np.shape(theta)[1]])
    for it in range(iterations):

        y_pred = predict(X,theta)
        delta_theta = np.zeros(np.shape(theta)) # the step we take
        # the derivative of the cost function with respect to the interc
ept
        delta_theta[0,0] = (1/m) * sum(y_pred - y_true) *learning_rate
        # the derivative of the cost function with respect to the slopes
* learning_rate
        delta_theta[0,1:] = (1/m)*learning_rate*( X.T.dot((y_pred - y_tr
ue)))
        theta = theta - delta_theta # update theta so we move down the g
radient
        theta_history[it] = theta[0]
        cost_history[it] = cost_function(X,y_true,theta[0])

    return theta[0], cost_history, theta_history
```

In [15]:
```
theta,cost_history,theta_hist = gradient_descent(df['x1'].values[:,np.ne
waxis],df['y'],[5.0,5.0],0.05,1500)
print(theta)
print(theta_hist)
```

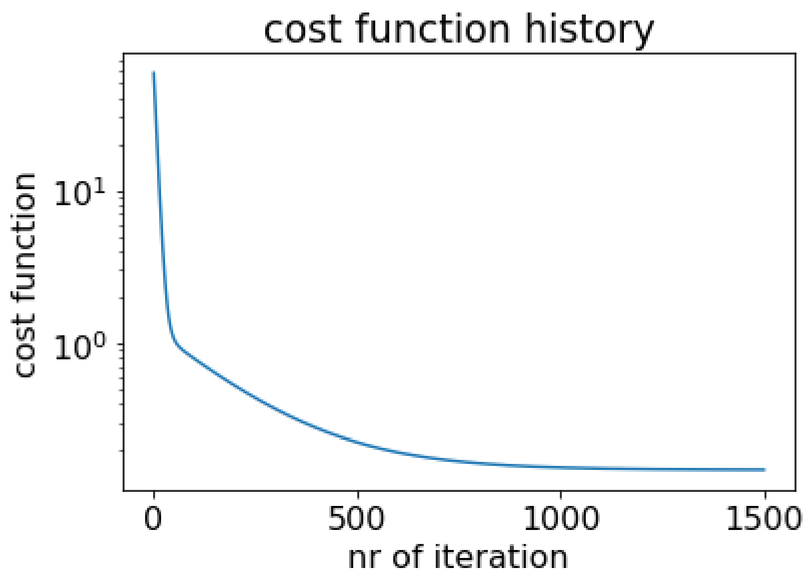
```
[ 0.81374506 -2.32315071]
[[ 4.60368338  4.77240776]
 [ 4.23299768  4.55868453]
 [ 3.88630699  4.35794734]
 ...
 [ 0.81353231 -2.3227565 ]
 [ 0.81363883 -2.32295387]
 [ 0.81374506 -2.32315071]]
```

In [16]:
```
plt.figure(figsize=(6.4,4.8))
ax = plt.gca()
extent = (np.min(theta0),np.max(theta0),np.min(theta1),np.max(theta1))
fig = ax.imshow(cost.T,origin='lower',extent=extent,vmin=0)
plt.colorbar(fig,label='cost function')
ax.contour(theta0,theta1,cost.T,levels=10,colors='black')
plt.plot(theta_hist[::20,0],theta_hist[::20,1],color='r',label='path')
plt.scatter(theta_hist[::20,0],theta_hist[::20,1],c='r')
plt.scatter(theta0[min_coords[0]],theta1[min_coords[1]],c='w',label='gri
d search result')
ax.xaxis.set_ticks_position("bottom")
plt.legend()
plt.xlabel('intercept')
plt.ylabel('slope')
plt.title('cost function parameter space')
plt.tight_layout()
plt.savefig('figures/cost_function_with_path.png',dpi=300)
plt.show()
```



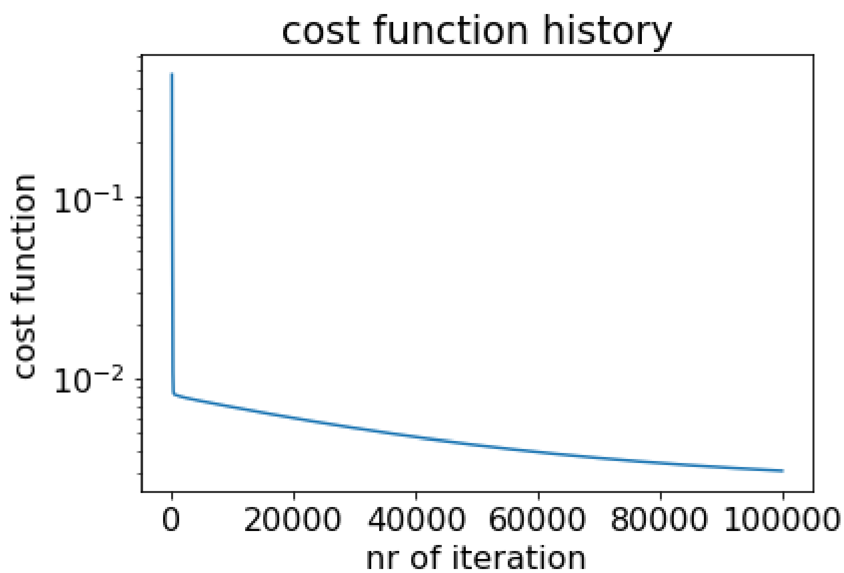

cost function parameter space
slope
intercept
cost function
path
grid search result
4
2
0
−2
−4
−4
−2
0
2
4
60
50
40
30
20
10
0

In [17]:
```
plt.plot(cost_history)
plt.semilogy()
plt.ylabel('cost function')
plt.xlabel('nr of iteration')
plt.title('cost function history')
plt.savefig('figures/cost_hist.png',dpi=300)
plt.show()
```



In [18]:
```
#theta,cost_history,theta_hist = gradient_descent(df[['x1','x2','x3','x4','x5']].values,df['y'],[1.1,-2.38,5.45,-44.7,75.33,-34.87],1.0,10000)
theta,cost_history,theta_hist = gradient_descent(df[['x1','x2','x3','x4','x5']].values,df['y'],[0,0,0,0,0,0],1.0,100000)
print(theta)

plt.plot(cost_history)
plt.semilogy()
plt.ylabel('cost function')
plt.xlabel('nr of iteration')
plt.title('cost function history')
plt.savefig('figures/cost_hist2.png',dpi=300)
plt.show()
```

```
[ 1.17809286 -1.46079625 -9.6913062   7.82929009  7.59160438 -5.4156485
4]
```




By now you can

- Describe the most commonly used regression metrics
- Describe what the cost function is
- Explain how a simple gradient descent algorithm works

In [ ]: