Welcome to Supervised Learning

Part 1: Introduction to machine learning and the bias-variance tradeoff

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https://github.com/azsom/Supervised-Learning (https://github.com/azsom/Supervised-Learning)

The topic of the course series: supervised Machine Learning (ML)

- how to build an ML pipeline from beginning to deployment
- we assume you already performed data cleaning
- this is the first course out of 6 courses
    - **Part 1: Introduction to machine learning and the bias-variance tradeoff**
    - Part 2: How to prepare your data for supervised machine learning
    - Part 3: Evaluation metrics in supervised machine learning
    - Part 4: SVMs, Random Forests, XGBoost
    - Part 5: Missing data in supervised ML
    - Part 6: Interpretability
- you can complete the courses in sequence or complete individual courses based on your interest

Tools

- we use python
    - pros: easy to use for a beginner programmer
    - cons: it is very difficult to write computationally efficient code
    - the divide between users and developers of python packages are wide
- packages we use: sklearn, pandas, numpy, matplotlib, XGBoost, SHAP
- if you are a python user, you need to know exactly what you are doing
    - carefully read the manual, work through the examples, test every line of code you write
        - good test of your understanding: could I write the function/method myself if I had to?
    - do not assume your code works, always test everything
    - there are two types of errors:
        - one that gives an error message
            - usually easy to fix

            - the error message tells you in which line the error occurs
            - read and understand the error message
            - if it's not obvious what the error is, read more on it on stackoverflow for example
        - sneaky errors without error message
            - these are tough!
            - your code runs and it gives some output but something is off
            - just staring at the code won't reveal the bug
            - print print print or use a debugger
            - check every line of code, trace issues through the code
    - to reduce the number of errors/bugs, do test-driven code development
        - first think about what the output of a function call/cell/piece of a piece of code should be
        - only then write the code
        - check if you got the expected output

Learning objectives of this course

By the end of the course, you will be able to

- describe how a task like spam filtering can be solved with explicit coding instructions vs. a machine learning algorithm that learns from examples (training data),
- summarize the similarities and differences between supervised and unsupervised ML,
- list the pros and cons of supervised machine learning,
- define the mathematical model behind linear and logistic regression,
- explain what the loss function is,
- describe the two main types of regularization and why it is important,
- perform a simple train/validation/test split on IID data,
- apply linear and logistic regression to datasets,
- tune the regularization hyperparameter,
- identify models with high bias and high variance,
- select the best model and measure its performance on a previously unseen dataset, the test set.

Module 1: Intro to Machine Learning

Learning objectives of this module:

- describe how a task like spam filtering can be solved with explicit coding instructions vs. a machine learning algorithm that learns from examples (training data),
- summarize the similarities and differences between supervised and unsupervised ML,
- list the pros and cons of supervised machine learning,

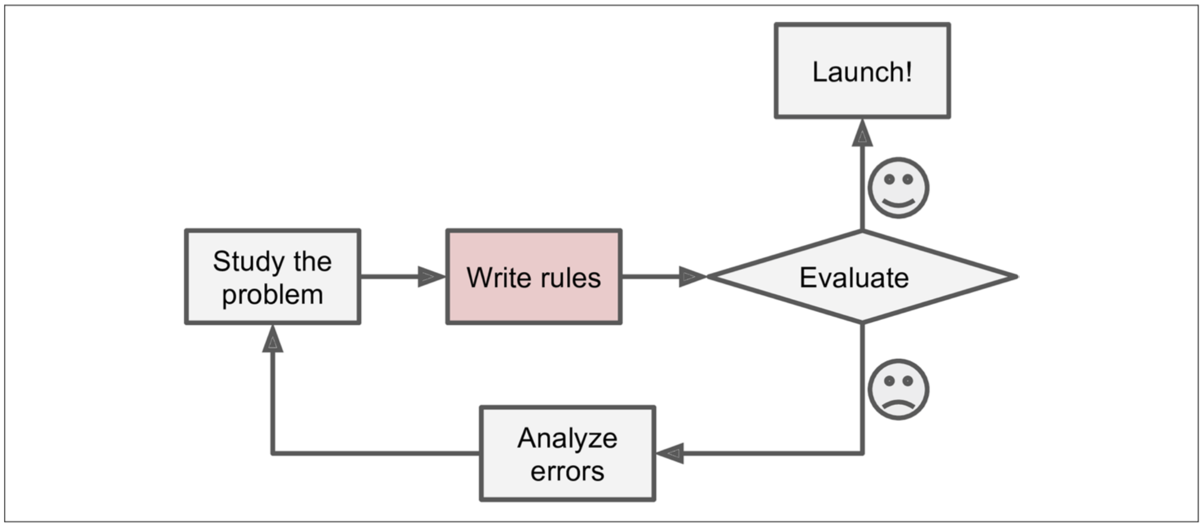
Supervised ML

- supervised ML is probably the most successful area in ML (based on economic value created)

  - **online advertising**: given an ad and user info, will the user click on the ad?
  - **real estate**: given home features, can we predict the house price?
  - **finance**: given an applicant and a finalcial product (e.g., a loan), will this applicant be able to successfully pay back the loan?
  - **health care**: given a patient, symptoms, and maybe test results, can we predict the illness?
  - ...
- supervised ML pros:
  - **automation**: computers perform calculations faster than humans (and computers are cheaper)
  - **learn from examples**: no need to explicitly tell the computer what to do. the computer figures out what to do based on examples (data)
- supervised ML con:
  - it can be difficult or labor-intensive to collect training data
  - there is no guarantee that you will be able to develop an accurate model based on the data you have

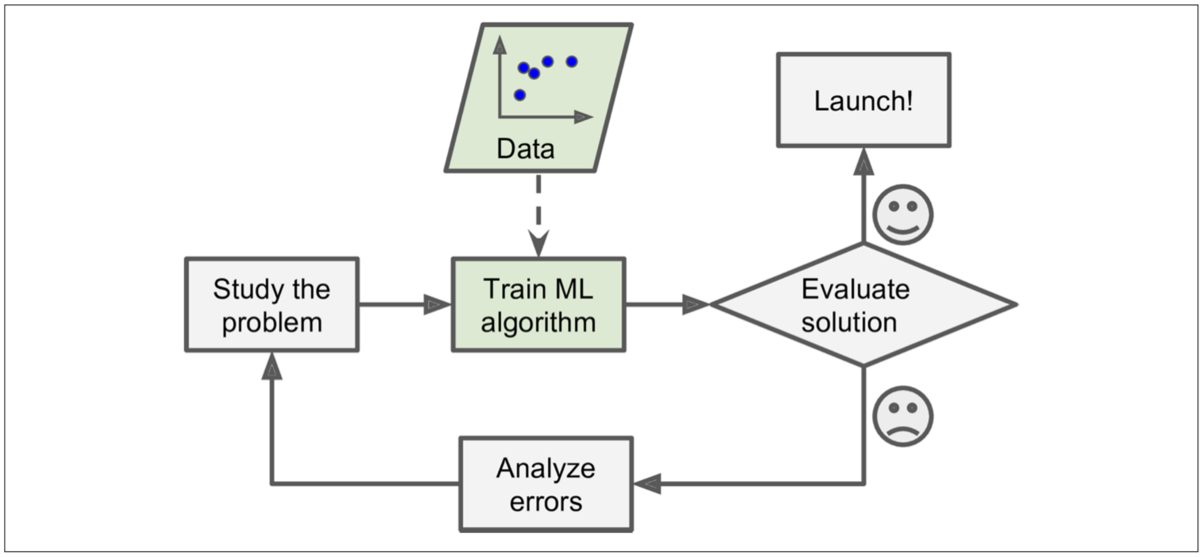
Example: spam filters

- Traditional coding pipeline with explicit instructions



Example: spam filters

- ML pipeline



- the data: feature matrix (X) and target variable (Y)
  - X can be structured (tabular data most commonly stored in excel and csv files or SQL databases)
  - X can be unstructured (e.g., images, text, voice recording, video)
  - Y can be categorical, the problem is **classification** (e.g., click or not click on an ad, sick or not sick)
  - Y can be continuous, the problem is **regression** (e.g., predict house price, stock price, age)
  - Y can be missing, the problem is **clustering**
- **we focus on structured data during the course series!**

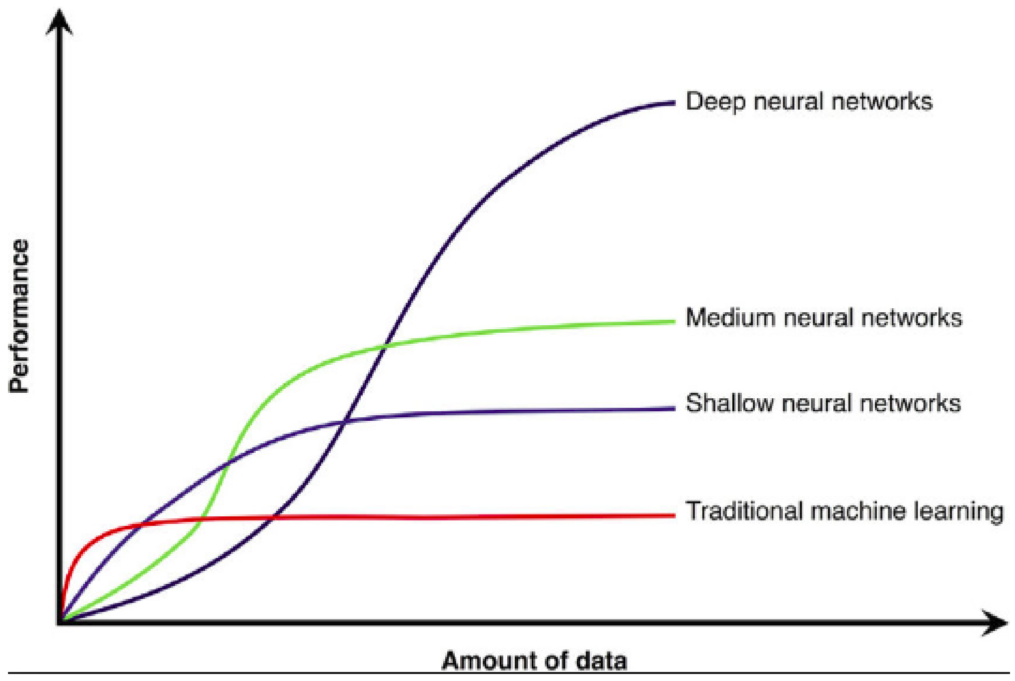
Structured data

X	**feature_1**	**feature_2**	**...**	**feature_j**	**...**	**feature_m**	**Y**
data_point_1	x_11	x_12	...	x_1j	...	x_1m	**y_1**
data_point_2	x_21	x_22	...	x_2j	...	x_2m	**y_2**
...	...	...	...	...	...	...	**...**
data_point_i	x_i1	x_i2	...	x_ij	...	x_im	**y_i**
...	...	...	...	...	...	...	**...**
data_point_n	x_n1	x_n2	...	x_nj	...	x_nm	**y_n**

Other areas of ML

- unsupervised ML
  - only the feature matrix X is available, there is no target variable
  - the goal is to find structure (clusters) in the data
  - often used in customer segmentation
- recommender systems
  - recommend products to a customer based on what products similar customers enjoyed

- reinforcement learning
    - the learning system, called an agent, can observe the environment, select and perform actions, and get rewards and penalties in return. Goal: come up with strategy to maximize rewards
    - often used when virtual environment is available (e.g., games like go or warcraft)
    - sounds appealing to use in real environments (like self-driving cars) but agents learn slow, lots of cars would need to be broken to teach an agent to drive this way
- deep learning
    - uses neural networks and often works with unstructured data
    - technically deep learning is supervised or unsupervised
    - extremely successful on large datasets



Module 2: Overview of linear and logistic regression with regularization

Learning objectives of this module:

- define the mathematical model behind linear and logistic regression,
- explain what the loss function is,
- describe the two main types of regularization and why it is important,

Supervised ML algorithms: three parts

- 1) **a mathematical model (f)** is used to convert the feature values into a prediction

$f(X_i) = y_i'$, where i is the ith data point in our sample. X_i is a vector and y_i' is a number.

```
- $f$ is your supervised ML algorithm
- it usually has a number of intrinsic parameters
```

- 2) **an optimization algorithm** is used to determine the intrinsic parameter values given the training set
  - there are various algorithms
  - e.g., gradient descent, backpropagation
- 3) the optimization algorithm minimizes a metric called **the cost function**
  - the cost function is used to determine the best intrinsic parameters of one model based on the training data

Linear Regression

In [ ]:
```python
# these lines are just illustration
# no X_train or y_train are defined yet so it won't run
from sklearn.linear_model import LinearRegression # import the model
LinReg = Linear_Regression() # initialize a simple linear regression mc
LinReg.fit(X_train,y_train) # we will learn now what happens when you i
```

- This is the **mathematical model**:

$$f(X_i) = y_i' = \theta_0 + X_{i1}\theta_1 + X_{i2}\theta_2 + \ldots = \theta_0 + \sum_{j=1}^{m} \theta_j X_{ij},$$

  where y_i' is the prediction of the linear regression model and θ are parameters.
- The **optimization algorithm** is some form of gradient descent
  - we won't go into detail but the basic idea is that gradient descent will find the θ values that minimize the cost function on the training data
- The **cost function** is MSE - mean squared error

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

Logistic Regression

In [ ]:
```python
from sklearn.linear_model import LogisticRegression
LogReg = LogisticRegression() # initialize a simple logistic regression
LogReg.fit(X_train,y_train) # we will learn what happens when you issue
```

- name is misleading, logistic regression is for classification problems!
- the model:

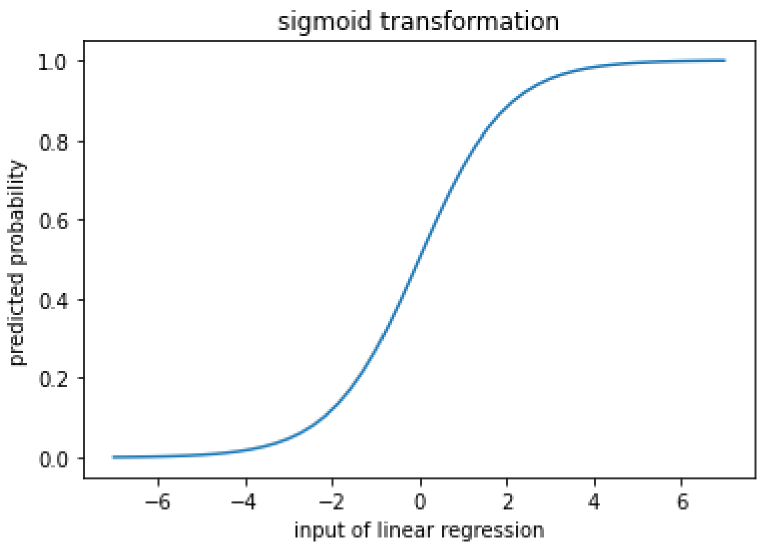
$$f(X_i) = y_i' = \frac{1}{1+e^{-z}}, \text{ where}$$
$$z = \theta_0 + \sum_{j=1}^{m} \theta_j x_{ij}$$

- $f(z) = \frac{1}{1+e^{-z}}$ is the sigmoid function which maps real values to be between 0 and 1 such that the real value 0 is mapped to 0.5.

- the output of a sigmoid function can be thought of as a predicted probability.

In [15]:
```python
import numpy as np
import matplotlib.pyplot as plt

def sigmoid(z):
    return 1/(1+np.exp(-z))

z = np.linspace(-7,7,50)
print(z)

plt.plot(z,sigmoid(z))
plt.xlabel('input of linear regression')
plt.ylabel('predicted probability')
plt.title('sigmoid transformation')
plt.savefig('figures/sigmoid_trans.png',dpi=300)
plt.show()
```

```
[-7.         -6.71428571 -6.42857143 -6.14285714 -5.85714286 -5.57142857
 -5.28571429 -5.         -4.71428571 -4.42857143 -4.14285714 -3.85714286
 -3.57142857 -3.28571429 -3.         -2.71428571 -2.42857143 -2.14285714
 -1.85714286 -1.57142857 -1.28571429 -1.         -0.71428571 -0.42857143
 -0.14285714  0.14285714  0.42857143  0.71428571  1.          1.28571429
  1.57142857  1.85714286  2.14285714  2.42857143  2.71428571  3.
  3.28571429  3.57142857  3.85714286  4.14285714  4.42857143  4.71428571
  5.          5.28571429  5.57142857  5.85714286  6.14285714  6.42857143
  6.71428571  7.        ]
```



- The **optimization algorithm** is some form of gradient descent
- the logloss metric is used as a **cost function** in logistic regression

$$L(\theta) = -\frac{1}{N}\sum_{i=1}^{n}[y_i \ln(y_i') + (1-y_i)\ln(1-y_i')]$$

- two scenarios:
  - y_i = 0 - left term disappears
  - y_i = 1 - right term disappears
- log(0) is undefined
  - y_i' is usually replaced with $\max(\min(y_i', 1-10^{-15}), 10^{-15})$ to avoid this issue

The extreme cases

- the classifier is confidently wrong
  - $y'_i = 10^{-15}$ for points in class 1
  - $y'_i = 1 - 10^{-15}$ for points in class 0

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

- the classifier is correct
  - $y'_i = 10^{-15}$ for points in class 0
  - $y'_i = 1 - 10^{-15}$ for points in class 1

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

- the logloss metric also needs to be minimized

Regularization

- models tend to overfit on the training data and such models don't perform well on previously unseen points
  - a sure sign of overfitting in linear and logistic regression is huge theta values, much larger than the typical ranges of your features and target variable
  - overfitting means that the model fits the noise rather than the underlying structure
    - e.g., fitting a high degree polinomial to a roughly linearly correlated set of points
- one way to address this shortcoming of ML models is regularization
- let's change the cost function and add a penalty term for large thetas
- **Lasso regression**: regularize using the l1 norm of theta:

$$L(\theta) = \text{original cost} + \frac{\alpha}{m}\sum_{j=0}^{m}|\theta_j|$$

- **Ridge regression**: regularize using the l2 norm of theta:

$$L(\theta) = \text{original cost} + \frac{\alpha}{m}\sum_{j=0}^{m}\theta_j^2$$

- α is the regularization parameter (0 or larger), it describes how much we penalize large thetas

Regulariztion in linear regression

- the original cost function is MSE and we add the penalty term
- **Lasso regression**: regularize using the l1 norm of theta:

$$L(\theta) = \frac{1}{n}\sum_{i=1}^{n}[(\theta_0 + \sum_{j=1}^{m}\theta_j x_{ij} - y_i)^2] + \frac{\alpha}{m}\sum_{j=0}^{m}|\theta_j|$$

- **Ridge regression**: regularize using the l2 norm of theta:

$$L(\theta) = \frac{1}{n}\sum_{i=1}^{n}[(\theta_0 + \sum_{j=1}^{m}\theta_j x_{ij} - y_i)^2] + \frac{\alpha}{m}\sum_{j=0}^{m}\theta_j^2$$

Regulariztion in logistic regression

- the original cost is logloss and we add the penalty term
- **Lasso regression**: regularize using the l1 norm of theta:

$$L(\theta) = -\frac{1}{N}\sum_{i=1}^{n}[y_i \ln(\frac{1}{1+e^{-\theta_0+\sum_{j=1}^{m}\ \theta_j x_{ij}}}) + (1-y_i)\ln(1-\frac{1}{1+e^{-\theta_0+\sum_{j=1}^{m}\ \theta_j x_{ij}}}))] + \frac{\alpha}{m}\sum_{j=0}^{m}|\theta_j|$$

- **Ridge regression**: regularize using the l2 norm of theta:

$$L(\theta) = -\frac{1}{N}\sum_{i=1}^{n}[y_i \ln(\frac{1}{1+e^{-\theta_0+\sum_{j=1}^{m}\ \theta_j x_{ij}}}) + (1-y_i)\ln(1-\frac{1}{1+e^{-\theta_0+\sum_{j=1}^{m}\ \theta_j x_{ij}}}))] + \frac{\alpha}{m}\sum_{j=0}^{m}\theta_j^2$$

Let's translate these concepts to code in the next module!

Module 3: The bias-variance tradeoff

Learning objectives of this module:

- perform a simple train/validation/test split on IID data,
- apply linear and logistic regression to datasets,
- tune the regularization hyperparameter,
- identify models with high bias and high variance,
- select the best model and measure its performance on a previously unseen dataset, the test set.

In [16]:

```python
# STEP 1: read in the data

# https://www4.stat.ncsu.edu/~boos/var.select/diabetes.html

# IID - independent and identically distributed dataset

import pandas as pd
df = pd.read_csv('https://www4.stat.ncsu.edu/~boos/var.select/diabetes.
print(df.head())

# separate out the feature matrix and the target variable
y = df.iloc[:,-1] # the last column is the target variable
X = df.iloc[:,:-1] # all but the last column are the features
print(y.head())
print(X.head())
```

```
   AGE  SEX   BMI     BP   S1     S2    S3   S4      S5  S6    Y
0   59    2  32.1  101.0  157   93.2  38.0  4.0  4.8598  87  151
1   48    1  21.6   87.0  183  103.2  70.0  3.0  3.8918  69   75
2   72    2  30.5   93.0  156   93.6  41.0  4.0  4.6728  85  141
3   24    1  25.3   84.0  198  131.4  40.0  5.0  4.8903  89  206
4   50    1  23.0  101.0  192  125.4  52.0  4.0  4.2905  80  135
0    151
1     75
2    141
3    206
4    135
Name: Y, dtype: int64
   AGE  SEX   BMI     BP   S1     S2    S3   S4      S5  S6
0   59    2  32.1  101.0  157   93.2  38.0  4.0  4.8598  87
1   48    1  21.6   87.0  183  103.2  70.0  3.0  3.8918  69
2   72    2  30.5   93.0  156   93.6  41.0  4.0  4.6728  85
3   24    1  25.3   84.0  198  131.4  40.0  5.0  4.8903  89
4   50    1  23.0  101.0  192  125.4  52.0  4.0  4.2905  80
```

In [11]:

```python
# STEP 2: split the data
from sklearn.model_selection import train_test_split

X_other, X_test, y_other, y_test = train_test_split(X,y,test_size=0.2,r
X_train, X_val, y_train, y_val = train_test_split(X_other,y_other,test_

# verify the results
print(X_train.shape) # 60% for training
print(X_val.shape) # 20% for validation
print(X_test.shape) # 20% for testing
```

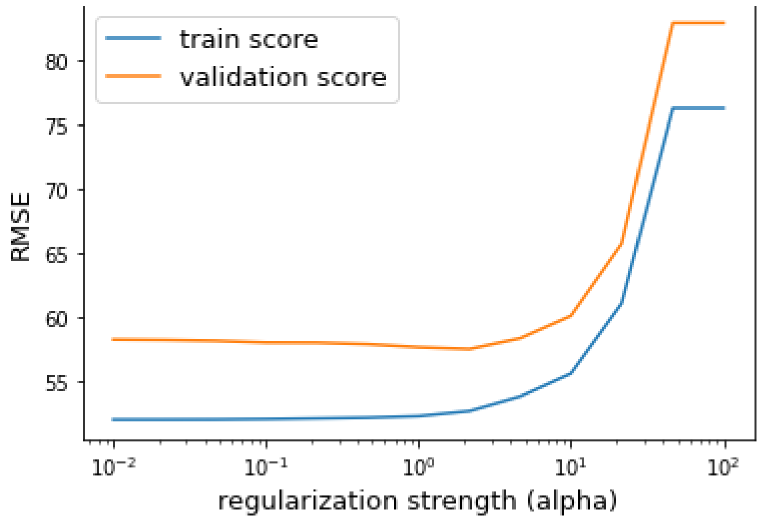
```
(264, 10)
(89, 10)
(89, 10)
```

In [12]:
```python
# STEP 3: preprocess the data
from sklearn.preprocessing import StandardScaler

scaler = StandardScaler() # initialize the scaler

X_train_prep = scaler.fit_transform(X_train)
X_val_prep = scaler.transform(X_val)
X_test_prep = scaler.transform(X_test)

# the _prep objects are now numpy arrays
# let's verify that all feature means are 0 and stds are 1
print(np.mean(X_train_prep,axis=0))
print(np.std(X_train_prep,axis=0))
print(np.mean(X_val_prep,axis=0)) # not exactly 0
print(np.std(X_val_prep,axis=0)) # not exactly 1
print(np.mean(X_test_prep,axis=0)) # not exactly 0
print(np.std(X_test_prep,axis=0)) # not exactly 1
```

```
[-1.88401483e-16  1.68215610e-16 -1.58122673e-16  2.85966537e-16
 -2.92695161e-16 -3.36431220e-17 -3.70074342e-17  4.47453522e-16
 -7.77156117e-16  4.97918205e-16]
[1. 1. 1. 1. 1. 1. 1. 1. 1. 1.]
[ 0.00482376 -0.03301861  0.12600247 -0.01374034  0.05696159  0.0065957
  0.14555163 -0.13140355 -0.02451996 -0.09520641]
[1.04300891 0.99719443 1.03188936 1.0245732  1.02866879 1.00032617
 0.91058225 0.8268551  1.07662793 1.04397869]
[ 0.0152835   0.05707869 -0.15068117 -0.09269383 -0.07121409 -0.08617701
  0.12650139 -0.15334999 -0.08066075 -0.18983855]
[1.03447167 1.00226924 0.94563471 0.99350518 1.00946002 1.04830518
 1.05149569 0.95477113 0.92799668 0.86719968]
```

In [13]:
```python
# STEP 4:
# train linear regression models
# tune the regularization parameter
# calculate and visualize train and validation scores
# select the model that performs best on the validation set
# calculate the generalization error using the test set

from sklearn.linear_model import Lasso
from sklearn.metrics import mean_squared_error

alphas = np.logspace(-2,2,13)
print(alphas)

train_scores = []
val_scores = []
models = []
for alpha in alphas:
    # initialize the model
    linreg = Lasso(alpha=alpha)
    # fit it to the training set
    linreg.fit(X_train_prep,y_train)
    # save the model
    models.append(linreg)
    # calculate and save train score
    y_train_pred = linreg.predict(X_train_prep)
    train_score = mean_squared_error(y_train,y_train_pred,squared=False
    train_scores.append(train_score)
    # calculate and save val score
    y_val_pred = linreg.predict(X_val_prep)
    val_score = mean_squared_error(y_val,y_val_pred,squared=False)
    val_scores.append(val_score)

# let's visualize the train and validation scores
plt.plot(alphas,train_scores,label='train score')
plt.plot(alphas,val_scores,label='validation score')
plt.xlabel('regularization strength (alpha)',fontsize=13)
plt.ylabel('RMSE',fontsize=13)
plt.semilogx()
plt.legend(fontsize=13)
plt.savefig('figures/bias-variance.png',dpi=300)
plt.show()
```

```
[1.00000000e-02 2.15443469e-02 4.64158883e-02 1.00000000e-01
 2.15443469e-01 4.64158883e-01 1.00000000e+00 2.15443469e+00
 4.64158883e+00 1.00000000e+01 2.15443469e+01 4.64158883e+01
 1.00000000e+02]
```



The bias-variance tradeoff

- high alpha (strong regularization):
    - the model is too simple
    - it performs poorly on both the training and validation sets (RMSEs are large)
    - high bias or low variance model
- low alpha (weak regularization)
    - the model is too complex
    - it performs very well on the training set but it performs comparatively poorly on the validation set
    - low bias or high variance model
- we are looking for the sweet spot in between
    - if your evaluation metric needs to be minimized (e.g., MSE, RMSE, logloss)
        - select the alpha with the smallest validation score
        - the corresponding model is the best
    - if your evaluation metric needs to be maximized (e.g., accuracy, R2)
        - select the alpha with the largest validation score
        - the corresponding model is the best

Let's select the best model and calculate the generalization error

In [14]:
```
indx = np.argmin(val_scores)
print('best alpha:',alphas[indx]) # the best alpha value
print('best validation score:',val_scores[indx]) # the validation score
final_model = models[indx] # pull out the best model
y_test_pred = final_model.predict(X_test_prep)
gen_error = mean_squared_error(y_test,y_test_pred,squared=False)
print('the generalization error:',gen_error) # the error we expect from
```

```
best alpha: 2.154434690031882
best validation score: 57.4873819354221
the generalization error: 54.72060685174691
```

Things we ignored but will cover in later courses

Things we ignored but will cover in later courses

- uncertainty due to splitting
  - different random states in train_test_split place different points in train/val/test
  - the random splitting of points introduces an uncertainty in the train/val/test scores and the best alpha values too
  - redo the whole pipeline with a couple of different random states to measure the uncertainty of generalization
- splitting
  - simple IID datasets like this are rare
  - part 2 covers more interesting splitting strategies
- preprocessing
  - this dataset is simple, all features are already numerical so preprocessing was easy (one standard scaler)
  - part 2 deals with more complex preprocessing pipelines
- more complex models have more than one hyperparameters to tune
  - nested for loops should be avoided
  - sklearn has excellent tools to do hyperparameter tuning over an arbitrary number of parameters
  - we cover this in part 4
- interpretability
  - predictions are often not enough!
  - you need to be able to explain how the model works and how it makes predictions
  - the doctor needs to be able to explain to the patient what factors influence the predicted disease progression in general but also for that patient in particular
  - part 6 covers this in detail

```
In [ ]:
```