ECE 20875

Python for Data Science

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(Adapted from material developed by Profs. Milind Kulkarni, Stanley Chan, Chris Brinton, David Inouye)

classification: logistic regression

regression with two classes

- With linear regression, we model the relationship between features and target with a linear equation:

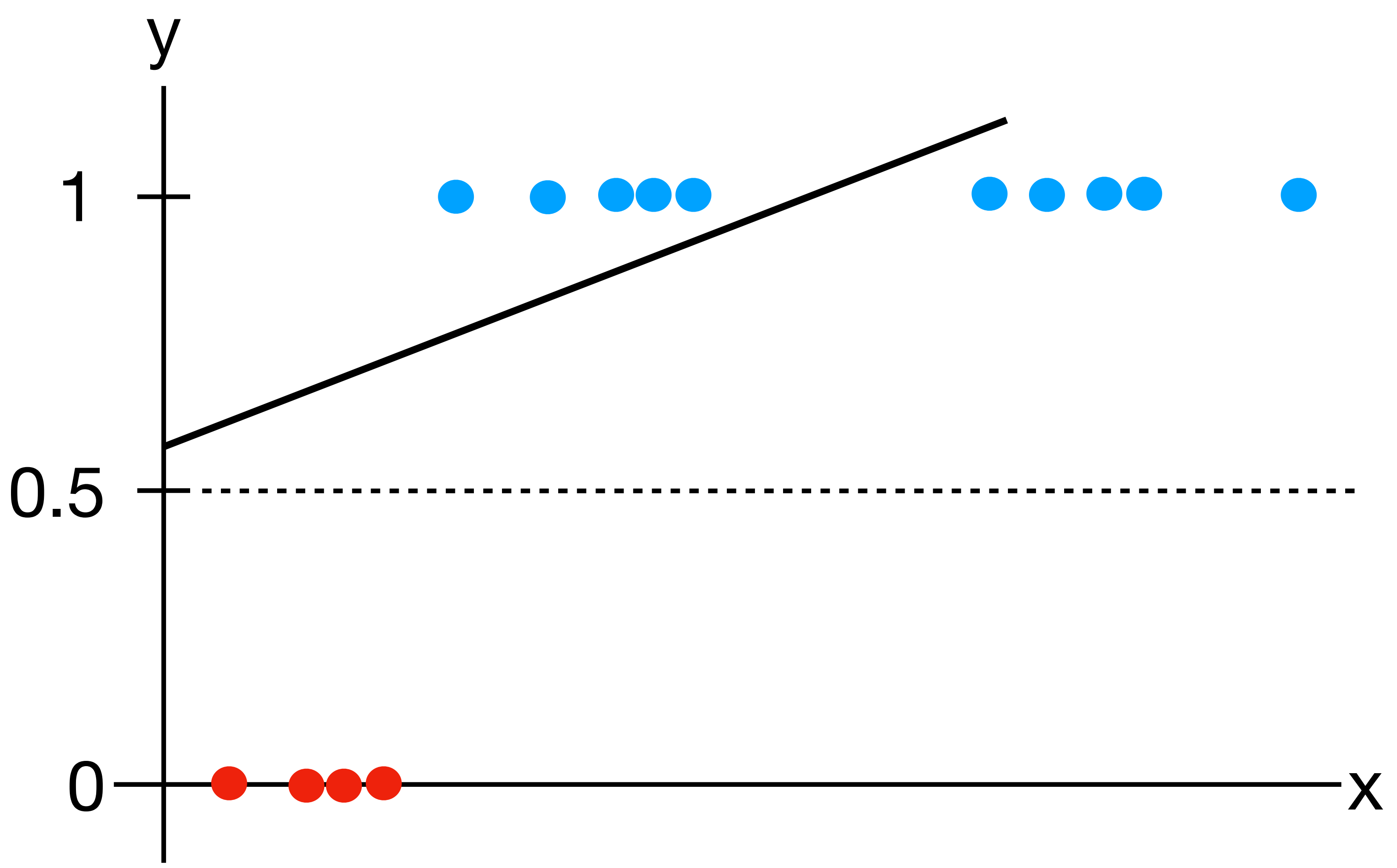
$$\hat{y}_i = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \cdots + \beta_m x_m$$

- Now, suppose we have two classes, i.e., $y \in \{0, 1\}$. We could use linear regression, but …

    - it will treat the classes as numbers, interpolating between the points

    - it cannot be interpreted as a probability

    - how would we generalize to multiple classes?



- Need a decision threshold, i.e., $y = 0.5$

- In this case, we would never predict the class $y = 0$, regardless of what x is!

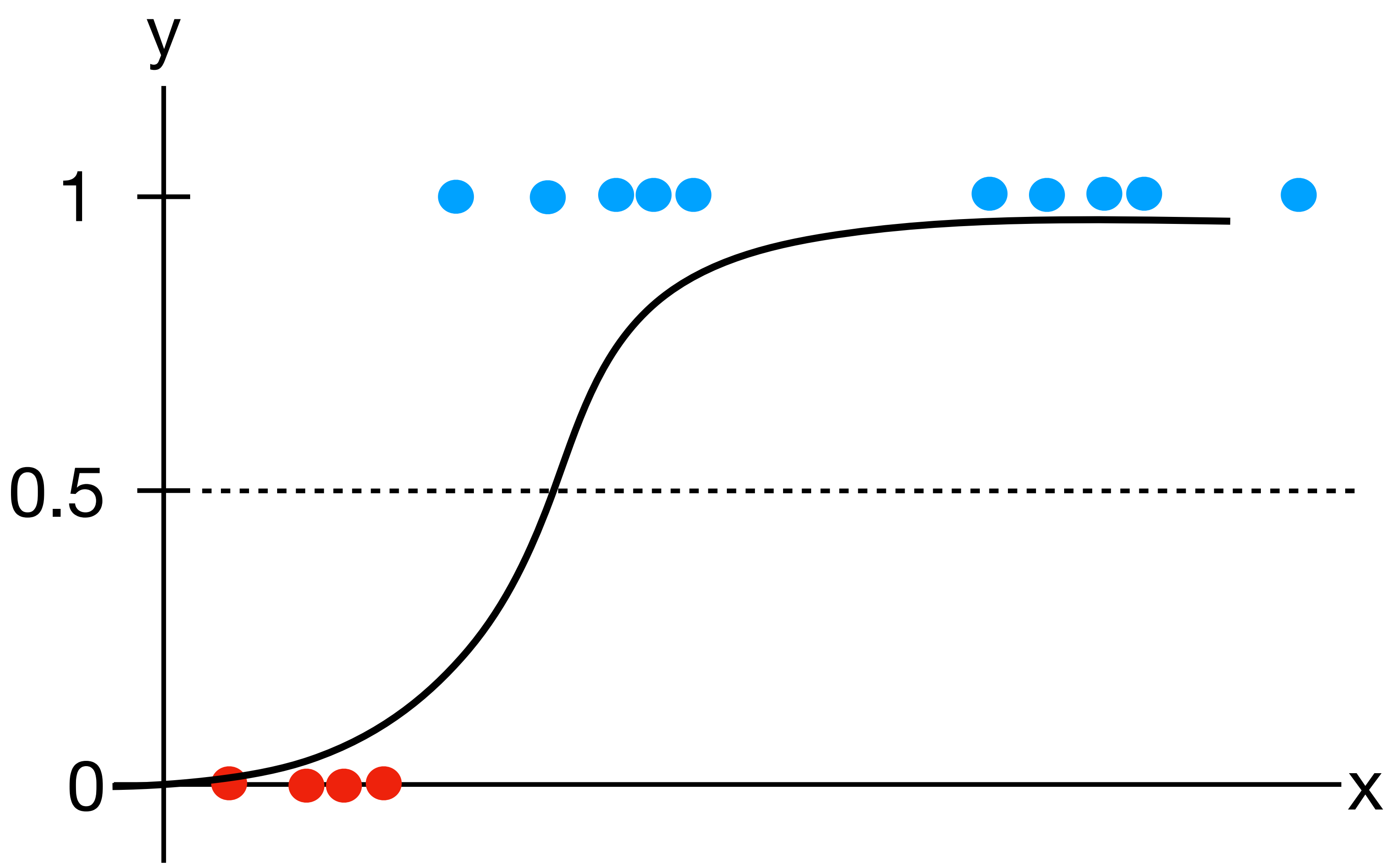
logistic regression model

- Instead of fitting a **hyperplane** (a line generalized to more than one dimension), use the **logistic function**

$$g(v) = \frac{1}{1 + e^{-v}}$$

to translate the output of linear regression to between 0 (as $v \to -\infty$) and 1 (as $v \to \infty$)

- Note that $1 - g(v) = \dfrac{e^{-v}}{1 + e^{-v}}$ (useful for derivations)



- This converts the outputs to probabilities:

$$\begin{aligned} f_\beta(x) &= g(\beta_0 + \beta^T x) = P(y = 1 \,|\, x) \\ &= \frac{1}{1 + \exp(-(\beta_0 + \beta_1 x_1 + \beta_2 x_2 + \cdots + \beta_m x_m))} \end{aligned}$$

- Now the **decision rule**
  - $\hat{y}(x) \geq 0.5 \to \hat{y} = 1$
  - $\hat{y}(x) < 0.5 \to \hat{y} = 0$

has a probabilistic interpretation

interpreting coefficients

- In linear regression, the effect of a coefficient is clear: $\beta_j x_j$ means for every unit change in x_j, the model changes by β_j
- For logistic regression, we need to find a different interpretation, since the weights no longer have a linear effect
- Consider the **odds**, i.e., the ratio $P(y=1\,|\,x)/P(y=0\,|\,x)$:
- $$\frac{P(y=1\,|\,x)}{P(y=0\,|\,x)} = \frac{1}{1+\exp(-(\beta_0+\beta_1x_1+\cdots+\beta_mx_m))}\cdot\frac{1+\exp(-(\beta_0+\beta_1x_1+\cdots+\beta_mx_m))}{\exp(-(\beta_0+\beta_1x_1+\cdots+\beta_mx_m))}$$

$$= \frac{1}{\exp(-(\beta_0+\beta_1x_1+\cdots+\beta_mx_m))} = \exp(\beta_0+\beta_1x_1+\cdots+\beta_mx_m)$$

interpreting coefficients

- Then we consider the ratio of the odds when x_j is increased by 1:

$$\frac{\text{odds}_{x_j+1}}{\text{odds}_{x_j}} = \frac{\exp(\cdots + \beta_j(x_j+1) + \cdots)}{\exp(\cdots + \beta_j x_j + \cdots)} = e^{\beta_j}$$

- Thus, a unit change in x_{ij} corresponds to a factor e^{β_j} change in the odds
  - $e^{\beta_j} > 1$: x_j increases the odds
  - $e^{\beta_j} < 1$: x_j decreases the odds

- Consider

$$\hat{y} = \frac{1}{1 + \exp(-(3 + 2x_1 + 0.5x_2 - 3x_3))}$$

- For this model …
  - x_1 and x_2 increase the odds
  - x_3 decreases the odds
  - x_3 has the largest factor impact on the odds (assuming the features are normalized!)

training logistic regression

- With linear regression, we can derive a closed-form solution for the parameters in terms of the least-squares equations

- For logistic regression, let's consider the **likelihood** of the model over data samples $i = 1,\ldots,n$:

$$L(\beta) = \prod_{i=1}^{n} p(y_i \,|\, x_i, \beta) = \prod_{i=1}^{n} (f_\beta(x_i))^{y_i} \cdot (1 - f_\beta(x_i))^{1-y_i}$$

when $y_i = 1$, we want to maximize $f_\beta(x_i)$, and
when $y_i = 0$, we want to maximize $1 - f_\beta(x_i)$

- And then the **log likelihood**, which is easier to optimize (like we did with GMMs):

$$l(\beta) = \sum_{i=1}^{n} \log \left[(f_\beta(x_i))^{y_i} \cdot (1 - f_\beta(x_i))^{1-y_i} \right] = \sum_{i=1}^{n} \left[y_i \log f_\beta(x_i) + (1 - y_i) \log(1 - f_\beta(x_i)) \right]$$

- There is no (known) closed form solution to maximize $l(\beta)$, given the $\log f_\beta(x_i)$ terms

gradient descent (ascent)

- We want to find β to *maximize* $l(\beta)$ but no closed-form exists.

- Consider the **gradient descent (ascent)** algorithm, an iterative procedure for finding a **local minimum (maximum)** of a function by moving away from (towards) the gradient:

$$\beta_j^{t+1} = \beta_j^t - \alpha^t \frac{\partial}{\partial \beta_j} l(\beta^t),$$

Gradient Descent

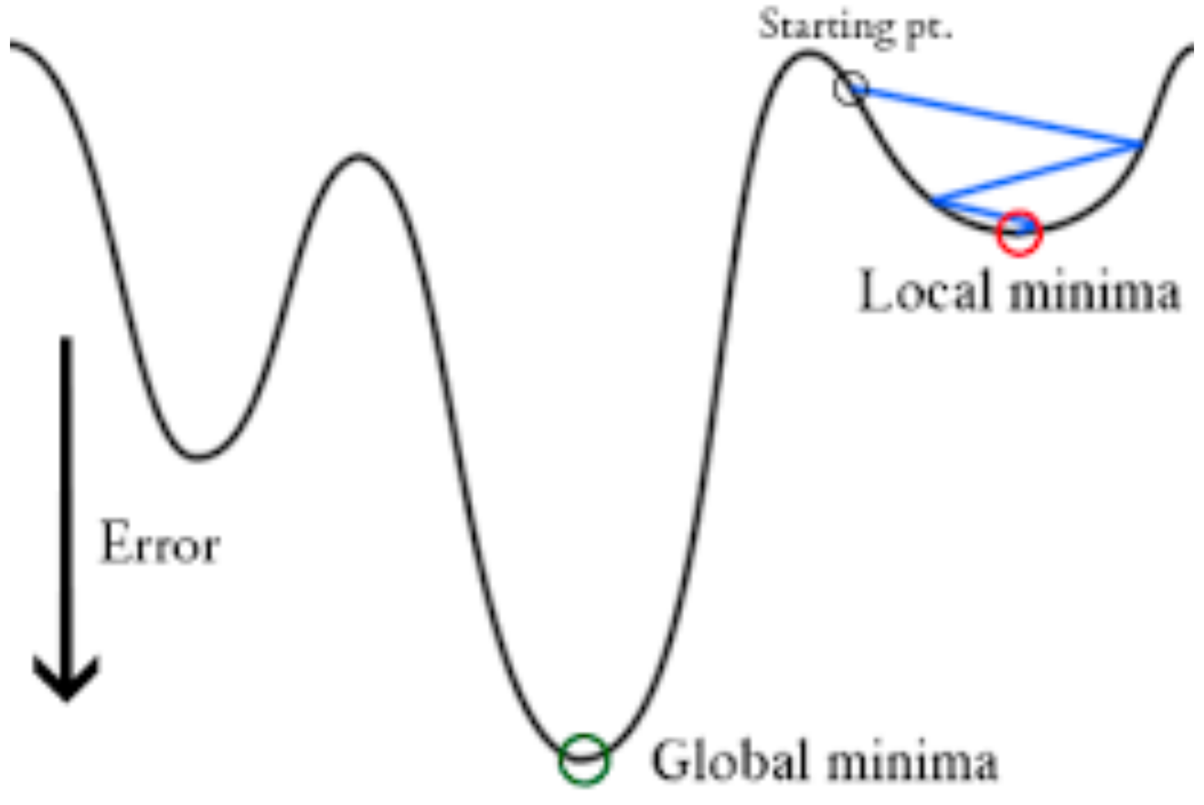
$$\boxed{\beta_j^{t+1} = \beta_j^t + \alpha^t \frac{\partial}{\partial \beta_j} l(\beta^t)}$$

Gradient Ascent

  - Here, α^t is the **step size** of the algorithm at time t

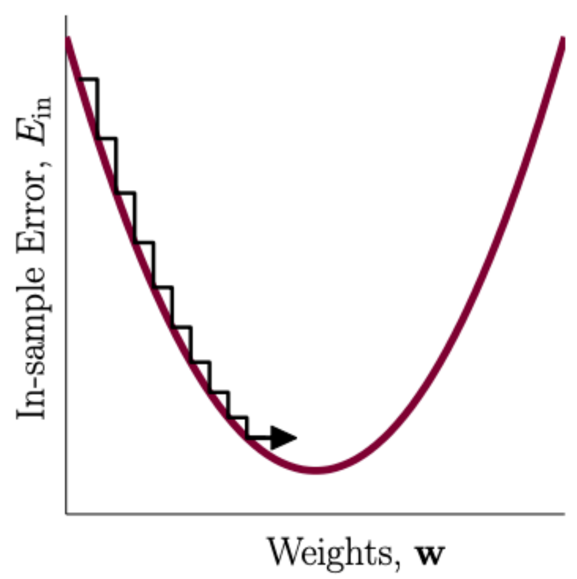
- Since $l(\beta)$ is a **concave** function, we can *guarantee* that gradient ascent will eventually converge to the **global maximum**, so long as certain conditions on α^t are met

for non-convex functions, no guarantee of convergence to optimum

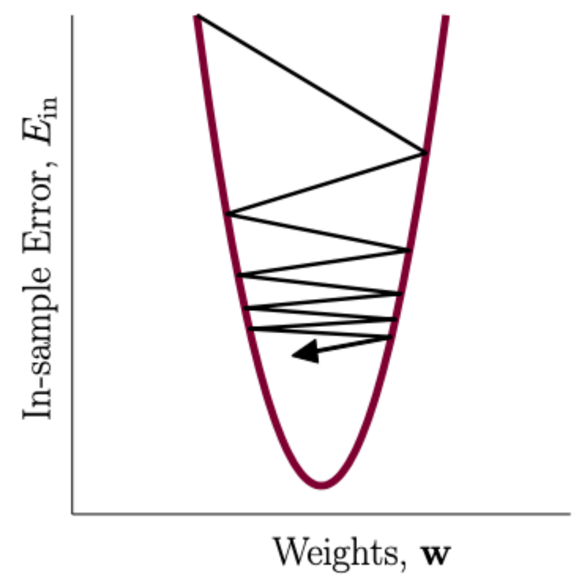


in general, the step size must be tuned correctly

η too small



η too large



gradient ascent t example

Suppose we have a single parameter b for some model we are trying to train. For this model, we find a log-likelihood function of

$$l(b) = -\left(\frac{b-m}{s}\right)^2$$

where m and s are constants. Derive the iterative procedure for determining the model parameters as a function of the step size α^t. Run the procedure for different values of α^t until $t = 10$ and compare the results.

solution

$$l(b) = -\left(\frac{b-m}{s}\right)^2$$

We always want to maximize the log-likelihood, so we use gradient *ascent*. Letting b^t be the value of b at iteration t, our update procedure will be:

$$b^{t+1} = b^t + \alpha^t \frac{d}{db} l(b^t)$$

Evaluating the derivative, this becomes:

$$b^{t+1} = b^t - 2\alpha^t \left(\frac{b^t - m}{s^2}\right)$$

Suppose $\alpha = 0.1$, $m = 5$, $s = 0.7$. If we start at $b^0 = 1.1$ (arbitrary), we get

$$b^1 = 1.1 - 2 \cdot 0.1 \cdot \left(\frac{1.1 - 5}{0.7^2}\right) = 2.692$$

$$b^2 = 2.692 - 2 \cdot 0.1 \cdot \left(\frac{2.692 - 5}{0.7^2}\right) = 3.634$$

…

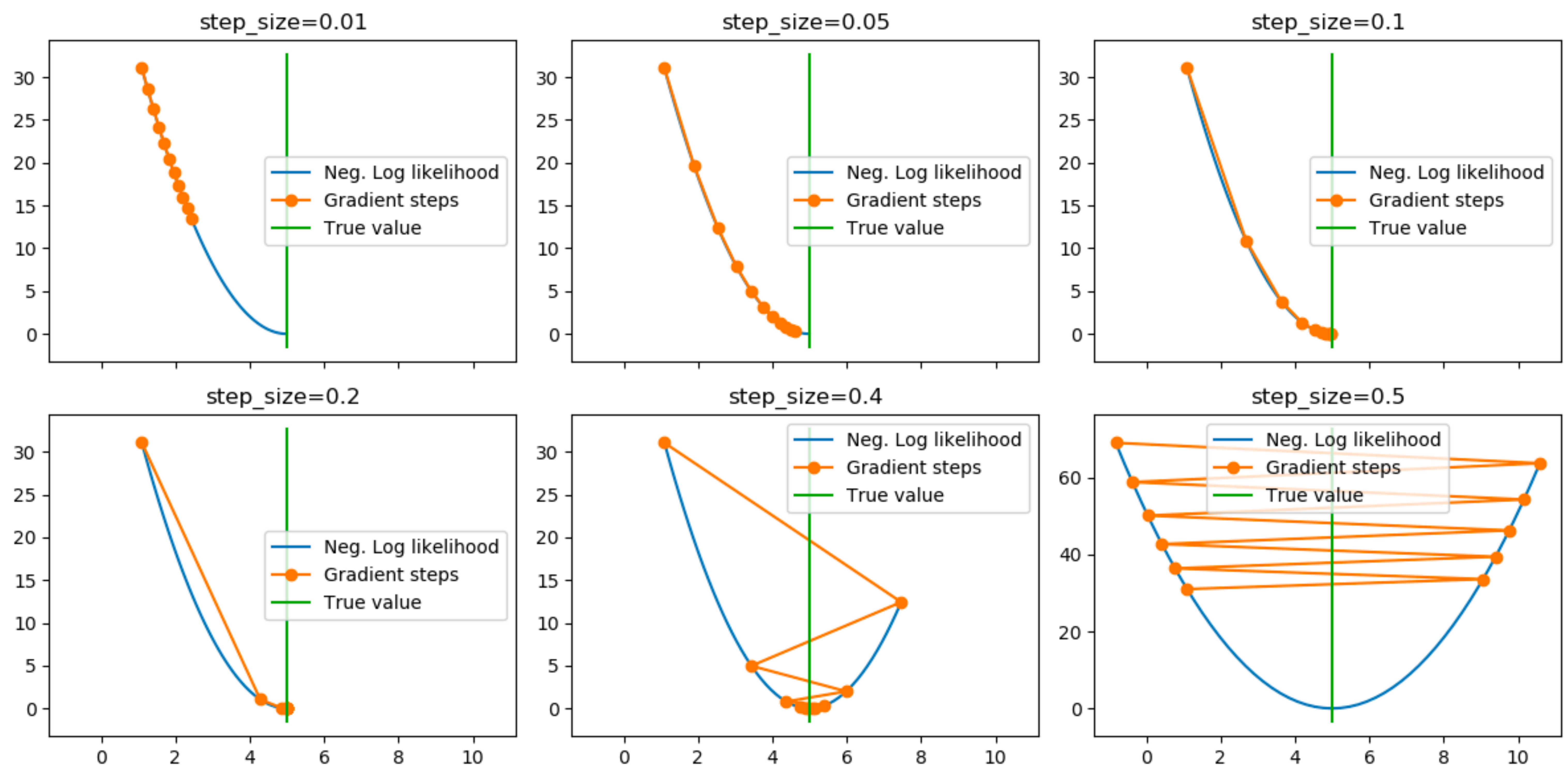
$$b^{10} = 4.965 - 2 \cdot 0.1 \cdot \left(\frac{4.965 - 5}{0.7^2}\right) = 4.979$$

solution

Below, we plot the evolution of b^t over t (see the Jupyter notebook), starting with $b^0 = 1.1$ for $\alpha^t = 0.01, 0.05, 0.1, 0.2, 0.4, 0.5$. Again, we set $m = 5$ and $s = 0.7$.

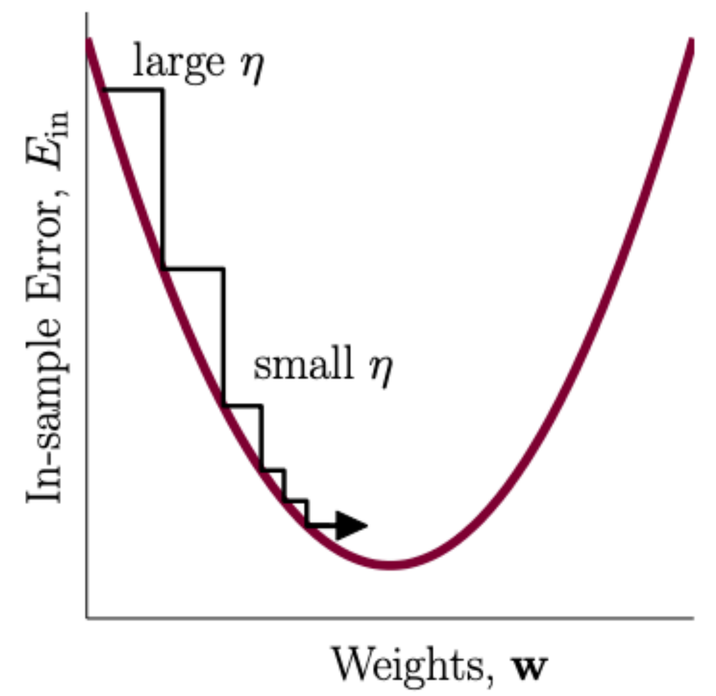
Here, the y-axis is actually $-l(b)$, to make the values positive. Maximizing the log-likelihood is equivalent to minimizing the negative log-likelihood.

Tuning α^t is a very important question!



gradient ascent for logistic regression

variable η_t – just right



- Back to logistic regression. Evaluating the partial derivative,

$$\frac{\partial}{\partial \beta_j} l(\beta) = \frac{\partial}{\partial \beta_j} \sum_{i=1}^{n} \left[y_i \log f_\beta(x_i) + (1 - y_i) \log(1 - f_\beta(x_i)) \right]$$

$$= \sum_{i=1}^{n} \left(\frac{y_i}{f_\beta(x_i)} - \frac{1 - y_i}{1 - f_\beta(x_i)} \right) \frac{\partial}{\partial \beta_j} f_\beta(x_i)$$

Partial derivative of loss with respect to $f_\beta(x_i)$

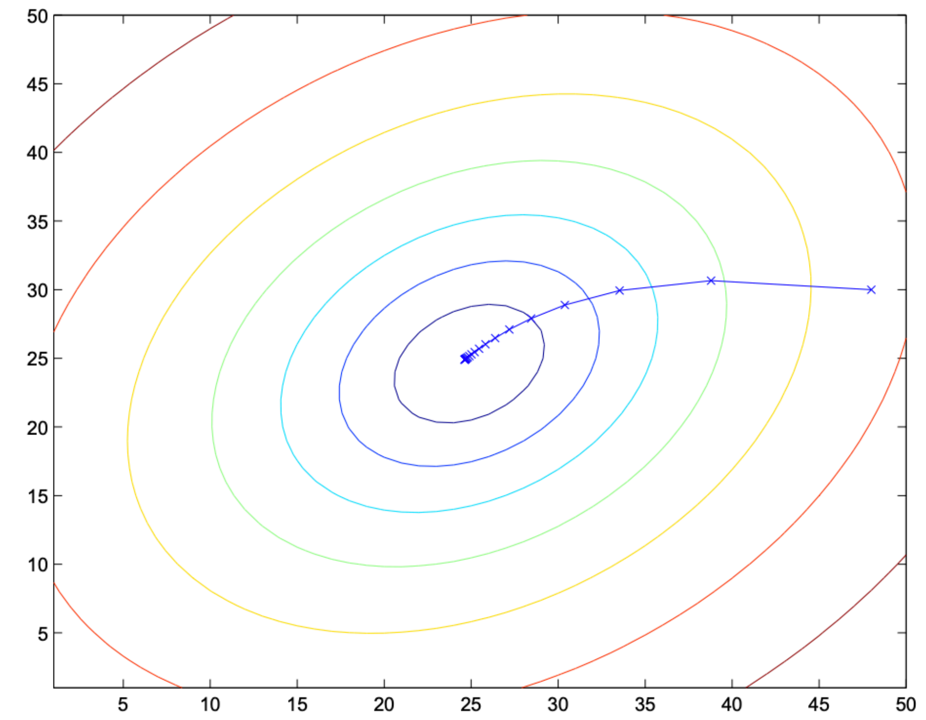
Partial derivative of logistic function $g(v)$ with respect to $v_i \equiv \beta_1 x_{i1} + \beta_2 x_{i2} + \ldots$

$$\frac{\partial}{\partial v} g(v) = \frac{\partial}{\partial v} (1 + e^{-v})^{-1} = -(1 + e^{-v})^{-2} e^{-v}(-1) = g(v)(1 - g(v))$$

$$= \sum_{i=1}^{n} \left(\frac{y_i}{f_\beta(x_i)} - \frac{1 - y_i}{1 - f_\beta(x_i)} \right) f_\beta(x_i)(1 - f_\beta(x_i)) \frac{\partial}{\partial \beta_j} (\cdots + \beta_j x_{ij} + \cdots)$$

Partial derivative of v_i with respect to β_j

$$= \sum_{i=1}^{n} \left(y_i (1 - f_\beta(x_i)) - (1 - y_i) f_\beta(x_i) \right) x_{ij} = \sum_{i=1}^{m} (y_i - f_\beta(x_i)) x_{ij}$$



- Thus, we get the following gradient ascent rule for logistic regression:

$$\beta_j^{t+1} = \beta_j^t + \alpha^t \left[\sum_{i=1}^{n} (y_i - f_\beta(x_i)) x_{ij} \right]$$

in python

- `from sklearn.linear_model import LogisticRegression`
  - https://scikit-learn.org/stable/modules/generated/sklearn.linear_model.LogisticRegression.html
- Most methods (`fit`, `predict`, …) are the same as linear regression
- One difference: Regularization parameter C
  - Higher C: *Less* regularization
  - Lower C: *More* regularization

```
from sklearn.linear_model
import LogisticRegression

from sklearn import metrics

logreg = LogisticRegression()

logreg.fit(X_train,y_train)

y_pred = logreg.predict(X_test)

metrics.accuracy_score(y_test,y
_pred)
```