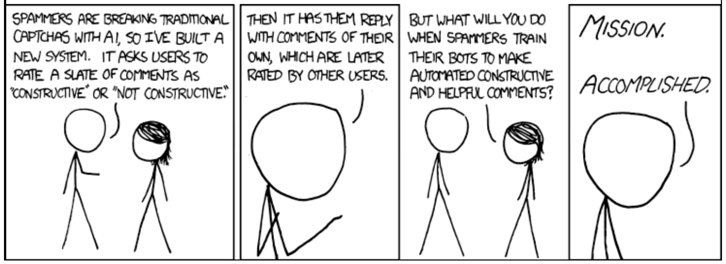
Linear models: Logistic regression

Chapter 3.3


SPAMMERS ARE BREAKING TRADITIONAL CAPTCHAS WITH A.I., SO I'VE BUILT A NEW SYSTEM. IT ASKS USERS TO RATE A SLATE OF COMMENTS AS "CONSTRUCTIVE" OR "NOT CONSTRUCTIVE."
THEN IT HAS THEM REPLY WITH COMMENTS OF THEIR OWN, WHICH ARE LATER RATED BY OTHER USERS.
BUT WHAT WILL YOU DO WHEN SPAMMERS TRAIN THEIR BOTS TO MAKE AUTOMATED CONSTRUCTIVE AND HELPFUL COMMENTS?
MISSION.
ACCOMPLISHED.

Predicting probabilities

Objective: learn to predict a probability $P(y \mid x)$ for a binary classification problem using a linear classifier

The target function: $f(\mathbf{x}) = \mathbb{P}[y = +1 \mid \mathbf{x}].$

$$P(y \mid \mathbf{x}) = \begin{cases} f(\mathbf{x}) & \text{for } y = +1; \\ 1 - f(\mathbf{x}) & \text{for } y = -1. \end{cases}$$

For positive examples $P(y = +1 \mid x) = 1$ whereas $P(y = +1 \mid x) = 0$ for negative examples.

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We'll assume a particular form for f(x).

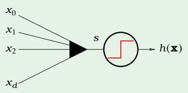
Can we assume that f(x) is linear?

Another linear model

The signal $s = \mathbf{w}^{\mathsf{T}}\mathbf{x}$ is the basis for several linear models:

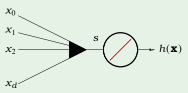
linear classification

$h(\mathbf{x}) = \text{sign}(s)$



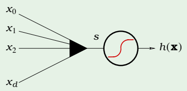
linear regression

$h(\mathbf{x}) = s$



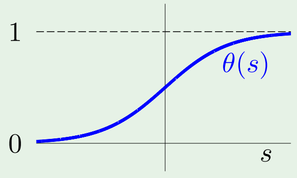
logistic regression

$h(\mathbf{x}) = \theta(s)$



The logistic function (aka squashing function):

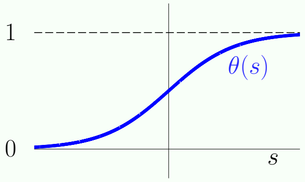
$$\theta(s) = \frac{e^s}{1 + e^s}$$



Properties of the logistic function

$$\theta(s) = \frac{e^s}{1+e^s} = \frac{1}{1+e^{-s}}.$$

$$\theta(-s) = \frac{e^{-s}}{1+e^{-s}} = \frac{1}{1+e^s} = 1-\theta(s).$$



Predicting probabilities

Fitting the data means finding a good hypothesis h

$$h \text{ is good if: } \begin{cases} h(\mathbf{x}_n) \approx 1 & \text{whenever } y_n = +1; \\ h(\mathbf{x}_n) \approx 0 & \text{whenever } y_n = -1. \end{cases}$$

Suppose that $h(\mathbf{x}) = \theta(\mathbf{w}^{\mathrm{T}}\mathbf{x})$ closely captures $\mathbb{P}[+1|\mathbf{x}]$:

$$P(y \mid \mathbf{x}) = \begin{cases} \theta(\mathbf{w}^{\mathrm{T}}\mathbf{x}) & \text{for } y = +1; \\ 1-\theta(\mathbf{w}^{\mathrm{T}}\mathbf{x}) & \text{for } y = -1. \end{cases}$$

Predicting probabilities

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$$P(y \mid \mathbf{x}) = \begin{cases} \theta(\mathbf{w}^{\mathrm{T}}\mathbf{x}) & \text{for } y = +1; \\ \theta(-\mathbf{w}^{\mathrm{T}}\mathbf{x}) & \text{for } y = -1. \end{cases}$$

More compactly: $P(y \mid \mathbf{x}) = \theta(y \cdot \mathbf{w}^{\mathrm{T}}\mathbf{x})$

Is logistic regression really linear?

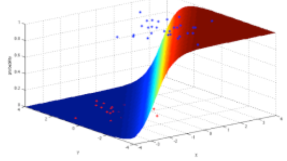
$$P(y=+1|\mathbf{x}) = \frac{\exp(\mathbf{w}^{\intercal}\mathbf{x})}{\exp(\mathbf{w}^{\intercal}\mathbf{x})+1}$$

$$P(y=-1|\mathbf{x}) = 1 - P(y=+1|\mathbf{x}) = \frac{1}{\exp(\mathbf{w}^{\intercal}\mathbf{x})+1}$$

To figure out how the decision boundary looks like consider:

$$\ln \frac{P(y=+1|\mathbf{x})}{P(y=-1|\mathbf{x})} = \mathbf{w}^{\intercal}\mathbf{x}$$

i.e. linear!



Maximum likelihood

We will find **w** using the principle of maximum likelihood.

Likelihood:
The probability of getting the $y_1, \ldots, y_N$ in $\mathcal{D}$ from the corresponding $\mathbf{x}_1, \ldots, \mathbf{x}_N$:

$$P(y_1, \ldots, y_N \mid \mathbf{x}_1, \ldots, \mathbf{x}_n) = \prod_{n=1}^{N} P(y_n \mid \mathbf{x}_n).$$

Valid since $(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_N, y_N)$ are independently generated

Maximizing the likelihood

$$\begin{aligned}
& \max && \textstyle\prod_{n=1}^{N} P(y_n \mid \mathbf{x}_n) \\
\Leftrightarrow\ & \max && \ln\left(\textstyle\prod_{n=1}^{N} P(y_n \mid \mathbf{x}_n)\right) \\
\equiv\ & \max && \textstyle\sum_{n=1}^{N} \ln P(y_n \mid \mathbf{x}_n) \\
\Leftrightarrow\ & \min && -\tfrac{1}{N}\textstyle\sum_{n=1}^{N} \ln P(y_n \mid \mathbf{x}_n) \\
\equiv\ & \min && \tfrac{1}{N}\textstyle\sum_{n=1}^{N} \ln \frac{1}{P(y_n \mid \mathbf{x}_n)} \\
\equiv\ & \min && \tfrac{1}{N}\textstyle\sum_{n=1}^{N} \ln \frac{1}{\theta(y_n \cdot \mathbf{w}^{\mathrm{T}}\mathbf{x}_n)} \\
\equiv\ & \min && \tfrac{1}{N}\textstyle\sum_{n=1}^{N} \ln(1 + e^{-y_n \cdot \mathbf{w}^{\mathrm{T}}\mathbf{x}_n})
\end{aligned}$$

Maximizing the likelihood

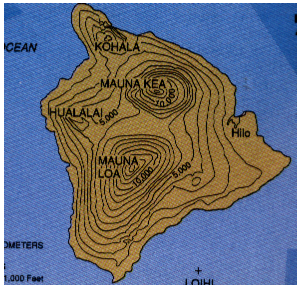
Summary: maximizing the likelihood is equivalent to

$$\text{minimize} \quad E_{\text{in}}(\mathbf{w}) = \frac{1}{N}\sum_{n=1}^{N} \underbrace{\ln\left(1 + e^{-y_n \mathbf{w}^{\mathrm{T}}\mathbf{x}_n}\right)}_{\mathrm{e}\left(h(\mathbf{x}_n), y_n\right)}$$

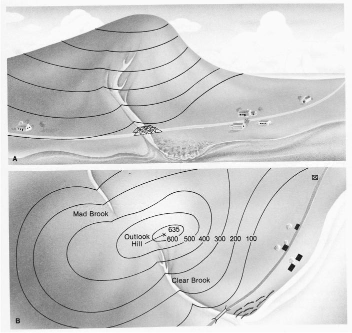
Cross entropy error

Digression: gradient descent

Topographical maps can give us some intuition about how to optimize a cost function



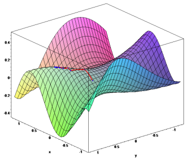
http://www.csus.edu/indiv/s/slaymaker/archives/geol101/shield1.jpg

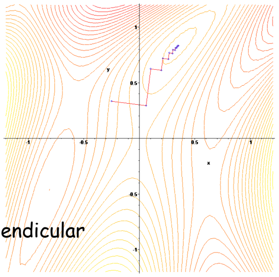


http://www.sir-ray.com/touro/IMG_0001_NEW.jpg

Digression: gradient descent

Given a function E(**w**), the gradient is the direction of steepest ascent
Therefore to minimize E(**w**), take a step in the direction of the negative of the gradient





Notice that the gradient is perpendicular to contours of equal E(**w**)

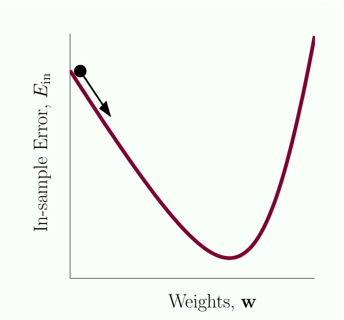
Images from http://en.wikipedia.org/wiki/Gradient_descent

Gradient descent

Gradient descent is an iterative process

$$\mathbf{w}(t+1) = \mathbf{w}(t) + \eta\hat{\mathbf{v}}$$

How to pick $\hat{\mathbf{v}}$?



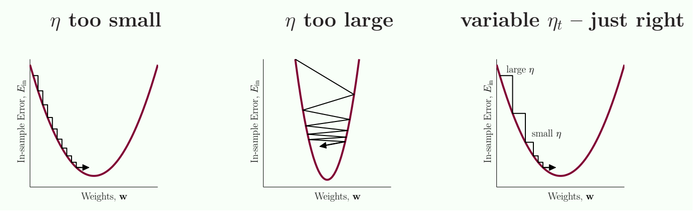
Gradient descent

The gradient is the best direction to take to optimize $E_{\text{in}}(\mathbf{w})$:

$$\begin{aligned}\Delta E_{\text{in}} &= E_{\text{in}}(\mathbf{w}(t+1)) - E_{\text{in}}(\mathbf{w}(t)) \\ &= E_{\text{in}}(\mathbf{w}(t)+\eta\hat{\mathbf{v}}) - E_{\text{in}}(\mathbf{w}(t)) \\ &= \eta\,\underbrace{\nabla E_{\text{in}}(\mathbf{w}(t))^{\mathrm{T}}\hat{\mathbf{v}}}_{\text{minimized at } \hat{\mathbf{v}} = -\frac{\nabla E_{\text{in}}(\mathbf{w}(t))}{\|\nabla E_{\text{in}}(\mathbf{w}(t))\|}} + O(\eta^2)\end{aligned}$$

Choosing the step size

The choice of the step size affects the rate of convergence:



Let's use a variable learning rate:

$$\mathbf{w}(t+1) = \mathbf{w}(t) + \eta_t\hat{\mathbf{v}}$$

$$\eta_t = \eta \cdot ||\nabla E_{\text{in}}(\mathbf{w}(t))||$$

When approaching the minimum:

$$||\nabla E_{\text{in}}(\mathbf{w}(t))|| \to 0$$

Choosing the step size

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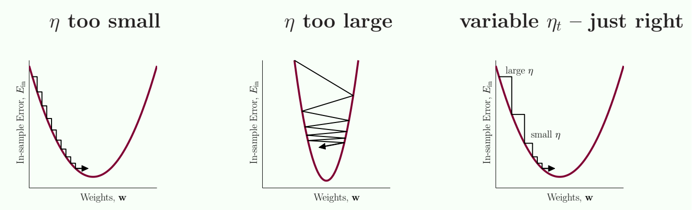


Let's use a variable learning rate:

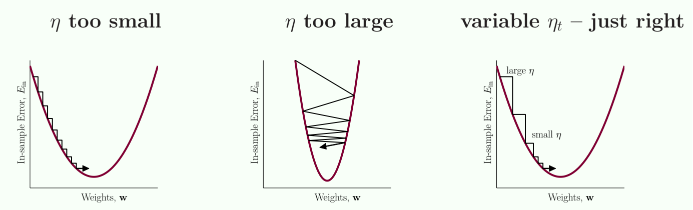
$$\mathbf{w}(t+1) = \mathbf{w}(t) + \eta_t \hat{\mathbf{v}}$$

$$\eta_t = \eta \cdot ||\nabla E_{\text{in}}(\mathbf{w}(t))||$$

$$\eta_t \hat{\mathbf{v}} = -\eta \cdot ||\nabla E_{\text{in}}(\mathbf{w}(t))|| \cdot \frac{\nabla E_{\text{in}}(\mathbf{w}(t))}{||\nabla E_{\text{in}}(\mathbf{w}(t))||} = -\eta \nabla E_{\text{in}}(\mathbf{w}(t))$$

The final form of gradient descent

The choice of the step size affects the rate of convergence:

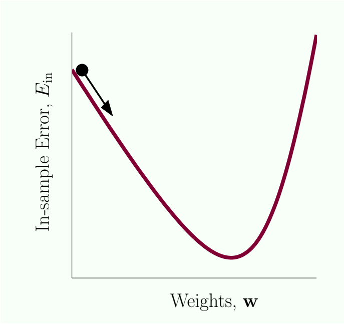


$$\mathbf{w}(t+1) = \mathbf{w}(t) - \eta \nabla E_{\text{in}}(\mathbf{w}(t))$$

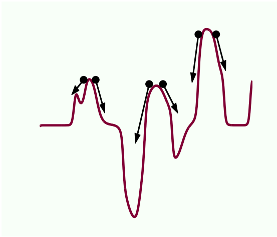
Logistic regression using gradient descent

We will use gradient descent to minimize our error function.

Fortunately, the logistic regression error function has a single global minimum:



So we don't need to worry about getting stuck in local minima



Logistic regression using gradient descent

Putting it all together:

```
Initialize at step $t = 0$ to $\mathbf{w}(0)$.
for $t = 0, 1, 2, \ldots$ do
    Compute the gradient
        $\mathbf{g}_t = \nabla E_{\text{in}}(\mathbf{w}(t))$.
    Move in the direction $\mathbf{v}_t = -\mathbf{g}_t$.
    Update the weights:
        $\mathbf{w}(t+1) = \mathbf{w}(t) + \eta \mathbf{v}_t$.
    Iterate 'until it is time to stop'.
end for
Return the final weights.
```

$$E_{\text{in}}(\mathbf{w}) = \frac{1}{N} \sum_{n=1}^{N} \underbrace{\ln\left(1 + e^{-y_n \mathbf{w}^{\mathsf{T}} \mathbf{x}_n}\right)}_{e(h(\mathbf{x}_n), y_n)}$$

$$\nabla E_{\text{in}} = -\frac{1}{N} \sum_{n=1}^{N} \frac{y_n \mathbf{x}_n}{1 + e^{y_n \mathbf{w}^{\mathsf{T}}(t) \mathbf{x}_n}}$$

Logistic regression

Comments:

- Assumptions: i.i.d. data and specific form of P(y | **x**). In practice logistic regression is solved by faster methods than gradient descent
- There is an extension to multi-class classification

Stochastic gradient descent

Variation on gradient descent that considers the error for a single training example:

$$E_{\text{in}}(\mathbf{w}) = \frac{1}{N}\sum_{n=1}^{N} \ln(1 + e^{-y_n \cdot \mathbf{w}^{\mathrm{T}}\mathbf{x}}) = \frac{1}{N}\sum_{n=1}^{N} e(\mathbf{w}, \mathbf{x}_n, y_n)$$

Pick a random data point $(\mathbf{x}_*, y_*)$

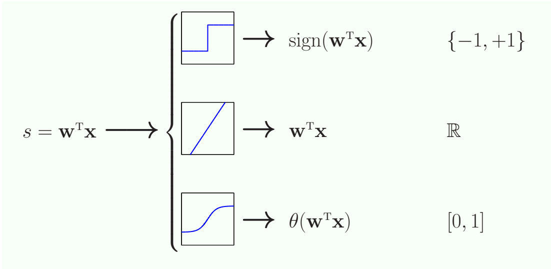
Run an iteration of GD on $e(\mathbf{w}, \mathbf{x}_*, y_*)$

$$\mathbf{w}(t+1) \leftarrow \mathbf{w}(t) - \eta \nabla_{\mathbf{w}} e(\mathbf{w}, \mathbf{x}_*, y_*)$$

$$\mathbf{w}(t+1) \leftarrow \mathbf{w}(t) + y_* \mathbf{x}_* \left(\frac{\eta}{1 + e^{y_* \mathbf{w}^{\mathrm{T}} \mathbf{x}_*}}\right)$$

Summary of linear models

Linear methods for classification and regression:



$s = \mathbf{w}^{\mathrm{T}}\mathbf{x} \longrightarrow$

$\longrightarrow \operatorname{sign}(\mathbf{w}^{\mathrm{T}}\mathbf{x})$ $\{-1, +1\}$

$\longrightarrow \mathbf{w}^{\mathrm{T}}\mathbf{x}$ $\mathbb{R}$

$\longrightarrow \theta(\mathbf{w}^{\mathrm{T}}\mathbf{x})$ $[0, 1]$

More to come!