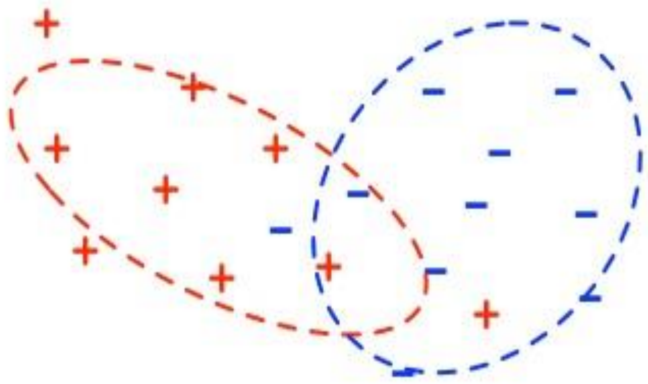
# Classification with discriminative models

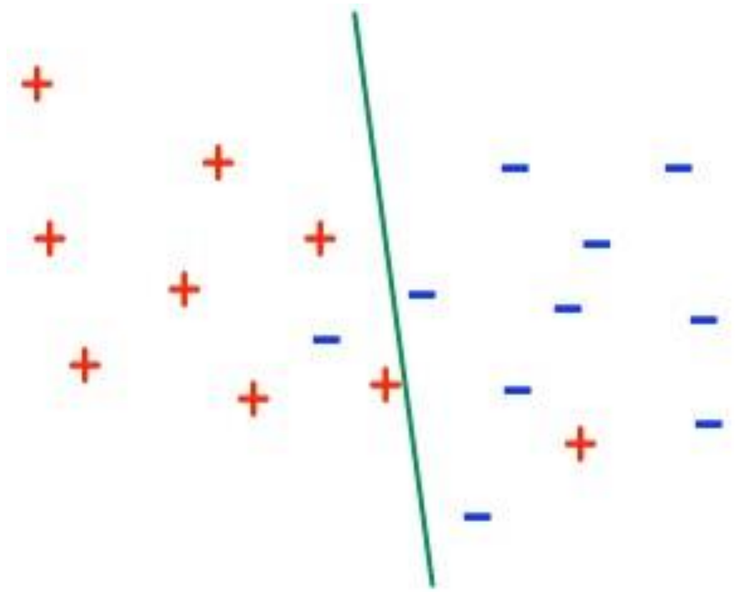
DSE 220

# Classification with parametrized models

Classifiers with a fixed number of parameters can represent a limited set of functions. Learning a model is about picking a good approximation.

Typically the *x* ’s are points in *p*-dimensional Euclidean space, $\mathbf{R}^p$





Two ways to classify:

- **Generative**: model the individual classes
- **Discriminative**: mode the decision boundary between the classes

# Generative models: pros and cons

Advantages:

- Multiclass is a breeze
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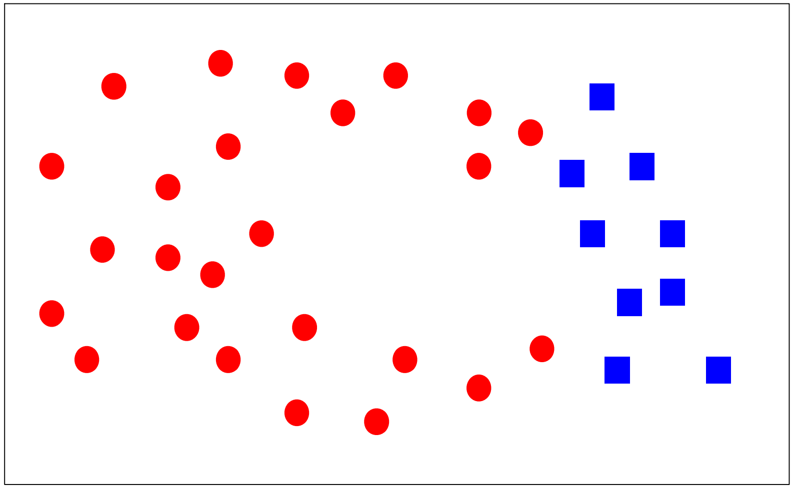
If we only care about classification, shouldn't we focus on the decision boundary rather than trying to model other aspects of the distribution of $x$ ?

# Generative versus discriminative



The generative way:

- Fit: $\pi_0$, $\pi_1$, $P_0$,$P_1$
- This determines a full joint distribution Pr($x$ , $y$ )
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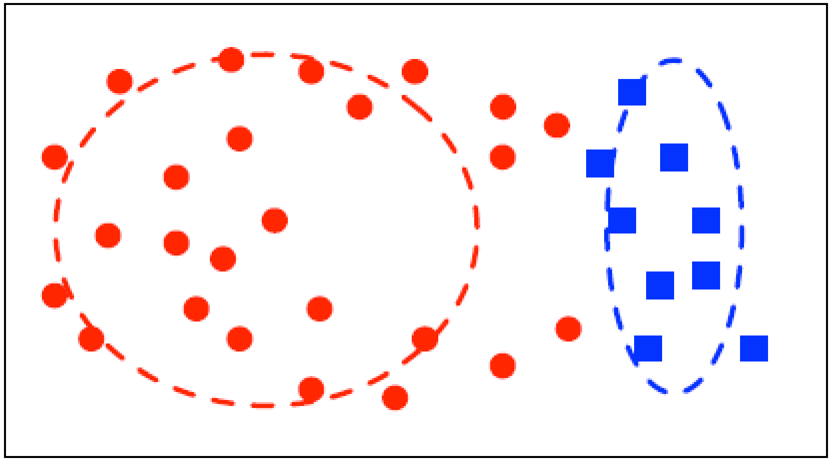

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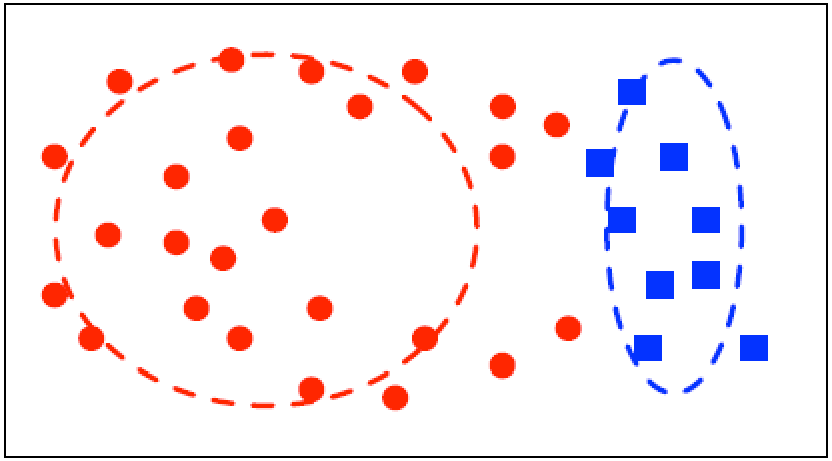

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The generative way: model Pr($y|x$) directly.
In our earlier terminology: forget about the $\mu$ (Prob. Distribution), just learn the $\eta$ (likelihood)

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$$\Pr(y = -1 \mid x) = \frac{1}{1 + e^{w \cdot x}}$$

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- More concisely,

$$\Pr(y \mid x) = \frac{1}{1 + e^{-y(w \cdot x)}}$$

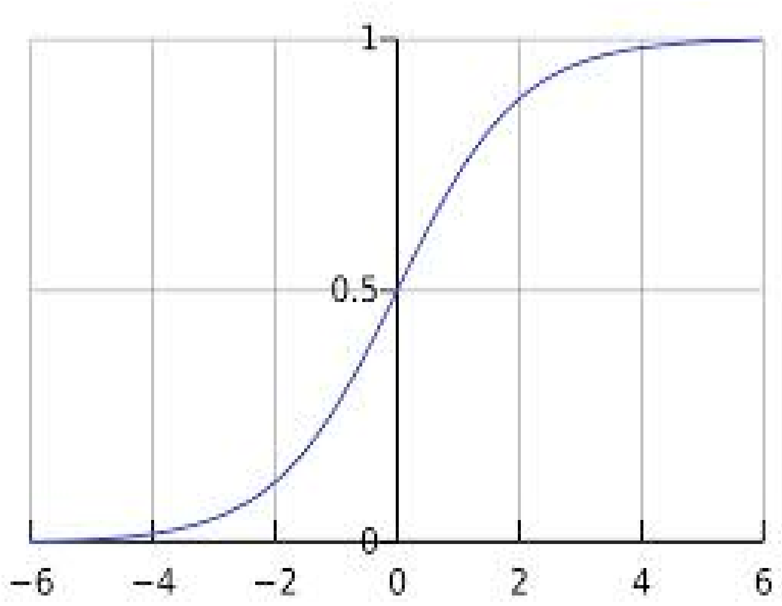
This is the **logistic regression model**, parametrized by $w$.

# The squashing function

Take $X = \mathbf{R}^p$ and $Y = \{-1, 1\}$. The model specified by $w \in \mathbf{R}^p$ is

$$\Pr_w(y \mid x) = \frac{1}{1 + e^{-y\,(w \cdot x)}} = g\,(y\,(w \cdot x)),$$

where $g\,(z) = 1/(1 + e^{-z})$ is the *squashing function*.



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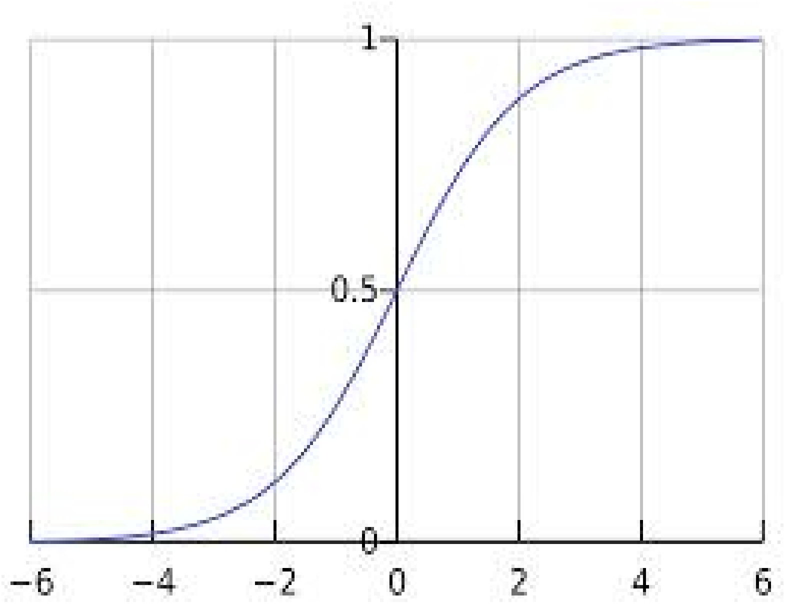


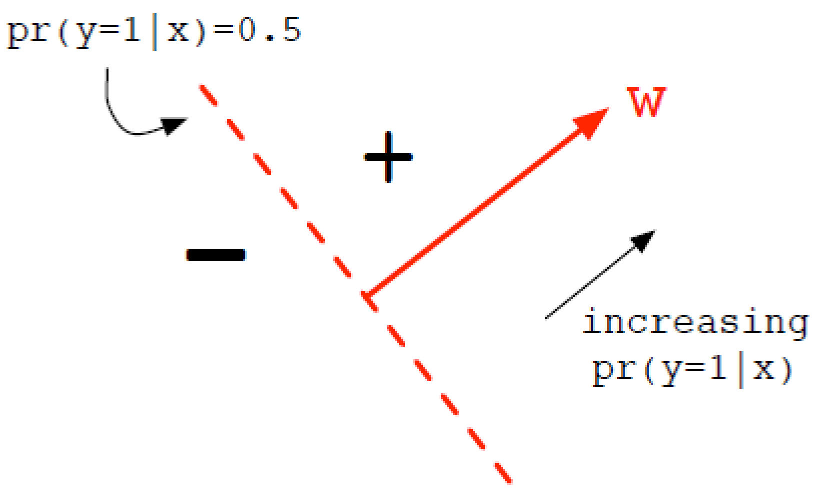

# Fitting $w$

The maximum-likelihood principle: given a data set

$$(x^{(1)}, y^{(1)}), \ldots, (x^{(n)}, y^{(n)}) \in \mathbb{R}^p \times \{-1, 1\},$$

pick the $w \in \mathbb{R}^p$ that maximizes

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$$L(w) \;=\; -\sum_{i=1}^{n} \ln \Pr_w(y^{(i)} \mid x^{(i)})$$

$$= \; -\sum_{i=1}^{n} \ln\left(\frac{1}{1 + e^{-y^{(i)}(w \cdot x^{(i)})}}\right) \;=\; \sum_{i=1}^{n} \ln(1 + e^{-y^{(i)}(w \cdot x^{(i)})})$$

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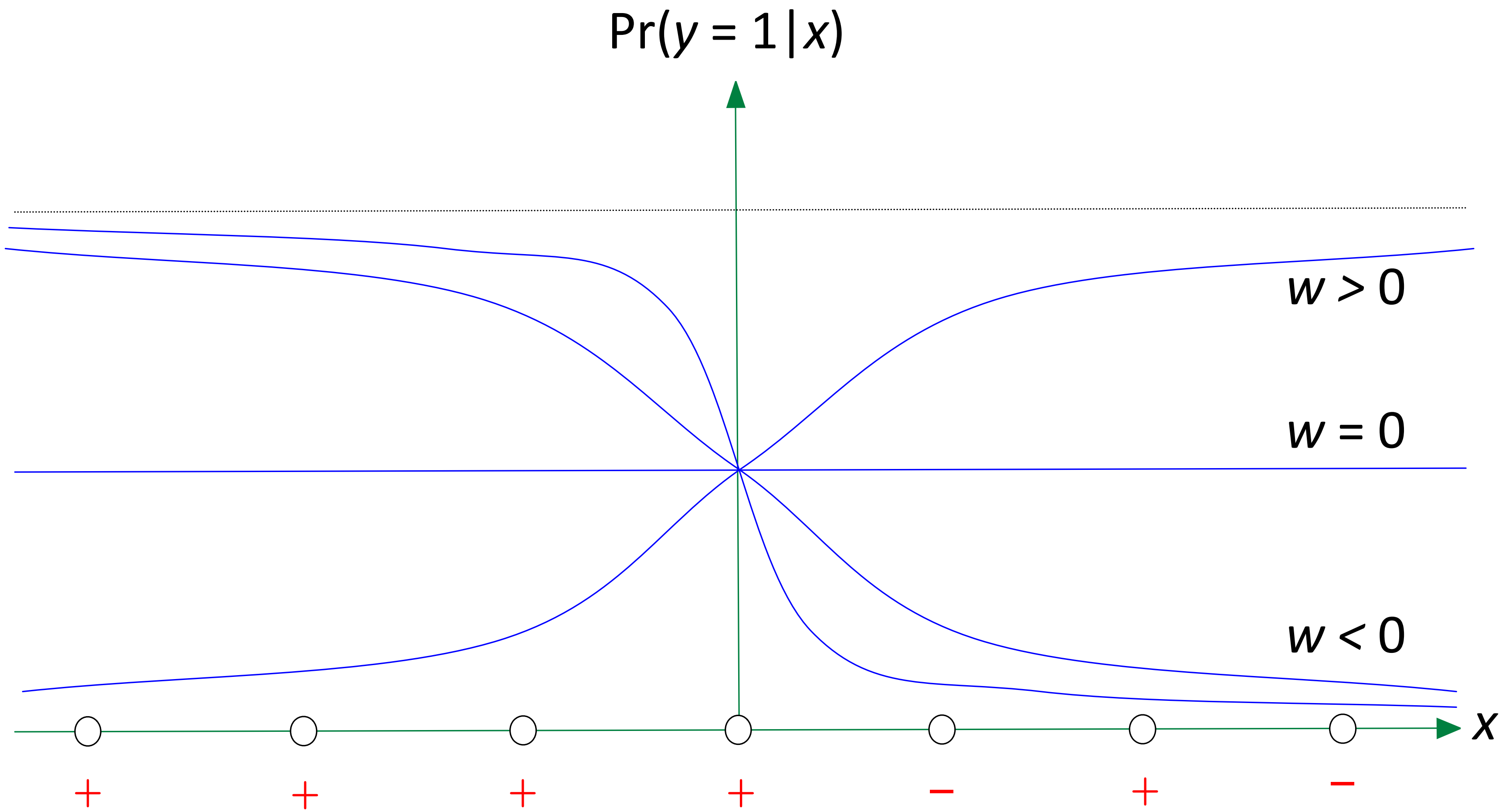
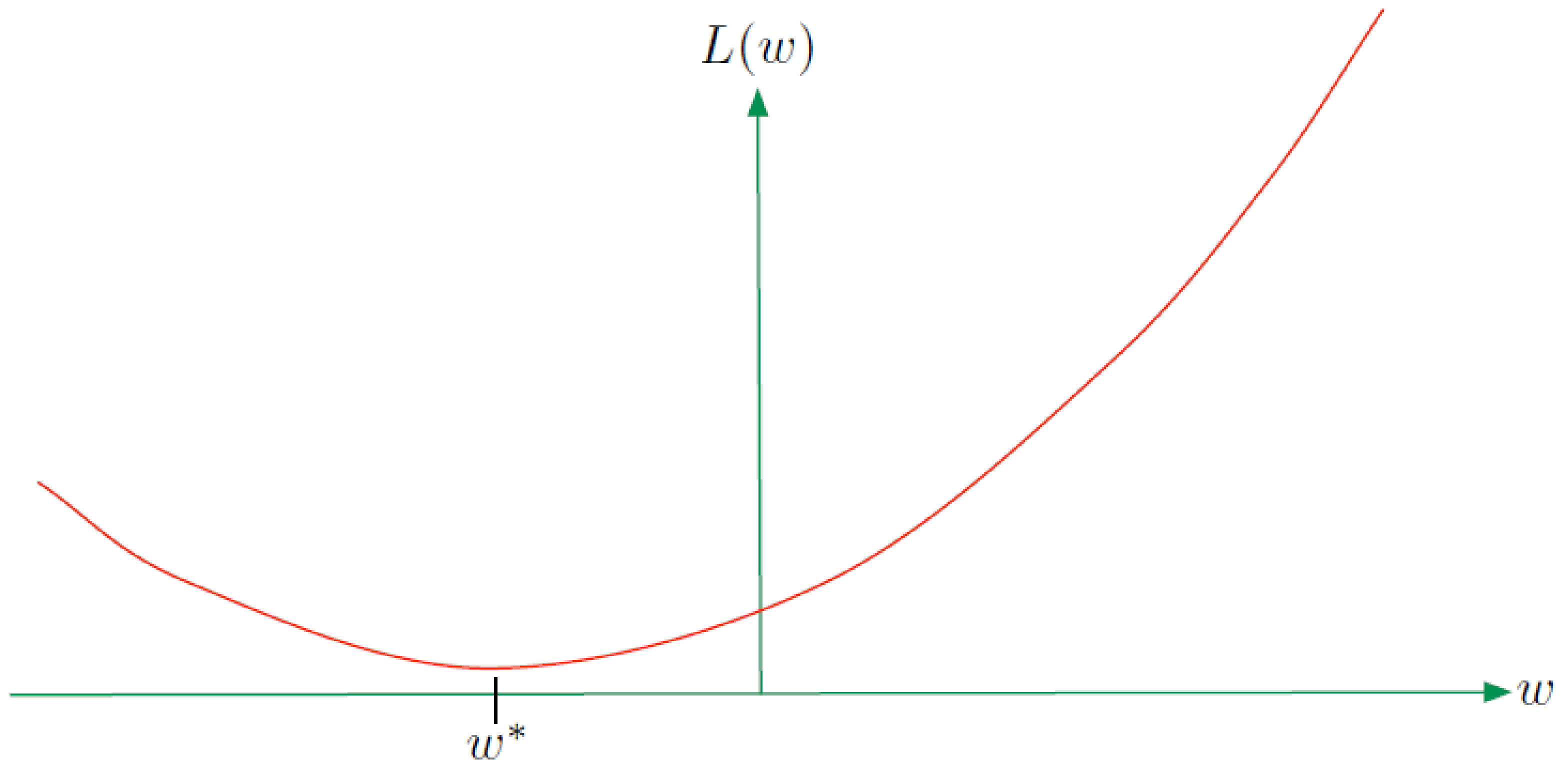
The good news: $L(w)$ is **convex** in $w$.

# One dimensional example

$$\Pr_w(y \mid x) = \frac{1}{1 + e^{-ywx}}, \quad w \in \mathbf{R}$$



# Example, cont'd




How to find the minimum of this convex function? A variety of options:

- Gradient descent
- Newton-Raphson

and many others.

# Gradient descent procedure for logistic regression

Given $(x^{(1)}, y^{(1)}), \ldots, (x^{(n)}, y^{(n)}) \in \mathbb{R}^p \times \{-1, 1\}$, find

$$\arg\min_{w \in \mathbb{R}^p} L(w) \;=\; \sum_{i=1}^{n} \ln(1 + e^{-y^{(i)}(w \cdot x^{(i)})})$$

- Set $w_0 = 0$
- For $t = 0, 1, 2, \ldots,$ until convergence:

$$w_{t+1} \;=\; w_t \;+\; \eta_t \sum_{i=1}^{n} y^{(i)} x^{(i)} \underbrace{\Pr_{w_t}(-y^{(i)} | x^{(i)})}_{\text{doubt}_t(x^{(i)}, y^{(i)})},$$

where $\eta_t$ is a step size chosen by line search to minimize $L(w_{t+1})$.

# Newton-Raphson procedure for logistic regression

- Set $w_0 = 0$
- For $t = 0, 1, 2, \ldots$, until convergence:

$$w_{t+1} \;=\; w_t \;+\; \eta_t \, (X^T D_t X)^{-1} \sum_{i=1}^{n} y^{(i)} x^{(i)} \mathrm{Pr}_{w_t}(-y^{(i)} | x^{(i)}),$$

  where
  - $X$ is the $n \times p$ data matrix with one point per row
  - $D_t$ is an $n \times n$ diagonal matrix with $(i, i)$ entry

$$D_{t,ii} \;=\; \mathrm{Pr}_{w_t}(1|x^{(i)}) \, \mathrm{Pr}_{w_t}(-1|x^{(i)})$$

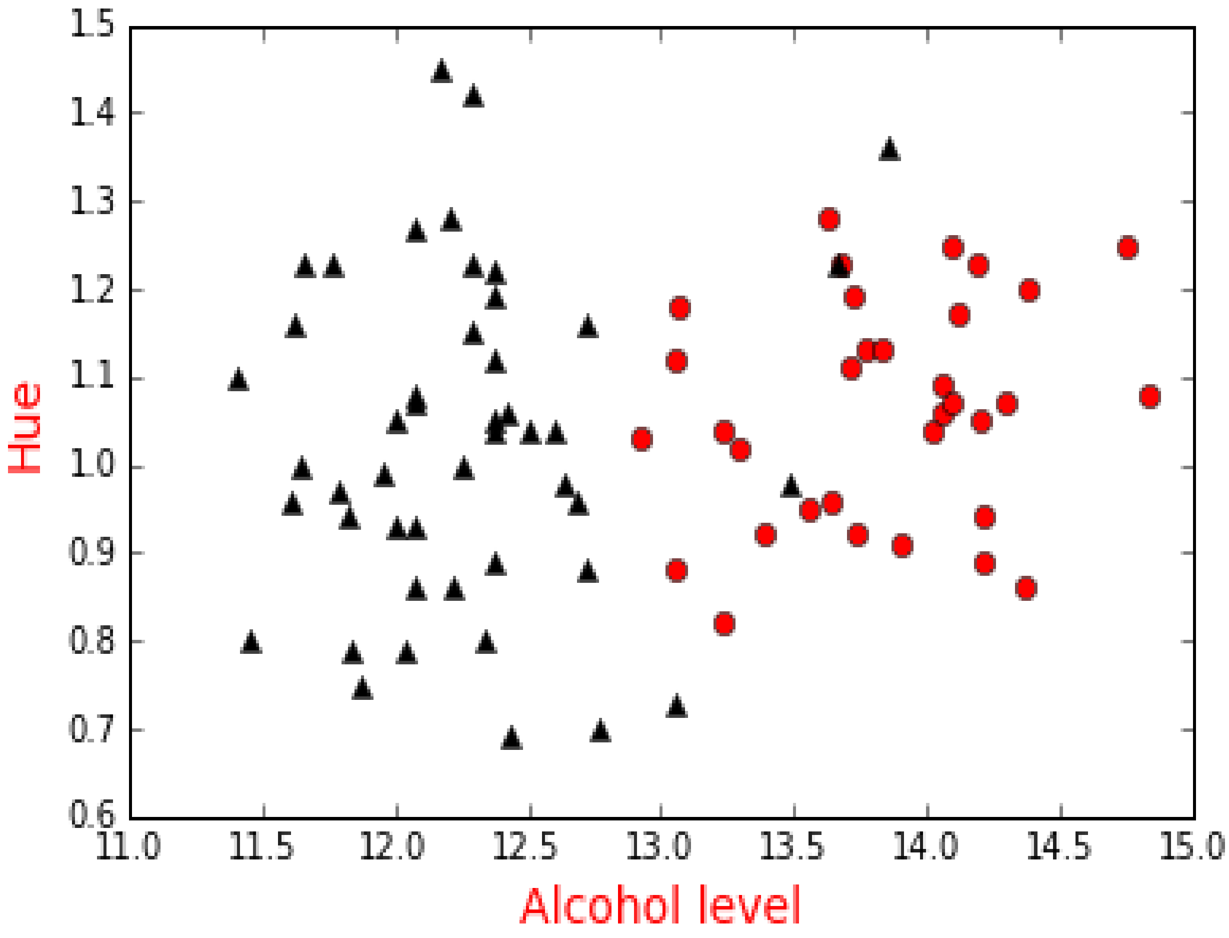
  - $\eta_t$ is a step size that is either fixed to 1 ("iterative reweighted least squares") or chosen by line search to minimize $L(w_{t+1})$.

# Example: “wine” data set

Recall: data from three wineries from the same region of Italy.

- 13 attributes: hue, color intensity, flavanoids, ash content, ...
- 178 instances in all: split into 118 train, 60 test

Pick two classes and just two attributes (hue, alcohol content).



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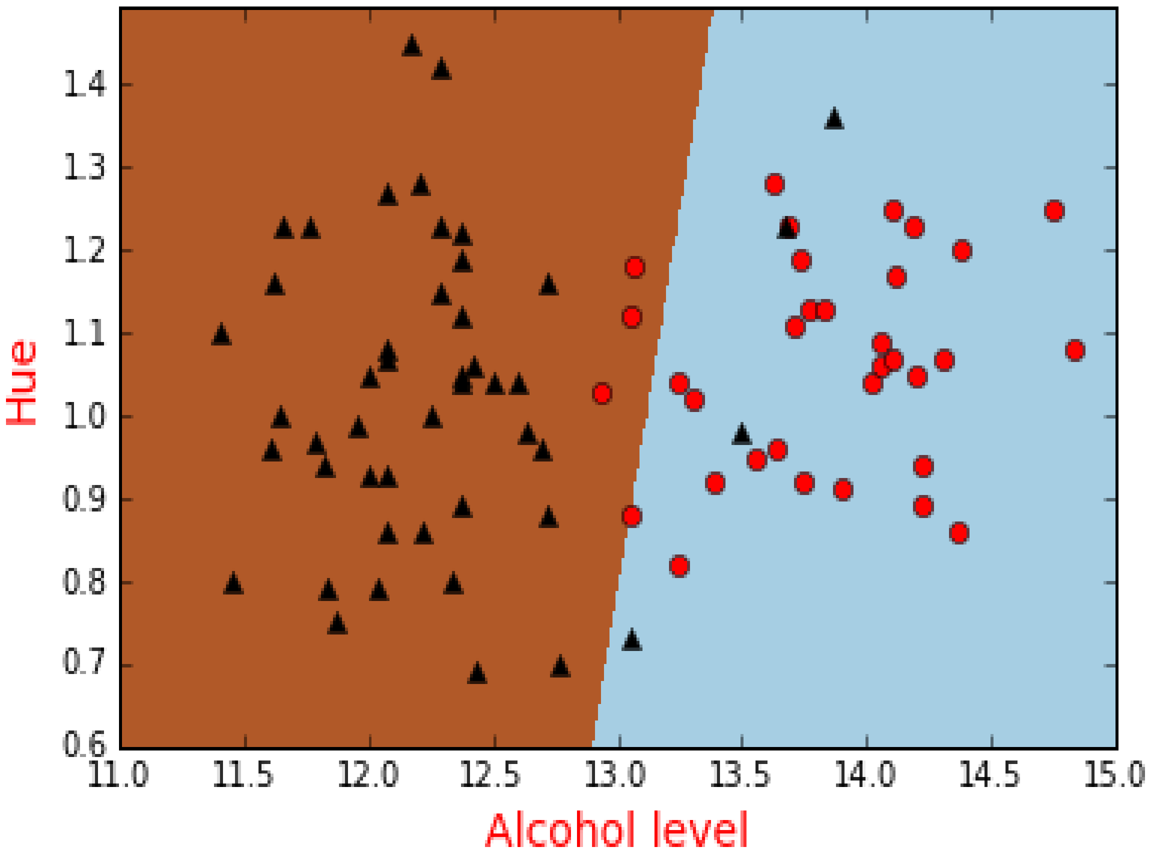


Test error using logistic regression: 10%.

# A closer look at the logistic loss

For $(x^{(1)}, y^{(1)}), \ldots, (x^{(n)}, y^{(n)}) \in \mathbb{R}^p \times \{-1, +1\}$,

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**First derivative**. There are $p$ partial derivatives $\partial L / \partial w_j$. Put into a vector:

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# A closer look at the logistic loss

For $(x^{(1)}, y^{(1)}), \ldots, (x^{(n)}, y^{(n)}) \in \mathbb{R}^p \times \{-1, +1\}$,

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Good news: $L(w)$ is **convex**, so local optimum implies global optimum.

# Quick quiz

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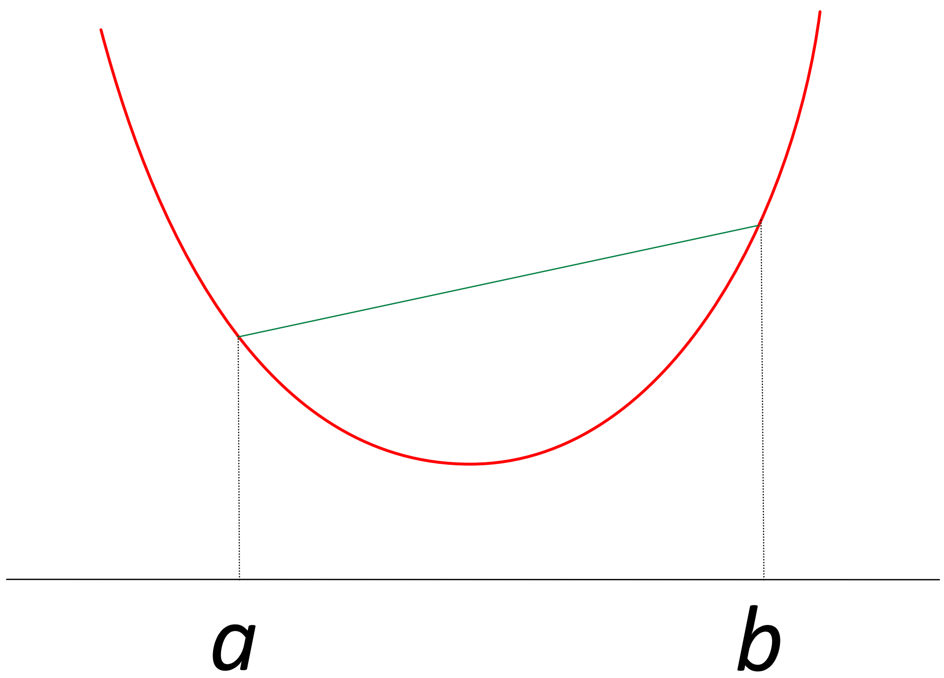
2. $F(w) = w^T w \rightarrow \boldsymbol{2w}$

# Convexity



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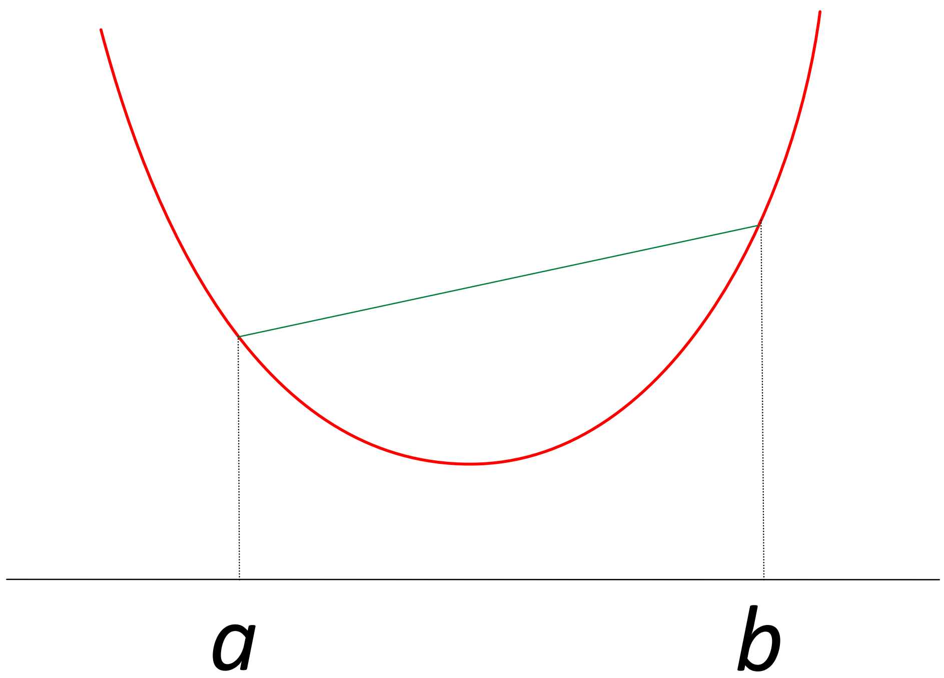


A function $f : \mathbb{R}^p \to \mathbb{R}$ is **convex** if for all $a, b \in \mathbb{R}^p$ and $0 < \theta < 1$,

$$f(\theta a + (1-\theta)b) \;\leq\; \theta f(a) + (1-\theta) f(b).$$

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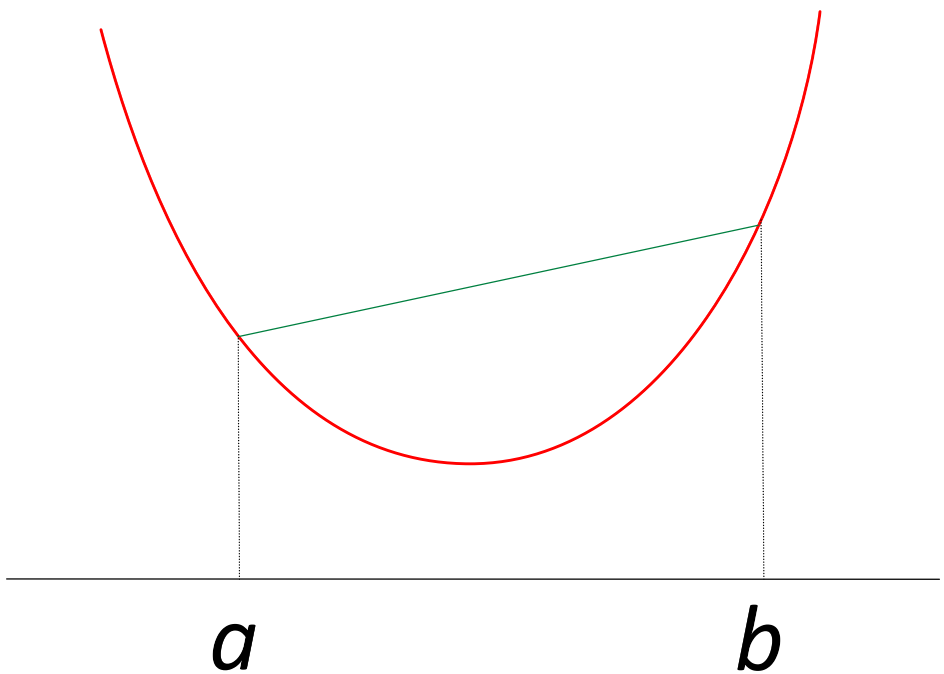


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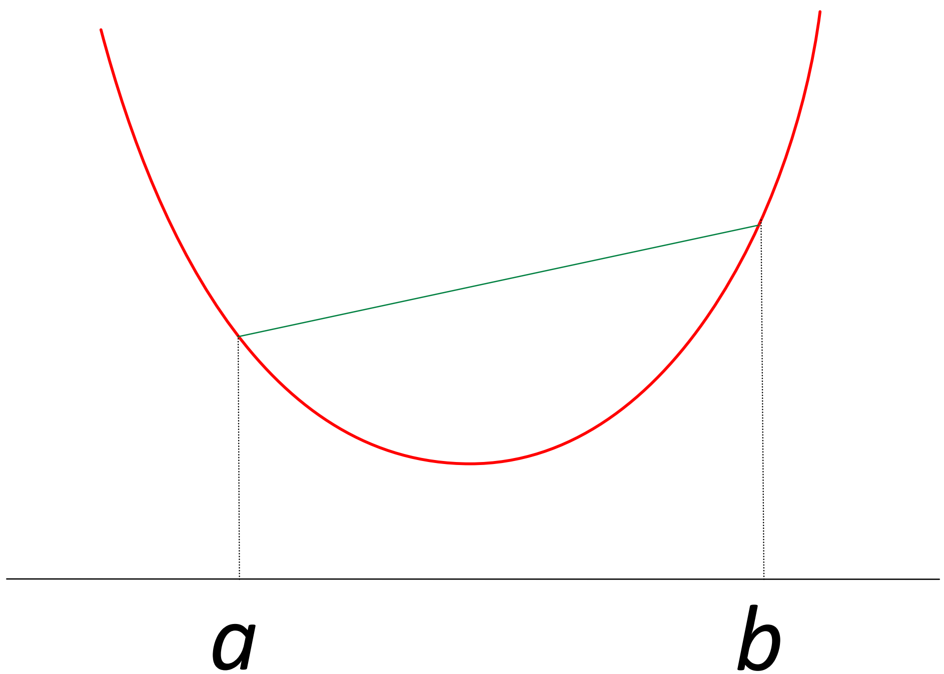


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$f$ is **concave** (resp., **strictly concave**) iff $-f$ is convex (resp., strictly convex).

# Second-derivative test for convexity

A function $f : \mathbb{R}^p \to \mathbb{R}$ has $p^2$ second partial derivatives $\frac{\partial^2 f}{\partial z_j \partial z_k}$ at any $z \in \mathbb{R}^p$ (assuming these exist).

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**Useful fact.** Suppose that for $f : \mathbb{R}^p \to \mathbb{R}$, the second partial derivatives exist everywhere and are continuous functions of $z$. Then:

1. $H(z)$ is a symmetric matrix.
2. $f$ is convex if and only if $H(z)$ is positive semidefinite for all $z \in \mathbb{R}^p$.

# Quick quiz

Is this function $f : \mathbb{R}^p \to \mathbb{R}$ convex?

$$f(z) = (u \cdot z)^2$$

(Here $u$ is some fixed vector in $\mathbb{R}^p$.)

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Yes

Calculate Hessian. It will be of the form $UU^T$

# Convexity of logistic regression loss function

Recall the loss function: for data $(x^{(i)}, y^{(i)}) \in \mathbb{R}^p \times \{-1, +1\}$,

$$L(w) \;=\; \sum_{i=1}^{n} \ln(1 + e^{-y^{(i)}(w \cdot x^{(i)})}).$$

We already know the first derivative:

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Second derivative: the $(j, k)$ entry of the Hessian $H(w)$ is

$$\begin{aligned}
\frac{\partial L}{\partial w_k \partial w_j} &= -\sum_{i=1}^{n} y^{(i)} x_j^{(i)} (-1) \frac{e^{y^{(i)}(w \cdot x^{(i)})}}{(1 + e^{y^{(i)}(w \cdot x^{(i)})})^2} y^{(i)} x_k^{(i)} \\
&= \sum_{i=1}^{n} x_j^{(i)} x_k^{(i)} \frac{e^{y^{(i)}(w \cdot x^{(i)})}}{(1 + e^{y^{(i)}(w \cdot x^{(i)})})^2} = \sum_{i=1}^{n} x_j^{(i)} x_k^{(i)} \, \frac{1}{1 + e^{w \cdot x^{(i)}}} \, \frac{1}{1 + e^{-w \cdot x^{(i)}}}
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$$\begin{aligned}\frac{\partial L}{\partial w_k \partial w_j} &= -\sum_{i=1}^{n} y^{(i)} x_j^{(i)} (-1) \frac{e^{y^{(i)}(w \cdot x^{(i)})}}{(1 + e^{y^{(i)}(w \cdot x^{(i)})})^2} y^{(i)} x_k^{(i)} \\ &= \sum_{i=1}^{n} x_j^{(i)} x_k^{(i)} \frac{e^{y^{(i)}(w \cdot x^{(i)})}}{(1 + e^{y^{(i)}(w \cdot x^{(i)})})^2} = \sum_{i=1}^{n} x_j^{(i)} x_k^{(i)} \frac{1}{1 + e^{w \cdot x^{(i)}}} \frac{1}{1 + e^{-w \cdot x^{(i)}}}\end{aligned}$$

This is $u_j \cdot u_k$, where vectors $u_1, \ldots, u_p \in \mathbb{R}^n$ are defined as follows:

$$u_j \text{ has } i\text{th coordinate } x_j^{(i)} \sqrt{\frac{1}{(1 + e^{w \cdot x^{(i)}})(1 + e^{-w \cdot x^{(i)}})}}.$$

# Convexity of logistic regression loss function

Recall the loss function: for data $(x^{(i)}, y^{(i)}) \in \mathbb{R}^p \times \{-1,+1\}$,

$$L(w) = \sum_{i=1}^{n} \ln(1 + e^{-y^{(i)}(w \cdot x^{(i)})}).$$

We already know the first derivative:

$$\frac{\partial L}{\partial w_j} = -\sum_{i=1}^{n} y^{(i)} x_j^{(i)} \frac{1}{1 + e^{y^{(i)}(w \cdot x^{(i)})}}.$$

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Therefore $H(w) = UU^T$, where $U$ is the matrix with rows $u_j$ $\Rightarrow$ convex.

# Gradient descent

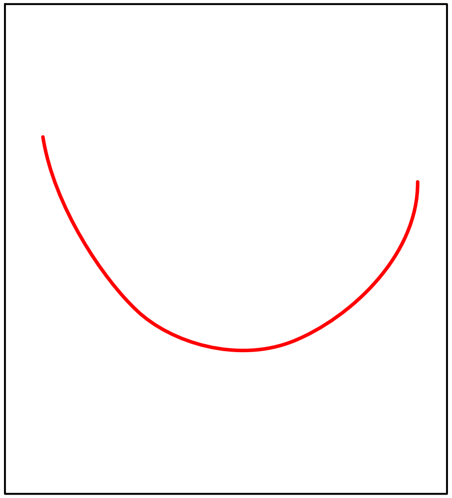
For minimizing a function $L(w)$:

- $w_o = 0,\ t = 0$
- while $\nabla L(w_t) \not\approx 0$:
  - $w_{t+1} = w_t - \eta_t \nabla L(w_t)$
  - $t = t + 1$

Here $\eta_t$ is the *step size* at time $t$.

# Gradient descent: rationale

"Differentiable" means "locally linear".



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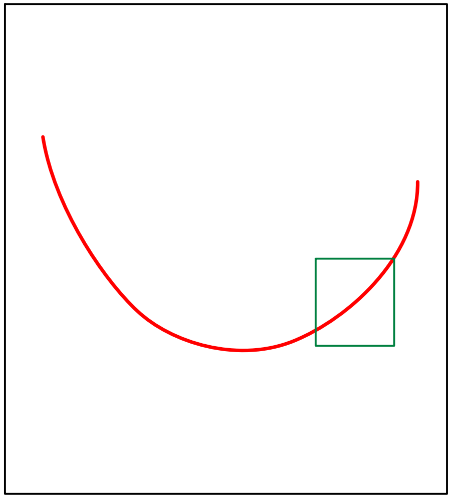

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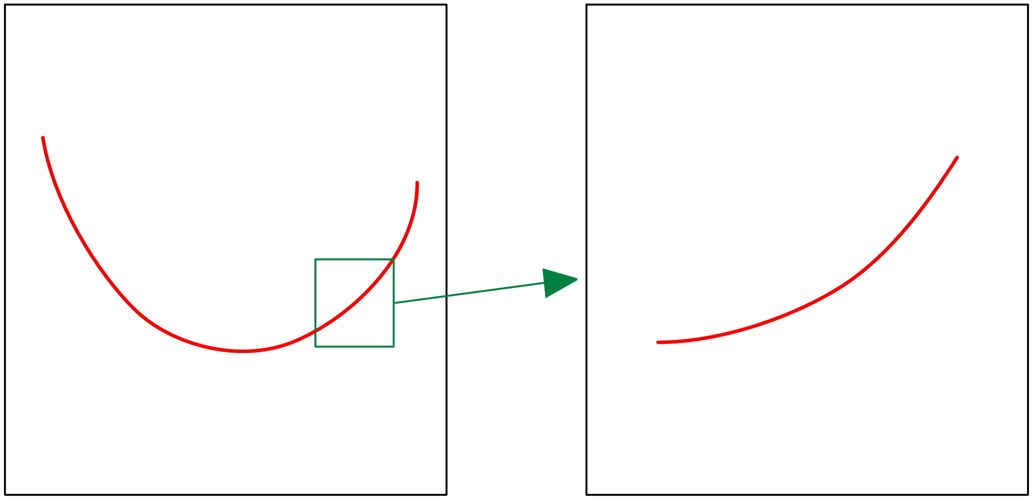

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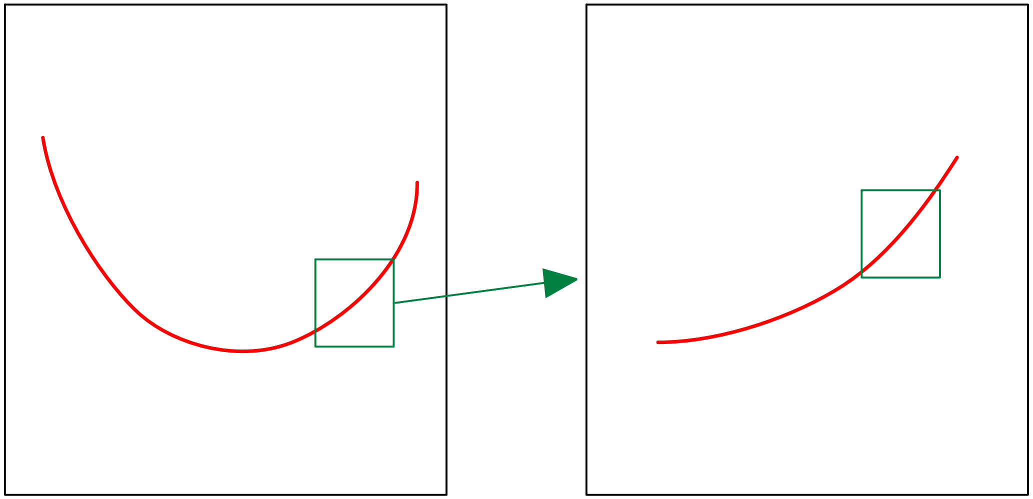

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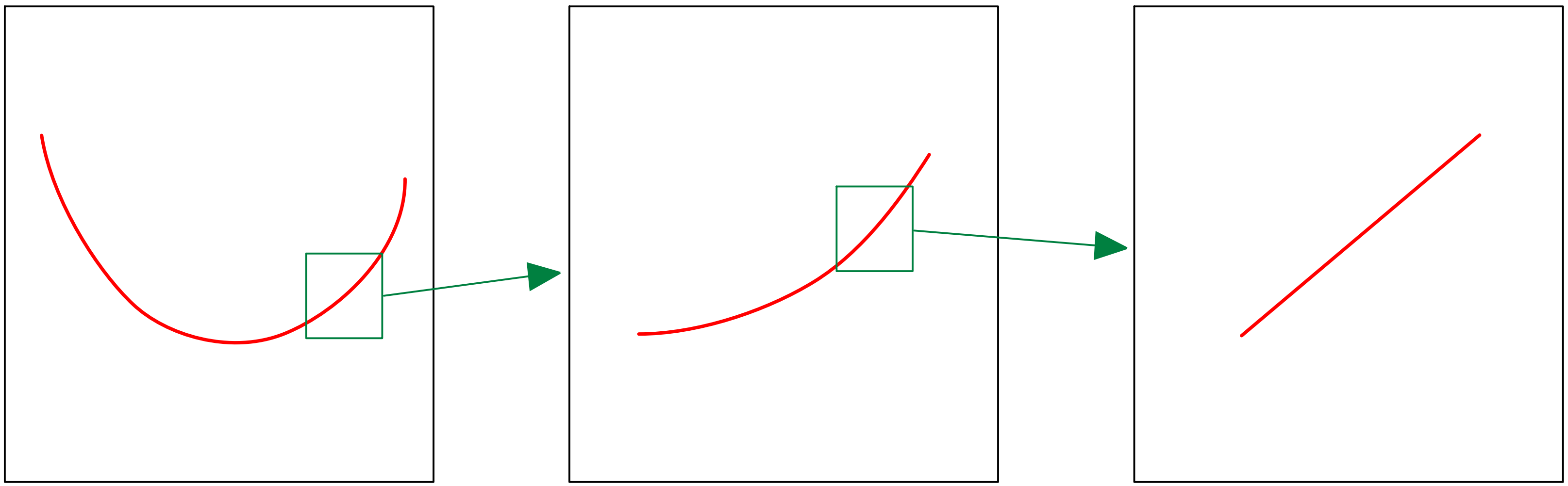

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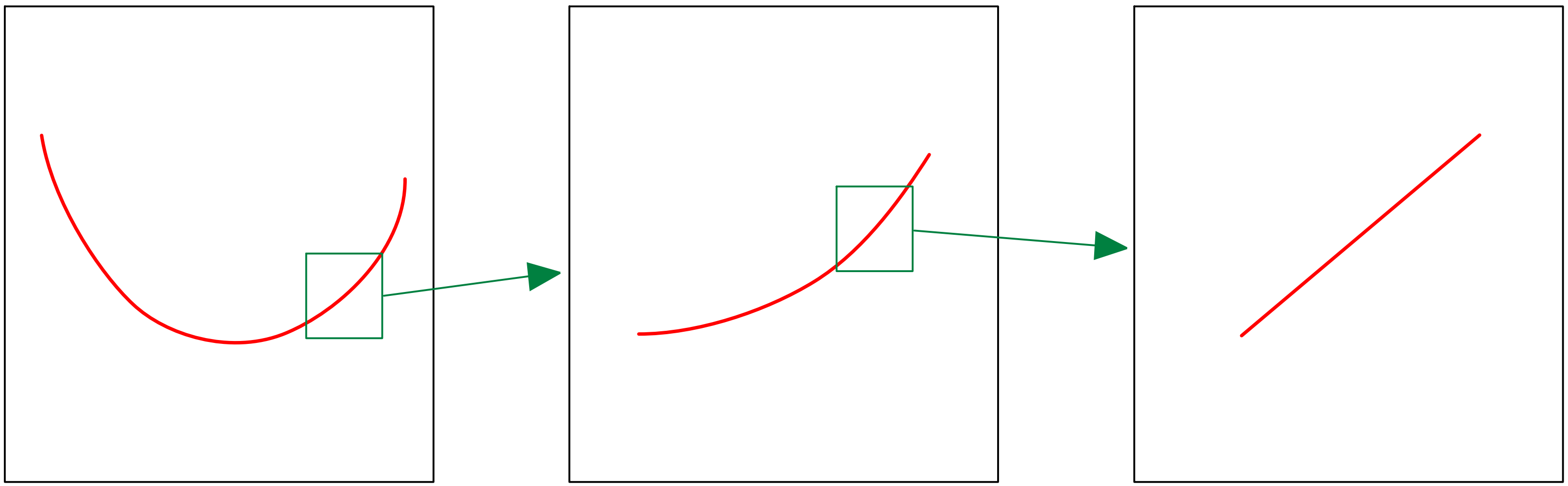


For *small* displacements $u \in \mathbb{R}^p$,

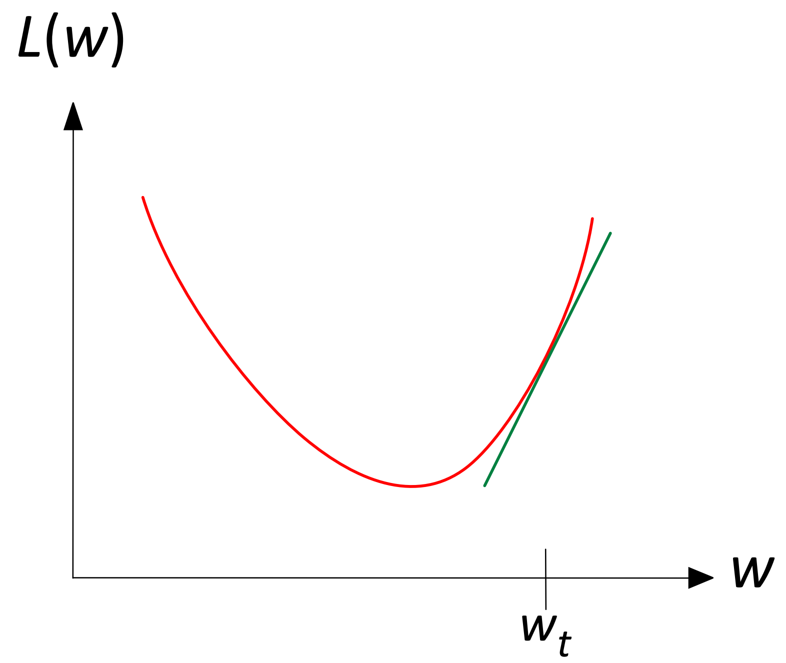
$$L(w+u) \;\approx\; L(w) + u \cdot \nabla L(w).$$

Therefore, if $u = -\eta \nabla L(w)$ is small,

$$L(w+u) \;\approx\; L(w) - \eta \|\nabla L(w)\|^2 \;<\; L(w).$$

# The step size matters

Gradient descent update: $w_{t+1} = w_t - \eta_t \nabla L(w_t)$.

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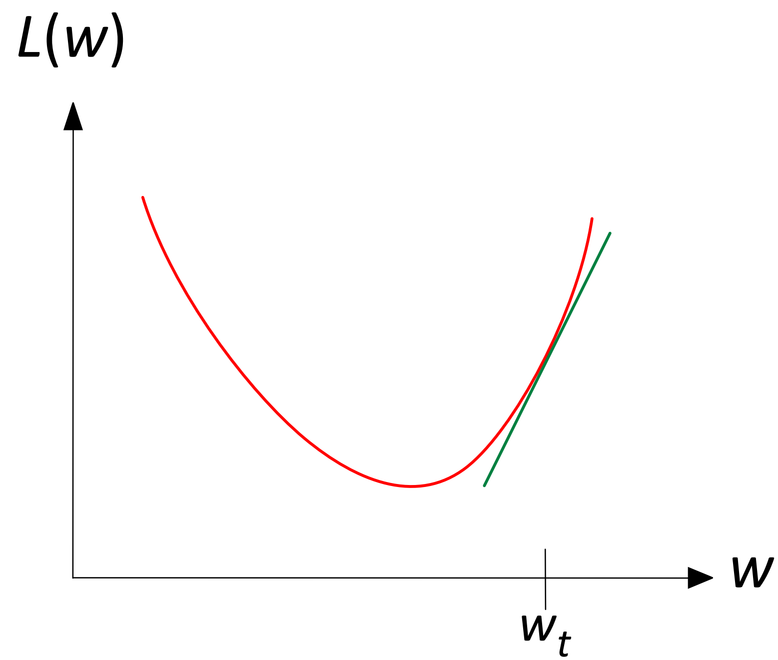


- Step size $\eta_t$ too small: not much progress
- Too large: overshoot the mark

One option: pick $\eta_t$ using a line search

$$\eta_t = \arg\min_{\alpha > 0} L(w_t - \alpha \nabla L(w_t)).$$

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- Set $t = 0$, $\alpha = 0.1$ (or anything random between 0 and 1)

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- Until $|| \nabla L(w_t)|| <$ some tolerance

This makes sure that $\alpha$ has a value that can lead us to the minimum value of $L(w_t)$.

# Variant: stochastic gradient descent

Recall gradient descent update for logistic regression: at time $t$

$$w_{t+1} = w_t + \eta_t \sum_{i=1}^{n} y^{(i)} x^{(i)} \underbrace{\Pr_{w_t}(-y^{(i)} | x^{(i)})}_{\text{doubt}_t(x^{(i)}, y^{(i)})}.$$

Each update involves the entire data set, which is inconvenient.

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**Stochastic gradient descent** makes updates based on just one point:

- Get next data point $(x, y)$ (e.g., keep cycling through the data set)
- $w_{t+1} = w_t + \eta_t \, y \, x \Pr_{w_t}(-y|x)$.

Convenient for very large data sets.

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Another option: make updates based on "mini-batches" of data points.

# Newton-Raphson

For minimizing a function $L(w)$:

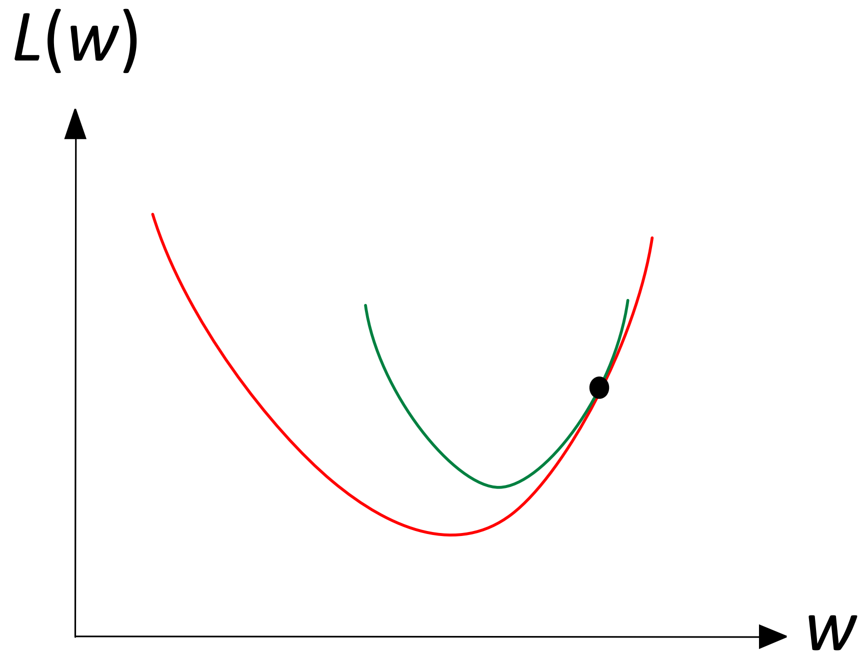
- $w_o = 0$, $t = 0$
- while $\nabla L(w_t) \not\approx 0$:
  - $w_{t+1} = w_t - \eta_t H^{-1}(w_t) \nabla L(w_t)$
  - $t = t + 1$

$H^{-1}(w)$ is the inverse of the Hessian at $w$

# Newton-Raphson: rationale

Second-order Taylor expansion: for small *u*,

$$L(w+u) \;\approx\; L(w) + u \cdot \nabla L(w) + \frac{1}{2} u^T H(w) u.$$



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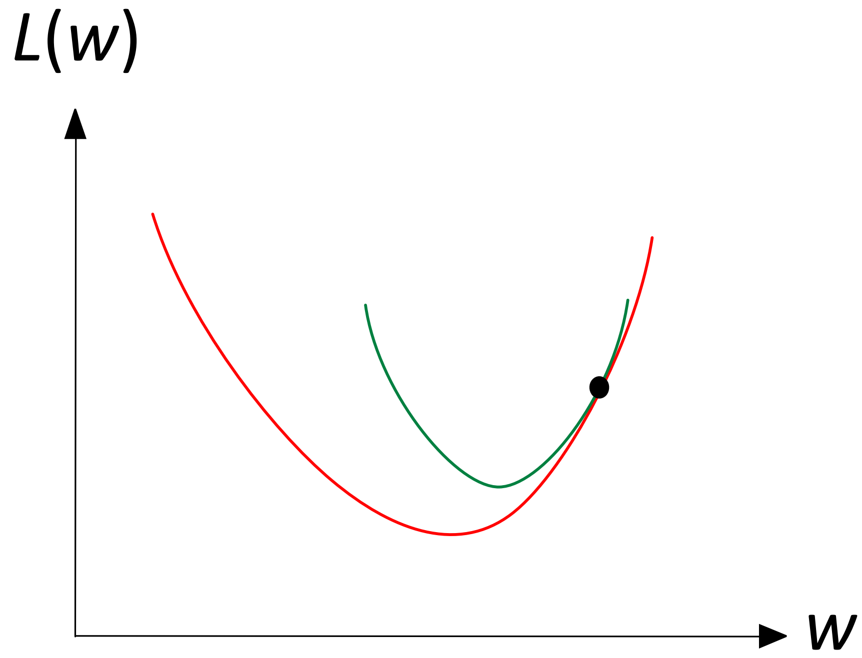


To minimize this quadratic approximation, set derivative to zero:

$$\nabla L(w) + H(w)u = 0 \;\Rightarrow\; u = -H^{-1}(w)\nabla L(w).$$

# Variant: quasi-Newton methods

For optimizing a function over $\mathbf{R}^p$ , the Newton update involves computing the $p \times p$ Hessian at each time step:

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Speed things up by using an approximation $B_t$ of $H^{-1}(w_t)$:

- Initialize it to the identity, say.
- Efficiently update $B_t \rightarrow B_{t+1}$ using a second-order approximation based on $w_{t+1}$, $w_t$, $\nabla L(w_t), \nabla L(w_{t+1})$.

Example: the BFGS (Broyden-Fletcher-Goldfarb-Shanno) procedure.

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Even better: instead of maintaining a dense matrix $B_t$, use an $O(p)$ – Sized approximation to it. Example: L-BFGS ("Limited memory BFGS").