Classification with discriminative models

DSE 220

So far..

- Introduction
- Nonparametric Methods
    - Decision Trees
    - kNN
- Parametric Methods
    - Generative Models
        - Naive Bayes
        - Binary Features, Multinomial Features
        - Gaussian Generative Model
        - Fisher Linear Discriminant Analysis
- Regression Analysis
- Evaluation Metrics
    - Accuracy, Recall, Precision, Sensitivity, Specificity,…
    - ROC Curves

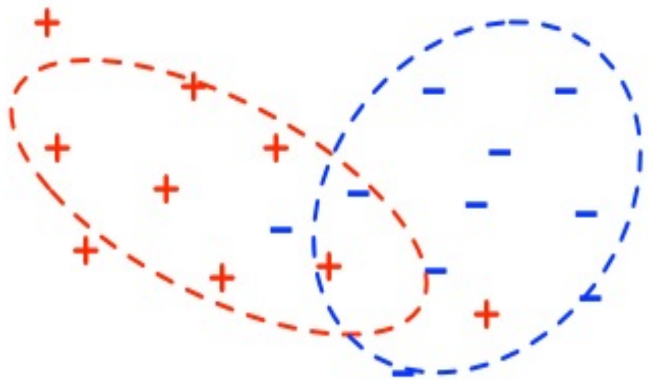
Today

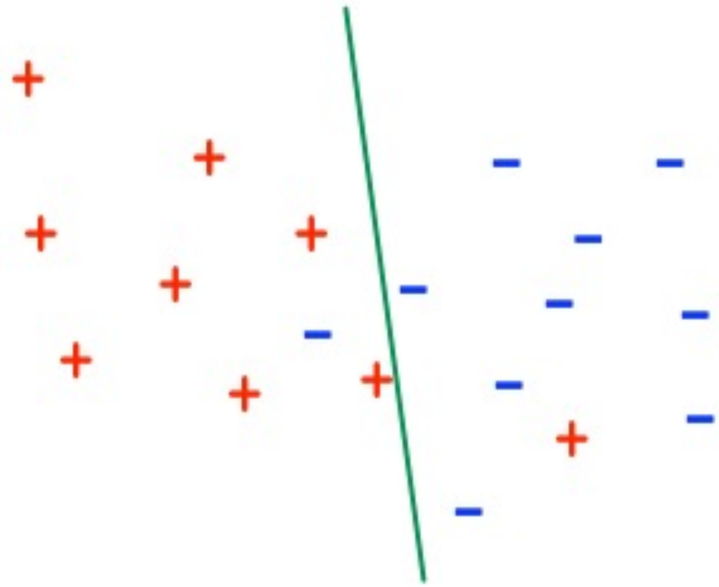
- Parametric Methods
    - Discriminative Methods
        - Logistic Regression
            - Gradient Descent
            - Newton-Raphson
        - ***Hands-On***
        - ***Self – practice***
        - Perceptron
        - SVMs
        - ***Hands-On***
        - ***Self – practice***
    - Kernels
        - ***Hands-On***
        - ***Self – practice***
    - Richer Output Spaces
        - ***Hands-On***
        - ***Self – practice***

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
- For many common models: converges fast
- Returns not just a classification but also a confidence $\Pr(y|x)$

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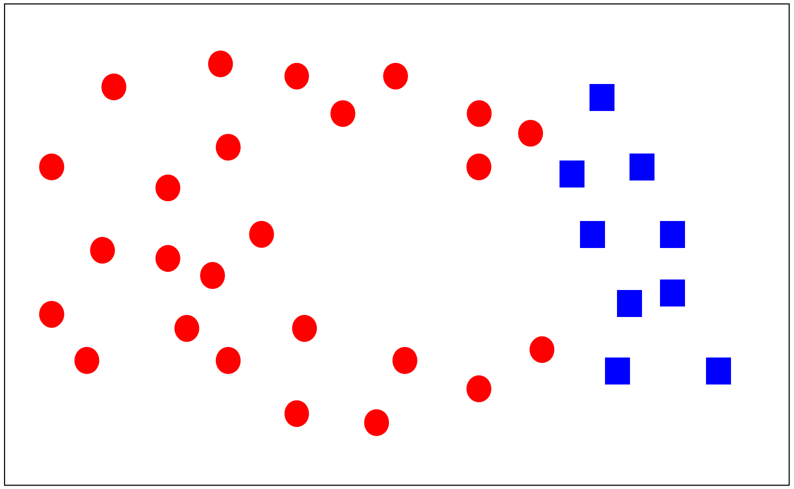
If we only care about classification, shouldn't we focus on the decision boundary rather than trying to model other aspects of the distribution of x ?

Generative versus discriminative



The generative way:

- Fit: π_0, π_1, P_0, P_1
- This determines a full joint distribution Pr(x , y)
- Use Bayes' rule to obtain Pr ($y|x$)

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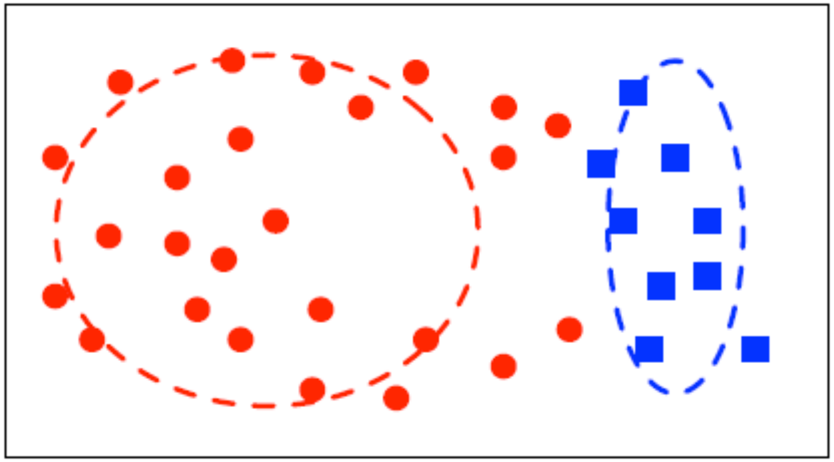

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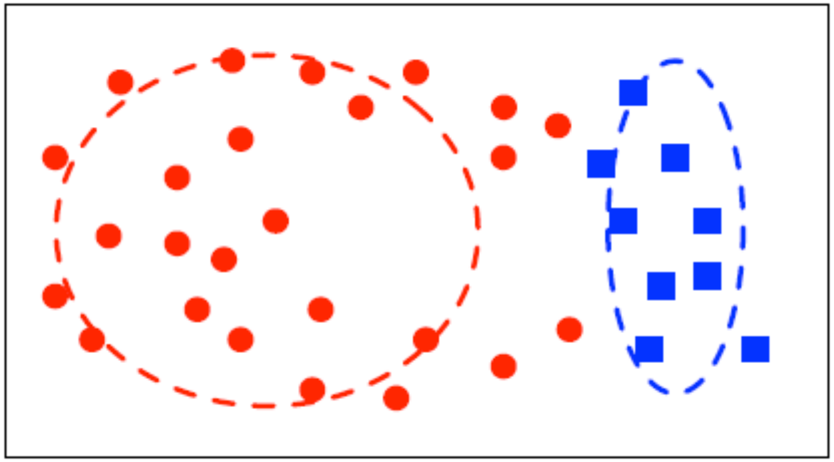

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The generative way: model Pr($y|x$) directly.
In our earlier terminology: forget about the μ (Prob. Distribution), just learn the η (likelihood)

Recall

- Binary Classification with Gaussian Generative Model

Binary classification with Gaussian generative model

Estimate class probabilities π_1, π_2 and fit a Gaussian to each class:

$$P_1 = N(\mu_1, \Sigma_1), P_2 = N(\mu_2, \Sigma_2)$$

E.g. If data points $x^{(1)}, \ldots, x^{(m)} \in \mathbb{R}^p$ are class 1:

$$\mu_1 \;=\; \frac{1}{m}\left(x^{(1)} + \cdots + x^{(m)}\right) \quad \text{and} \quad \Sigma_1 \;=\; \frac{1}{m}\sum_{i=1}^{m}(x^{(i)} - \mu_1)(x^{(i)} - \mu_1)^T$$

Given a new point x, predict class 1 iff:

$$\pi_1 P_1(x) > \pi_2 P_2(x) \quad \Leftrightarrow \quad x^T M x + 2w^T x \geq \theta,$$

where:

$$M = \frac{1}{2}(\Sigma_2^{-1} - \Sigma_1^{-1})$$
$$w = \Sigma_1^{-1}\mu_1 - \Sigma_2^{-1}\mu_2$$

and θ is a constant depending on the various parameters.

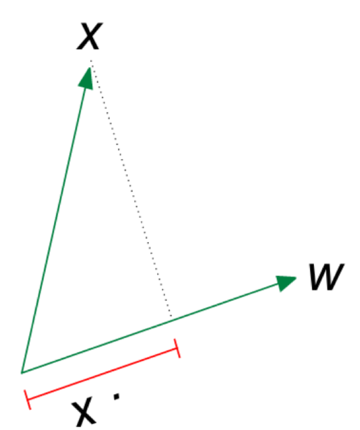
$\Sigma_1 = \Sigma_2$: linear decision boundary. Otherwise, quadratic boundary.

Linear decision boundary

When $\Sigma_1 = \Sigma_2 = \Sigma$: choose class 1 iff

$$x \cdot \underbrace{\Sigma^{-1}(\mu_1 - \mu_2)}_{w} \geq \theta.$$

Geometric picture: Suppose *w* is a unit vector (that is, $||w|| = 1$). Then $x \cdot w$ is the **projection** of vector *x* onto direction *w* .



And we can always make w a unit vector by dividing both sides of the inequality by $\|w\|$.

The logistic regression model

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- Say $\mathcal{Y} = \{-1, 1\}$. Recall: for Gaussians with common covariance,

$$\ln \frac{\Pr(y = 1 \mid x)}{\Pr(y = -1 \mid x)} = \underbrace{w \cdot x + \theta}_{\text{linear}}$$

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

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

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

- More concisely,

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

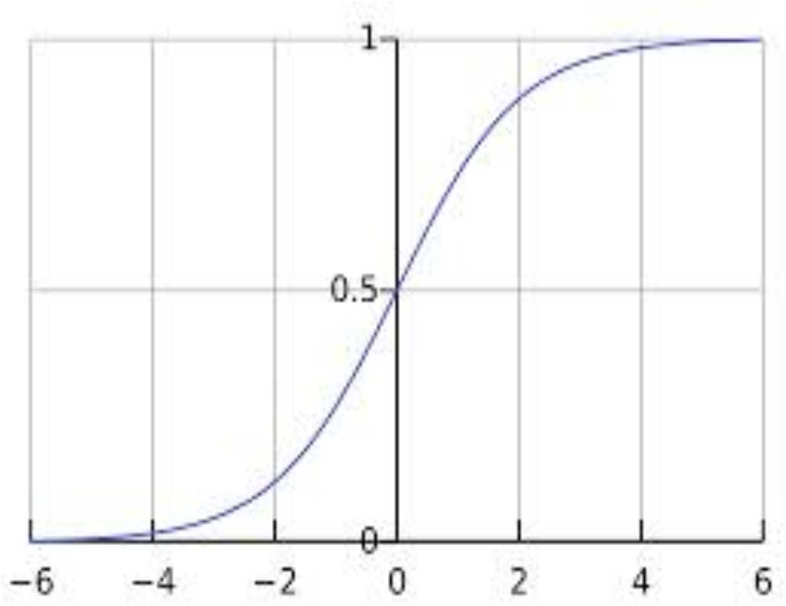
This is the **logistic regression model**, parametrized by w.

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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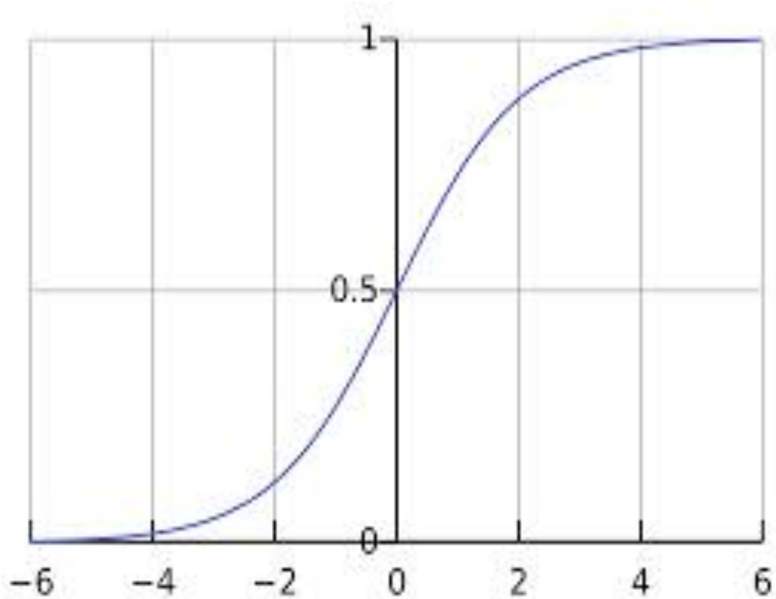

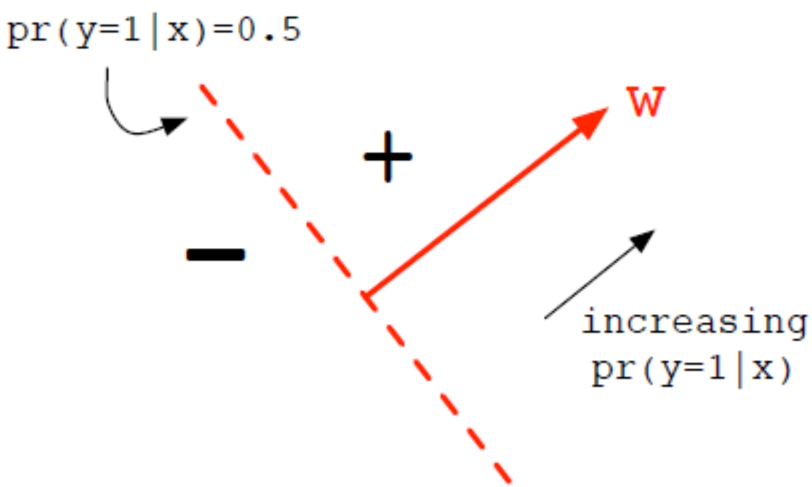

Fitting w

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

$$\prod_{i=1}^{n} \mathrm{Pr}_w(y^{(i)} \mid x^{(i)}).$$

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

Our goal is to minimize $L(w)$.

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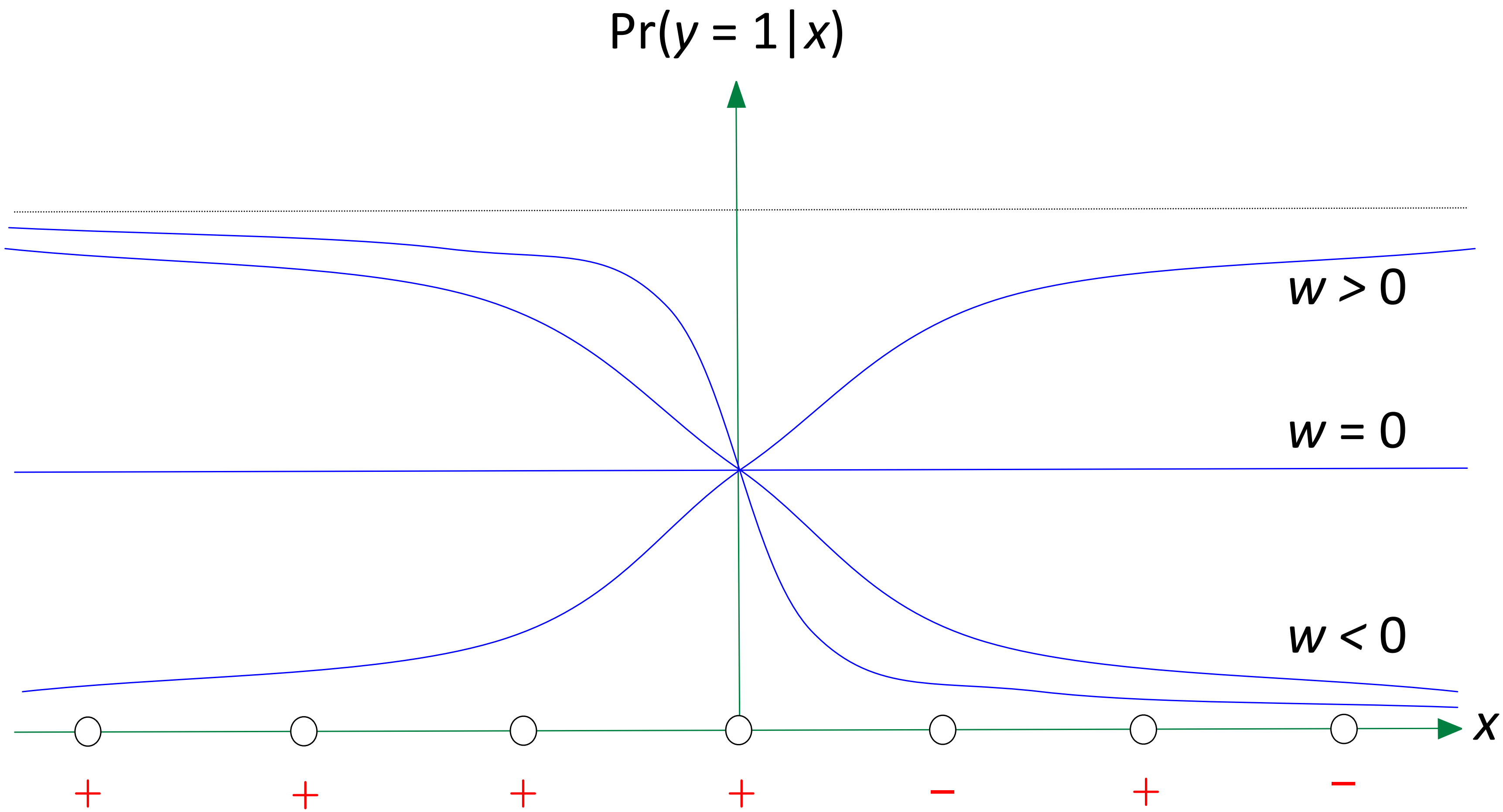
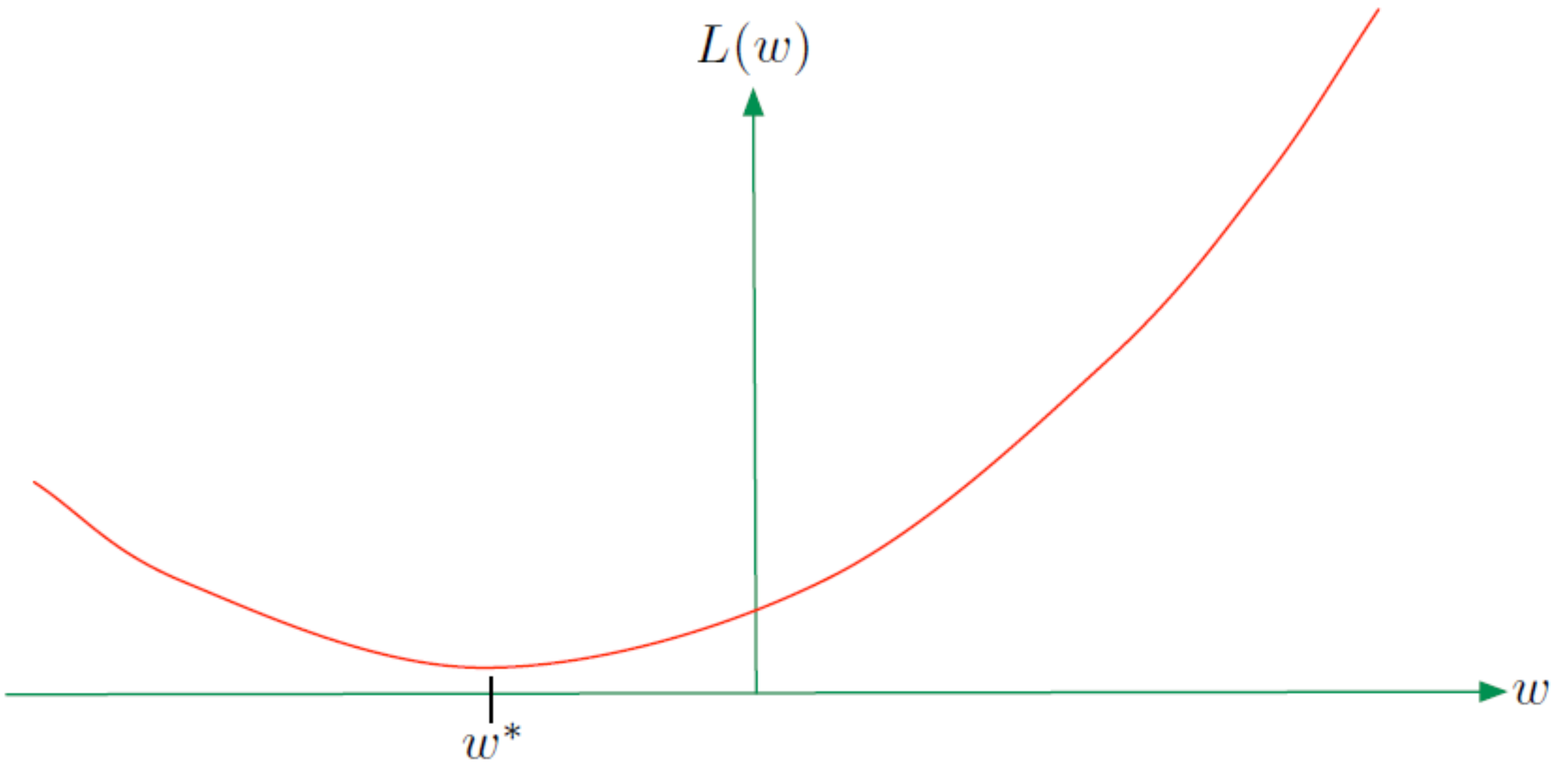
The good news: $L(w)$ is **convex** in w.

One dimensional example

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



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 η_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:

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

  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

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

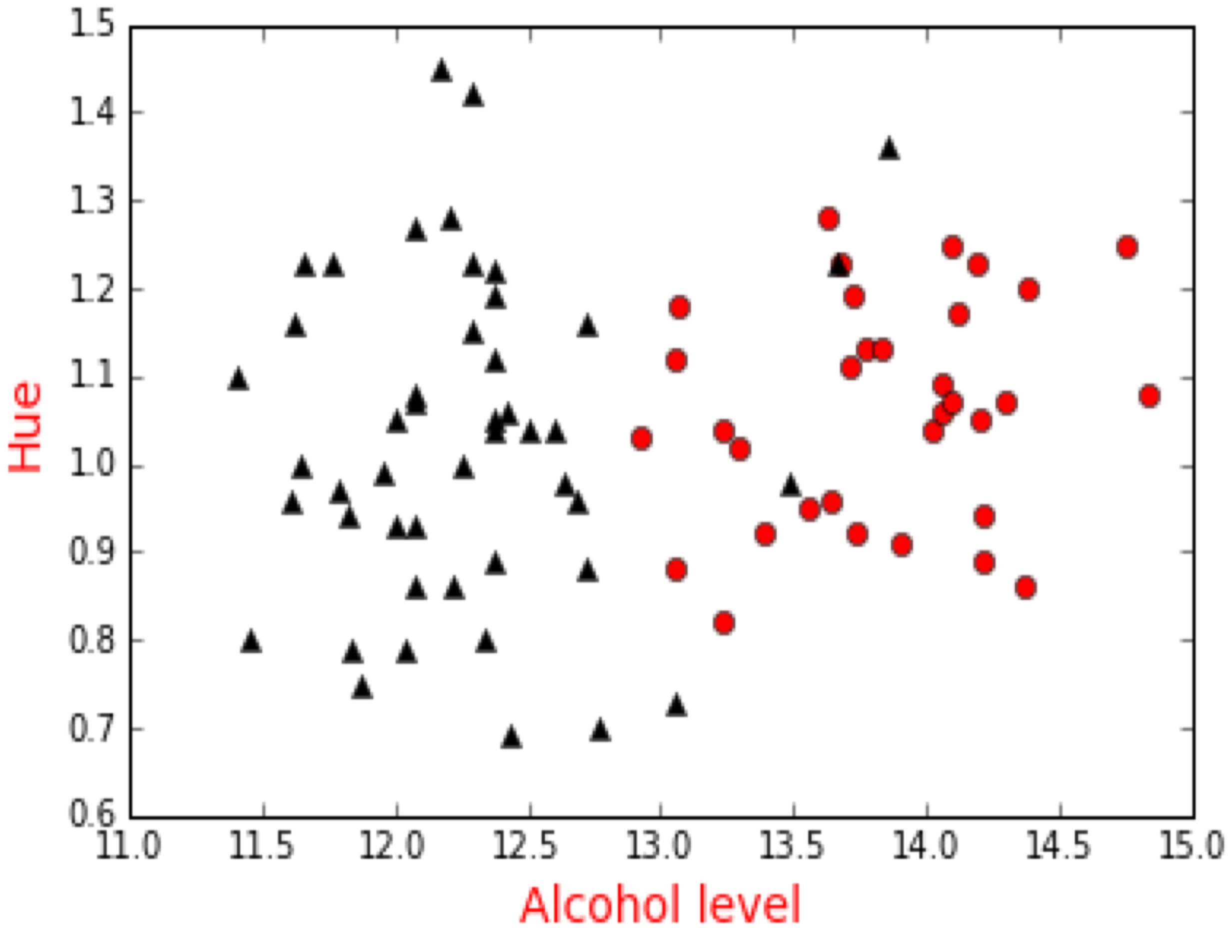
  - η_t is a step size that is either fixed to 1 ("iterative reweighted least squares") or chosen by line search to minimize $L(w_{t+1})$.

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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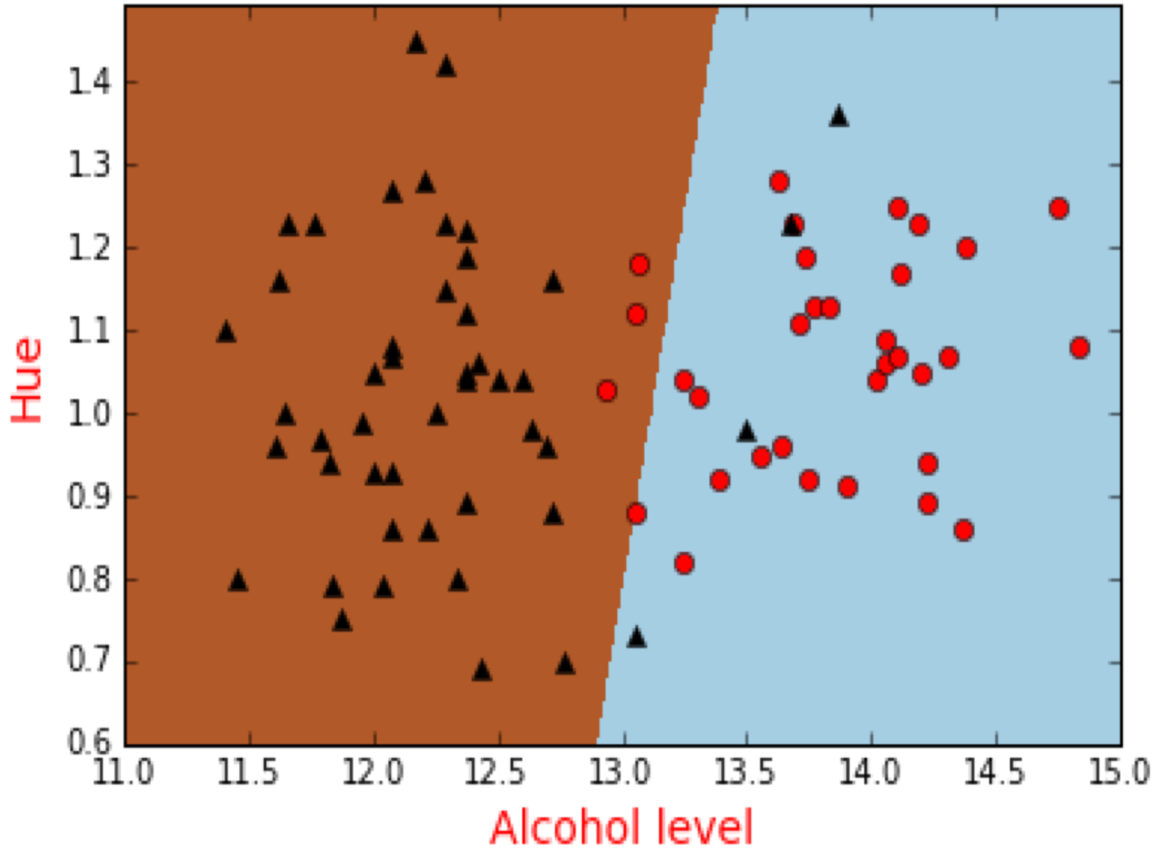

Test error using logistic regression: 10%.

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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Can't we just minimize this by calculus?

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A closer look at the logistic loss

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

Quick quiz

Compute the first derivative of the following functions on $\mathbf{R}^p$.

1. $F(w) = u \cdot w$, where $u \in \mathbf{R}^p$

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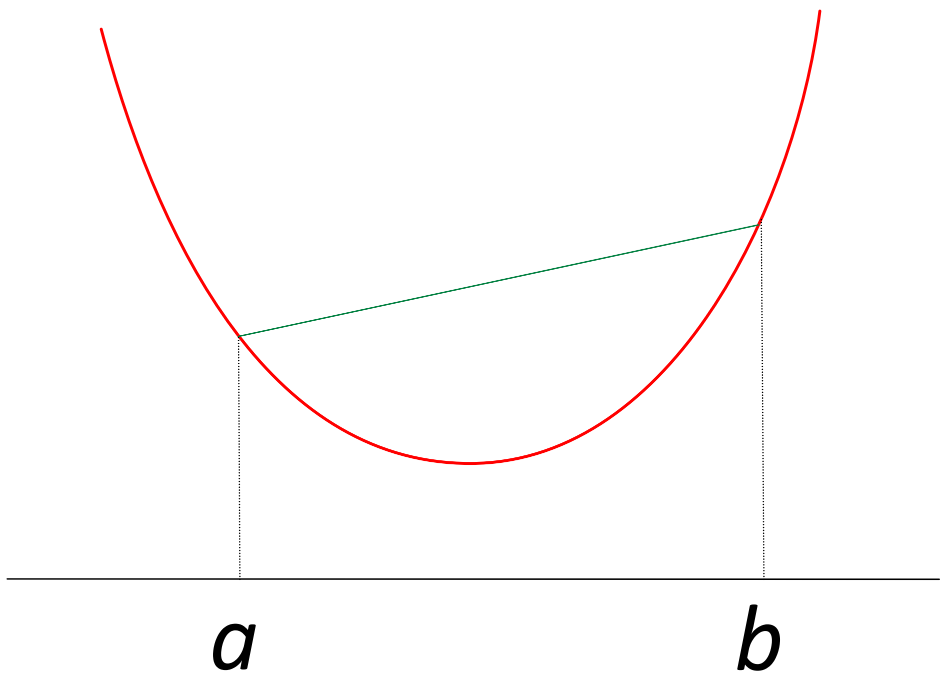
Convexity



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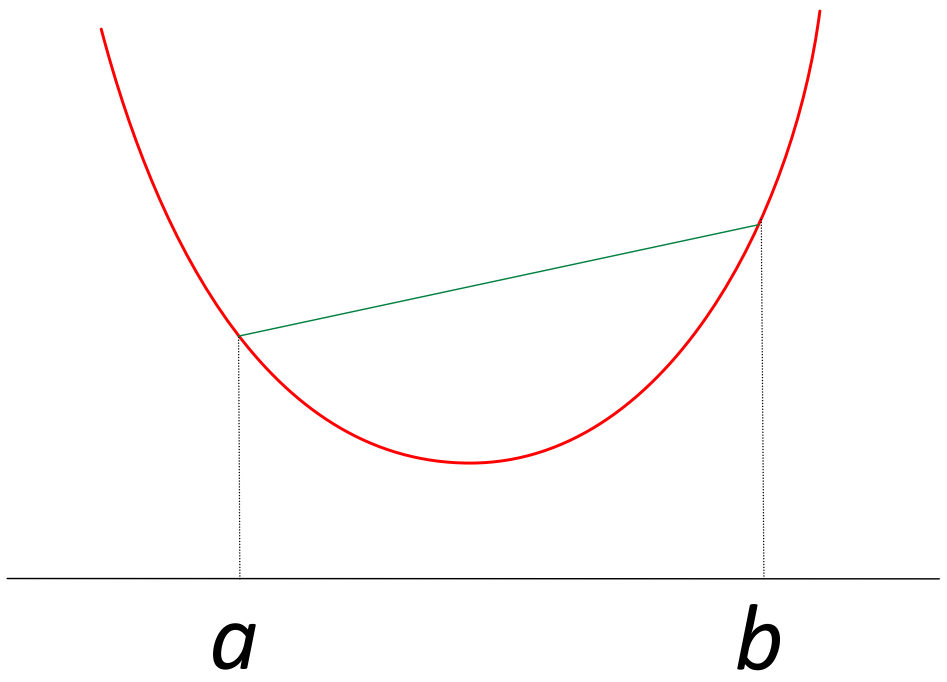

A function $f : \mathbb{R}^p \to \mathbb{R}$ is **convex** if for all $a, b \in \mathbb{R}^p$ and $0 < \theta < 1$,

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

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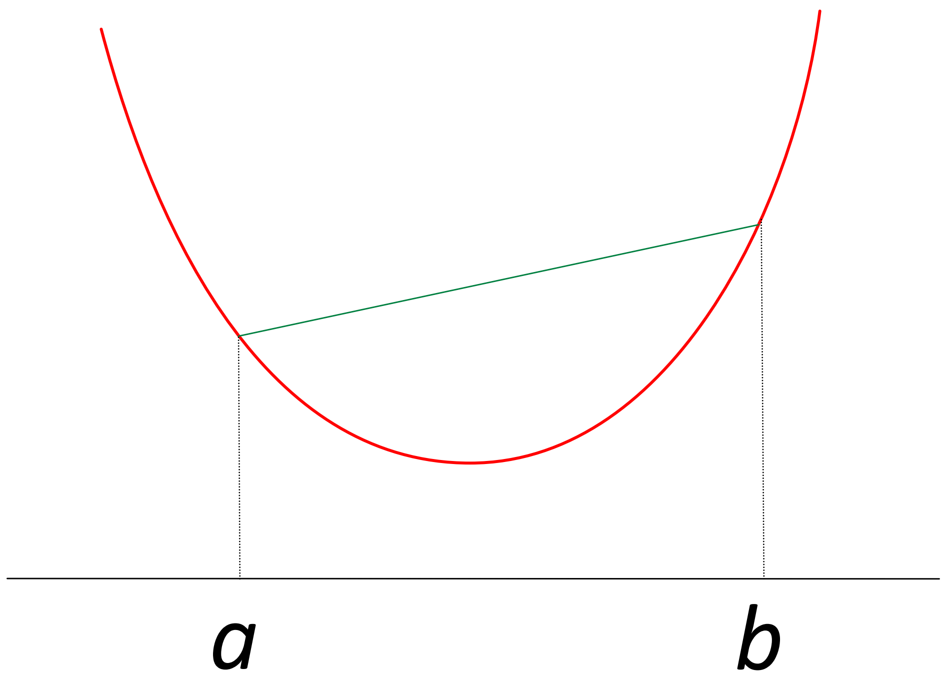

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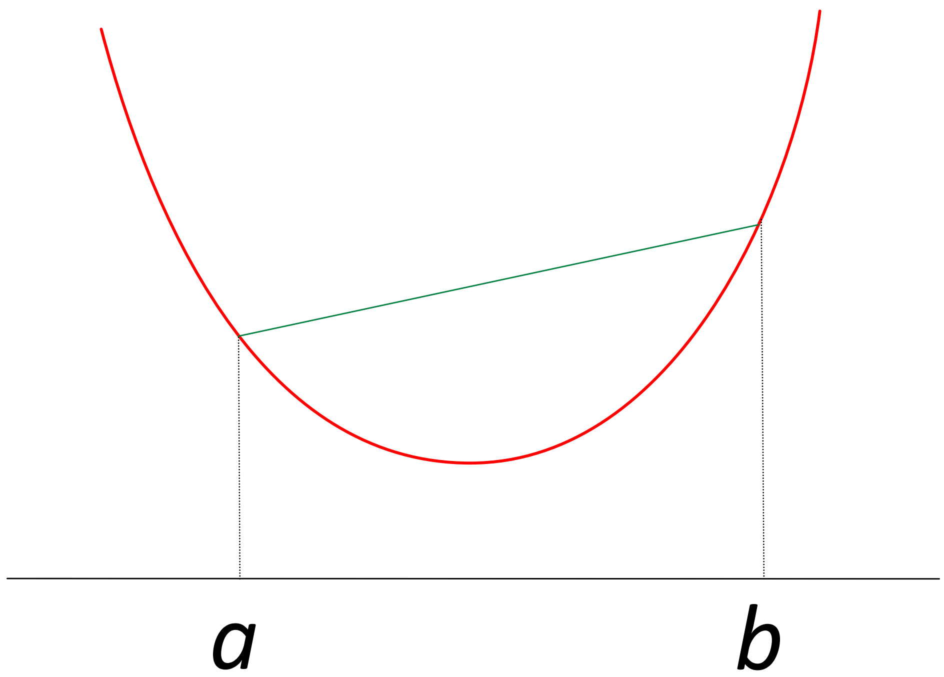

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f is **concave** (resp., **strictly concave**) iff $-f$ is convex (resp., strictly convex).

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:

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

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

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

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

Gradient descent

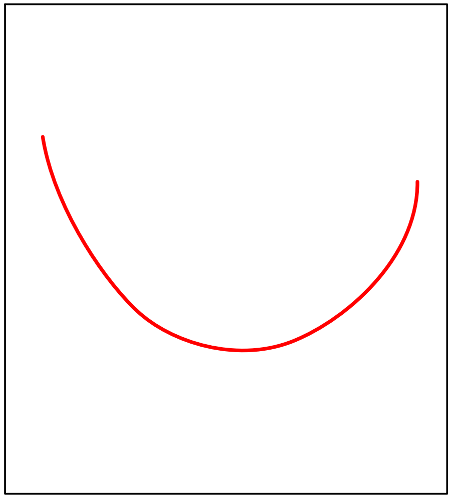
For minimizing a function $L(w)$:

- $w_o = 0, t = 0$
- while $\nabla L(w_t) \neq 0$:
  - $w_{t+1} = w_t - \eta_t \nabla L(w_t)$
  - $t = t + 1$

Here η_t is the *step size* at time t.

Gradient descent: rationale

“Differentiable” means “locally linear”.



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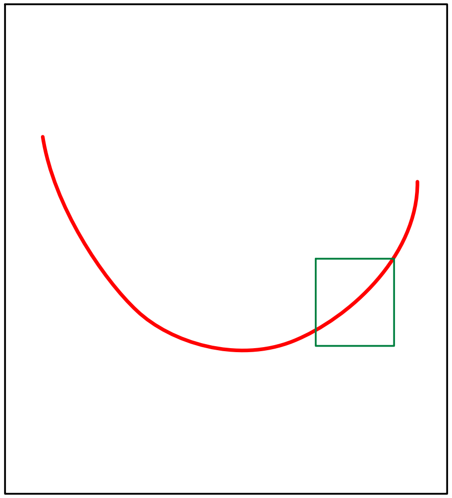

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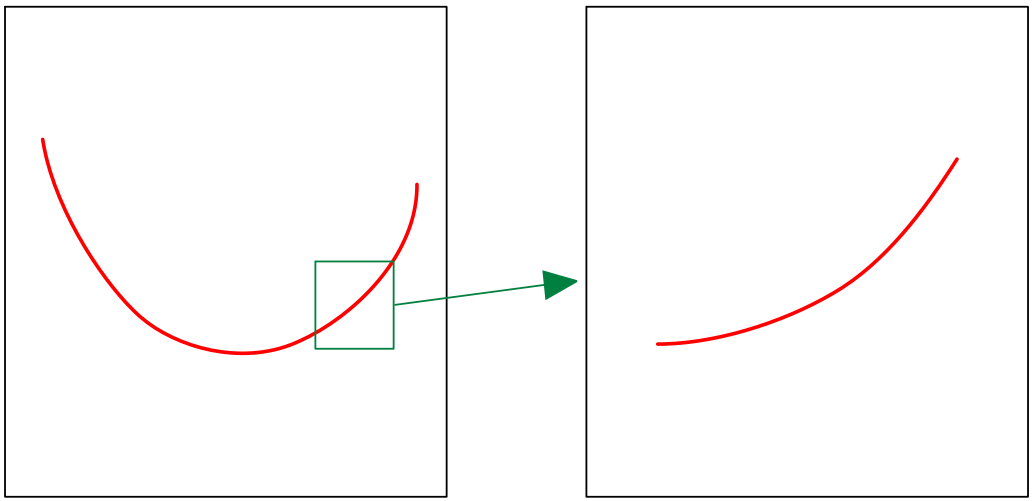

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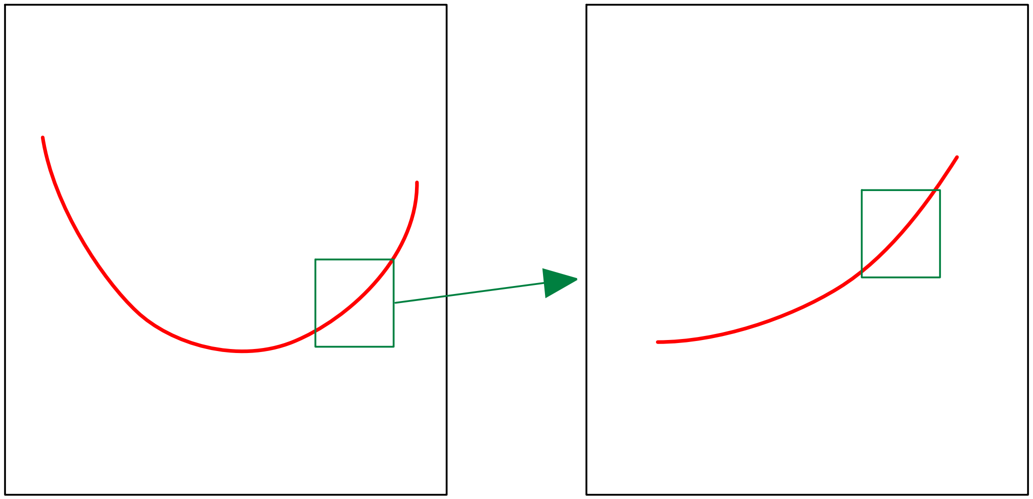

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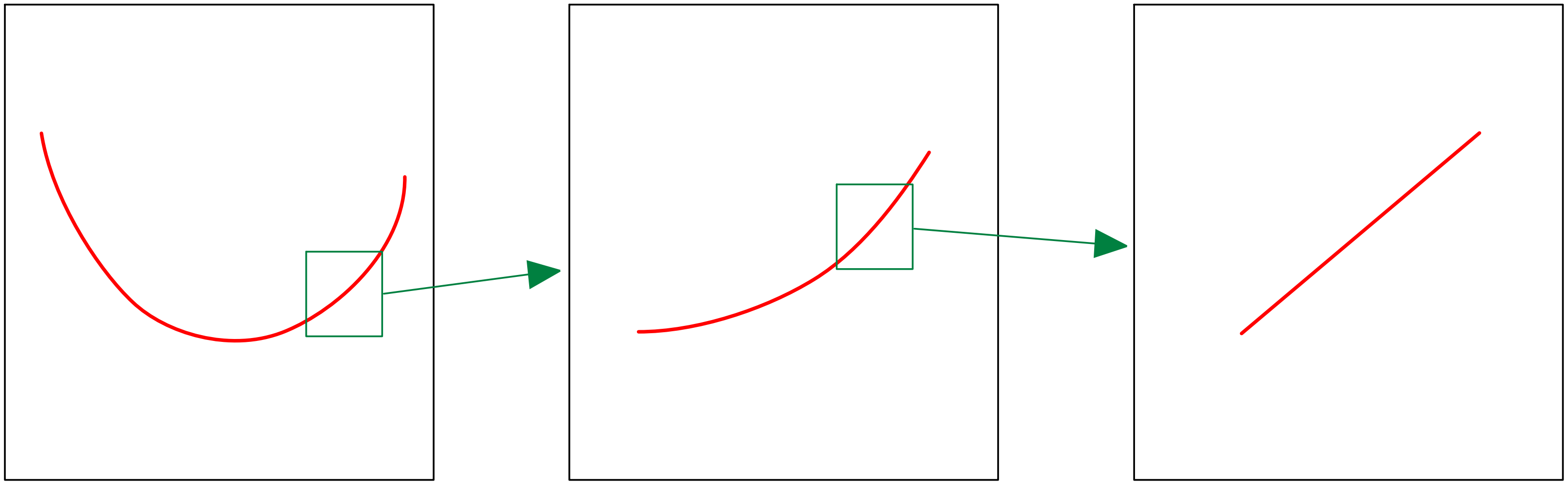

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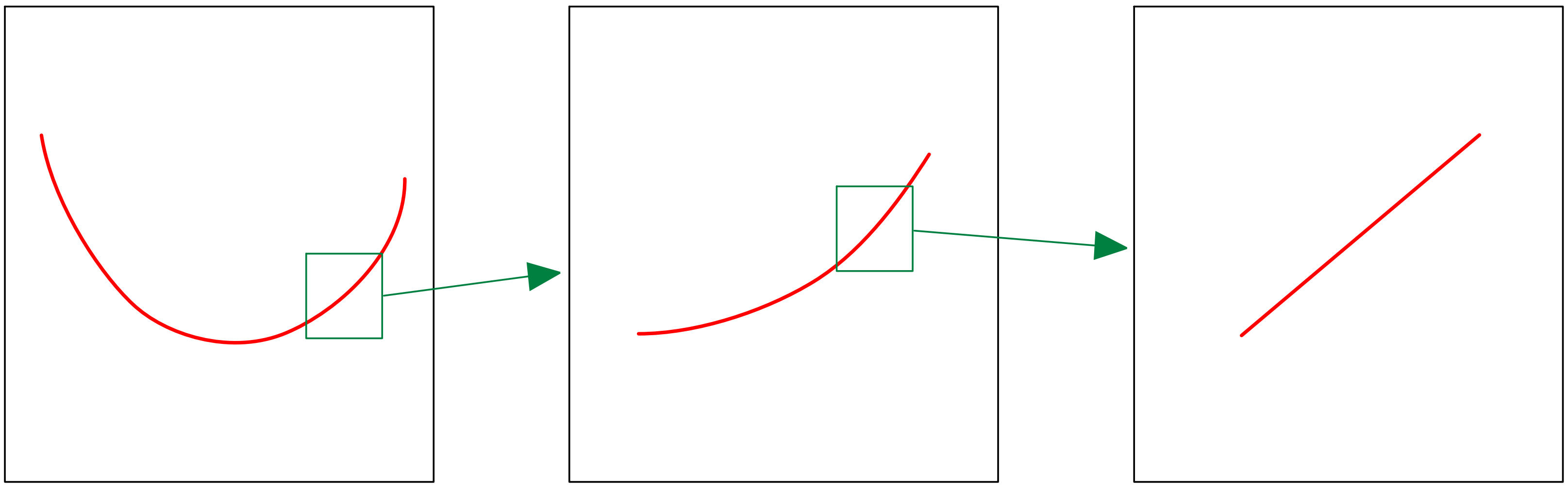


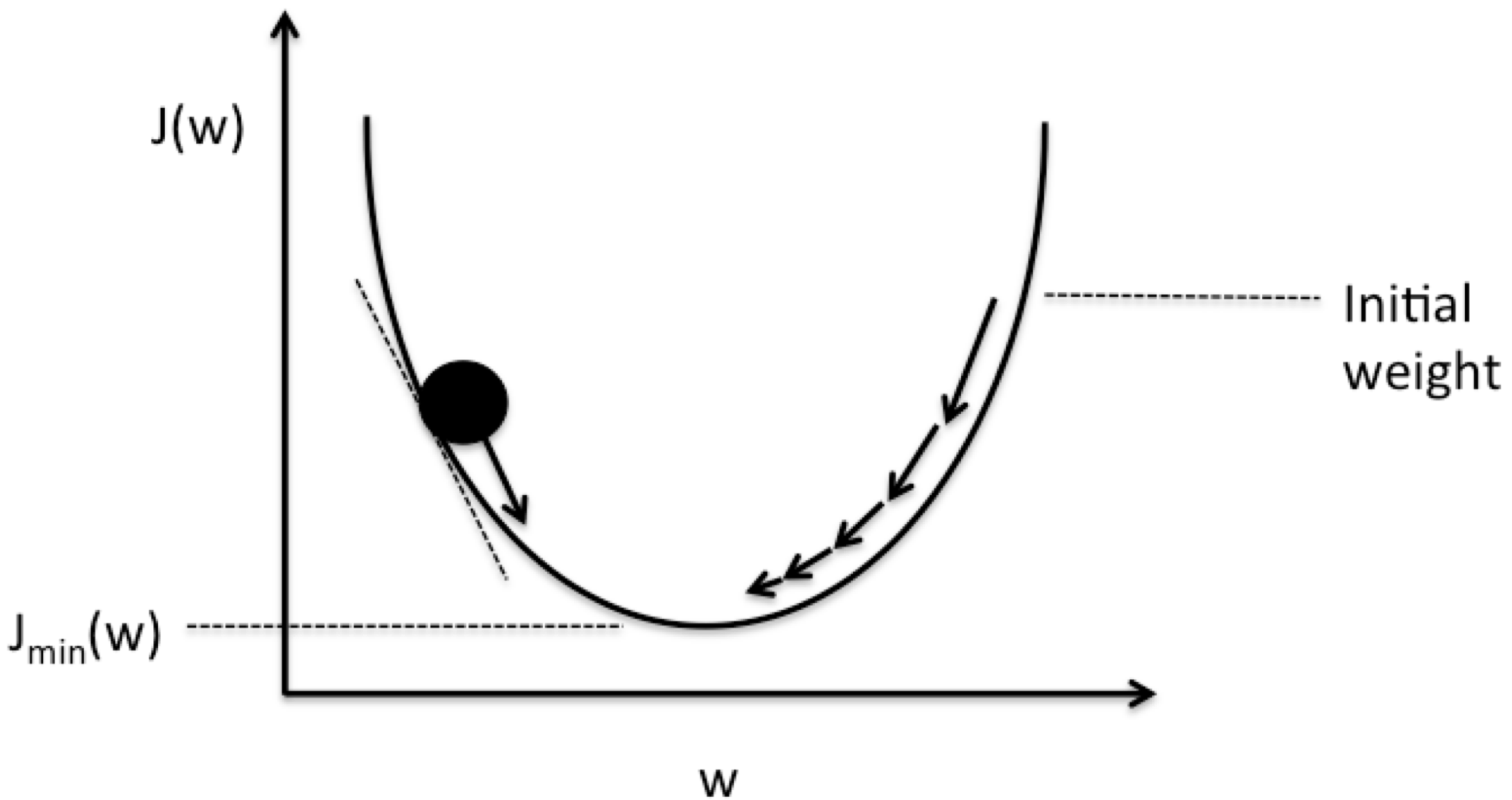
For *small* displacements $u \in \mathbb{R}^p$,

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

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

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

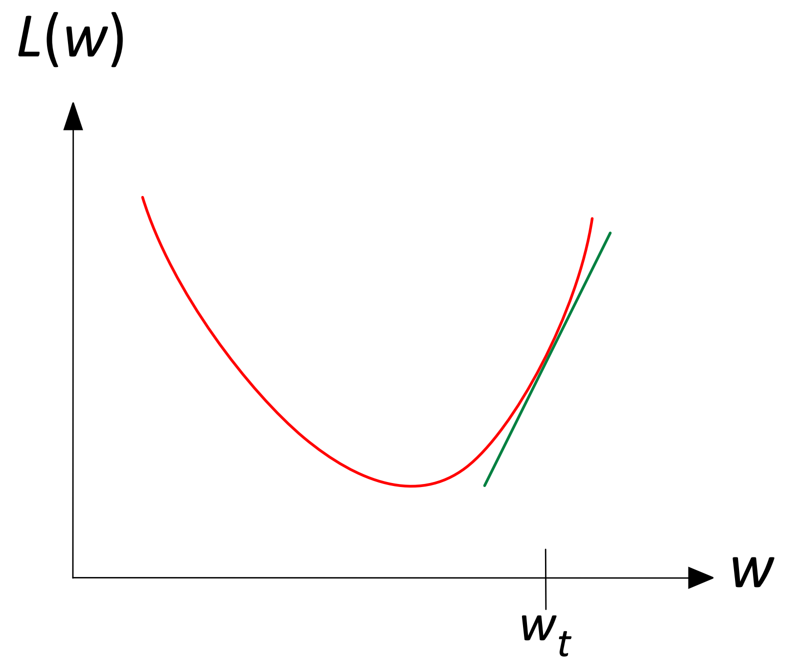
Gradient descent: rationale



Schematic of gradient descent.

The step size matters

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



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- Too large: overshoot the mark

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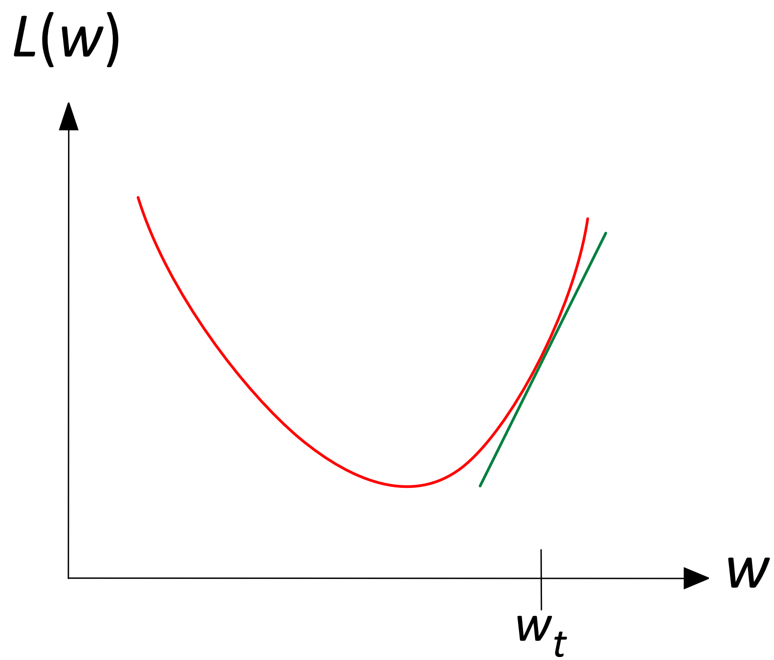

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One option: pick η_t using a line search

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

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

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This makes sure that α 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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Convenient for very large data sets.

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

Newton-Raphson

For minimizing a function $L(w)$:

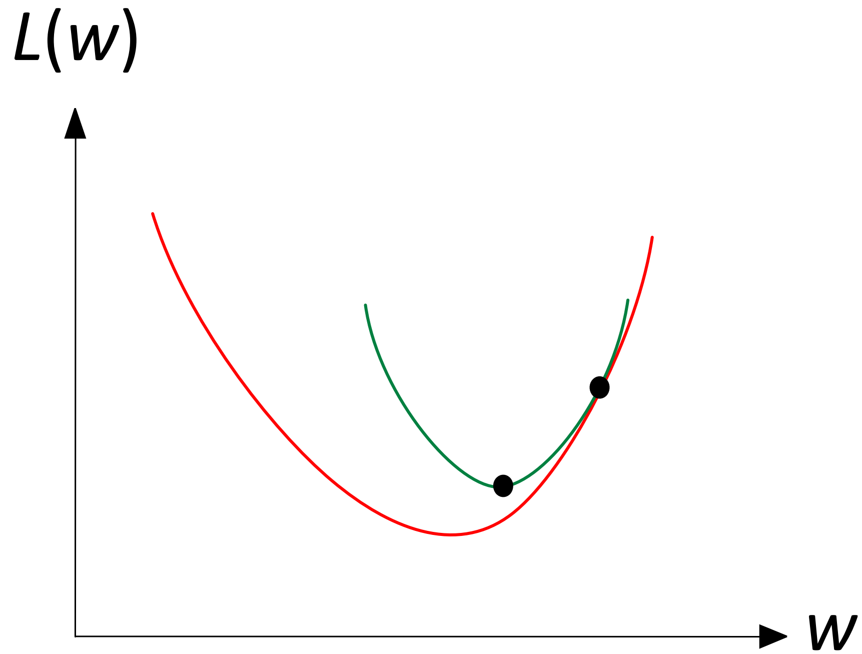
- $w_o = 0, t = 0$
- while $\nabla L(w_t) \not\approx 0$:
  - $w_{t+1} = w_t - \eta_t H^{-1}(w_t) \nabla L(w_t)$
  - $t = t + 1$

$H^{-1}(w)$ 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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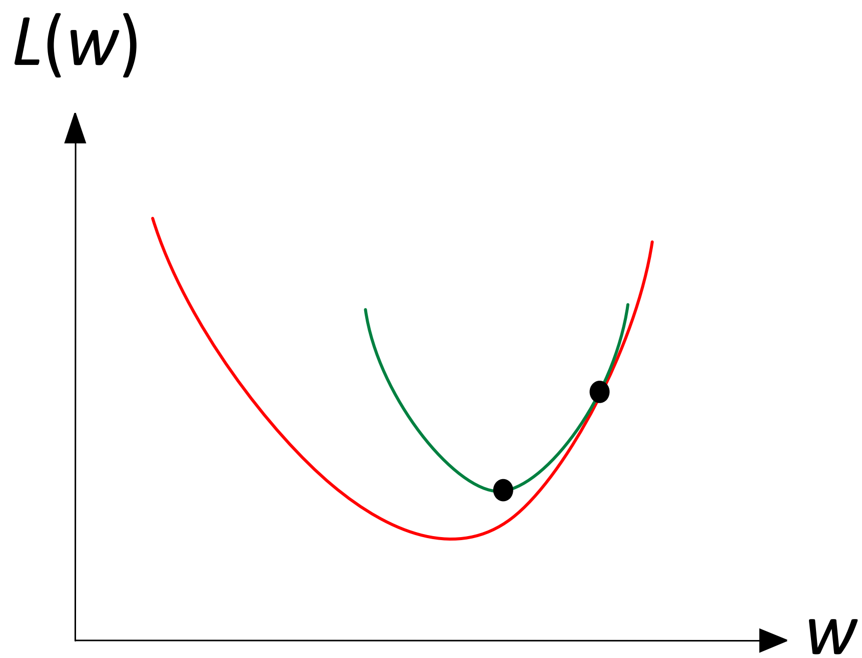

To minimize this quadratic approximation, set derivative to zero:

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

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").

Regularization: Selecting ‘Simple’ Model

1. A ‘simple’ model is one where weights has few non-zero parameters. (Only a few features are relevant.)

2. A ‘simple’ model is one where weights are almost uniform. (Only few features are significantly more relevant than others.)

Regularization

$L'(w) = L(w) + \alpha \, ||w||_1$ → l1 regularization (lasso)

$L'(w) = L(w) + \alpha \, ||w||_2^2$ → l2 regularization (ridge)

http://www.stat.cmu.edu/~larry/=sml/sparsity.pdf