CSCI567 Machine Learning (Fall 2018)

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U of Southern California

Sep 5, 2018

Administration

- HW 1 has been released.
- *Complete the GitHub survey ASAP* if you haven't.
- Follow Piazza for clarifications/typos of HW 1.
- DO NOT post your programming assignment outputs on Piazza.
- DEN problems should have been resolved.

Outline

Outline

Regression

Predicting a continuous outcome variable using past observations

- temperature, amount of rainfall, house price, etc.

Key difference from classification

- continuous vs discrete
- measure *prediction errors* differently.
- lead to quite different learning algorithms.

Linear Regression: regression with linear models: $f(\boldsymbol{w}) = \boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}$

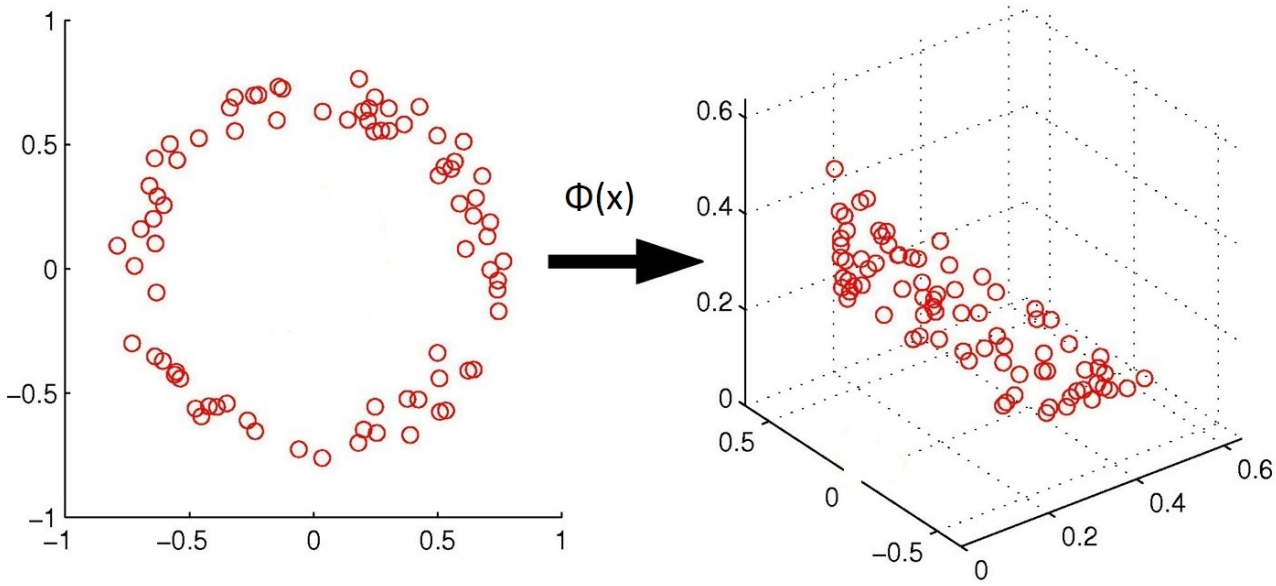
Least square solution

$$
\begin{aligned}
\boldsymbol{w}^* &= \underset{\boldsymbol{w}}{\operatorname{argmin}} \operatorname{RSS}(\boldsymbol{w}) \\
&= \underset{\boldsymbol{w}}{\operatorname{argmin}} \|\boldsymbol{X}\boldsymbol{w} - \boldsymbol{y}\|_2^2 \\
&= \left(\boldsymbol{X}^{\mathrm{T}}\boldsymbol{X}\right)^{-1}\boldsymbol{X}^{\mathrm{T}}\boldsymbol{y}
\end{aligned}
\qquad
\boldsymbol{X} = \begin{pmatrix} \boldsymbol{x}_1^{\mathrm{T}} \\ \boldsymbol{x}_2^{\mathrm{T}} \\ \vdots \\ \boldsymbol{x}_{\mathsf{N}}^{\mathrm{T}} \end{pmatrix}, \quad \boldsymbol{y} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_{\mathsf{N}} \end{pmatrix}
$$

Two approaches to find the minimum:

- find **stationary points** by setting gradient $= \mathbf{0}$
- "**complete the square**"

Regression with nonlinear basis



Model: $f(\boldsymbol{x}) = \boldsymbol{w}^{\mathrm{T}}\boldsymbol{\phi}(\boldsymbol{x})$ where $\boldsymbol{w} \in \mathbb{R}^M$

Similar least square solution: $\boldsymbol{w}^* = \left(\boldsymbol{\Phi}^{\mathrm{T}}\boldsymbol{\Phi}\right)^{-1}\boldsymbol{\Phi}^{\mathrm{T}}\boldsymbol{y}$

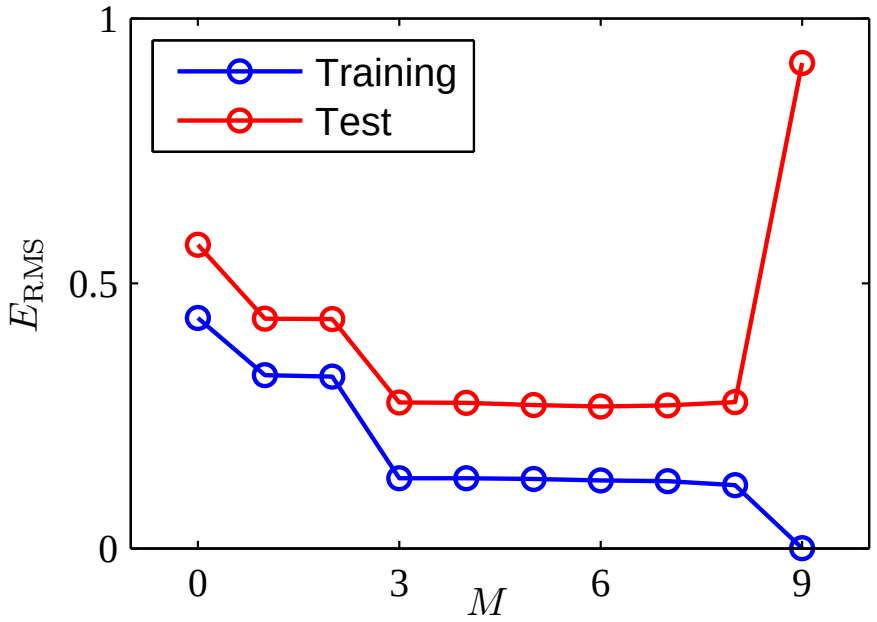
Underfitting and Overfitting

$M \leq 2$ is *underfitting* the data

- large training error
- large test error

$M \geq 9$ is *overfitting* the data

- small training error
- **large test error**



How to prevent overfitting? more data + regularization

$$\boldsymbol{w}^* = \underset{\boldsymbol{w}}{\operatorname{argmin}} \left(\mathrm{RSS}(\boldsymbol{w}) + \lambda \|\boldsymbol{w}\|_2^2 \right) = \left(\boldsymbol{\Phi}^{\mathrm{T}} \boldsymbol{\Phi} + \lambda \boldsymbol{I} \right)^{-1} \boldsymbol{\Phi}^{\mathrm{T}} \boldsymbol{y}$$

General idea to derive ML algorithms

Step 1. Pick a set of **models** $\mathcal{F}$

- e.g. $\mathcal{F} = \{f(\boldsymbol{x}) = \boldsymbol{w}^{\mathrm{T}}\boldsymbol{x} \mid \boldsymbol{w} \in \mathbb{R}^{\mathsf{D}}\}$
- e.g. $\mathcal{F} = \{f(\boldsymbol{x}) = \boldsymbol{w}^{\mathrm{T}}\boldsymbol{\Phi}(\boldsymbol{x}) \mid \boldsymbol{w} \in \mathbb{R}^{\mathsf{M}}\}$

Step 2. Define **error/loss** $L(y', y)$

Step 3. Find **empirical risk minimizer (ERM)**:

$$\boldsymbol{f}^* = \operatorname*{argmin}_{f \in \mathcal{F}} \sum_{n=1}^{N} L(f(x_n), y_n)$$

or **regularized empirical risk minimizer**:

$$\boldsymbol{f}^* = \operatorname*{argmin}_{f \in \mathcal{F}} \sum_{n=1}^{N} L(f(x_n), y_n) + \lambda R(f)$$

ML becomes optimization

Outline

Classification

Recall the setup:

- input (feature vector): $\boldsymbol{x} \in \mathbb{R}^{\mathsf{D}}$
- output (label): $y \in [\mathsf{C}] = \{1, 2, \cdots, \mathsf{C}\}$
- goal: learn a mapping $f : \mathbb{R}^{\mathsf{D}} \to [\mathsf{C}]$

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This lecture: **binary classification**

- Number of classes: $\mathsf{C} = 2$
- Labels: $\{-1, +1\}$ (cat or dog, fraud or not, price up or down...)

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We have discussed **nearest neighbor classifier**:

- require carrying the training set
- more like a heuristic

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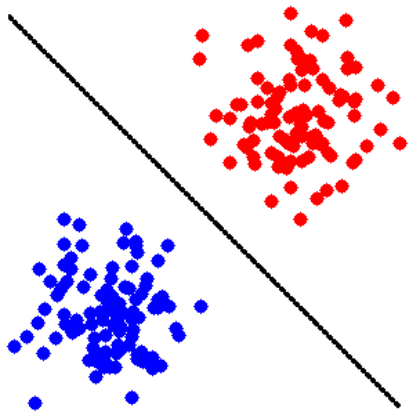

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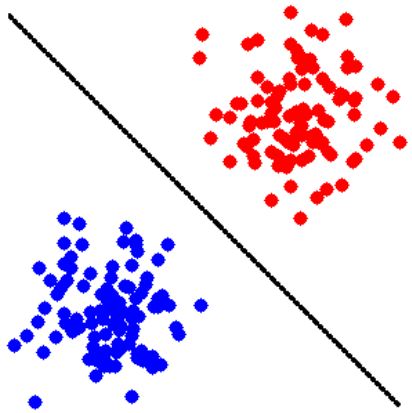
Sign of $\boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}$ predicts the label:

$$\text{sign}(\boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}) = \begin{cases} +1 & \text{if } \boldsymbol{w}^{\mathrm{T}}\boldsymbol{x} > 0 \\ -1 & \text{if } \boldsymbol{w}^{\mathrm{T}}\boldsymbol{x} \leq 0 \end{cases}$$

(Sometimes use sgn for sign too.)



The models

The set of **(separating) hyperplanes**:

$$\mathcal{F} = \{f(\boldsymbol{x}) = \mathsf{sgn}(\boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}) \mid \boldsymbol{w} \in \mathbb{R}^{\mathsf{D}}\}$$

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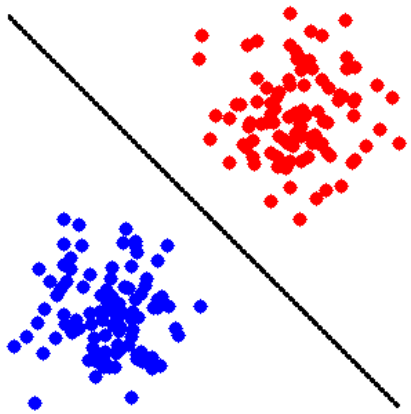
Good choice for *linearly separable* data, i.e., $\exists \boldsymbol{w}$ s.t.

$$\mathsf{sgn}(\boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}_{\boldsymbol{n}}) = y_n$$

for all $n \in [N]$.



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$$\mathsf{sgn}(\boldsymbol{w}^{\mathrm{T}}\boldsymbol{x_n}) = y_n \quad \text{or} \quad y_n \boldsymbol{w}^{\mathrm{T}}\boldsymbol{x_n} > 0$$

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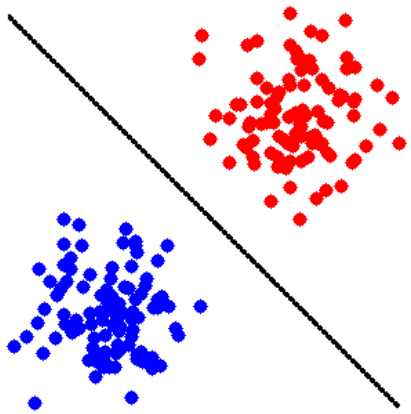
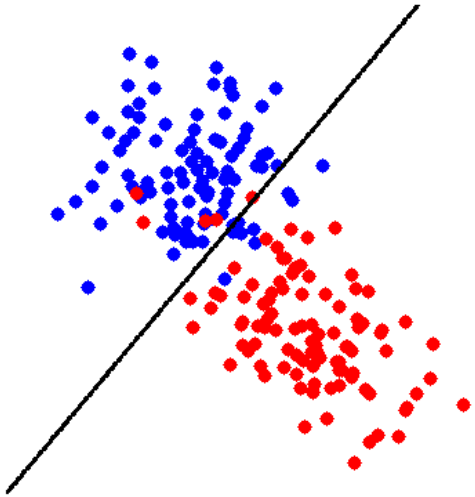


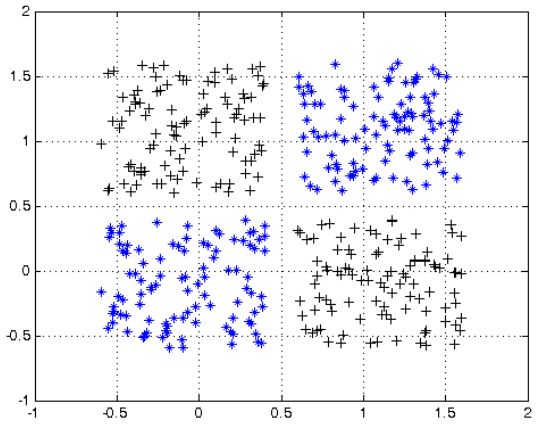
The models

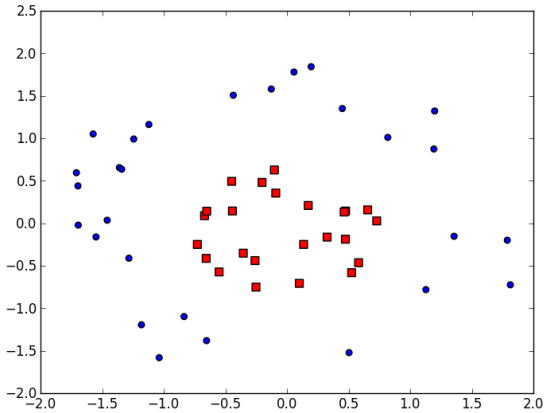
Still makes sense for "almost" linearly separable data



The models

For clearly not linearly separable data,





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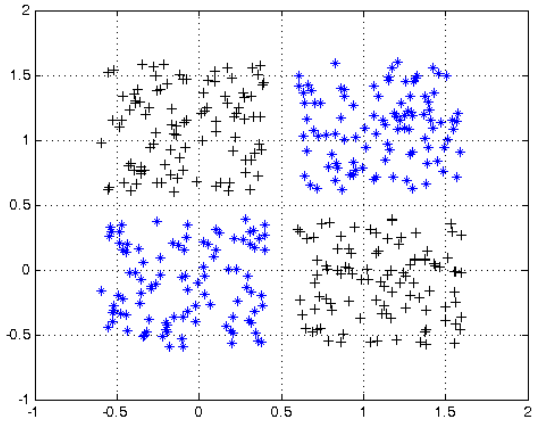

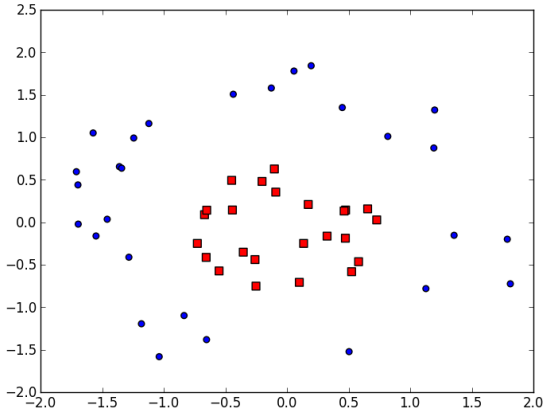

Again can apply a **nonlinear mapping** $\mathbf{\Phi}$:

$$\mathcal{F} = \{f(\boldsymbol{x}) = \mathsf{sgn}(\boldsymbol{w}^{\mathrm{T}}\mathbf{\Phi}(\boldsymbol{x})) \mid \boldsymbol{w} \in \mathbb{R}^{\mathsf{M}}\}$$

More discussions in the next two lectures.

0-1 Loss

Step 2. Define error/loss $L(y', y)$.

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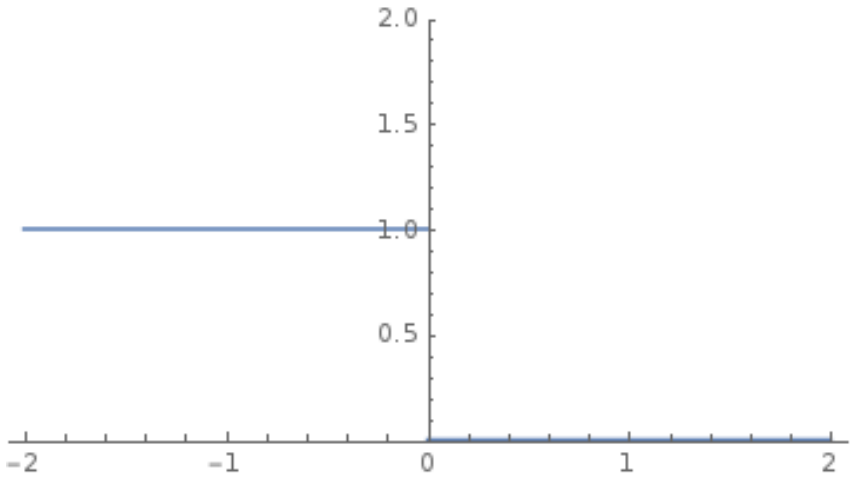
Most natural one for classification: **0-1 loss** $L(y', y) = \mathbb{I}[y' \neq y]$

For classification, more convenient to look at the loss **as a function of** $y\boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}$. That is, with

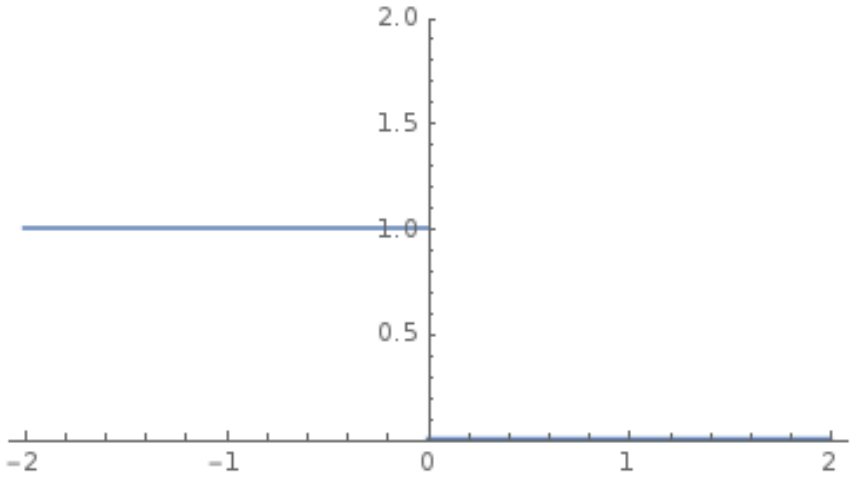
$$\ell_{0\text{-}1}(z) = \mathbb{I}[z \leq 0]$$



the loss for hyperplane $\boldsymbol{w}$ on example $(\boldsymbol{x}, y)$ is $\ell_{0\text{-}1}(y\boldsymbol{w}^{\mathrm{T}}\boldsymbol{x})$

Minimizing 0-1 loss is hard

However, 0-1 loss is *not convex*.



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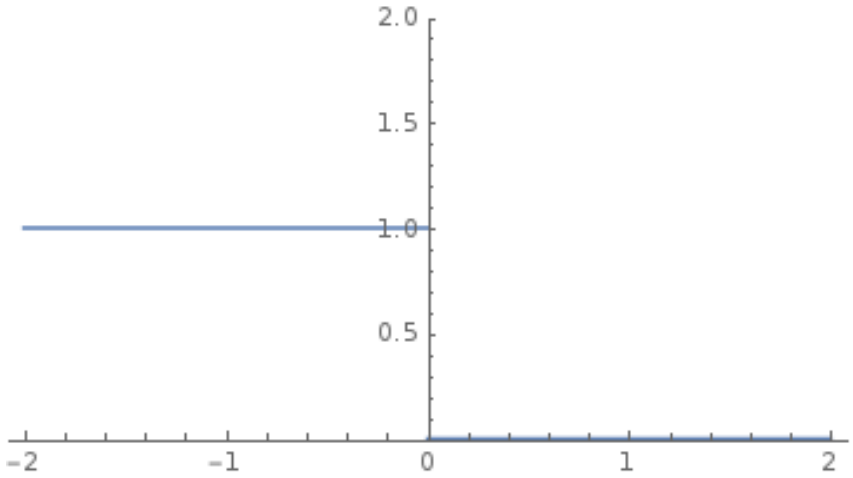
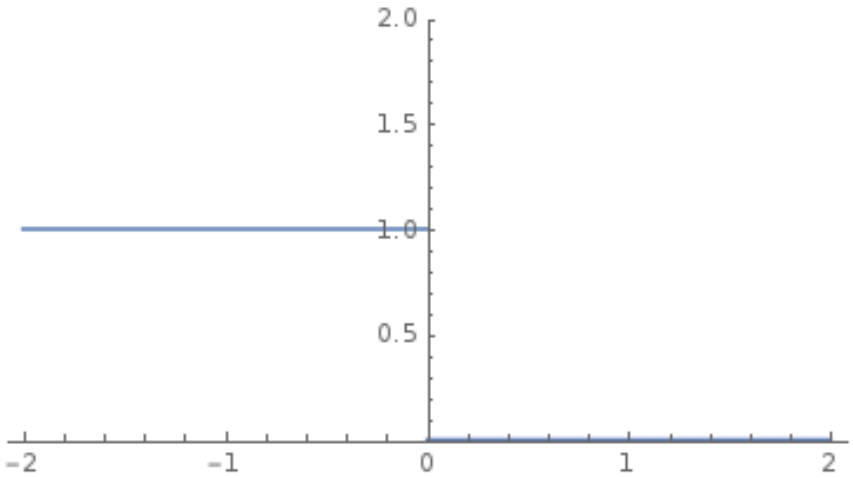


Even worse, minimizing 0-1 loss is *NP-hard in general*.

Surrogate Losses

Solution: find a **convex surrogate loss**



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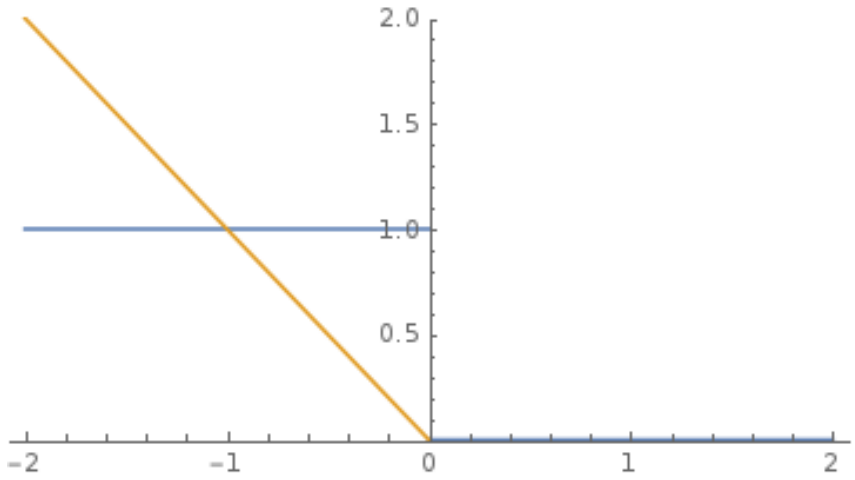

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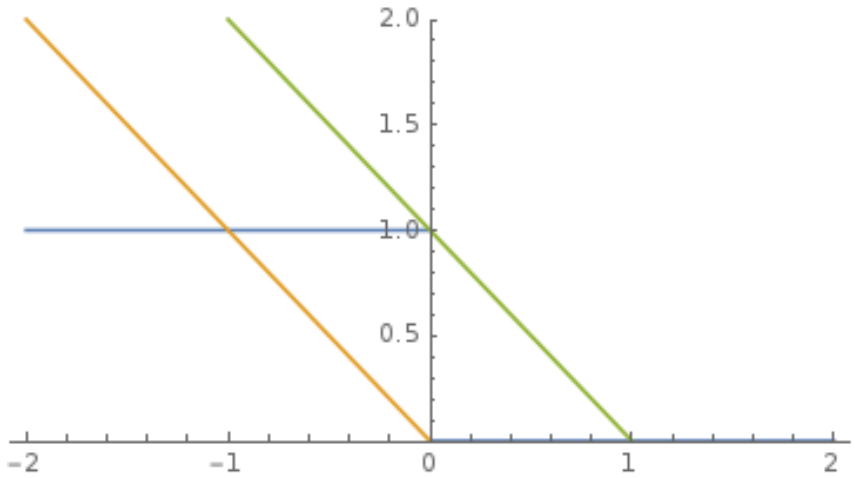

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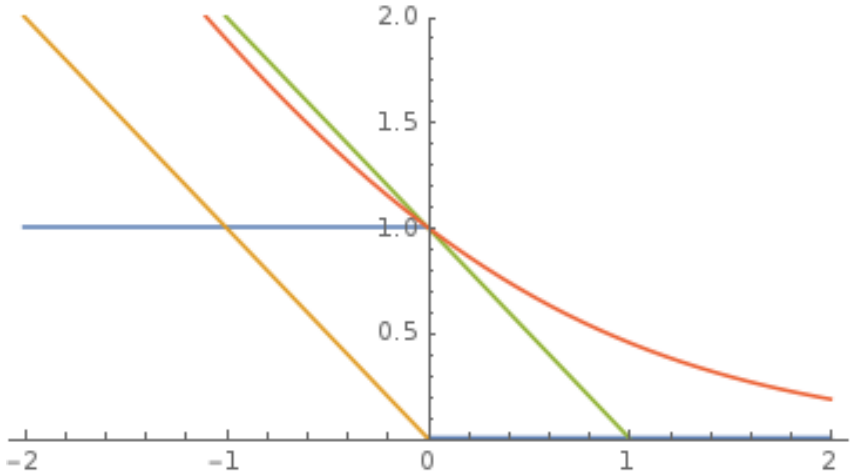

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- logistic loss $\ell_{\text{logistic}}(z) = \log(1 + \exp(-z))$ (used in logistic regression; the base of $\log$ doesn't matter)

ML becomes convex optimization

Step 3. Find ERM:

$$\boldsymbol{w}^* = \underset{\boldsymbol{w} \in \mathbb{R}^{\mathsf{D}}}{\operatorname{argmin}} \sum_{n=1}^{N} \ell(y_n \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n)$$

where $\ell(\cdot)$ can be perceptron/hinge/logistic loss

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Note: minimizing perceptron loss *does not really make sense* (try $\boldsymbol{w} = \mathbf{0}$), but the algorithm derived from this perspective does.

Outline

The Perceptron Algorithm

In one sentence: Stochastic Gradient Descent applied to perceptron loss

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i.e. find the minimizer of

$$F(\boldsymbol{w}) = \sum_{n=1}^{N} \ell_{\text{perceptron}}(y_n \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n)$$
$$= \sum_{n=1}^{N} \max\{0, -y_n \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n\}$$

using SGD

A detour of numerical optimization methods

We describe two simple yet extremely popular methods

- **Gradient Descent (GD)**: simple and fundamental
- **Stochastic Gradient Descent (SGD)**: faster, effective for large-scale problems

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- **Gradient Descent (GD)**: simple and fundamental
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Gradient is sometimes referred to as *first-order* information of a function. Therefore, these methods are called *first-order methods*.

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Goal: minimize $F(\boldsymbol{w})$

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where $\eta > 0$ is called step size or learning rate

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- in theory η should be set in terms of some parameters of F
- in practice we just try several small values

An example

Example: $F(\boldsymbol{w}) = 0.5(w_1^2 - w_2)^2 + 0.5(w_1 - 1)^2$.

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- do

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$$w_2^{(t+1)} \leftarrow w_2^{(t)} - \eta \left[-({w_1^{(t)}}^2 - w_2^{(t)}) \right]$$

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- until $F(\boldsymbol{w}^{(t)})$ **does not change much**

Why GD?

Intuition: by first-order **Taylor approximation**

$$F(\boldsymbol{w}) \approx F(\boldsymbol{w}^{(t)}) + \nabla F(\boldsymbol{w}^{(t)})^{\mathrm{T}}(\boldsymbol{w} - \boldsymbol{w}^{(t)})$$

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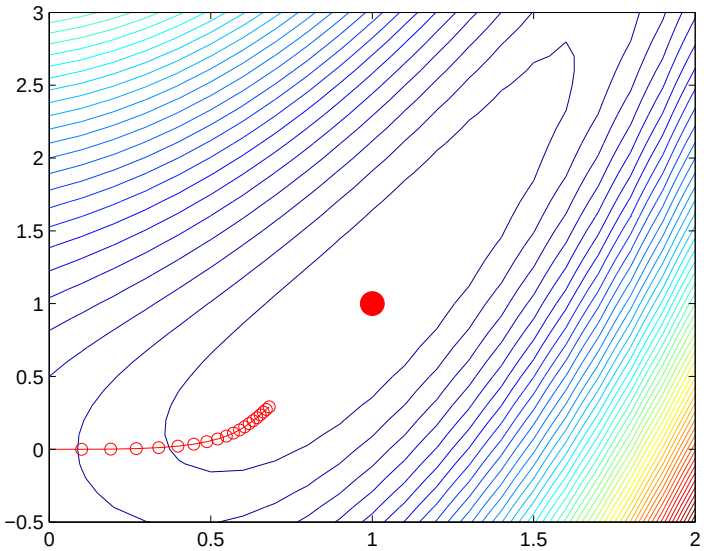

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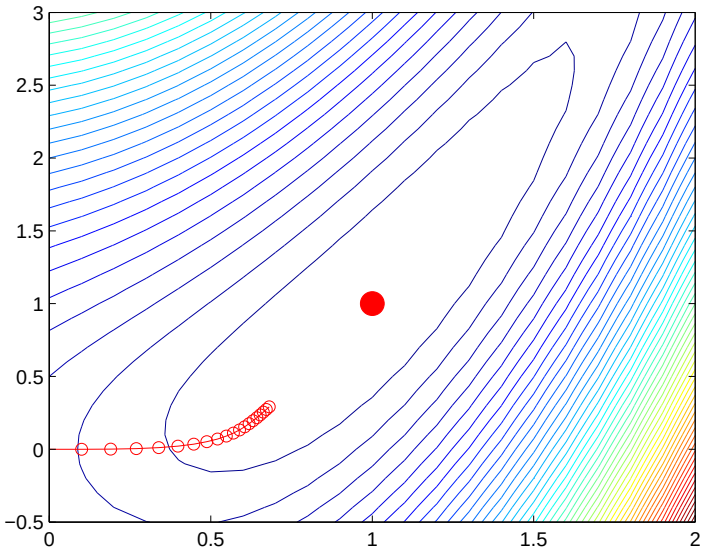

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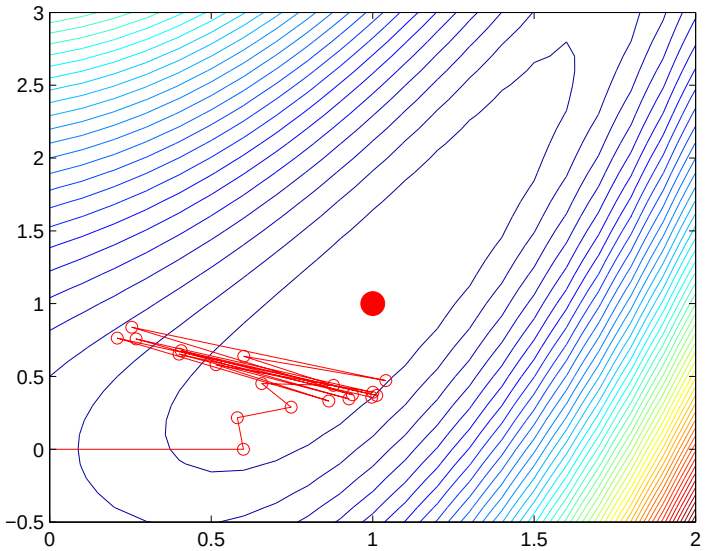

but large η is unstable

Stochastic Gradient Descent (SGD)

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$$\boldsymbol{w}^{(t+1)} \leftarrow \boldsymbol{w}^{(t)} - \eta \tilde{\nabla} F(\boldsymbol{w}^{(t)})$$

where $\tilde{\nabla} F(\boldsymbol{w}^{(t)})$ is a random variable (called **stochastic gradient**) s.t.

$$\mathbb{E}\left[\tilde{\nabla} F(\boldsymbol{w}^{(t)})\right] = \nabla F(\boldsymbol{w}^{(t)}) \qquad \text{(unbiasedness)}$$

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$$\mathbb{E}\left[\tilde{\nabla} F(\boldsymbol{w}^{(t)})\right] = \nabla F(\boldsymbol{w}^{(t)}) \qquad \text{(unbiasedness)}$$

Key point: it could be *much faster to obtain a stochastic gradient*!

Convergence Guarantees

Many for both GD and SGD on convex objectives.

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Even for *nonconvex objectives*, many recent works show effectiveness of GD/SGD.

Applying GD to perceptron loss

Objective

$$F(\boldsymbol{w}) = \sum_{n=1}^{N} \max\{0, -y_n \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n\}$$

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Slow: each update makes one pass of the entire training set!

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One common trick: pick one example $n \in [N]$ uniformly at random, let

$$\tilde{\nabla} F(\boldsymbol{w}^{(t)}) = -N \mathbb{I}[y_n \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n \leq 0] y_n \boldsymbol{x}_n$$

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Exercise: try SGD to minimize RSS for linear regression.

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- why $\eta = 1$? Does not really matter in terms of training error

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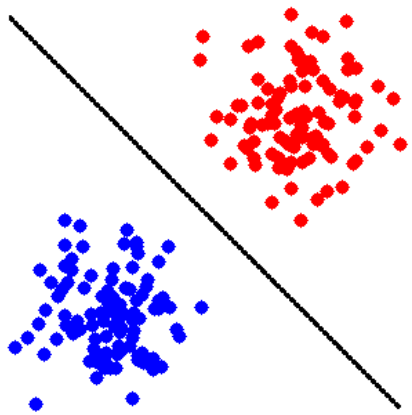
Thus it is more likely to get it right after the update.

Any theory?

(HW 1) If training set is linearly separable

- Perceptron *converges in a finite number of steps*
- training error is 0



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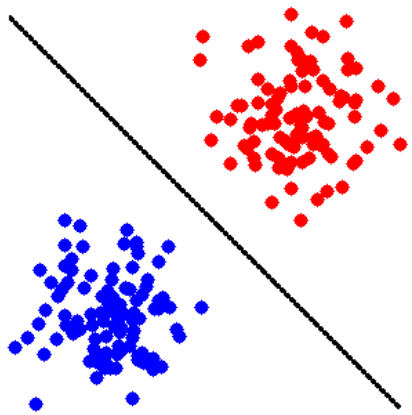

There are also guarantees when the data is not linearly separable.

Outline

A simple view

In one sentence: find the minimizer of

$$F(\boldsymbol{w}) = \sum_{n=1}^{N} \ell_{\text{logistic}}(y_n \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n)$$
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But why logistic loss? and why "regression"?

Predicting probability

Instead of predicting a discrete label, can we *predict the probability of each label?* i.e. regress the probabilities

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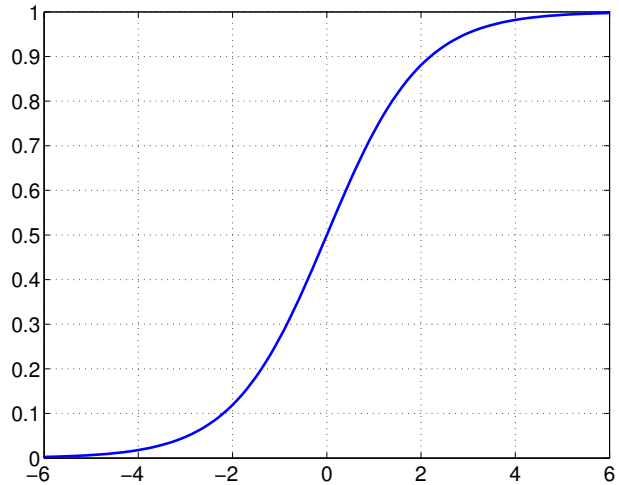
One way: **sigmoid function + linear model**

$$\mathbb{P}(y = +1 \mid \boldsymbol{x}; \boldsymbol{w}) = \sigma(\boldsymbol{w}^{\mathrm{T}} \boldsymbol{x})$$

where σ is the sigmoid function:

$$\sigma(z) = \frac{1}{1 + e^{-z}}$$



Properties

Properties of sigmoid $\sigma(z) = \frac{1}{1+e^{-z}}$

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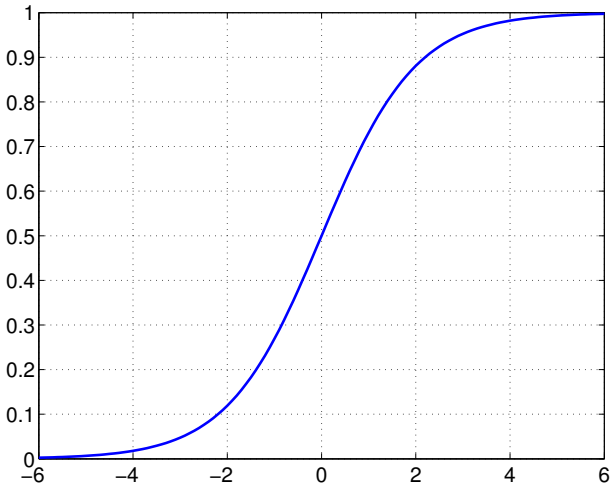

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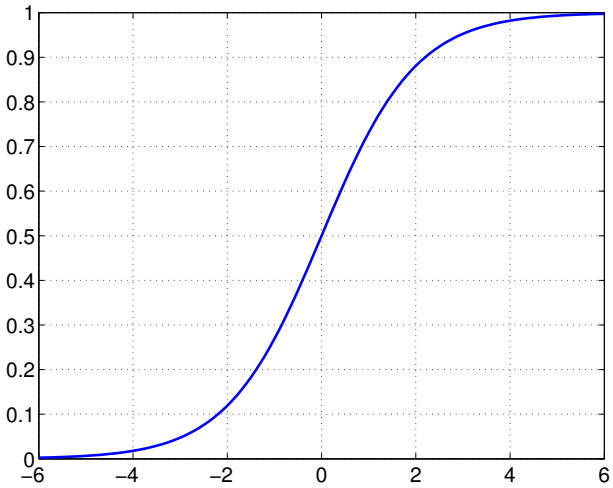

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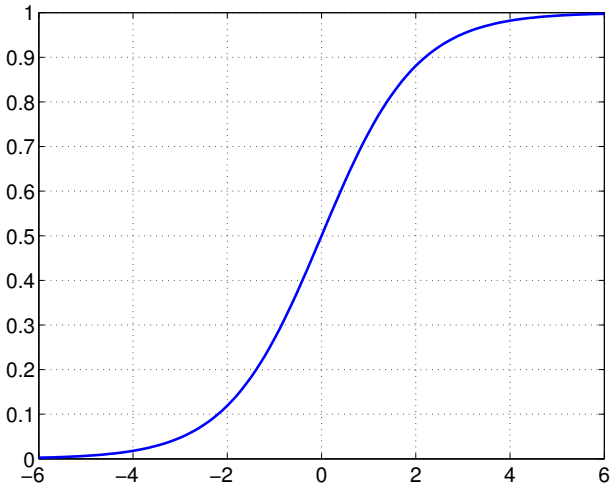

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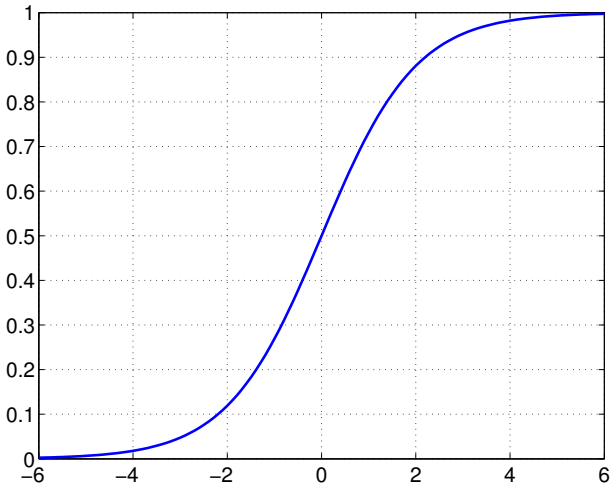

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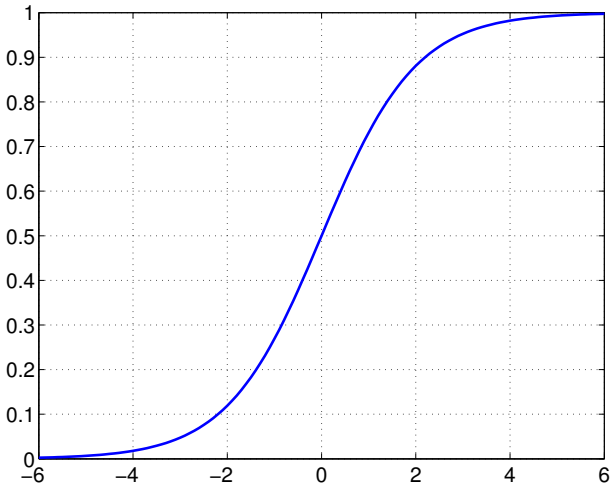

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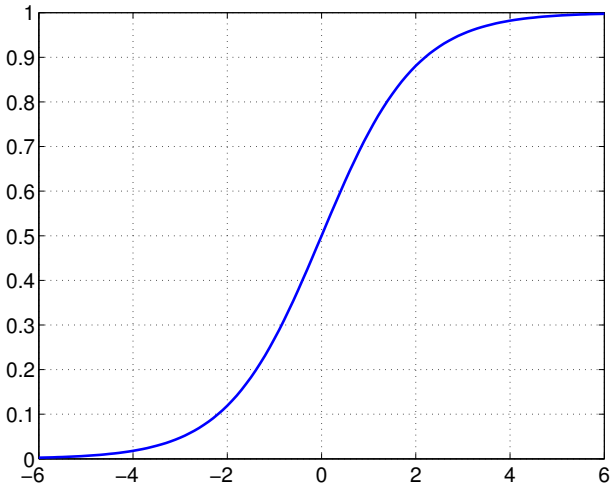

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and thus

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Specifically, what is the probability of seeing label $y_1, \cdots, y_n$ given $x_1, \cdots, x_n$, as a function of some $\boldsymbol{w}$?

$$P(\boldsymbol{w}) = \prod_{n=1}^{N} \mathbb{P}(y_n \mid \boldsymbol{x_n}; \boldsymbol{w})$$

MLE: find $\boldsymbol{w}^*$ that **maximizes the probability** $P(\boldsymbol{w})$

The MLE solution

$$\boldsymbol{w}^* = \underset{\boldsymbol{w}}{\operatorname{argmax}}\, P(\boldsymbol{w}) = \underset{\boldsymbol{w}}{\operatorname{argmax}} \prod_{n=1}^{N} \mathbb{P}(y_n \mid \boldsymbol{x_n}; \boldsymbol{w})$$

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&= \operatorname*{argmin}_{\boldsymbol{w}} F(\boldsymbol{w})
\end{aligned}
$$

i.e. *minimizing logistic loss is exactly doing MLE for the sigmoid model!*

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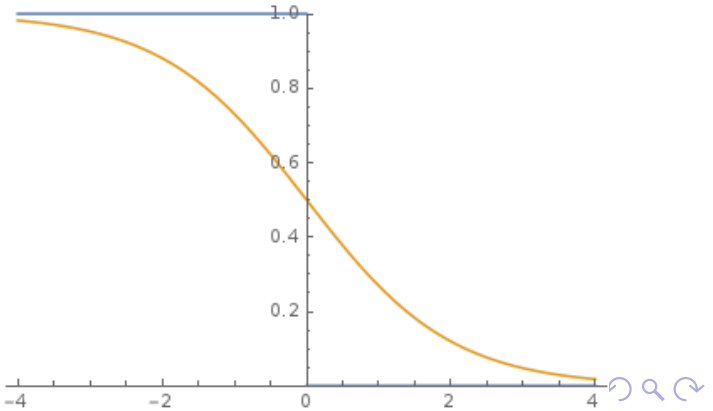
&= \boldsymbol{w} + \eta \mathbb{P}(-y_n \mid \boldsymbol{x}_n; \boldsymbol{w}) y_n \boldsymbol{x}_n
\end{aligned}
$$

This is a *soft version of Perceptron!*

$\mathbb{P}(-y_n | \boldsymbol{x}_n; \boldsymbol{w})$ versus $\mathbb{I}[y_n \neq \text{sgn}(\boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n)]$



A second-order method: Newton method

Recall the intuition of GD: we look at first-order **Taylor approximation**

$$F(\boldsymbol{w}) \approx F(\boldsymbol{w}^{(t)}) + \nabla F(\boldsymbol{w}^{(t)})^{\mathrm{T}}(\boldsymbol{w} - \boldsymbol{w}^{(t)})$$

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where $\boldsymbol{H}_t = \nabla^2 F(\boldsymbol{w}^{(t)}) \in \mathbb{R}^{\mathsf{D}\times\mathsf{D}}$ is the *Hessian* of F at $\boldsymbol{w}^{(t)}$, i.e.,

$$H_{t,ij} = \left.\frac{\partial^2 F(\boldsymbol{w})}{\partial w_i \partial w_j}\right|_{\boldsymbol{w}=\boldsymbol{w}^{(t)}}$$

(think "second derivative" when $D = 1$)

Deriving Newton method

If we minimize the second-order approximation (via "complete the square")

$$
\begin{aligned}
& F(\boldsymbol{w}) \\
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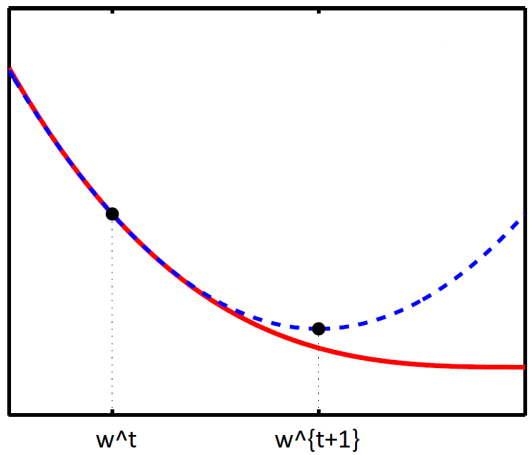

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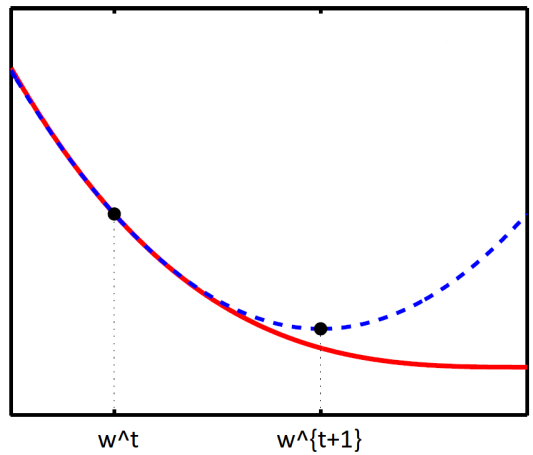
for convex F (so H_t is *positive semidefinite*)
we obtain **Newton method**:

$$\boldsymbol{w}^{(t+1)} \leftarrow \boldsymbol{w}^{(t)} - \boldsymbol{H}_t^{-1}\nabla F(\boldsymbol{w}^{(t)})$$



Comparing GD and Newton

$$\boldsymbol{w}^{(t+1)} \leftarrow \boldsymbol{w}^{(t)} - \eta \nabla F(\boldsymbol{w}^{(t)}) \quad \text{(GD)}$$

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  - e.g. how many iterations needed when applied to a quadratic?
- requires **second-order** information and is *slow* each iteration (there are many ways to improve it though)

Applying Newton to logistic loss

$$\nabla_{\boldsymbol{w}} \ell_{\text{logistic}}(y_n \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n) = -\sigma(-y_n \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n) y_n \boldsymbol{x}_n$$

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Exercises:

- why is the Hessian of logistic loss positive semidefinite?

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\end{aligned}$$

Exercises:

- why is the Hessian of logistic loss positive semidefinite?
- can we apply Newton method to perceptron/hinge loss?

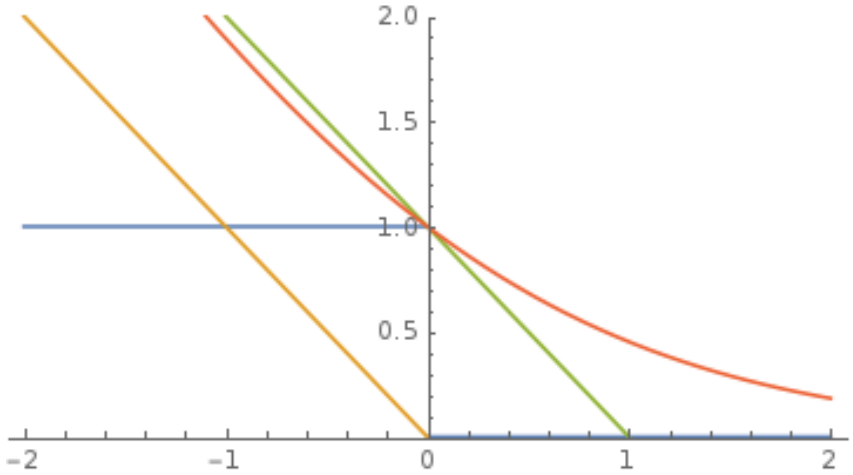
Summary

Linear models for classification:

Step 1. Model is the set of **separating hyperplanes**

$$\mathcal{F} = \{f(\boldsymbol{x}) = \mathsf{sgn}(\boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}) \mid \boldsymbol{w} \in \mathbb{R}^{\mathsf{D}}\}$$

Step 2. Pick the **surrogate loss**



- perceptron loss $\ell_{\text{perceptron}}(z) = \max\{0, -z\}$ (used in Perceptron)
- hinge loss $\ell_{\text{hinge}}(z) = \max\{0, 1 - z\}$(used in SVM and many others)
- logistic loss $\ell_{\text{logistic}}(z) = \log(1 + \exp(-z))$ (used in logistic regression)

Step 3. Find empirical risk minimizer (ERM):

$$\boldsymbol{w}^* = \underset{\boldsymbol{w} \in \mathbb{R}^{\mathsf{D}}}{\operatorname{argmin}} \sum_{n=1}^{N} \ell(y_n \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n)$$

using **GD/SGD/Newton**.