CSCI567 Machine Learning (Spring 2023)
Week 3: Linear Regression, Perceptron, Logistic Regression

Prof. Yan Liu

University of Southern California

Outline

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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

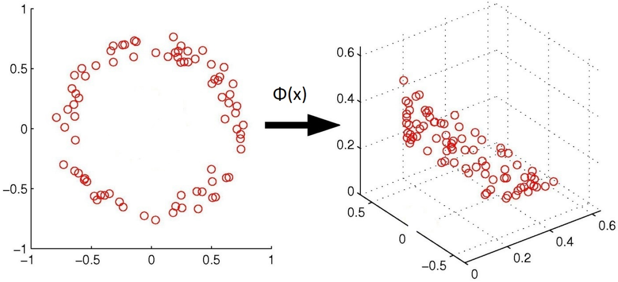
$$\begin{aligned} \boldsymbol{w}^* &= \operatorname*{argmin}_{\boldsymbol{w}} \mathrm{RSS}(\boldsymbol{w}) \\ &= \operatorname*{argmin}_{\boldsymbol{w}} \|\boldsymbol{X}\boldsymbol{w} - \boldsymbol{y}\|_2^2 \\ &= \left(\boldsymbol{X}^{\mathrm{T}}\boldsymbol{X}\right)^{-1}\boldsymbol{X}^{\mathrm{T}}\boldsymbol{y} \end{aligned}$$

$$\boldsymbol{X} = \begin{pmatrix} \boldsymbol{x}_1^{\mathrm{T}} \\ \boldsymbol{x}_2^{\mathrm{T}} \\ \vdots \\ \boldsymbol{x}_{\mathsf{N}}^{\mathrm{T}} \end{pmatrix}, \quad \boldsymbol{y} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_{\mathsf{N}} \end{pmatrix}$$

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

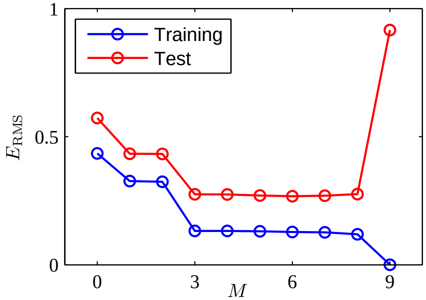
Underfitting and Overfitting

$M \leq 2$ 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

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Classification

Recall the setup:

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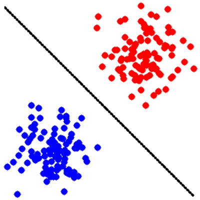

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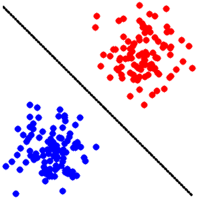
Sign of $\boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}$ predicts the label:

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

(Sometimes use sgn for sign too.)



The models

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

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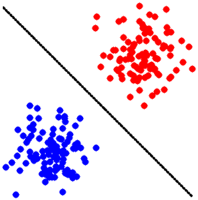
Good choice for *linearly separable* data, i.e., $\exists \boldsymbol{w}$ s.t.

$$\mathsf{sgn}(\boldsymbol{w}^{\mathrm{T}}\boldsymbol{x_n}) = y_n$$

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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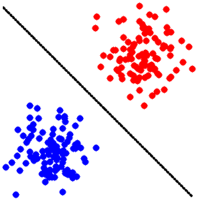
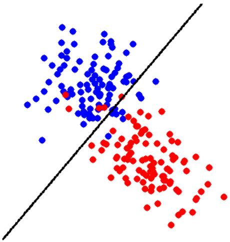


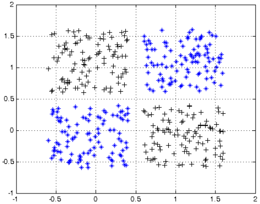
The models

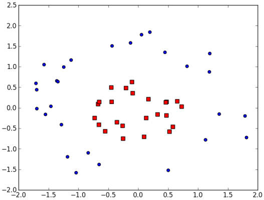
Still makes sense for "almost" linearly separable data



The models

For clearly not linearly separable data,





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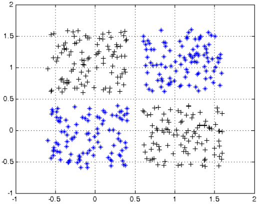

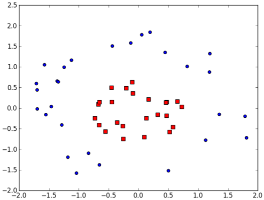

Again can apply a **nonlinear mapping** $\mathbf{\Phi}$:

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

More discussions in the next two lectures.

0-1 Loss

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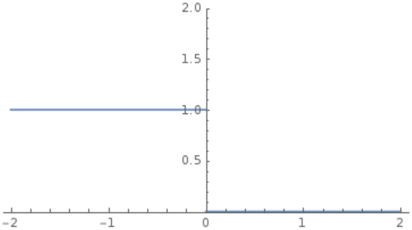
For classification, more convenient to look at the loss **as a function of $y\boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}$**. That is, with

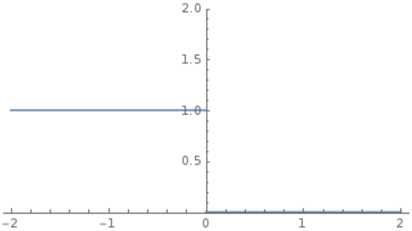
$$\ell_{\text{0-1}}(z) = \mathbb{I}[z \leq 0]$$



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

Minimizing 0-1 loss is hard

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



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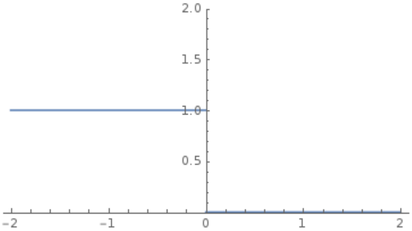
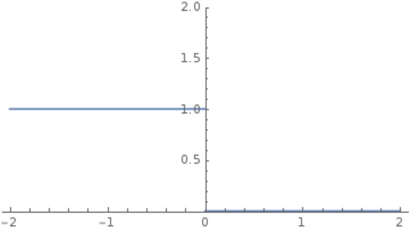


Even worse, minimizing 0-1 loss is *NP-hard in general*.

Surrogate Losses

Solution: find a **convex surrogate loss**



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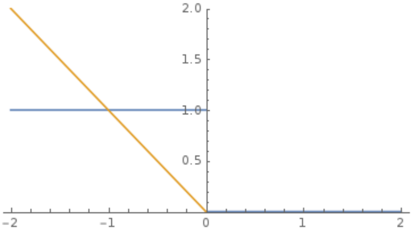

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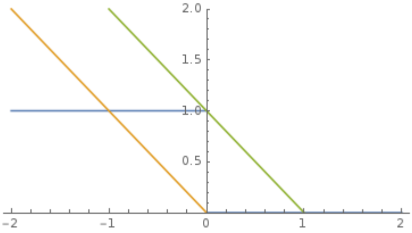

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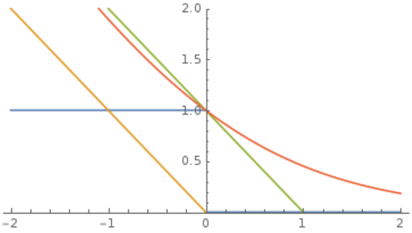

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- hinge loss $\ell_{\text{hinge}}(z) = \max\{0, 1 - z\}$(used in SVM and many others)
- logistic loss $\ell_{\text{logistic}}(z) = \log(1 + \exp(-z))$ (used in logistic regression; the base of $\log$ doesn't matter)

ML becomes convex optimization

Step 3. Find ERM:

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

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

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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

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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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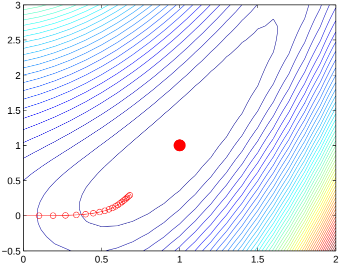

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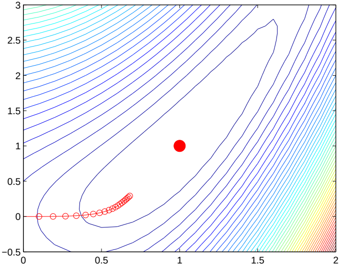

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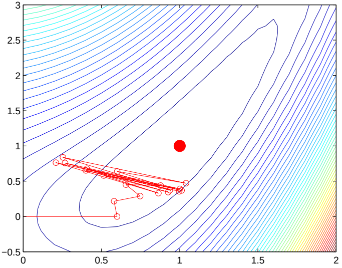

but large η is unstable

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

Convergence Guarantees

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

Applying GD to perceptron loss

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(only misclassified examples contribute to the gradient)

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GD update

$$\boldsymbol{w} \leftarrow \boldsymbol{w} + \eta \sum_{n=1}^{N} \mathbb{I}[y_n \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n \leq 0] y_n \boldsymbol{x}_n$$

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Gradient (or really *sub-gradient*) is

$$\nabla F(\boldsymbol{w}) = \sum_{n=1}^{N} -\mathbb{I}[y_n \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n \leq 0] y_n \boldsymbol{x}_n$$

(only misclassified examples contribute to the gradient)

GD update

$$\boldsymbol{w} \leftarrow \boldsymbol{w} + \eta \sum_{n=1}^{N} \mathbb{I}[y_n \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n \leq 0] y_n \boldsymbol{x}_n$$

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

Applying SGD to perceptron loss

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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

Why does it make sense?

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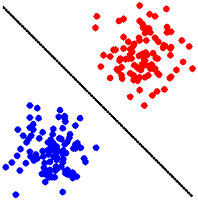
Thus it is more likely to get it right after the update.

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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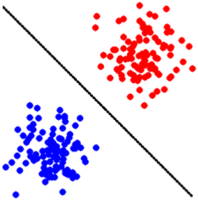

There are also guarantees when the data is not linearly separable.

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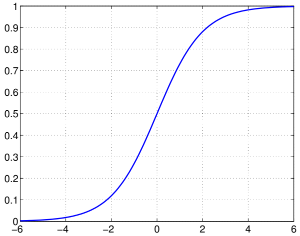
One way: **sigmoid function + linear model**

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

where σ is the sigmoid function:

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



Properties

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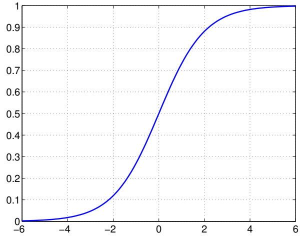
- between 0 and 1 (good as probability)



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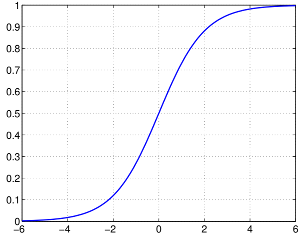

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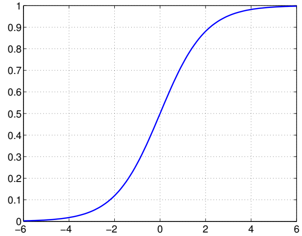

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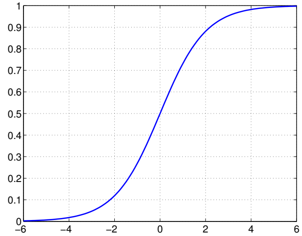

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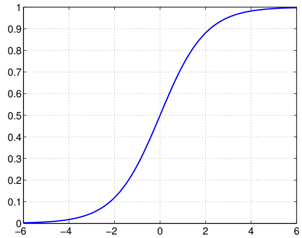

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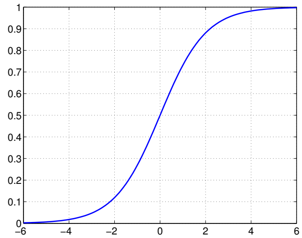

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and thus

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

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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** $P(w)$

The MLE solution

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

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&= \operatorname*{argmin}_{\boldsymbol{w}} F(\boldsymbol{w})
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i.e. *minimizing logistic loss is exactly doing MLE for the sigmoid model!*

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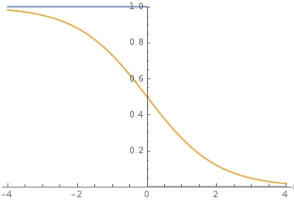
\end{aligned}$$

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 $D = 1$)

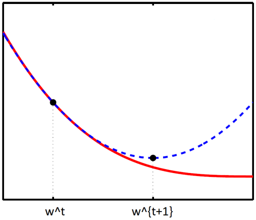
Deriving Newton method

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

$$F(\boldsymbol{w})$$

$$\approx F(\boldsymbol{w}^{(t)}) + \nabla F(\boldsymbol{w}^{(t)})^{\mathrm{T}}(\boldsymbol{w} - \boldsymbol{w}^{(t)}) + \frac{1}{2}(\boldsymbol{w} - \boldsymbol{w}^{(t)})^{\mathrm{T}} \boldsymbol{H}_t (\boldsymbol{w} - \boldsymbol{w}^{(t)})$$

$$= \frac{1}{2}\left(\boldsymbol{w} - \boldsymbol{w}^{(t)} + \boldsymbol{H}_t^{-1}\nabla F(\boldsymbol{w}^{(t)})\right)^{\mathrm{T}} \boldsymbol{H}_t \left(\boldsymbol{w} - \boldsymbol{w}^{(t)} + \boldsymbol{H}_t^{-1}\nabla F(\boldsymbol{w}^{(t)})\right) + \text{cnt.}$$



Deriving Newton method

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

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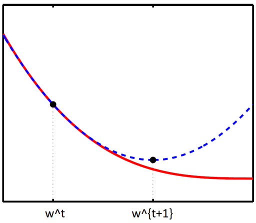
\end{aligned}
$$

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

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

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

Both are iterative optimization procedures,

Comparing GD and Newton

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- has no learning rate η (*so no tuning needed!*)
- converges *super fast* in terms of #iterations needed
  - 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

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

Applying Newton to logistic loss

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$$\nabla^2_{\boldsymbol{w}} \ell_{\mathsf{logistic}}(y_n \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n) = \left(\frac{\partial \sigma(z)}{\partial z} \bigg|_{z=-y_n \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n} \right) y_n^2 \boldsymbol{x}_n \boldsymbol{x}_n^{\mathrm{T}}$$

Applying Newton to logistic loss

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&= \sigma(y_n \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n) \left(1 - \sigma(y_n \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n)\right) \boldsymbol{x}_n \boldsymbol{x}_n^{\mathrm{T}}
\end{aligned}$$

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?

Applying Newton to logistic loss

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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?

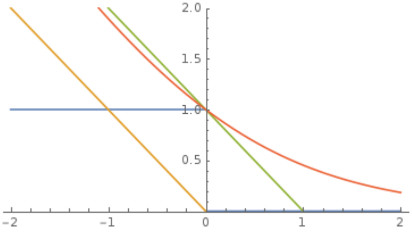
Summary

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):

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

using **GD/SGD/Newton**.