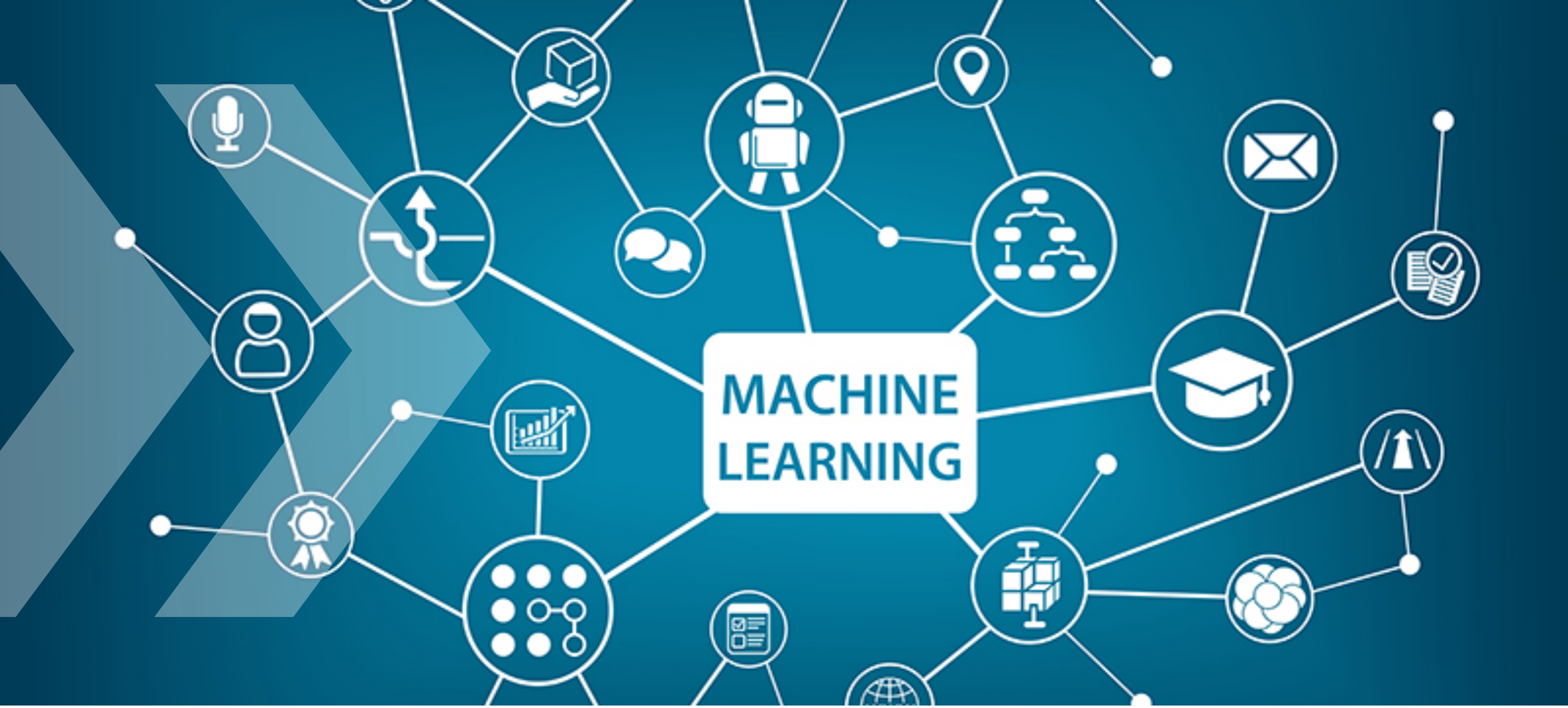

CS489/698: Intro to ML

Lecture 04: Logistic Regression

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Outline

- **Announcements**
- Baseline
- Learning “Machine Learning” Pyramid
- Regression or Classification (that’s it!)
- History of Classification
- History of Solvers (Analytical to Convex to “Non-Convex but smooth”)
- Convexity
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- Multiclass

Announcements

- Assignment 1 due next Tuesday

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Baseline

- Assuming Lin Alg Basics:

$$Ax = b$$

$$A = \begin{bmatrix} 4 & -5 \\ -2 & 3 \end{bmatrix}, \quad b = \begin{bmatrix} -13 \\ 9 \end{bmatrix}.$$

$$C = AB \in \mathbb{R}^{m\times p},$$

$$C_{ij} = \sum_{k=1}^{n} A_{ik} B_{kj}.$$

$$x = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}$$

$$(A^T)^T = A$$

$$(AB)^T = B^T A^T$$

$$(A+B)^T = A^T + B^T$$

$$\|x\|_2 = \sqrt{\sum_{i=1}^{n} x_i^2}.$$

$$x^T Ax = \sum_{i=1}^{n} x_i (Ax)_i = \sum_{i=1}^{n} x_i \left(\sum_{j=1}^{n} A_{ij} x_j \right) = \sum_{i=1}^{n} \sum_{j=1}^{n} A_{ij} x_i x_j \ .$$

$$x^T Ax = (x^T Ax)^T = x^T A^T x = x^T \left(\frac{1}{2} A + \frac{1}{2} A^T \right) x,$$

$$\nabla_A f(A) \in \mathbb{R}^{m\times n} = \begin{bmatrix} \frac{\partial f(A)}{\partial A_{11}} & \frac{\partial f(A)}{\partial A_{12}} & \cdots & \frac{\partial f(A)}{\partial A_{1n}} \\ \frac{\partial f(A)}{\partial A_{21}} & \frac{\partial f(A)}{\partial A_{22}} & \cdots & \frac{\partial f(A)}{\partial A_{2n}} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial f(A)}{\partial A_{m1}} & \frac{\partial f(A)}{\partial A_{m2}} & \cdots & \frac{\partial f(A)}{\partial A_{mn}} \end{bmatrix}$$

$$\nabla_x^2 f(x) \in \mathbb{R}^{n\times n} = \begin{bmatrix} \frac{\partial^2 f(x)}{\partial x_1^2} & \frac{\partial^2 f(x)}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f(x)}{\partial x_1 \partial x_n} \\ \frac{\partial^2 f(x)}{\partial x_2 \partial x_1} & \frac{\partial^2 f(x)}{\partial x_2^2} & \cdots & \frac{\partial^2 f(x)}{\partial x_2 \partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f(x)}{\partial x_n \partial x_1} & \frac{\partial^2 f(x)}{\partial x_n \partial x_2} & \cdots & \frac{\partial^2 f(x)}{\partial x_n^2} \end{bmatrix}.$$

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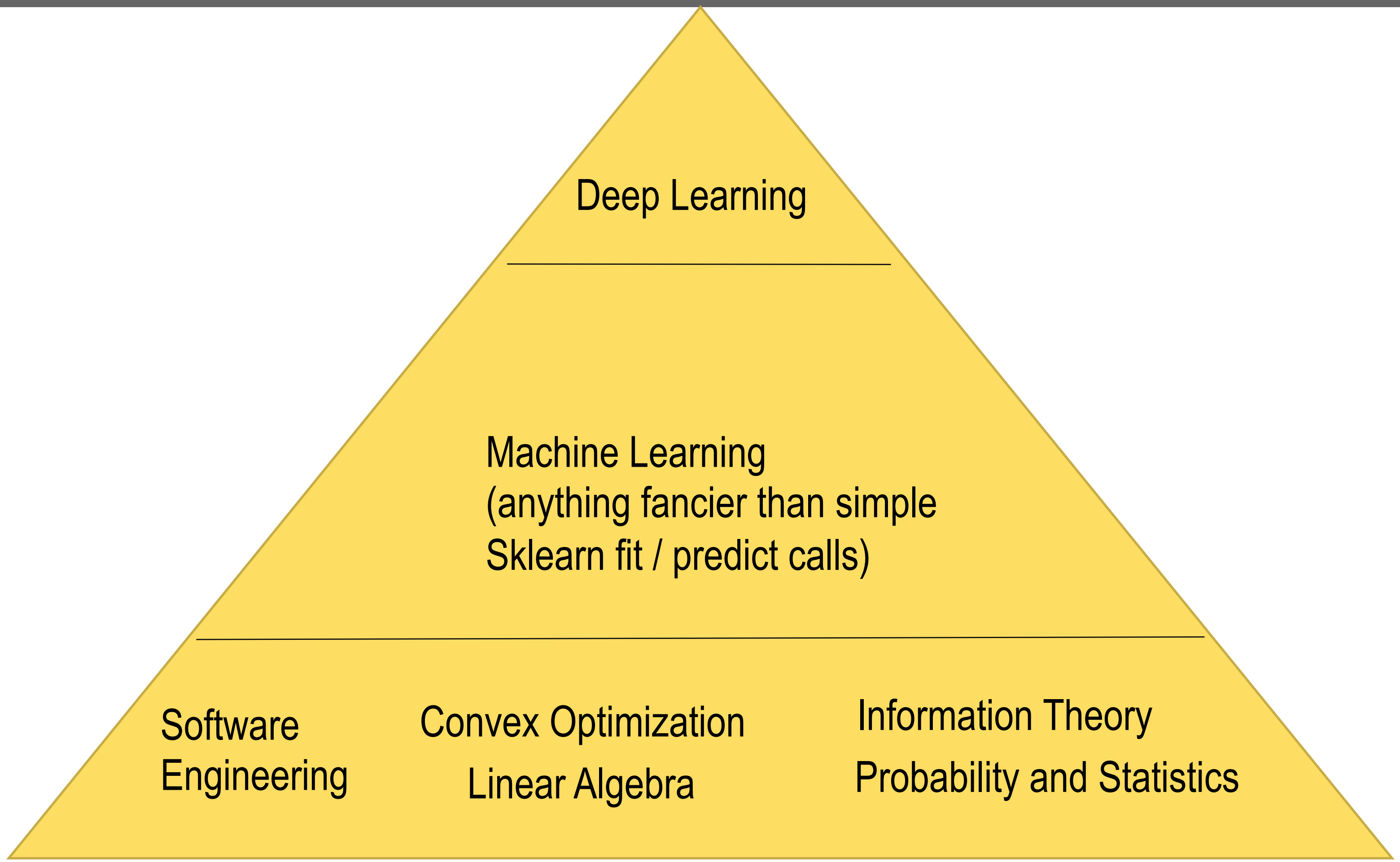
ML Pyramid



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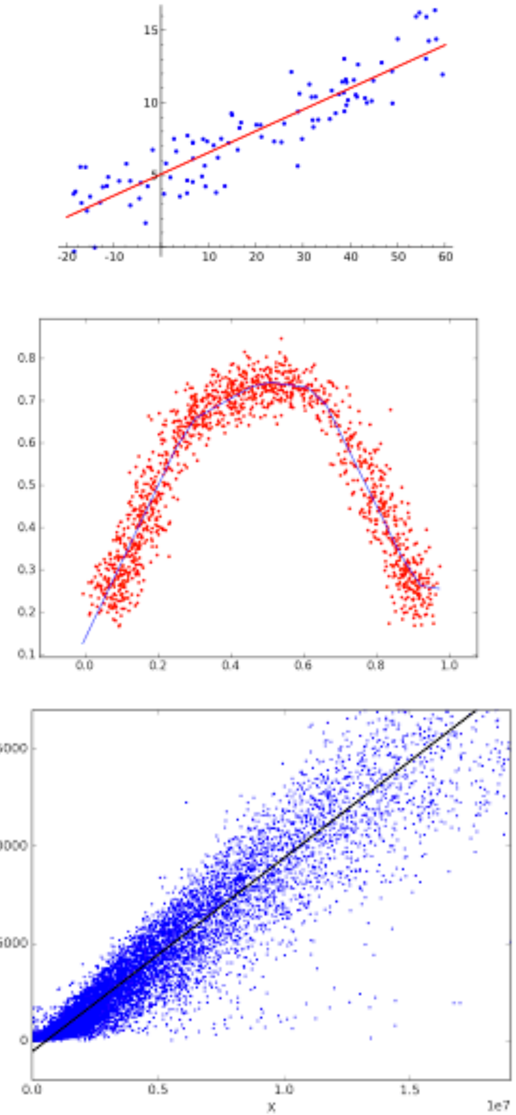
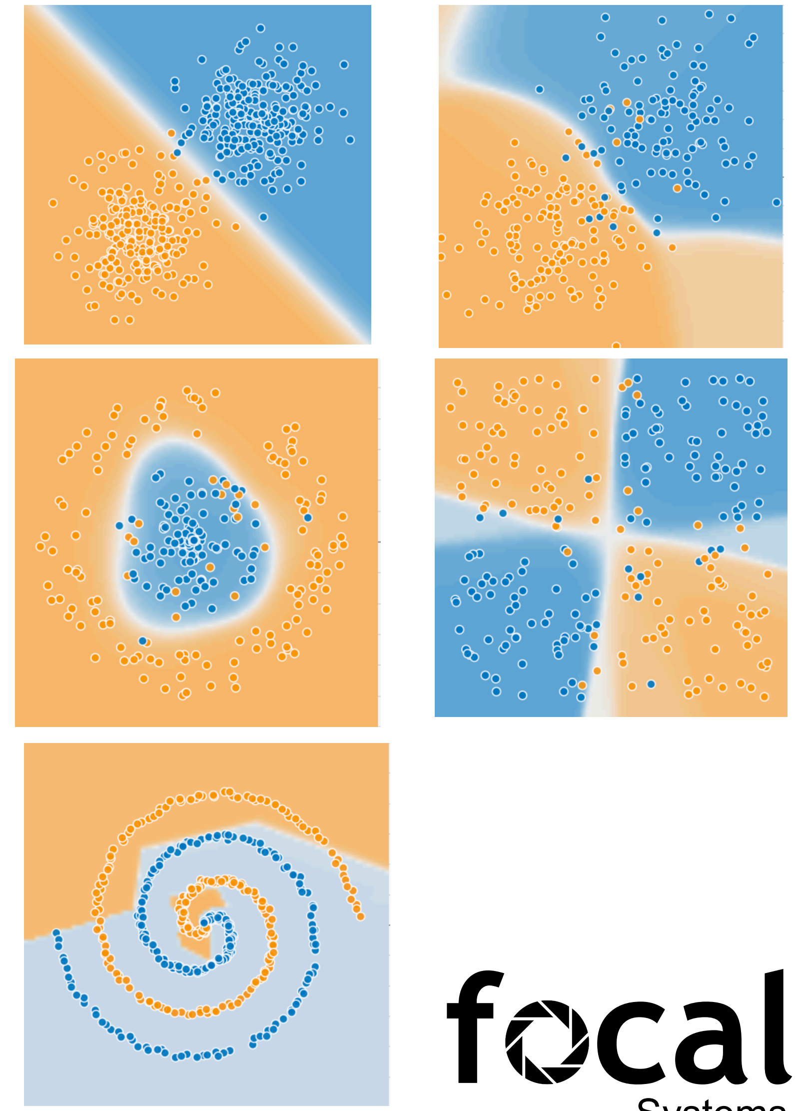
Regression or Classification



or



Francois Chaubard and Agastya Kalra

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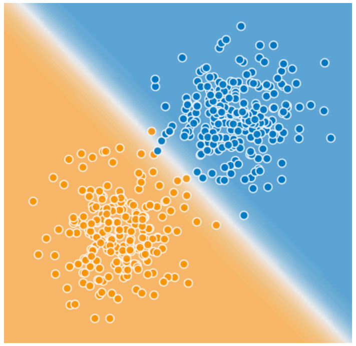
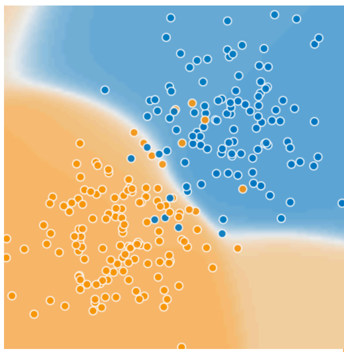
Classification

Higher “complexity” datasets need higher ”capacity” models
(Formally, higher VC-Dimensionality)

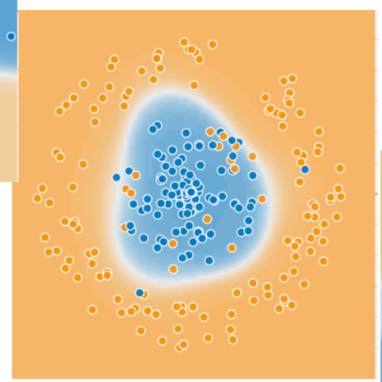


Perceptron



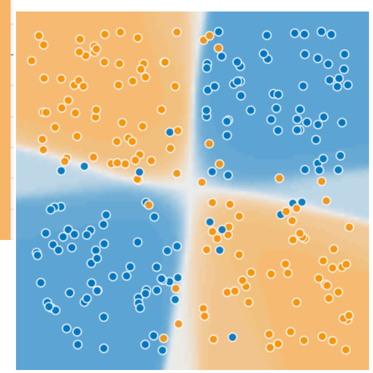
!Perceptron

Logistic Regression

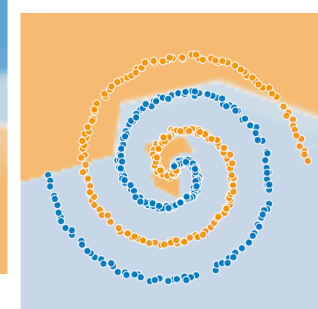


!Logistic Regression

MLP
Feature Eng
etc



etc



?

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History of Solvers

Closed Form <1950s

Least Squares

etc

Normal equation

$$\Theta = (X^T X)^{-1} X^T y$$

Iterative Methods+Convex 1950-2012

Interior Point Methods

Log Barrier

etc

Optimization problem in standard form

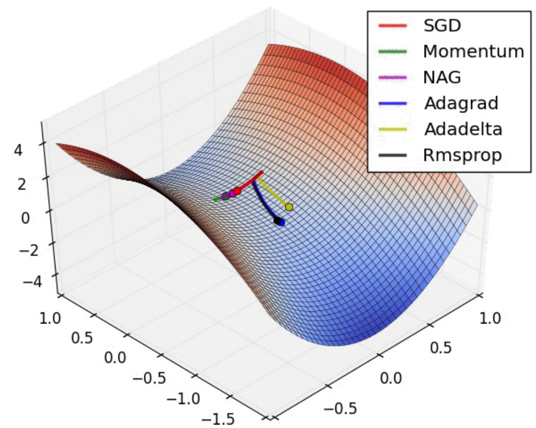
$$\begin{array}{ll} \text{minimize} & f_0(x) \\ \text{subject to} & f_i(x) \leq 0, \quad i = 1, \ldots, m \\ & h_i(x) = 0, \quad i = 1, \ldots, p \end{array}$$

- $x \in \mathbf{R}^n$ is the optimization variable
- $f_0 : \mathbf{R}^n \to \mathbf{R}$ is the objective or cost function
- $f_i : \mathbf{R}^n \to \mathbf{R}$, $i = 1, \ldots, m$, are the inequality constraint functions
- $h_i : \mathbf{R}^n \to \mathbf{R}$ are the equality constraint functions

Iterative Methods+Smooth 2012+

Deep Learning

etc



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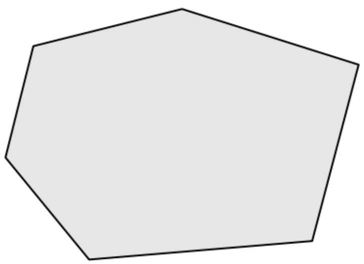
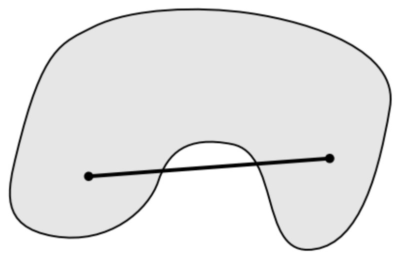
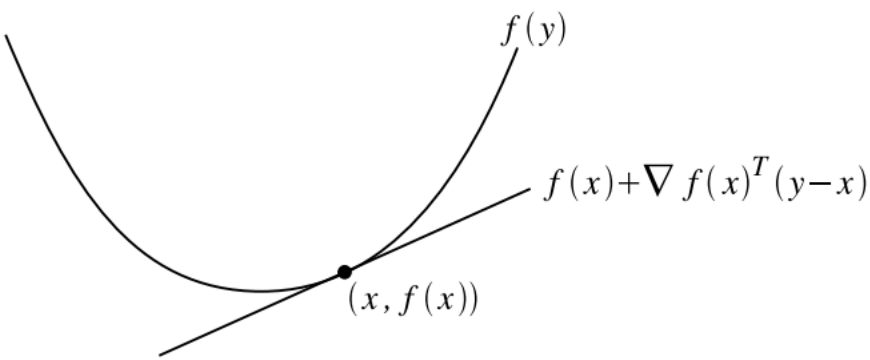
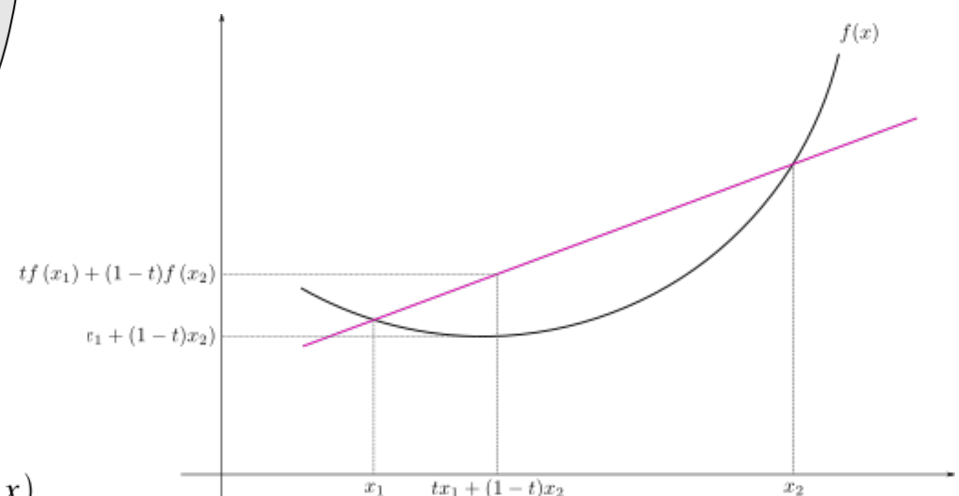
Convexity







Jensen's Inequality



$$f\left(tx_1 + (1-t)x_2\right) \leq tf(x_1) + (1-t)f(x_2).$$

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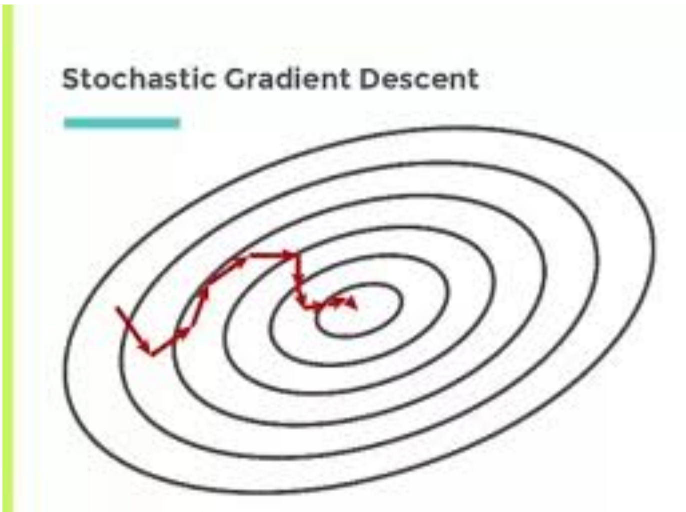
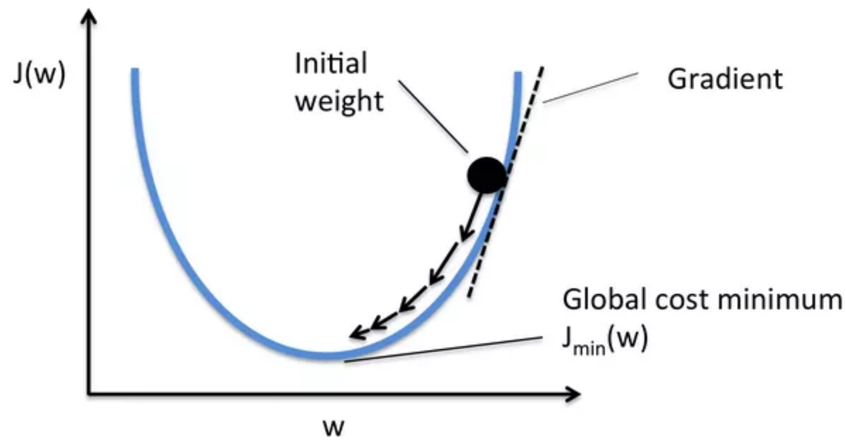
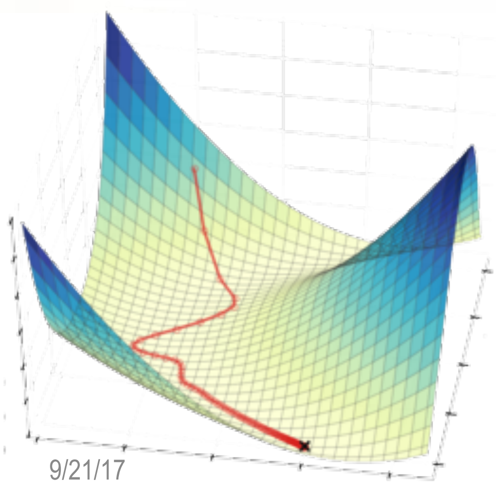
SGD





$$w := w - \eta \nabla Q_i(w).$$



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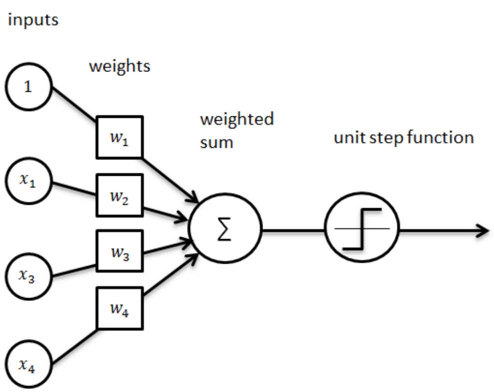
Perceptron

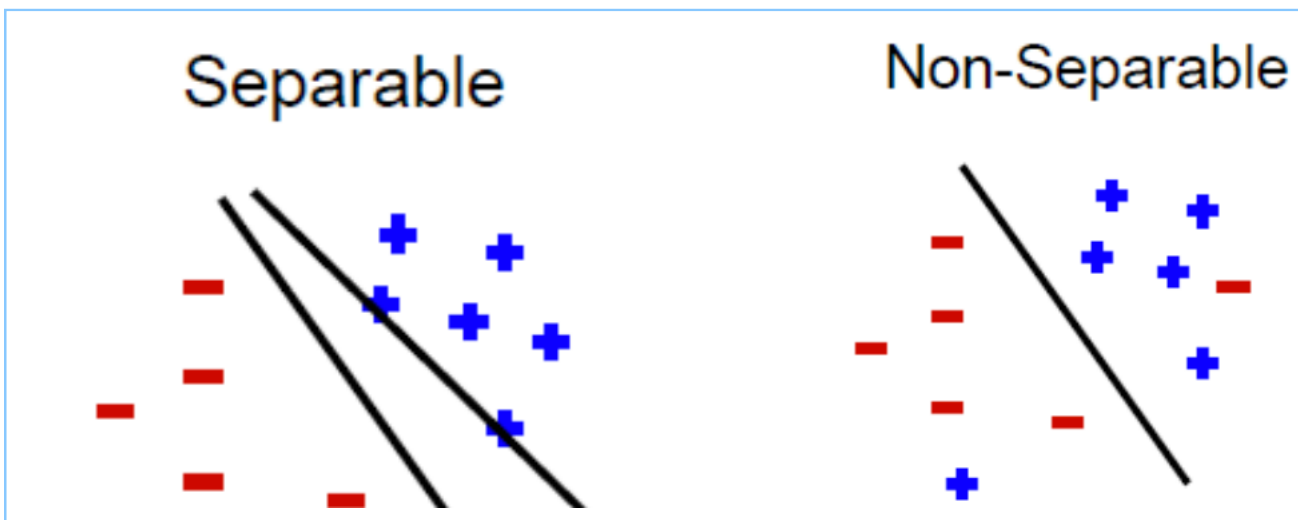


Algorithm 1: The perceptron algorithm (Rosenblatt 1958)

Input: $A \in \mathbb{R}^{(d+1)\times n}$, threshold $\delta \geq 0$, initialize $\mathbf{w}_0 \in \mathbb{R}^{d+1}$ arbitrarily

```
repeat
    select some column a of A;
    if ⟨a, w_t⟩ ≤ δ then
        w_{t+1} = w_t + a ;                    // up
        t ← t + 1
until convergence;
```

Issues:



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Bernoulli model

- Let P(Y=1 | X=**x**) = p(**x**; **w**), parameterized by **w**

- Conditional likelihood on $\{(\mathbf{x}_1, y_1), \ldots (\mathbf{x}_n, y_n)\}$:

$$\mathbf{P}(Y_1 = y_1, \ldots, Y_n = y_n | X_1 = \mathbf{x_1}, \ldots, X_n = \mathbf{x}_n)$$

  - simplifies if independence holds

$$\prod_{i=1}^{n} \mathbf{P}(Y_i = y_i | X_i = \mathbf{x}_i) = \prod_{i=1}^{n} p(\mathbf{x}_i; \mathbf{w})^{y_i} (1 - p(\mathbf{x}_i; \mathbf{w}))^{1-y_i}$$

  - Assuming y_i is {0,1}-valued

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Naïve solution

$$\prod_{i=1}^{n} p(\mathbf{x}_i; \mathbf{w})^{y_i} (1 - p(\mathbf{x}_i; \mathbf{w}))^{1-y_i}$$

- Find **w** to maximize conditional likelihood

- What is the solution if p(**x**; **w**) does not depend on **x**?

- What is the solution if p(**x**; **w**) does not depend on ?

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Generalized linear models (GLM)

- $y \sim \text{Bernoulli}(p)$; $p = p(\mathbf{x}; \mathbf{w})$ natural parameter
  - Logistic regression

- $y \sim \text{Normal}(\mu, \sigma^2)$; $\boldsymbol{\mu} = \boldsymbol{\mu}(\mathbf{x}; \mathbf{w})$
  - (weighted) least-squares regression

- GLM: $y \sim \exp(\, \theta\, \underbrace{\varphi(y)}_{\text{sufficient statistics}} - \underbrace{A(\theta)}_{\text{log-partition function}}\,)$

Logit transform

- $p(\mathbf{x}; \mathbf{w}) = \mathbf{w}^\top \mathbf{x}$? p >=0 not guaranteed…
- $\log p(\mathbf{x}; \mathbf{w}) = \mathbf{w}^\top \mathbf{x}$? better!
  - LHS negative, RHS real-valued…
- Logit transform $$\log \underbrace{\frac{p(\mathbf{x}; \mathbf{w})}{1 - p(\mathbf{x}; \mathbf{w})}}_{\text{odds ratio}} = \mathbf{w}^\top \mathbf{x}$$
- Or equivalently $$p(\mathbf{x}; \mathbf{w}) = \frac{1}{1 + \exp(-\mathbf{w}^\top \mathbf{x})}$$

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Prediction with confidence

$$p(\mathbf{x}; \mathbf{w}) = \frac{1}{1 + \exp(-\mathbf{w}^\top \mathbf{x})}$$

- $\hat{y} = 1$ if $p = P(Y=1 \mid X=x) > ½$ iff $\mathbf{w}^\top \mathbf{x} > 0$

- Decision boundary $\mathbf{w}^\top \mathbf{x} = 0$

- $\hat{y} = \mathrm{sign}(\mathbf{w}^\top \mathbf{x})$ as before, but with confidence $p(x; w)$

Not just a classification algorithm

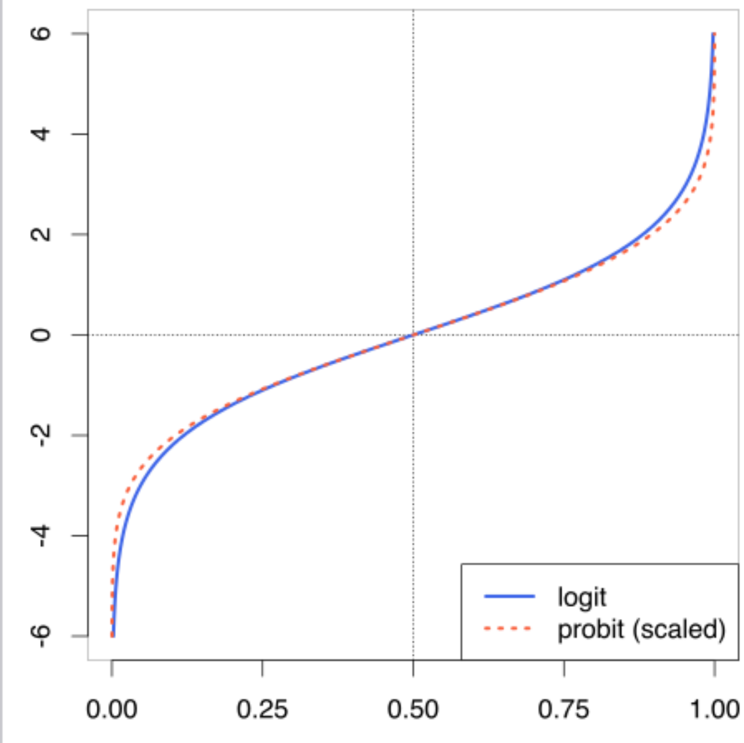
- Logistic regression does more than classification
  - it estimates conditional probabilities
  - under the logit transform assumption

- Having confidence in prediction is nice
  - the price is an assumption that may or may not hold

- If classification is the sole goal, then doing extra work
  - as shall see, SVM only estimates decision boundary

More than logistic regression

- F(p) transforms p from [0,1] to R
- Then, equating F(p) to a linear function $\mathbf{w}^T\mathbf{x}$
- But, there are many other choices for F!
  - precisely the inverse of any distribution function!



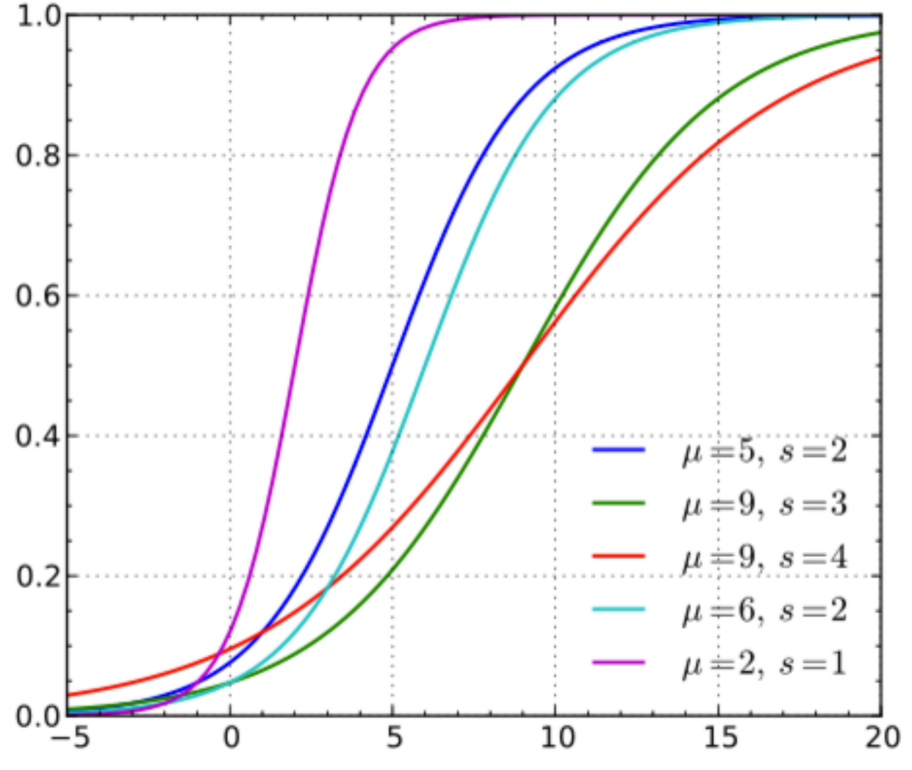
Comparison of the logit function with a scaled probit (i.e. the inverse CDF of the normal distribution), comparing $\operatorname{logit}(x)$ vs. $\Phi^{-1}(x)/\sqrt{\frac{\pi}{8}}$, which makes the slopes the same at the origin.

Logistic distribution

- Cumulative Distribution Function

$$F(x;\mu,s) = \frac{1}{1+\exp(-\frac{x-\mu}{s})}$$

- Mean mu, variance $s^2\pi^2/3$



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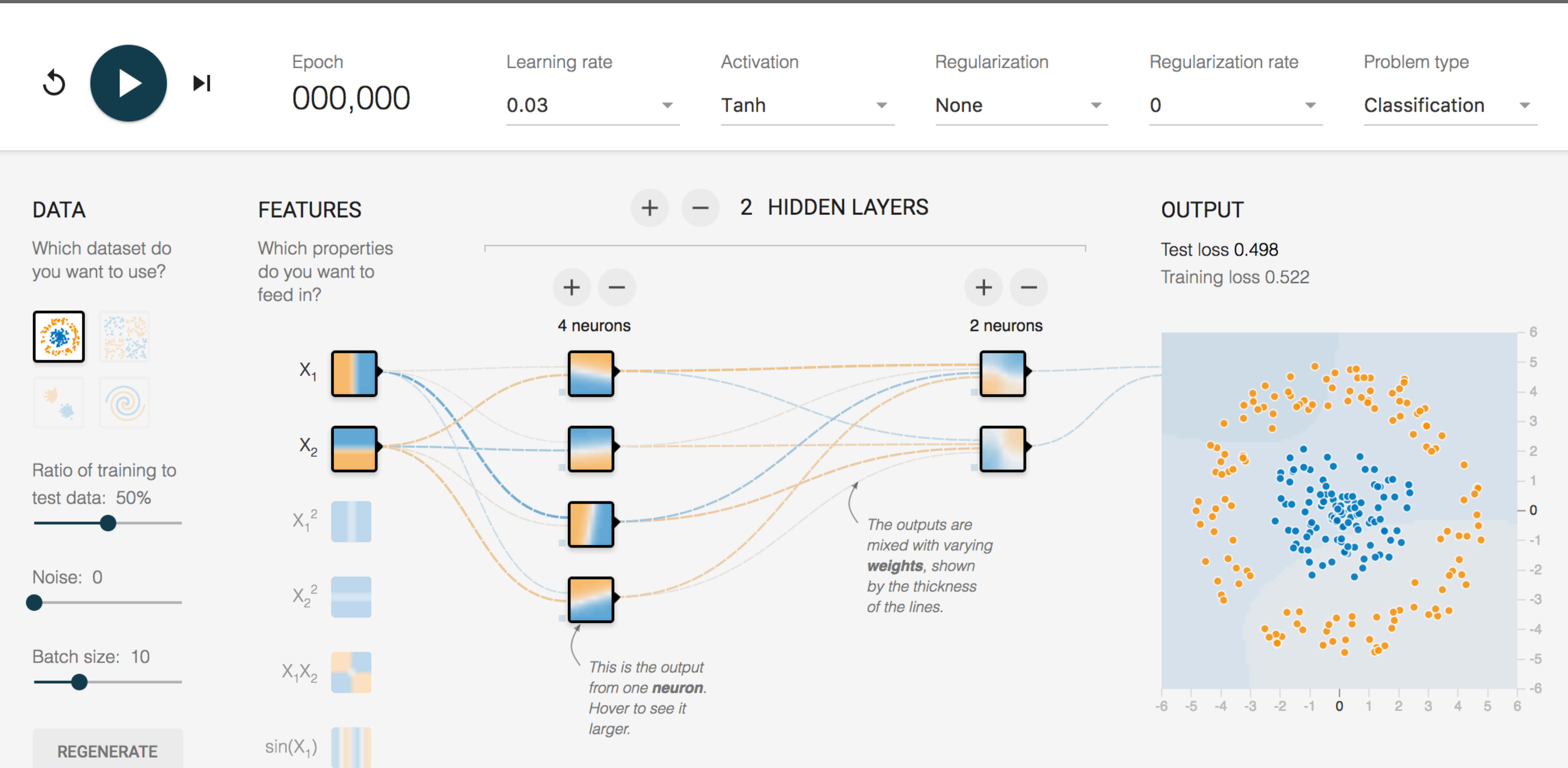
Playground



Epoch
000,000
Learning rate
0.03
Activation
Tanh
Regularization
None
Regularization rate
0
Problem type
Classification
DATA
Which dataset do you want to use?
Ratio of training to test data: 50%
Noise: 0
Batch size: 10
REGENERATE
FEATURES
Which properties do you want to feed in?
X1
X2
X1^2
X2^2
X1X2
sin(X1)
2 HIDDEN LAYERS
4 neurons
2 neurons
This is the output from one neuron. Hover to see it larger.
The outputs are mixed with varying weights, shown by the thickness of the lines.
OUTPUT
Test loss 0.498
Training loss 0.522

Tensorflow coding example

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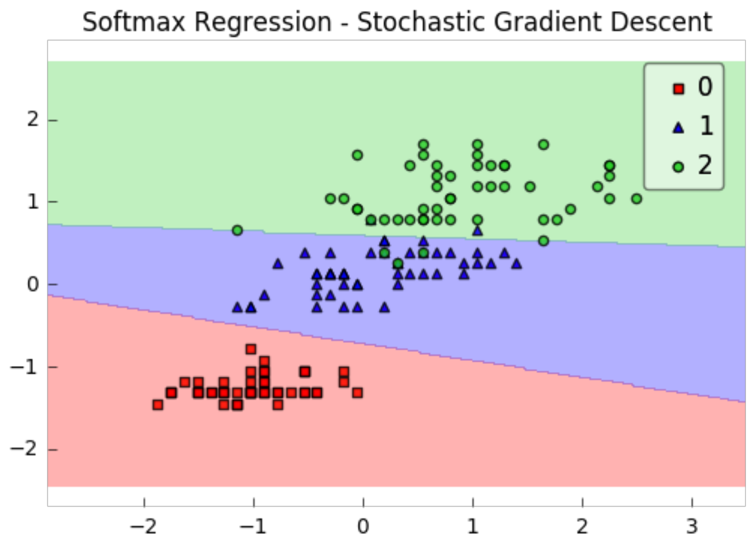
More than 2 classes

- Softmax

$$\mathbf{P}(Y = c|\mathbf{x}, W) = \frac{\exp(\mathbf{w}_c^\top \mathbf{x})}{\sum_{q=1}^{k} \exp(\mathbf{w}_q^\top \mathbf{x})}$$



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More than 2 classes

- Softmax

$$\mathbf{P}(Y = c|\mathbf{x}, W) = \frac{\exp(\mathbf{w}_c^\top \mathbf{x})}{\sum_{q=1}^k \exp(\mathbf{w}_q^\top \mathbf{x})}$$

- Again, nonnegative and sum to 1

- Negative log-likelihood (y is one-hot)

$$-\log \prod_{i=1}^n \prod_{c=1}^k p_{ic}^{y_{ic}} = -\sum_{i=1}^n \sum_{c=1}^k y_{ic} \log p_{ic}$$

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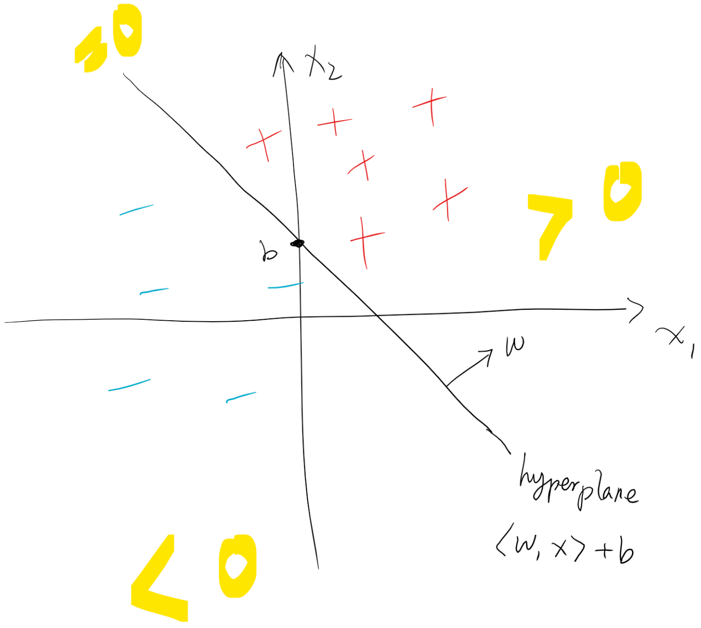
Questions?

backup

Classification revisited

- $\hat{y} = \text{sign}(\, \mathbf{x}^T\mathbf{w} + b\,)$
- How confident we are about $\hat{y}$?
- $|\mathbf{x}^T\mathbf{w} + b|$ seems a good indicator
  - real-valued; hard to interpret
  - ways to transform into [0,1]
- Better(?) idea: learn confidence directly



Conditional probability

- $P(Y=1 \mid X=\mathbf{x})$: conditional on seeing $\mathbf{x}$, what is the chance of this instance being positive, i.e., $Y=1$?
  - obviously, value in [0,1]

- $P(Y=0 \mid X=\mathbf{x}) = 1 - P(Y=1 \mid X=\mathbf{x})$, if two classes
  - more generally, sum to 1

Notation (Simplex). $\Delta_{k-1} := \{ \mathbf{p} \text{ in } R^k : \mathbf{p} \geq 0, \Sigma_i p_i = 1 \}$

Reduction to a harder problem

$$1_A = \begin{cases} 1, & A \text{ is true} \\ 0, & A \text{ is false} \end{cases}$$

- $P(Y=1 \mid X=\mathbf{x}) = E(1_{Y=1} \mid X=\mathbf{x})$

- Let $Z = 1_{Y=1}$, then regression function for (X, Z)
  - use linear regression for binary Z?

- Exploit **structure!**
  - conditional probabilities are in a simplex

- Never reduce to **unnecessarily harder** problem

Maximum likelihood

$$\prod_{i=1}^{n} p(\mathbf{x}_i; \mathbf{w})^{y_i} (1 - p(\mathbf{x}_i; \mathbf{w}))^{1-y_i}$$

$$p(\mathbf{x}; \mathbf{w}) = \frac{1}{1 + \exp(-\mathbf{w}^\top \mathbf{x})}$$

- Minimize negative log-likelihood

$$\sum_i \log(e^{(1-y_i)\mathbf{w}^\top \mathbf{x}_i} + e^{-y_i \mathbf{w}^\top \mathbf{x}_i}) \equiv \sum_i \log(1 + e^{-\tilde{y}_i \mathbf{w}^\top \mathbf{x}_i})$$

Newton's algorithm

$$\mathbf{w}_{t+1} \leftarrow \mathbf{w}_t - \eta_t [\nabla^2 f(\mathbf{w}_t)]^{-1} \cdot \nabla f(\mathbf{w}_t)$$

$$\nabla f(\mathbf{w}_t) = X^\top (\mathbf{p} - \mathbf{y})$$

$$\boxed{\nabla^2 f(\mathbf{w}_t) = \sum_i p_i(1 - p_i)\mathbf{x}_i \mathbf{x}_i^\top}$$

PSD

$$p_i = \frac{1}{1 + e^{-\mathbf{w}_t^\top \mathbf{x}_i}}$$

Uncertain predictions get bigger weight

- η = 1: iterative weighted least-squares

A word about implementation

- Numerically computing exponential can be tricky
  - easily underflows or overflows

- The usual trick
  - estimate the range of the exponents
  - shift the mean of the exponents to 0

Robustness

$$\ell(t) = \log(1 + e^t) \quad L(\hat{y}, y) = \ell(-\hat{y}y) \quad \hat{y} = \mathbf{w}^\top \mathbf{x}$$

- Bounded derivative

$$\ell'(t) = \frac{e^t}{1 + e^t} = \frac{1}{1 + e^{-t}}$$

- Variational exponential

Larger exp loss gets smaller weights

$$\log(1 + e^t) = \min_{0 \le \eta \le 1} \boxed{\eta e^t} - \log(\eta) + \eta - 1$$

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