

# COMP 3105 Introduction to Machine Learning

## Lecture 1: Linear Regression

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## Regression Examples: Estimate Real Numbers

Estimate fish weight

- ▶ Shape (length/width)  $\mapsto$  weight

Annual production of a corn farm

- ▶ Rainfall/sunshine/pest levels  $\mapsto$  production

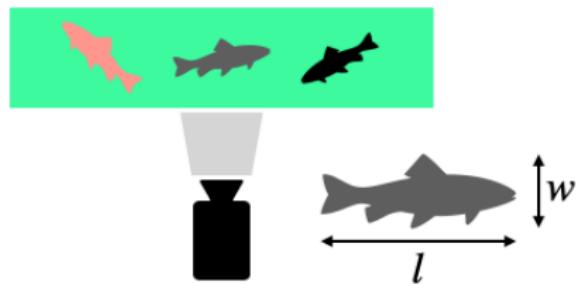
Glucose level of patients with diabetes

- ▶ Insulin injection, patient info  $\mapsto$  glucose level

Market price of a new product

- ▶ Cost/quality/transportation  $\mapsto$  price

## An Example: Estimate Fish Weight



Every fish is measured by [length, width]

- ▶ E.g., [70 cm, 18 cm]
- ▶ Captured by camera on the conveyor belt

Want to estimate its *weight*

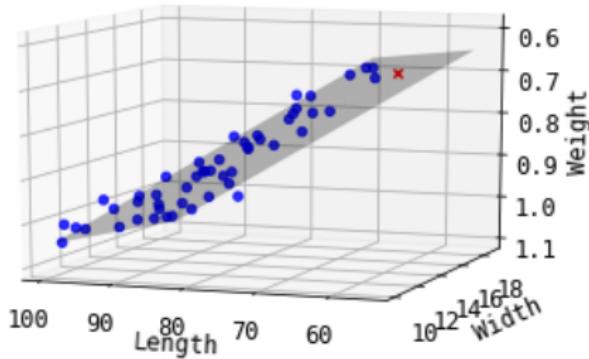
## An Example: Estimate Fish Weight (Cont.)

One possible formulation

- ▶ Represent each fish as a (column) vector  $\mathbf{x} = \begin{bmatrix} 1 \\ 70 \\ 18 \end{bmatrix}$  &  $y = 0.7$
- ▶ Plot what we know (blue points; three axes)
- ▶ Find a “plane” (with augmented  $\mathbf{x}$ ):

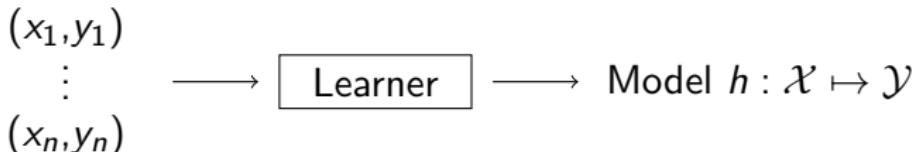
$$h(\mathbf{x}) = w_0 + w_1 x_1 + w_2 x_2 = \mathbf{x}_{1 \times 3}^\top \mathbf{w}_{3 \times 1}$$

- ▶ For new fish  $\mathbf{x}_0$ , predict  $\hat{y}_0 = h(\mathbf{x}_0)$



# General Framework: Supervised Learning

Training data



$x_i$ : input in domain  $\mathcal{X}$  (e.g., length and width  $\mathbb{R}^2$ )

- ▶ A.k.a. features, attributes, variables...
- ▶ Numeric (Length: 0.2, 1.3...)
- ▶ Categorical (Blood type: A/B/AB/O)
- ▶ Ordinal (Difficulty: easy/normal/hard; Discrete but rankable)

$y_i$ : output in range  $\mathcal{Y}$  (e.g., weight  $\mathbb{R}$ )

- ▶ A.k.a. ground-truth label (or simply label), target variable...
- ▶ Supervised: training data have both  $x$  and  $y$

Goal: Find  $h$  that predicts well for novel test  $x \in \mathcal{X}$

## The I.I.D. Assumption

ML requires certain assumption to work

Assume  $\{(x_i, y_i)\}_{i=1}^n$  are independently and identically distributed

- ▶ Independently:  $\forall i, (x_i, y_i)$  is freshly (independently) drawn from a probability distribution  $P(x, y)$
- ▶ Identical: All examples are drawn from the same  $P(x, y)$

The same applies to the novel test data (drawn from  $P(x, y)$ )

# Linear Regression Formulation

Suppose

- ▶ Input vector  $\mathbf{x}_i \in \mathcal{X} = \mathbb{R}^d$
- ▶ Output scalar  $y_i \in \mathcal{Y} = \mathbb{R}$  (regression)
- ▶ Linear model  $h_{\mathbf{w}}(\mathbf{x}) = \mathbf{x}^\top \mathbf{w}$  for some *parameters*  $\mathbf{w} \in \mathbb{R}^d$

Goal

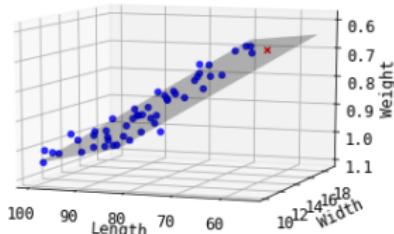
- ▶ Find a good  $\mathbf{w}$  so that  $\hat{y} \triangleq h_{\mathbf{w}}(\mathbf{x})$  is “close” to  $y$

Closeness? Loss function  $L(\hat{y}, y)$

- ▶ Absolute loss ( $L_1$  loss)  $L_1(\hat{y}, y) = |\hat{y} - y|$
- ▶ Squared loss ( $L_2$  loss)  $L_2(\hat{y}, y) = \frac{1}{2}(\hat{y} - y)^2$

Objective function: Empirical risk minimization (ERM)

$$\min_{\mathbf{w} \in \mathbb{R}^d} \quad \frac{1}{n} \sum_{i=1}^n L(\mathbf{x}_i^\top \mathbf{w}, y_i)$$



# Matrix/Vector Notations

The input matrix and output vector

$$X \triangleq \begin{bmatrix} -\mathbf{x}_1^\top & - \\ -\mathbf{x}_2^\top & - \\ \vdots & \\ -\mathbf{x}_n^\top & - \end{bmatrix} \in \mathbb{R}^{n \times d} \text{ and } \mathbf{y} \triangleq \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} \in \mathbb{R}^n$$

Then the prediction

$$\hat{\mathbf{y}} = X\mathbf{w} = \begin{bmatrix} -\mathbf{x}_1^\top & - \\ -\mathbf{x}_2^\top & - \\ \vdots & \\ -\mathbf{x}_n^\top & - \end{bmatrix} \begin{bmatrix} w_1 \\ w_2 \\ \vdots \\ w_d \end{bmatrix} \in \mathbb{R}^n$$

Want  $\hat{\mathbf{y}} \approx \mathbf{y}$

# Linear Regression Objective

$$\min_{\mathbf{w} \in \mathbb{R}^d} \frac{1}{n} \sum_{i=1}^n L(\mathbf{x}_i^\top \mathbf{w}, y_i)$$

Matrix/Vector notations

$$X \triangleq \begin{bmatrix} -\mathbf{x}_1^\top & - \\ -\mathbf{x}_2^\top & - \\ \vdots & \\ -\mathbf{x}_n^\top & - \end{bmatrix} \in \mathbb{R}^{n \times d} \text{ and } \mathbf{y} \triangleq \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} \in \mathbb{R}^n$$

- Want  $\hat{\mathbf{y}} = X\mathbf{w} \approx \mathbf{y}$

With  $L_2$  loss  $L_2(\hat{y}_i, y_i) = \frac{1}{2}(\hat{y}_i - y_i)^2 = \frac{1}{2}(\mathbf{x}_i^\top \mathbf{w} - y_i)^2$

- Recall (squared)  $L_2$  norm  $\|\mathbf{a}\|_2^2 = a_1^2 + a_2^2 + \cdots + a_n^2 = \mathbf{a}^\top \mathbf{a}$

$$\min_{\mathbf{w} \in \mathbb{R}^d} \frac{1}{2n} \|X\mathbf{w} - \mathbf{y}\|_2^2$$

## How to Solve It? Direct Approach

$$\min_{\mathbf{w} \in \mathbb{R}^d} J(\mathbf{w}) \triangleq \frac{1}{2n} \|X\mathbf{w} - \mathbf{y}\|_2^2 = \frac{1}{2n} (X\mathbf{w} - \mathbf{y})^\top (X\mathbf{w} - \mathbf{y})$$

Note that this objective function  $J$  is convex

Compute the gradient

$$\begin{aligned}\nabla J(\mathbf{w}) &= \frac{1}{2n} \nabla \left[ (X\mathbf{w} - \mathbf{y})^\top (X\mathbf{w} - \mathbf{y}) \right] \quad \text{if } f(u) = (au - b)^2, f'(u)? \text{ (chain rule)} \\ &= \frac{1}{n} (X\mathbf{w} - \mathbf{y}) \times ? \quad \nabla(X\mathbf{w} - \mathbf{y}) \quad \text{if } f(u) = au - b, f'(u)? \\ &= \frac{1}{n} \left( \underset{n \times d}{X} \underset{d \times 1}{\mathbf{w}} - \underset{n \times 1}{\mathbf{y}} \right) \times ? \quad \text{Dimension matched?} \\ &= \frac{1}{n} \underset{d \times n}{X^\top} \underset{n \times 1}{(X\mathbf{w} - \mathbf{y})} \quad \text{Grad shares the same dim as the params}\end{aligned}$$

Set it to zero to find the best  $\mathbf{w}$ . Assume that  $X^\top X$  is invertible

$$X^\top (X\mathbf{w} - \mathbf{y}) = \mathbf{0}_d \iff X^\top X\mathbf{w} = X^\top \mathbf{y} \iff \mathbf{w}^* = (X^\top X)^{-1} X^\top \mathbf{y}$$

## How to Solve It? Indirect Approach

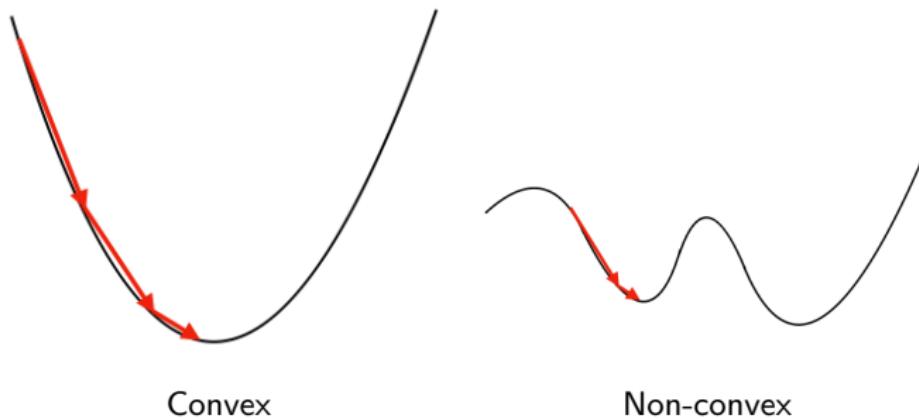
$$\mathbf{w}^* = \underset{\mathbf{w} \in \mathbb{R}^d}{\operatorname{argmin}} \frac{1}{2n} \|\mathbf{X}\mathbf{w} - \mathbf{y}\|_2^2 = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y}$$

Direct approach: compute the gradient and set to zero

- ▶ Not always possible

Indirect approach: iterative algorithm (gradient descent)

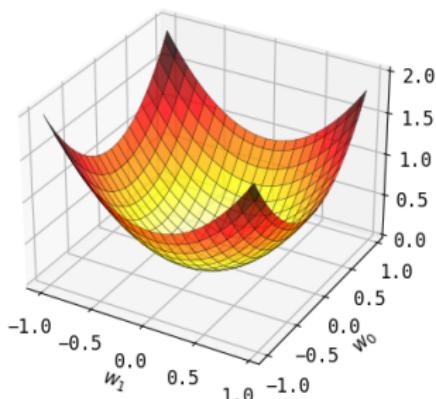
- ▶ Initial  $\mathbf{w}^{(0)}$  (e.g.  $\mathbf{w}^{(0)} = \mathbf{0}_d$ , a vector of all zeros)
- ▶  $\mathbf{w}^{(t+1)} = \mathbf{w}^{(t)} - \eta \nabla J(\mathbf{w}^{(t)})$  with step size  $\eta > 0$
- ▶ That's why convexity could be important



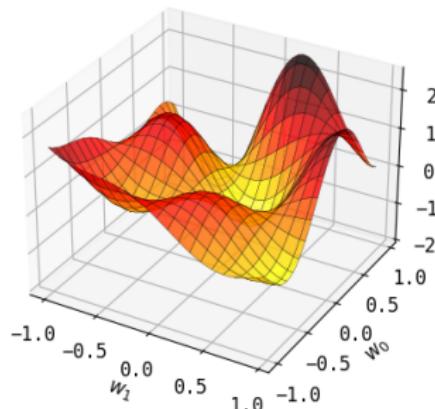
# How to Solve It? Indirect Approach

Gradient descent 3D visualization

- ▶  $\mathbf{w}^{(t+1)} = \mathbf{w}^{(t)} - \eta \nabla J(\mathbf{w}^{(t)})$  with step size  $\eta > 0$



Convex

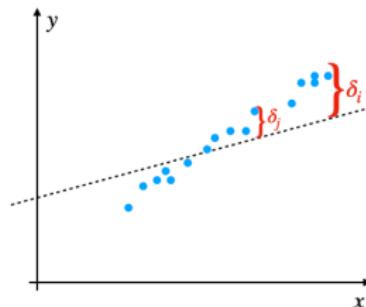


Non-convex

# How about Other Losses? $L_1$ Loss

$L_1$  loss minimization

$$\min_{\mathbf{w} \in \mathbb{R}^d} \quad \frac{1}{n} \sum_{i=1}^n |\mathbf{x}_i^\top \mathbf{w} - y_i|$$



- ▶ Convex but not *smooth* (abs not differentiable at 0)
- ▶ Direct approach is not possible

Other solvers?

- ▶ For point  $(\mathbf{x}_i, y_i)$ , defined a “tolerance”  $\delta_i \geq 0$

$$\begin{aligned} |\hat{y}_i - y_i| \leq \delta_i &\iff -\delta_i \leq \hat{y}_i - y_i \leq \delta_i \\ &\iff \mathbf{x}_i^\top \mathbf{w} - y_i \leq \delta_i \text{ and } y_i - \mathbf{x}_i^\top \mathbf{w} \leq \delta_i \end{aligned}$$

- ▶ Minimize sum of tolerances  $\min_{\mathbf{w}, \delta_i} \frac{1}{n} \sum_{i=1}^n \delta_i$

## $L_1$ Loss Minimization in Matrix Form

Using matrix/vector notations

- Recall  $L_1$  norm  $\|\mathbf{a}\|_1 = |a_1| + |a_2| + \cdots + |a_n|$

$$\min_{\mathbf{w} \in \mathbb{R}^d} \frac{1}{n} \|X\mathbf{w} - \mathbf{y}\|_1$$

Let  $\boldsymbol{\delta} \in \mathbb{R}_+^n$  be the “tolerance” between  $\hat{\mathbf{y}}$  and  $\mathbf{y}$

- Always non-negative  $\boldsymbol{\delta} \succeq \mathbf{0}_n$

$$\min_{\mathbf{w}, \boldsymbol{\delta}} \boldsymbol{\delta}^\top \mathbf{1}_n = \sum_{i=1}^n \delta_i \quad \text{Want tolerance sum to be small}$$

$$\text{s.t. } \boldsymbol{\delta} \succeq \mathbf{0}_n$$

$$X\mathbf{w} - \mathbf{y} \preceq \boldsymbol{\delta} \quad \text{Sandwich the difference}$$

$$\mathbf{y} - X\mathbf{w} \preceq \boldsymbol{\delta} \quad \text{on both sides} \Leftrightarrow |X\mathbf{w} - \mathbf{y}| \preceq \boldsymbol{\delta}$$

Linear programming (LP) problem (Why? Linear in both  $\mathbf{w}$  and  $\boldsymbol{\delta}$ ), which can be solved efficiently

## How about Other Losses? $L_\infty$ Loss

In general, the  $L_p$  loss:  $\|X\mathbf{w} - \mathbf{y}\|_p^p$ ,  $0 \leq p \leq \infty$

$L_\infty$  loss:  $\|X\mathbf{w} - \mathbf{y}\|_\infty \triangleq \max_{i=1,\dots,n} |\mathbf{x}_i^\top \mathbf{w} - y_i|$

- ▶ Control the maximum gap (worse point)

Let  $\delta \geq 0$  be the scalar "tolerance" (such that  $|\mathbf{x}_i^\top \mathbf{w} - y_i| \leq \delta$ )

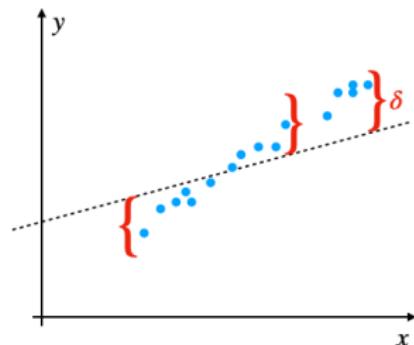
$$\min_{\mathbf{w}, \delta} \quad \delta$$

$$\text{s.t.} \quad \delta \geq 0$$

$$X\mathbf{w} - \mathbf{y} \preceq \delta \cdot \mathbf{1}_n$$

$$\mathbf{y} - X\mathbf{w} \preceq \delta \cdot \mathbf{1}_n$$

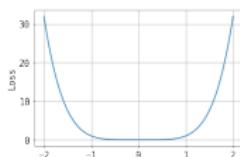
Again, an LP problem



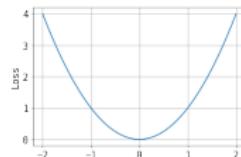
# Which Loss to Use?

Different  $p$  values give different models  $\mathbf{w}^*$

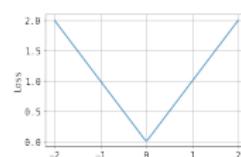
- ▶  $1 \leq p \leq \infty$ : objective function is convex
- ▶  $1 < p < \infty$ : objective function is smooth and differentiable
- ▶  $0 < p < 1$ : *not* convex, but grow slowly as  $\hat{y}$  deviates from  $y$ 
  - ▶ More robust, not affected much by outliers



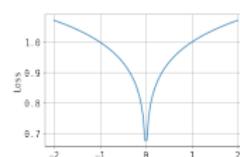
$$p = 5$$



$$p = 2$$



$$p = 1$$

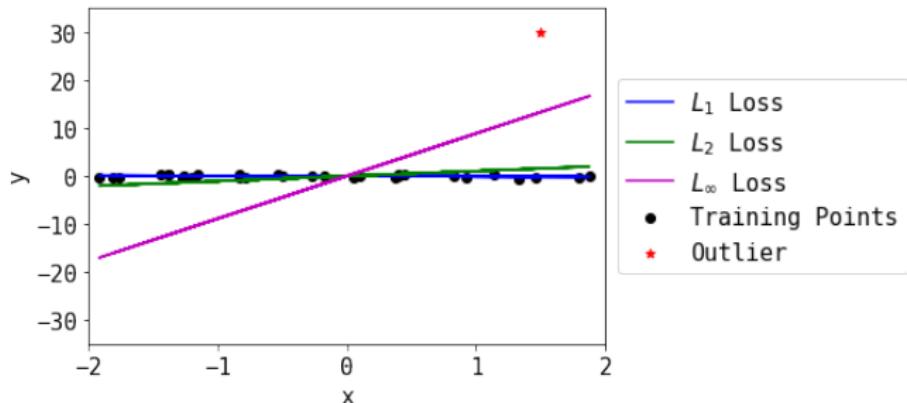


$$p = 0.1$$

Loss with different  $p$  values for one data point ( $x$ -axis:  $\hat{y} - y$ )

# Which Loss to Use?

An example: Learning with outliers



- ▶ Large  $p$  ( $L_\infty$ ) chases the outlier (focus on the worse error)
- ▶ Small  $p$  ( $L_1$ ) is robust (treat every error equally)

Always use small  $p$ ? No, because...

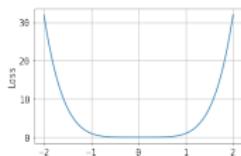
- ▶  $p < 1$  is not convex and difficult to minimize

# Which Loss to Use?

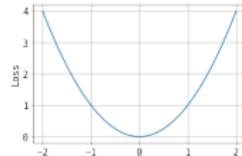
No free lunch

Pros and cons of convex versus robust losses

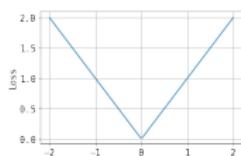
Loss type	Pros 	Cons 
Convex loss $p \in [1, \infty]$	Efficient optimization	Sensitive to outlier
Robust loss $p \in [0, 1)$	Slow growth, robust	Difficult to optimize



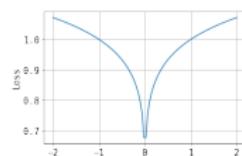
$$p = 5$$



$$p = 2$$



$$p = 1$$



$$p = 0.1$$

## Recap

This lecture: linear regression models  $\mathbf{y} \approx X\mathbf{w}$

- ▶  $L_2$  loss  $\rightarrow$  analytic solution
- ▶  $L_1$  &  $L_\infty$  losses  $\rightarrow$  linear programming (LP)
- ▶ Different  $p$ : convex versus robust losses

## References

Bishop and Nasrabadi (2006, Sec.3.1)  
Hastie et al. (2009, Sec.2.3.1 & Sec.3.2)

- Bishop, C. M. and Nasrabadi, N. M. (2006). *Pattern recognition and machine learning*, volume 4. Springer.
- Hastie, T., Tibshirani, R., Friedman, J. H., and Friedman, J. H. (2009). *The elements of statistical learning: data mining, inference, and prediction*, volume 2. Springer.

## Appendix: CVXOPT LP Formulation for $L_1$ Loss

$$\begin{array}{ll} \min_{\mathbf{w}, \boldsymbol{\delta}} & \boldsymbol{\delta}^\top \mathbf{1}_n \\ \text{s.t.} & \boldsymbol{\delta} \succeq \mathbf{0}_n \\ & X\mathbf{w} - \mathbf{y} \preceq \boldsymbol{\delta} \\ & \mathbf{y} - X\mathbf{w} \preceq \boldsymbol{\delta} \end{array} \quad \begin{array}{ll} \min_{\mathbf{x}} & \mathbf{c}^\top \mathbf{x} \\ \text{s.t.} & G\mathbf{x} \preceq \mathbf{h} \end{array}$$

$\mathbf{x}$  in CVXOPT means unknowns (not a training input vector)

$$\mathbf{x} = \begin{bmatrix} \mathbf{w} \\ \boldsymbol{\delta} \end{bmatrix} \in \mathbb{R}^{d+n}$$

Want  $\mathbf{c}^\top \mathbf{x} = \boldsymbol{\delta}^\top \mathbf{1}_n = \sum_{i=1}^n \delta_i$ . What is  $\mathbf{c} \in \mathbb{R}^{d+n}$  then?

$$\mathbf{c}^\top \mathbf{x} = \left[ \underbrace{0, 0, \dots, 0}_{d \text{ zeros}}, \underbrace{1, 1, \dots, 1}_{n \text{ ones}} \right] \begin{bmatrix} \mathbf{w} \\ \boldsymbol{\delta} \end{bmatrix} = \boldsymbol{\delta}^\top \mathbf{1}_n$$

## Appendix: CVXOPT LP Formulation for $L_1$ Loss

$$\text{s.t. } \delta \succeq \mathbf{0}_n$$

$$\text{s.t. } G\mathbf{x} \preceq \mathbf{h}$$

$$X\mathbf{w} - \mathbf{y} \preceq \delta$$

$$\mathbf{y} - X\mathbf{w} \preceq \delta$$

Constraints in CVXOPT

$$G\mathbf{x} = \begin{bmatrix} -G_{1:} & - \\ -G_{2:} & - \\ \vdots & \\ -G_{k:} & - \end{bmatrix} \mathbf{x} \preceq \begin{bmatrix} h_1 \\ h_2 \\ \vdots \\ h_k \end{bmatrix} = \mathbf{h}$$

Each row is a constraint

$$G_{i:}\mathbf{x} \leq h_i \quad i = 1, 2, \dots, k$$

## Appendix: CVXOPT LP Formulation for $L_1$ Loss

$$\text{s.t. } \delta \succeq \mathbf{0}_n \iff -\delta \preceq \mathbf{0}_n \quad \text{s.t. } G\mathbf{x} \preceq \mathbf{h}$$

$$X\mathbf{w} - \mathbf{y} \preceq \delta$$

$$\mathbf{y} - X\mathbf{w} \preceq \delta$$

Three sets of constraints (color coded)

$$G_{3n \times (d+n)} \cdot \mathbf{x}_{(d+n) \times 1} = \begin{bmatrix} G^{(1)} \\ G^{(2)} \\ G^{(3)} \end{bmatrix}_{n \times (d+n)} \begin{bmatrix} \mathbf{w} \\ \delta \end{bmatrix} \preceq \begin{bmatrix} \mathbf{h}^{(1)} \\ \mathbf{h}^{(2)} \\ \mathbf{h}^{(3)} \end{bmatrix}_{n \times 1} = \mathbf{h}$$

Want  $G_{n \times (d+n)} \cdot \begin{bmatrix} \mathbf{w} \\ \delta \end{bmatrix} \preceq \mathbf{h}^{(1)} \Leftrightarrow -\delta \preceq \mathbf{0}_n$ . What are  $G^{(1)}$  and  $\mathbf{h}^{(1)}$ ?

$$\begin{bmatrix} G^{(11)} & G^{(12)} \end{bmatrix}_{n \times d} \cdot \begin{bmatrix} \mathbf{w} \\ \delta \end{bmatrix}_{d \times 1} = G^{(11)}_{n \times d} \mathbf{w}_{d \times 1} + G^{(12)}_{n \times n} \delta_{n \times 1} = -\delta \preceq \mathbf{0}_n = \mathbf{h}^{(1)}$$

So  $G^{(11)} = \mathbf{0}_{n \times d}$ ,  $G^{(12)} = -I_n$  and  $\mathbf{h}^{(1)} = \mathbf{0}_n$

## Appendix: CVXOPT LP Formulation for $L_1$ Loss

$$\text{s.t. } \delta \succeq \mathbf{0}_n \iff -\delta \preceq \mathbf{0}_n \quad \text{s.t. } G\mathbf{x} \preceq \mathbf{h}$$

$$X\mathbf{w} - \mathbf{y} \preceq \delta$$

$$\mathbf{y} - X\mathbf{w} \preceq \delta$$

Three sets of constraints (color coded)

$$G_{3n \times (d+n)} \cdot \mathbf{x}_{(d+n) \times 1} = \begin{bmatrix} G^{(1)} \\ G^{(2)} \\ G^{(3)} \end{bmatrix}_{n \times (d+n)} \begin{bmatrix} \mathbf{w} \\ \delta \end{bmatrix} \preceq \begin{bmatrix} \mathbf{h}^{(1)} \\ \mathbf{h}^{(2)} \\ \mathbf{h}^{(3)} \end{bmatrix}_{n \times 1} = \mathbf{h}$$

Want  $G^{(2)}_{n \times (d+n)} \cdot \begin{bmatrix} \mathbf{w} \\ \delta \end{bmatrix} \preceq \mathbf{h}^{(2)}_{n \times 1} \Leftrightarrow X\mathbf{w} - \delta \preceq \mathbf{y}$ . What are  $G^{(2)}, \mathbf{h}^{(2)}$ ?

$$\begin{bmatrix} G^{(21)} & G^{(22)} \end{bmatrix}_{n \times d} \cdot \begin{bmatrix} \mathbf{w} \\ \delta \end{bmatrix}_{d \times 1} = G^{(21)}_{n \times d} \mathbf{w}_{d \times 1} + G^{(22)}_{n \times n} \delta_{n \times 1} = X\mathbf{w} - \delta \preceq \mathbf{y} = \mathbf{h}^{(2)}$$

So  $G^{(21)} = X$ ,  $G^{(22)} = -I_n$  and  $\mathbf{h}^{(2)} = \mathbf{y}$

## Appendix: CVXOPT LP Formulation for $L_1$ Loss

$$\text{s.t. } \delta \succeq \mathbf{0}_n \iff -\delta \preceq \mathbf{0}_n \quad \text{s.t. } G\mathbf{x} \preceq \mathbf{h}$$

$$X\mathbf{w} - \mathbf{y} \preceq \delta$$

$$\mathbf{y} - X\mathbf{w} \preceq \delta$$

Three sets of constraints (color coded)

$$G_{3n \times (d+n)} \cdot \mathbf{x}_{(d+n) \times 1} = \begin{bmatrix} G^{(1)} \\ G^{(2)} \\ G^{(3)} \end{bmatrix}_{n \times (d+n)} \begin{bmatrix} \mathbf{w} \\ \delta \end{bmatrix} \preceq \begin{bmatrix} \mathbf{h}^{(1)} \\ \mathbf{h}^{(2)} \\ \mathbf{h}^{(3)} \end{bmatrix}_{n \times 1} = \mathbf{h}$$

Want  $G^{(3)}_{n \times (d+n)} \cdot \begin{bmatrix} \mathbf{w} \\ \delta \end{bmatrix}_{n \times 1} \preceq \mathbf{h}^{(3)} \Leftrightarrow -X\mathbf{w} - \delta \preceq -\mathbf{y}$ . Then  $G^{(3)}, \mathbf{h}^{(3)}$ ?

$$\begin{bmatrix} G^{(31)} & G^{(32)} \end{bmatrix}_{n \times d} \cdot \begin{bmatrix} \mathbf{w} \\ \delta \end{bmatrix}_{d \times 1} = G^{(31)}_{n \times d} \mathbf{w}_{d \times 1} + G^{(32)}_{n \times n} \delta_{n \times 1} = -X\mathbf{w} - \delta \preceq -\mathbf{y} = \mathbf{h}^{(3)}$$

So  $G^{(31)} = -X$ ,  $G^{(32)} = -I_n$  and  $\mathbf{h}^{(3)} = -\mathbf{y}$

## Appendix: CVXOPT LP Formulation for $L_1$ Loss

To summarize

$$\begin{aligned} \min_{\mathbf{x}} \quad & \underbrace{[0, 0, \dots, 0, 1, 1, \dots, 1]}_{\mathbf{c}^\top} \cdot \underbrace{\begin{bmatrix} \mathbf{w} \\ \delta \end{bmatrix}}_{\mathbf{x}} \\ \text{s.t.} \quad & \underbrace{\begin{bmatrix} \mathbf{0}_{n \times d} & -I_n \\ X & -I_n \\ -X & -I_n \end{bmatrix}}_G \cdot \underbrace{\begin{bmatrix} \mathbf{w} \\ \delta \end{bmatrix}}_{\mathbf{x}} \preceq \underbrace{\begin{bmatrix} \mathbf{0}_n \\ \mathbf{y} \\ -\mathbf{y} \end{bmatrix}}_h \end{aligned}$$

After solving  $\mathbf{x} = \begin{bmatrix} \mathbf{w} \\ \delta \end{bmatrix}$

- ▶  $\mathbf{w}$  model parameters
- ▶  $\delta$  tolerances

Exercise/Assignment:  $L_\infty$  loss