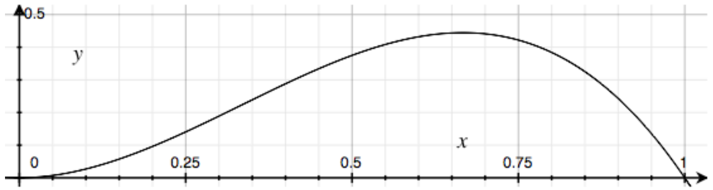
CPSC 340:
Machine Learning and Data Mining

MLE and MAP

Last Time: Maximum Likelihood Estimation (MLE)

- Maximum likelihood estimation (MLE) for fitting probabilistic models.
  - We have a given fixed dataset D.
  - We pick a statistical model with unknown parameters 'w'.
  - We define the likelihood function as a probability mass/density p(D | w).
  - We choose the model $\hat{w}$ that maximizes the likelihood:



$$\hat{w} \in \underset{w}{\operatorname{argmax}} \{p(D|w)\}$$

- Appealing "consistency" properties as n goes to infinity (take STAT 4XX).
  - "This is a reasonable thing to do for large data sets".

- Gives naïve Bayes "counting" estimates we used. $\hat{w} = \frac{\text{\# of ones}}{\text{\# of examples}}$

Minimizing the Negative Log-Likelihood (NLL)

- To compute maximize likelihood estimate (MLE), usually we equivalently minimize the negative "log-likelihood" (NLL):
  - "Log-likelihood" is short for "logarithm of the likelihood".

$$\hat{w} \in \underset{w}{\operatorname{argmax}} \{p(D \mid w)\} \equiv \underset{w}{\operatorname{argmin}} \{-\log(p(D \mid w))\}$$

"equivalent"

- Why are these equivalent?
  - Logarithm is strictly monotonic: if $\alpha > \beta$, then $\log(\alpha) > \log(\beta)$.
    - So location of maximum doesn't change if we take logarithm.
  - Changing sign flips max to min.

- See [Max and Argmax](#) notes if this seems strange.

Minimizing the Negative Log-Likelihood (NLL)

- We use log-likelihood because it turns multiplication into addition:

$$\log(\alpha\beta) = \log(\alpha) + \log(\beta)$$

- More generally: $\log\left(\prod_{i=1}^{n} a_i\right) = \sum_{i=1}^{n} \log(a_i)$

- If data is 'n' IID samples then $p(D \mid w) = \prod_{i=1}^{n} \underbrace{p(D_i \mid w)}_{\text{likelihood of example 'i'}}$

and our MLE is $\hat{w} \in \underset{w}{\operatorname{argmax}} \left\{ \prod_{i=1}^{n} p(D_i \mid w) \right\} \equiv \underset{w}{\operatorname{argmin}} \left\{ -\sum_{i=1}^{n} \log(p(D_i \mid w)) \right\}$

Next Topic: Least Squares and MLE

Least Squares is Gaussian MLE

- It turns out that most objectives have an MLE interpretation:
  - For example, consider minimizing the squared error:

$$f(w) = \frac{1}{2}\|Xw - y\|^2$$

  - This gives MLE of a linear model with IID noise from a normal distribution:

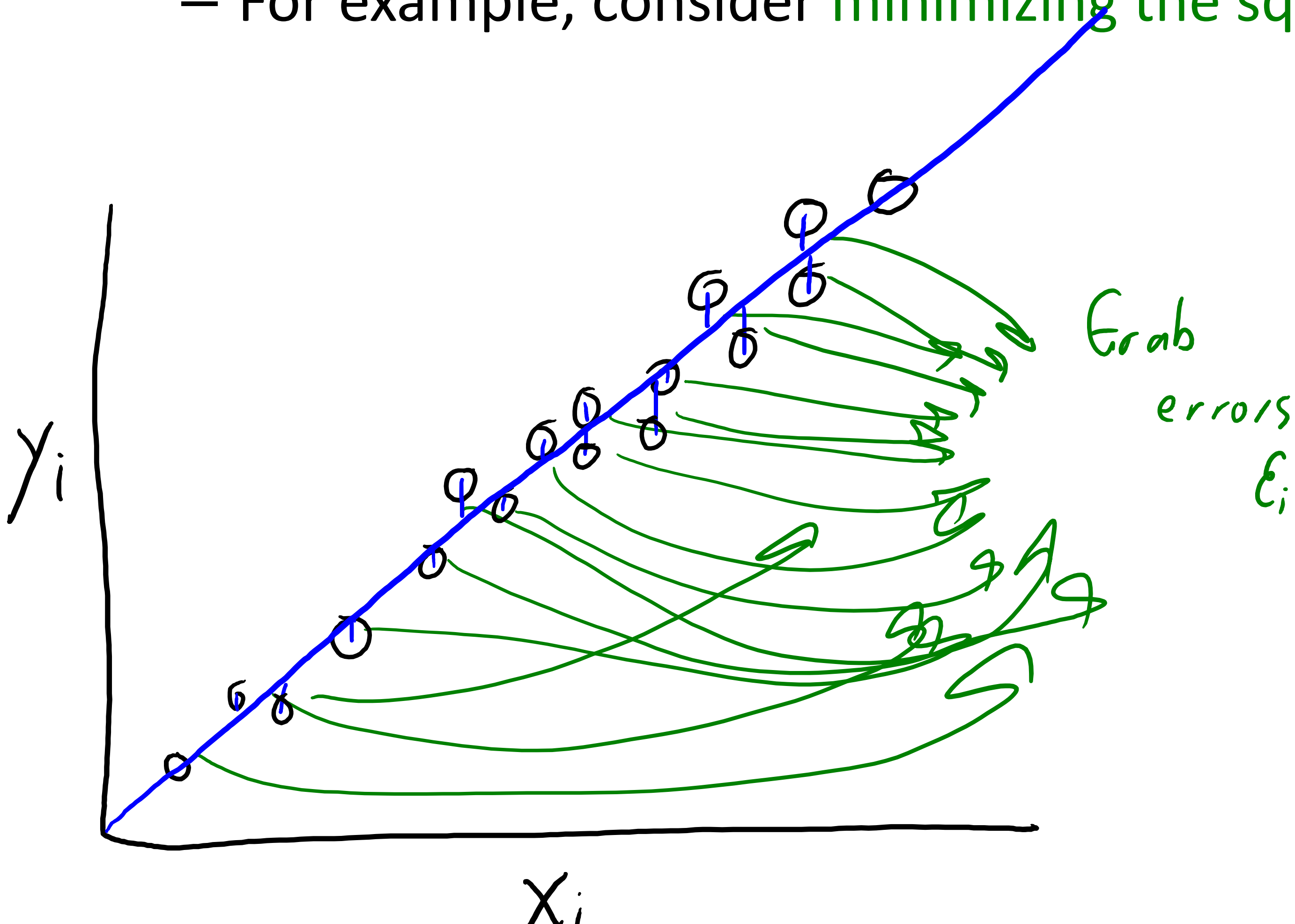
$$y_i = w^T x_i + \varepsilon_i$$

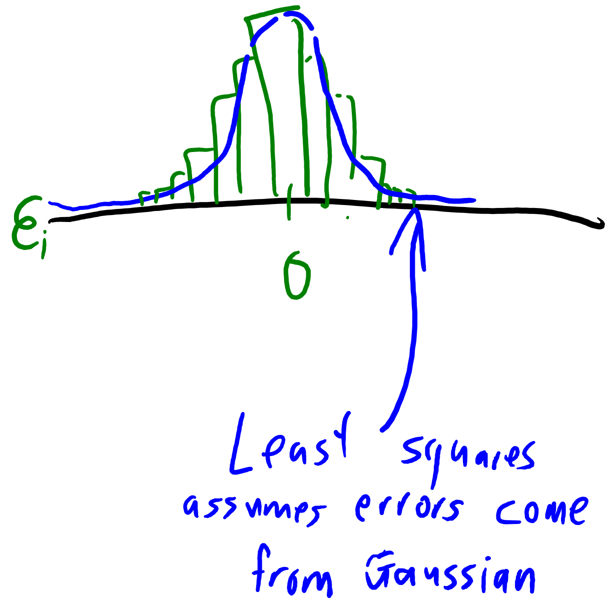
where each ε_i is sampled independently from standard normal

    - "Gaussian" is another name for the "normal" distribution.
  - Remember that least squares solution is called the "normal equations".

Least Squares is Gaussian MLE

- It turns out that most objectives have an MLE interpretation:
  - For example, consider minimizing the squared error:





Least Squares is Gaussian MLE (Gory Details)

- Let's assume that $y_i = w^T x_i + \varepsilon_i$, with ε_i following $\underbrace{\text{standard normal}}_{\text{also known as "Gaussian" distribution}}$:

$$p(\varepsilon_i) = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{\varepsilon_i^2}{2}\right)$$

- This leads to a Gaussian likelihood for example 'i' of the form:

$$p(y_i \mid x_i, w) = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{(w^T x_i - y_i)^2}{2}\right)$$

- Finding MLE (minimizing NLL) is least squares:

$$f(w) = -\sum_{i=1}^n \log(p(y_i \mid w, x_i))$$

$$= -\sum_{i=1}^n \log\left(\frac{1}{\sqrt{2\pi}} \exp\left(-\frac{(w^T x_i - y_i)^2}{2}\right)\right)$$

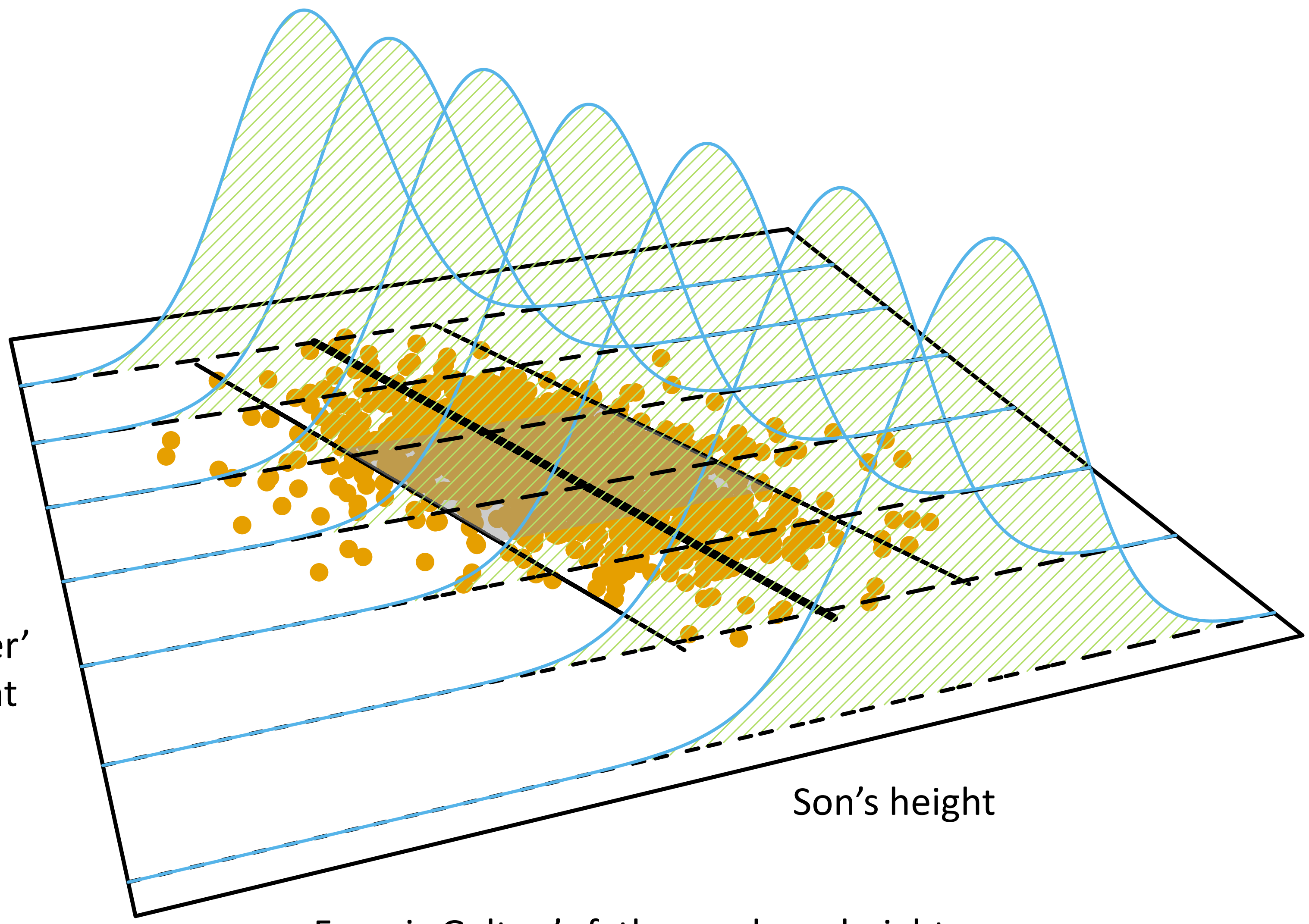
$$= -\sum_{i=1}^n \left[\underbrace{\log\left(\frac{1}{\sqrt{2\pi}}\right)}_{\text{constant in 'w'}} + \underbrace{\log(\exp}_{\text{operations cancel}}\left(-\frac{(w^T x_i - y_i)^2}{2}\right))\right]$$

$$= -\sum_{i=1}^n \left[(\text{constant}) - \frac{1}{2}(w^T x_i - y_i)^2\right]$$

$$= (\text{constant}) + \frac{1}{2}\sum_{i=1}^n (w^T x_i - y_i)^2$$

$$= (\text{constant}) + \frac{1}{2}\|Xw - y\|^2$$

Gaussian Errors and Linear Regression



Francis Galton's father and son heights

$\epsilon_i = w^T x_i - y_i$ follows a normal distribution $N(0, \sigma^2)$

The variance is the same across different x_i

Estimating $\boldsymbol{\sigma}$

Recall the NLL is

$$\mathsf{NLL}(\boldsymbol{\beta}, \sigma^2) = \sum_{i=1}^{N} \left(\frac{1}{2}(\log(2\pi) + \log(\sigma^2)) + \frac{1}{2\sigma^2}(y_i - \mathbf{x}_i^{\mathrm{T}}\boldsymbol{\beta})^2 \right)$$

So we can solve σ^2 to get

$$\hat{\sigma}^2 = \frac{1}{N}(\mathbf{y} - \mathbf{X}\boldsymbol{\beta})^{\mathrm{T}}(\mathbf{y} - \mathbf{X}\boldsymbol{\beta}) = \frac{1}{N} \cdot \mathsf{RSS}$$

An unbiased version is typically used:

$$\hat{\sigma}^2 = \frac{1}{N - D - 1}(\mathbf{y} - \mathbf{X}\boldsymbol{\beta})^{\mathrm{T}}(\mathbf{y} - \mathbf{X}\boldsymbol{\beta}) = \frac{1}{N - D - 1} \cdot \mathsf{RSS}$$

$\hat{\sigma}$ is called the 'residual standard error' or 'root mean squared error'

Digression: “Generative” vs. “Discriminative”

- Notice, that we maximized conditional p(y | X, w), not the joint p(y, X | w).
  - We did MLE “conditioned” on the features ‘X’ being fixed (no “likelihood of X”).
  - This is called a “discriminative” supervised learning model.
  - A “generative” model (like naïve Bayes) would optimize p(y, X | w).

- Discriminative probabilistic models:
  - Least squares, robust regression, logistic regression.
  - Can use complicated features because you don’t model ‘X’.

- Example of generative probabilistic models:
  - Naïve Bayes, linear discriminant analysis (makes Gaussian assumption).
  - Often need strong assumption because they model ‘X’.

- “Folk” belief: generative models are often better with small ‘n’.

Loss Functions and Maximum Likelihood Estimation

- So least squares is MLE under Gaussian likelihood.

If $p(y_i | x_i, w) = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{(w^T x_i - y_i)^2}{2}\right)$

then MLE of 'w' is minimum of $f(w) = \frac{1}{2}\|Xw - y\|^2$

- With a Laplace likelihood you would get absolute error.

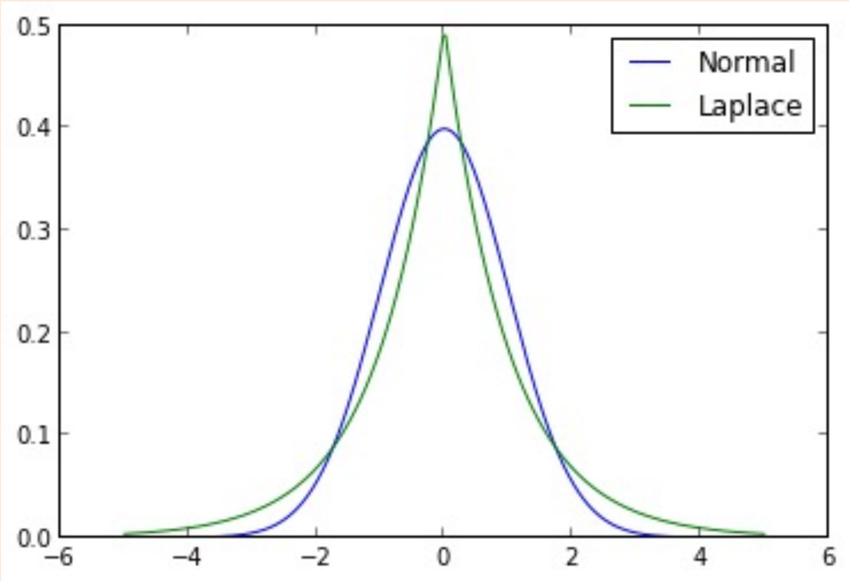
If $p(y_i | x_i, w) = \frac{1}{2} \exp(-|w^T x_i - y_i|)$

then MLE is minimum of $f(w) = \|Xw - y\|_1$

- Other likelihoods lead to different errors ("sigmoid" -> logistic loss).

"Heavy" Tails vs. "Light" Tails

- We know that L1-norm is more robust than L2-norm.
  – What does this mean in terms of probabilities?



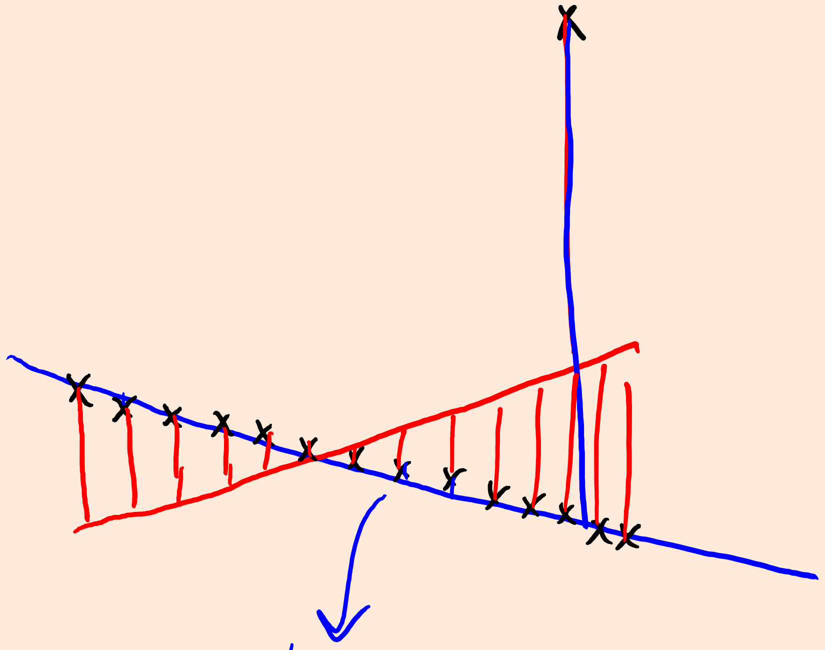
Here "tail" means "mass of the distribution away from the mean."

  – Gaussian has "light tails": assumes everything is close to mean.
  – Laplace has "heavy tails": assumes some data is far from mean.
  – Student 't' is even more heavy-tailed/robust, but NLL is non-convex.

http://austinrochford.com/posts/2013-09-02-prior-distributions-for-bayesian-regression-using-pymc.html

“Heavy” Tails vs. “Light” Tails

- Laplace distribution is robust to outliers

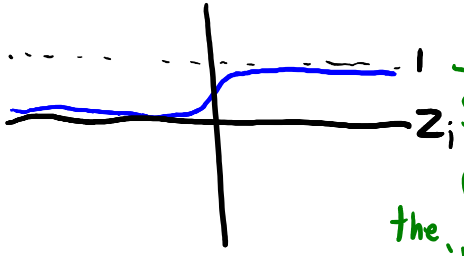


Linear model 'w' minimizing $f(w) = \|Xw - y\|_1 = \sum_{i=1}^{n} |w^T x_i - y_i|$

Sigmoid: transforming w^Tx_i to a probability

- Recall we got probabilities from binary linear models with sigmoid:
  1. The linear model w^Tx_i gives us a number z_i in $(-\infty, \infty)$.
  2. We'll map $z_i=w^Tx_i$ to a probability with the sigmoid function.

$$h(z_i) = \frac{1}{1+\exp(-z_i)}$$



Gives values in the range (0,1) that we'll interpret as probabilities

- We can show that MLE with this model gives logistic loss.

Sigmoid: transforming w^Tx_i to a probability

- We'll define $p(y_i = +1 \mid z_i) = h(z_i)$, where 'h' is the sigmoid function.

So $p(y_i = -1 \mid z_i) = 1 - p(y_i = +1 \mid z_i)$

$= 1 - h(z_i)$

$= h(-z_i)$

can show from definition of 'h'

- With y_i in $\{-1,+1\}$, we can write both cases as $p(y_i \mid z_i) = h(y_iz_i)$.
- So we convert $z_i=w^Tx_i$ into "probability of y_i" using:

$$p(y_i \mid w, x_i) = h(y_i \underbrace{w^Tx_i}_{z_i})$$

$$= \frac{1}{1 + \exp(-y_iw^Tx_i)}$$

- MLE with this likelihood is equivalent to minimizing logistic loss.

MLE Interpretation of Logistic Regression

- For IID regression problems the conditional NLL can be written:

$$\underbrace{-\log(p(y \mid X, w))}_{NLL} = -\log\Big(\underbrace{\prod_{i=1}^{n} p(y_i \mid x_i, w)}_{\text{IID assumption}}\Big) = -\underbrace{\sum_{i=1}^{n}}_{\substack{\text{log turns}\\ \text{product into sum}}} \log(p(y_i \mid x_i, w))$$

- Logistic regression assumes sigmoid($w^T x_i$) conditional likelihood:

$$p(y_i \mid x_i, w) = h(y_i w^T x_i) \quad \text{where} \quad h(z_i) = \frac{1}{1+\exp(-z_i)}$$

- Plugging in the sigmoid likelihood, the NLL is the logistic loss:

$$NLL(w) = -\sum_{i=1}^{n} \log\left(\frac{1}{1+\exp(-y_i w^T x_i)}\right) = \sum_{i=1}^{n} \log(1+\exp(-y_i w^T x_i))$$

(since $\log(1) = 0$)

MLE Interpretation of Logistic Regression

- We just derived the logistic loss from the perspective of MLE.
  - Instead of "smooth convex approximation of 0-1 loss", we now have that logistic regression is doing MLE in a probabilistic model.
  - The training and prediction would be the same as before.
    - We still minimize the logistic loss in terms of 'w'.
  - But MLE justifies sigmoid for "probability that e-mail is important":

$$p(y_i \mid x_i, w) = \frac{1}{1 + \exp(-y_i w^T x_i)}$$

  - Similarly, NLL under the softmax likelihood is the softmax loss (for multi-class).

Next Topic: MAP Estimation

Maximum Likelihood Estimation and Overfitting

- In our abstract setting with data D the MLE is:

$$\hat{w} \in \underset{w}{\text{argmax}} \{p(D \mid w)\}$$

- But conceptually MLE is a bit weird:
  - "Find the 'w' that makes 'D' have the highest probability given 'w'."

- And MLE often leads to overfitting:
  - Data could be very likely for some very unlikely 'w'.
  - For example, a complex model that overfits by memorizing the data.

- What we really want:
  - "Find the 'w' that has the highest probability given the data D."

Maximum a Posteriori (MAP) Estimation

- Maximum a posteriori (MAP) estimate maximizes the reverse probability:

$$\hat{w} \in \underset{w}{\text{argmax}}\{p(w|D)\}$$

  - This is what we want: the probability of 'w' given our data.

- MLE and MAP are connected by Bayes rule:

$$\underbrace{p(w|D)}_{\text{posterior}} = \frac{p(D|w)p(w)}{p(D)} \propto \underbrace{p(D|w)}_{\text{likelihood}}\underbrace{p(w)}_{\text{prior}}$$

- So MAP maximizes the likelihood p(D|w) times the prior p(w):
  - Prior is our "belief" that 'w' is correct before seeing data.
  - Prior can reflect that complex models are likely to overfit.

MAP Estimation and Regularization

- From Bayes rule, the MAP estimate with IID examples D_i is:

$$\hat{w} \in \underset{w}{\operatorname{argmax}} \{ p(w \mid D) \} \equiv \underset{w}{\operatorname{argmax}} \left\{ \prod_{i=1}^{n} \left[p(D_i \mid w) \right] p(w) \right\}$$

- By again taking the negative of the logarithm as before we get:

$$\hat{w} \in \underset{w}{\operatorname{argmin}} \left\{ - \sum_{i=1}^{n} \left[\underbrace{\log(p(D_i \mid w))}_{\text{loss}} \right] - \underbrace{\log(p(w))}_{\text{regularizer}} \right\}$$

- So we can view the negative log-prior as a regularizer:
  - Many regularizers are equivalent to negative log-priors.

L2-Regularization and MAP Estimation

- We obtain L2-regularization under an independent Gaussian assumption:

Assume each w_j comes from a Gaussian with mean 0 and variance $1/\lambda$

- This implies that:

Gaussian assumption

$$p(w) \underset{\text{independence}}{=} \prod_{j=1}^{d} p(w_j) \propto \prod_{j=1}^{d} \exp\left(-\frac{\lambda}{2}w_j^2\right) \underset{e^{\alpha}e^{\beta}=e^{\alpha+\beta}}{=} \exp\left(-\frac{\lambda}{2}\sum_{j=1}^{d} w_j^2\right)$$

- So we have that:

$$-\log(p(w)) = -\log\left(\exp\left(-\frac{\lambda}{2}\|w\|^2\right)\right) + (\text{constant}) = \frac{\lambda}{2}\|w\|^2 + (\text{constant})$$

- With this prior, the MAP estimate with IID training examples would be

$$\hat{w} \in \underset{w}{\text{argmin}}\left\{-\log(p(y|X,w)) - \log(p(w))\right\} \equiv \underset{w}{\text{argmin}}\left\{-\sum_{i=1}^{n}\left[\log(p(y_i|x_i,w))\right] + \frac{\lambda}{2}\|w\|^2\right\}$$

MAP Estimation and Regularization

- MAP estimation gives link between probabilities and loss functions.
  - Gaussian likelihood (σ = 1) + Gaussian prior gives L2-regularized least squares.

If $p(y_i \mid x_i, w) \propto \exp\left(-\frac{(w^Tx_i - y_i)^2}{2}\right)$ $\quad p(w_j) \propto \exp\left(-\frac{\lambda}{2} w_j^2\right)$

then MAP estimation is equivalent to minimizing $f(w) = \frac{1}{2}\|Xw - y\|^2 + \frac{\lambda}{2}\|w\|^2$

  - Laplace likelihood (σ = 1) + Gaussian prior give L2-regularized robust regression:

If $p(y_i \mid x_i, w) \propto \exp(-|w^Tx_i - y_i|)$ $\quad p(w) \propto \exp\left(-\frac{\lambda}{2} w_j^2\right)$

then MAP estimation is equivalent to minimizing $f(w) = \|Xw - y\|_1 + \frac{\lambda}{2}\|w\|^2$

  - As 'n' goes to infinity, effect of prior/regularizer goes to zero.
  - Unlike with MLE, the choice of σ changes the MAP solution for these models.

Common Linear Regressions and GLMs

Likelihood	Prior	Posterior	Name
Gaussian	Uniform	Point	Least squares
Student	Uniform	Point	Robust regression
Laplace	Uniform	Point	Robust regression
Gaussian	Gaussian	Point	Ridge
Gaussian	Laplace	Point	Lasso
Gaussian	Gauss-Gamma	Gauss-Gamma	Bayesian lin. reg

- For other y such as counts, we may use e.g., Poisson regression, negative binomial regression.
- We may use binomial regression for proportional data, etc.
- If you want to learn more, you can read “Generalized Linear Models” and the “Exponential Family” distributions.

Next Topic: Wrapping up Part 3

End of Part 3: Key Concepts

- Linear models predict based on linear combination(s) of features:

$$w^T x_i = w_1 x_{i1} + w_2 x_{i2} + \cdots + w_d x_{id}$$

- We model non-linear effects using a change of basis:
  - Replace d-dimensional x_i with k-dimensional z_i and use $v^T z_i$.
  - Examples include polynomial basis and (non-parametric) RBFs.

- Regression is supervised learning with continuous labels.
  - Logical error measure for regression is squared error:

$$f(w) = \frac{1}{2}\|Xw - y\|^2$$

  - Can be solved as a system of linear equations.

End of Part 3: Key Concepts

- Gradient descent finds local minimum of smooth objectives.
  - Converges to a global optimum for convex functions.
  - Can use smooth approximations (Huber, log-sum-exp)
- Stochastic gradient methods allow huge/infinite 'n'.
  - Though very sensitive to the step-size.
- Kernels let us use similarity between examples, instead of features.
  - Lets us use some exponential- or infinite-dimensional features.
- Feature selection is a messy topic.
  - Classic method is forward selection based on L0-norm.
  - L1-regularization simultaneously regularizes and selects features.

End of Part 3: Key Concepts

- We can reduce over-fitting by using regularization:

$$f(w) = \frac{1}{2}\|Xw - y\|^2 + \frac{\lambda}{2}\|w\|^2$$

- Squared error is not always right measure:
  - Absolute error is less sensitive to outliers.
  - Logistic loss and hinge loss are better for binary y_i.
  - Softmax loss is better for multi-class y_i.
- MLE/MAP perspective:
  - We can view loss as log-likelihood and regularizer as log-prior.
  - Allows us to define losses based on probabilities.

The Story So Far…

- Part 1: Supervised Learning.
  - Methods based on counting and distances.
- Part 2: Unsupervised Learning.
  - Methods based on counting and distances.
- Part 3: Supervised Learning (just finished).
  - Methods based on linear models and gradient descent.
- Part 4: Unsupervised Learning.
  - Methods based on linear models and gradient descent.

Summary

- Maximum likelihood estimation viewpoint of common models.
  - The choice of likelihood corresponds to the choice of loss: Gaussian/Laplace likelihood leads to squared/absolute error.

- MAP estimation directly models $p(w \mid X, y)$.
  - The choice of prior corresponds to the choice of regularizer: Gaussian/Laplace prior leads to L2/L1-regularization.

- Next time:
  - What 'parts' are your personality made of?

Regularizing Other Models

- We can view priors in other models as regularizers.

- Remember the problem with MLE for naïve Bayes:
  - The MLE of p('lactase' = 1| 'spam') is: count(spam,lactase)/count(spam).
  - But this caused problems if count(spam,lactase) = 0.

- Our solution was Laplace smoothing:
  - Add "+1" to our estimates: (count(spam,lactase)+1)/(counts(spam)+2).
  - This corresponds to a "Beta" prior so Laplace smoothing is a regularizer.

Why do we care about MLE and MAP?

- Unified way of thinking about many of our tricks?
  - Probabilistic interpretation of logistic loss.
  - Laplace smoothing and L2-regularization are doing the same thing.

- Remember our two ways to reduce overfitting in complicated models:
  - Model averaging (ensemble methods).
  - Regularization (linear models).

- "Fully"-Bayesian methods (CPSC 440) combine both of these.
  - Average over all models, weighted by posterior (including regularizer).
  - Can use extremely-complicated models without overfitting.

Losses for Other Discrete Labels

- MLE/MAP gives loss for classification with basic labels:
  - Least squares and absolute loss for regression.
  - Logistic regression for binary labels {“spam”, “not spam”}.
  - Softmax regression for multi-class {“spam”, “not spam”, “important”}.

- But MLE/MAP lead to losses with other discrete labels (bonus):
  - Ordinal: {1 star, 2 stars, 3 stars, 4 stars, 5 stars}.
  - Counts: 602 ‘likes’.
  - Survival rate: 60% of patients were still alive after 3 years.
  - Unbalanced classes: 99.9% of examples are classified as +1.
- Define likelihood of labels, and use NLL as the loss function.

- We can also use ratios of probabilities to define more losses (bonus):
  - Binary SVMs, multi-class SVMs, and “pairwise preferences” (ranking) models.

Discussion: Least Squares and Gaussian Assumption

- Classic justifications for the Gaussian assumption underlying least squares:
  - Your noise might really be Gaussian. (It probably isn't, but maybe it's a good enough approximation.)
  - The central limit theorem (CLT) from probability theory. (If you add up enough IID random variables, the estimate of their mean converges to a Gaussian distribution.)

- I think the CLT justification is wrong as we've never assumed that the x_{ij} are IID across 'j' values. We only assumed that the examples x_i are IID across 'i' values, so the CLT implies that our estimate of 'w' would be a Gaussian distribution under different samplings of the data, but this says nothing about the distribution of y_i given w^Tx_i.

- On the other hand, there are reasons *not* to use a Gaussian assumption, like it's sensitivity to outliers. This was (apparently) what lead Laplace to propose the Laplace distribution as a more robust model of the noise.
- The "student t" distribution (published anonymously by Gosset while working at the Guiness beer company) is even more robust, but doesn't lead to a convex objective.

Binary vs. Multi-Class Logistic

- How does multi-class logistic generalize the binary logistic model?
- We can re-parameterize softmax in terms of (k-1) values of z_c:

$$p(y \mid z_1, z_2, \dots, z_{k-1}) = \frac{\exp(z_y)}{1 + \sum_{c=1}^{k-1} \exp(z_c)} \text{ if } y \neq k \quad \text{and} \quad p(y \mid z_1, z_2, \dots, z_{k-1}) = \frac{1}{1 + \sum_{c=1}^{k-1} \exp(z_c)} \text{ if } y = k$$

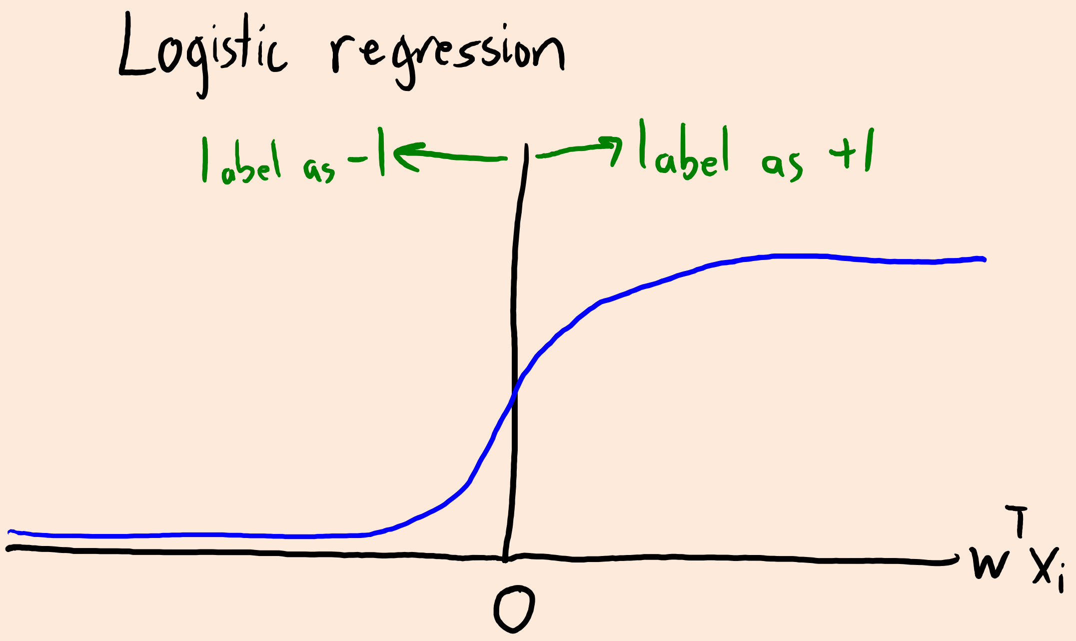
  – This is due to the "sum to 1" property (one of the z_c values is redundant).
  – So if k=2, we don't need a z_2 and only need a single 'z'.
  – Further, when k=2 the probabilities can be written as:

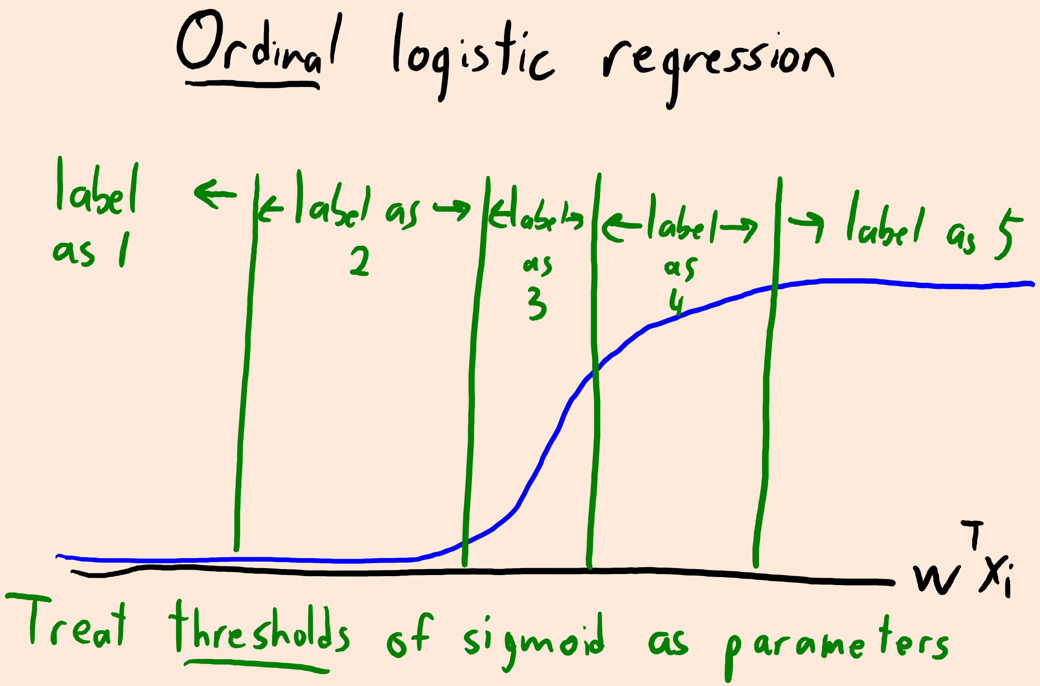
$$p(y=1 \mid z) = \frac{\exp(z)}{1+\exp(z)} = \frac{1}{1+\exp(-z)} \qquad p(y=2 \mid z) = \frac{1}{1+\exp(z)}$$

  – Renaming '2' as '-1', we get the binary logistic regression probabilities.

Ordinal Labels

- Ordinal data: categorical data where the order matters:
  - Rating hotels as {'1 star', '2 stars', '3 stars', '4 stars', '5 stars'}.
  - Softmax would ignore order.
- Can use 'ordinal logistic regression'.





Count Labels

- Count data: predict the number of times something happens.
  - For example, y_i = "602" Facebook likes.
- Softmax requires finite number of possible labels.
- We probably don't want separate parameter for '654' and '655'.
- Poisson regression: use probability from Poisson count distribution.
  - Many variations exist, a lot of people think this isn't the best likelihood.

Censored Survival Analysis (Cox Partial Likelihood)

- Censored survival analysis:
  - Target y_i is last time at which we know person is alive.
    - But some people are still alive (so they have the same y_i values).
    - The y_i values (time at which they die) are "censored".
  - We use v_i=0 is they are still alive and otherwise we set v_i = 1.

- Cox partial likelihood assumes "instantaneous" rate of dying depends on x_i but not on total time they've been alive (not that realistic). Leads to likelihood of the "censored" data of the form:

$$p(y_i, v_i \mid x_i, w) = \exp(v_i w^T x_i)\exp(-y_i \exp(w^T x_i))$$

- There are many extensions and alternative likelihoods.

Other Parsimonious Parameterizations

- Sigmoid isn't the way to model a binary $p(y_i \mid x_i, w)$:
  - Probit (uses CDF of normal distribution, very similar to logistic).
  - Noisy-Or (simpler to specify probabilities by hand).
  - Extreme-value loss (good with class imbalance).
  - Cauchit, Gosset, and many others exist…

Unbalanced Training Sets

- Consider the case of binary classification where your training set has 99% class -1 and only 1% class +1.
  - This is called an "unbalanced" training set
- Question: is this a problem?
- Answer: it depends!
  - If these proportions are representative of the test set proportions, and you care about both types of errors equally, then "no" it's not a problem.
    - You can get 99% accuracy by just always predicting -1, so ML can only help with the 1%.
  - But it's a problem if the test set is not like the training set (e.g. your data collection process was biased because it was easier to get -1's)
  - It's also a problem if you care more about one type of error, e.g. if mislabeling a +1 as a -1 is much more of a problem than the opposite
    - For example if +1 represents "tumor" and -1 is "no tumor"

Unbalanced Training Sets

- This issue comes up a lot in practice!
- How to fix the problem of unbalanced training sets?
  – Common strategy is to build a "weighted" model:
    - Put higher weight on the training examples with y_i=+1.

$$f(w) = \sum_{i=1}^{n} v_i \log(1+\exp(-y_i w^T x_i))$$

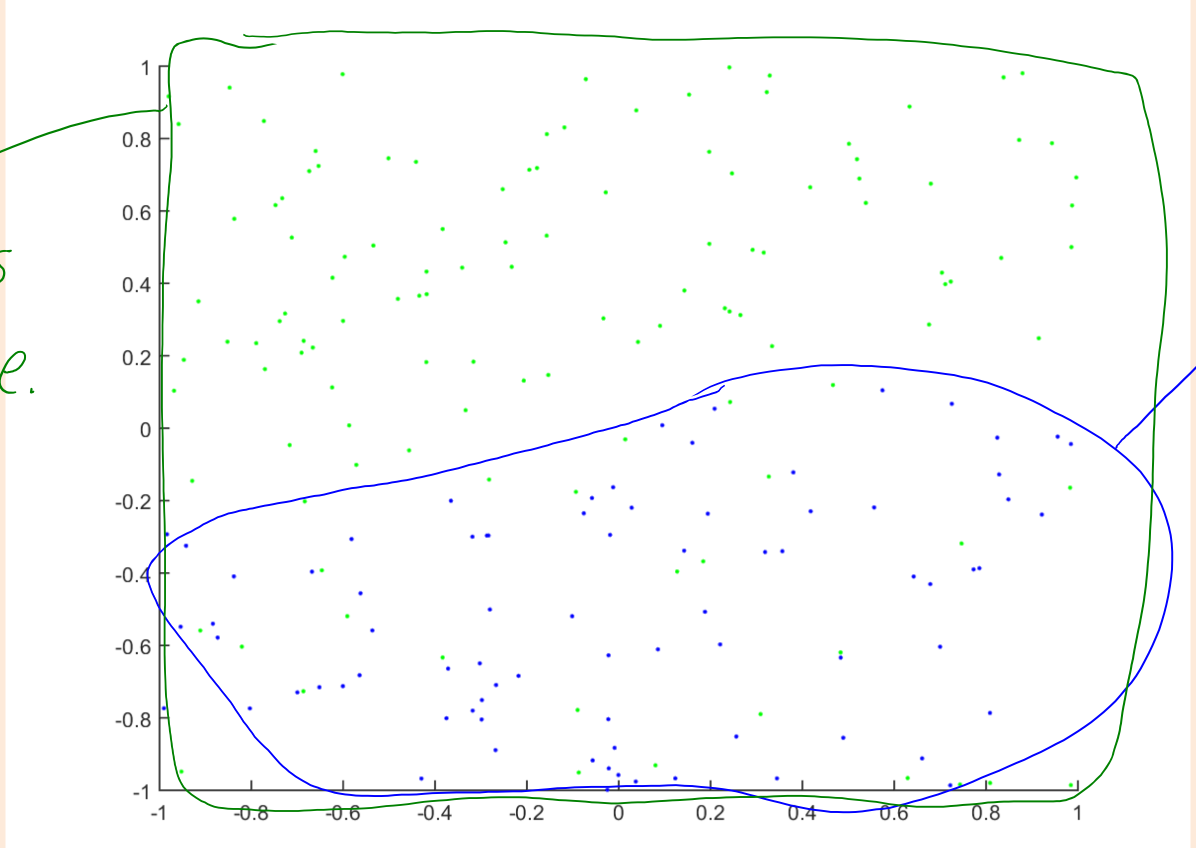
Make this weight bigger for under-represented class

    - This is equivalent to replicating those examples in the training set.
    - You could also subsample the majority class to make things more balanced.
    - Boostrap: create a dataset of size 'n' where n/2 are sampled from +1, n/2 from -1.
  – Another approach is to try to make "fake" data to fill in minority class.
  – Another option is to change to an asymmetric loss function (next slides) that penalizes one type of error more than the other.
  – Some discussion of different methods here.

Unbalanced Data and Extreme-Value Loss

- Consider binary case where:
  - One class overwhelms the other class ('unbalanced' data).
  - Really important to find the minority class (e.g., minority class is tumor).

"majority" class
is everywhere.



important "minority"
class

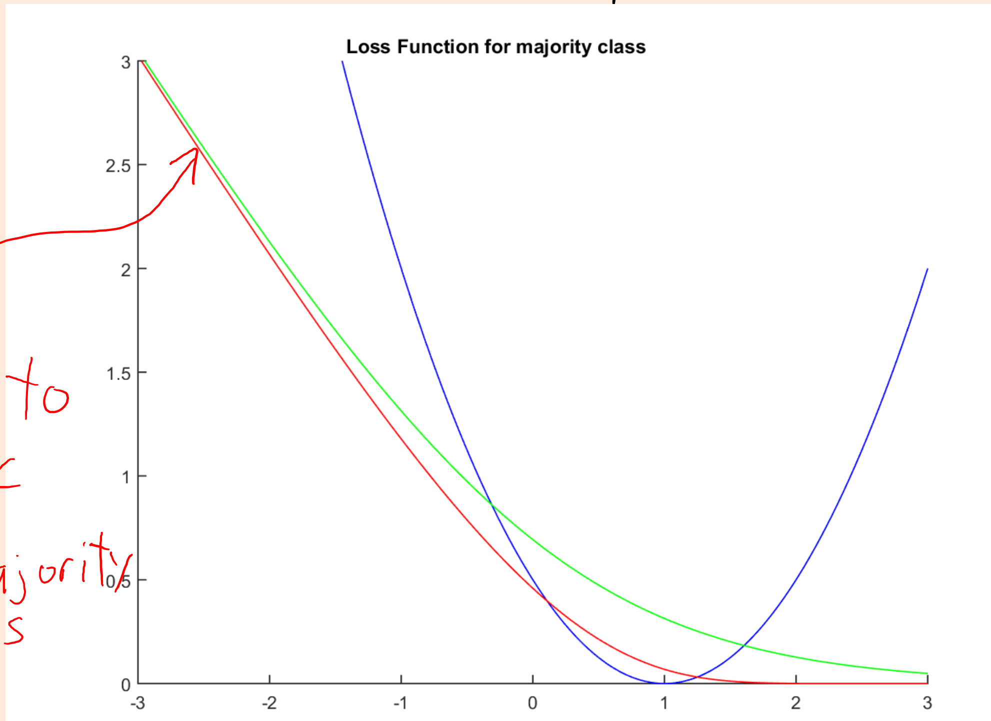
Unbalanced Data and Extreme-Value Loss

- Extreme-value distribution:

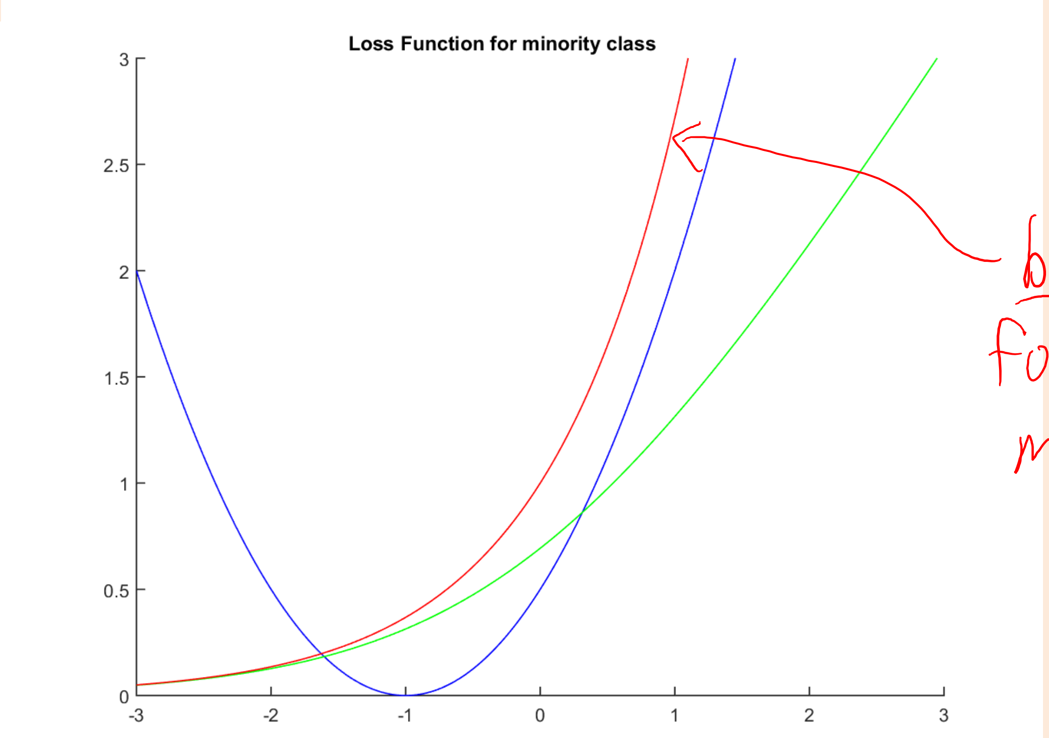
$$p(y_i = +1 \mid \hat{y}_i) = 1 - \exp(-\exp(\hat{y}_i)) \quad [+1 \text{ is majority class}]$$

To make it a probability, $p(y_i = -1 \mid \hat{y}_i) = \exp(-\exp(\hat{y}_i))$

asymmetric



Similar to logistic for majority class



big penalty for getting minority class wrong.

Unbalanced Data and Extreme-Value Loss

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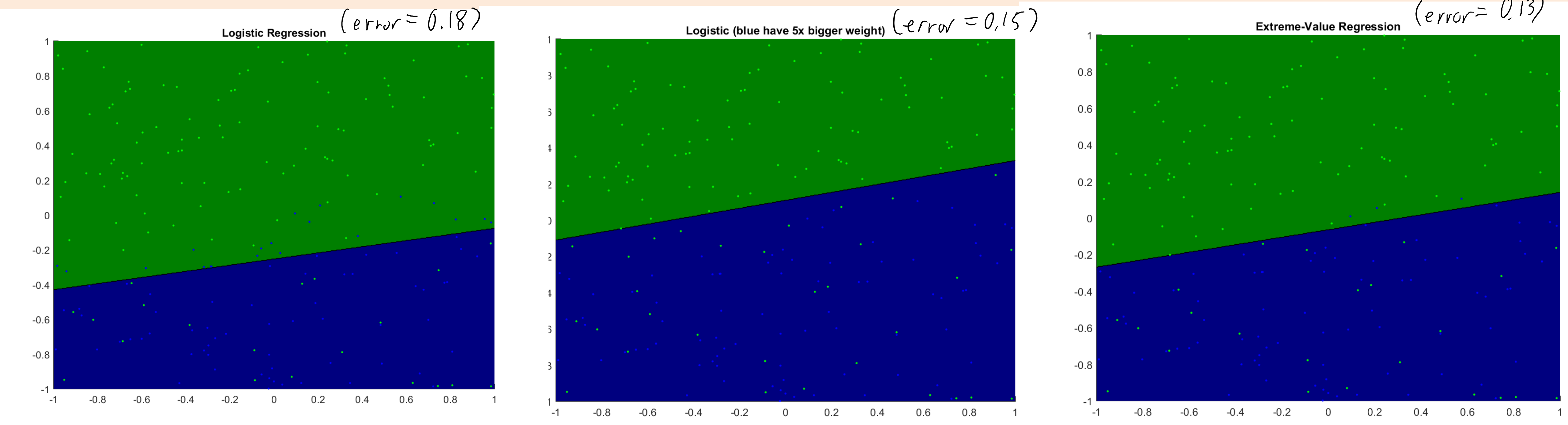

Loss Functions from Probability Ratios

- We've seen that loss functions can come from probabilities:
  - Gaussian => squared loss, Laplace => absolute loss, sigmoid => logistic.
- Most other loss functions can be derived from probability ratios.
  - Example: sigmoid => hinge.

$$p(y_i \mid x_i, w) = \frac{1}{1 + \exp(-y_i w^T x_i)} = \frac{\exp(\frac{1}{2} y_i w^T x_i)}{\underbrace{\exp(\frac{1}{2} y_i w^T x_i) + \exp(-\frac{1}{2} y_i w^T x_i)}_{\text{Same normalizing constant for } y_i = +1 \text{ and } x_i = -1}} \propto \exp(\tfrac{1}{2} y_i w^T x_i)$$

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$$p(y_i \mid x_i, w) \propto \exp\left(\frac{1}{2} y_i w^T x_i\right)$$

To classify y_i correctly, it's sufficient to have $\underbrace{\frac{p(y_i \mid x_i, w)}{p(-y_i \mid x_i, w)}} \geq \beta$ for some 'β' > 1

Notice that normalizing constant doesn't matter:

$$\frac{\exp\left(\frac{1}{2} y_i w^T x_i\right)}{\exp\left(-\frac{1}{2} y_i w^T x_i\right)} \geq \beta$$

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$$p(y_i \mid x_i, w) \propto \exp\left(\tfrac{1}{2} y_i w^T x_i\right)$$

We need: $\dfrac{\exp(\frac{1}{2} y_i w^T x_i)}{\exp(-\frac{1}{2} y_i w^T x_i)} \geq \beta$

Take log:

$$\log\left(\frac{\exp(\frac{1}{2} y_i w^T x_i)}{\exp(-\frac{1}{2} y_i w^T x_i)}\right) \geq \log(\beta) \iff \frac{1}{2} y_i w^T x_i + \frac{1}{2} y_i w^T x_i \geq \log(\beta)$$

$$\Updownarrow$$

$y_i w^T x_i \geq 1$ (if we choose $\log(\beta) = 1$)

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- Most other loss functions can be derived from probability ratios.
  - Example: sigmoid => hinge.

$p(y_i | x_i, w) \propto \exp(\frac{1}{2} y_i w^T x_i)$

We need: $\frac{\exp(\frac{1}{2} y_i w^T x_i)}{\exp(-\frac{1}{2} y_i w^T x_i)} \geq \beta$

Or equivalently:

$y_i w^T x_i \geq 1$ (for $\beta = \exp(1)$)

Define a loss function by amount of constraint violation:

$\max\{0, 1 - y_i w^T x_i\}$

when $1 - y_i w^T x_i \leq 0$ when $1 - y_i w^T x_i \geq 0$

We get SVMs by looking at regularized average loss:

$f(w) = \sum_{i=1}^{n} \max\{0, 1 - y_i w^T x_i\} + \frac{\lambda}{2} \|w\|^2$

Loss Functions from Probability Ratios

- General approach for defining losses using probability ratios:
  1. Define constraint based on probability ratios.
  2. Minimize violation of logarithm of constraint.
- Example: softmax => multi-class SVMs.

Assume: $p(y_i = c \mid x_i, w) \propto \exp(w_c^T x_i)$

Want: $\dfrac{p(y_i \mid x_i, w)}{p(y_i = c' \mid x_i, w)} \geq \beta$ for all c' and some $\beta > 1$

For $\beta = \exp(1)$ equivalent to

$$w_{y_i}^T x_i - w_{c'}^T x_i \geq 1$$

for all $c' \neq y_i$

Option 1: penalize all violations:

$$\sum_{c'=1}^{K} \max\{0, 1 - w_{y_i}^T x_i + w_{c'}^T x_i\}$$

Option 2: penalize only max violation:

$$\max_{c' \neq c} \{\max\{0, 1 - w_{y_i}^T x_i + w_{c'}^T x_i\}\}$$

Supervised Ranking with Pairwise Preferences

- Ranking with pairwise preferences:
  - We aren't given any explicit y_i values.
  - Instead we're given list of objects (i,j) where $y_i > y_j$.

Assume $p(y_i \mid X, w) \propto \exp(w^T x_i)$ is probability that object 'i' has highest rank.

Want: $\frac{p(y_i \mid X, w)}{p(y_j \mid X, w)} \geq \beta$ for all preferences (i,j)

For $\beta = \exp(1)$ equivalent to

$$w^T x_i - w^T x_j \geq 1$$

for preferences (i,j)

We can use $f(w) = \sum_{(i,j) \in R} \max\{0, 1 - w^T x_i + w^T x_j\}$

This approach can also be used to define losses for total/partial orderings. (but this information is hard to get)