ORIE 4741: Learning with Big Messy Data

Loss functions

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Outline

Maximum likelihood estimation

Regression

Classification

The prediction space

Multiclass classification

Ordinal regression

Beyond linear models
Probabilistic setup

- suppose you know a function \( p : \mathbb{R} \rightarrow [0, 1] \) so that
  \[ P(y_i = y \mid x_i, w) = p(y; x_i, w) \]
- for example, if \( y_i = w^T x_i + \varepsilon_i, \varepsilon_i \sim \mathcal{N}(0, \sigma^2) \), then
  \[ P(y_i = y \mid x_i, w) \sim \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(y_i - w^T x_i)^2}{2\sigma^2}\right) \]
- likelihood of data given parameter \( w \) is
  \[ L(D; w) = \prod_{i=1}^{n} P(y_i = y \mid x_i, w) \]
- for example, for linear model with Gaussian error,
  \[ L(D; w) \sim \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(y_i - w^T x_i)^2}{2\sigma^2}\right) \]
Maximum Likelihood Estimation (MLE)

MLE: choose \( w \) to maximize \( L(D; w) \)

- likelihood

\[
L(D; w) = \prod_{i=1}^{n} p(y_i; x_i, w)
\]

- negative log likelihood

\[
\ell(D; w) = -\log L(D; w)
\]

- maximize \( L(D; w) \) \( \iff \) minimize \( \ell(D; w) \)
Example: Maximum Likelihood Estimation (MLE)

- for linear model with Gaussian error,

\[
\ell(D; w) \sim -\log \left( \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi\sigma^2}} \exp \left( -\frac{(y_i - w^T x_i)^2}{2\sigma^2} \right) \right)
\]

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

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

\[
= \frac{n}{2} \log(2\pi\sigma^2) + \sum_{i=1}^{n} \frac{1}{2\sigma^2} (y_i - w^T x_i)^2
\]

\[
= \frac{n}{2} \log(2\pi\sigma^2) + \frac{1}{2\sigma^2} \sum_{i=1}^{n} (y_i - w^T x_i)^2
\]

- so maximize \( L(D; w) \iff \text{minimize} \sum_{i=1}^{n} (y_i - w^T x_i)^2 \)
what if I have beliefs about what $w$ should be before I begin?

- $w$ should be small
- $w$ should be sparse
- $w$ should be nonnegative

**idea:** impose **prior** on $w$ to specify

$$P(w)$$

before seeing any data
Maximum-a-posteriori estimation

after I see data, compute posterior probability

\[ P(D; w) = P(D \mid w) P(w) \]

maximum a posteriori (MAP estimation): choose \( w \) to maximize posterior probability
Maximum-a-posteriori estimation

after I see data, compute posterior probability

\[ P(D; w) = P(D | w) P(w) \]

maximum a posteriori (MAP estimation): choose \( w \) to maximize posterior probability

n.b. this is not what a true Bayesian would do
(see, e.g., Bishop, Pattern Recognition and Machine Learning)
Ridge regression: interpretation as MAP estimator

- prior probability of model $w \sim \mathcal{N}(0, I_d)$
- noise $\epsilon_i \sim \mathcal{N}(0, \sigma^2)$, $i = 1, \ldots, n$
- response $y_i = w^T x_i + \epsilon_i$, $i = 1, \ldots, n$

\[
P(D; w) = P(D \mid w) P(w)
\]
\[
\approx \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(\frac{-(y_i - w^T x_i)^2}{2\sigma^2}\right) \prod_{i=1}^{d} \frac{1}{\sqrt{2\pi}} \exp\left(\frac{-w_i^2}{2}\right)
\]
\[
= (2\pi\sigma^2)^{-\frac{n}{2}} \prod_{i=1}^{n} \left(\exp\left(\frac{-(y_i - w^T x_i)^2}{2\sigma^2}\right)\right) (2\pi)^{-\frac{d}{2}} \prod_{i=1}^{d} \left(\exp\left(\frac{-w_i^2}{2}\right)\right)
\]
\[
\ell(D; w) = -\log(P(D; w))
\]
\[
= \frac{n}{2} \log(2\pi\sigma^2) + \frac{d}{2} \log(2\pi) + \frac{1}{2\sigma^2} \sum_{i=1}^{n} (y_i - w^T x_i)^2 + \frac{1}{2} \sum_{i=1}^{d} w_i^2
\]
Ridge regression: interpretation as MAP estimator

- prior probability of model $w \sim \mathcal{N}(0, I_d)$
- noise $\epsilon_i \sim \mathcal{N}(0, \sigma^2)$, $i = 1, \ldots, n$
- response $y_i = w^T x_i + \epsilon_i$, $i = 1, \ldots, n$

$$
\mathbb{P}(D; w) = \mathbb{P}(D \mid w) \mathbb{P}(w)
\approx \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(\frac{-(y_i - w^T x_i)^2}{2\sigma^2}\right) \prod_{i=1}^{d} \frac{1}{\sqrt{2\pi}} \exp\left(\frac{-w_i^2}{2}\right)
= (2\pi\sigma^2)^{-\frac{n}{2}} \prod_{i=1}^{n} \left(\exp\left(\frac{-(y_i - w^T x_i)^2}{2\sigma^2}\right)\right) (2\pi)^{-\frac{d}{2}} \prod_{i=1}^{d} \left(\exp\left(\frac{-w_i^2}{2}\right)\right)
$$

$$
\ell(D; w) = -\log(\mathbb{P}(D; w))
= \frac{n}{2} \log(2\pi\sigma^2) + \frac{d}{2} \log(2\pi) + \frac{1}{2\sigma^2} \sum_{i=1}^{n} (y_i - w^T x_i)^2 + \frac{1}{2} \sum_{i=1}^{d} w_i^2
$$

... aha! and we have ridge regression with $\lambda = \sigma^2$
Recap: regularized empirical risk minimization

choose model by solving

\[
\text{minimize } \frac{1}{n} \sum_{i=1}^{n} \ell(x_i, y_i; w) + r(w)
\]

with variable \( w \in \mathbb{R}^d \)

- parameter vector \( w \in \mathbb{R}^d \)
- loss function \( \ell : \mathcal{X} \times \mathcal{Y} \times \mathbb{R}^d \to \mathbb{R} \)
- regularizer \( r : \mathbb{R}^d \to \mathbb{R} \)
Recap: regularized empirical risk minimization

choose model by solving

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why?

- want to minimize the risk \( \mathbb{E}_{(x,y) \sim \mathcal{P}} \ell(x, y; w) \)
- approximate it by the empirical risk \( \sum_{i=1}^{n} \ell(x, y; w) \)
- add regularizer to help model generalize
Loss functions

what kind of loss functions should we use?
depends on type of data

- real
- boolean
- ordinal
- nominal
- ...

and on noise in data

- small?
- large but sparse?
- from some probabilistic model?
- ...


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Beyond linear models
Loss functions for real-valued data

- quadratic
- $\ell_1$
- huber
- quantile
- ...
Least squares regression finds the mean

least squares ($\ell_2$) regression:

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

special case: no covariates. what is

$$\arg\min_w \frac{1}{n} \sum_{i=1}^{n} (y_i - w)^2?$$
Least squares regression finds the mean

Least squares ($\ell_2$) regression:

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

special case: no covariates. what is

$$\text{argmin}_w \quad \frac{1}{n} \sum_{i=1}^{n} (y_i - w)^2$$?

A: mean($y$)!
\( \ell_1 \) regression finds the median

\( \ell_1 \) regression:

\[
\text{minimize } \frac{1}{n} \sum_{i=1}^{n} |y_i - w^T x_i| + r(w)
\]

special case: no covariates. what is

\[
\text{argmin}_w \frac{1}{n} \sum_{i=1}^{n} |y_i - w|?
\]
$\ell_1$ regression finds the median

$\ell_1$ regression:

\[
\text{minimize } \frac{1}{n} \sum_{i=1}^{n} |y_i - w^T x_i| + r(w)
\]

special case: no covariates. what is

\[
\arg\min_w \frac{1}{n} \sum_{i=1}^{n} |y_i - w|
\]

- if $pn$ of the $y_i$’s are bigger than $w$,
- then as $w$ increases to $w + \delta$,
- $\frac{1}{n} \sum_{i:y_i > w} |y_i - w|$ decreases by $p\delta$
- $\frac{1}{n} \sum_{i:y_i < w} |y_i - w|$ increases by $(1 - p)\delta$
- if $p = \frac{1}{2}$, objective stays the same
\( \ell_1 \) regression finds the median

\( \ell_1 \) regression:

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\text{minimize} \quad \frac{1}{n} \sum_{i=1}^{n} |y_i - w^T x_i| + r(w)
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\[
\arg\min_{w} \frac{1}{n} \sum_{i=1}^{n} |y_i - w|?
\]

- if \( pn \) of the \( y_i \)'s are bigger than \( w \),
- then as \( w \) increases to \( w + \delta \),
- \( \frac{1}{n} \sum_{i:y_i > w} |y_i - w| \) decreases by \( p\delta \)
- \( \frac{1}{n} \sum_{i:y_i < w} |y_i - w| \) increases by \( (1 - p)\delta \)
- if \( p = \frac{1}{2} \), objective stays the same

**A:** \( w = \text{median}(y) \)!
Huber regression

Huber regression:

$$\text{minimize} \quad \frac{1}{n} \sum_{i=1}^{n} \text{huber}(y_i - w^T x_i) + r(w)$$

where we define the Huber function

$$\text{huber}(z) = \begin{cases} 
\frac{1}{2}z^2 & |z| \leq 1 \\
|z| - \frac{1}{2} & |z| > 1 
\end{cases}$$
Huber regression

Huber regression:

\[
\text{minimize} \quad \frac{1}{n} \sum_{i=1}^{n} \text{huber}(y_i - w^T x_i) + r(w)
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where we define the Huber function

\[
\text{huber}(z) = \begin{cases} 
\frac{1}{2}z^2 & |z| \leq 1 \\
|z| - \frac{1}{2} & |z| > 1 
\end{cases}
\]

Huber decomposes error into a small (Gaussian) part and a large (robust) part

\[
\text{huber}(x) = \inf_{s+n=x} |s| + \frac{1}{2}n^2
\]

(proof: take derivative)
Robust statistics

Q: when would you want to use a robust loss function?
Robust statistics

Q: when would you want to use a robust loss function?
A: for robustness in the presence of large outliers
  ▶ large, infrequent sensor malfunctions
  ▶ people lying on surveys
  ▶ anything that’s not a sum of small iid random variables
define the positive and negative parts of $x \in \mathbb{R}$

$$(x)_+ = \max(x, 0), \quad (x)_- = \max(-x, 0)$$
Quantile regression finds the right quantile

Quantile regression: for $\alpha \in (0, 1)$,

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

special case: no covariates. what is

$$\text{argmin}_w \frac{1}{n} \sum_{i=1}^{n} \alpha (y_i - w)_+ + (1 - \alpha) (y_i - w)_-?$$
Quantile regression finds the right quantile

Quantile regression: for \( \alpha \in (0, 1) \),

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\[
\arg\min_w \frac{1}{n} \sum_{i=1}^{n} \alpha (y_i - w)_+ + (1 - \alpha) (y_i - w)_- 
\]

- if \( pn \) of the \( y_i \)’s are bigger than \( w \),
- then as \( w \) increases to \( w + \delta \),
- first term decreases by \( p \alpha \delta \)
- second term increases by \( (1 - p)(1 - \alpha)\delta \)
- so if \( p = 1 - \alpha \), objective stays the same
Quantile regression finds the right quantile

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\textbf{A: } w \text{ is the } \alpha \text{th quantile of } y!
Demo: robust regression
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Beyond linear models
Loss functions for classification

suppose \( \mathcal{Y} = \{-1, 1\} \). let \( \ell(x, y; w) = \)
Loss functions for classification

suppose $\mathcal{Y} = \{-1, 1\}$. let $\ell(x, y; w) =$

- 0-1 loss $\mathbb{1}(y \neq \text{sign}(w^T x))$
- quadratic loss $(y - w^T x)^2$
- hinge loss $(1 - yw^T x)_+$
- logistic loss $\log(1 + \exp(-w^T x))$
- ...

trade off dislike of false positives vs false negatives
Loss functions for classification

\[ y = 1 \]
Loss functions for classification

\[ y = 1 \]
Loss functions for classification

\[ y = -1 \]
Loss functions for classification

\[ y = -1 \]
Losses for classification

- hinge loss
  \[ \ell_{\text{hinge}}(x, y; w) = (1 - yw^T x)_+ \]

- logistic loss
  \[ \ell_{\text{logistic}}(x, y; w) = \log(1 + \exp\left(-yw^T x\right)) \]
Logistic loss: interpretation

- logistic function maps real numbers to probabilities
  \[ \text{logistic}(u) = \frac{\exp(u)}{1 + \exp(u)} = \frac{1}{1 + \exp(-u)} \]

- suppose that given \( w^T x \), \( y \) is a Bernoulli random variable
  \[ y = \begin{cases} 
    1 & \text{with prob } \text{logistic}(w^T x) \\
    -1 & \text{with prob } (1 - \text{logistic}(w^T x)) = \text{logistic}(-w^T x) 
  \end{cases} \]

  notice \( \mathbb{P}(y|w, x) = \text{logistic}(yw^T x) \)

- logistic loss is \(-\log \mathbb{P}(y|w, x)\)
  \[
  \ell_{\text{logistic}}(x, y; w) = -\log(\text{logistic}(yw^T x)) \\
  = -\log \left( \frac{1}{1 + \exp(-yw^T x)} \right) \\
  = \log \left( 1 + \exp(-yw^T x) \right)
  \]
Hinge loss: interpretation

suppose we solve

\[
\begin{align*}
\text{minimize} & \quad \|w\|^2 \\
\text{subject to} & \quad \sum_{i=1}^n \ell_{\text{hinge}}(x_i, y_i; w) = 0
\end{align*}
\]

(recall \( \ell_{\text{hinge}}(x, y; w) = (1 - yw^T x)_+ \))

- solution classifies every point correctly, with a safety margin: for every \( i = 1, \ldots, n, \)

\[
1 \leq y_i w^T x_i
\]

- compare to perceptron
- as \( \|w\| \) gets smaller, the distance \( \Delta x \) to classification boundary gets bigger
  - let difference between two lines be \( \Delta x = \alpha w \)
  - suppose \( w^T x^0 = 0, \ w^T x^1 = 1, \) and \( x^1 = x^0 + \Delta x \)
  - compute (by subtraction) \( 1 = w^T \Delta x = w^T (\alpha w) = \alpha \|w\|^2 \)
  - so \( \|\Delta x\| = \|\alpha w\| = \alpha \|w\| = 1/\|w\| \)
Hinge loss: interpretation

solid line: $w^T x = 0$; dashed lines: $w^T x = \pm 1$
Support Vector Machine (SVM)

Now instead solve the support vector machine problem (SVM)

\[
\text{minimize} \quad \sum_{i=1}^{n} \ell_{\text{hinge}}(x_i, y_i; w) + \lambda \| w \|^2
\]

- allows some mistakes
- trades off the severity of mistakes with the safety margin
Loss functions for classification

suppose $\mathcal{Y} = \{-1, 1\}$. let $\ell(x, y; w) =$
Loss functions for classification

suppose \( \mathcal{Y} = \{-1, 1\} \). let \( \ell(x, y; w) = \)

- 0-1 loss \( \mathbb{1}(y \neq \text{sign}(w^T x)) \)
- quadratic loss \( (y - w^T x)^2 \)
- hinge loss \( (1 - yw^T x)_+ \)
- logistic loss \( \log(1 + \exp(-w^T x)) \)
- ...

trade off dislike of false positives vs false negatives
Loss functions for classification

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trade off dislike of false positives vs false negatives

properties:

- continuous?
suppose $\mathcal{Y} = \{-1, 1\}$. let $\ell(x, y; w) =$

- 0-1 loss $\mathbb{1}(y \neq \text{sign}(w^T x))$
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trade off dislike of false positives vs false negatives

properties:

- continuous? quadratic, hinge, logistic
- differentiable?
Loss functions for classification

suppose \( \mathcal{Y} = \{-1, 1\} \). let \( \ell(x, y; w) = \)

- 0-1 loss \( \mathbb{1}(y \neq \text{sign}(w^T x)) \)
- quadratic loss \( (y - w^T x)^2 \)
- hinge loss \( (1 - yw^T x)_+ \)
- logistic loss \( \log(1 + \exp(-w^T x)) \)
- ...

trade off dislike of false positives vs false negatives

properties:

- continuous? quadratic, hinge, logistic
- differentiable? quadratic, logistic
- insensitive to outliers?
Loss functions for classification

suppose $\mathcal{Y} = \{-1, 1\}$. let $\ell(x, y; w) =$

- 0-1 loss $\mathbb{I}(y \neq \text{sign}(w^T x))$
- quadratic loss $(y - w^T x)^2$
- hinge loss $(1 - yw^T x)_+$
- logistic loss $\log(1 + \exp(-w^T x))$
- ... 

trade off dislike of false positives vs false negatives

properties:

- continuous? quadratic, hinge, logistic
- differentiable? quadratic, logistic
- insensitive to outliers? 0-1
- sensitive to outliers?
Loss functions for classification

suppose \( \mathcal{Y} = \{-1, 1\} \). let \( \ell(x, y; w) = \)

- 0-1 loss \( \mathbb{1}(y \neq \text{sign}(w^T x)) \)
- quadratic loss \( (y - w^T x)^2 \)
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- ... 

trade off dislike of false positives vs false negatives

properties:

- continuous? quadratic, hinge, logistic
- differentiable? quadratic, logistic
- insensitive to outliers? 0-1
- sensitive to outliers? quadratic
- quadratic?
Loss functions for classification

suppose \( \mathcal{Y} = \{-1, 1\} \). let \( \ell(x, y; w) = \)

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- ... 

trade off dislike of false positives vs false negatives 

properties:

- continuous? quadratic, hinge, logistic
- differentiable? quadratic, logistic
- insensitive to outliers? 0-1
- sensitive to outliers? quadratic
- quadratic? quadratic
- probabilistic interpretation?
Loss functions for classification

Suppose \( \mathcal{Y} = \{ -1, 1 \} \). Let \( \ell(x, y; w) = \)

- 0-1 loss \( 1(y \neq \text{sign}(w^T x)) \)
- quadratic loss \( (y - w^T x)^2 \)
- hinge loss \( (1 - yw^T x)_+ \)
- logistic loss \( \log(1 + \exp(-w^T x)) \)

... trade off dislike of false positives vs false negatives

Properties:

- Continuous? quadratic, hinge, logistic
- Differentiable? quadratic, logistic
- Insensitive to outliers? 0-1
- Sensitive to outliers? quadratic
- Quadratic? quadratic
- Probabilistic interpretation? logistic
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Beyond linear models
Recap linear models

- input space $\mathbb{R}^d$
- output space $\mathcal{Y}$
  - regression: $\mathcal{Y} = \mathbb{R}$
  - classification: $\mathcal{Y} = \{-1, 1\}$
- parameter space $\mathbb{R}^d$
- hypothesis class $h \in \mathcal{H}$

$$\mathcal{H} = \{ h : \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R} \}$$

e.g., $\mathcal{H} = \{ h : h(x; w) = w^T x \}$

- rewrite the objective using this notation

$$\text{minimize} \quad \frac{1}{n} \sum_{i=1}^{n} \ell(y_i, h(x_i; w)) + r(w)$$

with variable $w \in \mathbb{R}^d$
The prediction space

- input space $\mathcal{X}$
- output space $\mathcal{Y}$
- parameter space $\mathcal{W}$
- prediction space $\mathcal{Z}$
- hypothesis class $h \in \mathcal{H}$

$$\mathcal{H} = \{ h : \mathcal{X} \times \mathcal{W} \to \mathcal{Z} \}$$

- rewrite the objective using this notation

$$\text{minimize} \quad \frac{1}{n} \sum_{i=1}^{n} \ell(y_i, h(x_i; w)) + r(w)$$

with variable $w \in \mathcal{W}$

- loss function $\ell : \mathcal{Y} \times \mathcal{Z} \to \mathbb{R}$ maps between prediction space and output space
How to predict?

given

- a loss function $\ell: \mathcal{Y} \times \mathcal{Z} \to \mathbb{R}$
- a hypothesis class $h: \mathcal{X} \times \mathcal{W}$, and
- model parameters $w \in \mathcal{W}$ fit to data

**Q:** how to predict $\hat{y}$ for a new sample $x$?
How to predict?

given

- a loss function $\ell : \mathcal{Y} \times \mathcal{Z} \rightarrow \mathbb{R}$
- a hypothesis class $h : \mathcal{X} \times \mathcal{W}$, and
- model parameters $w \in \mathcal{W}$ fit to data

**Q:** how to predict $\hat{y}$ for a new sample $x$?

**A:** predict $\hat{y}$ by solving

$$
\hat{y} = \arg\min_{y \in \mathcal{Y}} \ell(y, h(x; w))
$$

**MLE interpretation:** if $z = w^T x$, $\ell(y, z) = -\log P(y \mid z)$, then $\hat{y}$ is *most probable* $y \in \mathcal{Y}$ given $z = w^T x$. 
Prediction: examples

given
  ▶ a loss function $\ell : \mathcal{Y} \times \mathcal{Z} \rightarrow \mathbb{R}$
  ▶ a hypothesis class $h : \mathcal{X} \times \mathcal{W}$, and
  ▶ model parameters $w \in \mathcal{W}$ fit to data

predict $\hat{y}$ by solving

$$\hat{y} = \arg\min_{y \in \mathcal{Y}} \ell(y, h(x; w))$$

▶ for quadratic loss,
Prediction: examples

given

- a loss function $\ell : \mathcal{Y} \times \mathcal{Z} \rightarrow \mathbb{R}$
- a hypothesis class $h : \mathcal{X} \times \mathcal{W}$, and
- model parameters $w \in \mathcal{W}$ fit to data

predict $\hat{y}$ by solving

$$\hat{y} = \arg\min_{y \in \mathcal{Y}} \ell(y, h(x; w))$$

- for quadratic loss, $\mathcal{Y} = \mathcal{Z}$, and $\hat{y} = w^T x$
- for $\ell_1$, Huber loss, or quantile loss,
Prediction: examples

given

- a loss function \( \ell : \mathcal{Y} \times \mathcal{Z} \to \mathbf{R} \)
- a hypothesis class \( h : \mathcal{X} \times \mathcal{W}, \) and
- model parameters \( w \in \mathcal{W} \) fit to data

predict \( \hat{y} \) by solving

\[
\hat{y} = \arg\min_{y \in \mathcal{Y}} \ell(y, h(x; w))
\]

- for quadratic loss, \( \mathcal{Y} = \mathcal{Z} \), and \( \hat{y} = w^T x \)
- for \( \ell_1 \), Huber loss, or quantile loss, \( \mathcal{Y} = \mathcal{Z} \), and \( \hat{y} = w^T x \)
- for hinge loss \( \ell(y, h(x; w)) = (1 - yw^T x)_+ \),
Prediction: examples

given

- a loss function $\ell : \mathcal{Y} \times \mathcal{Z} \rightarrow \mathbb{R}$
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  $\mathcal{Y} = \{-1, 1\}$
Prediction: examples

given

- a loss function \( \ell : \mathcal{Y} \times \mathcal{Z} \to \mathbb{R} \)
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- for hinge loss \( \ell(y, h(x; w)) = (1 - yw^T x)_+ \), \( \mathcal{Y} = \{-1, 1\} \) and \( \hat{y} = \text{sign}(w^T x) \)
- for logistic loss \( \ell(y, h(x; w)) = \log(1 + \exp(-yw^T x)) \), \( \mathcal{Y} = \{-1, 1\} \)
Prediction: examples

given

- a loss function $\ell : \mathcal{Y} \times \mathcal{Z} \rightarrow \mathbb{R}$
- a hypothesis class $h : \mathcal{X} \times \mathcal{W}$, and
- model parameters $w \in \mathcal{W}$ fit to data

predict $\hat{y}$ by solving

$$\hat{y} = \arg\min_{y \in \mathcal{Y}} \ell(y, h(x; w))$$

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- for $\ell_1$, Huber loss, or quantile loss, $\mathcal{Y} = \mathcal{Z}$, and $\hat{y} = w^T x$
- for hinge loss $\ell(y, h(x; w)) = (1 - yw^T x)_+$, $\mathcal{Y} = \{-1, 1\}$ and $\hat{y} = \text{sign}(w^T x)$
- for logistic loss $\ell(y, h(x; w)) = \log(1 + \exp(-yw^T x))$, $\mathcal{Y} = \{-1, 1\}$ and $\hat{y} = \text{sign}(w^T x)$
Outline

Maximum likelihood estimation

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Multiclass classification

Ordinal regression

Beyond linear models
Multiclass classification

how to predict nominal values?
Multiclass classification

how to predict **nominal** values?

▸ **idea 1: classification**
  1. encode \( y \in \mathcal{Y} \) as a vector \( \psi(y) \)
  2. predict entries of \( \psi(y) \)
  3. each entry of \( z = h(x; w) \) will predict corresponding entry of \( \psi(y) \)
Multiclass classification

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▶ idea 2: learning probabilities
1. learn the probability \( \mathbb{P}(y = y' \mid x) \) for every \( y' \in \mathcal{Y} \)
2. predict \( y = \text{argmax}_{y' \in \mathcal{Y}} \mathbb{P}(y = y' \mid x) \)
3. \( z = h(x; w) \) will parametrize probability distribution
Multiclass classification: examples

examples:

- classifying which breed of dog is present in an image
- classifying the type of heart disease given a electrocardiogram (EKG)
- predicting if a water well is ok, needs repair, or is defunct
- more examples from projects?
Multiclass classification via binary classification

idea 1: classification

1. encode $y \in \mathcal{Y}$ as a vector $\psi(y)$
2. predict entries of $\psi(y)$
3. each entry of $z = h(x; w)$ will predict corresponding entry of $\psi(y)$

Q: how to pick $\psi(y)$? (suppose $\mathcal{Y} = \{1, \ldots, k\}$)
Multiclass classification via binary classification

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Q: how to pick \( \psi(y) \)? (suppose \( \mathcal{Y} = \{1, \ldots, k\} \))

- one-hot encoding:
  \[
  \psi(y) = (-1, \ldots, \hat{1}, \ldots, -1) \in \{-1, 1\}^k
  \]
  (resulting scheme is called **one-vs-all** classification)
Multiclass classification via binary classification

idea 1: classification

1. encode $y \in \mathcal{Y}$ as a vector $\psi(y)$
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- one-hot encoding:
  
  $\psi(y) = (-1, \ldots, 1, \ldots, -1) \in \{-1, 1\}^k$

  (resulting scheme is called **one-vs-all** classification)

- binary codes:
  
  - define binary expansion of $y$, $\text{bin}(y) \in \{-1, 1\}^{\log(k)}$
  - let $\psi(y) = 2 \text{bin}(y) - 1 \in \{-1, 1\}^{\log(k)}$
Multiclass classification via binary classification

**idea 1: classification**

1. encode $y \in \mathcal{Y}$ as a vector $\psi(y)$
2. predict entries of $\psi(y)$
3. each entry of $z = h(x; w)$ will predict corresponding entry of $\psi(y)$

**Q:** how to pick $\psi(y)$? (suppose $\mathcal{Y} = \{1, \ldots, k\}$)

- one-hot encoding:
  
  $y$th entry
  
  $\psi(y) = (-1, \ldots, \overset{\land}{1}, \ldots, -1) \in \{-1, 1\}^k$

  (resulting scheme is called **one-vs-all** classification)

- binary codes:
  
  - define binary expansion of $y$, bin($y$) $\in \{-1, 1\}^{\log(k)}$
  
  - let $\psi(y) = 2 \text{bin}(y) - 1 \in \{-1, 1\}^{\log(k)}$

- error-correcting codes
Multiclass classification via binary classification

idea 1: classification

1. encode $y \in \mathcal{Y}$ as a vector $\psi(y)$
2. predict entries of $\psi(y)$
3. each entry of $z = h(x; w)$ will predict corresponding entry of $\psi(y)$

Q: how to pick $\psi(y)$? (suppose $\mathcal{Y} = \{1, \ldots, k\}$)

▶ one-hot encoding:

\[ \psi(y) = (-1, \ldots, 1, \ldots, -1) \in \{-1, 1\}^k \]

(resulting scheme is called one-vs-all classification)

▶ binary codes:

▶ define binary expansion of $y$, $\text{bin}(y) \in \{-1, 1\}^{\log(k)}$

▶ let $\psi(y) = 2 \text{bin}(y) - 1 \in \{-1, 1\}^{\log(k)}$

▶ error-correcting codes

these vary in the dimension of $\psi(y) = \text{dimension of } z$
Multiclass classification via binary classification

idea 1: classification

1. encode $y \in \mathcal{Y}$ as a vector $\psi(y) \in \{-1, 1\}^k$
2. predict entries of $\psi(y)$
3. each entry of $z = h(x; w)$ will predict corresponding entry of $\psi(y)$

**Q:** how to predict entries of $\psi(y) \in \{-1, 1\}^k$?
Multiclass classification via binary classification

**idea 1: classification**

1. encode $y \in \mathcal{Y}$ as a vector $\psi(y) \in \{-1, 1\}^k$
2. predict entries of $\psi(y)$
3. each entry of $z = h(x; w)$ will predict corresponding entry of $\psi(y)$

**Q:** how to predict entries of $\psi(y) \in \{-1, 1\}^k$?

- reduce to a bunch of binary problems!
- let $W \in \mathbb{R}^{k \times d}$, so $z = Wx \in \mathbb{R}^k$
- pick your favorite loss function $\ell^{\text{bin}}$ for binary classification
- fit parameter $W$ by minimizing loss function

$$\ell^{\text{nom}}(y, z) = \sum_{i=1}^{k} \ell^{\text{bin}}(\psi(y)_i, z_i)$$
One-vs-All classification

\[ x_1 \]
\[ x_2 \]

\[ 1 \text{ vs } 2,3 \]
\[ 3 \text{ vs } 1,2 \]
\[ 2 \text{ vs } 1,3 \]
Multiclass classification via learning probabilities

(for concreteness, suppose $\mathcal{Y} = \{1, \ldots, k\}$) idea 2: learning probabilities

1. learn the probability $P(y = y' \mid x)$ for every $y' \in \mathcal{Y}$
2. predict $y = \arg\max_{y' \in \mathcal{Y}} P(y = y' \mid x)$
3. $z = h(x; w) \in \mathbb{R}^k$ will parametrize probability distribution

Q: how to predict probabilities?
Multiclass classification via learning probabilities

- let $W \in \mathbb{R}^{k \times d}$, so $Wx \in \mathbb{R}^{k}$

- **multinomial logit** takes a hint from logistic:
  let $z = h(x; W) = Wx$, and suppose
  
  $$
  P(y = i \mid z) = \frac{\exp(z_i)}{\sum_{j=1}^{k} \exp(z_j)}
  $$

  (ensures probabilities are positive and sum to 1)

- fit by minimizing negative log likelihood

  $$
  \ell(y, z) = -\log(P(y \mid z)) = -\log\left(\frac{\exp(z_y)}{\sum_{j=1}^{k} \exp(z_j)}\right)
  $$
Multinomial classification

![Graph showing data points and lines for various comparisons.]

- 1 vs 2, 3
- 2 vs 1, 3
- 3 vs 1, 2
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Beyond linear models
Ordinal regression

how to predict ordinal values?
Ordinal regression

how to predict ordinal values?

▶ idea 0: regression
  1. encode \( y \in \mathcal{Y} \) in \( \mathbb{R} \)
how to predict **ordinal** values?

- **idea 0: regression**
  1. encode $y \in \mathcal{Y}$ in $\mathbb{R}$

- **idea 1: classification**
  1. encode $y \in \mathcal{Y}$ as a vector $\psi(y)$
  2. predict entries of $\psi(y)$
  3. each entry of $z = h(x; w)$ will predict corresponding entry of $\psi(y)$
Ordinal regression

how to predict ordinal values?

▶ idea 0: regression
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3. $z = h(x; w)$ will parametrize probability distribution
Ordinal regression

(for concreteness, suppose $Y = \{1, \ldots, k\}$) idea 0: regression

1. encode $y \in Y$ in $\mathbb{R}$
2. predict with $Z = \mathbb{R}$

- quadratic loss

$$\ell(y, z) = (y - z)^2$$

- ordinal hinge loss

$$\ell(y, z) = \sum_{y' = 1}^{y-1} (1 - z + y')_+ + \sum_{y' = y+1}^{k} (1 + z - y')_+$$
Ordinal regression via predicting a vector

idea 1: classification

1. encode $y \in \mathcal{Y}$ as a vector $\psi(y)$
2. predict entries of $\psi(y)$
3. each entry of $z = h(x; w)$ will predict corresponding entry of $\psi(y)$

(for concreteness, suppose $\mathcal{Y} = \{1, \ldots, k\}$)

- how to encode $y$ as a vector?
Ordinal regression via predicting a vector

idea 1: classification

1. encode \( y \in \mathcal{Y} \) as a vector \( \psi(y) \)
2. predict entries of \( \psi(y) \)
3. each entry of \( z = h(x; w) \) will predict corresponding entry of \( \psi(y) \)

(for concreteness, suppose \( \mathcal{Y} = \{1, \ldots, k\} \))

- how to encode \( y \) as a vector? how about

\[
\psi(y) = (1, \ldots, 1, -1, \ldots, -1) \in \{-1, 1\}^{k-1}
\]

- let \( W \in \mathbb{R}^{k-1 \times d} \), so \( z = Wx \in \mathbb{R}^{k-1} \)
- pick your favorite loss function \( \ell^{\text{bin}} \) for binary classification
- fit model \( W \) by minimizing loss function

\[
\ell^{\text{ord}}(y; z) = \sum_{i=1}^{k-1} \ell^{\text{bin}}(\psi(y)_i; z_i)
\]
Ordinal regression via predicting a vector

- set $\psi(y) = (1, \ldots, 1, -1, \ldots, -1) \in \{-1, 1\}^{k-1}$
- let $W \in \mathbb{R}^{k-1 \times d}$, so $z = Wx \in \mathbb{R}^{k-1}$
- fit parameter $W$ by minimizing loss function

$$
\ell^{\text{ord}}(y; z) = \sum_{i=1}^{k-1} \ell^{\text{bin}}(\psi(y)_i, z_i)
$$

- $i$th column of $W$ defines a line separating levels $y \leq i$ from levels $y > i$

**Q:** How to predict $\hat{y}$ given $x$ and $W$?
Ordinal regression via predicting a vector

- set \( \psi(y) = (1, \ldots, 1, -1, \ldots, -1) \in \{-1, 1\}^{k-1} \)
- let \( W \in \mathbb{R}^{k-1 \times d} \), so \( z = Wx \in \mathbb{R}^{k-1} \)
- fit parameter \( W \) by minimizing loss function
  \[
  \ell^{\text{ord}}(y; z) = \sum_{i=1}^{k-1} \ell^{\text{bin}}(\psi(y)_i, z_i)
  \]
- \( i \)th column of \( W \) defines a line separating levels \( y \leq i \) from levels \( y > i \)

Q: How to predict \( \hat{y} \) given \( x \) and \( W \)?
A: Compute \( z = Wx \), and predict
  \[
  \hat{y} = \arg\min_{y \in Y} \ell^{\text{ord}}(y; z)
  \]
Ordinal regression
Regularization for ordinal regression

▶ need to ensure that

\[ P(y > 1 \mid z) \geq P(y > 2 \mid z) \geq \ldots \geq P(y > k - 1 \mid z) \]

▶ since \( P(y > i \mid z) \sim \exp (() z_i) \), need to ensure that

\[ z_1 \geq z_2 \geq \ldots \geq z_{k-1} \]

▶ can do this by insisting that

\[ W = \begin{bmatrix} w^T & b_1 \\ w^T & b_2 \\ \vdots & \vdots \\ w^T & b_{k-1} \end{bmatrix} \]

and \( b_1 \geq b_2 \geq \cdots \geq b_{k-1} \)

▶ then \( z = Wx \) satisfies \( z_1 \geq z_2 \geq \cdots \geq z_{k-1} \)

▶ this is a kind of \textbf{regularization} on \( W \)!
Outline

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Coding and decoding

we now have four different spaces

▶ input space $\mathcal{X}$
▶ output space $\mathcal{Y}$
▶ parameter space $\mathcal{W}$
▶ prediction space $\mathcal{Z}$

a model is given by a choice of

▶ loss function $l : \mathcal{Y} \times \mathcal{Z} \rightarrow \mathbb{R}$,
▶ regularizer $r : \mathcal{W} \rightarrow \mathbb{R}$, and
▶ hypothesis class $h : \mathcal{X} \times \mathcal{W} \rightarrow \mathcal{Z}$
we fit the model by solving

$$\text{minimize } \frac{1}{n} \sum_{i=1}^{n} \ell(y_i, h(x_i; w)) + r(w)$$

to find $w \in \mathcal{W}$

given a parameter $w \in \mathcal{W}$ and a new input $x \in \mathcal{X}$, we predict $y \in \mathcal{Y}$ by solving

$$y = \arg\min_{y \in \mathcal{Y}} \ell(y, h(x_i; w))$$
What models fit in this framework?

- linear models
- linear models with feature transformations
- decision trees
- neural networks
- generalized additive models
- unsupervised learning (!)
- ...
Resources

- quantile regression https://www.cscu.cornell.edu/news/statnews/stnews70.pdf