ORIE 4741: Learning with Big Messy Data

Loss functions

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Outline

3.36pt

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

$$\mathbb{P}(y_i = y \mid x_i, w) = p(y; x_i, w)$$

▶ for example, if $y_i = w^T x_i + \varepsilon_i$, $\varepsilon_i \sim \mathcal{N}(0, \sigma^2)$, then

$$\mathbb{P}(y_i = y \mid x_i, w) \sim \frac{1}{\sqrt{2\pi\sigma^2}} \exp \left( -\frac{(y_i - w^T x_i)^2}{2\sigma^2} \right)$$

▶ likelihood of data given parameter $w$ is

$$L(D; w) = \prod_{i=1}^{n} \mathbb{P}(y_i = y \mid x_i, w)$$

▶ 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 $L(\mathcal{D}; w)$

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

- **negative log likelihood**
  \[
  \ell(\mathcal{D}; w) = -\log L(\mathcal{D}; w)
  \]

- **maximize $L(\mathcal{D}; w)$ \iff minimize $\ell(\mathcal{D}; w)$**
Example: Maximum Likelihood Estimation (MLE)

- for linear model with Gaussian error,

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

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

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

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

- 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

$$P(D; w) = P(D | w) P(w)$$

maximum a posteriori (MAP estimation): choose $w$ to maximize posterior probability
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 $y_i = w^T x_i + \epsilon_i$, $i = 1, \ldots, n$

\[
\mathbb{P}(D; w) = \mathbb{P}(D \mid w) \mathbb{P}(w)
\]
\[
\approx \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi\sigma^2}} \exp \left( \frac{-(y_i - w^T x_i)^2}{2\sigma^2} \right) \prod_{i=1}^{d} \frac{1}{\sqrt{2\pi}} \exp \left( \frac{-w_i^2}{2} \right)
\]
\[
= (2\pi\sigma^2)^{-\frac{n}{2}} \prod_{i=1}^{n} \left( \exp \left( \frac{-(y_i - w^T x_i)^2}{2\sigma^2} \right) \right) (2\pi)^{-\frac{d}{2}} \prod_{i=1}^{d} \left( \exp \left( \frac{-w_i^2}{2} \right) \right)
\]
\[
\ell(D; w) = -\log \left( \mathbb{P}(D; w) \right)
\]
\[
= \frac{n}{2} \log(2\pi\sigma^2) + \frac{d}{2} \log(2\pi) + \frac{1}{2\sigma^2} \sum_{i=1}^{n} (y_i - w^T x_i)^2 + \frac{1}{2} \sum_{i=1}^{d} w_i^2
\]
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 $y_i = w^T x_i + \epsilon_i$, $i = 1, \ldots, n$

$$P(D; w) = P(D \mid w) P(w)$$

$$\sim \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi\sigma^2}} \exp \left( -\frac{(y_i - w^T x_i)^2}{2\sigma^2} \right) \prod_{i=1}^{d} \frac{1}{\sqrt{2\pi}} \exp \left( -\frac{w_i^2}{2} \right)$$

$$= (2\pi\sigma^2)^{-\frac{n}{2}} \prod_{i=1}^{n} \left( \exp \left( -\frac{(y_i - w^T x_i)^2}{2\sigma^2} \right) \right) (2\pi)^{-\frac{d}{2}} \prod_{i=1}^{d} \left( \exp \left( -\frac{w_i^2}{2} \right) \right)$$

$$\ell(D; w) = -\log (P(D; w))$$

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

... 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 \( \ell : \mathcal{X} \times \mathcal{Y} \times \mathbb{R}^d \rightarrow \mathbb{R} \)
- regularizer \( r : \mathbb{R}^d \rightarrow \mathbb{R} \)
Recap: regularized empirical risk minimization

choose model by solving

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why?

- want to minimize the risk \( \mathbb{E}_{(x,y) \sim P} \ell(x, y; w) \)
- 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

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

least squares ($\ell_2$) regression:

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

special case: no covariates. what is

$$\arg\min_w \frac{1}{n} \sum_{i=1}^{n} (y_i - w)^2$$

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

\(\ell_1\) regression:

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

special case: no covariates. what is

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

\( \ell_1 \) regression:

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\]

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
\( l_1 \) regression finds the median

\( l_1 \) regression:

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

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 \( \alpha \in (0, 1) \),

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

special case: no covariates. what is

\[
\arg\min_w \frac{1}{n} \sum_{i=1}^{n} \alpha (y_i - w)_+ + (1 - \alpha)(y_i - w)_-?
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Quantile regression finds the right quantile

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

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- if $pn$ of the $y_i$’s are bigger than $w$,
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**A:** $w$ is the $\alpha$th quantile of $y$!
Demo: robust regression
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3.36pt

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

\[ \ell_{\text{logistic}}(x, y; w) = \log(1 + \exp(-yw^T x)) \]
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 \(-\log \mathbb{P}(y|w, x)\)

\[
\ell_{\text{logistic}}(x, y; w) = -\log(\text{logistic}(yw^T x)) = -\log \left( \frac{1}{1 + \exp(-yw^T x)} \right) = \log \left( 1 + \exp \left( -yw^T x \right) \right)
\]
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: \( w^T x = \pm 1 \)
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 $\mathbb{I}(y \neq \text{sign}(w^T x))$
- quadratic loss $(y - w^T x)^2$
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- ...

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

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trade off dislike of false positives vs false negatives

properties:

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

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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 $\ell(x, y; w) =$

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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?
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?
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 \( \ell(x, y; w) = \)

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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? 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 $h \in \mathcal{H}$

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

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

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

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 $\ell : \mathcal{Y} \times \mathcal{Z} \rightarrow \mathbb{R}$
- 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 $x$?
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 $x$?

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

$$\hat{y} = \text{argmin}_{y \in \mathcal{Y}} \ell(y, h(x; w))$$

**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

$$\hat{y} = \operatorname{argmin}_{y \in \mathcal{Y}} \ell(y, h(x; w))$$

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

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  $$
  \ell(y, h(x; w)) = (1 - yw^T x)_+,
  \mathcal{Y} = \{-1, 1\}$$
Prediction: examples

given

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$\mathcal{Y} = \{-1, 1\}$ 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 \( \ell : \mathcal{Y} \times \mathcal{Z} \to \mathbb{R} \)
- 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 quadratic loss, \( \mathcal{Y} = \mathcal{Z} \), and \( \hat{y} = w^T x \)
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- 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

Regression

Classification

The prediction space

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 $y = \arg\max_{y' \in \mathcal{Y}} \mathbb{P}(y = y' \mid x)$
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

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

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▶ one-hot encoding:

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

(resulting scheme is called \textbf{one-vs-all} classification)
Multiclass classification via binary classification

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- **one-hot encoding:**
  
  \[ \psi(y) = (-1, \ldots, \underbrace{1}_{y} \ldots, -1) \in \{-1, 1\}^k \]

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

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

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▶ error-correcting codes
Multiclass classification via binary classification

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- one-hot encoding:
  \[
  \psi(y) = (-1, \ldots, 1, \ldots, -1) \in \{-1, 1\}^k
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- binary codes:
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  - 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 \( y \in Y \) 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

The diagram illustrates the classification process using a two-dimensional dataset. The axes are labeled $x_1$ and $x_2$. The lines and markers indicate different classification scenarios:

- Red line: $1$ vs $2,3$
- Green line: $3$ vs $1,2$
- Blue line: $2$ vs $1,3$

Points are marked according to these classifications, with different symbols representing each class.
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 $y = \text{argmax}_{y' \in \mathcal{Y}} P(y = y' \mid x)$
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

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

3.36pt

Maximum likelihood estimation
Regression
Classification
The prediction space
Multiclass classification
Ordinal regression
Beyond linear models
Ordinal regression

how to predict **ordinal** values?
how to predict **ordinal** values?

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

how to predict **ordinal** values?

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  1. encode $y \in \mathcal{Y}$ as a vector $\psi(y)$
  2. predict entries of $\psi(y)$
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Ordinal regression

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 $\psi(y)$

▶ idea 2: learning probabilities
  1. learn the probability $\mathbb{P}(y = y' \mid x)$ for every $y' \in \mathcal{Y}$
  2. predict $y = \arg\max_{y' \in \mathcal{Y}} \mathbb{P}(y = y' \mid x)$
  3. $z = h(x; w)$ will parametrize probability distribution
Ordinal regression

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

**idea 0: regression**

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

- quadratic loss
  \[
  \ell(y, z) = (y - z)^2
  \]
- ordinal hinge loss
  \[
  \ell(y, z) = \sum_{y' = 1}^{y-1} (1 - z + y')_+ + \sum_{y' = y+1}^{k} (1 + z - y')_+
  \]

\[
\begin{array}{c}
\text{a = 1} \\
1 2 3 4 5
\end{array}
\begin{array}{c}
\text{a = 2} \\
1 2 3 4 5
\end{array}
\begin{array}{c}
\text{a = 3} \\
1 2 3 4 5
\end{array}
\begin{array}{c}
\text{a = 4} \\
1 2 3 4 5
\end{array}
\begin{array}{c}
\text{a = 5} \\
1 2 3 4 5
\end{array}
\]

\(1 2 3 4 5\)

\(a = 1\)

\(a = 2\)

\(a = 3\)

\(a = 4\)

\(a = 5\)
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 \( \psi(y) = (1, \ldots, 1, \overset{\text{ith column}}{-1}, \ldots, -1) \in \{-1, 1\}^{k-1} \)
- 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

$$
\hat{y} = \arg\min_{y \in \mathcal{Y}} \ell^{\text{ord}}(y; z)
$$
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 \( b_1 \geq b_2 \geq \ldots \geq b_{k-1} \)
- then \( z = Wx \) satisfies \( z_1 \geq z_2 \geq \ldots \geq z_{k-1} \)
- this is a kind of \textbf{regularization} on \( W \)!
Outline

3.36pt

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Beyond linear models
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 $\ell : \mathcal{Y} \times \mathcal{Z} \to \mathbb{R}$,
▶ regularizer $r : \mathcal{W} \to \mathbb{R}$, and
▶ hypothesis class $h : \mathcal{X} \times \mathcal{W} \to \mathcal{Z}$
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