ORIE 4741: Learning with Big Messy Data

Regularization

Professor Udell
Operations Research and Information Engineering
Cornell

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Regularized empirical risk minimization

choose model by solving

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

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 \( r : \mathbb{R}^d \rightarrow \mathbb{R} \)
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- regularizer $r : \mathbb{R}^d \rightarrow \mathbb{R}$

why?

- want to minimize the \textbf{risk} $\mathbb{E}_{(x,y) \sim P} \ell(x, y; w)$
- approximate it by the \textbf{empirical risk} $\sum_{i=1}^{n} \ell(x, y; w)$
- add regularizer to help model generalize
Example: regularized least squares

find best model by solving

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

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

ridge regression, aka quadratically regularized least squares:

- loss function $\ell(x, y; w) = (y - w^T x)^2$
- regularizer $r(w) = \|w\|^2$
Outline

Maximum likelihood estimation

Regularizers

Quadratic regularization

$l_1$ regularization

Nonnegative regularizer
Probabilistic setup

▶ suppose you know a function $p : \mathbb{R} \rightarrow [0, 1]$ so that

$$P(y_i = y \mid x_i, w) \sim p(y; x_i, w)$$

▶ 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

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

▶ for example, for linear model with Gaussian error,

$$L(D; w) = \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi\sigma^2}} \exp \left( -\frac{(y_i - w^T x_i)^2}{2\sigma^2} \right)$$
**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,

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

= \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
Example: Maximum Likelihood Estimation (MLE)

for linear model with Gaussian error,

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

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

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

so maximize \( L(D; w) \iff \text{minimize} \sum_{i=1}^{n} (y_i - w^T x_i)^2 \)
(for fixed \( \sigma \))
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 $\mathbb{P}(w)$

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
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

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 $y_i = w^T x_i + \epsilon_i$, $i = 1, \ldots, n$

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

\ldots aha! and we have \textbf{ridge regression} with $\lambda = \sigma^2$
Outline

Maximum likelihood estimation

Regularizers

Quadratic regularization

$\ell_1$ regularization

Nonnegative regularizer
Regularization

why regularize?

▶ reduce variance of the model
▶ impose prior structural knowledge
▶ improve interpretability
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▶ reduce variance of the model
▶ impose prior structural knowledge
▶ improve interpretability

why not regularize?

▶ *Gauss-Markov theorem*:
  least squares is the best linear unbiased estimator
▶ regularization increases bias
Regularizers: a tour

we might choose regularizer so models will be

▶ small
▶ sparse
▶ nonnegative
▶ smooth
▶ ...

compare with forward- and backward-stepwise selection (e.g., AIC, BIC): regularized models tend to have lower variance.
(see Elements of Statistical Learning (Hastie, Tibshirani, Friedman) for more information.)
Regularizers: a tour

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- smooth
- ...

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Quadratic regularizer

quadratic regularizer

\[ r(w) = \lambda \sum_{i=1}^{n} w_i^2 \]

ridge regression

minimize \[ \sum_{i=1}^{n} (y_i - w^T x_i)^2 + \lambda \sum_{i=1}^{n} w_i^2 \]

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

solution \( w = (X^T X + \lambda I)^{-1} X^T y \)
Quadratic regularizer

- shrinks coefficients towards 0
- shrinks more in the direction of the smallest singular values of $X$
Is least squares scaling invariant?

suppose Alice and Bob do the same experiment

- Alice measures distance in mm
- Bob measures distance in km

they each compute an estimator with least squares and compare their predictions

Q: Do they make the same predictions?
A: Yes!
Is least squares scaling invariant?

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Q: Do they make the same predictions?
A: Yes!
Least squares is scaling invariant

if \( \beta \in \mathbb{R} \), \( D \in \mathbb{R}^{d \times d} \) is diagonal, and Alice’s measurements \((X', y')\) are related to Bob’s \((X, y)\) by

\[
y' = \beta y, \quad X' = XD,
\]

then the resulting least squares models are

\[
w = (X^T X)^{-1} X^T y, \quad w' = (X'^T X')^{-1} X'^T y'
\]

and they make the same predictions:

\[
X'w' = X'(X'^T X')^{-1} X'^T y' = XD(D^T X^T XD)^{-1} D^T X^T \beta y
\]
\[
= XDD^{-1}(X^T X)^{-1}(D^T)^{-1} D^T X^T \beta y
\]
\[
= \beta X(X^T X)^{-1} X^T y = \beta Xw
\]
Least squares is scaling invariant

if $\beta \in \mathbb{R}$, $D \in \mathbb{R}^{d \times d}$ is diagonal, and Alice’s measurements $(X', y')$ are related to Bob’s $(X, y)$ by

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$$= XDD^{-1}(X^T X)^{-1}(D^T)^{-1} D^T X^T \beta y$$

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

we say least squares is **invariant under scaling**
Is ridge regression scaling invariant?

Suppose Alice and Bob do the same experiment

- Alice measures distance in mm
- Bob measures distance in km

They each compute an estimator with ridge regression and compare their predictions.
Is ridge regression scaling invariant?

suppose Alice and Bob do the same experiment

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Q: Do they make the same predictions?
Is ridge regression scaling invariant?

suppose Alice and Bob do the same experiment

- Alice measures distance in mm
- Bob measures distance in km

they each compute an estimator with ridge regression and compare their predictions

Q: Do they make the same predictions?
A: No!
Ridge regression is not scaling invariant

if $\beta \in \mathbb{R}$, $D \in \mathbb{R}^{d \times d}$ is diagonal, and Alice’s measurements $(X', y')$ are related to Bob’s $(X, y)$ by

$$y' = \beta y, \quad X' = XD,$$

then the resulting ridge regression models are

$$w = (X^T X + \lambda I)^{-1} X^T y, \quad w' = (X'^T X' + \lambda I)^{-1} X'^T y'$$

and the predictions are

$$Xw = X(X^T X + \lambda I)^{-1} X^T y, \quad X'w' = X'(X'^T X' + \lambda I)^{-1} X'^T y'$$

ridge regression is not invariant under coordinate transformations
Scaling and offsets

to get the same answer no matter the units of measurement, 
standardize the data: for each column of $X$ and of $y$

▶ demean: subtract column mean
▶ standardize: divide by column standard deviation

let

$$\mu_j = \frac{1}{n} \sum_{i=1}^{n} X_{ij}, \quad \mu = \frac{1}{n} \sum_{i=1}^{n} y_i$$

$$\sigma^2_j = \frac{1}{n} \sum_{i=1}^{n} (X_{ij} - \mu_j)^2, \quad \sigma^2 = \frac{1}{n} \sum_{i=1}^{n} (y_i - \mu)^2$$

solve

$$\text{minimize} \quad \sum_{i=1}^{n} \left( \frac{y_i - \mu}{\sigma} - \sum_{j=1}^{d} w_j \frac{X_{ij} - \mu_j}{\sigma_j} \right)^2 + \lambda \sum_{j=1}^{d} w_j^2$$
Scale the regularizer, not the data

instead of

\[
\minimize \sum_{i=1}^{n} \left( \frac{y_i - \mu}{\sigma} - \sum_{j=1}^{d} w_j \frac{X_{ij} - \mu_i}{\sigma_i} \right)^2 + \sum_{j=1}^{d} w_j^2,
\]

▶ multiply through by \( \sigma^2 \)
▶ reparametrize \( w'_j = \frac{\sigma}{\sigma_j} w_j \)

to find the equivalent problem

\[
\minimize \sum_{i=1}^{n} (y_i - \sum_{j=1}^{d} w'_j X_{ij} + c(w'))^2 + \sum_{j=1}^{d} \sigma_j^2 (w'_j)^2,
\]

where \( c(w') \) is some linear function of \( w' \)
finally absorb \( c(w') \) into the constant term in the model

\[
\minimize \| y - Xw' \|^2 + \lambda \sum_{j=1}^{d} \sigma_j^2 (w'_j)^2,
\]
Scaling and offsets

a different solution to scaling and offsets: take the MAP view

- \( r(w) \) is negative log prior on \( w \)
- with a gaussian prior,

\[
   r(w) = \sum_{i=1}^{n} \sigma_i^2 w_i^2
\]

where \( \frac{1}{\sigma_i} \) is the variance of the prior on the \( i \)th entry of \( w \)

- if you believe the noise in the \( i \)th features is large, penalize the \( i \)th entry more (\( \sigma_i \) big);
- if you believe the noise in the \( i \)th features is small, penalize the \( i \)th entry less (\( \sigma_i \) small);
- if you measure \( X \) or \( y \) in different units, your prior on \( w \) should change accordingly
Scaling and offsets

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- $r(w)$ is negative log prior on $w$
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$$r(w) = \sum_{i=1}^{n} \sigma_i^2 w_i^2$$

where $\frac{1}{\sigma_i}$ is the variance of the prior on the $i$th entry of $w$

- if you believe the noise in the $i$th features is large, penalize the $i$th entry more ($\sigma_i$ big);
- if you believe the noise in the $i$th features is small, penalize the $i$th entry less ($\sigma_i$ small);
- if you measure $X$ or $y$ in different units, your prior on $w$ should change accordingly

example: don’t penalize the offset $w_n$ of the model ($\sigma_n \to \infty$)

$$r(w) = \sum_{i=1}^{n-1} w_i^2$$
Outline

Maximum likelihood estimation

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$l_1$ regularization

Nonnegative regularizer
\( \ell_1 \) regularization

\( \ell_1 \) regularizer

\[
r(w) = \lambda \sum_{i=1}^{n} |w_i|
\]

lasso problem

\[
\text{minimize } \sum_{i=1}^{n} (y_i - w^T x_i)^2 + \lambda \sum_{i=1}^{n} |w_i|
\]

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

- penalizes large \( w \) less than ridge regression
- no closed form solution
Recall $\ell_p$ norms

$\ell_p$ norm $\|w\|_p$ for $p \in (0, \infty)$ is defined as

$$\|w\|_p = \left( \sum_{i=1}^{d} |w|^p \right)^{1/p}$$

examples:

- $\ell_1$ norm is $\|w\|_1 = \sum_{i=1}^{d} |w|$
- $\ell_2$ norm is $\|w\|_2 = \sqrt{\sum_{i=1}^{d} w^2}$

for $p = 0$ or $p = \infty$, $\ell_p$ norm is defined by taking limit:

- $\ell_\infty$ norm is $\|w\|_\infty = \lim_{p \to \infty} (\sum_{i=1}^{d} |w|^p)^{1/p} = \max_i |w_i|$  
- $\ell_0$ norm is $\|w\|_0 = \lim_{p \to 0} (\sum_{i=1}^{d} |w|^p)^{1/p} = \text{card}(w)$, number of nonzeros in $w$

note: $\ell_0$ is not actually a norm  
(not absolutely homogeneous since $\|\alpha w\|_0 = \|w\|_0$ for $\alpha \neq 0$)
\( \ell_1 \) regularization

why use \( \ell_1 \)?

- best convex lower bound for \( \ell_0 \) on the \( \ell_\infty \) unit ball
- tends to produce sparse solution

example:

- suppose \( X_1 = y \), \( X_2 = \alpha y \) for some \( 0 < \alpha < 1 \)
- fit lasso model and ridge regression model as \( \lambda \to 0 \)

\[
\begin{align*}
\hat{w}^{\text{ridge}} &= \lim_{\lambda \to 0} \arg\min_w \|y - Xw\|_2^2 + \lambda \|w\|_2^2 \\
\hat{w}^{\text{lasso}} &= \lim_{\lambda \to 0} \arg\min_w \|y - Xw\|_2^2 + \lambda \|w\|_1
\end{align*}
\]

- as \( \lambda \to 0 \), solution solves least squares \( \implies \hat{w}_1 + \alpha \hat{w}_2 = 1 \)
\( \ell_1 \) regularization

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\mathbf{w}^{\text{ridge}} &= \lim_{\lambda \to 0} \arg\min_{\mathbf{w}} \|\mathbf{y} - \mathbf{X}\mathbf{w}\|^2 + \lambda \|\mathbf{w}\|_2^2 \\
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\end{align*}
\]

- as \( \lambda \to 0 \), solution solves least squares \( \implies \mathbf{w}_1 + \alpha \mathbf{w}_2 = 1 \)
- ridge regression minimizes \( \mathbf{w}_1^2 + \mathbf{w}_2^2 \) \( \implies \mathbf{w}_1 = \mathbf{w}_2 = \frac{1}{1+\alpha} \)
- lasso minimizes \( |\mathbf{w}_1| + |\mathbf{w}_2| \) \( \implies \mathbf{w}_1 = 1, \mathbf{w}_2 = 0 \)
Sparsity

why would you want sparsity?

▶ credit card application: requires less info from applicant
▶ medical diagnosis: easier to explain model to doctor
▶ genomic study: which genes to investigate?
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**Convex indicator**

define *convex indicator* \( 1 : \{ \text{true, false} \} \rightarrow \mathbb{R} \cup \{ \infty \} \)

\[
1(z) = \begin{cases} 
0 & \text{if } z \text{ is true} \\
\infty & \text{if } z \text{ is false}
\end{cases}
\]

define *convex indicator* of set \( C \)

\[
1_C(x) = 1(x \in C) = \begin{cases} 
0 & x \in C \\
\infty & \text{otherwise}
\end{cases}
\]
Convex indicator

define **convex indicator** $1 : \{ \text{true, false} \} \rightarrow \mathbb{R} \cup \{ \infty \}$

$$1(z) = \begin{cases} 0 & z \text{ is true} \\ \infty & z \text{ is false} \end{cases}$$

define **convex indicator** of set $C$

$$1_C(x) = 1(x \in C) = \begin{cases} 0 & x \in C \\ \infty & \text{otherwise} \end{cases}$$

don’t confuse this with the boolean indicator $\mathbb{1}(z)$ (no standard notation...)
Nonnegative regularization

nonnegative regularizer

\[ r(w) = \sum_{i=1}^{n} 1(w_i \geq 0) \]

nonnegative least squares problem (NNLS)

\[
\text{minimize} \quad \sum_{i=1}^{n} (y_i - w^T x_i)^2 + \sum_{i=1}^{n} 1(w_i \geq 0)
\]

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

- value is \( \infty \) if \( w_i < 0 \)
- so solution is \textbf{always} nonnegative
- often, solution is also sparse
Nonnegative coefficients

why would you want nonnegativity?
Nonnegative coefficients

why would you want nonnegativity?

▶ electricity usage: how often is device turned on?
  ▶ n = times, d = electric devices,
  ▶ y = usage, X = which devices use power at which times
  ▶ w = devices used by household

▶ hyperspectral imaging: which species are present?
  ▶ n = frequencies, d = possible materials,
  ▶ y = observed spectrum, X = known spectrum of each material
  ▶ w = material composition of location

▶ logistics: which routes to run?
  ▶ n = locations, d = possible routes,
  ▶ y = demand, X = which routes visit which locations
  ▶ w = size of truck to send on each route
Nonnegative coefficients

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► logistics: which routes to run?
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Demo: Regularized Regression

https://github.com/ORIE4741/demos/
RegularizedRegression.ipynb
Smooth coefficients

smooth regularizer

\[
    r(w) = \sum_{i=1}^{d-1} (w_{i+1} - w_i)^2 = \|Dw\|^2
\]

where \( D \in \mathbb{R}^{(d-1) \times d} \) is the first order difference operator

\[
    D_{ij} = \begin{cases} 
        1 & j = i \\
        -1 & j = i + 1 \\
        0 & \text{else}
    \end{cases}
\]

smoothed least squares problem

\[
    \text{minimize} \quad \sum_{i=1}^{n} (y_i - w^T x_i)^2 + \lambda \|Dw\|^2
\]
Why smooth?

- allow model to change over space or time
  - *e.g.*, different years in tax data
- interpolates between one model and separate models for different domains
  - *e.g.*, counties in tax data
- can couple *any* pairs of model coefficients, not just $(i, i + 1)$