COMS 4721: Machine Learning for Data Science Lecture 4, 1/26/2017

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.

REGRESSION WITH/WITHOUT REGULARIZATION

y pairs ndormations data response Given: A data set $(x_1, y_1), \ldots, (x_n, y_n)$, where $x \in \mathbb{R}^d$ and $y \in \mathbb{R}$. We standardize such that each dimension of x is zero mean unit variance, and y is zero mean. such that we work without Model: We define a model of the form We particularly focus on the case where $f(x; w) = x^T w$. [x exclusive of x, y, y.] Learning: We can learn the model by minimizing the objective (aka, "loss") function $\mathcal{L} = \sum_{i=1}^{n} (y_i - x_i^T w)^2 + \lambda w^T w \Leftrightarrow \mathcal{L} = \|y - Xw\|^2 + \lambda \|w\|^2$ We've focused on $\lambda = 0$ (least squares) and $\lambda > 0$ (ridge regression).

BIAS-VARIANCE TRADE-OFF

BIAS-VARIANCE FOR LINEAR REGRESSION SE cofficient x > [each co.variatevector] having covariance of [N-dimnedor We can go further and hypothesize a *generative* model $y \sim N(XW, \sigma^2 I)$ and some true (but unknown) and the some true (but unknown) are the some true (but some true (but unknown) underlying value for the parameter vector w. I we believe that there is some time vector w generating out that the variate out data. We hypothesize this but don't have it's -• We saw how the least squares solution, $w_{LS} = (X^T X)^{-1} X^T y$, is unbiased but potentially has high variance: (by wivin 2ing x wood framing that he expected when you However, the variance of $\mathbb{E}[w_{\rm LS}]=w$, ${\rm Var}[w_{\rm LS}]=\sigma^2(X^TX)^{-1}$. Leader that we will be a provided by the property of the property of the property of the provided by the property of the property of the provided by the property of the provided by the pro lexhacted votice of our By contrast, the ridge regression solution is $w_{RR} = (\lambda I + X^T X)^{-1} X^T y_{RR}$ Using the same procedure as for least squares, we can show that the expeded de repression soft subtention model hypothesis N(Xu)625) $\mathbb{E}[w_{RR}] = (\lambda I + X^T X)^{-1} X^T X w, \quad \text{Var}[w_{RR}] = \sigma^2 Z (X^T X)^{-1} Z^T,$ where $Z = (I + \lambda (X^{T}X)^{-1})^{-1}$.

Covariate: a variable that is possibly predictive of the outcome under the study.

vector W by p	that our expected ridge solution relates to the true remultiplying by this matrix.
letting x	-> 0, experted, variance pevent to least square values.
V	experted, variance fevert to least square
	values.

*unbiased expected get " is the moth,

The expectation and covariance of w_{LS} and w_{RR} gives insight into how well we can hope to learn w in the case where our model assumption is correct. (manipular $y \sim N(xu) = 1$) is the consect model assumption.)

- ► Least squares solution: <u>unbiased</u>, but potentially high variance
- Ridge regression solution: biased, but lower variance than LS

So which is preferable?

Ultimately, we really care about how well our solution for w generalizes to new data. Let (x_0, y_0) be future data for which we have x_0 , but not y_0 .

- ▶ Least squares predicts $y_0 = x_0^T w_{LS}$ for new deta
- Ridge regression predicts $y_0 = x_0^T w_{RR}$

This who we care about how well are us going to do with future dota.

So inthis the model assumption that we've going to make, then the performance that we use on the new data to massive street gradity of sol should also take into

In keeping with the square error measure of performance, we could calculate squered ervor. the expected squared error of our prediction: given allogher previous de une ve seen oxplain.

$$\mathbb{E}\left[(y_0-x_0^T\hat{w})^2|X,x_0\right] = \int_{\mathbb{R}}\int_{\mathbb{R}^n}(y_0-x_0^T\hat{w})^2p(y|X,w)p(y_0|x_0,w)\,dy\,dy_0.$$
 Squared everyon fraction. Independing one has so the vertex Y ?

- ▶ The estimate \hat{w} is either w_{LS} or w_{RR} .
- ► The distributions on y, y_0 are Gaussian with the true (but unknown) $w_{response}$ • We condition on knowing x_0, x_1, \ldots, x_n . windsles post
- expones to test solacc. to distribution which distribution where welrove seen in the but & what In words this is saying:
 - Imagine I know X, x_0 and assume some true underlying w. Let re quity to see
 - ▶ I generate $y \sim N(Xw, \sigma^2 I)$ and approximate w with $\hat{w} = w_{LS}$ or $w_{RR}^{0^*}$.
 - But I don't get see to yourd ▶ I then predict $y_0 \sim N(x_0^T w, \sigma^2)$ using $y_0 \approx x_0^T \hat{w}$.

What is the expected squared error of my prediction?

W whole y!

We integrate over both the distribution of Y given X and W. So for a part and W, we calculate the distribution on Y. * * distribution of new restourse given true but unknown vector W. Was depended on vector y and motrix X.

So when we're integrating out Y-that integral is going to impact how

my functions in this meter is. I didn't understand, wouldy part come out? P3M: me're quine to see now this expected squared er vor of any rediction changes as a function of the data we have the con visite, xo has and also some true but unknown underlying regression coefficient vector don't get this) how can we live i neasure me wantying coefficient.

Calculations imply we're conditioning on n & no

Is the model considered in

We can calculate this as follows (assume conditioning on x_0 and X),

$$\mathbb{E}[(y_0-x_0^T\hat{w})^2]=\mathbb{E}[y_0^2]-2\mathbb{E}[y_0]x_0^T\mathbb{E}[\hat{w}]+x_0^T\mathbb{E}[\hat{w}\hat{w}^T]x_0$$

$$\text{we can say that the consequent of the single expectation.} \qquad \text{we con say that the expectation given } x$$

$$\mathbb{E}[x_0]=\mathbb{E}[y_0]\mathbb{E}[\hat{w}] = \mathbb{E}[y_0]\mathbb{E}[\hat{w}] = \mathbb{E}[y_0]\mathbb$$

wediction?



We can calculate this as follows (assume conditioning on x_0 and X),

$$\mathbb{E}[(y_0 - x_0^T \hat{w})^2] = \mathbb{E}[y_0^2] - 2\mathbb{E}[y_0]x_0^T \mathbb{E}[\hat{w}] + x_0^T \mathbb{E}[\hat{w}\hat{w}^T]x_0$$

- ► Since y_0 and \hat{w} are independent, $\mathbb{E}[y_0\hat{w}] = \mathbb{E}[y_0]\mathbb{E}[\hat{w}]$.
- ► Remember: $\mathbb{E}[\hat{w}\hat{w}^T] = \text{Var}[\hat{w}] + \mathbb{E}[\hat{w}]\mathbb{E}[\hat{w}]^T$

Plugging these values in:
$$\mathbb{E}[y_0^2] = \sigma^2 + (x_0^T w)^2$$
 where you with its now
$$\mathbb{E}[(y_0 - x_0^T \hat{w})^2] = \sigma^2 + (x_0^T w)^2 - 2(x_0^T w)(x_0^T \mathbb{E}[\hat{w}]) + (x_0^T \mathbb{E}[\hat{w}])^2 + x_0^T \text{Var}[\hat{w}]x_0$$

$$= \sigma^2 + x_0^T (w - \mathbb{E}[\hat{w}])(w - \mathbb{E}[\hat{w}])^T x_0 + x_0^T \text{Var}[\hat{w}]x_0$$
 shy ground that we will nearly whate the properties of the least squares / richer various of experiences of the desired values of the properties of the pr

We have shown that if

- 1. $y \sim N(Xw, \sigma^2)$ and $y_0 \sim N(x_0^T w, \sigma^2)$, and
- 2. we approximate w with \hat{w} according to some algorithm, then

$$\mathbb{E}[(y_0 - x_0^T \hat{w}$$

then
$$\mathbb{E}[(y_0 - x_0^T \hat{w})^2 | X, x_0] = \sigma^2 + x_0^T (w - \mathbb{E}[\hat{w}])(w - \mathbb{E}[\hat{w}])^T x_0 + x_0^T Var[\hat{w}] x_0$$

$$\text{Now rade off changes here.}$$

Now we see that the generalization error is a combination of three factors:

We see that the generalization error is a combination of three factors:

We see that the *generalization error* is a combination of three factors:

- 1. Measurement noise we can't control this given the model.
- 2. Model bias how close to the solution we expect to be on average. (UM)
- 3. Model variance how sensitive our solution is to the data.

We saw how we can find $\mathbb{E}[\hat{w}]$ and $\text{Var}[\hat{w}]$ for the LS and RR solutions.

then well we expect to do on new data given the algorithm that we used to approximate is with old data; is going to take into
that we used to approximate is with old data, is going to take into
CILICATOR I NOTE I POSE TERRILIS.
O simply the noise which we can never get nid of.
It's the noise of the ansor.
Of The second term is how close we expect our soll to be to the
_ trush. How hi ared is our solution.
3 The third term how much variance is therein our solution.
So a sold with low blas and very high variance, so no bias a bery high
So a sold with low blow but very high variance, so no bias I very high variance. We have I'm form equation but I red term night se manive.
ejudtoo but I've term night be marrive.
whereas, another rolly like the nide vegrenion solly. which has
some bigs but botentially much smaller variance, can trade off some
non-negative (naritive) value here (Ind ferm) for very migreduation
of the value here (TI) raterm) fonthe LS sda.
so that's the bias voicance tradeof.
n n

So we can, again, calculate the variance. So we can compare the variance of the ridge regression solution to the least-square solution. However, for the ridge regression solution, we don't know what w is. And so even though we can calculate this term, this entire term for least squares because w cancels here, for ridge regression, we still have w in this term. And so the bias really depends on what the value of w is. So we can make some statements, potentially about values for w that works out very well, or values of w where this term blows up. And also, the relationship of our solution to the new observation that we're trying to make a prediction for is factored in by using x-naught here.

BIAS-VARIANCE TRADE-OFF

This idea is more general:

- ▶ Imagine we have a model: $y = f(x; w) + \epsilon$, $\mathbb{E}(\epsilon) = 0$, $Var(\epsilon) = \sigma^2$
- We approximate f by minimizing a loss function: $\hat{f} = \arg \min_{f} \mathcal{L}_{f}$.
- We apply \hat{f} to new data, $y_0 \approx \hat{f}(x_0) \equiv \hat{f}_0$.

Then integrating everything out (y, X, y_0, x_0) :

$$\mathbb{E}[(y_0 - \hat{f}_0)^2] = \mathbb{E}[y_0^2] - 2\mathbb{E}[y_0\hat{f}_0] + \mathbb{E}[\hat{f}_0^2]$$

$$= \sigma^2 + f_0^2 - 2f_0\mathbb{E}[\hat{f}_0] + \mathbb{E}[\hat{f}_0]^2 + \operatorname{Var}[\hat{f}_0]$$

$$= \underbrace{\sigma^2}_{noise} + \underbrace{(f_0 - \mathbb{E}[\hat{f}_0])^2}_{squared \ bias} + \underbrace{\operatorname{Var}[\hat{f}_0]}_{variance}$$

This is interesting in principle, but is deliberately vague (What is f?) and usually can't be calculated (What is the distribution on the data?)

CROSS-VALIDATION

An easier way to evaluate the model is to use cross-validation.

The procedure for *K*-fold cross-validation is very simple:

- 1. Randomly split the data into *K* roughly equal groups.
- 2. Learn the model on K-1 groups and predict the held-out Kth group.
- 3. Do this *K* times, holding out each group once.
- 4. Evaluate performance using the cumulative set of predictions. The masters of how our model milestorm on unser dotal. For the case of the regularization parameter λ , the above sequence can be run for several values with the best-performing value of λ chosen.

The data you test the model on should never be used to train the model.

1	2	3	4	5	just the sum of
Train	Train	Validation	Train	Train	references on each leld-out

BAYES RULE

very useful for quantifying our unertainity in model parameters.

-> discurs it in the context of linear regression broblems so for.

PRIOR INFORMATION/BELIEF

Motiving through ridge regression. is not this just a constraint july are you industry thin the a measure of how measure of greating the we work with the vector with the detail which is detailed in the detail the detail

idge regression objective function that we have, the data
$$\mathcal{L} = \sum_{i=1}^{n} (y_i - x_i^T w)^2 + \lambda w^T w$$
. It is shown a wind that $y_i = 1$ in a sever it constraints w. It imposes who half of on the independent of the shown is dear that the

The regularization term $\lambda w^T w$ was imposed to penalize values in w that are large. This reduced potential high-variance predictions from least squares.

In a sense, we are imposing a "prior belief" about what values of w we consider to be good.

Question: Is there a mathematical way to formalize this?

Answer: Using probability we can frame this via Bayes rule.

REVIEW: PROBABILITY STATEMENTS

Imagine we have two events, A and B, that may or may not be related, e.g.,

- ightharpoonup A = "It is raining"
- ► B = "The ground is wet"

We can talk about probabilities of these events,

- ightharpoonup P(A) = Probability it is raining
- ▶ P(B) = Probability the ground is wet

We can also talk about their conditional probabilities,

- ▶ P(A|B) = Probability it is raining *given* that the ground is wet
- ▶ P(B|A) = Probability the ground is wet *given* that it is raining

We can also talk about their *joint* probabilities,

▶ P(A, B) = Probability it is raining *and* the ground is wet

CALCULUS OF PROBABILITY

There are simple rules from moving from one probability to another

1.
$$P(A,B) = P(A|B)P(B) = P(B|A)P(A)$$

1.
$$P(A,B)=P(A|B)P(B)=P(B|A)P(A)$$
2. $P(A)=\sum_b P(A,B=b)$ - Marginal probability. (When you add that extra word may not 3. $P(B)=\sum_a P(A=a,B)$ you're inhiping there's some additional event

that you've integrating or summing out. Using these three equalities, we automatically can say

$$P(A|B) = \frac{P(B|A)P(A)}{P(B)} = \frac{P(B|A)P(A)}{\sum_{a} P(B|A = a)P(A = a)}$$

$$P(B|A) = \frac{P(A|B)P(B)}{P(A)} = \frac{P(A|B)P(B)}{\sum_{b} P(A|B = b)P(B = b)}$$

This is known as "Bayes rule." Tallows us to grantify that we don't know want was. distributions. is marginal policy of a be joint washifty of a be

BAYES RULE

P(B|A) -> Porterior belief of unknown b, given the observation a.
P(A|B) -> Likelihood of socing what we saw given a contain setting for b.

Bayes rule lets us quantify what we don't know. Imagine we want to say something about the probability of B given that A happened. Ji keli hood of observing what we say Bayes rule says that the probability of B after knowing A is: P(B|A) = P(A|B)P(B) / P(A)The posterior likelihood prior marginal and the probability of B is the probability of B we have the probability of B and B we have the posterior likelihood prior marginal and the probability of B is the posterior of the posterior likelihood prior marginal and the probability of B is the posterior likelihood prior marginal and the probability of B is the posterior likelihood prior marginal and the probability of B is the posterior likelihood prior marginal and the probability of B is the posterior likelihood prior marginal and the probability of B is the probability of B is the posterior likelihood prior marginal and B is the probability of B is the

Notice that with this perspective, these probabilities take on new meanings.

That is, P(B|A) and P(A|B) are both "conditional probabilities," but they have different significance.

when we think about what we do and don't know. These menipulations on previous slide which are just simply conditional fjoint and marginal probabilities take on new meanitys.

BAYES RULE WITH CONTINUOUS VARIABLES

Bayes rule generalizes to continuous-valued random variables as follows. However, instead of probabilities we work with densities.

- ► Let θ be a continuous-valued model parameter. Si kelihood of dota.

 ► Let X be data we possess. Then by Bayes rule.

 Prior probability of model.

$$p(\theta|X) = \frac{p(X|\theta)p(\theta)}{\int p(X|\theta)p(\theta)d\theta} = \frac{p(X|\theta)p(\theta)}{\int p(X)} \quad \text{which it y of model}$$
 Posterior probability of the model parameter/variable given the values of the model. In this equation, dela we've observed.

So in this case, using Bayer rule for model Jeaning too possess, just maighted probabilities of the definition of the dotter.

$$p(X|\theta) \text{ is the likelihood, known from the model definition} \quad \text{of the dotter.}$$

- $\triangleright p(X|\theta)$ is the likelihood, known from the model definition.
- \triangleright $p(\theta)$ is a prior distribution that we define.
- ▶ Given these two, we can (in principle) calculate $p(\theta|X)$.

So for examp the likeliho generative di v uniables.	le the probability of the data given the model variable, which is od is known from the model definition. So we define some stribution on our data, given some model with its unknown.
b(0) → T	re by or wasability on the model variable & is also something

b(9) → The prior probability on the model variable s is also something that we're going to define.

p(O(x) > So what we want is the posterior probability of all model variables , and we can write that in terms of things that we know. And then the only question is whether we can calculate this integral (p(x(0)pcos) in the denominator in order to give a closel form analytic expression for the posterior brobability.

EXAMPLE: COIN BIAS (example) We are trying to learn the bias of the coin.

What it means to be independent: X. - Xn an independent of each other if the likelihood of all data is just equal to the product of likelihood of each observation.

We have a coin with bias π towards "heads". (Encode: heads = 1, tails = 0) independently

We flip the coin many times and get a sequence of n numbers $(\bar{x_1}, \dots, x_n)$. Assume the flips are independent, meaning

Bun oulli random vanishe
$$p(x_1,\ldots,x_n|\pi) = \prod_{i=1}^n p(x_i|\pi) = \prod_{i=1}^n \pi^{x_i} (1-\pi)^{1-x_i}.$$

We choose a prior for π which we define to be a beta distribution,

Q, b
$$> O$$
 (strictly positive)
$$p(\pi) = Beta(\pi|a,b) = \frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)}\pi^{a-1}(1-\pi)^{b-1}.$$

What is the posterior distribution of π given x_1, \ldots, x_n ? (the sequence that we've observed)

EXAMPLE: COIN BIAS

From Bayes rule,

likelihood of aparticulars equena given the coin bois stimes the prior on the coin bias.

$$p(\pi|x_1,\ldots,x_n) = \frac{p(x_1,\ldots,x_n|\pi)p(\pi)}{\int_0^1 p(x_1,\ldots,x_n|\pi)p(\pi)d\pi}.$$

There is a trick that is often useful:

 τ i sategradorer all pensible values τ can take.

- ► The denominator only normalizes the numerator, doesn't depend on π . ▶ We can write $p(\pi|x) \propto p(x|\pi)p(\pi)$. (" \propto " → "proportional to") is a functional to "when the two and see if we recognize anything:
 - (itely hood

$$\begin{array}{lll} p(\pi|x_1,\ldots,x_n) & \propto & \left[\prod_{i=1}^n \pi^{x_i} (1-\pi)^{1-x_i}\right] \left[\frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)} \pi^{a-1} (1-\pi)^{b-1}\right] \text{ removed to} \\ & \propto & \pi^{\sum_{i=1}^n x_i + a - 1} (1-\pi)^{\sum_{i=1}^n (1-x_i) + b - 1} \end{array}$$
 since we are washing with

We recognize this as $p(\pi|x_1,\ldots,x_n)=Beta(\sum_{i=1}^n x_i+a,\sum_{i=1}^n (1-x_i)+b)$

remaine the product of these I terms this remaining to appear was mumerature denominator, it's gama canadad.

So if we're	only interested in giving the bosterior as a function that's
brobondial.	Meaning the posterior is equal to this function times some no. It integrates to 1, we don't have to wany about any term like _ lied ordo function of bi, that doesn't i make bi.
Such that i	t integrates to 1, we don't have to worm about any term like _
that well's	und and a meeting of his that doesn't i make pi.
· · · · · · · · · · · · · · · · · · ·	med source footstation of bit, then was
Po we re	rguize any distributions that are proportial to this function.
	0 0
<u> </u>	Deta Beta
Andso her	e we have a posterior probability distribution on the bias
of the con	n takes justo account the prior and the data and gives
	•
us a me	asure of the uncertainity of what This as represented by
-	
this fun	ction.
5.13 400 .	O V - · · · ·

(we can now relate ridge regression to a probability distribution)

MAXIMUM A POSTERIORI

LIKELIHOOD MODEL

Least squares and maximum likelihood

When we modeled data pairs (x_i, y_i) with a linear model, $y_i \approx x_i^T w$, we saw that the least squares solution, (the value of w that whim zes to sum of squared errors.)

$$w_{LS} = \arg\min_{w} (y - Xw)^{T} (y - Xw),$$

was equivalent to the maximum likelihood solution when $y \sim N(Xw, \sigma^2 I)$. So we can view the LS soly probabilistic dry as being a max. Histilihood soly probabilistic connection can be made of the detailed of the connection can be made of the connection can be connected as the connection can be made of the connection can be connected as the connec for the ridge regression problem.

PRIOR MODEL

First, make an assumption of a prior model for the vector w.

y is greet ed from a multi-variate
Ridge regression and Bayesian modeling.

The likelihood model is $y \sim N(Xw, \sigma^2 I)$. What about a prior for w?

Let us assume that the prior for w is Gaussian, $w \sim N(0, \lambda^{-1}I)$. Then do not function and distribution $p(w) = \left(\frac{\lambda}{2\pi}\right)^{\frac{d}{2}} \mathrm{e}^{-\frac{\lambda}{2}w^T w}.$

We can now try to find a w that satisfies both the data likelihood, and our prior conditions about w.

MAXIMUM A POSERIORI ESTIMATION

Maximum a poseriori (MAP) estimation seeks the most probable value w

under the posterior: $\begin{array}{ll} \text{posterior A istribution of we given} \\ \text{So this is what we maximise} \\ \text{want to with mattery maximise} \\ \text{over w.} \end{array} = \arg\max_{w} \ln \frac{p(y|w,X)p(w)}{p(y|X)}$

Contrast this with ML. which only focuses on the likelihood. Ty given X we have added 2 terms. O (or of prior) Additional turn that armit actually instrum. The normalizing constant term $\ln p(y|X)$ doesn't involve w. Therefore, we can maximize the first two terms alone of w that maximize (ay max) & w

▶ In many models we don't know $\ln p(y|X)$, so this fact is useful.

(innowy models we court calculate this integral in dosed form.

MAP FOR LINEAR REGRESSION

MAP using our defined prior gives:

Ji Wellhood Prior. $w_{\text{MAP}} = \arg \max_{w} \ln p(y|w,X) + \ln p(w)$ $= \arg \max_{w} -\frac{1}{2\sigma^{2}}(y - Xw)^{T}(y - Xw) - \frac{\lambda}{2}w^{T}w + \text{const.}$

Calling this objective \mathcal{L} , then as before we find w such that removed (austral) that don't import was gradient of $\nabla_w \mathcal{L} = \frac{1}{\sigma^2} X^T y - \frac{1}{\sigma^2} X^T X w - \lambda w = 0$ the sol $^{\text{L}}$.

- ► The solution is $w_{\text{MAP}} = (\lambda \sigma^2 I + X^T X)^{-1} X^T v$.
- Notice that $w_{\text{MAP}} = w_{\text{RR}}$ (modulo a switch from λ to $\lambda \sigma^2$)
- Trust like least squares soft maximizes the posterior, while LS maximizes the likelihood. I trust like least squares soft maximizes the idelihood. So it conepado to mox. Likelihood soft Ridge regression maximizes the posterior under Comply redefined original formation converbables the map soft. Uls = WML WRE = Wmap to is the individual original policy of the individual original original