

Regularization for linear models

L1 (Lasso), L2 (Ridge)

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MIGHT BE MOST POPULAR
INTERVIEW QUESTION



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Motivation for regularization

- 3 main problems with least-squares (OLS) regression:
 - Model with “too many” parameters (e.g., neural nets) will overfit
 - Data sets w/outliers can skew line too much to fit outliers; bad generalization
 - Data sets w/many features can get extreme coefficients in linear models (see notebook “L1 regularization with normalization”)
- Often unregularized models work but we get extreme coefficients (extreme negative and positive coefficients must be canceling out)
- L1 (Lasso) regularization also has the advantage that it allows superfluous coefficients to shrink to zero
- Having zero coefficients helps reduce model complexity (fewer coefficients), improving interpretability and usually improving generality

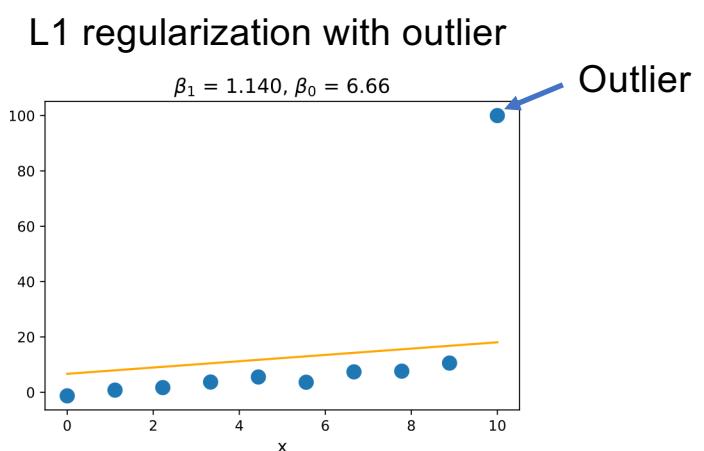
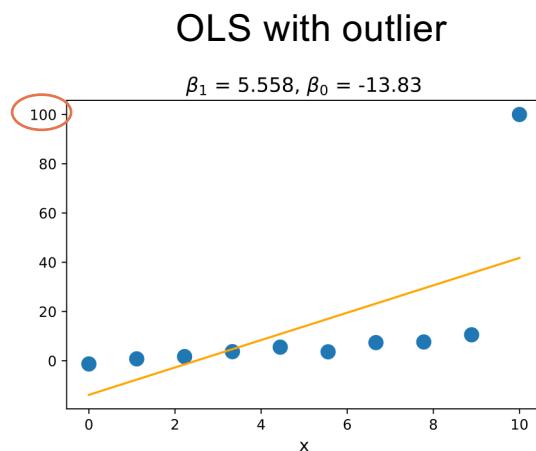
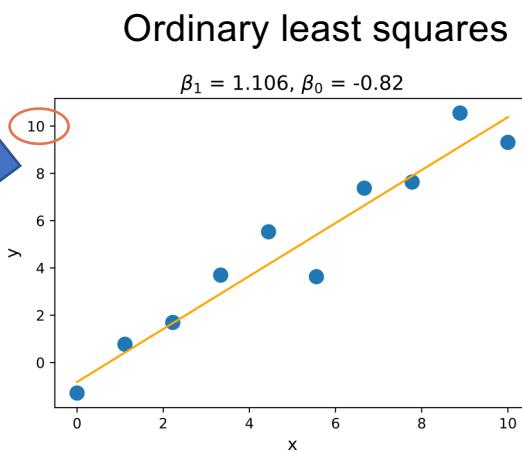
See <https://github.com/parrt/msds621/blob/master/notebooks/linear-models/regressor-regularization.ipynb>

Regularization premise

- Extreme coefficients are unlikely to yield good generalization
- So, we're simply going to constrain model coefficient magnitudes
- Same technique works for linear and logistic regression
(logistic is just a sigmoid of output of linear model anyway)
- Preview: add L1 or L2 norm of β coefficient vector to loss function

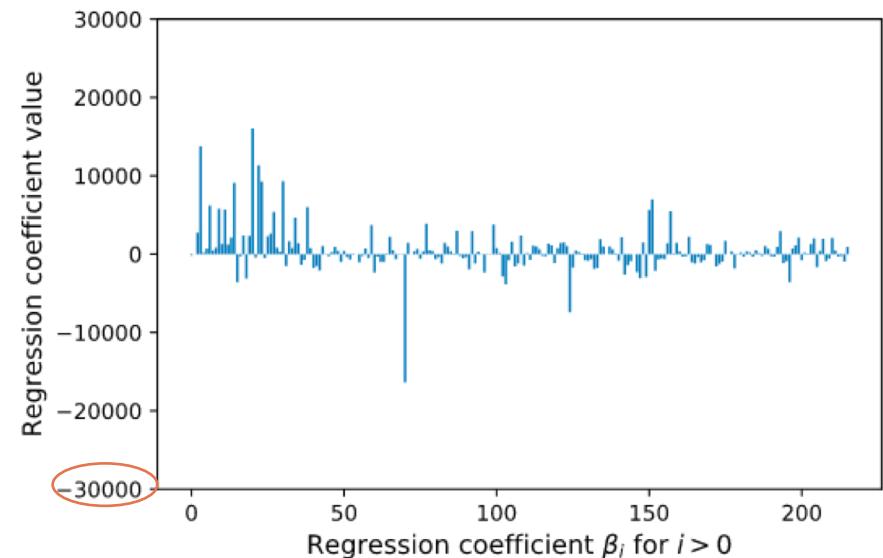
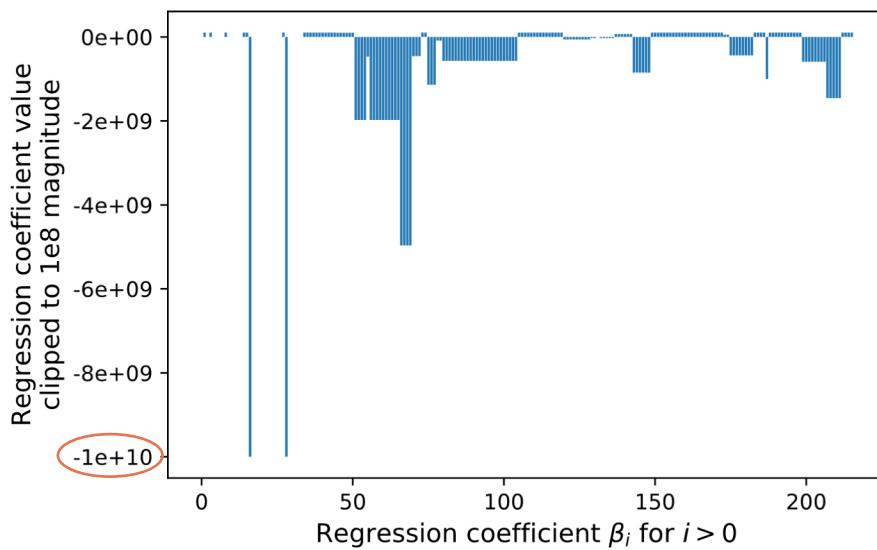
Let's make a deal!

- Let's trade some model bias for improved generality
- Consider an example of a simple data set with OLS fit
- Now, send $y[x==10]$ to 100; we get skewed line & bad R^2
- Regularization brings slope back down but with some bias



Ames housing data set (regressor)

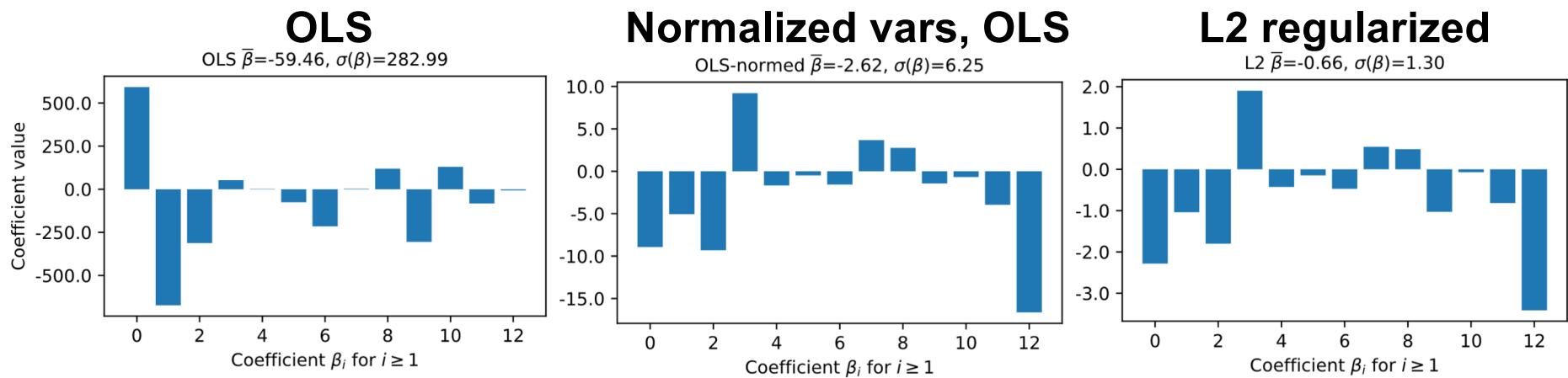
- With dummy vars, number of columns explodes from 81 to 216
- Compare scale of coeff (huge coefficients don't generalize)
- Regressor test R² is -1e6 w/o L2 regularization and ~0.82 with



See <https://github.com/parrt/msds621/blob/master/notebooks/linear-models/regressor-regularization.ipynb>

Wine classifier less accurate w/o reg.

- Wine data set (130 records, 14 numeric vars)
- Test accur=.96 (normalized data) w/OLS; accur=1.0 w/regularization
- L2 regularization 1.0 test score
- L1 regularization still .96 but can drop 4 coefficients from model



See <https://github.com/parrt/msds621/blob/master/notebooks/linear-models/classifier-regularization.ipynb>

Example: classifier w/ too many features

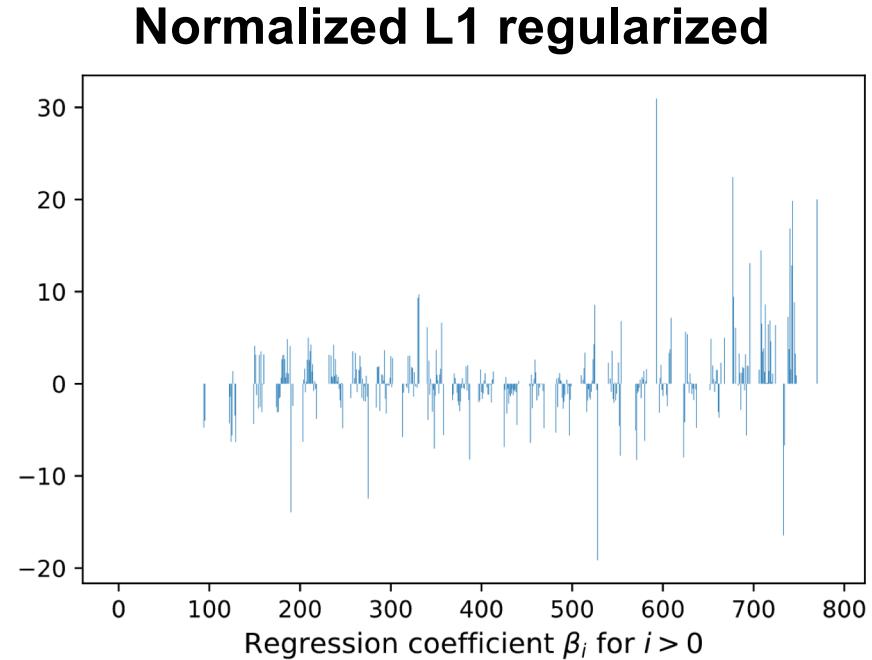
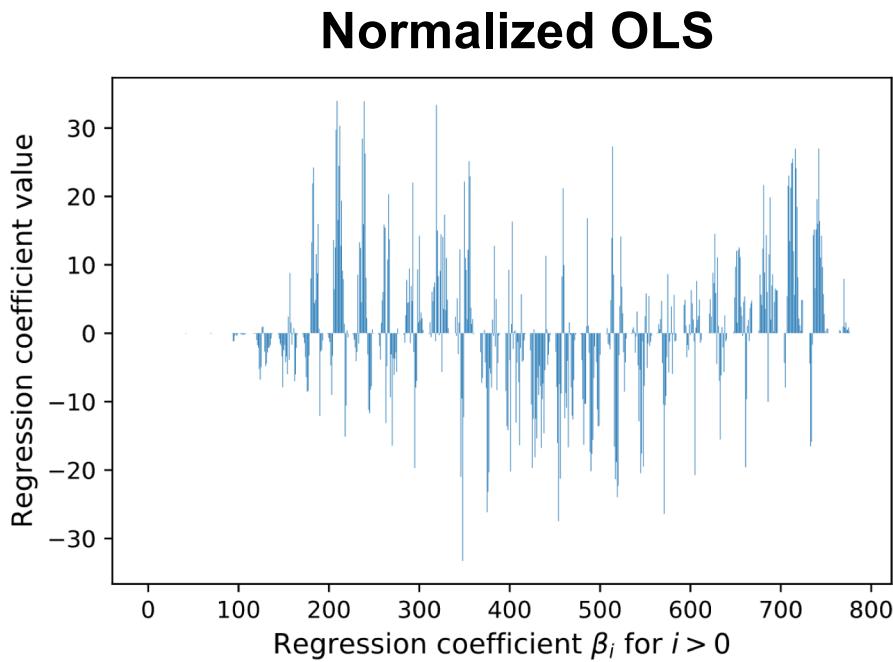
- Distinguish between ones and sevens (MNIST dataset)

MNIST sample	ones sample	sevens sample
3 8 6 9 6	1 1 1 1 1	7 7 7 7 7
4 5 3 8 4	1 1 1 1 1	7 7 7 7 7
5 2 3 8 4	1 1 1 1 1	7 7 7 7 7
8 1 5 0 5	1 1 1 1 1	7 7 7 7 7
9 7 4 1 0	1 1 1 1 1	7 7 7 7 7

See <https://github.com/parrt/msds621/blob/master/notebooks/linear-models/classifier-regularization.ipynb>

Compare coefficients w/o & with L1 reg

- Test accur=0.96 (normalized data) w/OLS and w/L1 but log loss drops a lot
- L1 regularization has zeroed out lots of coefficients and still accurate!



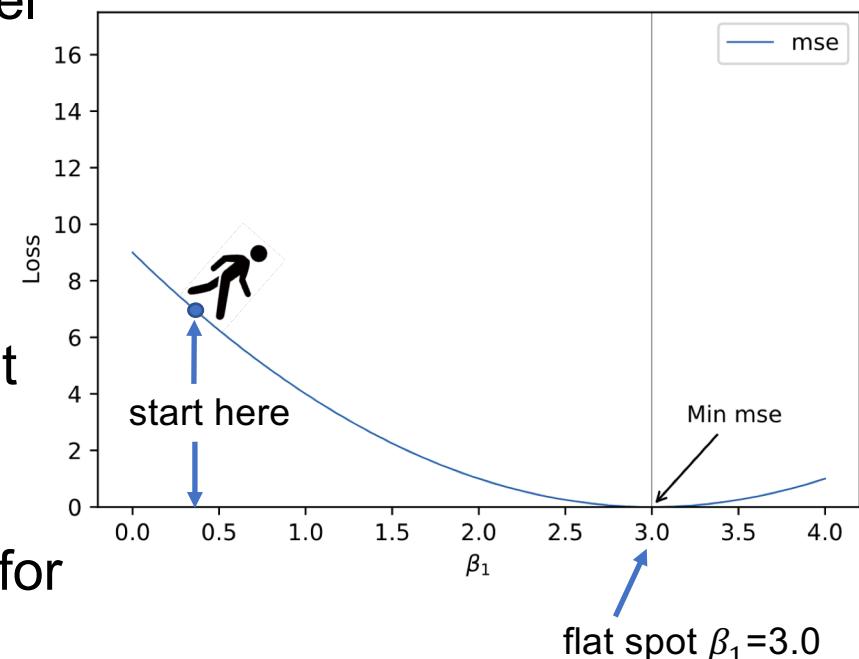
The regularization mechanism

The goal: Don't let optimization get too specific to training data; inhibit best fit

The cost: Sacrifice some model bias (underfit) for generality

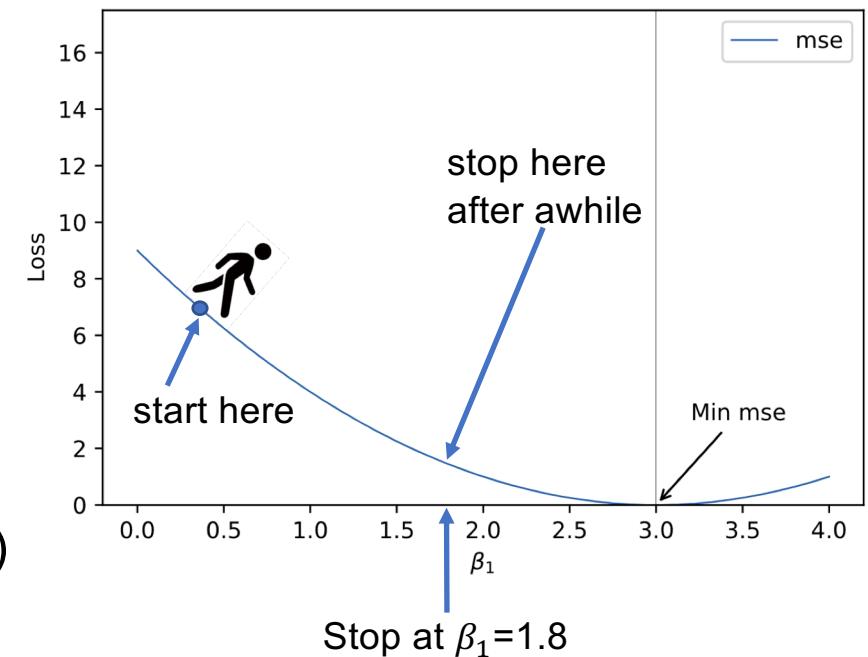
Detour: How training works in 1 dimension

- Loss function (cost) is a function of model parameters (betas) and data set
- Minimize MSE loss computed on the **training set**
- Loss is a quadratic $(y - \hat{y})^2$ so pick a random starting point for β_1 and then just walk β_1 downhill until you hit flat spot
- The derivative/slope of loss function is 0 at the minimum loss
- The β_1 at loss minimum is best fit coeff. for training set
- (We'll have full lecture on gradient descent, don't worry!)



Simplest regularization

- Just terminate minimization process early; don't let the coefficients fully reach the minimal loss location
- (Called *early stopping* in neural nets)
- Walk “downhill” on training set loss curve until either:
 - You run out of AWS CPU credits
 - After fixed amount of time (you're bored)
 - Loss on **validation set** starts going up, not down

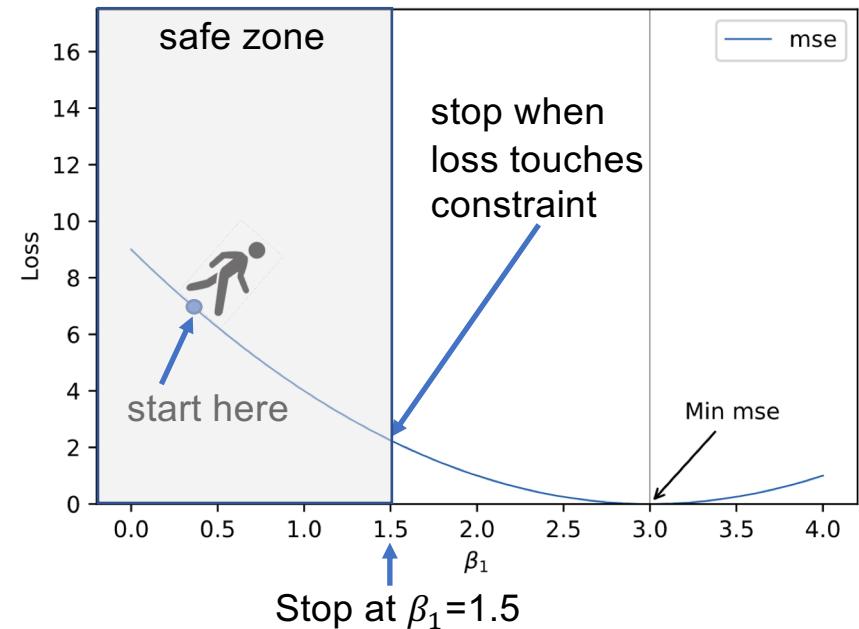


Improving early termination of training

- Stopping after fixed amount of time depends on how fast our “hiker” moves along loss curve and it’s hard to pick duration
- Instead, let’s just restrict magnitude of $\beta_1 < t$ for some t
- Pick initial β_1 in $[0,t)$ and go downhill and stop at minimum or when $\beta_1 \geq t$

Minimizing subject to a *hard constraint*

- Let $t=1.5$, which defines “safe zone”
- Stop at min loss point or $\beta_1 = t$
- The “best” coefficient is where constraint t and loss function meet, if min loss is outside safe zone
- If min loss is in safe zone, then regularization constraint wasn’t needed (same as OLS)



Minimizing in 2D subject to hard constraint

- Spin line segment $[0,t]$ around origin 360° , gives a circle
- Recall formula for circle; constrain β_i such that $\beta_1^2 + \beta_2^2 < t$ where t is radius squared
- The “best” coefficient is min loss function **on constraint curve** (if loss min outside zone)
- If loss min inside radius, same as OLS
- Pick initial $[\beta_1, \beta_2]$ inside safe zone, then start walking downhill, stop at min loss or edge of the safe zone
- **This is L2 (Ridge) regularization**
$$\sum_{j=1}^p \beta_j^2 < t$$

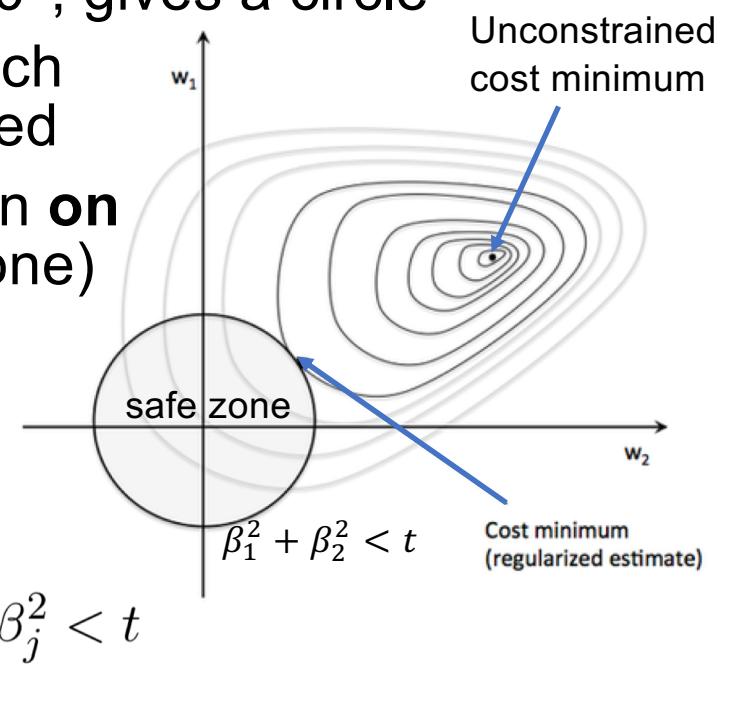


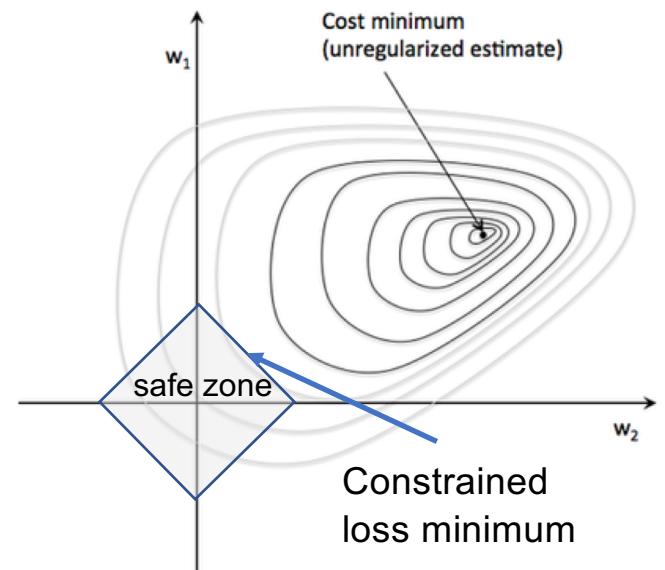
Image credit: <https://www.kdnuggets.com/2016/06/regularization-logistic-regression.html>

Minimizing L1 in 2D (hard constraint)

- Instead, we can sum the $|\beta_i|$'s not β_i^2 's, giving diamond-shaped safe zone
- **This is L1 (Lasso) regularization**

$$\sum_{j=1}^p |\beta_j| < t$$

- Notice how statisticians have this backwards; L1 constraint zone looks like a ridge not lasso, and L2 safe zone (circle) looks like a lasso



Fitting regularized linear model (Conceptually)

- Minimize the usual MSE loss function:

$$\mathcal{L}(\beta) = \sum_{i=1}^n (y^{(i)} - (\mathbf{x}'^{(i)} \cdot \beta))^2$$

- Subject to either (L2 or L1):

$$\sum_{j=1}^p \beta_j^2 < t \quad \text{or} \quad \sum_{j=1}^p |\beta_j| < t$$

- Problem is “subject to” constraint is hard to implement

Detour: Lagrange Multipliers

- Magic of Lagrange multipliers lets us incorporate constraint into loss function:

$$\mathcal{L}(\beta) \text{ s.t. } \sum_{j=1}^p \beta_j^2 \leq t \text{ same as}$$

$$\mathcal{L}(\beta, \lambda) = \mathcal{L}(\beta) + \lambda \left(\sum_{j=1}^p \beta_j^2 - t \right) \text{ for some } \lambda$$

(λ and t are related one-to-one per ESLII book
but by no relationship I can find)

How we *actually* fit regularized models

- Minimizing loss function subject to a constraint is harder to implement than just function minimization
- Invoke magic of Lagrange

$$\text{For L2: } \mathcal{L}(\beta) + \lambda \sum_{j=1}^p \beta_j^2$$

$$\text{For L1: } \mathcal{L}(\beta) + \lambda \sum_{j=1}^p |\beta_j|$$

- Drop t since t is constant & doesn't affect minimizing
- This is a **soft constraint** and penalty increases as β_i 's move away from origin; *there's no hard cutoff!*
- Net effect is that regularization pulls min loss location closer to origin!

Fitting both β_i 's and hyperparameter λ

- λ is unknown like t but at least we have a single function now
- Find λ by finding minimum loss for different λ values, pick λ that gets min loss on validation set

$$\mathcal{L}(\beta) + \lambda \sum_{j=1}^p \beta_j^2$$

$$\mathcal{L}(\beta) + \lambda \sum_{j=1}^p |\beta_j|$$

- β_0 is just \bar{y} , assuming zero-centered data set (next slide)
- **Note:** β_0 is NOT included in penalty, but is used in $\mathcal{L}(\beta)$

Normalizing/standardizing data

- Regularization requires that you normalize your data set
- Zero center each variable and divide by the standard deviation

$$x^{(i)} = \frac{(x^{(i)} - \bar{x})}{\sigma_x}$$

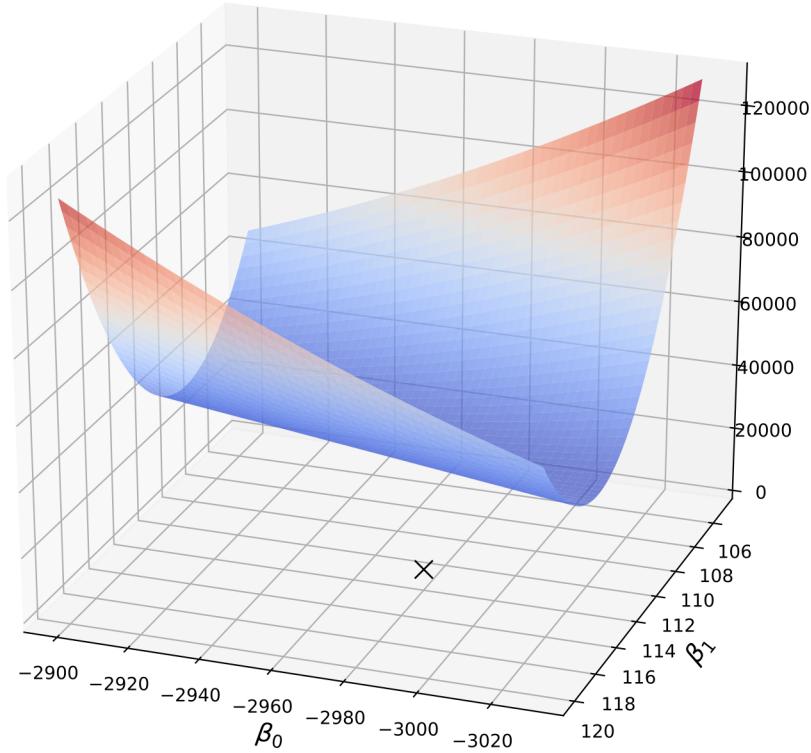
- Computing β_0 as simply mean(y) for L1/L2 linear regression requires normalization

More reasons to standardize variables

- We have just one λ for all coefficients so vars must be in same range or big β 's prevent regularization of small coefficients (big var ranges cause big β 's)
- Finding coefficients is often more efficient for normalized data
 - Loss contours for normalized vars are less erratic due to nature of finite precision floating point; operations (like subtraction) on data in very different ranges are ill-conditioned
 - Loss contours for normalized vars are more spherical and yield gradients that point more directly at min loss
 - If x_1 is in [0, 100] and x_2 in [0, 0.001], then a **single** learning rate, η , that is small enough for x_2 (so we converge) is too slow for x_1

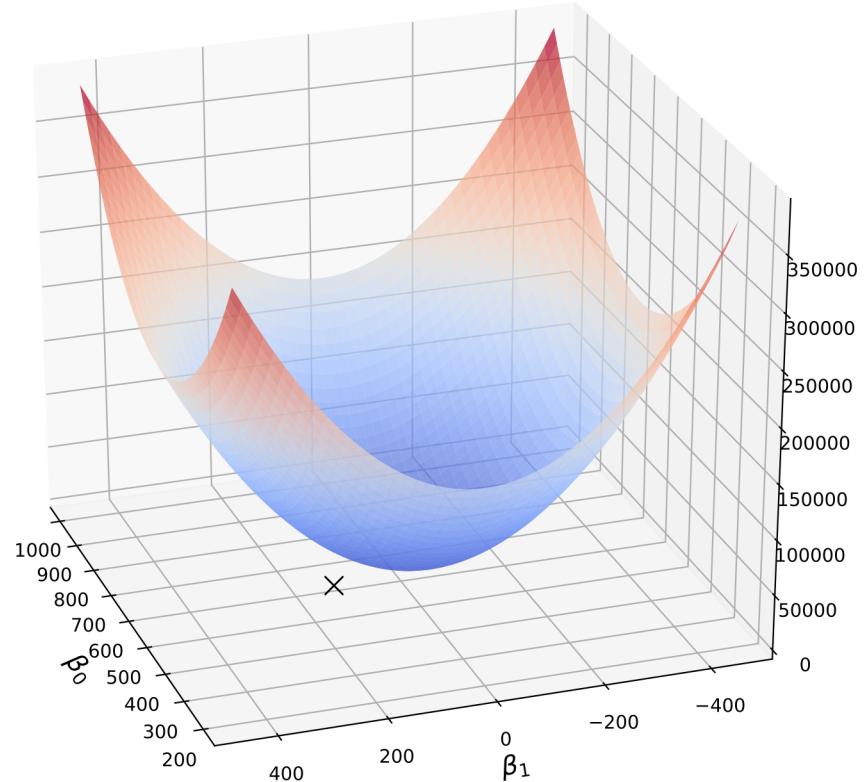
$$\lambda \sum_{j=1}^p \beta_j^2$$

Loss function shape for normalized vars



Untouched variables

Cheese consumption vs bedsheets strangulation death data set

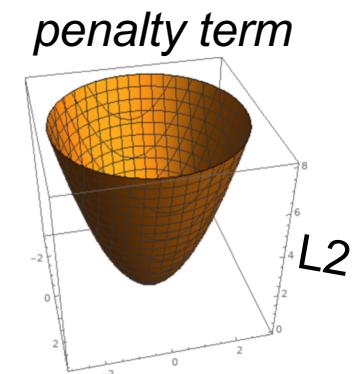


Normalized variables

See <https://github.com/parrt/msds621/blob/master/notebooks/linear-models/viz-gradient-descent.ipynb>

How penalty term restricts β_i 's

- Think of regularization as two different cost functions, MSE and regularization, added together
- L2 loss increases with the sum of squared coefficients
- L1 loss increases with sum of coefficient magnitudes
- Regularization penalty term **increases loss** but skews min loss β_i location towards origin as penalty curve is anchored at origin
- L1&L2 **shift** β_i 's **towards 0** because penalty approaches 0 only at $\beta=0$
- Soft constraint makes larger β_i very unlikely due to increased penalty away from origin (hard constraint makes large coefficients $> t$ impossible)

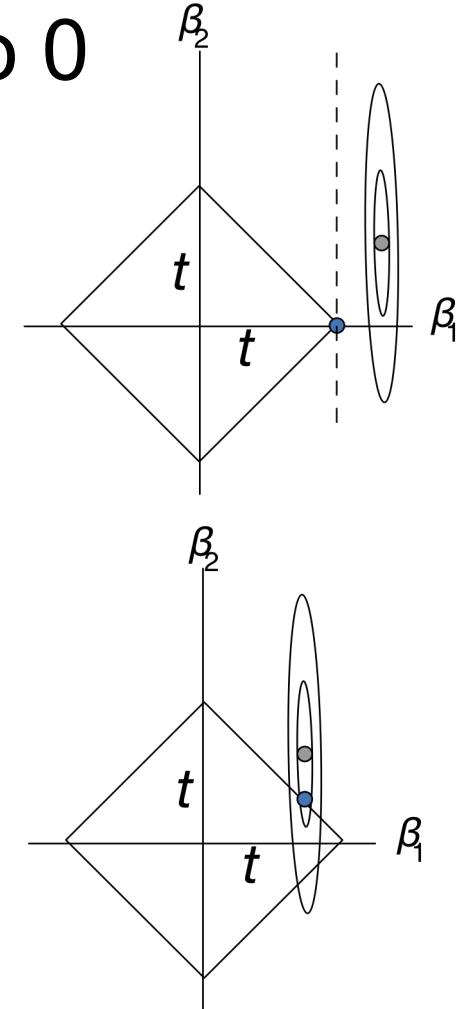
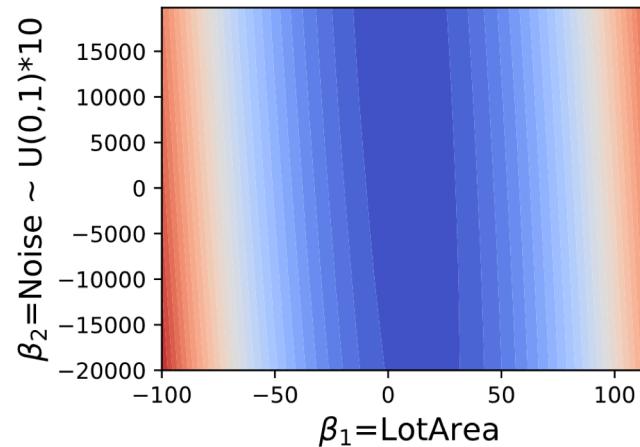


The effect of regularization

- What happens when λ is 0? Regularization is turned off
- What happens when we crank up λ ? Loss function strives for small β
- Pushing λ higher with L1 pushes more coefficients to 0
- L1 does not discourage β_i from fading to 0, but L2 discourages
- Squaring coefficients for L2 in constraint discourages any single β_i from getting much bigger than the others; squeezes β_i 's together
- λ is independent of training data, so can reduce model's dependence on data during fit, which regularizes model

L1 shifts non-predictive coefficients to 0

- Assume we have 2 vars, β_1 is useful but β_2 is noise
- Loss function contours are elliptical with vertical or nearly vertical major axis
- Moving in β_2 dir doesn't cost much but β_1 movement is very expensive so L1 regularization will sacrifice β_2 before β_1
- Ames example,
 $(\text{LotArea}, \text{Noise}) \rightarrow y$
loss function



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Theoretical support

Rosset, S., Zhu, J. & Hastie, T. : Boosting as a regularized path to a maximum margin classifier.
Journal of Machine Learning Research **5** (2004) (Aug):941-973

Appendix B. Uniqueness and Existence Results:

$$\min_{\|\beta\|_1 \leq c} \sum_{i=1}^n C(y_i, \beta' h(\mathbf{x}_i)) \quad (33)$$

Theorem 3 Assume that the unconstrained solution for problem (33) has l_1 norm bigger than c . Then there exists a solution of (33) which has at most n non-zero coefficients.

So, if the min location is outside of “safe zone”, then at most all coeff are non-zero but they go on to point out we get more zeros as size of safe zone increases:

4. Convergence of the solutions to sparse solution, as c increases

Lab time

- Exploring regularization for linear regression
<https://nbviewer.jupyter.org/github/parrt/msds621/blob/master/labs/linear-models/regularization-regr.ipynb>
- Note: that link is for viewing since github screws that up; you will need to go to the course repo to get interactive labs
<https://github.com/parrt/msds621/tree/master/labs/linear-models>

Regularized logistic regression

Optimizing likelihood with penalty terms

- Same mechanism, minimizing (**negation** of maximum likelihood) via Lagrangian interpretation:

$$\mathcal{L}(\beta, \lambda) = - \sum_{i=1}^n \left\{ y^{(i)} \mathbf{x}'^{(i)} \beta - \log(1 + e^{\mathbf{x}' \beta}) \right\} + \lambda \sum_{j=1}^p \beta_j^2$$

$$\mathcal{L}(\beta, \lambda) = - \sum_{i=1}^n \left\{ y^{(i)} \mathbf{x}'^{(i)} \beta - \log(1 + e^{\mathbf{x}' \beta}) \right\} + \lambda \sum_{j=1}^p |\beta_j|$$

Note: β_0 is NOT included in penalty, but is used in $\mathcal{L}(\beta)$ term

Fitting logistic regression β_i 's and λ

- ESLII book p125 says to find L1 β_0 and $\beta_{1..p}$ that maximize:

$$\max_{\beta_0, \beta} \left\{ \sum_{i=1}^N \left[y_i(\beta_0 + \beta^T x_i) - \log(1 + e^{\beta_0 + \beta^T x_i}) \right] - \lambda \sum_{j=1}^p |\beta_j| \right\}. \quad (4.31)$$

- We minimize the negative of that to find β of max likelihood
- Means we must find β_0 differently than for $\beta_{1..p}$
- As before, find λ by computing minimum loss for different λ values, pick λ that gets min loss on validation set

L1 Logistic gradient is tricky to get right

Algorithm: $L1NegLogLikelihood(\mathbf{X}', \mathbf{y}, \beta')$

$err = \mathbf{y} - \sigma(\mathbf{X}' \cdot \beta')$ (*error vector is $n \times 1$ column vector*)
 $\frac{\partial}{\partial \beta_0} = mean(err)$ (*usual log-likelihood gradient; use current β'*)
 $r = \lambda \text{sign}(\beta')$ (*regularization term $p + 1 \times 1$ column vector*)
 $r[0] = 0$ (*kill β_0 position but keep as $p + 1 \times 1$ vector*)
 $\nabla = \frac{1}{n} \left\{ \mathbf{X}'^T err - r \right\}$
return $- \begin{bmatrix} \frac{\partial}{\partial \beta_0} \\ \nabla_1 \\ \vdots \\ \nabla_p \end{bmatrix}$

Resources with code

- <https://aimotion.blogspot.com/2011/11/machine-learning-with-python-logistic.html>
- <https://stackoverflow.com/questions/38853370/matlab-regularized-logistic-regression-how-to-compute-gradient>
- You may look at but not cut-paste from these examples for your project (and I think there are some bugs too)

Key takeaways

- Regularization increases generality at cost of some bias
- Does so by restricting size of coefficients with hard constraint (conceptually) or soft constraint using penalty term (impl.)
- For hard constraint, min loss inside safe zone or on zone border
- Soft constraint penalty just makes bigger parameters less likely
- L2 discourages any β_i from getting much bigger than the others
- L1 does not discourage β_i from fading to 0, but L2 discourages
- For $\beta < 1$, β^2 gets smaller, not bigger; L2 can't push β to left very much near 0 as it's shifting by fraction of β
- In practice, we see L1 zero out unpredictive vars

Key implementation details

- Minimize $\mathcal{L}(\beta, \lambda)$ by trying multiple λ and choosing parameters from fitted model getting lowest **validation** error
- Always normalize X before fitting models
- If 0-centered x_i then $\beta_0 = \text{mean}(y)$ for L1 and L2 regression
- Logistic regression has no closed form for β_0
- OLS & L2 regularized linear regression have symbolic solutions
- L1 linear regression and L1/L2 logistic regression require iterative solution: usually some gradient descent variation

Interview questions (L1 vs L2)

- Both L1 and L2 increase bias (reduce "accuracy" of fit, predictions)
- L1 useful for variable / feature selection as some β_i go to 0
- L2 useful when you have collinear features (e.g., both tumor radius and tumor circumference features)
 - Collinearity increases coefficient variance, making them unreliable
 - And L2 reduces variance of β_i estimate which counteracts effect of collinearity
- With regularization, we don't get unbiased β_i estimates
 - Expected value of β_i estimate is no longer β_i since we've constrained β_i 's
 - Consequence: we no longer know effect of x_i on target y via β_i
- In my experiments, regularization improves regression much more than classification in terms of R^2 and simple accuracy; (due to sigmoid constraining the solutions to the loss function?)

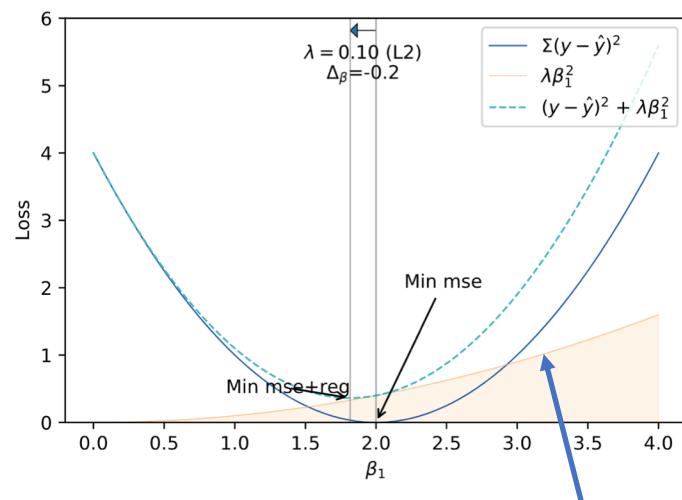
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EPILOGUE:

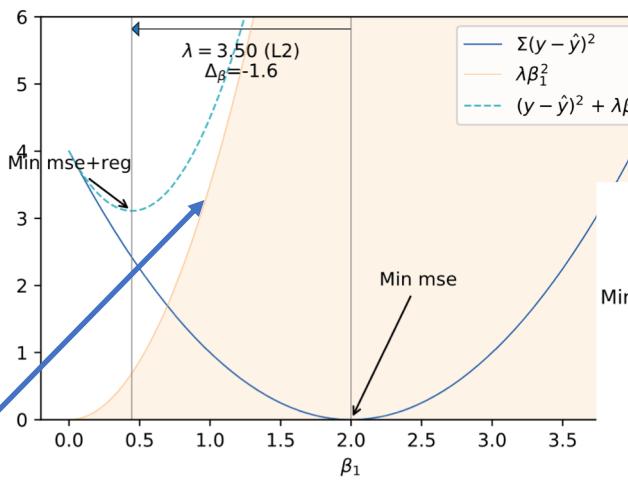
More on the effect of increasing hyper parameter λ

Visual effect of increasing λ for L2 (single variable)

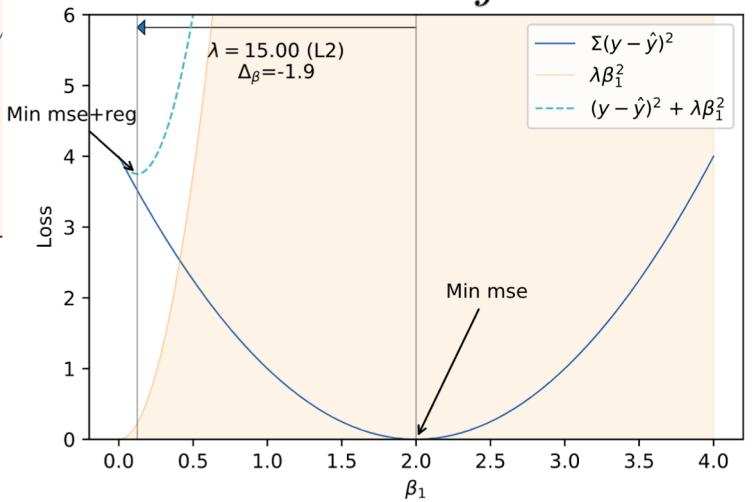


Takes roughly $\lambda = 300$ to get β_1 to 0!

$$\mathcal{L}(\beta) + \lambda \sum_{j=1}^p \beta_j^2$$



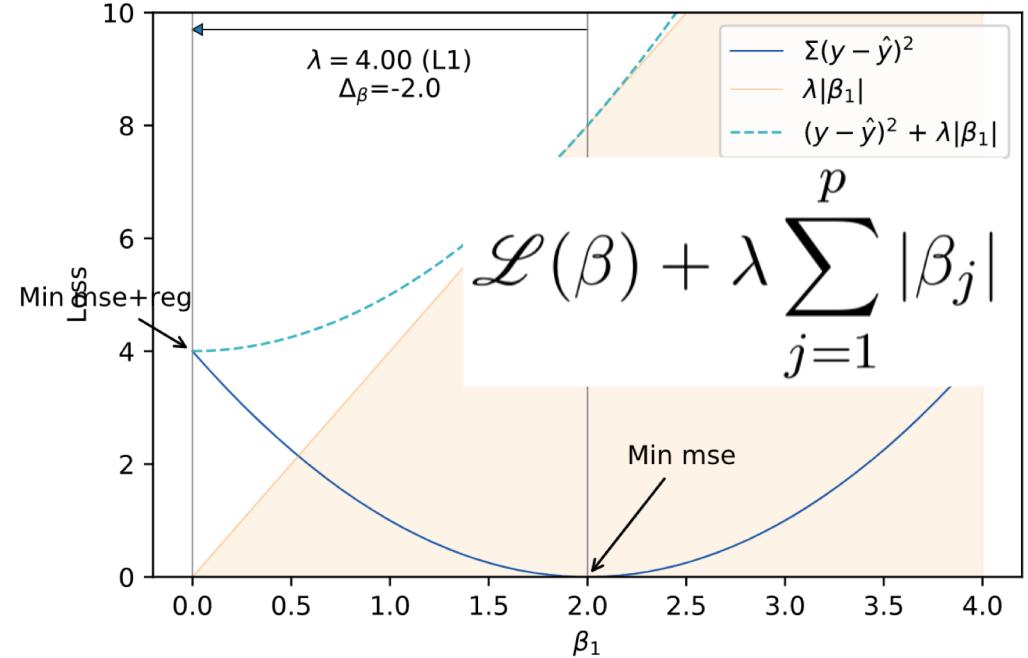
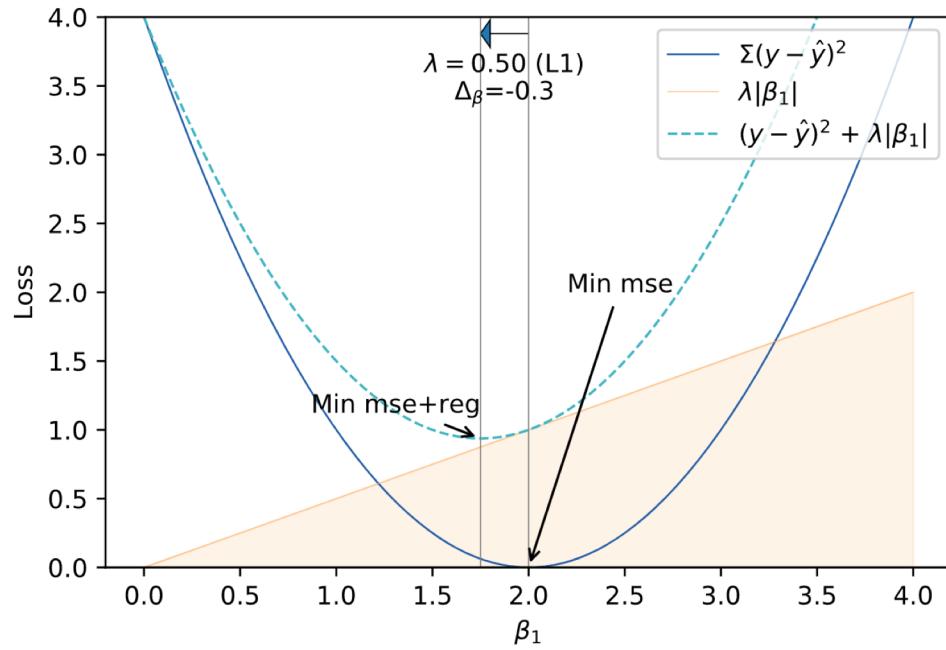
Decelerating increase in loss,
decelerating shift of β_1 towards 0



See <https://github.com/parrt/msds621/blob/master/notebooks/linear-models/viz-regularization.ipynb>

Visual effect of increasing λ for L1

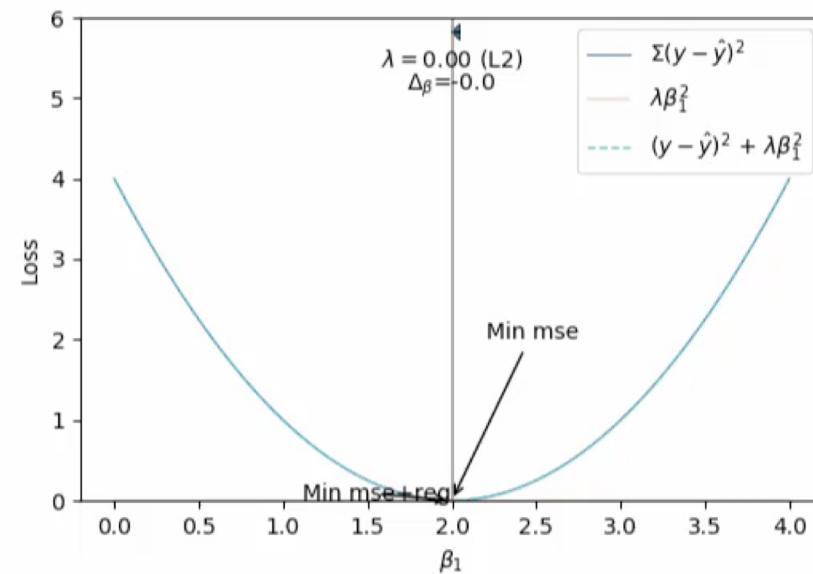
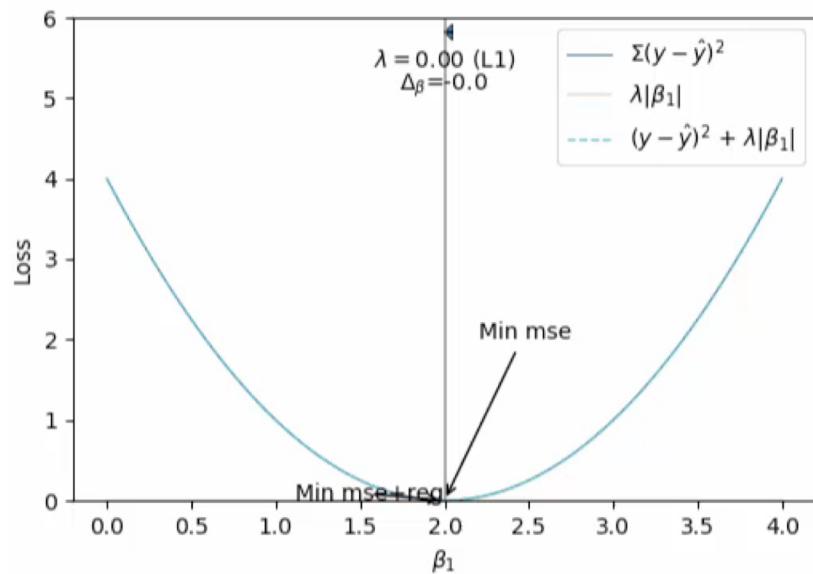
Smooth/linear increase in loss and shift of β_1 towards 0
Doesn't take huge λ to get β_1 to 0



See <https://github.com/parrt/msds621/blob/master/notebooks/linear-models/viz-regularization.ipynb>

L1 vs L2 regularization visually

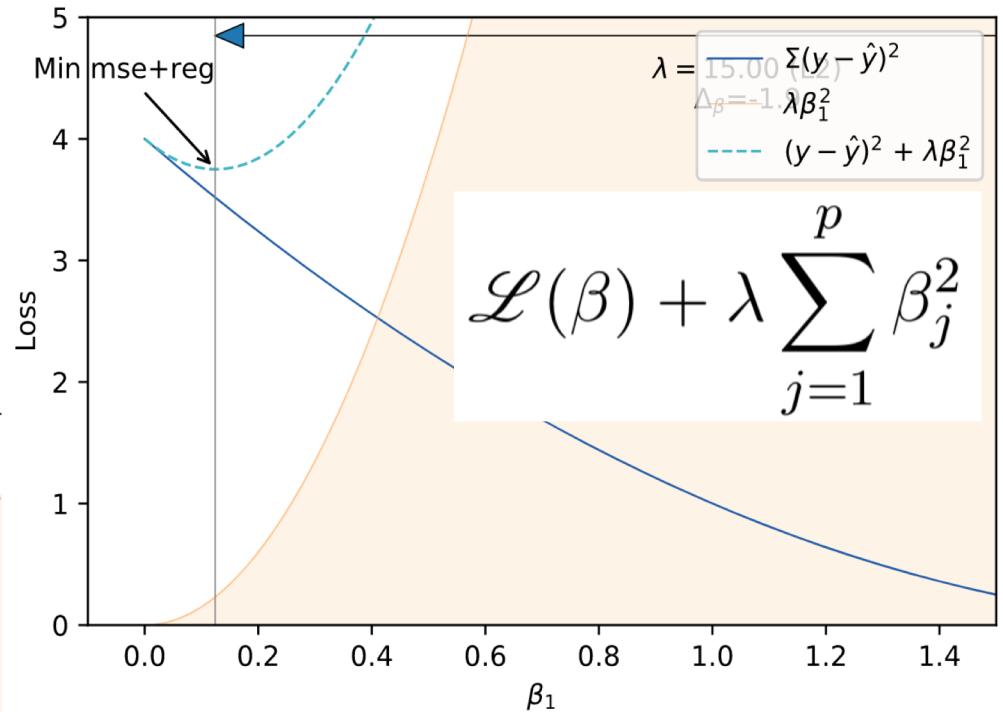
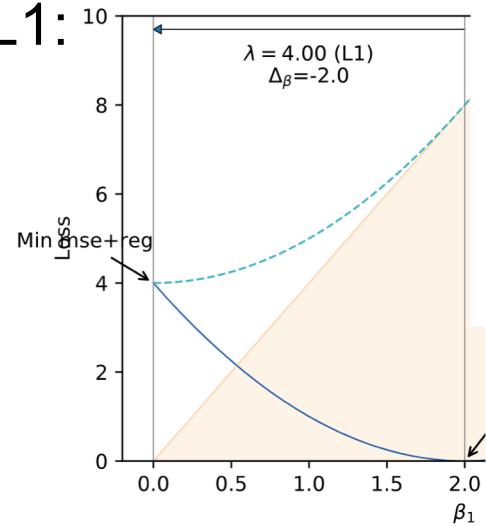
- Notice how L1 has no problem pushing β to 0 whereas L2 struggles to get there (this is a video page)



Animations from: <https://github.com/parrt/msds621/blob/master/notebooks/linear-models/viz-regularization.ipynb>

Zoom in on L2 trying to push β to 0

- For $\beta < 1$, β^2 gets smaller, not bigger
- Since β decelerates, L2 can't push β to left quickly near 0
- Compare to L1:



Why L1 can yield $\beta_i=0$ (and why not L2?)

- (p=1) Derivative of L2 penalty term w.r.t β is $2\lambda\beta$, which is the increase in loss due to penalty term; $2\lambda\beta$ vanishes as $\beta \rightarrow 0$
- When $\beta < 1$, L2 adds a fraction of λ to loss each time; asymptotic
- The closer it comes to 0, the slower the increase in loss & shift in β associated with min loss
- For L1, derivative is just $\lambda\text{sign}(\beta)$, independent of β magnitude, so loss increases at same rate (λ) even near $\beta = 0$

$$\mathcal{L}(\beta) + \lambda \sum_{j=1}^p \beta_j^2$$

$$\mathcal{L}(\beta) + \lambda \sum_{j=1}^p |\beta_j|$$

Why/when L1 encourages 0 coefficients

- In practice, we see L1 zero out unpredictive variables for large p (p is number of features) or when λ gets big enough
- There's a theorem that says $P(\beta_i = 0) \rightarrow 1$ as $p \rightarrow \infty$
- As $p \rightarrow \infty$, diamond shape collapses in on itself to a point
- Distance between discontinuities (feasibility points / axis crossings) approaches zero, making it less likely β_i sits on an edge of the diamond; mostly likely sits at a discontinuity
- Uminsky drew a picture that convinced me 0's are more likely and I came up with a drawing showing 0's more likely for nonpredictive variables...(but we're way off our scope here 😊)