

Regularization for linear models

L1 (Lasso), L2 (Ridge)

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MIGHT BE MOST POPULAR
INTERVIEW QUESTION



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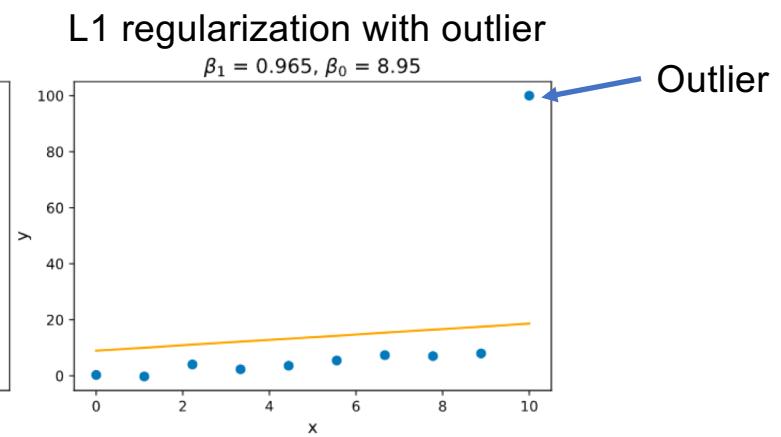
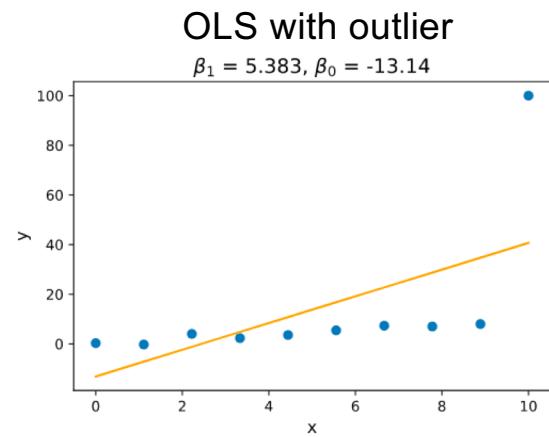
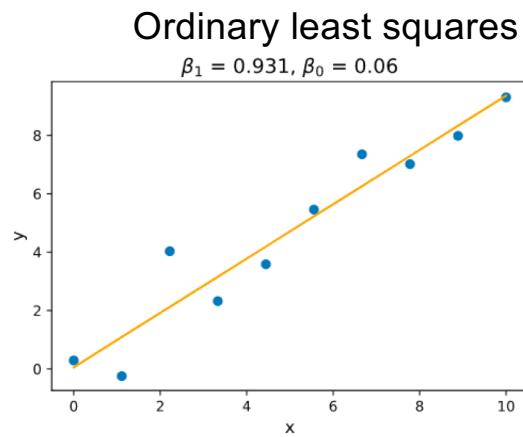
Motivation for regularization

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

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

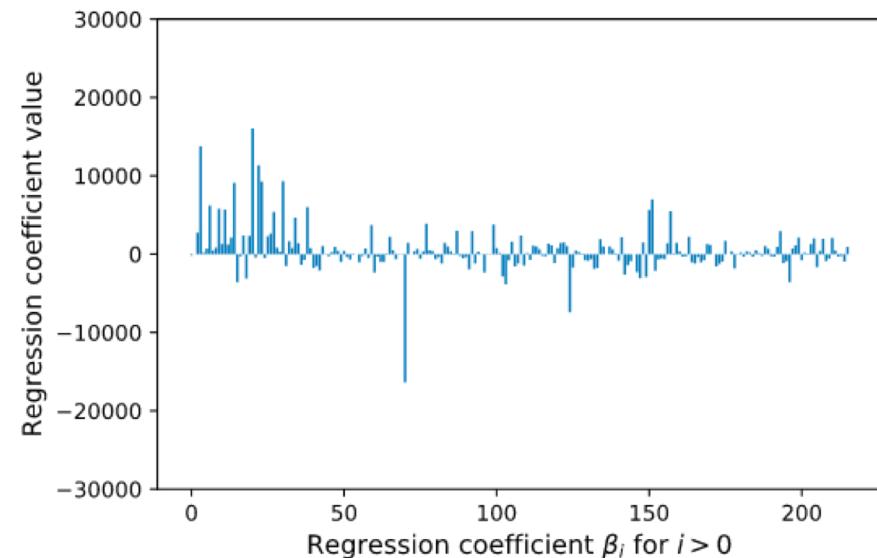
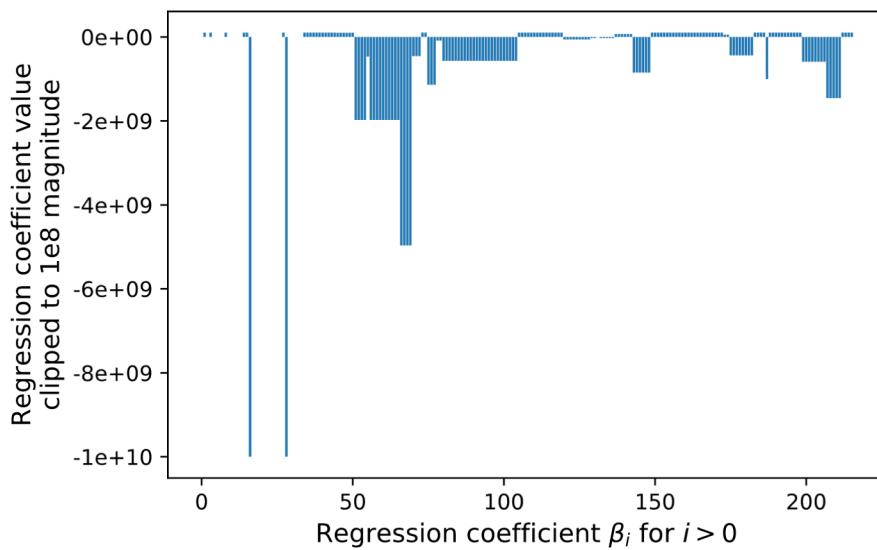
Let's make a deal!

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



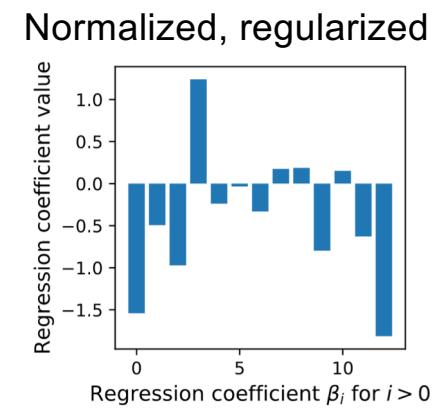
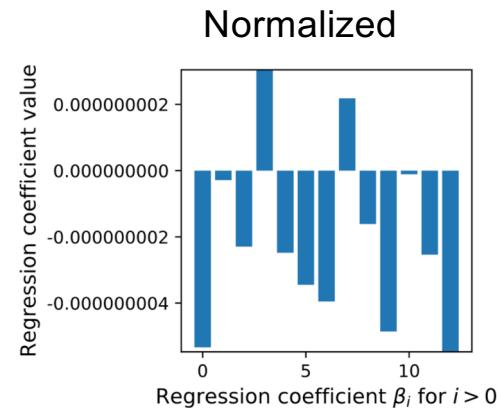
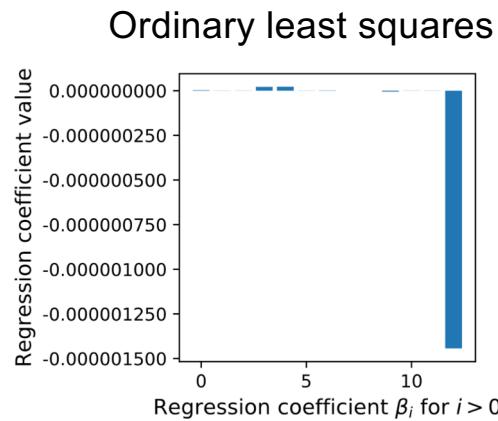
Ames housing data set (regressor)

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



Wine classifier fails w/o regularization

- Wine data set (130 records, 14 numeric vars)
- Test accur=0.59 (normalized data) w/OLS; accur=.98 w/regularization
- Normalizing also helps coefficient interpretation
- Regularization constrains coefficients to sane range



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

Example: classifier w/ too many features

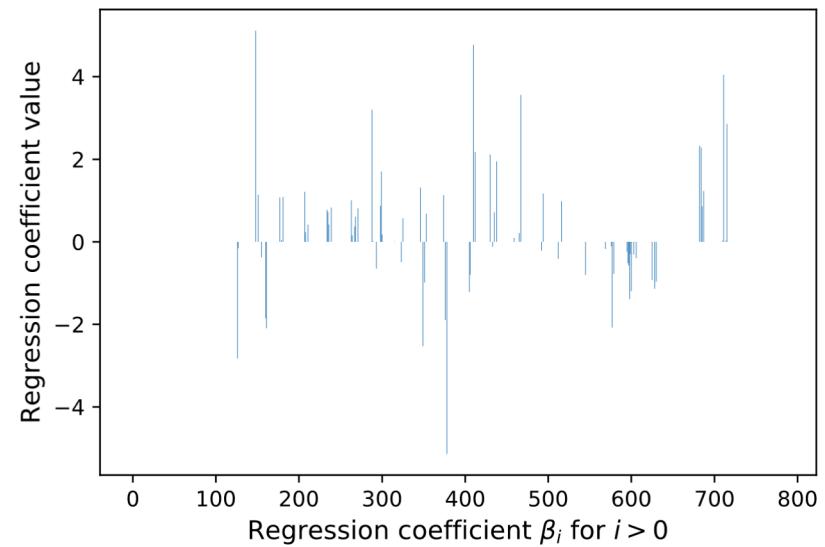
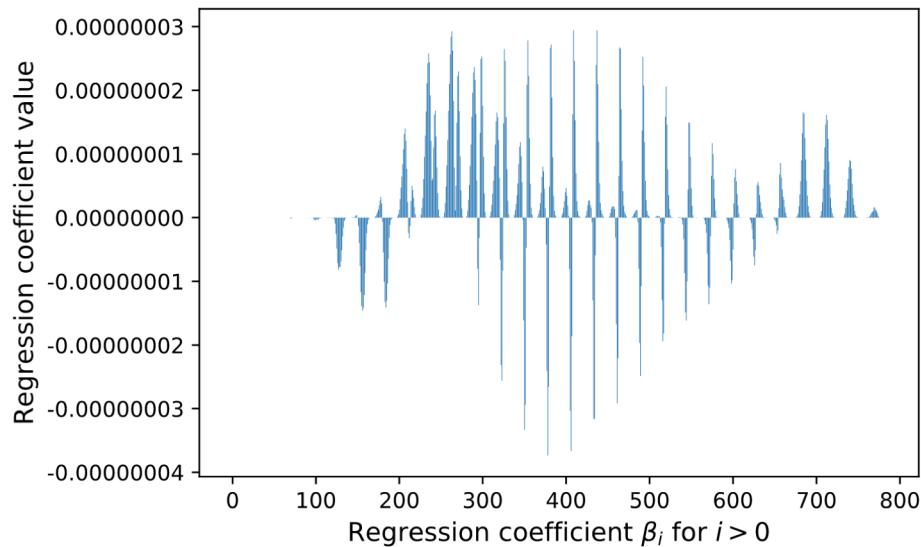
- Distinguish between ones and sevens (MNIST dataset)
- W/o regularization, accuracy score = .50 (same as guessing)

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

Check out the scale difference and how reg (L1) kills off some variables
Test accur=0.49 (normalized data) w/OLS; accur=.98 w/regularization (L1)



Note out L1 regularization has zeroed out lots of coefficients

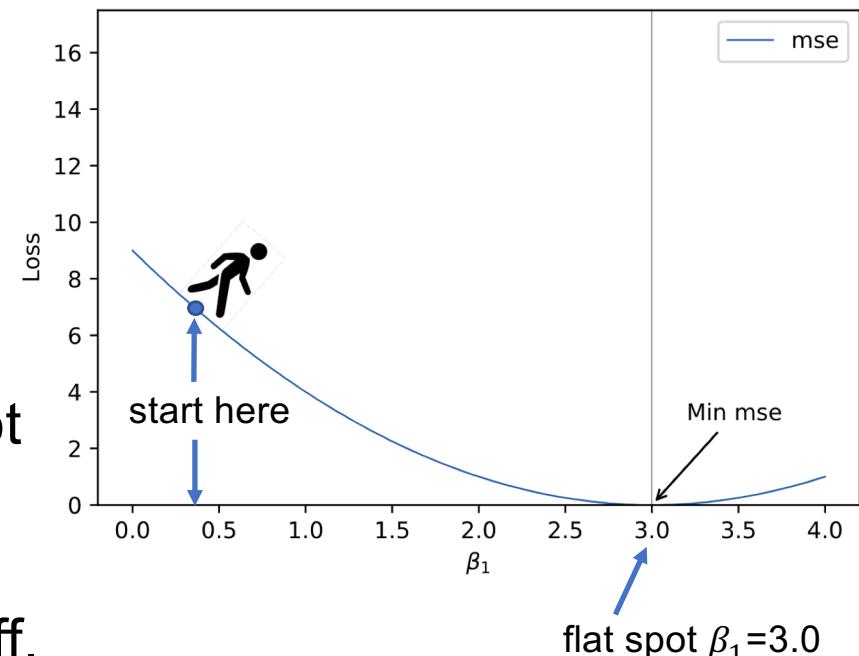
The regularization mechanism

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

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

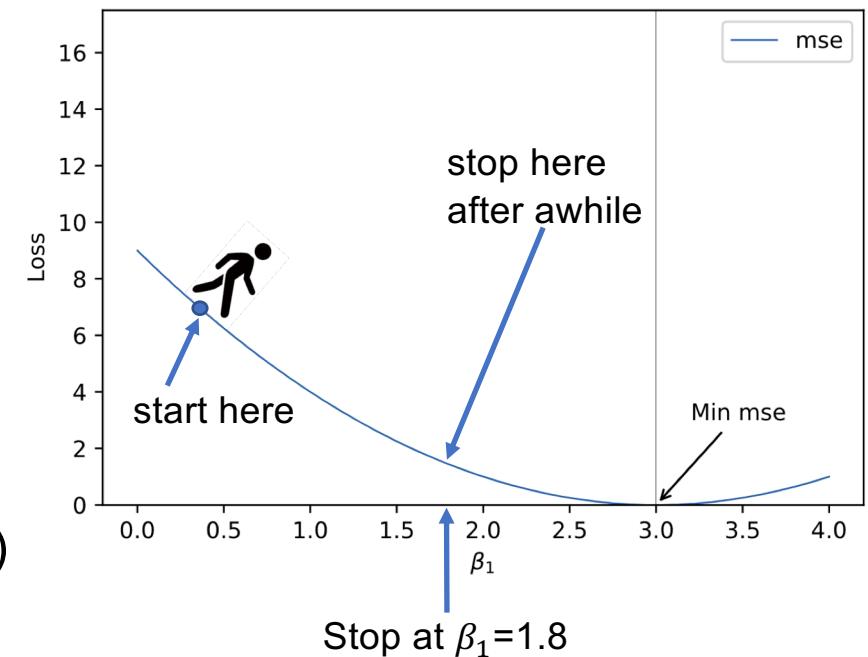
Detour: How training works in 1 dimension

- Loss function (cost) is a function of model parameters (betas), data set
- Minimize 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 downhill until you hit flat spot
- The derivative of loss function is 0 at the minimum loss
- The β_1 at loss minimum is best fit coeff. for training set



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

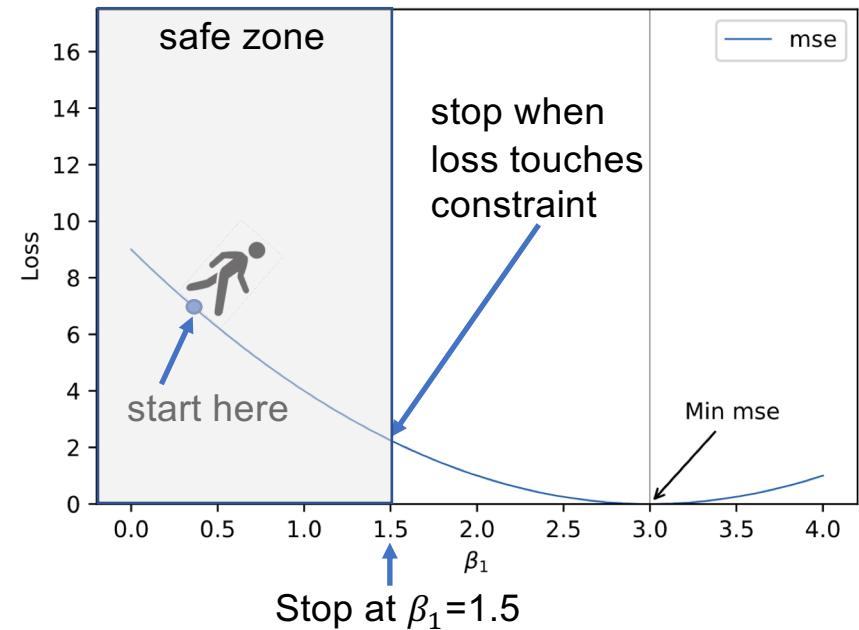


Improving early termination of training

- Stopping after fixed amount of time depends on how fast our "hiker" moves along loss curve and hard to pick duration
- Checking if the loss on **validation set** starts going up is more expensive; each iteration must compute loss on another set
- 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
- It could be min loss is in safe zone, meaning regularization wasn’t req’d



Minimizing in 2D subject to hard constraint

- Spinning segment $[0,t]$ around origin 360° yields 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**

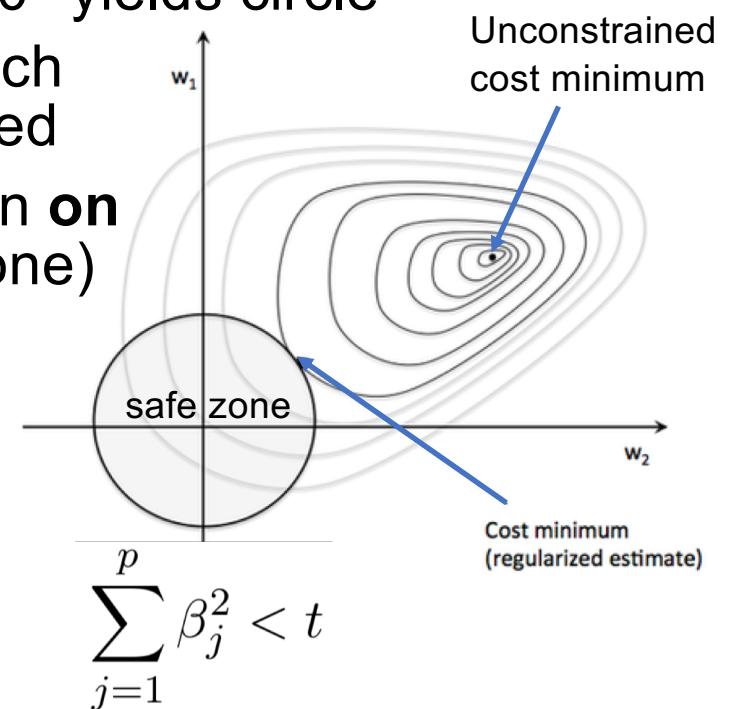
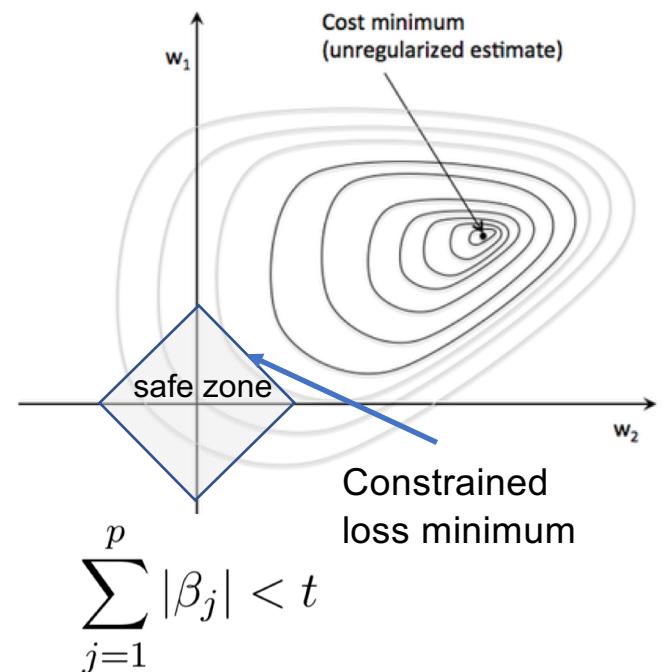


Image credit: <https://www.kdnuggets.com/2016/06/regularization-logistic-regression.html>

Minimizing in 2D subject to hard constraint

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



Notice statisticians have this backwards; L1 constraint zone looks like a ridge not lasso  UNIVERSITY OF SAN FRANCISCO and L2 safe zone (circle) looks like a lasso

Fitting regularized linear model (Conceptually)

- Minimize the loss function:

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

- Subject to either (L2 or L1):

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

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 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

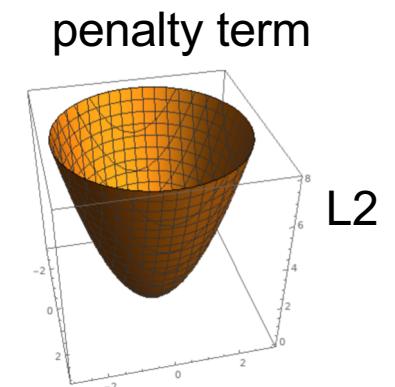
$$\text{For L2: } \mathcal{L}(\beta) + \lambda \sum_{j=1}^p \beta_j^2$$

- 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

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

How penalty term restricts β_i 's

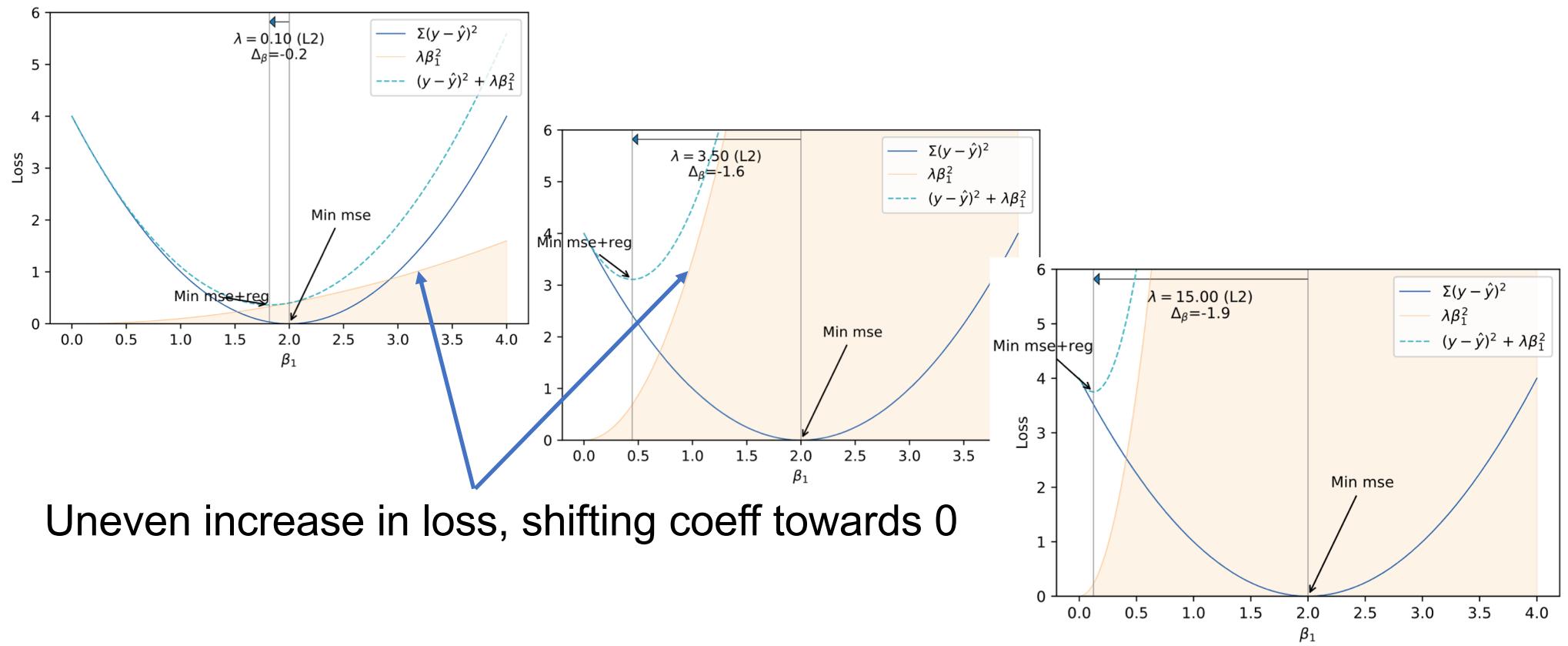
- Think of regularization as two different cost functions, MSE and regularization, added together
- L2 loss increases with the sum of squared coefficients
- L1 increases with sum of coefficient magnitudes
- Regularization penalty term **increases loss** but skews it towards origin as penalty curve is anchored at origin; that **shifts β_i 's to towards 0**
- Soft constraint makes larger β_i very unlikely due to increased penalty away from origin



The effect of regularization

- λ is independent of training data, so can reduce model's dependence on data during fit, which regularizes model
- 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 to 0
- L1 does not discourage β_i from fading to 0, but L2 discourages
- Squaring coefficients for L2 in constraint discourages any β_i from getting much bigger than the others; squeezes β_i together

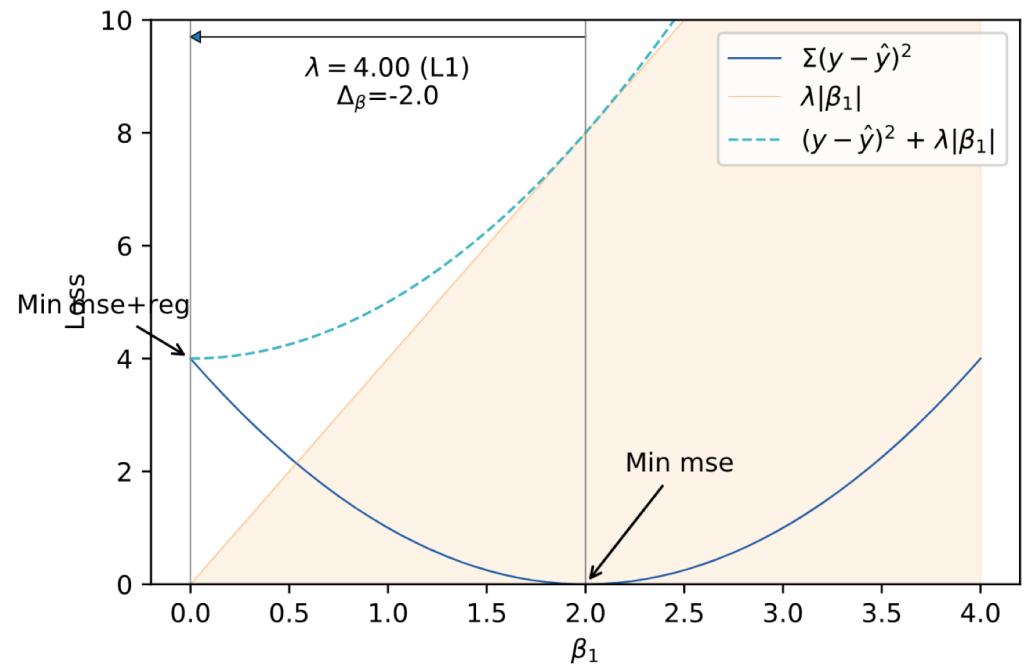
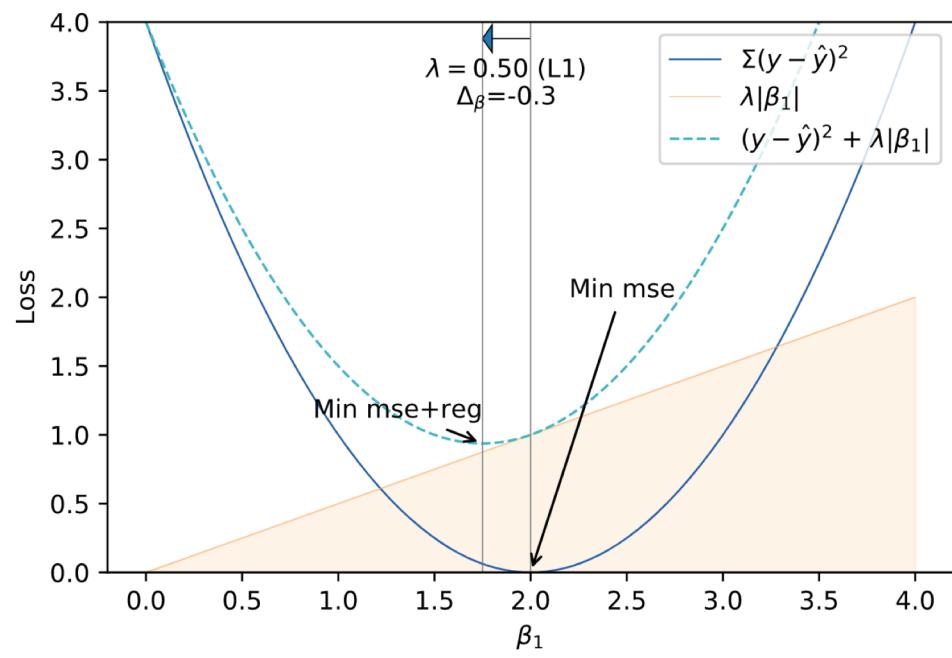
L2 Visually



Uneven increase in loss, shifting coeff towards 0

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

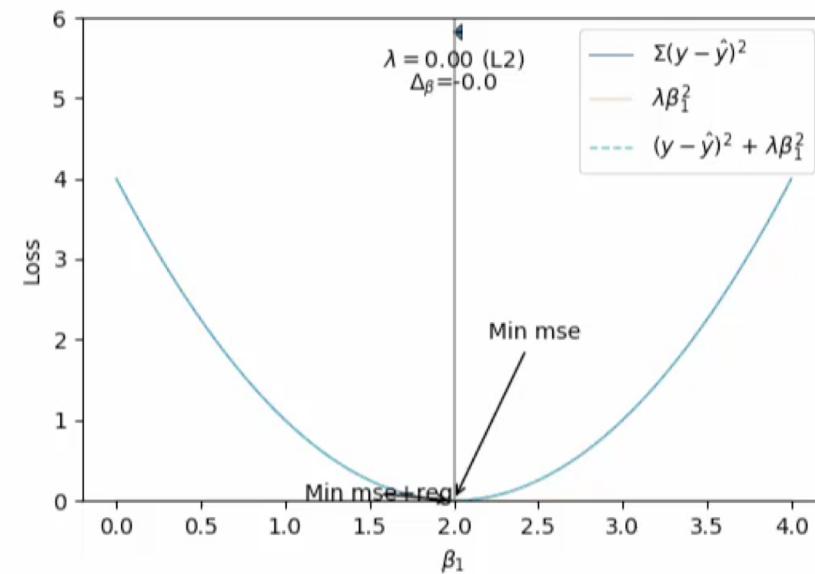
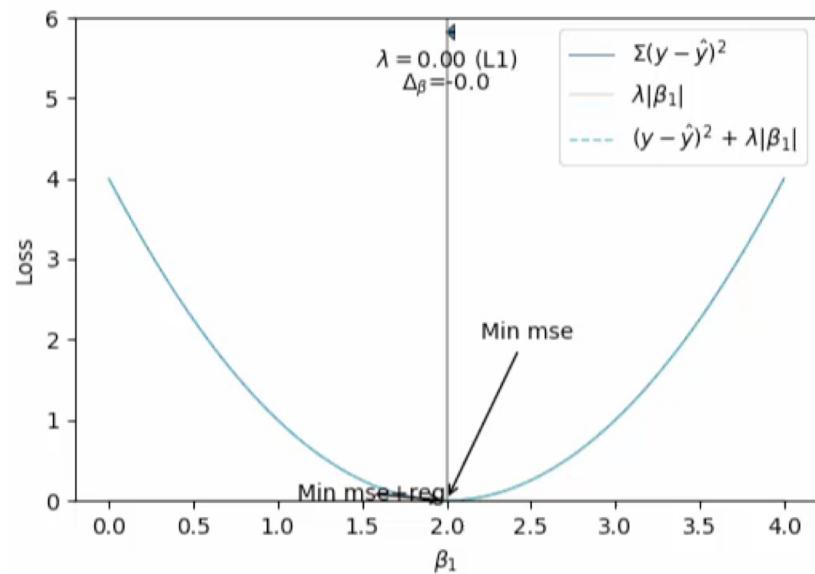
L1 Visually



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

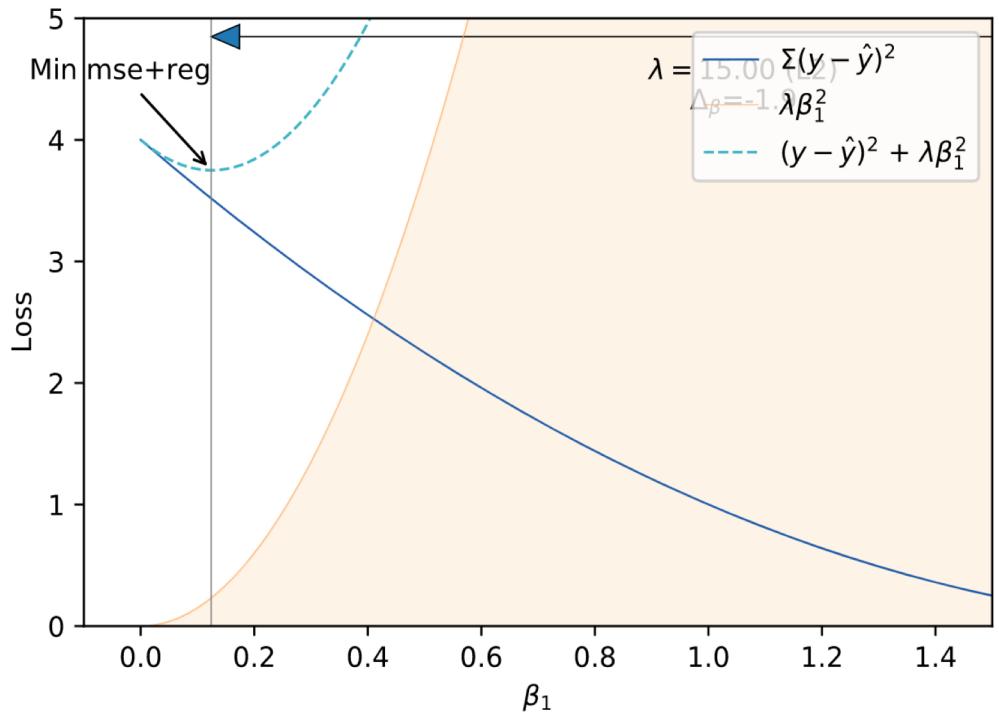
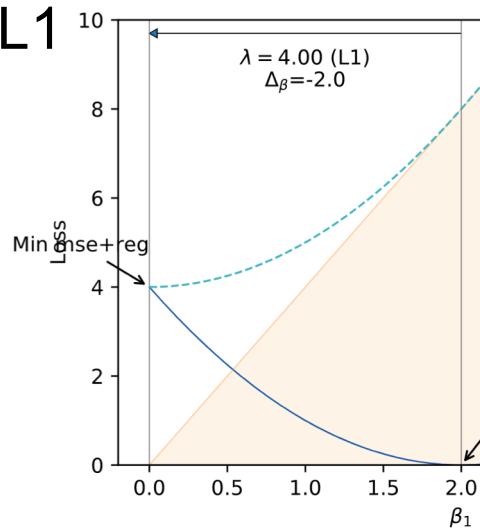
L1 vs L2 regularization visually

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



Zoom in on L2 trying to push β to 0

- For $\beta < 1$, β^2 gets smaller, not bigger
- L2 can't push loss up, β to left very much near 0
- Compare to L1



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

- (p=1) Derivative of penalty term w.r.t β is $2\lambda\beta$ for L2, 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
- For L1, derivative is just $\lambda\text{sign}(\beta)$, independent of β magnitude, so increases loss at same rate (λ) even near 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

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 computing minimum loss for different λ values, pick λ that gets min loss on validation set

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

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

Normalizing data

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

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

- Reasons:
 - One λ for all coefficients so must be in same range or big coefficients prevent regularization of small coefficients
 - Finding coefficients is often more efficient for normalized data sets
 - Allows us to compute β_0 as simply mean(y) for L1/L2 linear regression

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

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:

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

- Means we must find β_0 differently than for $\beta_{1..p}$
- Find λ by computing minimum loss for different λ values, pick λ that gets min loss on validation set
- We'll examine the implementation in gradient descent lecture

Key takeaways

- Regularization increases generality at cost of some bias
- Does so by restricting size of parameters with hard constraint (conceptually) or soft constraint using penalty term
- 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