Regularization for linear models

L1 (Lasso), L2 (Ridge)

MIGHT BE MOST POPULAR INTERVIEW QUESTION

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In depth reading:
https://explained.ai/regularization/index.html

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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”)
- 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
- Often, unregularized models work but we get extreme coefficients 🤔 (extreme negative and positive coefficients must be canceling out)

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

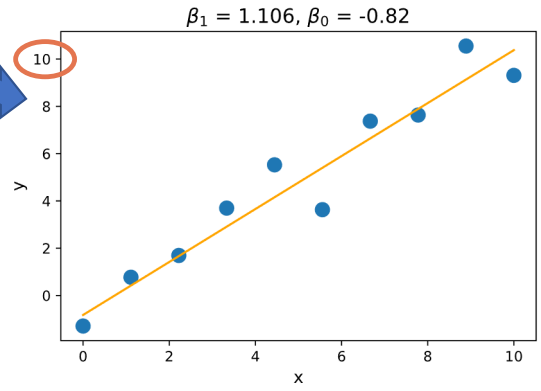
Regularization premise

- **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 applied to output of linear model anyway)
- Preview: add L1 or L2 norm of β coefficient vector to loss function, so loss functions are now a function of known y, predicted y, **AND** model parameters

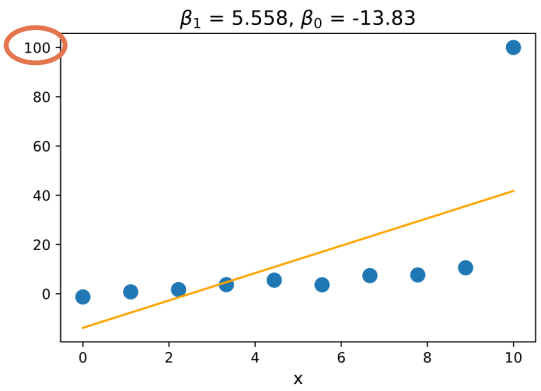
Let's make a deal!

- Let's trade some model bias (accuracy) 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

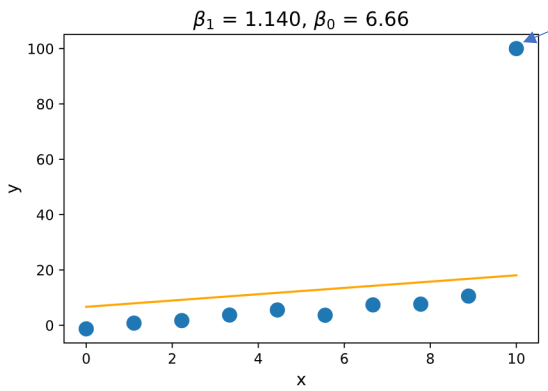
Ordinary least squares



OLS with outlier



L1 regularization with outlier



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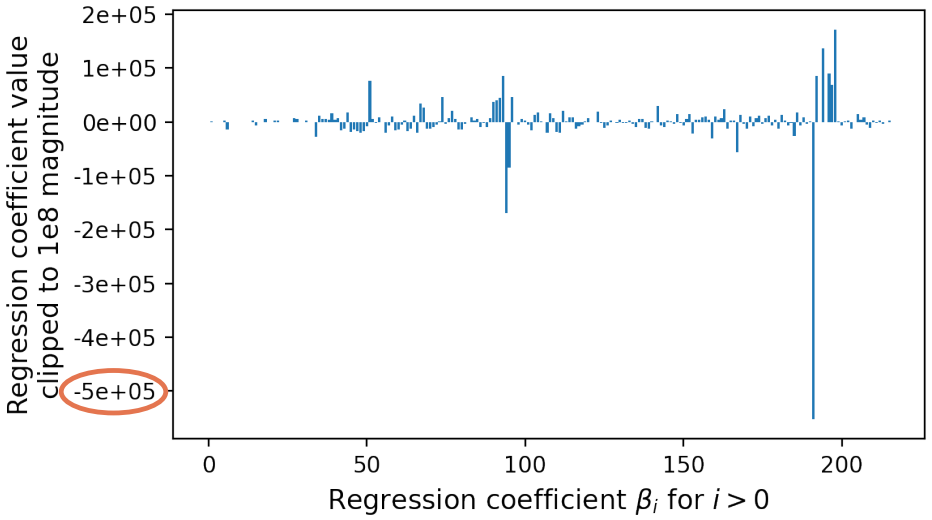
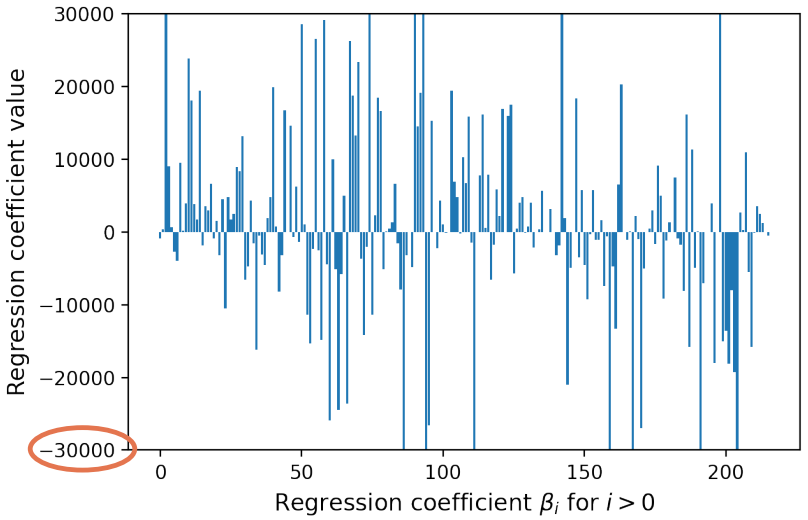
Ames housing data set (regressor)

- With dummy vars, number of columns explodes from 81 to 216
- Compare scale of coeff (huge coefficients don't generalize)
- Regressor test R^2 is -3e20 w/o regularization and ~0.85 with L1



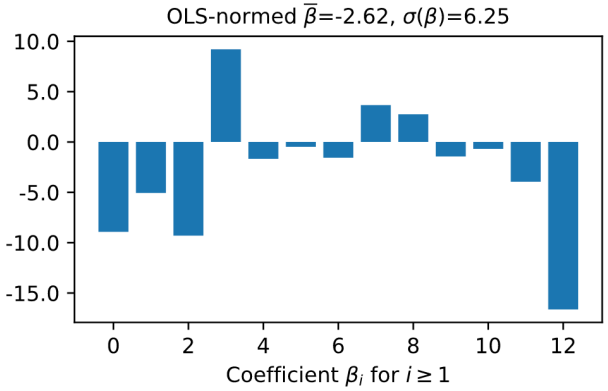


See https://github.com/parrt/msds621/blob/master/notebooks/linear-models/regressor-regularization.ipynb

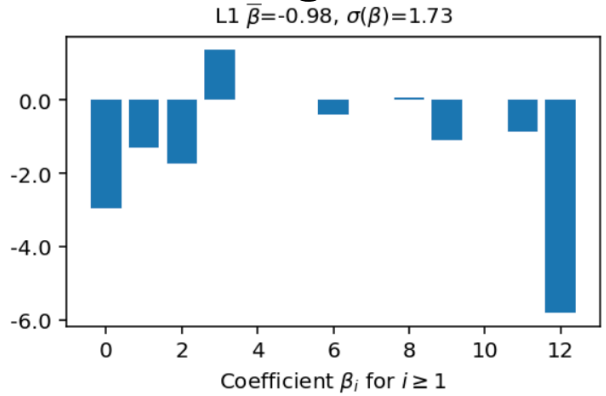
Wine classifier less accurate w/o reg.

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

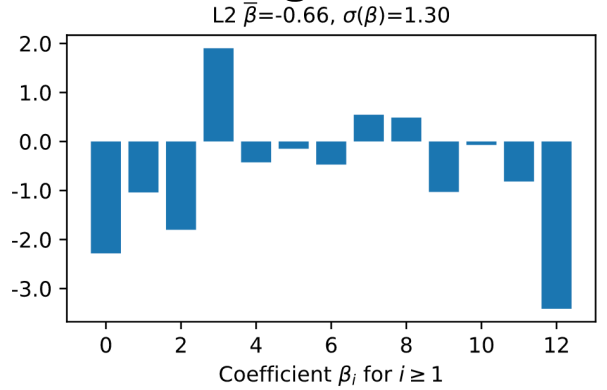
Normalized vars, OLS



L1 regularized



L2 regularized

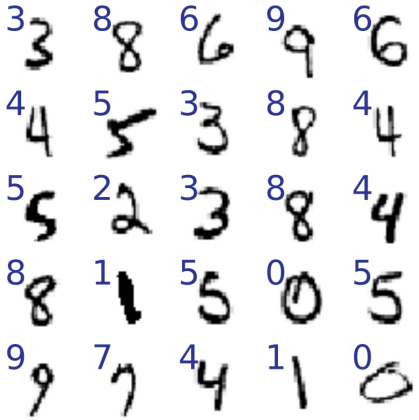


See https://github.com/parrt/msds621/blob/master/notebooks/linear-models/classifier-regularization.ipynb

Example: classifier with many features

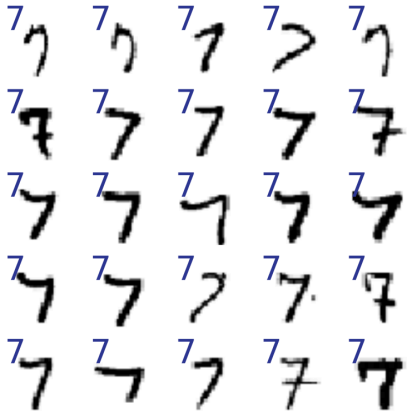
- Distinguish between ones and sevens (MNIST dataset)

MNIST sample



ones sample

sevens sample

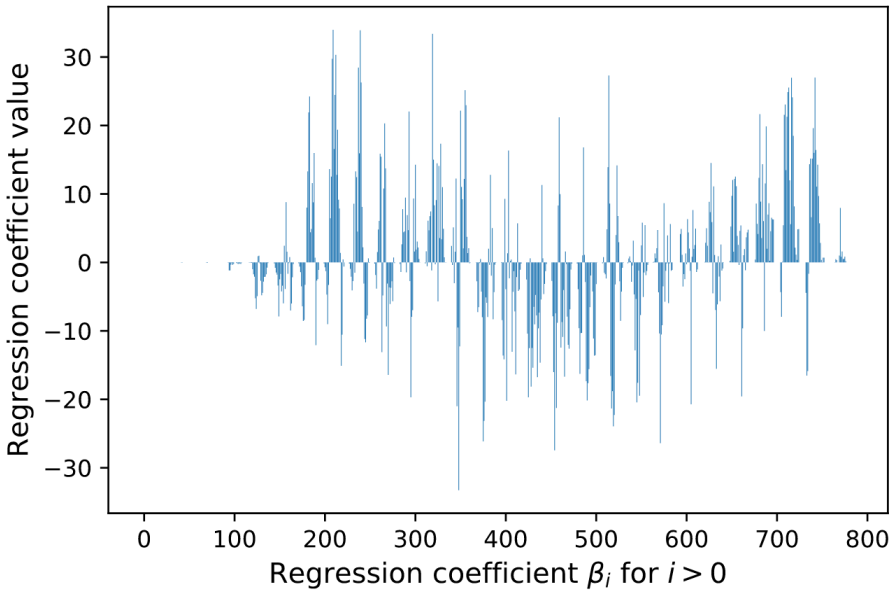


See https://github.com/parrt/msds621/blob/master/notebooks/linear-models/classifier-regularization.ipynb

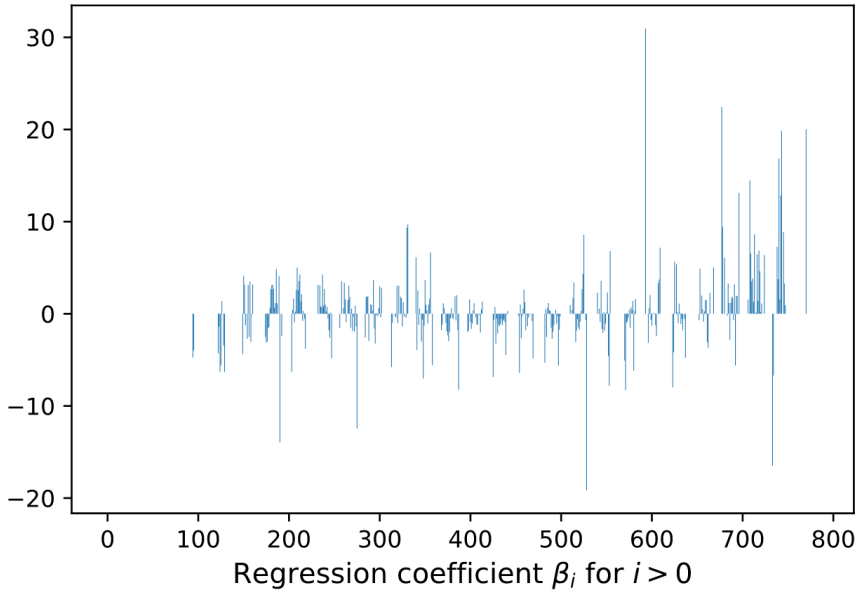
Compare coefficients w/o & with L1 reg

- Test accur=96% w/OLS and L1 but **log loss** improves a lot
- Also L1 regularization has zeroed out 423 coefficients and still accurate!

OLS logistic



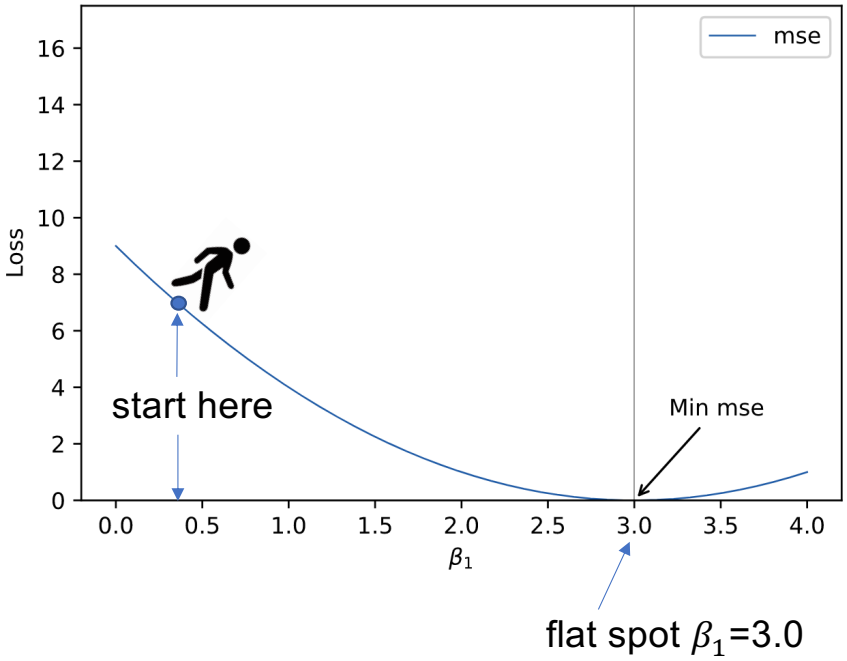
L1 regularized logistic



Quick detour:
Training models by walking downhill and normalizing data

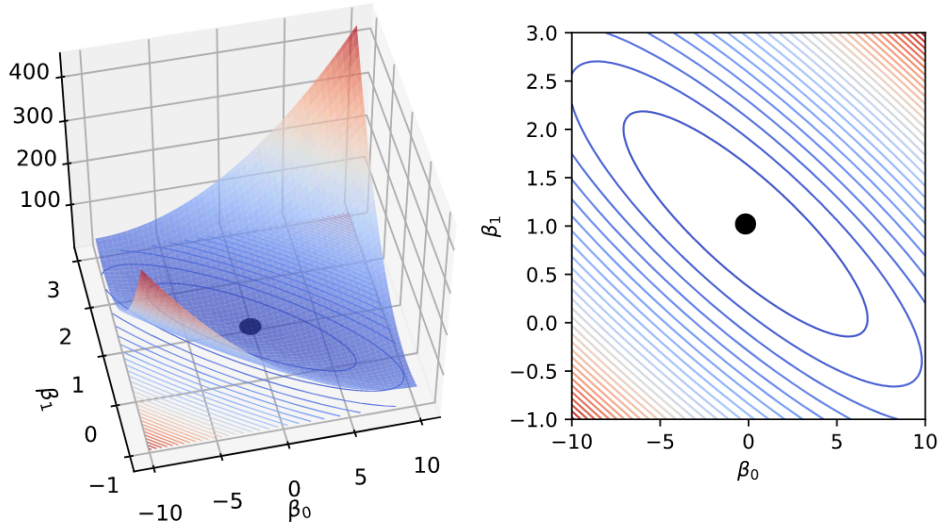
How training works in 1 dimension

- Loss function (cost) is a function of model predictions $\hat{y}$, known y values
- 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 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 coefficient for training set



Training in 2D; loss function shape

- We still walk downhill, but different directions can have different slopes
- Move search "particle" in 2D to find coefficients associated with minimum loss
- Think of dropping marble on surface and letting it roll down to low point
- (We'll have full lecture on gradient descent, don't worry!)



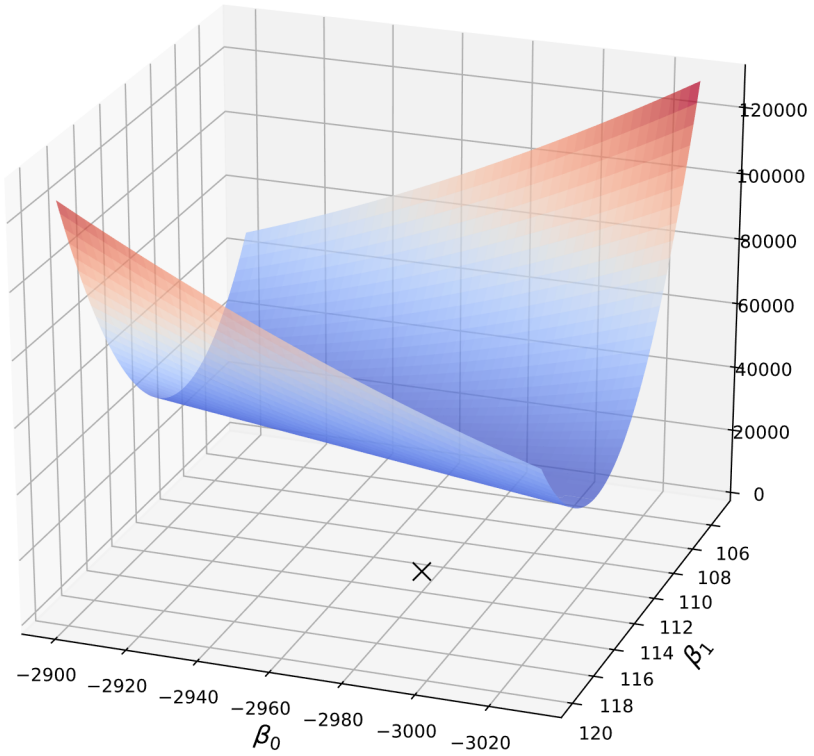
See https://github.com/parrt/msds621/blob/master/notebooks/linear-models/viz-gradient-descent.ipynb

For training linear models, always normalize/standardize data

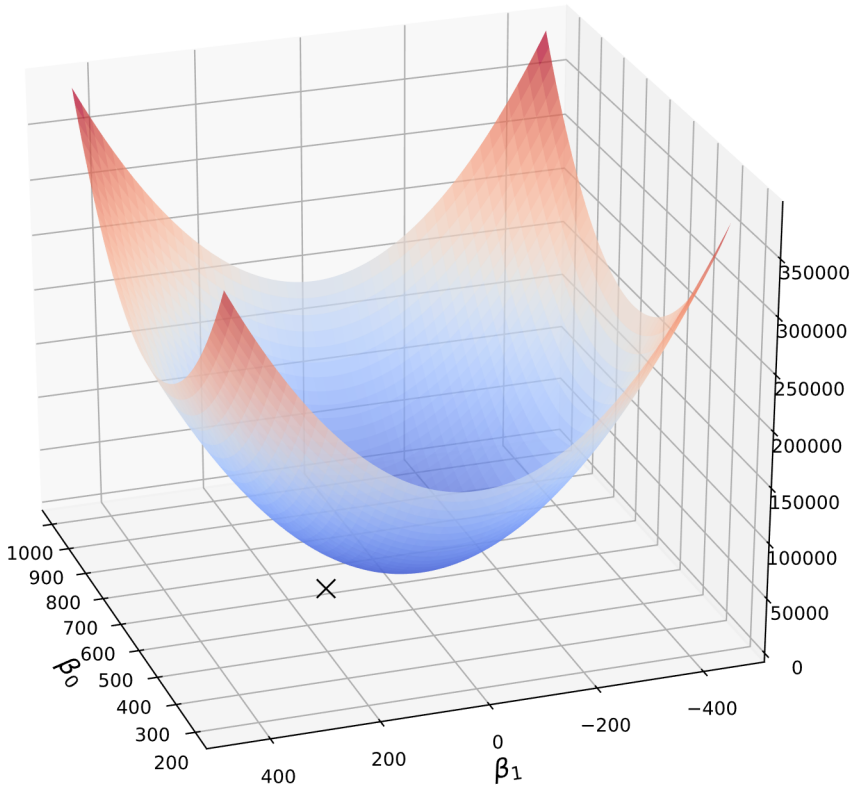
- First, standardization leads to faster training
- Second, regularization requires standardization, otherwise regularization shrinks coefficients disproportionately
- Zero center each variable and divide by the standard deviation

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

2D loss function shape for normalized vars



Untouched variables



Normalized variables

Cheese consumption vs bedsheet strangulation death data set

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

Standardization yields faster training

- 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, leading to faster convergence
- 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 (AdaGrad helps here as it has a learning rate per var)

See http://yann.lecun.com/exdb/publis/pdf/lecun-98b.pdf

Must standardize for regularized training

- 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)

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

- Also β_0 is simply mean(y) for L1/L2 linear regression if we standardize variables
- (We'll examine regularization next)
- **Q**. When do we NOT do normalization of variables?

  It's always safe to do it, but if all we care about is predictive analytics, rather than analysis of parameters, then it's okay not to normalize; on the other hand we often need regularization for generalization purposes, which requires normalization

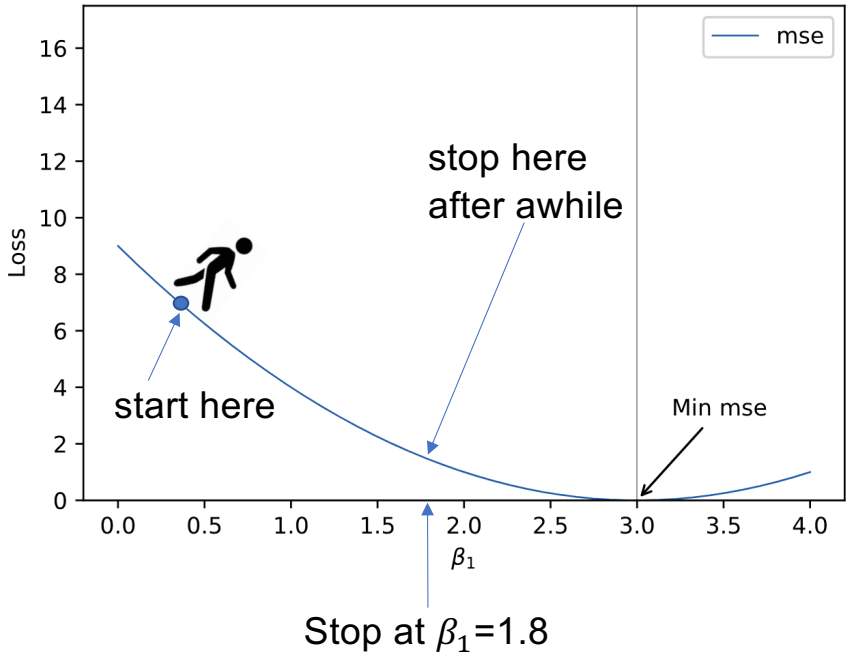
The regularization mechanism

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

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

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** (a moving avg thereof) starts going up, not down

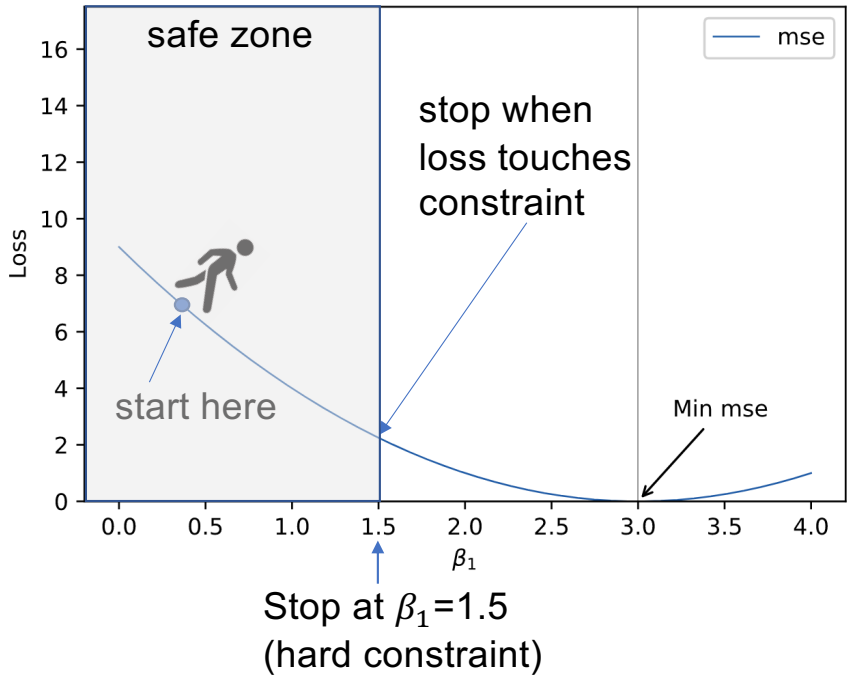


Improving early termination of training

- 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
- We agreed earlier that extreme β coefficients would likely be bad for generality
- Strategy: Pick initial β_1 in $[0, t)$ for some max t and go downhill and stop at minimum or when $\beta_1 \geq t$

Minimizing loss, 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

- Spinning 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** $\sum_{j=1}^{p} \beta_j^2 < t$

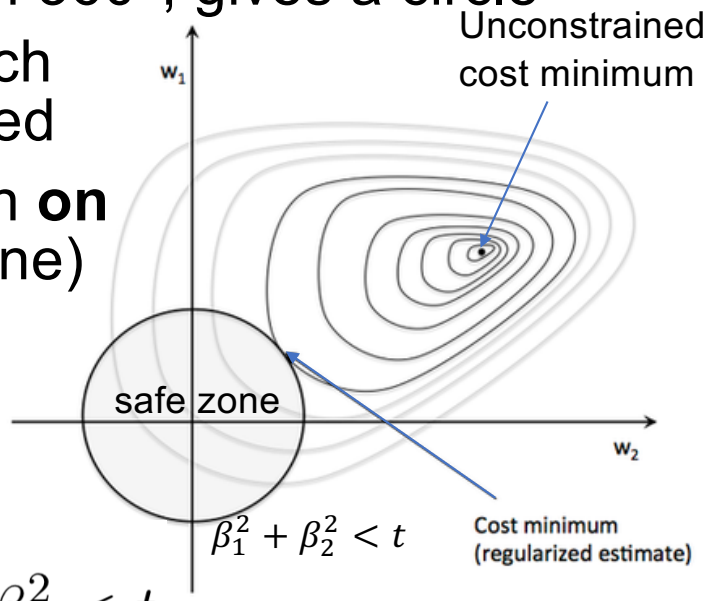
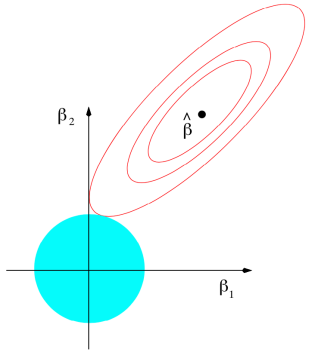


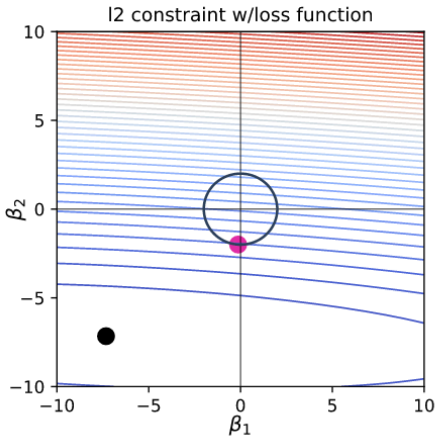
Image credit: https://www.kdnuggets.com/2016/06/regularization-logistic-regression.html

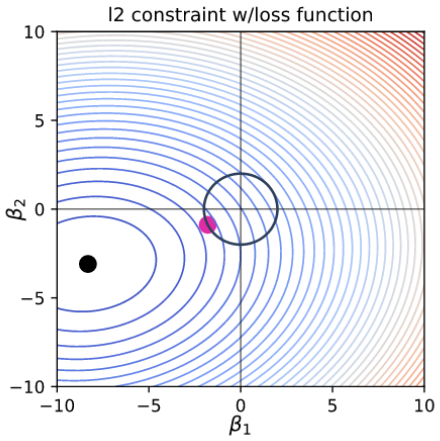
L2 regularization examples

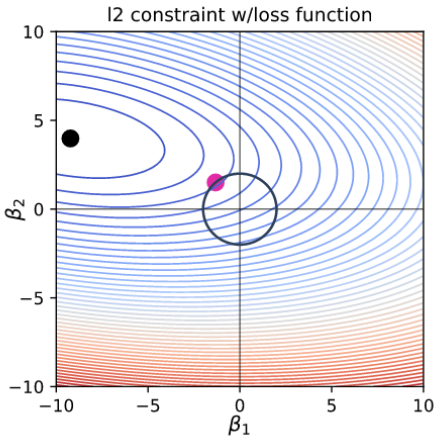
- The L2 regularized coefficients sit on the L2 boundary circle where the loss function has the minimum value.
- Walk around the circle and identify the location with the minimum loss function value

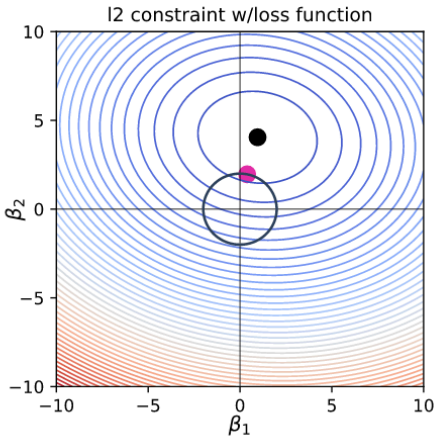


Hard constraint illustration from ESL page 71.









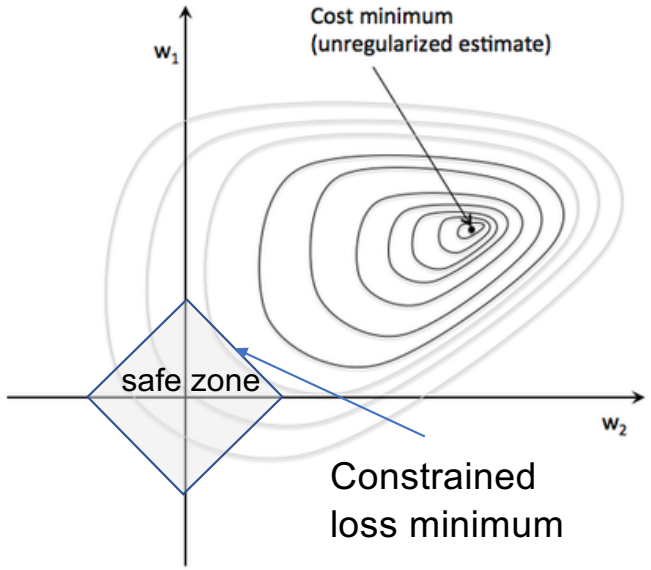
These are topo maps; see https://en.wikipedia.org/wiki/Topographic_map

Minimizing L1 in 2D (hard constraint)

- Instead of β_i^2's, we can sum $|\beta_i|$'s, giving diamond-shaped safe zone
- **This is L1 (*Lasso*) regularization**

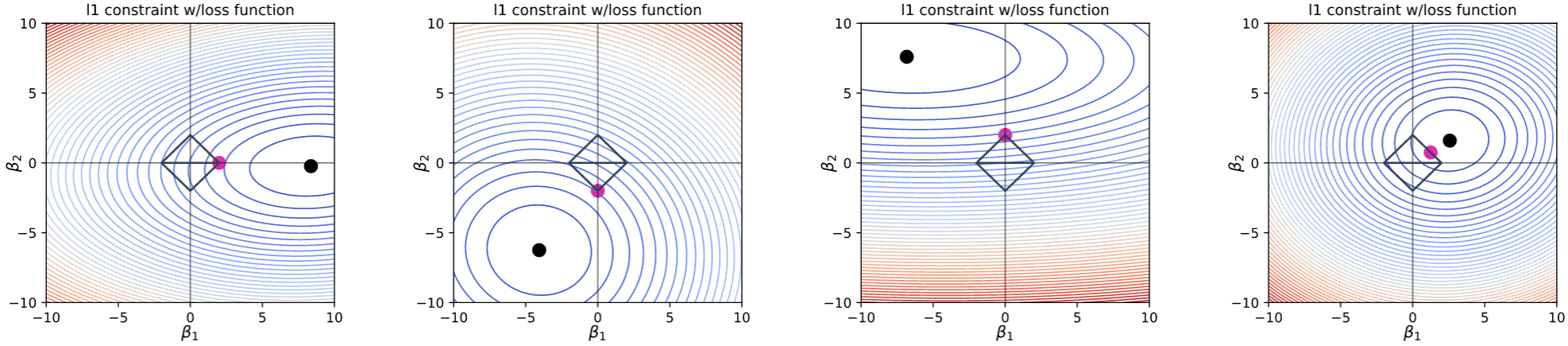
$$\sum_{j=1}^{p} |\beta_j| < t$$

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



L1 regularization examples

- The L1 regularized coefficients sit on the L1 boundary diamond where the loss function has the minimum value.
- Walk around the diamond and identify the location with the minimum loss function value



Please note how often the red dot sits at a diamond corner, with a $\beta_i = 0$

Questions

- Do we want to make the model parameters as small as possible? E.g., are we trying to drive them to zero?

  We are constraining the coefficient magnitude rather than trying to drive them to 0; driving all to 0 would mean creating a model that always predicted 0

- When do we choose L1 vs L2 regularization?

  L1 when you want to reduce the number of features

- Is L1 always better than L2 or vice versa?

  Not that I have experienced

- Is it okay to get rid of L1 parameters that go to zero?

  Sure. Remember that there are always exogenous variables we are implicitly "dropping"

Fitting regularized linear model (Conceptually)

- Minimize the usual MSE loss function (assume β has β_0):

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

- **Subject to** either (L2 or L1):

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

- Problem is "**subject to**" constraint is tough to implement

Detour: Lagrange Multipliers

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

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

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

(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 more complicated to implement than just function minimization so…
- Invoke magic of Lagrange multipliers:

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

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

- 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 combined loss location closer to origin!

Fitting β_i's and picking hyperparameter λ

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

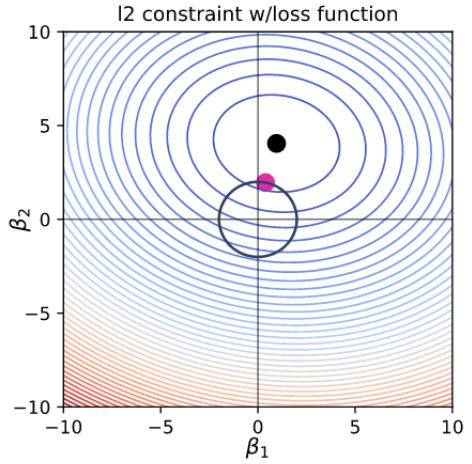
$$\mathscr{L}(\beta) + \lambda \sum_{j=1}^{p} \beta_j^2 \qquad\qquad \mathscr{L}(\beta) + \lambda \sum_{j=1}^{p} |\beta_j|$$

- β_0 is just $\overline{y}$, assuming zero-centered data set
- **Note**: β_0 is NOT included in penalty

Hard vs soft constraints in 2D

Hard constraint

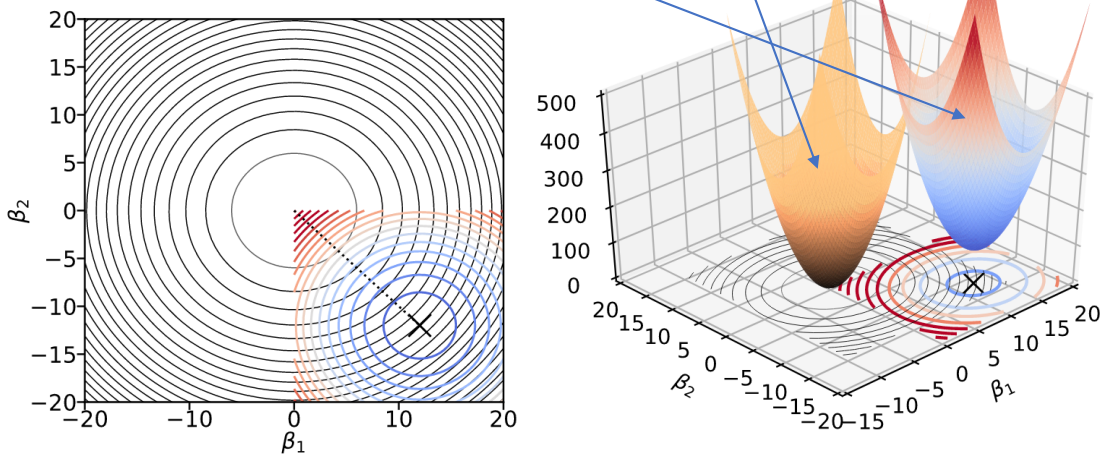
$$\mathscr{L}(\beta) \text{ s.t.} \sum_{j=1}^{p} \beta_j^2 \leq t$$



Constrained loss function

Soft constraint

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

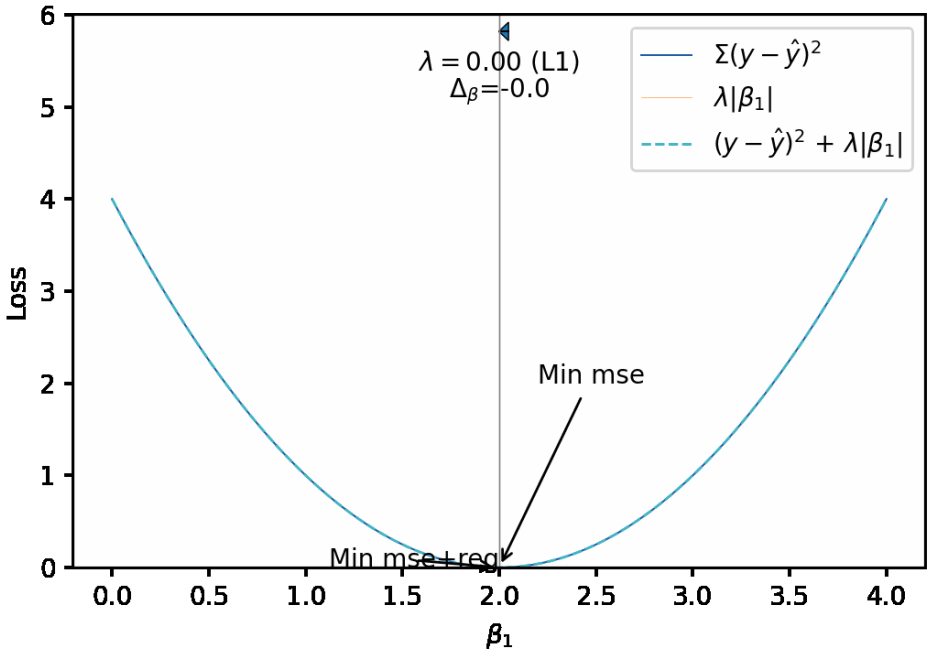


Sum of loss and penalty functions

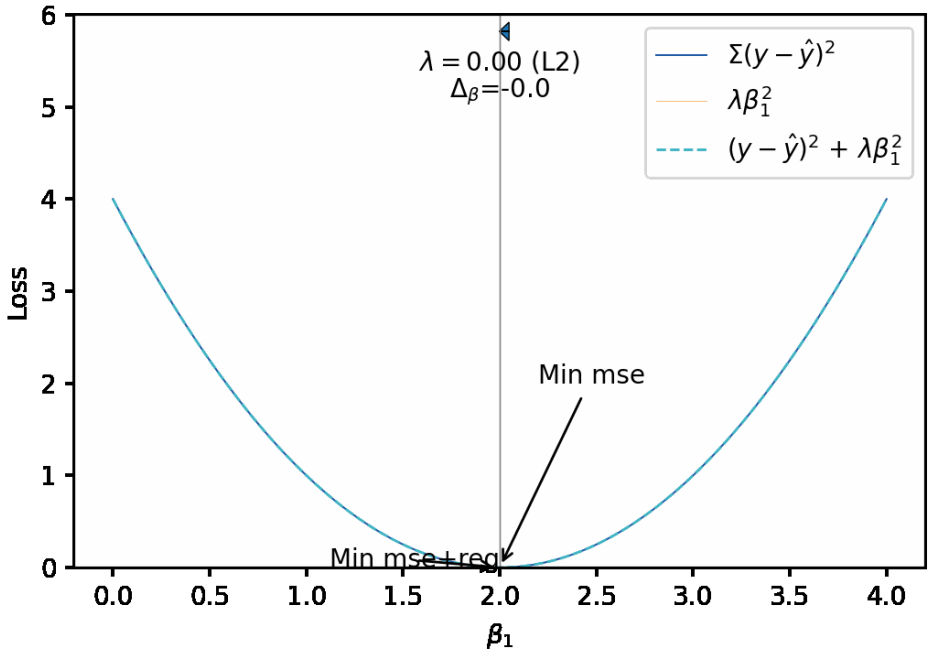
See https://explained.ai/regularization/index.html

1D example of loss+penalty curves

L1 β_1 can quickly converge to 0 for large λ

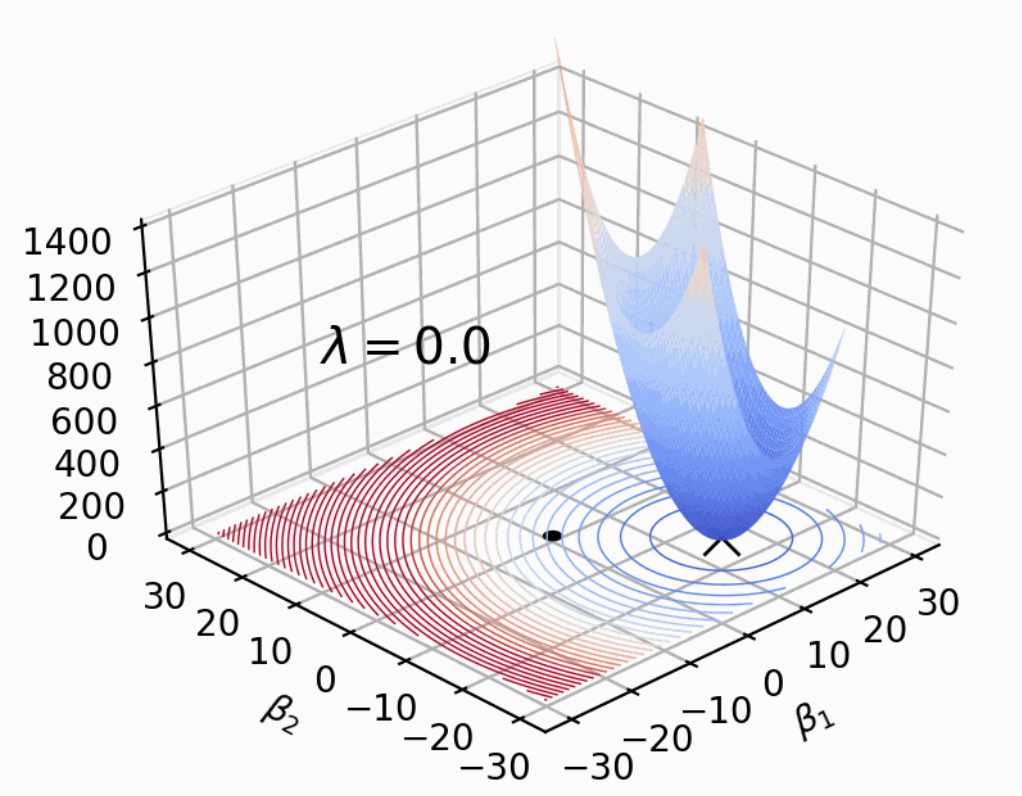


L2 β_1 struggles to converge to 0 for large λ



Affect of λ on combined loss function

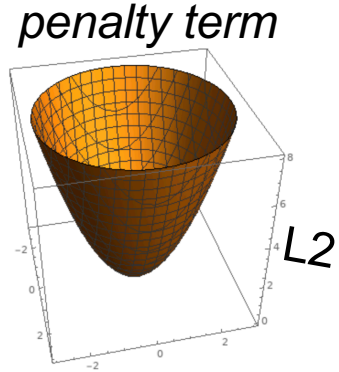
- MSE loss function + soft constraint as λ varies from 0 to 6
- Same training data so MSE loss surface is the same
- Only λ is changing here, increasing penalty for same β_i coefficients
- Combined loss function moves upwards and towards the origin



See https://explained.ai/regularization/index.html

How penalty term restricts β_i's

- Think of regularization as two different cost functions, MSE and regularization, added together
- Regularization penalty term **increases loss** but skews min loss β_i location towards origin as penalty curve is anchored at origin
- Soft constraint makes larger β_i very unlikely due to increased penalty away from origin (whereas hard constraint makes large coefficients > t impossible)
- L1&L2 **shift** β_i**'s towards 0** because penalty approaches 0 only at β=0
- **Q.** How can L1 *soft* constraint still drive β to 0?



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
- L1 tends to shrink coefficients to zero; useful for feature selection since we can drop features with zero coefficients
- L2 tends to shrink coefficients evenly; discourages any single β_i from getting much bigger than the others
- L2 useful when you have collinear/codependent features
  - e.g., **gender** and **ispregnant**
  - codependence tends to increase coefficient variance, making coefficients unreliable/unstable, which hurts model generality
  - L2 reduces the variance of these coefficient estimates

Comparing L1 and L2 regularization

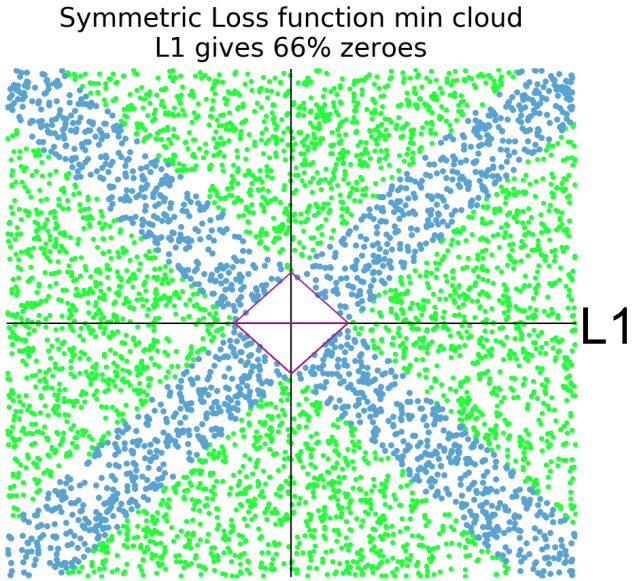
See https://explained.ai/regularization/L1vsL2.html

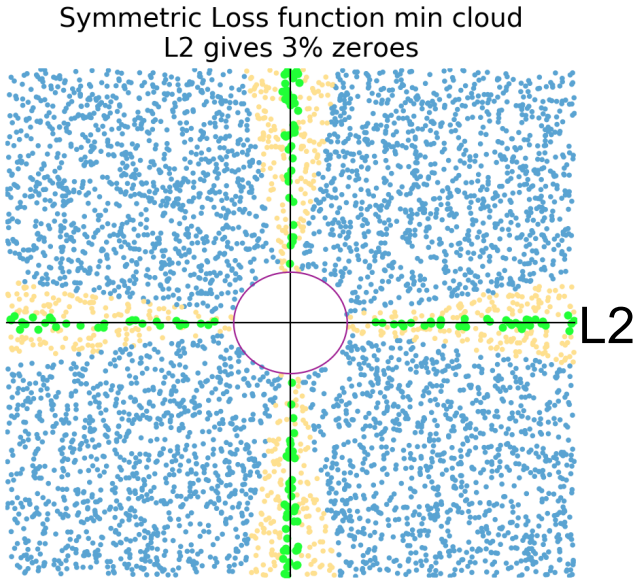
L1 regularization encourages coefficients=0

L1 has many more zero parameters than L2 for symmetric loss functions

- Simulate random symmetric two-variable quadratic loss functions at random locations

Dots: loss function minimum locations; green: a zero coefficient, blue no zeros, orange a coeff close to 0

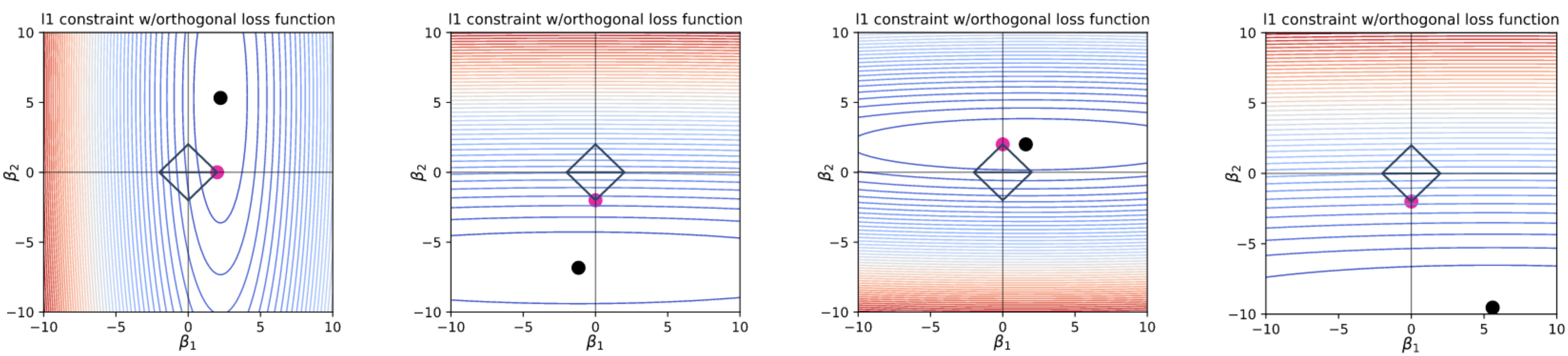




See https://explained.ai/regularization/index.html

L1 regularization strongly encourages zero coefficients for less predictive features

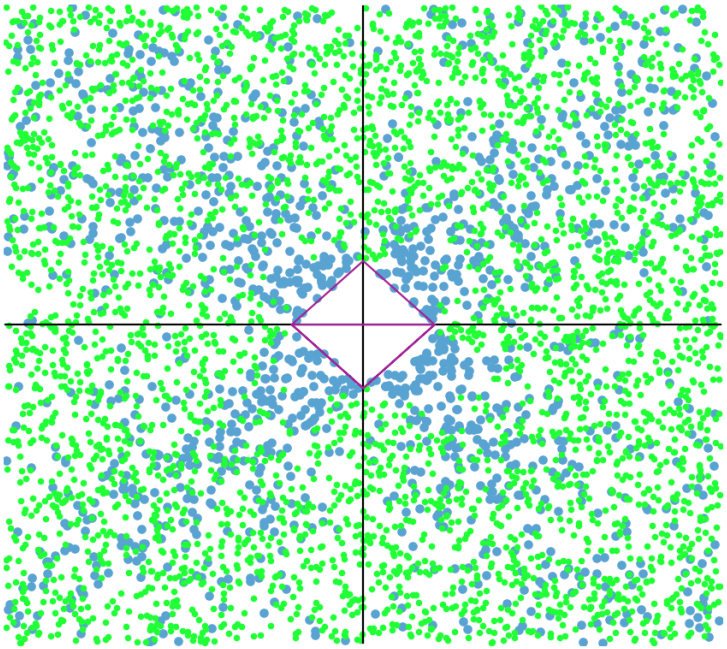
- Imagine one of two features is very important and the other isn't
- Implies loss function looks like a taco shell or canoe, and at or close to 90 degrees to one of the axes
- Movement in one direction is much more expensive than movement in the other



Random asymmetric, angled loss functions

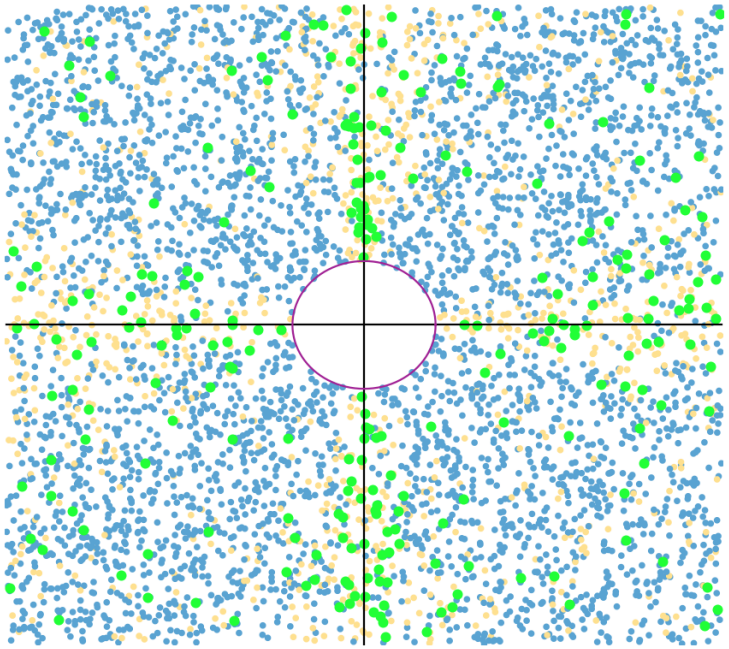
L1 still has many more zero parameters than L2 for arbitrary loss functions

Loss function min cloud
L1 gives 72% zeroes



L1

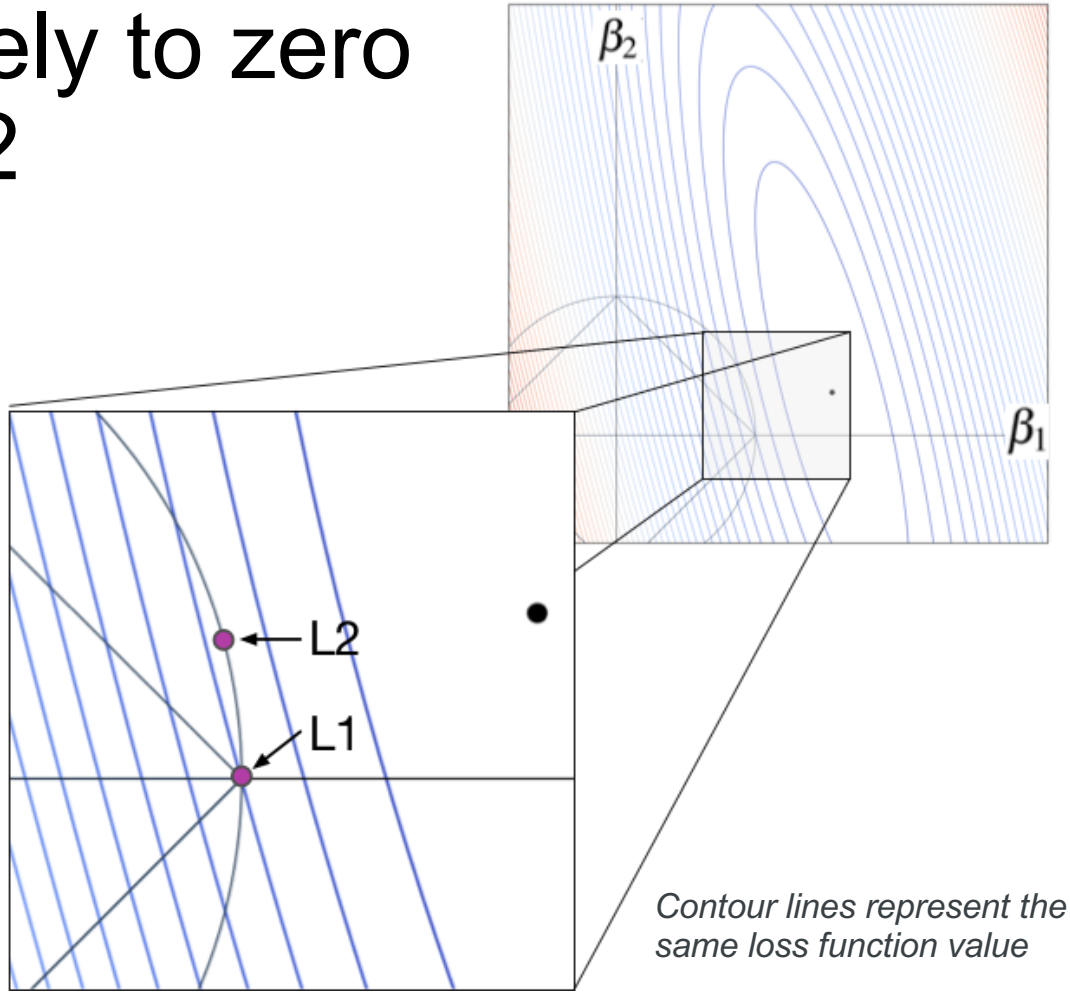
Loss function min cloud
L2 gives 5% zeroes



L2

Why L1 is more likely to zero coefficients than L2

- Moving away from the L1 diamond point immediately increases loss
- L2 can move upwards a bit before moving leftward away from loss function minimum
- As black dot approaches β_1 axis, L2 purple dot approaches β_1 axis, but L1 gets $\beta_2 = 0$ even when loss min location far from axis



Contour lines represent the same loss function value

See https://explained.ai/regularization/index.html

Lab time

- Exploring regularization for linear regression
  https://github.com/parrt/msds621/tree/master/labs/linear-models/regularization-regr.ipynb

Regularized logistic regression

Optimizing likelihood with penalty terms

(Logistic regularization is **not** required for your project, but L1 is an option)

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

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

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

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

Fitting L1 logistic regression β_i's and picking λ

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

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

- We minimize the negative of that to find β with min loss
- 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; see gradient descent lecture

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 is inside safe zone or on zone border
- Soft constraint penalty discourages bigger parameters
- L2 discourages any β_i from getting much bigger than the others
- L1 encourages zero β_i; in practice, we see L1 zero out unpredictive vars

Key implementation details

- Minimize $\mathcal{L}(\beta, \lambda)$ by trying multiple λ and choosing parameter ... tted model getting lowest **validation** error
- Normalize numeric variables in X before fitting linear models
- If 0-centered x_i then $\beta_0 = mean(y)$ 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 much less likely to get zero coefficients
- 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?)

Lab time

- Regularization for logistic regression
  https://github.com/parrt/msds621/blob/master/labs/linear-models/regularization-logi.ipynb