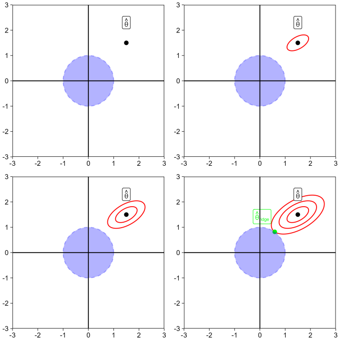
Introduction to Machine Learning

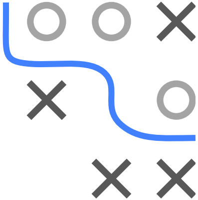
Regularization
Ridge Regression



Learning goals

- Regularized linear model
- Ridge regression / *L*2 penalty
- Understand parameter shrinkage
- Understand correspondence to constrained optimization

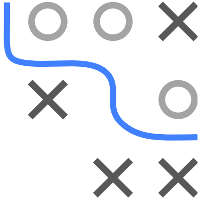
REGULARIZATION IN LM



- Can also overfit if p large and n small(er)
- OLS estimator requires full-rank design matrix
- For highly correlated features, OLS becomes sensitive to random errors in response, results in large variance in fit
- We now add a complexity penalty to the loss:

$$\mathcal{R}_{\text{reg}}(\boldsymbol{\theta}) = \sum_{i=1}^{n} \left(y^{(i)} - \boldsymbol{\theta}^\top \mathbf{x}^{(i)}\right)^2 + \lambda \cdot J(\boldsymbol{\theta}).$$

RIDGE REGRESSION / L2 PENALTY



Intuitive measure of model complexity is deviation from 0-origin; coeffs then have no or a weak effect. So we measure $J(\boldsymbol{\theta})$ through a vector norm, shrinking coeffs closer to 0.

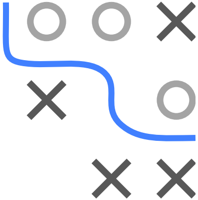
$$\begin{aligned}\hat{\theta}_{\text{ridge}} &= \arg\min_{\boldsymbol{\theta}} \sum_{i=1}^{n} \left(y^{(i)} - \boldsymbol{\theta}^T \mathbf{x}^{(i)}\right)^2 + \lambda \sum_{j=1}^{p} \theta_j^2 \\ &= \arg\min_{\boldsymbol{\theta}} \|\mathbf{y} - \mathbf{X}\boldsymbol{\theta}\|_2^2 + \lambda\|\boldsymbol{\theta}\|_2^2\end{aligned}$$

Can still analytically solve this:

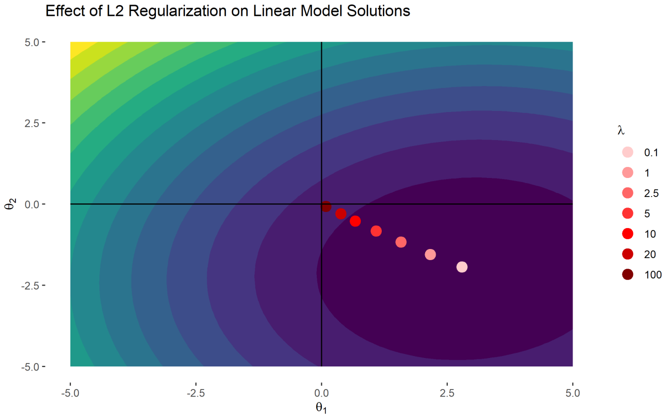
$$\hat{\theta}_{\text{ridge}} = (\mathbf{X}^T\mathbf{X} + \lambda \boldsymbol{I})^{-1}\mathbf{X}^T\mathbf{y}$$

Name: We add pos. entries along the diagonal "ridge" of $\mathbf{X}^T\mathbf{X}$

RIDGE REGRESSION / L2 PENALTY / 2



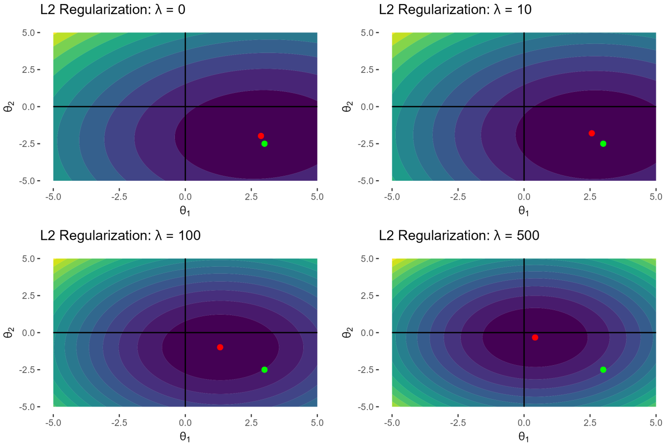
Let $y = 3x_1 - 2x_2 + \epsilon$, $\epsilon \sim N(0, 1)$. The true minimizer is $\theta^* = (3, -2)^T$, with $\hat{\theta}_{\text{ridge}} = \arg\min_{\boldsymbol{\theta}} \|\mathbf{y} - \mathbf{X}\boldsymbol{\theta}\|^2 + \lambda\|\boldsymbol{\theta}\|^2$.



With increasing regularization, $\hat{\theta}_{ridge}$ is pulled back to the origin (contour lines show unregularized objective).

RIDGE REGRESSION / L2 PENALTY / 3

Contours of regularized objective for different λ values.
$\hat{\theta}_{\text{ridge}} = \arg\min_{\boldsymbol{\theta}} \|\mathbf{y} - \mathbf{X}\boldsymbol{\theta}\|^2 + \lambda\|\boldsymbol{\theta}\|^2$.

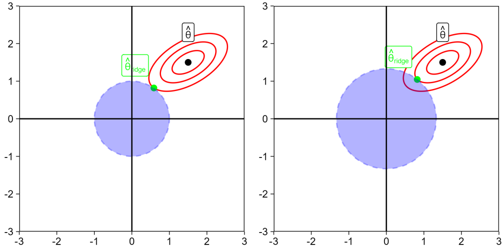


Green = true coefs of the DGP and red = ridge solution.

RIDGE REGRESSION / L2 PENALTY / 4

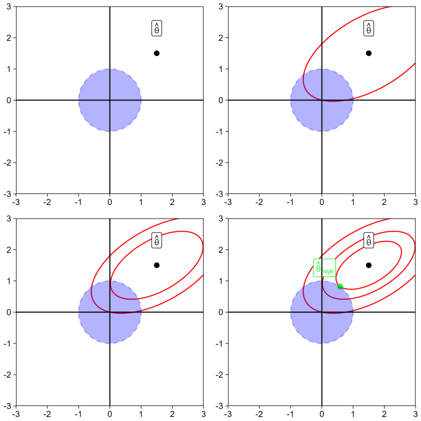
We understand the geometry of these 2 mixed components in our regularized risk objective much better, if we formulate the optimization as a constrained problem (see this as Lagrange multipliers in reverse).

$$
\begin{aligned}
\min_{\boldsymbol{\theta}} \quad & \sum_{i=1}^{n} \left(y^{(i)} - f\left(\mathbf{x}^{(i)} \mid \boldsymbol{\theta}\right)\right)^2 \\
\text{s.t.} \quad & \|\boldsymbol{\theta}\|_2^2 \leq t
\end{aligned}
$$



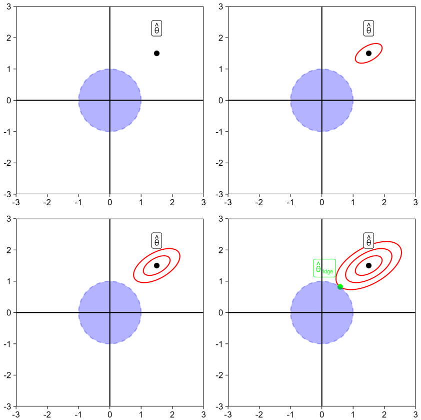
NB: There is a bijective relationship between λ and t: $\lambda \uparrow \Rightarrow \; t \downarrow$ and vice versa.

RIDGE REGRESSION / L2 PENALTY / 5



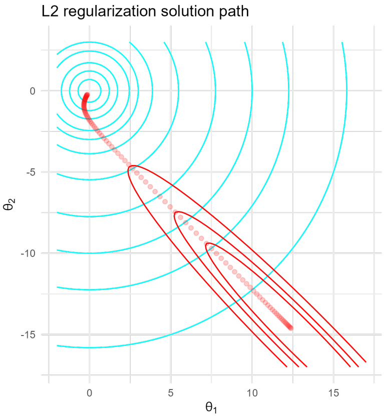
- Inside constraints perspective: From origin, jump from contour line to contour line (better) until you become infeasible, stop before.
- We still optimize the $\mathcal{R}_{\text{emp}}(\boldsymbol{\theta})$, but cannot leave a ball around the origin.
- $\mathcal{R}_{\text{emp}}(\boldsymbol{\theta})$ grows monotonically if we move away from $\hat{\theta}$ (elliptic contours).
- Solution path moves from origin to border of feasible region with minimal L_2 distance.

RIDGE REGRESSION / L2 PENALTY / 6



- Outside constraints perspective: From $\hat{\theta}$, jump from contour line to contour line (worse) until you become feasible, stop then.
- So our new optimum will lie on the boundary of that ball.
- Solution path moves from unregularized estimate to feasible region of regularized objective with minimal L_2 distance.

RIDGE REGRESSION / L2 PENALTY / 7



- Here we can see entire solution path for ridge regression
- Cyan contours indicate feasible regions induced by different λs
- Red contour lines indicate different levels of the unreg. objective
- Ridge solution (red points) gets pulled toward origin for increasing λ

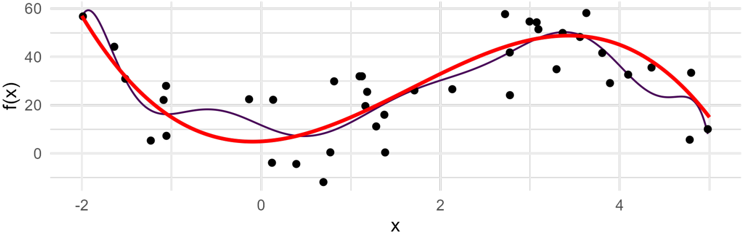
EXAMPLE: POLYNOMIAL RIDGE REGRESSION

Consider $y = f(x) + \epsilon$ where the true (unknown) function is $f(x) = 5 + 2x + 10x^2 - 2x^3$ (in red).

Let's use a dth-order polynomial

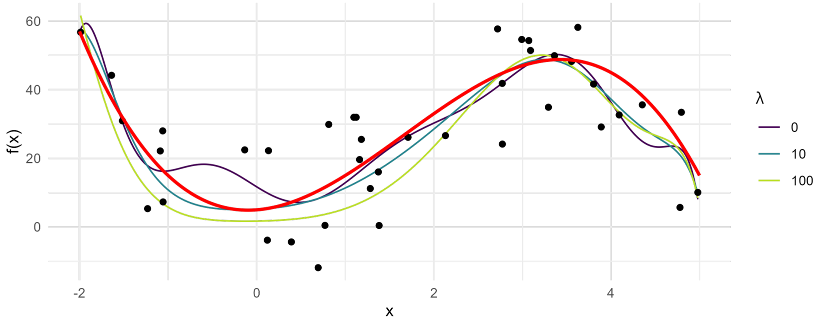
$$f(x) = \theta_0 + \theta_1 x + \cdots + \theta_d x^d = \sum_{j=0}^{d} \theta_j x^j.$$

Using model complexity $d = 10$ overfits:



EXAMPLE: POLYNOMIAL RIDGE REGRESSION / 2

With an *L*2 penalty we can now select *d* "too large" but regularize our model by shrinking its coefficients. Otherwise we have to optimize over the discrete *d*.



λ	θ_0	θ_1	θ_2	θ_3	θ_4	θ_5	θ_6	θ_7	θ_8	θ_9	θ_{10}
0.00	12.00	-16.00	4.80	23.00	-5.40	-9.30	4.20	0.53	-0.63	0.13	-0.01
10.00	5.20	1.30	3.70	0.69	1.90	-2.00	0.47	0.20	-0.14	0.03	-0.00
100.00	1.70	0.46	1.80	0.25	1.80	-0.94	0.34	-0.01	-0.06	0.02	-0.00