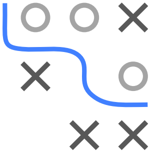
Overview

Regularization

Introduction to Machine Learning

Regularization
Introduction

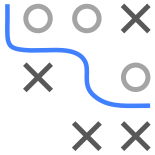


Learning goals

- Overfitting
- Motivation of regularization
- First overview of techniques
- Pattern of regularized ERM formula

WHAT IS REGULARIZATION?

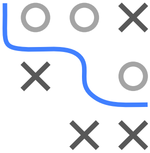
Methods that add **inductive bias** to model, usually some “low complexity” priors (shrinkage and sparsity) to reduce overfitting and get better bias-variance tradeoff



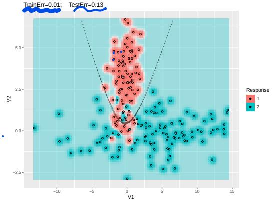
- **Explicit regularization**: penalize explicit measure of model complexity in ERM (e.g., $L1/L2$)
- **Implicit regularization**: early stopping, data augmentation, parameter sharing, dropout or ensembling
- **Structured regularization**: structural prior knowledge over groups of parameters or subnetworks (e.g., group lasso Yuan and Lin 2006)

RECAP: OVERFITTING

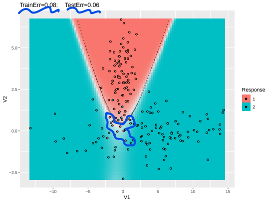
- Occurs when model reflects noise or artifacts in training data
- Model often then does not generalize well (small train error, high test error) – or at least works better on train than on test data



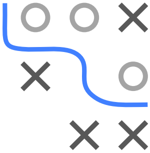
Overfitted model



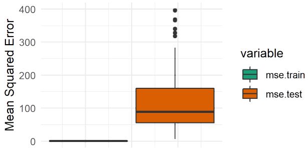
Appropriate model



EXAMPLE I: OVERFITTING



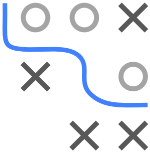
- Data set: daily maximum **ozone level** in LA; $n = 50$
- 12 features: time (weekday, month); weather (temperature at stations, humidity, wind speed); pressure gradient
- Orig. data was subsetted, so it feels "high-dim." now (low n in relation to p)
- LM with all features (L2 loss)
- MSE evaluation under 10×10 REP-CV



Model fits train data well, but generalizes poorly.

EXAMPLE II: OVERFITTING

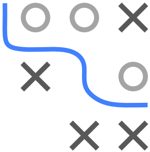
- We train an MLP and a CART on the mtcars data
- Both models are not regularized
- And configured to make overfitting more likely



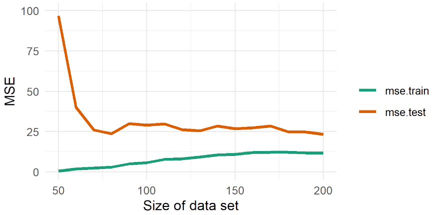
	Train MSE	Test MSE
Neural Network	3.68	19.98
CART	0.00	10.21

(And we now switch back to the Ozone example...)

AVOIDING OVERFITTING – COLLECT MORE DATA

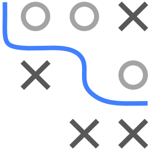


We explore our results for increased dataset size.



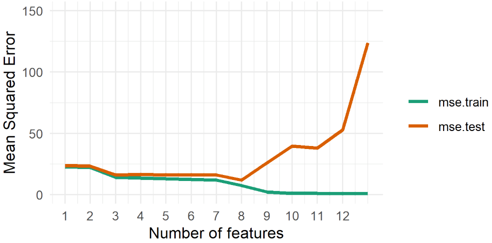
Fit slightly worsens, but test error decreases.
But: Often not feasible in practice.

AVOIDING OVERFITTING – REDUCE COMPLEXITY



We try the simplest model: a constant. So for $L2$ loss the mean of $y^{(i)}$.

We then increase complexity by adding one feature at a time.



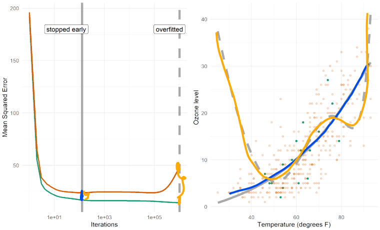
NB: We added features in a specific (clever) order, so we cheated a bit.

AVOIDING OVERFITTING – OPTIMIZE LESS

Now: polynomial regression with temperature as single feature

$$f(\mathbf{x} \mid \boldsymbol{\theta}) = \sum_{k=0}^{d} \theta_k \cdot (x_T)^k$$

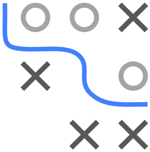
We set $d = 15$ to overfit to small data. To investigate early stopping, we don't analytically solve the OLS problem, but run GD stepwise.



We see: Early stopping GD can improve results.

NB: GD for poly-regr usually needs many iters before it starts to overfit, so we used a very small training set.

REGULARIZED EMPIRICAL RISK MINIMIZATION



We have contradictory goals:

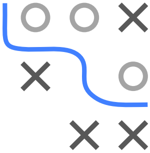
- **maximizing fit** (minimizing the train loss)
- **minimizing complexity** of the model

We saw how we can include features in a binary fashion.
But we would rather control complexity **on a continuum**.

REGULARIZED EMPIRICAL RISK MINIMIZATION

Common pattern:

θ+θx+θ



$$\mathcal{R}_{\text{reg}}(f) = \mathcal{R}_{\text{emp}}(f) + \lambda \cdot J(f) = \sum_{i=1}^{n} L\left(y^{(i)}, f\left(\mathbf{x}^{(i)}\right)\right) + \lambda \cdot J(f)$$

- $J(f)$: **complexity penalty**, **roughness penalty** or **regularizer**
- $\lambda \geq 0$: **complexity control** parameter
- The higher λ, the more we penalize complexity
- $\lambda = 0$: We just do simple ERM; $\lambda \to \infty$: we don't care about loss, models become as "simple" as possible
- λ is hard to set manually and is usually selected via CV
- As for $\mathcal{R}_{\text{emp}}$, $\mathcal{R}_{\text{reg}}$ and J are often defined in terms of $\boldsymbol{\theta}$:

$J(f)$ penalty

regularization term

$\theta_0 + \theta_1 x_1 + \theta_2 x_2$

$$\mathcal{R}_{\text{reg}}(\boldsymbol{\theta}) = \mathcal{R}_{\text{emp}}(\boldsymbol{\theta}) + \lambda \cdot J(\boldsymbol{\theta})$$

$\lambda = 1$

$2 + 12 \cdot 1 = 14$

12

$3 + 4x_1 + 5x^2$

$\theta_0 + \theta_1 + \theta_2$

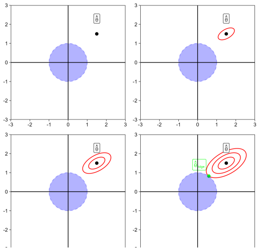
$10 + 1 \cdot 2.001$

2.001

$0 + 2x + 0.001x^2$

Introduction to Machine Learning

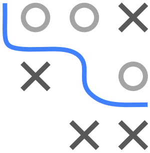
Regularization
Ridge Regression



Learning goals

- Regularized linear model
- Ridge regression / *L2* 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.

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

$3 + 2x + 4x^2$

$3^2 + 2^2 + 4^2$

Can still analytically solve this:

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

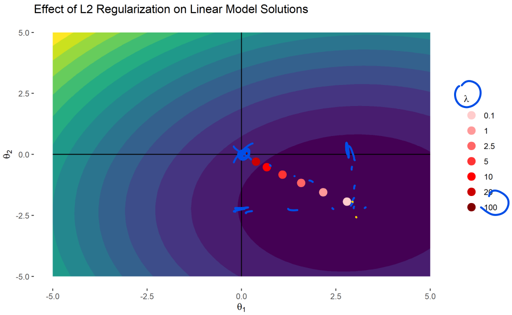
Name: We add pos. entries along the diagonal "ridge" of $\mathbf{X}^T\mathbf{X}$

$\|\theta\| = |3| + |2| + |4| =$

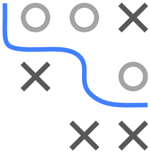
$= 9$

RIDGE REGRESSION / L2 PENALTY

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

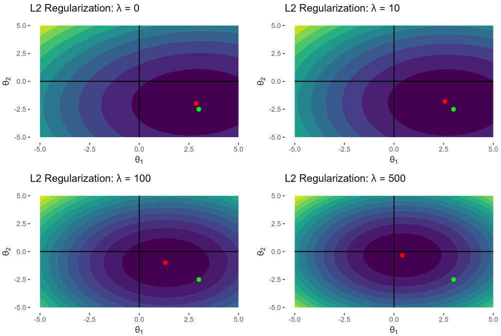


With increasing regularization, $\hat{\theta}_{ridge}$ is pulled back to the origin (contour lines show unregularized objective).



RIDGE REGRESSION / L2 PENALTY

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

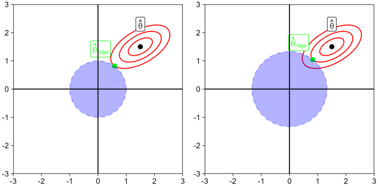


Green = true coefs of the DGP and red = ridge solution.

RIDGE REGRESSION / L2 PENALTY

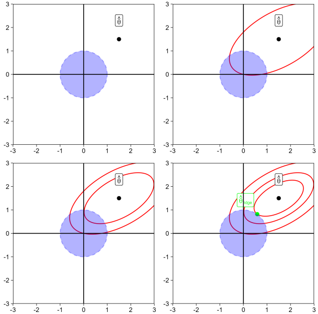
We understand the geometry of these 2 mixed components in our regularized risk objective much better, if we formulate the optimization as a constrained problem (see this as Lagrange multipliers in reverse).

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



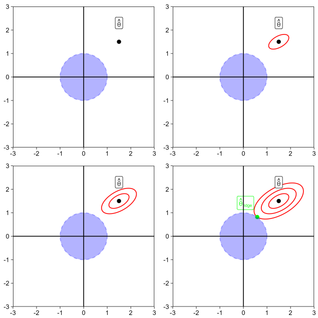
NB: There is a bijective relationship between λ and t: $\lambda \uparrow \Rightarrow \; t \downarrow$ and vice versa.

RIDGE REGRESSION / L2 PENALTY



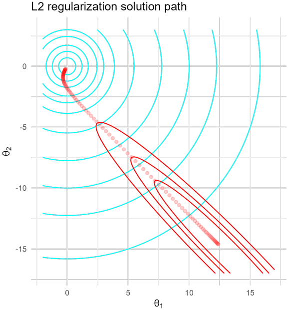
- Inside constraints perspective: From origin, jump from contour line to contour line (better) until you become infeasible, stop before.
- We still optimize the $\mathcal{R}_{\text{emp}}(\boldsymbol{\theta})$, but cannot leave a ball around the origin.
- $\mathcal{R}_{\text{emp}}(\boldsymbol{\theta})$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

RIDGE REGRESSION / L2 PENALTY



- 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



- 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

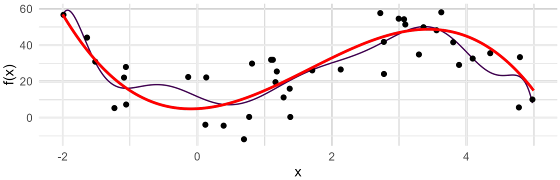
EXAMPLE: POLYNOMIAL RIDGE REGRESSION

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

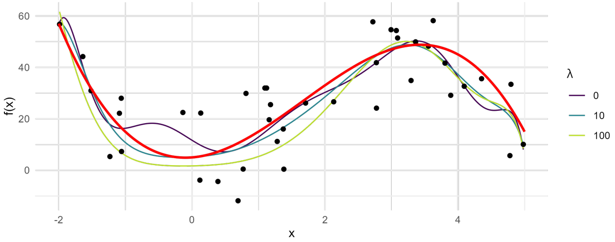
$$f(x) = \theta_0 + \theta_1 x + \cdots + \theta_d x^d = \sum_{j=0}^{d} \theta_j x^j.$$

Using model complexity $d = 10$ overfits:



EXAMPLE: POLYNOMIAL RIDGE REGRESSION

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*.

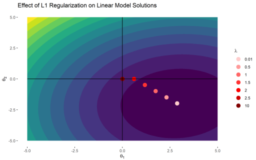


λ	θ_0	θ_1	θ_2	θ_3	θ_4	θ_5	θ_6	θ_7	θ_8	θ_9	θ_{10}
0.00	12.00	-16.00	4.80	23.00	-5.40	-9.30	4.20	0.53	-0.63	0.13	-0.01
10.00	5.20	1.30	3.70	0.69	1.90	-2.00	0.47	0.20	-0.14	0.03	-0.00
100.00	1.70	0.46	1.80	0.25	1.80	-0.94	0.34	-0.01	-0.06	0.02	-0.00

Introduction to Machine Learning

Regularization
Lasso Regression

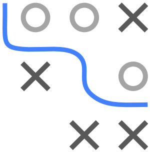
$|\theta|$



Learning goals

- Lasso regression / $L1$ penalty
- Know that lasso selects features
- Support recovery

LASSO REGRESSION



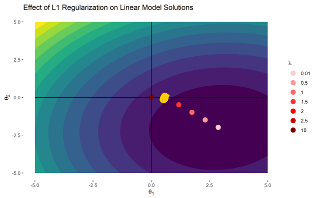
Another shrinkage method is the so-called **lasso regression** (least absolute shrinkage and selection operator), which uses an $L1$ penalty on $\boldsymbol{\theta}$:

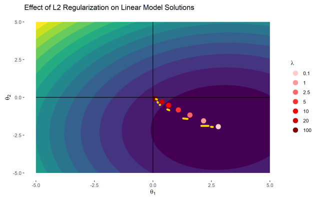
$$\begin{aligned}\hat{\boldsymbol{\theta}}_{\text{lasso}} &= \arg\min_{\boldsymbol{\theta}} \sum_{i=1}^{n} \left(y^{(i)} - \boldsymbol{\theta}^T \mathbf{x}^{(i)}\right)^2 + \lambda \sum_{j=1}^{p} |\theta_j| \\ &= \arg\min_{\boldsymbol{\theta}} (\mathbf{y} - \mathbf{X}\boldsymbol{\theta})^\top (\mathbf{y} - \mathbf{X}\boldsymbol{\theta}) + \lambda \|\boldsymbol{\theta}\|_1\end{aligned}$$

Optimization is much harder now. $\mathcal{R}_{\text{reg}}(\boldsymbol{\theta})$ is still convex, but in general there is no analytical solution and it is non-differentiable.

LASSO REGRESSION

Let $y = 3x_1 - 2x_2 + \epsilon$, $\epsilon \sim N(0, 1)$. The true minimizer is $\theta^* = (3, -2)^T$. LHS = $L1$ regularization; RHS = $L2$

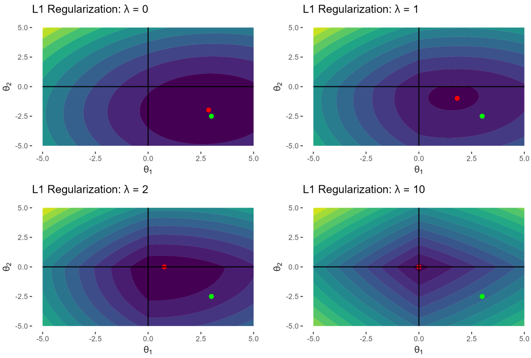


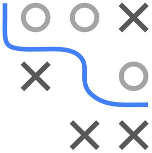


With increasing regularization, $\hat{\theta}_{lasso}$ is pulled back to the origin, but takes a different “route”. θ_2 eventually becomes 0!

LASSO REGRESSION

Contours of regularized objective for different λ values.





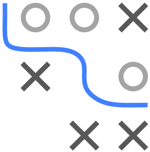
Green = true minimizer of the unreg.objective and red = lasso solution.

Feature Scaling

$ft^2 \to 1-8000 \to \times 2$

$a\{yrs\} \to 1-5 \to \times 200$

REGULARIZATION AND FEATURE SCALING

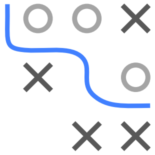


- Typically we omit θ_0 in penalty $J(\boldsymbol{\theta})$ so that the "infinitely" regularized model is the constant model (but can be implementation-dependent).
- Unregularized LM has **rescaling equivariance**, if you scale some features, can simply "anti-scale" coefs and risk does not change.
- Not true for Reg-LM: if you down-scale features, coeffs become larger to counteract. They are then penalized stronger in $J(\boldsymbol{\theta})$, making them less attractive without any relevenat reason.
- **So: usually standardize features in regularized models, whether linear or non-linear!**

REGULARIZATION AND FEATURE SCALING

- Let the DGP be $y = \sum_{j=1}^{5} \theta_j x_j + \varepsilon$ for $\boldsymbol{\theta} = (1, 2, 3, 4, 5)^\top$, $\varepsilon \sim \mathcal{N}(0, 1)$
- Suppose x_5 was measured in *m* but we change the unit to *cm* ($\tilde{x}_5 = 100 \cdot x_5$):

Method	$\hat{\theta}_1$	$\hat{\theta}_2$	$\hat{\theta}_3$	$\hat{\theta}_4$	$\hat{\theta}_5$	MSE
OLS	0.984	2.147	3.006	3.918	**5.205**	0.812
OLS Rescaled	0.984	2.147	3.006	3.918	**0.052**	0.812



$x_5 \cdot 5.2.$

$100 x_5 \cdot \frac{5.2}{100}$

- Estimate $\hat{\theta}_5$ gets scaled by $1/100$ while other estimates and MSE are invariant
- Running ridge regression with $\lambda = 10$ on same data shows that rescaling of of x_5 does not result in inverse rescaling of $\hat{\theta}_5$ (everything changes!)
- This is because $\hat{\theta}_5$ now lives on small scale while $L2$ constraint stays the same. Hence remaining estimates can "afford" larger magnitudes.

Method	$\hat{\theta}_1$	$\hat{\theta}_2$	$\hat{\theta}_3$	$\hat{\theta}_4$	$\hat{\theta}_5$	MSE
Ridge	0.709	1.874	2.661	3.558	**4.636**	1.366
Ridge Rescaled	0.802	1.943	2.675	3.569	**0.051**	1.08

30%

0.3

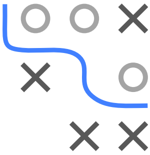
- For lasso, especially for very correlated features, we could arbitrarily force a feature out of the model through a unit change.

Weight Decay

WEIGHT DECAY VS. L2 REGULARIZATION

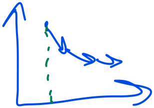
Let's optimize $L2$-regularized risk of a model $f(\mathbf{x} \mid \boldsymbol{\theta})$

$$\min_{\boldsymbol{\theta}} \mathcal{R}_{\text{reg}}(\boldsymbol{\theta}) = \min_{\boldsymbol{\theta}} \mathcal{R}_{\text{emp}}(\boldsymbol{\theta}) + \frac{\lambda}{2}\|\boldsymbol{\theta}\|_2^2$$



by GD. The gradient is

$$\nabla_{\boldsymbol{\theta}} \mathcal{R}_{\text{reg}}(\boldsymbol{\theta}) = \nabla_{\boldsymbol{\theta}} \mathcal{R}_{\text{emp}}(\boldsymbol{\theta}) + \lambda \boldsymbol{\theta}$$



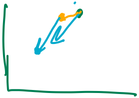
We iteratively update $\boldsymbol{\theta}$ by step size α times the negative gradient

$$(\alpha + \beta)' = \alpha' + \beta'$$

$$\begin{aligned} \boldsymbol{\theta}^{[\text{new}]} &= \boldsymbol{\theta}^{[\text{old}]} - \alpha \left(\nabla_{\boldsymbol{\theta}} \mathcal{R}_{\text{emp}}(\boldsymbol{\theta}^{[\text{old}]}) + \lambda \boldsymbol{\theta}^{[\text{old}]} \right) \\ &= \boldsymbol{\theta}^{[\text{old}]}(1 - \underbrace{\alpha\lambda)}_{<1} - \alpha \nabla_{\boldsymbol{\theta}} \mathcal{R}_{\text{emp}}(\boldsymbol{\theta}^{[\text{old}]}) \end{aligned}$$

$$\theta^{\text{old}} - \lambda \left(\nabla \mathcal{R}_{\text{emp}}(\theta^{\text{old}}) + \lambda \cdot \theta \right)$$

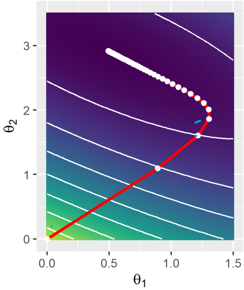
We see how $\boldsymbol{\theta}^{[old]}$ decays in magnitude – for small α and λ – before we do the gradient step. Performing the decay directly, under this name, is a very well-known technique in DL - and simply $L2$ regularization in disguise (for GD).



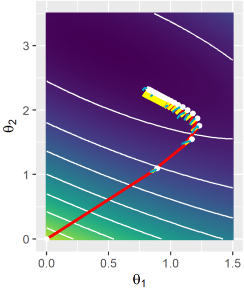
0.9

WEIGHT DECAY VS. L2 REGULARIZATION / 2

In GD With WD, we slide down neg. gradients of $\mathcal{R}_{\text{emp}}$, but in every step, we are pulled back to origin.



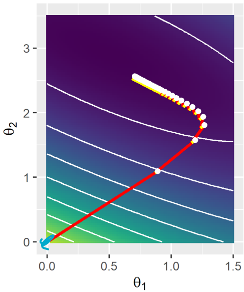
Without WD



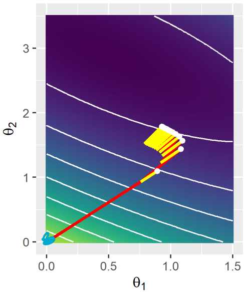
With GD

WEIGHT DECAY VS. L2 REGULARIZATION / 3

How strongly we are pulled back (for fixed α) depends on λ:



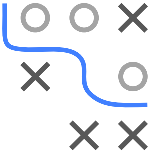
Small λ



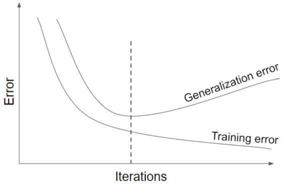
Large λ

Early Stopping

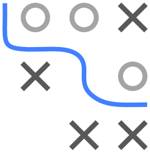
EARLY STOPPING



- Especially for complex nonlinear models we can easily overfit
- In optimization: Often, after a certain number of iterations, generalization error begins to increase even though training error continues to decrease



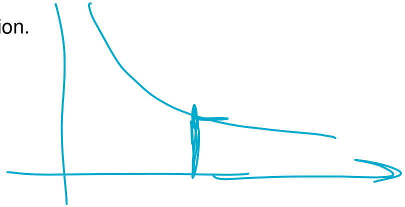
EARLY STOPPING / 2



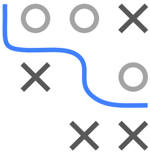
For iterative optimizers like SGD,
we can monitor this step-by-step over small iterations:

1. Split train data $\mathcal{D}_{\text{train}}$ into $\mathcal{D}_{\text{subtrain}}$ and $\mathcal{D}_{\text{val}}$ (e.g. with ratio of 2:1)
2. Train on $\mathcal{D}_{\text{subtrain}}$ and eval model on $\mathcal{D}_{\text{val}}$
3. Stop when validation error stops decreasing
(after a range of “patience” steps)
4. Use parameters of the previous step for the actual model

More sophisticated forms also apply cross-validation.



EARLY STOPPING AND *L*2 Goodfellow, Bengio, and Courville 2016



Strengths	Weaknesses
Effective and simple	Periodical evaluation of validation error
Applicable to almost any model without adjustment	Temporary copy of $\boldsymbol{\theta}$ (we have to save the whole model each time validation error improves)
Combinable with other regularization methods	Less data for training $\rightarrow$ include $\mathcal{D}_{\text{val}}$ afterwards

- For simple case of LM with squared loss and GD optim initialized at $\boldsymbol{\theta} = 0$: Early stopping has exact correspondence with *L*2 regularization/WD: optimal early-stopping iter T_{stop} inversely proportional to λ scaled by step-size α

$$T_{\text{stop}} \approx \frac{1}{\alpha\lambda} \Leftrightarrow \lambda \approx \frac{1}{T_{\text{stop}}\alpha}$$

- Small λ (regu. $\downarrow$) $\Rightarrow$ large T_{stop} (complexity $\uparrow$) and vice versa