# MIT 9.520/6.7910
# Statistical Learning Theory and Applications

## Class 05: Implicit Regularization

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# Learning algorithm design so far

Pick a representation, then:

- ERM, penalized/constrained,

$$\min_{w \in \mathbb{R}^d} \underbrace{\frac{1}{n} \sum_{i=1}^{n} \ell(y_i, w^\top x_i) + \lambda \|w\|^2}_{\widehat{L}^\lambda(w)}.$$

- Optimization by GD/SGD,

$$w_{t+1} = w_t - \gamma \nabla \widehat{L}^\lambda(w_t).$$

# Beyond ERM

- Are there other algorithm design principles?

- So far statistics/regularization separate from computations.

Today we will see how *optimization regularizes implicitly*.

# Least squares recap: minimal norm

Recall that for least squares

$$\widehat{X}w = \widehat{Y}$$

$$\underbrace{\min_{w\in\mathbb{R}^d} \frac{1}{n}\left\|\widehat{Y} - \widehat{X}w\right\|^2}_{n>d} \qquad \underbrace{\min_{w\in\mathbb{R}^d} \|w\|, \quad \text{subj. to} \quad \widehat{X}w = \widehat{Y}}_{n<d}$$

$$\Rightarrow \quad \widehat{w}^\dagger = \widehat{X}^\dagger \widehat{Y}.$$

# Least squares recap: pernalized ERM

$$\min_{w \in \mathbb{R}^d} \frac{1}{n} \left\| \widehat{Y} - \widehat{X} w \right\|^2 + \lambda \|w\|^2$$

$$\Rightarrow \quad \widehat{w}_\lambda = (\widehat{X}^\top \widehat{X} + \lambda n I)^{-1} \widehat{X}^\top \widehat{Y} = \widehat{X}^\top (\widehat{X} \widehat{X}^\top + \lambda n I)^{-1} \widehat{Y}$$

$$\lim_{\lambda \to 0} (\widehat{X}^\top \widehat{X} + \lambda n I)^{-1} \widehat{X}^\top = \widehat{X}^\dagger \quad \Rightarrow \quad \lim_{\lambda \to 0} \widehat{w}_\lambda = \widehat{w}^\dagger$$

# Outline

The implicit bias of gradient descent

Gradient descent stability and early stopping

# Least squares learning with gradient descent

We want to understand the learning properties of

$$\widehat{w}_{t+1} = \widehat{w}_t - \gamma \frac{1}{n} \widehat{X}^\top (\widehat{X}\widehat{w}_t - \widehat{Y}),$$

the gradient descent iteration for the empirical risk,

$$\widehat{L}(w) = \frac{1}{2n} \left\| \widehat{Y} - \widehat{X}w \right\|^2.$$

No penalties no constraints (!): what can we hope for?

# Implicit bias of gradient descent

We know that, for suitable $\gamma$

$$\lim_{t \to \infty} \widehat{w}_t = \arg\min \widehat{L}(w).$$

In fact, we can show that

$$\lim_{t \to \infty} \widehat{w}_t = \widehat{w}^{\dagger}.$$

# Understanding the implicit bias of GD for LS

$$\widehat{w}_{t+1} = \widehat{w}_t - \gamma \frac{2}{n} \widehat{X}^\top (\widehat{X}\widehat{w}_t - \widehat{Y}),$$

If $w_0 \in \text{Range}(\widehat{X}^\top)$ (e.g. $w_0 = 0$), then $\widehat{w}_t \in \text{Range}(\widehat{X}^\top)$ for all $t$.

$\Rightarrow$ GD converges to a solution in $\text{Range}(\widehat{X}^\top)$.

[1] Recall that $\text{Range}(\widehat{X}^\top) = \text{Null}(\widehat{X})^\perp$

# Understanding the implicit bias of GD for LS

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$\Rightarrow$ GD converges to a solution in $\text{Range}(\widehat{X}^\top)$.

The minimal norm solution $\widehat{w}^\dagger$ is the unique solution in[1] $\text{Range}(\widehat{X}^\top)$.

Then,

$$\lim_{t \to \infty} \widehat{w}_t = \widehat{w}^\dagger.$$

[1] Recall that $\text{Range}(\widehat{X}^\top) = \text{Null}(\widehat{X})^\perp$

# Implicit bias/regularization

Compare

$$\lim_{t \to \infty} \widehat{w}_t = \widehat{w}^\dagger,$$

to

$$\lim_{\lambda \to 0} \widehat{w}^\lambda = \widehat{w}^\dagger.$$

- Gradient descent explores solutions with a *bias* towards small norms.
- The bias is *implicit* in the sense that there are no explicit constraint/penalties.

# Implicit bias for other loss functions

Regression

Consider $\ell(x^\top w - y)$ and

$$\widehat{w}_{t+1} = \widehat{w}_t - \gamma_t \frac{1}{n} \sum_{i=1}^{n} x_i \ell'(x_i^\top w - y_i),$$

Then $w_t \in \text{Range}(\widehat{X}^\top)$, and if $\ell(0) = 0$ and $n > d$ then $\widehat{w}_t \to \widehat{w}^\dagger$ (why?).

# Implicit bias for other loss functions

## Regression

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## Classification

Consider $\ell(x^\top wy)$ and

$$\widehat{w}_{t+1} = \widehat{w}_t - \gamma_t \frac{1}{n} \sum_{i=1}^{n} x_i \ell'(x_i^\top w y_i).$$

Then $w_t \in \text{Range}(\widehat{X}^\top)$. Convergence to max margin solutions can be ensured in some cases.

# Terminology: regularization and pseudosolutions?

- In signal processing minimal norm solutions are called regularization.
- In classical regularization theory, they are called pseudosolutions.
- Regularization refers to a family of solutions converging to pseudosolutions, e.g. Tikhonov.

# Outline

The implicit bias of gradient descent

Gradient descent stability and early stopping

# Back for more regularization

- There are problems in which $\widehat{w}^\dagger$ is unstable.

- Regularization: define a family of solutions + select one ensuring stability.

Tikhonov regularization

$$\widehat{w}^\lambda \to \widehat{w}^\dagger,$$

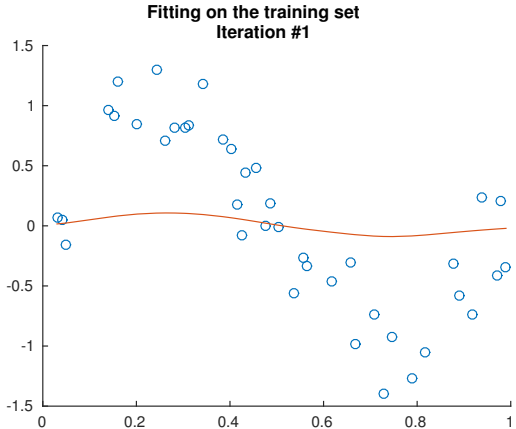
as $\lambda \to 0$. Choose $\lambda \neq 0$ if needed.

# Regularization by gradient descent?

Gradient descent converges to the minimal norm solution, but:

- does it define a family of meaningful regularized solutions?
- Where is the regularization parameter?

# An intuition: early stopping



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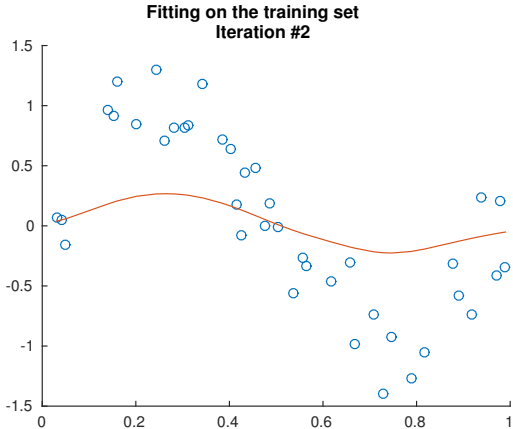

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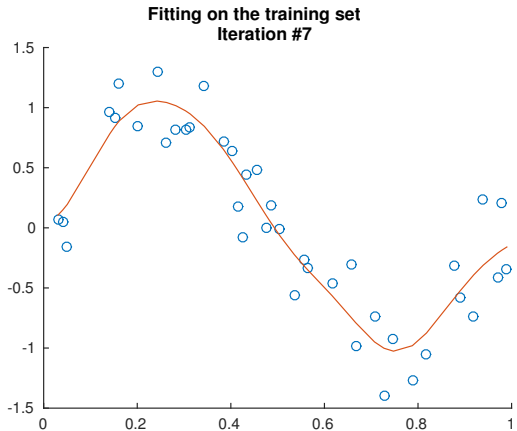

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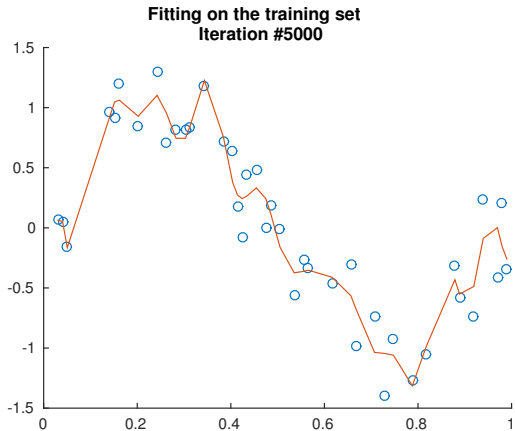

Is there a way to formalize this intuition?

# Interlude: geometric series

Recall for $|a| < 1$

$$\sum_{j=0}^{\infty} a^j = (1-a)^{-1}, \qquad \sum_{j=0}^{t} a^j = (1-a^t)(1-a)^{-1}.$$

# Interlude: geometric series

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Equivalently for $|b| < 1$

$$\sum_{j=0}^{\infty} (1-b)^j = b^{-1}, \qquad \sum_{j=0}^{t} (1-b)^j = (1-(1-b)^t)b^{-1}.$$

# Interlude II: Neumann series

Assume $I - A$ invertible matrix and $\|A\| < 1$

$$\sum_{j=0}^{\infty} A^j = (I - A)^{-1}, \qquad \sum_{j=0}^{t} A^j = (I - A^t)(I - A)^{-1}.$$

[2] Argument can be extended to pseudoinverses.

# Interlude II: Neumann series

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$$\sum_{j=0}^{\infty} A^j = (I - A)^{-1}, \qquad \sum_{j=0}^{t} A^j = (I - A^t)(I - A)^{-1}.$$

Equivalently for $B$ invertible[2] and $\|B\| < 1$

$$\sum_{j=0}^{\infty} (I - B)^j = B^{-1}, \qquad \sum_{j=0}^{t} (I - B)^j = (I - (I - B)^t)B^{-1}.$$

[2] Argument can be extended to pseudoinverses.

# Rewriting GD

For $w_0 = 0$, by induction

$$\widehat{w}_{t+1} = \widehat{w}_t - \frac{\gamma}{n}\widehat{X}^\top(\widehat{X}\widehat{w}_t - \widehat{Y}),$$

can be written as

$$\widehat{w}_{t+1} = \frac{\gamma}{n}\sum_{j=0}^{t}(I - \gamma\widehat{X}^\top\widehat{X})^j\widehat{X}^\top\widehat{Y}.$$

# Rewriting GD (cont.)

- Write

$$\widehat{w}_{t+1} = \widehat{w}_t - \frac{\gamma}{n}\widehat{X}^\top(\widehat{X}\widehat{w}_t - \widehat{Y}) = (I - \frac{\gamma}{n}\widehat{X}^\top\widehat{X})\widehat{w}_t + \frac{\gamma}{n}\widehat{X}^\top\widehat{Y}.$$

# Rewriting GD (cont.)

- Write

$$\widehat{w}_{t+1} = \widehat{w}_t - \frac{\gamma}{n}\widehat{X}^\top(\widehat{X}\widehat{w}_t - \widehat{Y}) = (I - \frac{\gamma}{n}\widehat{X}^\top\widehat{X})\widehat{w}_t + \frac{\gamma}{n}\widehat{X}^\top\widehat{Y}.$$

- Assume

$$\widehat{w}_t = \frac{\gamma}{n}\sum_{j=0}^{t-1}(I - \frac{\gamma}{n}\widehat{X}^\top\widehat{X})^j\widehat{X}^\top\widehat{Y}.$$

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- Assume

$$\widehat{w}_t = \frac{\gamma}{n}\sum_{j=0}^{t-1}(I - \frac{\gamma}{n}\widehat{X}^\top\widehat{X})^j\widehat{X}^\top\widehat{Y}.$$

- Then

$$\begin{aligned}\widehat{w}_{t+1} &= (I - \frac{\gamma}{n}\widehat{X}^\top\widehat{X})\frac{\gamma}{n}\sum_{j=0}^{t-1}(I - \frac{\gamma}{n}\widehat{X}^\top\widehat{X})^j\widehat{X}^\top\widehat{Y} + \frac{\gamma}{n}\widehat{X}^\top\widehat{Y} \\ &= \frac{\gamma}{n}\sum_{j=0}^{t}(I - \frac{\gamma}{n}\widehat{X}^\top\widehat{X})^j\widehat{X}^\top\widehat{Y}.\end{aligned}$$

# Neumann series and GD

$$\widehat{w}_{t+1} = \frac{\gamma}{n}\sum_{j=0}^{t}(I - \frac{\gamma}{n}\widehat{X}^\top\widehat{X})^j\widehat{X}^\top\widehat{Y}.$$

GD is a truncated power series approximation of the pseudoinverse!

If $\gamma$ is such that[3] $\left\|I - \frac{\gamma}{n}\widehat{X}^\top\widehat{X}\right\| < 1$, then for large $t$

$$\frac{\gamma}{n}\sum_{j=0}^{t}(I - \frac{\gamma}{n}\widehat{X}^\top\widehat{X})^j\widehat{X}^\top \approx \widehat{X}^\dagger$$

and we recover $\widehat{w}_t \to \widehat{w}^\dagger$.

[3] Compare to classic conditions.

# Stability properties of GD

For any $t$

$$\widehat{w}_t = (I - (I - \frac{\gamma}{n}\widehat{X}^\top \widehat{X})^t)(\widehat{X}^\top \widehat{X})^{-1}\widehat{X}^\top \widehat{Y}$$

(assume invertibility for simplicity).

Then

$$\underbrace{\widehat{w}_t \approx (\widehat{X}^\top \widehat{X})^{-1}\widehat{X}^\top \widehat{Y}}_{\text{large } t}, \qquad \underbrace{\widehat{w}_t \approx \frac{\gamma}{n}\widehat{X}^\top \widehat{Y}}_{\text{small } t}.$$

Compare to Tikhonov $\widehat{w}_\lambda = (\widehat{X}^\top \widehat{X} + \lambda n I)^{-1}\widehat{X}^\top \widehat{Y}$

$$\underbrace{\widehat{w}_\lambda \approx (\widehat{X}^\top \widehat{X})^{-1}\widehat{Y}}_{\text{small } \lambda}, \qquad \underbrace{\widehat{w}_\lambda \approx \lambda n \widehat{X}^\top \widehat{Y}}_{\text{large } \lambda}.$$

# Spectral view and filtering

Recall for Tikhonov

$$\widehat{w}^{\lambda} = \sum_{j=1}^{r} \frac{s_j}{s_j^2 + \lambda} (u_j^{\top} \widehat{Y}) v_j.$$

# Spectral view and filtering

Recall for Tikhonov

$$\widehat{w}^{\lambda} = \sum_{j=1}^{r} \frac{s_j}{s_j^2 + \lambda} (u_j^{\top} \widehat{Y}) v_j.$$

For GD

$$\widehat{w}^{\lambda} = \sum_{j=1}^{r} \frac{(1 - (1 - \frac{\gamma}{n} s_j^2)^t)}{s_j} (u_j^{\top} \widehat{Y}) v_j.$$

# Spectral view and filtering

Recall for Tikhonov

$$\widehat{w}^{\lambda} = \sum_{j=1}^{r} \frac{s_j}{s_j^2 + \lambda} (u_j^\top \widehat{Y}) v_j.$$

For GD

$$\widehat{w}^{\lambda} = \sum_{j=1}^{r} \frac{(1 - (1 - \frac{\gamma}{n} s_j^2)^t)}{s_j} (u_j^\top \widehat{Y}) v_j.$$

Both methods can be seen as performing spectral filtering

$$\widehat{w}^{\lambda} = \sum_{j=1}^{r} F(s_j)(u_j^\top \widehat{Y}) v_j,$$

for some suitable filter function $F$.

# Implicit regularization and early stopping

The stability of GD decreases with $t$, i.e. higher condition number for

$$(I - (I - \frac{\gamma}{n}\widehat{X}^\top \widehat{X})^t)(\widehat{X}^\top \widehat{X})^{-1}\widehat{X}^\top.$$

*Early-stopping* the iteration as a (implicit) regularization effect.

# Summary so far

$$\widehat{w}_{t+1} = \widehat{w}_t - \frac{\gamma}{n}\widehat{X}^\top(\widehat{X}\widehat{w} - \widehat{Y}) = \frac{\gamma}{n}\sum_{j=0}^{t}(I - \gamma\widehat{X}^\top\widehat{X})^j\widehat{X}^\top\widehat{Y}.$$

- Implicit bias: gradient descent converges to the minimal norm solution.
- Stability: the number of iteration is a regularization parameter.

Name game: gradient descent, Landweber iteration, $L^2$-Boosting.

# A bit of history

These ideas are fashionable now but have also a long history.

- The idea that iterations converge to pseudosolutions is from the 50's.
- The observation that iterations control stability dates back at least to the 80's.

Classic name is iterative regularization (there are books about it).

# Why is it back in fashion?

- Early stopping is used as a heuristic while training neural nets.
- Convergence to minimal norm solutions could help understanding generalization in deep learning?
- New perspective on algorithm design merging statistics and optimization.

# Statistics meets optimization

- Training time= model complexity?
- Iterations control statistical accuracy *and* numerical complexity.
- This kind of regularization is also called computational or algorithmic.

# Beyond linear least squares

- Other forms of optimization?
- Other loss functions?
- Other class of functions?
- Other norms?

# Other forms of optimization

Largely unexplored, there are some results on:

- Accelerated methods and conjugate gradient.
- Stochastic/incremental gradient methods.

Mostly for least squares.

It is clear that other parameters control regularization/stability, e.g step-size, mini-batch-size, averaging etc.

# Other loss functions

There are some results.

For $\ell$ convex, let

$$\widehat{L}(w) = \frac{1}{n} \sum_{i=1}^{n} \ell(y_i, w^\top x_i).$$

The gradient/subgradient descent iteration is

$$\widehat{w}_{t+1} = \widehat{w}_t - \gamma_t \nabla \widehat{L}(\widehat{w}_t).$$

# Other loss functions (cont.)

$$\widehat{w}_{t+1} = \widehat{w}_t - \gamma_t \nabla \widehat{L}(\widehat{w}_t)$$

An intuition: note that, if $\sup_t \left\| \nabla \widehat{L}(\widehat{w}_t) \right\| \leq B$,

$$\|\widehat{w}_t\| \leq \sum_t \gamma_t B,$$

the number of iterations/stepsize control the norm of the iterates.

# Representer theorem for GD

$$\widehat{w}_{t+1} = \widehat{w}_t - \gamma_t \frac{1}{n} \sum_{i=1}^{n} x_i \ell'(x_i^\top w, y_i).$$

It is easy to show that by induction that

$$\widehat{w}_t = \sum_{i=1}^{n} x_i (c_t)_i, \Leftrightarrow \hat{f}_t(x) = x^\top \widehat{w}_t = \sum_{i=1}^{n} x^\top x_i (c_t)_i$$

$$c_{t+1} = \widehat{w}_t - \gamma_t \frac{1}{n} \sum_{i=1}^{n} e_i \ell'(x_i^\top \widehat{w}_t, y_i),$$

This will give us kernels! Neural nets is trickier...

# Other norms

Some results.

- Gradient descent needs be replaced to bias iterations towards desired norms.

- Bregman iterations, mirror descent, proximal gradients can be used.

# Summing up

- A different way to design algorithms.
- Implicit/iterative regularization.
- Iterative regularization for least squares.
- Extensions.