Implicit Regularization

A Statistical View

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Machine learning

$$\text{test error} \leq \text{training error} + \sqrt{\frac{\text{complexity}}{n}}$$

- optimization <= gradient methods
- generalization <= complexity control

Machine learning

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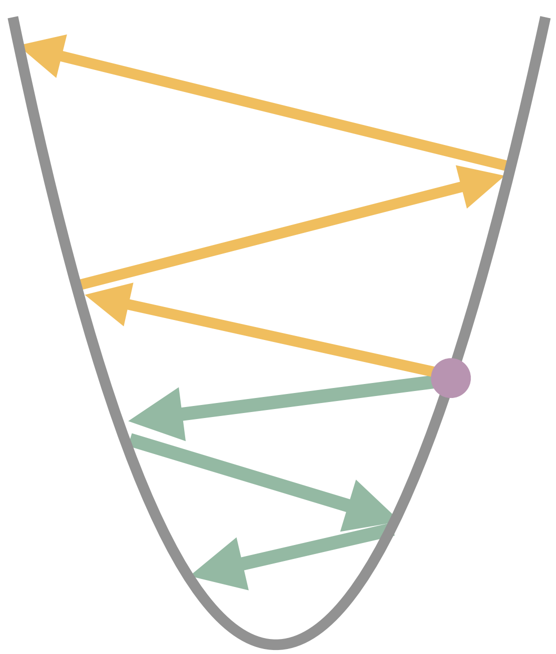
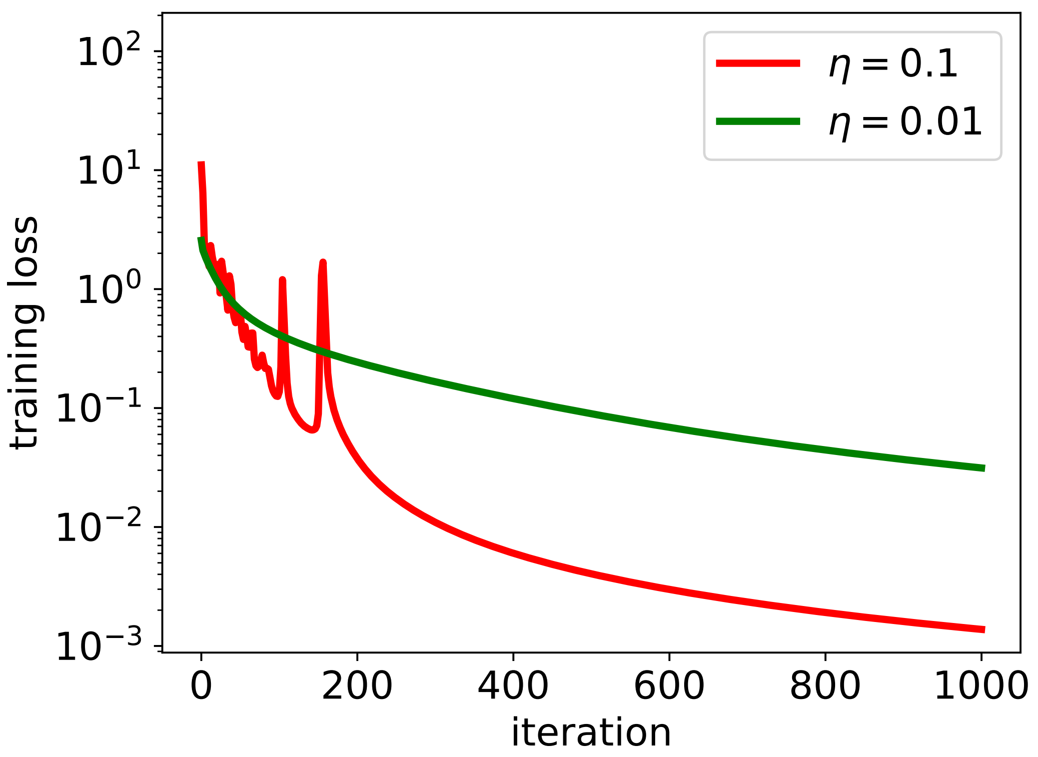
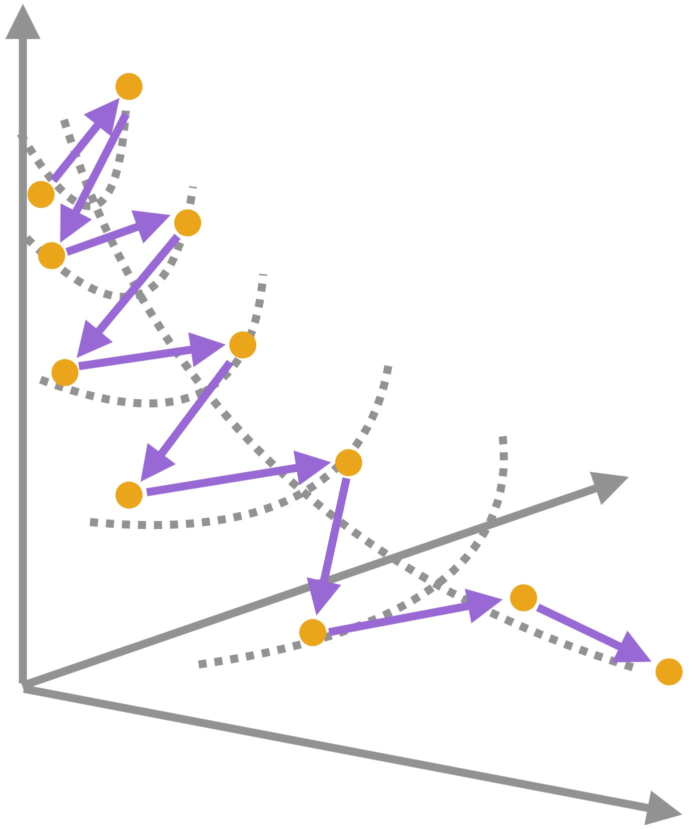
- optimization <= gradient methods

past work: large stepsize accelerates GD for logistic regression







Machine learning

$$\text{test error} \leq \text{training error} + \sqrt{\frac{\text{complexity}}{n}}$$

- optimization <= gradient methods
- generalization <= complexity control

this talk: generalization, done together with optimization

Complexity control

classical answer: **explicit control**

- model family
- norm regularization
- ...

deep learning: **implicit control via opt algo**

- early stopping
- stochastic averaging
- ...

how good is implicit regularization?

Bartlett. "For valid generalization the size of the weights is more important than the size of the network." NeurIPS 1996

One of our results

For all Gaussian linear regression problems:

early stopping is

- always no worse
- sometimes much better

than ℓ_2-regularization.

Our approach

Instance-wise risk comparison ← instead of minimax

← high dimension

- GD vs ridge regression
- GD vs (online) SGD

Peter Bartlett

Jason Lee

Sham Kakade

Bin Yu

Wu, Bartlett*, Lee*, Kakade*, Yu*. "Risk comparisons in linear regression: implicit regularization dominates explicit regularization." arXiv 2025

Linear regression

finite signal-to-noise ratio

$$x \sim \mathrm{N}(0, \Sigma), \quad y = x^\top w^* + \mathrm{N}(0, 1) \text{ for } \|w^*\|_\Sigma \lesssim 1$$

problem determined by (Σ, w^*)

excess risk / prediction error

$$\begin{aligned} R(w) &= \mathbb{E}(y - x^\top w)^2 - \mathbb{E}(y - x^\top w^*)^2 \\ &= \|w - w^*\|_\Sigma^2 \end{aligned}$$

n iid samples $(x_1, y_1), \ldots, (x_n, y_n)$

$$X = \begin{bmatrix} x_1^\top \\ \vdots \\ x_n^\top \end{bmatrix} \quad Y = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix}$$

Explicit / implicit regularization

ridge regression hyperparameter: $\lambda \geq 0$

$$w_\lambda^{\text{ridge}} = \arg\min \frac{1}{n}\sum_{i=1}^{n} \|x_i^\top w - y_i\|^2 + \lambda\|w\|^2$$
$$= (X^\top X + n\lambda I)^{-1} X^\top Y$$

gradient descent hyperparameter: $t \geq 0$

- $w_0 = 0$
- for $s = 1, \ldots, t$,
$$w_s = w_{s-1} - \frac{\eta}{n} X^\top (X w_{s-1} - Y)$$
- $w_t^{\text{gd}} = w_t$

Notation

- SVD

$$\Sigma = \sum_{i \geq 1} \lambda_i u_i u_i^\top \qquad \lambda_1 \geq \lambda_2 \geq \ldots$$

- head and tail divided by k

$$\Sigma_{0:k} = \sum_{i \leq k} \lambda_i u_i u_i^\top \qquad \Sigma_{k:\infty} = \sum_{i > k} \lambda_i u_i u_i^\top$$

- matrix M, vector v

M^{-1} = pseudoinverse of M $\qquad \|v\|_M^2 = v^\top M v$

Bounds for ridge

*possible to pin down constants via RMT

Theorem. For all $\lambda \geq 0$, in expectation

$$\mathbb{E}R\left(w_\lambda^{\text{ridge}}\right) \gtrsim \tilde{\lambda}^2 \|w^*\|^2_{\Sigma^{-1}_{0:k^*}} + \|w^*\|^2_{\Sigma_{k^*:\infty}} + \min\left\{\frac{D}{n}, 1\right\}$$

"$\mathbb{E}$" can be made "w.h.p."

same upper bound holds w.h.p.

critical index $\quad k^* = \min\left\{k : \lambda + \frac{\sum_{i>k} \lambda_i}{n} \geq c\lambda_{k+1}\right\}$

effective regularization $\quad \tilde{\lambda} = \lambda + \frac{\sum_{i>k^*} \lambda_i}{n}$

effective dimension $\quad D = k^* + \frac{1}{\tilde{\lambda}^2} \sum_{i>k^*} \lambda_i^2$

Tsigler & Bartlett. "Benign overfitting in ridge regression." JMLR 2023

A ridge-type bound for GD

Theorem [**W**BLKY'25]**.** For all $0 < \eta \lesssim 1/\mathrm{tr}(\Sigma)$ and $t \geq 0$, w.h.p.

$$R\left(w_t^{\mathrm{gd}}\right) \lesssim \tilde{\lambda}^2 \|w^*\|^2_{\Sigma^{-1}_{0:k^*}} + \|w^*\|^2_{\Sigma_{k^*:\infty}} + \frac{D}{n}$$

was $\min\left\{\frac{D}{n}, 1\right\}$

critical index $\quad k^* = \min\left\{k : \frac{1}{\eta t} + \frac{\sum_{i>k} \lambda_i}{n} \geq c\lambda_{k+1}\right\}$

effective regularization $\quad \tilde{\lambda} = \frac{1}{\eta t} + \frac{\sum_{i>k^*} \lambda_i}{n}$

was λ

effective dimension $\quad D = k^* + \frac{1}{\tilde{\lambda}^2} \sum_{i>k^*} \lambda_i^2$

GD is no worse than ridge.

Proof. If $D > n$, set $t = 0$; otherwise, set $t = 1/(\eta\lambda)$.

GD dominates ridge

$$x \sim \mathrm{N}(0, \Sigma), \quad y = x^\top w^* + \mathrm{N}(0,1) \ \text{ for } \ \|w^*\|_\Sigma \lesssim 1$$

Theorem [**W**BLKY'25]**.** For **every** Gaussian linear regression, $n \geq 1$, and $\lambda \geq 0$, there is t such that: w.h.p.

$$R\left(w_t^{\mathrm{gd}}\right) \lesssim \mathbb{E} R\left(w_\lambda^{\mathrm{ridge}}\right)$$

Prior work. Assume an isotropic prior, $\mathbb{E} w^{*\otimes 2} \propto I$

$$\inf_\lambda \mathbb{E} R\left(w_\lambda^{\mathrm{ridge}}\right) \leq \mathbb{E} R\left(w_t^{\mathrm{gd}}\right) \leq 1.69 \mathbb{E} R\left(w_\lambda^{\mathrm{ridge}}\right)$$

next: GD can be much better than ridge

Ali, Kolter, Tibshirani. "A continuous-time view of early stopping for least squares regression." AISTATS 2019

Power law class

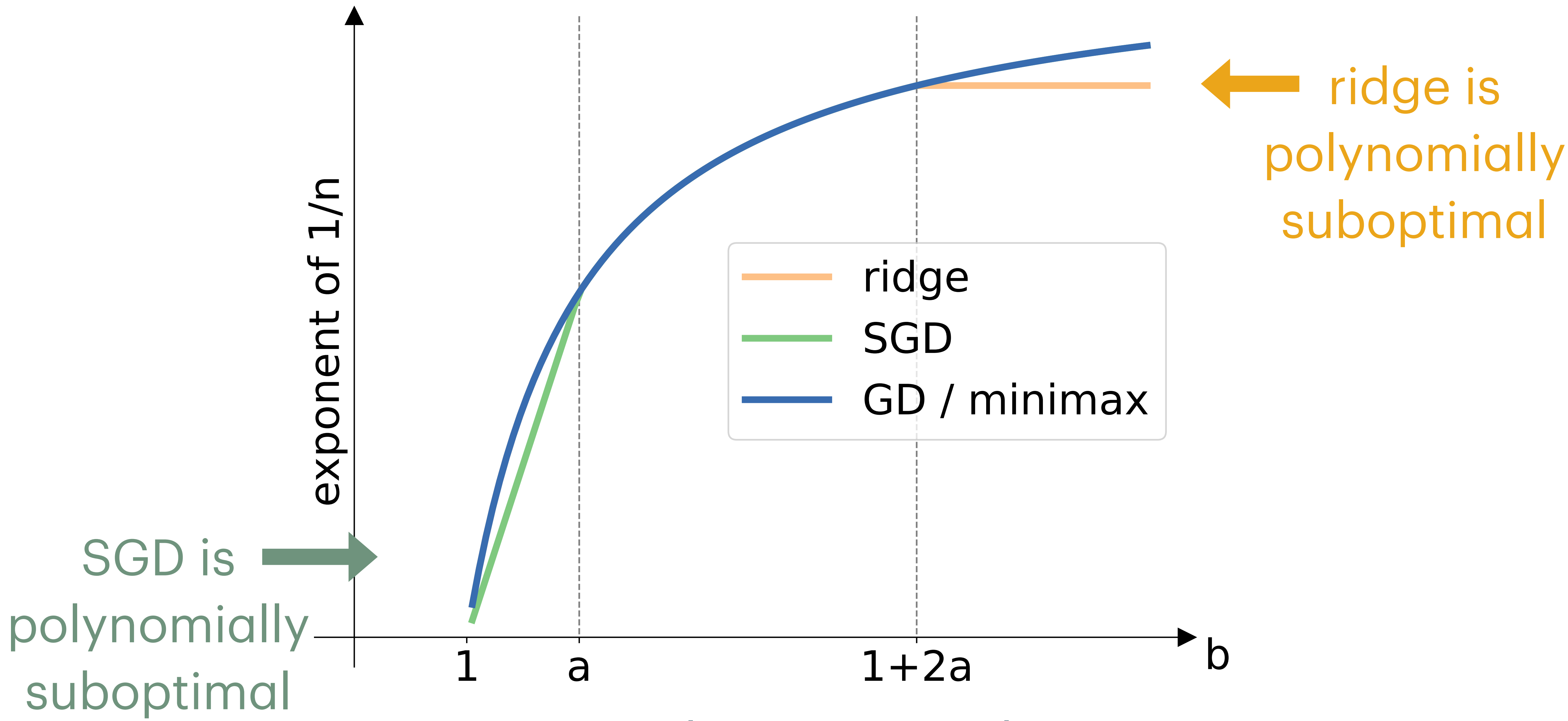
$$\lambda_i \eqsim i^{-a} \qquad \lambda_i (u_i^\top w^*)^2 \eqsim i^{-b} \qquad \text{for } a, b > 1$$

	1<b<a	a<b<1+2a	b>1+2a
ridge	$O\left(n^{-\frac{b-1}{b}}\right)$		$\Omega\left(n^{-\frac{2a}{1+2a}}\right)$
SGD	$\tilde{\Omega}\left(n^{-\frac{b-1}{a}}\right)$	$\tilde{O}\left(n^{-\frac{b-1}{b}}\right)$	
GD	$O\left(n^{-\frac{b-1}{b}}\right)$		
minimax	$\Omega\left(n^{-\frac{b-1}{b}}\right)$		

GD is always optimal
ridge/SGD is only partially optimal

Power law class

$\lambda_i \approx i^{-a}$ $\quad$ $\lambda_i (u_i^\top w^*)^2 \approx i^{-b}$ $\quad$ for $a, b > 1$



GD is always optimal

(best of ridge and SGD is also optimal)

Results so far

GD dominates ridge

- always no worse
- sometimes much better

remark (computation)

multi-pass SGD (sample with replacement)

- multi-pass SGD is no better than GD
- with correct stepsizes, multi-pass SGD $\approx$ GD

Why not known earlier?

fixed design is easy [DFKU’13, 6 pages]

but random design is hard

- instance-wise, not worst-case
- high-dim is surprising [BLLT’20, 44 pages]
- right tools 2019+

more surprise: GD vs (online) SGD

Dhillon, Foster, Kakade, Unga. “A risk comparison of ordinary least squares vs ridge regression.” JMLR 2013

Bartlett, Long, Lugosi, Tsigler. “Benign overfitting in linear regression.” PNAS 2020

Batch / online

gradient descent

- $w_0 = 0$
- for $s = 1, \ldots, t$,

$$w_s = w_{s-1} - \frac{\eta}{n} X^\top (X w_{s-1} - Y)$$

- $w_t^{\text{gd}} = w_t$

hyperparameter: $t \geq 0$

stochastic gradient descent

- $w_0 = 0, \eta_0 = \eta, N = n / \log n$
- for $i = 1, \ldots, n$,

$$\eta_i = \begin{cases} 0.1 \eta_{i-1} & \text{if } i \,\%\, N = 0 \\ \eta_{i-1} & \text{else} \end{cases}$$

$$w_i = w_{i-1} - \eta_i (x_i^\top w_{i-1} - y_i) x_i$$

- $w_\eta^{\text{sgd}} = w_n$

hyperparameter: $0 < \eta \lesssim 1/\text{tr}(\Sigma)$

compare implicit regularization: batch vs online

Bounds for SGD

Theorem. For all $0 < \eta \lesssim 1/\mathrm{tr}(\Sigma)$, in expectation

$$\mathbb{E}R\left(w_\eta^{\mathsf{sgd}}\right) \eqsim \left\| \prod_{i=1}^{n} (I - \eta_i \Sigma) w^* \right\|_\Sigma^2 + \frac{D}{N}$$

matching upper / lower bounds

effective steps $N = n/\log n$ "N" can be made "n"

critical index $k^* := \min\left\{ \frac{1}{\eta N} \geq c\lambda_{k+1} \right\}$

effective dimension $D = k^* + \eta^2 N^2 \sum_{i>k^*} \lambda_i^2$

effective regularization

Zou*, **Wu***, Braverman, Gu, Kakade. "Benign overfitting of constant-stepsize SGD for linear regression." COLT 2021

Wu*, Zou*, Braverman, Gu, Kakade. "Last iterate risk bounds of SGD with decaying stepsize for overparameterized linear regression." ICML 2022

SGD vs ridge

excess risk = bias + D/N

	SGD	ridge
bias	$\lVert e^{-\Theta(\eta N)\Sigma_{0:k^*}} w^* \rVert^2_{\Sigma_{0:k^*}} + \lVert w^* \rVert^2_{\Sigma_{k^*:\infty}}$ bias decays faster	$\tilde{\lambda}^2 \lVert w^* \rVert^2_{\Sigma^{-1}_{0:k^*}} + \lVert w^* \rVert^2_{\Sigma_{k^*:\infty}}$
effective steps	$N = n/\log n$	$N = n$
critical index	$\lambda_{k^*} \gtrsim \frac{1}{\eta N} \gtrsim \lambda_{k^*+1}$	$\lambda_{k^*} \gtrsim \lambda + \frac{\sum_{i>k^*} \lambda_i}{n} \gtrsim \lambda_{k^*+1}$
effective regularization	$\tilde{\lambda} = \frac{1}{\eta N}$ constraint	$\tilde{\lambda} = \lambda + \frac{\sum_{i>k^*} \lambda_i}{n}$ constraint
effective dimension	$\eta \lesssim 1/\mathrm{tr}(\Sigma)$ $D = k^* + \frac{1}{\tilde{\lambda}^2} \sum_{i>k^*} \lambda_i^2$	heavy tail

GD dominates ridge; *would GD dominate SGD?*

GD does not dominate SGD

Theorem [**W**BLKY'25]**.** $n \geq 1$. For a sequence of d-dim problems

$$d \geq n^2 \qquad w^* = \begin{bmatrix} n^{0.45} \\ 0 \\ \vdots \\ 0 \end{bmatrix} \qquad \Sigma = \begin{bmatrix} n^{-0.9} & & & \\ & 1/d & & \\ & & \ddots & \\ & & & 1/d \end{bmatrix}$$

we have $\|w^*\|_\Sigma^2 \leq 1$, moreover

- for all $0 < \eta \lesssim 1$ and $t \geq 0$, $\quad \mathbb{E}R\left(w_t^{\text{gd}}\right) = \Omega\left(n^{-0.2}\right)$
- for $\eta \eqsim 1$, $\quad \mathbb{E}R\left(w_\eta^{\text{sgd}}\right) = O\left(\log(n)/n\right)$

in high-dim
online learning can be poly better than batch!

A lower bound for GD

Theorem [**W**BLKY'25]**.** For all $0 < \eta \lesssim 1/\mathrm{tr}(\Sigma)$ and $t \geq 0$

$$\mathbb{E}R\left(w_t^{\mathsf{gd}}\right) \gtrsim \left(\frac{\sum_{i>\ell^*} \lambda_i}{n}\right)^2 \|w^*\|^2_{\Sigma^{-1}_{0:\ell^*}} + \|w^*\|^2_{\Sigma_{\ell^*:\infty}} + \min\left\{\frac{D}{n}, 1\right\}$$

effective dimension $\quad D = k^* + \frac{1}{\tilde{\lambda}^2} \sum_{i>k^*} \lambda_i^2$ *as before…*

benign overfitting index $\quad \ell^* = \min\left\{k : \frac{\sum_{i>k} \lambda_i}{n} \geq c\lambda_{k+1}\right\}$

GD variance = ridge variance
GD bias ≥ OLS bias

in high-dim
OLS bias can be large

when would GD dominate SGD?

A SGD-type bound for GD

Theorem [**W**BLKY'25]**.** For all $0 < \eta \lesssim 1/\mathrm{tr}(\Sigma)$ and $0 \le t \lesssim n$, w.h.p.

$$R\left(w_t^{\mathsf{gd}}\right) \lesssim \left\| (I - \eta\Sigma)^{t/2} w^* \right\|_\Sigma^2 + \frac{D}{n} + \left(\frac{D_1}{n}\right)^2$$

critical index $\quad k^* := \min \left\{ \frac{1}{\eta t} \ge c\lambda_{k+1} \right\}$

effective dimension $\quad D = k^* + \eta^2 t^2 \sum_{i>k^*} \lambda_i^2$

same as SGD when $t = \Theta(N)$

order-1 effective dim $\quad D_1 = k^* + \eta t \sum_{i>k^*} \lambda_i$

- $D \le D_1$, always
- in the hard example, $D \ll D_1$

when would $D_1 \lesssim D$?

Spectrum condition

Assumption. Spectrum decays *fast* and *continuously*

$$\text{for all } \tau > 1, \quad \tau \sum_{\lambda_i < 1/\tau} \lambda_i \lesssim \#\{\lambda_i \geq 1/\tau\}$$

satisfied by

- $\lambda_i \eqsim a^{-i}$ for $a > 1$
- $\lambda_i \eqsim i^{-a}$ for $a > 1$

violated by

- $\lambda_i \eqsim i^{-1} \log^{-a}(i)$ for $a > 1$
- $(\lambda_i)_{i \geq 1}$ in the hard example

$$(n^{-0.9}, 1/d, \ldots, 1/d) \text{ for } d \geq n^2$$

- rules out benign overfitting
- implies $D_1 \lesssim k^* \leq D$

GD dominates SGD in a subclass

Assumption. Spectrum decays fast and continuously

$$\text{for all } \tau > 1, \quad \tau \sum_{\lambda_i < 1/\tau} \lambda_i \lesssim \#\{\lambda_i \geq 1/\tau\}$$

$$x \sim \mathrm{N}(0, \Sigma), \quad y = x^\top w^* + \mathrm{N}(0,1) \ \text{ for } \ \|w^*\|_\Sigma \lesssim 1$$

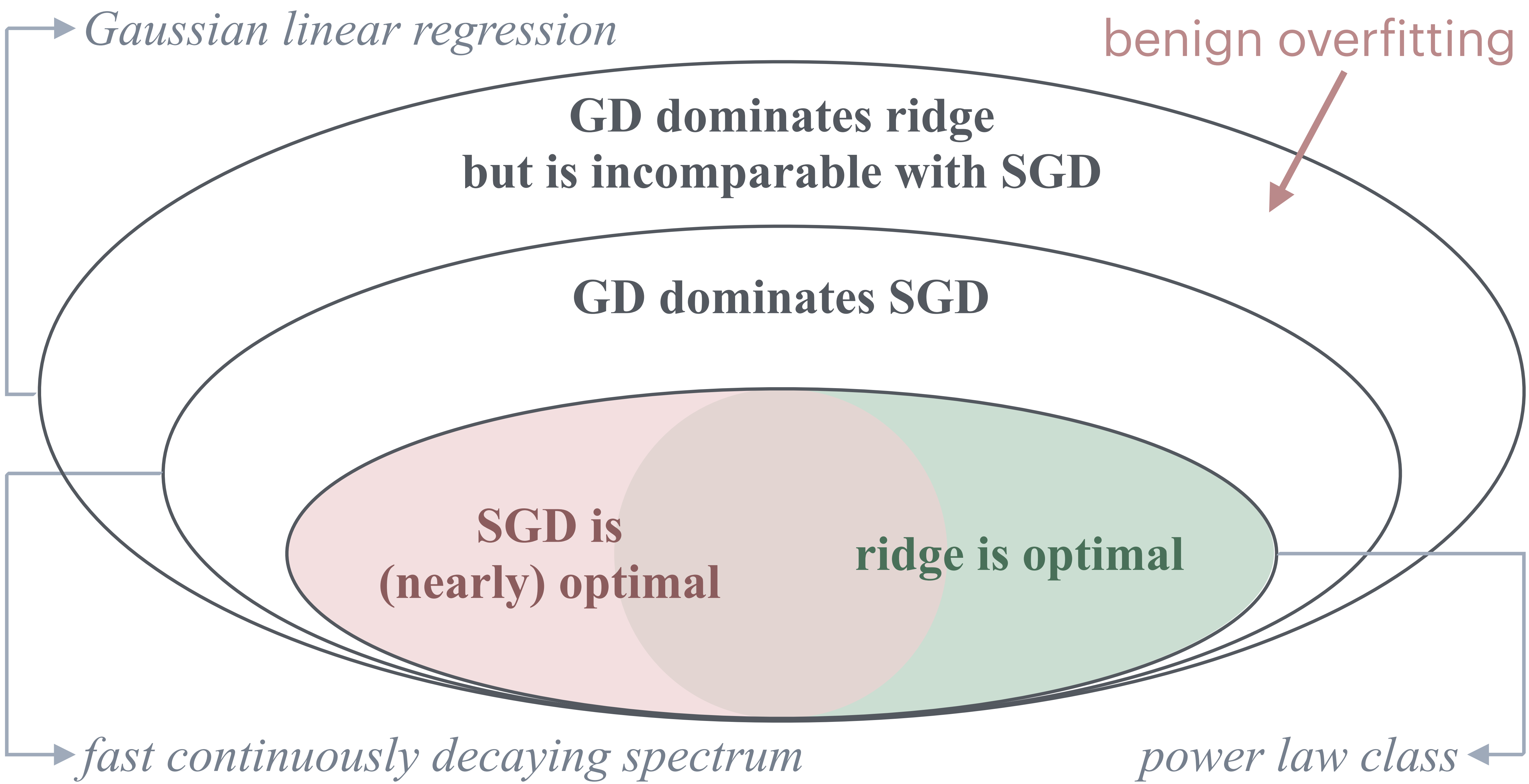
Theorem [**W**BLKY'25]**.** For every Gaussian linear regression satisfying the above, $n \geq 1$, and $0 \leq \eta \lesssim 1$, there is t such that

$$\mathbb{E}R\left(w_t^{\mathsf{gd}}\right) \lesssim \mathbb{E}R\left(w_\eta^{\mathsf{sgd}}\right)$$

Proof. Assumption implies $D_1 \lesssim k^* \leq D$.

no constraint on w^*

Contributions



“dominance”: always no worse, sometimes much better

How to reuse data?

- GD and SGD are incomparable
- multi-pass SGD is no better than GD
- but multi-epoch SGD (sample without replacement) dominates both
    - first epoch recovers SGD
    - continuous limit $\eta \to 0$ recovers GF

data reuse strategy makes poly differences
call for a new theory!