The Implicit Regularization of Stochastic Gradient Flow for Least Squares

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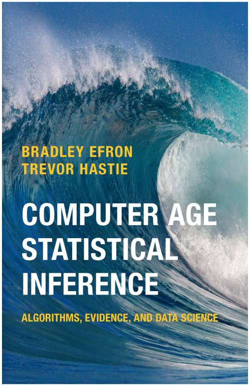
Outline

Introduction



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Algorithms and Inference

Statistics is the science of learning from experience, particularly experience that arrives a little bit at a time: the successes and failures of a new experimental drug, the uncertain measurements of an asteroid's path toward Earth. It may seem surprising that any one theory can cover such an amorphous target as "learning from experience." In fact, there are *two* main statistical theories, Bayesianism and frequentism, whose connections and disagreements animate many of the succeeding chapters.

Introduction

Given the sizes of modern data sets, stochastic gradient descent is one of the most widely used optimization algorithms today

- Computational and statistical properties have been studied for decades (Robbins & Monro, 1951; Fabian, 1968; Ruppert, 1988; Kushner & Yin, 2003; Polyak & Juditsky, 1992; ...)

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Recent interest in implicit regularization [Mahoney and Orecchia, 2011, Mahoney, 2012, Gleich and Mahoney, 2014, Martin and Mahoney, 2018, Soudry et al., 2018, Rosasco and Villa, 2015, Lin et al., 2016, Lin and Rosasco, 2017, Neu and Rosasco, 2018] etc

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In particular, a line of work showing (early-stopped) gradient descent is linked to ℓ_2 regularization [Nacson et al., 2018, Gunasekar et al., 2018, Suggala et al., 2018, Ali et al., 2018, Poggio et al., 2019, Ji and Telgarsky, 2019] etc

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"Double win"

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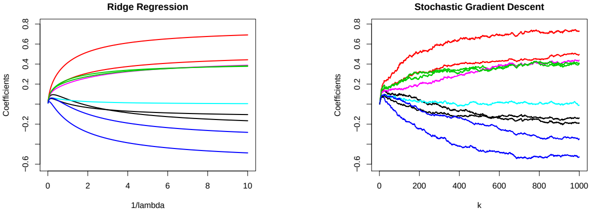
Why might there be a connection, at all?

Compare the paths for least squares regression



Here we focus on least squares regression

Introduction

Main tool for making the connection: a stochastic differential equation that we call stochastic gradient flow

Linked to SGD with a constant step size; more on this later

We give a bound on the excess risk of stochastic gradient flow at time t, over ridge regression with tuning parameter $\lambda = 1/t$

Result(s) hold across the entire optimization path
Results do not place strong conditions on the features
Proofs are simpler than in discrete-time (hard to handle var.)

Outline

Stochastic gradient flow

Stochastic gradient flow

Least squares regression (response $y \in \mathbb{R}^n$; data $X \in \mathbb{R}^{n \times p}$)

$$\underset{\beta \in \mathbb{R}^p}{\text{minimize}} \ \frac{1}{2n}\|y - X\beta\|_2^2 = \frac{1}{n}\sum_{i=1}^{n}(y_i - x_i^\top \beta)^2 := F(\beta)$$

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Mini-batch SGD: $k = 1, 2, 3, \ldots$, $\eta > 0$ fixed step size, m mini-batch size w/ replacement, $\beta^{(0)} = 0$

$$\beta^{(k)} = \beta^{(k-1)} + \frac{\eta}{m} \cdot \sum_{i \in \mathcal{I}_k} (y_i - x_i^\top \beta^{(k-1)}) x_i$$

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Add+subtract gradient:

$$\begin{aligned} \beta^{(k)} &= \beta^{(k-1)} + \frac{\eta}{n} \cdot X^\top (y - X\beta^{(k-1)}) \\ &+ \eta \cdot \left(\frac{1}{m} X_{\mathcal{I}_k}^\top (y_{\mathcal{I}_k} - X_{\mathcal{I}_k} \beta^{(k-1)}) - \frac{1}{n} X^\top (y - X\beta^{(k-1)}) \right). \end{aligned}$$

Stochastic gradient flow

Motivates the stochastic differential equation [Mandt et al., 2015, Hu et al., 2017, Feng et al., 2017, Li et al., 2019, Feng et al., 2019]

$$d\beta_t = \underbrace{\frac{1}{n} X^\top (y - X\beta_t)\, dt}_{\substack{\text{just the gradient for} \\ \text{least squares regression}}} + \underbrace{Q_\eta(\beta_t)^{1/2}\, dW(t)}_{\substack{\text{fluctuations are governed by the} \\ \text{cov. of the stochastic gradients}}}, \tag{1}$$

where $\beta_0 = 0$,

$$Q_\eta(\beta) = \eta \cdot \mathrm{Cov}_{\mathcal{I}} \left(\frac{1}{m} X_{\mathcal{I}}^\top (y_{\mathcal{I}} - X_{\mathcal{I}} \beta) \right)$$

is the diffusion coefficient, $\mathcal{I} \subseteq \{1, \ldots, n\}$ is a mini-batch, and $\eta > 0$ is a (fixed) step size

We call (1) stochastic gradient flow

Has a few nice properties, and bears several connections to SGD with a constant step size; more on this next

Stochastic gradient flow

Lemma: the Euler discretization of stochastic gradient flow $\tilde{\beta}^{(k)}$, and constant step size SGD $\beta^{(k)}$, share first and second moments, i.e.,

$$\mathbb{E}(\tilde{\beta}^{(k)}) = \mathbb{E}(\beta^{(k)}) \quad \text{and} \quad \mathrm{Cov}(\tilde{\beta}^{(k)}) = \mathrm{Cov}(\beta^{(k)})$$

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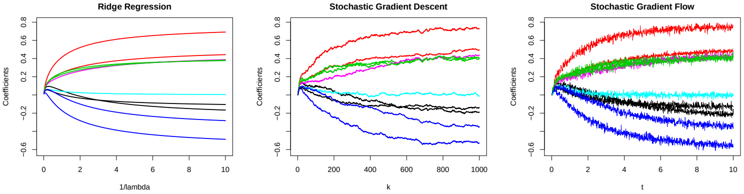
Sanity check: revisiting the solution/optimization paths from earlier



Stochastic gradient flow

A number of works consider instead the constant covariance process,

$$d\beta_t = \frac{1}{n} X^\top (y - X\beta_t)\, dt + \boxed{\left(\frac{\eta}{m} \cdot \hat{\Sigma}\right)^{1/2} dW(t)}, \qquad (2)$$

where $\hat{\Sigma} = X^\top X/n$ [Mandt et al., 2017, Wang, 2017, Dieuleveut et al., 2017, Fan et al., 2018]

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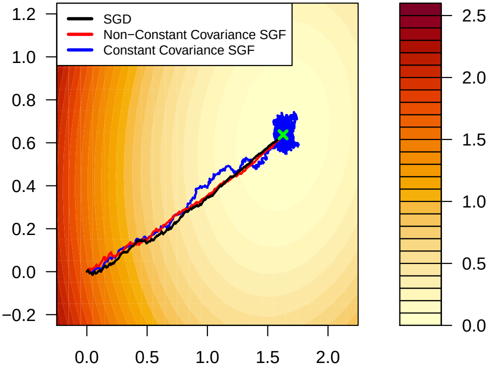
Stochastic Gradient Langevin dynamics (SGLD) takes diffusion coeff as τI [Geman and Hwang, 1986, Seung et al., 1992, Neal, 2011, Welling and Teh, 2011, Sato and Nakagawa, 2014, Teh et al., 2016, Raginsky et al., 2017, Cheng et al., 2019]

Stochastic gradient flow

Stochastic gradient flow is a more accurate approximation



Outline

Statistical Setup

Assume a standard regression model

$$y = X\beta_* + \varepsilon, \quad \varepsilon \sim (0, \sigma^2 I)$$

Fix X; let $s_i, i = 1, \ldots, p$, denote the eigenvalues of $X^\top X/n$

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Recall a useful result for (batch) gradient flow (Ali et al., 2018)

For least squares regression, gradient flow is

$$\dot{\beta}_t = \frac{1}{n} X^\top (y - X\beta_t) dt, \quad \beta_0 = 0$$

Has the solution

$$\hat{\beta}_t^{\mathrm{gf}} = (X^\top X)^+ (I - \exp(-tX^\top X/n)) X^\top y$$

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$$\hat{\beta}_t^{\mathrm{gf}} = (X^\top X)^+ (I - \exp(-tX^\top X/n)) X^\top y$$

Then, for any time $t \geq 0$ (note the correspondence with λ),

$\mathrm{Bias}^2(\hat{\beta}_t^{\mathrm{gf}}; \beta_*) \leq \mathrm{Bias}^2(\hat{\beta}_{1/t}^{\mathrm{ridge}}; \beta_*)$ and

$\mathrm{Var}(\hat{\beta}_t^{\mathrm{gf}}) \leq 1.6862 \cdot \mathrm{Var}(\hat{\beta}_{1/t}^{\mathrm{ridge}})$, so that

$\mathrm{Risk}(\hat{\beta}_t^{\mathrm{gf}}; \beta_*) \leq 1.6862 \cdot \mathrm{Risk}(\hat{\beta}_{1/t}^{\mathrm{ridge}}; \beta_*)$

Excess risk bound (over ridge)

Thm.: for any time $t > 0$ (provided the step size is small enough),

$$
\begin{aligned}
&\mathrm{Risk}(\hat\beta_t^{\mathrm{sgf}};\beta_*) - \mathrm{Risk}(\hat\beta_{1/t}^{\mathrm{ridge}};\beta_*) \\
&\quad \le 0.6862 \cdot \mathrm{Var}_\varepsilon(\hat\beta_{1/t}^{\mathrm{ridge}}) && \text{(scaled ridge variance)} \\
&\qquad + \eta \cdot \frac{n}{m} \sum_{i=1}^{p} \mathbb{E}_\varepsilon\left[\frac{\exp(\delta_y) s_i}{s_i - \alpha/2}\big(\exp(-\alpha t) - \exp(-2ts_i)\big)\right] \\
&&& \text{(``price of stochasticity'')} \\
&\qquad + \eta \cdot \frac{n}{m} \sum_{i=1}^{p} \mathbb{E}_\varepsilon\Big[\gamma_y\big(1 - \exp(-2ts_i)\big)\Big] && \text{(limiting opt. error)}
\end{aligned}
$$

η, m denote the step size and mini-batch size, respectively

s_i denote the eigenvalues of the sample covariance matrix

$\alpha, \gamma_y, \delta_y$ depend on n, p, m, η, s_i, y, but not t (see paper for details)

Implications/observations

$t = 1/\lambda$ scaling...

Appears in Rosasco & Poggio's papers and lectures
The implicit regularization of GD, and the connection to ridge, is, in their presentations, a key toy example for "why GD works in deep learning"
- `youtube.com/watch?v=4yLCuZnhkdI&t=3982` ..."number of iterations becomes $1/\lambda$"

Implications/observations

Result(s) hold across the entire optimization path

No strong conditions placed on the data matrix X

Also, have the following lower bound under oracle tuning

$$\inf_{\lambda \geq 0} \mathrm{Risk}(\hat{\beta}^{\mathrm{ridge}}_{\lambda}; \beta_*) \leq \inf_{t \geq 0} \mathrm{Risk}(\hat{\beta}^{\mathrm{sgf}}_{t}; \beta_*)$$

Implications/observations

Proof: stochastic calculus (Ito's rule) uses the special covariance structure of the diffusion coefficient $Q_\eta(\beta_t)$ for least squares

$$\mathrm{Risk}(\hat{\beta}_t^{\mathrm{sgf}}) = \mathrm{Bias}^2(\hat{\beta}_t^{\mathrm{sgf}}) + \mathrm{Var}_\varepsilon(\hat{\beta}_t^{\mathrm{gf}}) + \mathrm{tr}\,\mathbb{E}_\varepsilon[\mathrm{Cov}_I(\hat{\beta}_t^{\mathrm{sgf}})|\varepsilon].$$

$$\mathrm{tr}\,\mathrm{Cov}_I(\hat{\beta}_t^{\mathrm{sgf}}) = O\left(\int_0^t \mathrm{tr}\,Q_\eta(\hat{\beta}_t^{\mathrm{sgf}}) \cdot \mathrm{tr}\,\hat{\Sigma}\exp[2(\tau - t)\hat{\Sigma}]d\tau\right)$$

$$\mathrm{tr}\left(Q_\eta(\beta)\right) = O\left(F(\beta)\right)$$

Implications/observations

The second and third (variance) terms ...

- Depend on the signal-to-noise ratio; this is different from gradient flow (and linear smoothers in general, because stochastic gradient flow/descent are actually *randomized* linear smoothers)
- The second term decreases with time, just as a bias would (but is a variance); this is different from gradient flow (see lemma in the paper)

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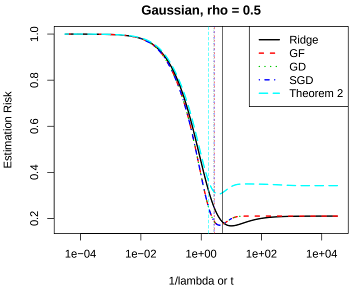
Third term vanishes (equals zero) if $p \geq n$ (can interpolate with overparametrization); "optimization variance smaller"

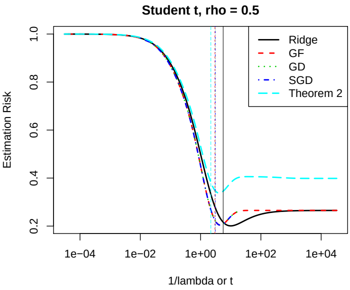
Outline

Synthetic data

Below, we show $n = 100, p = 10, m = 10$

- The bound (Theorem 2) tracks ridge's (and SGD's) risk(s) closely
- The bound / SGD achieve risk comparable to grad flow in less time
- See paper for other settings (e.g., high dimensions), coefficient error





Outline

Conclusion

Gave theoretical and empirical evidence showing stochastic gradient flow is closely related to ℓ_2 regularization - "why SGD works in statistical learning"

Interesting directions for future work

- Showing that stochastic gradient flow and SGD are, in fact, close
- Making the computational-statistical trade-off precise
- General convex losses
- Adaptive stochastic gradient methods

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Thanks for listening!

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