Dropout Regularization Versus ℓ_2-Penalization in the Linear Model

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Joint work with Sophie Langer and Johannes Schmidt-Hieber

G.C., Sophie Langer, and Johannes Schmidt-Hieber. "Dropout Regularization Versus ℓ_2-Penalization in the Linear Model." *arXiv preprint: 2306.10529* (2023).

Motivation: Model Averaging

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Problem: Combinatorial Explosion!

Dropout in Neural Networks

Proposed Solution: Dropout![1]

[1]Srivastava N. et al. "Dropout: a simple way to prevent neural networks from overfitting." *Journal of Machine Learning Research* (2014).

Dropout in Neural Networks

Proposed Solution: Dropout![1]

- Randomly exclude connections from training at every step of the gradient descent
- Re-scale trained weights appropriately

$\Longrightarrow$ Approximates model averaging while being tractable

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Dropout in Neural Networks

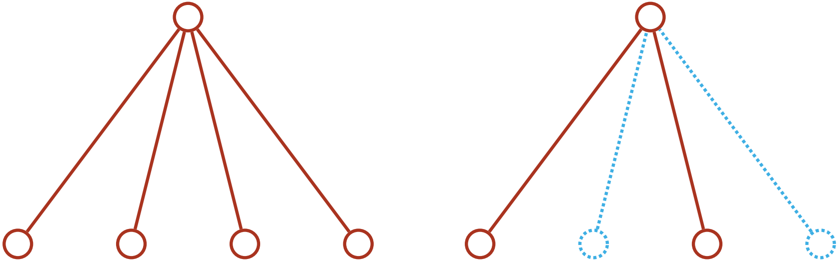

Figure: Regular neuron (left) and one sample of a neuron with dropout (right).

Why Study the Linear Model?

Canonical piece of wisdom: adding dropout noise to linear regression performs ridge regression/ℓ_2-penalization/Thikhonov regularization!

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Proposition (Srivastava et al. Section 9)

Dropout matrix $D_{ii} \overset{i.i.d.}{\sim} \mathrm{Ber}(p)$*; linear model* $Y = X\beta_\star + \varepsilon$ *with standard normal noise independent of* D*, then*

$$\arg\min_\beta \mathbb{E}\Big[\|Y - XD\beta\|_2^2 \mid Y\Big] = \Big(pX^{\mathrm{t}}X + (1-p)\mathrm{Diag}\big(X^{\mathrm{t}}X\big)\Big)^{-1} X^{\mathrm{t}}Y$$

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Intuition:

- Re-scaled minimizer of the averaged loss performs weighted ridge regression:

$$p\tilde{\beta} = \arg\min_{\beta} \left(\|Y - X\beta\|_2^2 + \left(\frac{1}{p} - 1\right) \cdot \left\|\sqrt{\mathrm{Diag}(X^{\mathsf{t}}X)}\beta\right\|_2^2\right)$$

- Small $p \implies$ strong regularization

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Problems:

- No explicit gradient descent
- No access to variance $\implies$ no statistical analysis

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Problems:

- No explicit gradient descent
- No access to variance $\implies$ no statistical analysis
- Conditional expectation $\mathbb{E}[\,\cdot \mid Y]$ represents loss of information $\implies$ $\tilde{\beta}$ may not capture gradient descent dynamics

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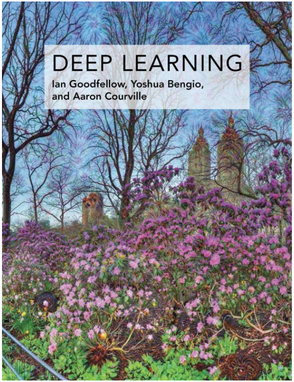

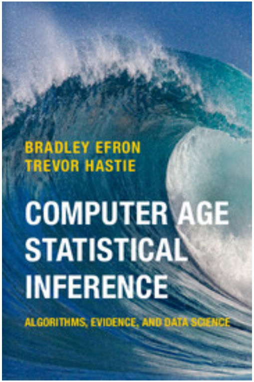

Some Definitions

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$$\begin{aligned}
\mathbb{X} &:= X^{\mathrm{t}} X \\
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($\mathbb{X}_p$ invertible if $\min_i \mathbb{X}_{ii} > 0$)

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- *Averaged dropout estimator*: $\tilde{\beta} = \mathbb{X}_p^{-1} X^{\mathrm{t}} Y$ (minimizer from proposition)

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- *Averaged dropout estimator*: $\tilde{\beta} = \mathbb{X}_p^{-1} X^{\mathrm{t}} Y$
- Euclidean norm $\|\cdot\|_2$ on vectors; spectral norm $\|\cdot\|$ on matrices

Incorporating Dropout with Gradient Descent

Standard Gradient Descent:

$$\beta_{k+1} = \beta_k - \frac{\alpha}{2} \nabla_{\beta_k} \left\| Y - X\beta_k \right\|_2^2$$

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On-Line Dropout:

$$\tilde{\beta}_{k+1} = \tilde{\beta}_k - \frac{\alpha}{2} \nabla_{\tilde{\beta}_k} \left\| Y - XD_{k+1}\tilde{\beta}_k \right\|_2^2$$

A new $i.i.d.$ dropout matrix is sampled every iteration!

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Questions:

- Convergence towards $\tilde{\beta}$?
- Statistical optimality?

Convergence of Expectation

Proposition

If $\alpha p \|\mathbb{X}\| < 1$ *and* $\min_i \mathbb{X}_{ii} > 0$*, then*

$$\left\|\mathbb{E}[\tilde{\beta}_k - \tilde{\beta}]\right\|_2 \leq \left\|I - \alpha p \mathbb{X}_p\right\|^k \cdot \left\|\mathbb{E}[\tilde{\beta}_0 - \tilde{\beta}]\right\|_2$$

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Intuition:

- Exponential decay, as in regular gradient descent
- Expected learning rate αp

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Idea of proof:

- Rewrite

$$\tilde{\beta}_k - \tilde{\beta} = \left(I - \alpha D_k \mathbb{X} D_k\right)\left(\tilde{\beta}_{k-1} - \tilde{\beta}\right) + \alpha D_k \overline{\mathbb{X}}\left(pI - D_k\right)\tilde{\beta}$$

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- Compute

$$\mathbb{E}\big[D_k \mathbb{X} D_k\big] = p\mathbb{X}_p$$
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- Now $\mathbb{E}\left[\tilde{\beta}_k - \tilde{\beta}\right] = (I - \alpha p \mathbb{X}_p)\mathbb{E}\left[\tilde{\beta}_{k-1} - \tilde{\beta}\right]$; finish with induction!

Second-Order Dynamics I

Lemma

Up to exponentially decaying remainder ρ_k, second moment of $\tilde{\beta}_k - \tilde{\beta}$ evolves as affine dynamical system

$$\mathbb{E}\Big[(\tilde{\beta}_k - \tilde{\beta})(\tilde{\beta}_k - \tilde{\beta})^{\mathsf{t}}\Big] = S\Big(\mathbb{E}\Big[(\tilde{\beta}_{k-1} - \tilde{\beta})(\tilde{\beta}_{k-1} - \tilde{\beta})^{\mathsf{t}}\Big]\Big) + \rho_{k-1}$$

pushed forward by affine operator S on matrices.

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Intuition:

- Interaction between GD dynamics and on-line dropout encapsulated in S
- This structure remains hidden when considering averaged estimator $\tilde{\beta}$

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Exact Definition:

$$\begin{aligned} S(A) = {} & (I - \alpha p \mathbb{X}_p) A (I - \alpha p \mathbb{X}_p) + \alpha^2 p(1-p) \mathrm{Diag}(\mathbb{X}_p A \mathbb{X}_p) \\ & + \alpha^2 p^2 (1-p)^2 \overline{\mathbb{X}} \odot \left(A + \mathbb{E}[\tilde{\beta}\tilde{\beta}^{\mathrm{t}}]\right) \odot \overline{\mathbb{X}} \\ & + \alpha^2 p^2 (1-p) \Big(\overline{\mathbb{X}} \mathrm{Diag}\big(A + \mathbb{E}[\tilde{\beta}\tilde{\beta}^{\mathrm{t}}]\big) \overline{\mathbb{X}}\Big)_p \\ & + \alpha^2 p^2 (1-p) \Big(\overline{\mathbb{X}} \mathrm{Diag}(\mathbb{X}_p A) + \mathrm{Diag}(\mathbb{X}_p A) \overline{\mathbb{X}}\Big) \end{aligned}$$

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Notes on Proof:

- S has complex expression due to dependence structure in

$$\tilde{\beta}_k - \tilde{\beta} = \big(I - \alpha D_k \mathbb{X} D_k\big)\big(\tilde{\beta}_{k-1} - \tilde{\beta}\big) + \alpha D_k \overline{\mathbb{X}}\big(pI - D_k\big)\tilde{\beta}$$

- Proof requires computing 4^{th} order moments of the form $\mathbb{E}\big[D_k A D_k B D_k C D_k\big]$

Second-Order Dynamics II

Theorem

For sufficiently small $\alpha := \alpha(\mathbb{X}, p)$, $S_0 := S(0)$, *and* $S_{\mathrm{lin}} := S - S_0$

$$\left\| \mathbb{E}\Big[(\tilde{\beta}_k - \tilde{\beta})(\tilde{\beta}_k - \tilde{\beta})^{\mathrm{t}}\Big] - \big(\mathrm{id} - S_{\mathrm{lin}}\big)^{-1} S_0 \right\| = O\Big(k \|I - \alpha p \mathbb{X}_p\|^{k-1}\Big)$$

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Notes:

- Limit characterized by intercept S_0 and linear part S_{lin} of S
- Small $\alpha \implies$ operator norm of S_{lin} less than 1

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Corollary I:

- $\mathrm{Cov}\big(\tilde{\beta}_k\big) = \mathrm{Cov}\big(\tilde{\beta}\big) + \big(\mathrm{id} - S_{\text{lin}}\big)^{-1} S_0 + O\Big(k \|I - \alpha p \mathbb{X}_p\|^{k-1}\Big)$

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- Unfortunately, $\left(\mathrm{id} - S_{\mathrm{lin}}\right)^{-1} S_0 > 0$ in general, so $\tilde{\beta}_k$ does not attain the optimal variance!

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Corollary II:

- In general, $\tilde{\beta}_k$ does not converge to $\tilde{\beta}$ in L_2 since

$$\mathrm{Tr}\Big(\mathbb{E}\Big[(\tilde{\beta}_k - \tilde{\beta})(\tilde{\beta}_k - \tilde{\beta})^{\mathrm{t}} \Big] \Big) = \mathbb{E}\Big[\| \tilde{\beta}_k - \tilde{\beta} \|_2^2 \Big].$$

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- Second-order analysis of gradient descent with dropout is already rather technical in the linear model.
- Elementary — yet complicated — linear algebra is necessary at first to compute the basic objects, then a more abstract perspective can be applied.
- Second-order dynamics are only visible through direct study of on-line iterates.
- Often cited connection with ridge regression is more nuanced for the variance.

For more details:

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Thanks for your attention!