Linear Models

Numerical Methods for Deep Learning

Learning Problem

Given examples (inputs)

$$\mathbf{Y} = \begin{pmatrix} \mathbf{y}_1 & \mathbf{y}_2 & \cdots & \mathbf{y}_n \end{pmatrix} \in \mathbb{R}^{n_f \times n}$$

and labels (outputs)

$$\mathbf{C} = \begin{pmatrix} \mathbf{c}_1 & \mathbf{c}_2 & \cdots & \mathbf{c}_n \end{pmatrix} \in \mathbb{R}^{n_c \times n},$$

find a classification/prediction function $f(\cdot, \boldsymbol{\theta})$, i.e.,

$$f(\mathbf{y}_j, \boldsymbol{\theta}) \approx \mathbf{c}_j, \quad j = 1, \ldots, n.$$

Regression and Least-Squares

Simplest option, a linear model with $\boldsymbol{\theta} = (\mathbf{W}, \mathbf{b})$ and

$$f(\mathbf{Y}, \mathbf{W}, \mathbf{b}) = \mathbf{W}\mathbf{Y} + \mathbf{b}\mathbf{e}_n^\top \approx \mathbf{C}$$

- $\mathbf{W} \in \mathbb{R}^{n_c \times n_f}$ are *weights*
- $\mathbf{b} \in \mathbb{R}^{n_c}$ are *biases*
- $\mathbf{e}_n \in \mathbb{R}^n$ is a vector of ones

Equivalent notation:

$$f(\mathbf{Y}, \mathbf{W}, \mathbf{b}) = \begin{pmatrix} \mathbf{W} & \mathbf{b} \end{pmatrix} \begin{pmatrix} \mathbf{Y} \\ \mathbf{e}_n^\top \end{pmatrix} \approx \mathbf{C}$$

Problem may not have a solution, or may have infinite solutions (when?). Solve through optimization

$$\min_{\mathbf{W}} \frac{1}{2} \|\mathbf{W}\mathbf{Y} - \mathbf{C}\|_F^2$$

(Frobenius norm: $\|\mathbf{A}\|_F^2 = \mathrm{trace}(\mathbf{A}^\top \mathbf{A}) = \sum_{i,j} \mathbf{A}_{i,j}^2$.)

Remark: Relation to Least-Squares

Consider the regression problem

$$\min_{\mathbf{W}} \frac{1}{2}\|\mathbf{W}\mathbf{Y} - \mathbf{C}\|_F^2.$$

It is easy to see that this is equivalent to

$$\min_{\mathbf{W}} \frac{1}{2}\|\mathbf{Y}^\top\mathbf{W}^\top - \mathbf{C}^\top\|_F^2,$$

which can be solved separately for each row in $\mathbf{W}$

$$\mathbf{W}(j,:)^\top = \arg\min_{\mathbf{w}} \frac{1}{2}\|\mathbf{Y}^\top\mathbf{w} - \mathbf{C}(j,:)^\top\|_F^2.$$

Notation: Let $\mathbf{A} = \mathbf{Y}^\top$ and $\mathbf{X} = \mathbf{W}^\top$ (easy to add bias here), we solve

$$\min_{\mathbf{X}} \frac{1}{2}\|\mathbf{A}\mathbf{X} - \mathbf{C}^\top\|_F^2$$

Optimality Conditions for Least-Squares

To minimize a function need to differentiate and equate to 0

$$\frac{\partial \left(\frac{1}{2}\|\mathbf{AX} - \mathbf{C}^\top\|_F^2\right)}{\partial \mathbf{X}} = 0$$

Compute the derivatives in three steps

1. $$\frac{\partial \left(\frac{1}{2}\|\mathbf{R}\|_F^2\right)}{\partial \mathbf{R}} = ???$$
2. $$\frac{\partial \left(\mathbf{AX}\right)}{\partial \mathbf{X}} = ???$$
3. Use chain rule

Least-Squares: Normal Equations

The necessary and sufficient optimality conditions for the least-squares problem are

$$\frac{\partial\left(\frac{1}{2}\|\mathbf{AX}-\mathbf{C}^\top\|_F^2\right)}{\partial \mathbf{X}} = \mathbf{A}^\top(\mathbf{AX}-\mathbf{C}^\top) = 0$$

Reorganize to obtain the **normal equations**

$$\mathbf{X} = (\mathbf{A}^\top\mathbf{A})^{-1}(\mathbf{A}^\top\mathbf{C}^\top).$$

Here, $\mathbf{A}^\top\mathbf{A} \in \mathbb{R}^{n_f \times n_f}$ must be invertible, i.e.,

- sufficient amount of data $(n > n_f)$
- data is linearly independent

Coding: Least-Squares Regression

1. Write a code for solving

$$\min_{\mathbf{W},\mathbf{b}} \frac{1}{2}\|\mathbf{W}\mathbf{Y} + \mathbf{b}\mathbf{e}_n^\top - \mathbf{C}\|^2$$

   and apply it to some of our test data (MNIST / CIFAR10)
2. Solve the problem using the normal equations derived above.
3. Use optimal weights to predict labels for test data. How well does your solution generalize?

Ill-posedness and the SVD

If the data is linearly dependent or close to be linearly dependent, least-squares problem gives no good solution [2, 4, 3].
Understanding can be gained by the *Singular Value Decomposition* (SVD) (e.g., [1, Ch. 8])

$$\mathbf{A} = \mathbf{U}\boldsymbol{\Sigma}\mathbf{V}^\top$$

where $\mathbf{U} \in \mathbb{R}^{n_f \times n_f}, \mathbf{V} \in \mathbb{R}^{n_f \times n}$ satisfy

$$\mathbf{U}^\top\mathbf{U} = \mathbf{I}, \quad \text{and} \quad \mathbf{V}^\top\mathbf{V} = \mathbf{I}$$

Diagonal of $\boldsymbol{\Sigma}$ contains the singular values $\sigma_1 \geq ...\sigma_{n_f} \geq 0$

$$\boldsymbol{\Sigma} = \begin{pmatrix} \sigma_1 & & \\ & \ddots & \\ & & \sigma_{n_f} \end{pmatrix}$$

Ill-posedness and Regularization

Important is the *effective rank*: If $\sigma_j \ll \sigma_1$ for all $j \geq k$, then the effective rank of the problem is k.

If $k < n_f$, the least squares problem is ill-posed, i.e., solution does not exist or is unstable.
Small perturbations in $\mathbf{C}$ or $\mathbf{A} = \mathbf{Y}^\top$ yield large perturbations in $\mathbf{X} = \mathbf{W}^\top$

Solve regularized problem: For $\lambda > 0$

$$\min_{\mathbf{X}} \frac{1}{2}\|\mathbf{AX} - \mathbf{C}^\top\|_F^2 + \frac{\lambda}{2}\|\mathbf{X}\|_F^2$$

Exercise: solve the regularized least-squares problem

Ill-posedness and Regularization

Important is the *effective rank*: If $\sigma_j \ll \sigma_1$ for all $j \geq k$, then the effective rank of the problem is k.

If $k < n_f$, the least squares problem is ill-posed, i.e., solution does not exist or is unstable.
Small perturbations in $\mathbf{C}$ or $\mathbf{A} = \mathbf{Y}^\top$ yield large perturbations in $\mathbf{X} = \mathbf{W}^\top$

Solve regularized problem: For $\lambda > 0$

$$\min_{\mathbf{X}} \frac{1}{2}\|\mathbf{AX} - \mathbf{C}^\top\|_F^2 + \frac{\lambda}{2}\|\mathbf{X}\|_F^2$$

Exercise: solve the regularized least-squares problem

$$\mathbf{X} = (\mathbf{A}^\top\mathbf{A} + \lambda\mathbf{I})^{-1}\mathbf{A}^\top\mathbf{C}^\top$$

The Bias-Variance Decomposition

Assume $\mathbf{C}^\top = \mathbf{A}\mathbf{X}_{\text{true}} + \epsilon$, $\epsilon \sim \mathcal{N}(0, \sigma\mathbf{I})$, $\lambda > 0$ fixed.
Then setting $\mathbf{A}_\lambda^\dagger = (\mathbf{A}^\top\mathbf{A} + \lambda\mathbf{I})^{-1}$

$$\begin{aligned}
\mathbf{X} - \mathbf{X}_{\text{true}} &= \mathbf{A}_\lambda^\dagger\mathbf{A}^\top\mathbf{C}^\top - \mathbf{X}_{\text{true}} \\
&= \left(\mathbf{A}_\lambda^\dagger\mathbf{A}^\top\mathbf{A} - \mathbf{I}\right)\mathbf{X}_{\text{true}} + \mathbf{A}_\lambda^\dagger\mathbf{A}^\top\epsilon \\
&= -\lambda\mathbf{A}_\lambda^\dagger\mathbf{X}_{\text{true}} + \mathbf{A}_\lambda^\dagger\mathbf{A}^\top\epsilon
\end{aligned}$$

The Bias-Variance Decomposition

Assume $\mathbf{C}^\top = \mathbf{A}\mathbf{X}_{\text{true}} + \epsilon$, $\epsilon \sim \mathcal{N}(0, \sigma\mathbf{I})$, $\lambda > 0$ fixed.
Then setting $\mathbf{A}^\dagger_\lambda = (\mathbf{A}^\top\mathbf{A} + \lambda\mathbf{I})^{-1}$

$$
\begin{aligned}
\mathbf{X} - \mathbf{X}_{\text{true}} &= \mathbf{A}^\dagger_\lambda \mathbf{A}^\top \mathbf{C}^\top - \mathbf{X}_{\text{true}} \\
&= \left(\mathbf{A}^\dagger_\lambda \mathbf{A}^\top \mathbf{A} - \mathbf{I}\right) \mathbf{X}_{\text{true}} + \mathbf{A}^\dagger_\lambda \mathbf{A}^\top \epsilon \\
&= -\lambda \mathbf{A}^\dagger_\lambda \mathbf{X}_{\text{true}} + \mathbf{A}^\dagger_\lambda \mathbf{A}^\top \epsilon
\end{aligned}
$$

Error depends on $\epsilon \rightsquigarrow$ take expectation

$$
\begin{aligned}
\mathbb{E}\|\mathbf{X} - \mathbf{X}_{\text{true}}\|_F^2 &= \mathbb{E}\|\mathbf{A}^\dagger_\lambda \mathbf{A}^\top \epsilon - \lambda \mathbf{A}^\dagger_\lambda \mathbf{X}_{\text{true}}\|_F^2 \\
&= \overbrace{\lambda^2 \|\mathbf{A}^\dagger_\lambda \mathbf{X}_{\text{true}}\|_F^2}^{\|\text{bias}\|_{\text{F}}^2} + \overbrace{\sigma^2 \text{trace}\left(\mathbf{A}\mathbf{A}^{\dagger^T}_\lambda \mathbf{A}^\dagger_\lambda \mathbf{A}^\top\right)}^{\text{variance}}
\end{aligned}
$$

The Bias-Variance Decomposition

Assume $\mathbf{C}^\top = \mathbf{A}\mathbf{X}_{\text{true}} + \epsilon$, $\epsilon \sim \mathcal{N}(0, \sigma\mathbf{I})$, $\lambda > 0$ fixed.
Then setting $\mathbf{A}_\lambda^\dagger = (\mathbf{A}^\top\mathbf{A} + \lambda\mathbf{I})^{-1}$

$$\begin{aligned}
\mathbf{X} - \mathbf{X}_{\text{true}} &= \mathbf{A}_\lambda^\dagger \mathbf{A}^\top \mathbf{C}^\top - \mathbf{X}_{\text{true}} \\
&= \left(\mathbf{A}_\lambda^\dagger \mathbf{A}^\top \mathbf{A} - \mathbf{I}\right) \mathbf{X}_{\text{true}} + \mathbf{A}_\lambda^\dagger \mathbf{A}^\top \epsilon \\
&= -\lambda \mathbf{A}_\lambda^\dagger \mathbf{X}_{\text{true}} + \mathbf{A}_\lambda^\dagger \mathbf{A}^\top \epsilon
\end{aligned}$$

Error depends on $\epsilon \rightsquigarrow$ take expectation

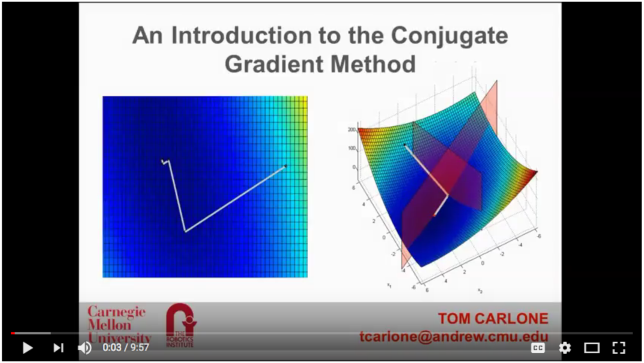
$$\begin{aligned}
\mathbb{E}\|\mathbf{X} - \mathbf{X}_{\text{true}}\|_F^2 &= \mathbb{E}\|\mathbf{A}_\lambda^\dagger \mathbf{A}^\top \epsilon - \lambda \mathbf{A}_\lambda^\dagger \mathbf{X}_{\text{true}}\|_F^2 \\
&= \overbrace{\lambda^2 \|\mathbf{A}_\lambda^\dagger \mathbf{X}_{\text{true}}\|_F^2}^{\|\text{bias}\|_\text{F}^2} + \overbrace{\sigma^2 \text{trace}\left(\mathbf{A}\mathbf{A}_\lambda^{\dagger T} \mathbf{A}_\lambda^\dagger \mathbf{A}^\top\right)}^{\text{variance}}
\end{aligned}$$

Take home: No such thing as exact recovery!

Next Time

Solving large-scale least-squares problems.

Watch: `https://www.youtube.com/watch?v=eAYohMUpPMA`



Overview of Conjugate Gradient Method

References

[1] U. M. Ascher and C. Greif. A First Course on Numerical Methods. SIAM, Philadelphia, 2011.

[2] P. C. Hansen. *Rank-deficient and discrete ill-posed problems*. SIAM Monographs on Mathematical Modeling and Computation. Society for Industrial and Applied Mathematics (SIAM), Philadelphia, PA, 1998.

[3] P. C. Hansen. *Discrete inverse problems*, volume 7 of *Fundamentals of Algorithms*. Society for Industrial and Applied Mathematics (SIAM), Philadelphia, PA, 2010.

[4] C. R. Vogel. *Computational Methods for Inverse Problems*. SIAM, Philadelphia, 2002.