Regularizations

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The ℓ_2-Norm Regularization

Linear Regression

Input: feature matrix $\mathbf{X} \in \mathbb{R}^{n \times d}$ and labels $\mathbf{y} \in \mathbb{R}^n$.

Output: vector $\mathbf{w} \in \mathbb{R}^d$ such that $\mathbf{X}\mathbf{w} \approx \mathbf{y}$.

Task

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Task

- Least squares regression:

$$\min_{\mathbf{w}} \ \frac{1}{n} \left|\left|\mathbf{X}\mathbf{w} - \mathbf{y}\right|\right|_2^2 .$$

- Ridge regression:

$$\min_{\mathbf{w}} \ \frac{1}{n} \left|\left|\mathbf{X}\mathbf{w} - \mathbf{y}\right|\right|_2^2 + \gamma \left|\left|\mathbf{w}\right|\right|_2^2 .$$

Methods

Loss Function

Regularization

Ridge Regression: Algorithms

- **Analytical solution:** $\mathbf{w}^\star = (\mathbf{X}^T\mathbf{X} + n\gamma\mathbf{I}_d)^{-1}\mathbf{X}^T\mathbf{y}$.
  - Time complexity: $O(nd^2 + d^3)$.

Ridge Regression: Algorithms

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  - Time complexity: $O(nd^2 + d^3)$.
- Derivations:
  - The objective function is $f(\mathbf{w}) = \frac{1}{n}\left\|\mathbf{X}\mathbf{w} - \mathbf{y}\right\|_2^2 + \gamma\left\|\mathbf{w}\right\|_2^2$.
  - The gradient is $\nabla f(\mathbf{w}) = \frac{2}{n}\mathbf{X}^T(\mathbf{X}\mathbf{w} - \mathbf{y}) + 2\gamma\mathbf{w}$.
  - Set $\nabla f(\mathbf{w}) = 0$ leads to $\frac{2}{n}(\mathbf{X}^T\mathbf{X} + n\gamma\mathbf{I}_d)\mathbf{w} = \frac{2}{n}\mathbf{X}^T\mathbf{y}$.
- Time complexity:
  - $O(nd^2)$ time for the multiplication $\mathbf{X}^T\mathbf{X}$.
  - $O(d^3)$ time for the inversion of the $d \times d$ matrix $\mathbf{X}^T\mathbf{X} + n\gamma\mathbf{I}_d$.

Ridge Regression: Algorithms

- **Conjugate gradient (CG)**
  - $O\left(\sqrt{\kappa}\log\frac{1}{\epsilon}\right)$ iterations to reach ϵ precision.
  - $O(nd)$ per-iteration time complexity (for computing the gradient).
  - Hessian matrix: $\nabla^2 f(\mathbf{w}) = \frac{2}{n}(\mathbf{X}^T\mathbf{X} + n\gamma\mathbf{I}_d)$.
  - $\kappa = \frac{\lambda_{\max}(\mathbf{X}^T\mathbf{X}) + n\gamma}{\lambda_{\min}(\mathbf{X}^T\mathbf{X}) + n\gamma}$ is the condition number of the Hessian.

Usefulness of Regularization

Question: Why do we use the ℓ_2-norm regularization?

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- Reason 1: easier to optimize.
  - Conjugate gradient (CG) requires $O\left(\sqrt{\kappa}\log\frac{1}{\epsilon}\right)$ iterations to reach ϵ precision.
  - Least squares: $\kappa = \frac{\lambda_{\max}(\mathbf{X}^T\mathbf{X})}{\lambda_{\min}(\mathbf{X}^T\mathbf{X})}$.
  - Ridge regression: $\kappa = \frac{\lambda_{\max}(\mathbf{X}^T\mathbf{X}) + n\gamma}{\lambda_{\min}(\mathbf{X}^T\mathbf{X}) + n\gamma}$ (decrease as γ increases).
  - ➡ CG converges faster as γ increases.

Usefulness of Regularization

Question: Why do we use the ℓ_2-norm regularization?

- Reason 1: easier to optimize.
- Reason 2: better generalization.
  - Least squares has better training error (due to the optimality).
  - Ridge regression makes better prediction on test set (due to *bias-variance decomposition*).

The ℓ_1-Norm Regularization

Motivations

$$\mathbf{x} \in \mathbb{R}^d \xrightarrow{\text{prediction}} y \in \mathbb{R}$$

Fact 1: y can be independent of some of the d feature.

Fact 2: if $d \gg n$, linear models are likely to overfit.

Example: Use genomic data to predict disease.

- d is huge: human has 20K protein-coding genes.
- n is small: tens or hundreds of human participants in an experiment.
- Most genes are irrelevant to a specific disease.

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Goal 1: Select the features relevant to y.

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Fact 1: y can be independent of some of the d feature.

Fact 2: if $d \gg n$, linear models are likely to overfit.

Goal 1: Select the features relevant to y.

Goal 2: Prevent overfitting for large d, small n problems.

The ℓ_1-Norm Constraint

- LASSO: $\min_{\mathbf{w}} \frac{1}{2n} ||\mathbf{X}\mathbf{w} - \mathbf{y}||_2^2;$ $\boxed{\text{s.t. } ||\mathbf{w}||_1 \leq t.}$

The feasible set $\{\mathbf{w}: \; ||\mathbf{w}||_1 \leq t\}$ is convex.

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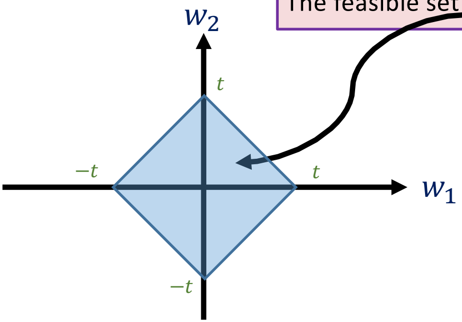

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  - The optimal solution $\mathbf{w}^\star$ is **sparse** (i.e., most entries are zeros).
  - Smaller t ➔ sparser $\mathbf{w}^\star$.

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  - Smaller t ➔ sparser $\mathbf{w}^\star$.
  - Sparsity ⬌ feature selection. Why?
    - Let $\mathbf{x}'$ be a test feature vector.
    - The prediction is $\mathbf{x}'^T \mathbf{w}^\star$.
    - If $w_1^\star = 0$, then the prediction is independent of x_1'.

The ℓ_1-Norm Regularization

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- **Another form**: $\min_{\mathbf{w}} \quad \frac{1}{2n}\|\mathbf{X}\mathbf{w}-\mathbf{y}\|_2^2 + \gamma\|\mathbf{w}\|_1.$

Loss Function

Regularization

Summary

Regularized ERM

- Regularized empirical risk minimization:

$$\min_{\mathbf{w}\in\mathbb{R}^d} \quad \frac{1}{n}\sum_{i=1}^{n} L(\mathbf{w};\ \mathbf{x}_i, y_i) \quad + \quad R(\mathbf{w}).$$

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Loss Function

- Linear regression: $L(\mathbf{w};\ \mathbf{x}_i, y_i) = \frac{1}{2}(\mathbf{w}^T\mathbf{x}_i - y_i)^2$
- Logistic regression: $L(\mathbf{w};\ \mathbf{x}_i, y_i) = \log(1 + \exp(-y_i\mathbf{w}^T\mathbf{x}_i))$
- SVM: $L(\mathbf{w};\ \mathbf{x}_i, y_i) = \max\{0,\ 1 - y_i\mathbf{w}^T\mathbf{x}_i\}$

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Regularization

- ℓ_1-norm: $R(\mathbf{w}) = \gamma||\mathbf{w}||_1$
- ℓ_2-norm: $R(\mathbf{w}) = \gamma||\mathbf{w}||_2^2$
- Elastic net: $R(\mathbf{w}) = \gamma_1||\mathbf{w}||_1 + \gamma_2||\mathbf{w}||_2^2$