Empirical Risk Minimization
Announcements
Recap on Linear Regression

Given dataset \( \mathcal{D} = \{x_i, y_i\}, x_i \in \mathbb{R}^d, y_i \in \mathbb{R} \)
Recap on Linear Regression

Given dataset $\mathcal{D} = \{x_i, y_i\}, x_i \in \mathbb{R}^d, y_i \in \mathbb{R}$

Least Regression with squared loss:

$$\arg \min_w \sum_{i=1}^{n} (w^T x_i - y_i)^2$$
Recap on Linear Regression

Given dataset $\mathcal{D} = \{x_i, y_i\}, x_i \in \mathbb{R}^d, y_i \in \mathbb{R}$

Derivation of Normal equation:

$$L(w) := \sum_{i=1}^{n} (w^T x_i - y_i)^2$$

$$\nabla_w L(w) = \chi^T \chi w - \chi^T \gamma$$

$$\chi = \begin{bmatrix} x_1 & x_2 & \cdots & x_n \end{bmatrix} \quad \gamma = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$
Recap on SVM

Given dataset $\mathcal{D} = \{x_i, y_i\}, x_i \in \mathbb{R}^d, y_i \in \{+1, -1\}$

Hard margin SVM:

$$
\min_{w,b} \|w\|_2^2 \\
\forall i : y_i(w^T x_i + b) \geq 1
$$
Recap on SVM

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Width of the “street”: $\frac{1}{\|w\|_2}$
Recap on SVM

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Hard margin SVM:

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$$\forall i : y_i(w^T x_i + b) \geq 1$$

Width of the “street”:

$$\frac{2}{\|w\|_2}$$
Recap on SVM

Given dataset $\mathcal{D} = \{x_i, y_i\}$, $x_i \in \mathbb{R}^d$, $y_i \in \{+1, -1\}$

Hard margin SVM:

$$
\min_{w,b} \|w\|_2^2
$$

$$
\forall i : y_i(w^T x_i + b) \geq 1
$$

Width of the “street”:

$$
\frac{2}{\|w\|_2}
$$

Find a “street” that has largest width, while keep all the points outside of the street.
Outline for Today

1. Empirical Risk Minimization

2. Examples on loss & hypothesis classes

3. Regularization
ERM

Recall the general supervised learning setting:
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We have some distribution $P$, dataset $\mathcal{D} = \{x_i, y_i\}_{i=1}^n$
ERM

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Hypothesis $h : \mathcal{X} \rightarrow \mathbb{R}$, & hypothesis class $\mathcal{H} := \{ h \} \subset \mathcal{X} \rightarrow \mathbb{R}$
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Hypothesis $h : \mathcal{X} \rightarrow \mathbb{R}$, & hypothesis class $\mathcal{H} := \{h\} \subset \mathcal{X} \rightarrow \mathbb{R}$

Loss function: $\ell(h(x), y)$
ERM

The ultimate objective function:

\[
\arg \min_{h \in \mathcal{H}} \mathbb{E}_{x,y \sim P} \left[ \ell(h(x), y) \right]
\]
The ultimate objective function:

$$\arg \min_{h \in \mathcal{H}} \mathbb{E}_{x,y \sim P} [\ell(h(x), y)]$$
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$$\text{arg min}_{h \in \mathcal{H}} \mathbb{E}_{x,y \sim P}[\ell(h(x), y)]$$

Instead we have its \textit{empirical} version:

$$\text{arg min}_{h \in \mathcal{H}} \sum_{x,y} \ell(h(x), y)$$
The ultimate objective function:

$$\arg \min_{h \in \mathcal{H}} \mathbb{E}_{x,y \sim P} \left[ \ell(h(x), y) \right]$$

Instead we have its **empirical** version

$$\arg \min_{h \in \mathcal{H}} \frac{1}{n} \sum_{i=1}^{n} \left[ \ell(h(x_i), y_i) \right]$$
The ultimate objective function:

$$\arg\min_{h \in \mathcal{H}} \mathbb{E}_{x,y \sim P}[\ell(h(x), y)]$$

Instead we have its empirical version

$$\arg\min_{h \in \mathcal{H}} \frac{1}{n} \sum_{i=1}^{n} [\ell(h(x_i), y_i)]$$

Empirical risk / Empirical error
The generalization error of ERM solution

\[ \hat{h}_{ERM} := \arg \min_{h \in \mathcal{H}} \frac{1}{n} \sum_{i=1}^{n} [\ell(h(x_i), y_i)] \]
The generalization error of ERM solution

\[ \hat{h}_{ERM} := \arg \min_{h \in \mathcal{H}} \frac{1}{n} \sum_{i=1}^{n} \ell(h(x_i), y_i) \]

We often are interested in the true performance of \( \hat{h}_{ERM} \):
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We often are interested in the true performance of \( \hat{h}_{ERM} \):

\[ \mathbb{E}_D \left[ \mathbb{E}_{x,y \sim P} \ell (\hat{h}_{ERM}(x), y) \right] \]
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We often are interested in the true performance of \( \hat{h}_{ERM} \):

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Note \( \hat{h}_{ERM} \) is a random quantity as it depends on data \( \mathcal{D} \).
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\[ \mathbb{E}_D \left[ \mathbb{E}_{x,y \sim P} \ell(\hat{h}_{ERM}(x), y) \right] \]

Note \( \hat{h}_{ERM} \) is a random quantity as it depends on data \( D \)

e.g., In LR: \( \hat{w} = (XX^T)^{-1}XY \).
The generalization error of ERM solution

Ideally, we want the true loss of ERM to be small:

$$\mathbb{E}_{\mathcal{D}} \left[ \mathbb{E}_{x,y \sim P} \ell(\hat{h}_{ERM}(x), y) \right] \approx \min_{h \in \mathcal{H}} \mathbb{E}_{x,y \sim P} \ell(h(x), y)$$
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The Minimum expected loss we could get if we knew \( P \)
The generalization error of ERM solution

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\]

The Minimum expected loss we could get if we knew \( P \)

However, this may not hold if we are not careful about designing \( \mathcal{H} \)
Example:

\[ P: x \text{ uniformly distribution over the square;} \]
Label: blue if inside the smaller square, else red
Consider a hypothesis class $\mathcal{H}$ contains ALL mappings from $x \rightarrow y$. 

$P$: $x$ uniformly distribution over the square; Label: blue if inside the smaller square, else red.
Example:

Consider a hypothesis class $\mathcal{H}$ contains ALL mappings from $x \rightarrow y$

Zero one loss $\ell(h(x), y) = 1(h(x) \neq y)$

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**Example:**

Consider a hypothesis class $\mathcal{H}$ contains ALL mappings from $x \to y$

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Let us consider this solution that memorizes data:

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Example:

Consider a hypothesis class $\mathcal{H}$ contains ALL mappings from $x \rightarrow y$

Zero one loss $\ell(h(x), y) = 1(h(x) \neq y)$

Let us consider this solution that memorizes data:

$$h(x) = \begin{cases} 
    y_i & \text{if } \exists i, x_i = x \\
    +1 & \text{else}
\end{cases}$$
Example:

\[ P: x \text{ uniformly distribution over the square; Label: blue if inside the dashed square, else red} \]

\[ \hat{h}(x) = \begin{cases} y_i & \text{if } \exists i, x_i = x \\ +1 & \text{else} \end{cases} \]

\[ \Rightarrow \frac{1}{n} \sum_{i=1}^{n} \ell(\hat{h}(x_i), y_i) = 0 \]
Example:

$P$: $x$ uniformly distribution over the square;
Label: blue if inside the dashed square, else red

\[
\hat{h}(x) = \begin{cases} 
  y_i & \text{if } \exists i, x_i = x \\
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\end{cases}
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\[
\Rightarrow \quad \frac{1}{n} \sum_{i=1}^{n} \ell(\hat{h}(x_i), y_i) = 0
\]

Q: But what’s the true expected error of this $\hat{h}$?
Example:

\[ \hat{h}(x) = \begin{cases} y_i & \text{if } \exists i, x_i = x \\ +1 & \text{else} \end{cases} \]

\[ \Rightarrow \frac{1}{n} \sum_{i=1}^{n} \ell(\hat{h}(x_i), y_i) = 0 \]

Q: But what’s the true expected error of this \( \hat{h} \)?

A: area of smaller box / total area
ERM with inductive bias

A common solution is to restrict the search space (i.e., hypothesis class)

\[ \hat{h}_{ERM} := \arg \min_{h \in \mathcal{H}} \frac{1}{n} \sum_{i=1}^{n} [\ell(h(x_i), y_i)] \]
ERM with inductive bias

A common solution is to restrict the search space (i.e., hypothesis class)

\[ \hat{h}_{ERM} := \arg \min_{h \in \mathcal{H}} \frac{1}{n} \sum_{i=1}^{n} [\ell(h(x_i), y_i)] \]

By restricting to \( \mathcal{H} \), we bias towards solutions from \( \mathcal{H} \)
Example:

\( P: x \) uniformly distribution over the square;
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Unrestricted hypothesis class did not work;
Example:

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However, if we restrict $\mathcal{H}$ to contains ALL axis-aligned rectangles, then ERM will succeed, i.e.,
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Unrestricted hypothesis class did not work;

However, if we restrict $\mathcal{H}$ to contains ALL axis-aligned rectangles, then ERM will succeed, i.e.,

$$\mathbb{E}_\mathcal{D} \left[ \mathbb{E}_{x,y \sim P} \ell(\hat{h}_{\text{ERM}}(x), y) \right] \leq \min_{h \in \mathcal{H}} \mathbb{E}_{x,y \sim P} \ell(h(x), y) + O(1/\sqrt{n})$$

\[= 0\]
\( P: x \) uniformly distribution over the square; Label: blue if inside the dashed square, else red

Example:

Unrestricted hypothesis class did not work;

However, if we restrict \( \mathcal{H} \) to contains ALL axis-aligned rectangles, then ERM will succeed, i.e.,

\[
\mathbb{E}_\mathcal{D} \left[ \mathbb{E}_{x,y \sim \mathcal{D}} (\hat{h}_{\text{ERM}}(x), y) \right] \\
\leq \min_{h \in \mathcal{H}} \mathbb{E}_{x,y \sim \mathcal{D}} (h(x), y) + O(1/\sqrt{n}) \\
\leq O(1/\sqrt{n})
\]
Example:

Unrestricted hypothesis class did not work;

However, if we restrict $\mathcal{H}$ to contains ALL axis-aligned rectangles, then ERM will succeed, i.e.,

$$\mathbb{E}_\mathcal{D} \left[ \mathbb{E}_{x,y \sim P} \ell(\hat{h}_{\text{ERM}}(x), y) \right] \leq \min_{h \in \mathcal{H}} \mathbb{E}_{x,y \sim P} \ell(h(x), y) + O(1/\sqrt{n})$$

$$\leq O(1/\sqrt{n})$$

(Exact proof out of the scope of this class — see CS 4783/5783)

$P$: $x$ uniformly distribution over the square; Label: blue if inside the dashed square, else red
Summary so far

ERM with unrestricted hypothesis class could fail (i.e., overfitting)

To guarantee small test error, we need to restrict $\mathcal{H}$
Outline for Today

1. Empirical Risk Minimization

2. Examples on loss & hypothesis classes

3. Regularization
ERM with restricted hypothesis class

\[
\min_h \frac{1}{n} \sum_{i=1}^{n} [\ell(h(x_i), y_i)]
\]

s.t. \( h \in \mathcal{H} \)

Let’s go through several examples on Constraints under the linear regression context
Linear Regression: squared loss + $\ell_2$ constraint

$$\min_w \frac{1}{n} \sum_{i=1}^{n} (w^T x_i - y_i)^2$$
Linear Regression: squared loss + $\ell_2$ constraint

$$\min_w \frac{1}{n} \sum_{i=1}^{n} (w^T x_i - y_i)^2$$

s.t. $\|w\|^2_2 \leq B$
Linear Regression: squared loss + $\ell_2$ constraint

\[
\min_{w} \frac{1}{n} \sum_{i=1}^{n} (w^T x_i - y_i)^2 \\
\text{s.t. } \|w\|_2^2 \leq B
\]
Linear Regression: squared loss + $\ell_1$ constraint

$$\min_w \frac{1}{n} \sum_{i=1}^{n} (w^T x_i - y_i)^2$$

s.t. $\|w\|_1 \leq B$

$$\|w\|_1 = \sum_{i=1}^{d} |w_i|$$
Linear Regression: squared loss + $\ell_1$ constraint

$$\min_w \frac{1}{n} \sum_{i=1}^{n} (w^T x_i - y_i)^2$$

s.t. $\|w\|_1 \leq B$

Advantage: give sparse solution
Linear Regression: squared loss + $\ell_p$ constraint

\[
\min_w \frac{1}{n} \sum_{i=1}^{n} (w^T x_i - y_i)^2 \quad \text{s.t. } \|w\|_p \leq B
\]

\[
0 < p < 1
\]

\[
\|w\|_p = \left( \sum_{i=1}^{d} |w_i|^p \right)^{\frac{1}{p}}
\]
Linear Regression: squared loss + $\ell_p$ constraint

$$\min_w \frac{1}{n} \sum_{i=1}^{n} (w^\top x_i - y_i)^2$$

s.t. $\|w\|_p \leq B$

$0 < p < 1$

Advantage of $\ell_p$ constraint: very sparse solution

Disadvantage: Non-convex
Constraints help avoid overfitting

Without constraint, we might overfit to an outlier
Constraints help avoid overfitting

Without constraint, we might overfit to an outlier

With constraint $\|w\|^2_2 \leq B$, we can avoid overfitting (i.e., force us to not pay too much attention to minimizing loss)
Constraints help avoid overfitting

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With constraint $\|w\|_2^2 \leq B$, we can avoid overfitting (i.e., force us to not pay too much attention to minimizing loss)
Constraints help avoid overfitting

Without constraint, we might overfit to an outlier

With constraint $\|w\|_2^2 \leq B$, we can avoid overfitting (i.e., force us to not pay too much attention to minimizing loss)

(More details in next lecture)
Other loss functions with linear regression

Absolute loss:

$$\min_{w} \frac{1}{n} \sum_{i=1}^{n} |w^T x_i - y_i|$$

s.t. $R(w) \leq B$

$R(w) = \|w\|_2$

$R(w) = \|w\|_1$

$z := w^T x - y$
Other loss functions with linear regression

Absolute loss:

$$\min_w \frac{1}{n} \sum_{i=1}^{n} |w^T x_i - y_i|$$

s.t. $R(w) \leq B$

Advantage: less sensitive to outliers
Other loss functions with linear regression

Absolute loss:

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s.t. $R(w) \leq B$

Advantage: less sensitive to outliers

Disadvantage: no closed-form solution, non-differentiable at 0
Other loss functions with linear regression

Huber loss:

\[
\min_w \frac{1}{n} \sum_{i=1}^{n} L_\delta(w^T x - y)
\]

s.t. \( R(w) \leq B \)

Where

\[
L_\delta(z) = \begin{cases} 
  z^2/2 & \text{if } |z| \leq \delta \\
  \delta(|z| - \delta/2) & \text{else}
\end{cases}
\]
Other loss functions with linear regression

Huber loss:

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Where

$$L_\delta(z) = \begin{cases} 
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\delta(|z| - \delta/2) & \text{else}
\end{cases}$$

Advantage: best of both worlds
Other loss functions with linear regression

Huber loss:

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Where

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L_\delta(z) = \begin{cases} 
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  \delta(|z| - \delta/2) & \text{else}
\end{cases}
\]

Advantage: best of both worlds

Disadvantage: additional parameter \( \delta \) to tune
Linear classification: Hinge loss + constraint

\[
\min_{w,b} \frac{1}{n} \sum_{i=1}^{n} \max \left\{ 0, 1 - y_i (w^T x_i + b) \right\}
\]

\[
\text{s.t. } \|w\|_2^2 \leq B
\]
Linear classification: Hinge loss + constraint

\[
\min_{w,b} \frac{1}{n} \sum_{i=1}^{n} \max\{0, 1 - y_i(w^T x_i + b)\}
\]

s.t. \( \|w\|_2^2 \leq B \)

\( z := y(w^T x + b) \)

(Correct)
Linear classification: Hinge loss + constraint

\[
\min_{w,b} \frac{1}{n} \sum_{i=1}^{n} \max \left\{ 0, 1 - y_i(w^T x_i + b) \right\}
\]

s.t. \( \|w\|_2^2 \leq B \)

Constraint avoids overfit:
(Recall: small \( \|w\|_2 \) should have large street width)

\[ z := y(w^T x + b) \]

(max\{0,1 − z\})

(wrong)

(Correct)
Linear classification: Log-loss + constraints

$$\min_{w,b} \frac{1}{n} \sum_{i=1}^{n} \ln \left( 1 + \exp(-y_i(w^T x_i + b)) \right)$$

s.t. $\|w\|_2^2 \leq B$
Linear classification: Log-loss + constraints

\[
\min_{w,b} \frac{1}{n} \sum_{i=1}^{n} \ln \left( 1 + \exp(-y_i(w^T x_i + b)) \right) \\
\text{s.t. } \|w\|_2^2 \leq B
\]
Linear classification: Exponential loss + constraints

$$\min_{w,b} \frac{1}{n} \sum_{i=1}^{n} \exp \left( -y_i (w^T x_i + b) \right)$$

s.t. $\|w\|_2^2 \leq B$
Linear classification: Exponential loss + constraints

\[
\min_{w,b} \frac{1}{n} \sum_{i=1}^{n} \exp \left( -y_i (w^T x_i + b) \right)
\]

s.t. \( \|w\|_2^2 \leq B \)

(Later, AdaBoost uses this loss)
Linear classification: Exponential loss + constraints

\[
\min_{w,b} \frac{1}{n} \sum_{i=1}^{n} \exp \left( -y_i (w^T x_i + b) \right)
\]

s.t. \( \|w\|_2^2 \leq B \)

(Later, AdaBoost uses this loss)

Very aggressive loss (but may overfit w/ noisy data)
Outline for Today

1. Empirical Risk Minimization

2. Examples on loss & hypothesis classes

3. Regularization
Regularization

We can turn constraint optimization problem into unconstrained using Lagrange multiplier

Example:
Regularization

We can turn constraint optimization problem into unconstrained using Lagrange multiplier

Example:

\[
\min_{\mathbf{w}} \frac{1}{n} \sum_{i=1}^{n} (\mathbf{w}^\top \mathbf{x}_i - y_i)^2 \\
\text{s.t. } \|\mathbf{w}\|_1 \leq B
\]
Regularization

We can turn constraint optimization problem into unconstrained using Lagrange multiplier

Example:

\[
\min_w \frac{1}{n} \sum_{i=1}^{n} (w^T x_i - y_i)^2 \\
\text{s.t. } \|w\|_1 \leq B
\]

\[
\min_w \frac{1}{n} \sum_{i=1}^{n} (w^T x_i - y_i)^2 + \lambda \|w\|_2^2
\]
Regularization

We can turn constraint optimization problem into unconstrained using Lagrange multiplier

Example:

$$\min_w \frac{1}{n} \sum_{i=1}^{n} (w^T x_i - y_i)^2$$

s.t. $\|w\|_1 \leq B$

$$\min_w \frac{1}{n} \sum_{i=1}^{n} (w^T x_i - y_i)^2 + \lambda \|w\|_2^2$$

(More details about Lagrange multiplier in Anil’s optimization class CS4220)
Examples:

Soft-margin SVM:

$$\min_{w,b} \sum_{i=1}^{n} \max \left\{ 0, 1 - y_i(w^T x_i + b) \right\} + \lambda \|w\|_2^2$$
Examples:

Soft-margin SVM:

\[
\min_{w,b} \sum_{i=1}^{n} \max \left\{ 0, 1 - y_i (w^T x_i + b) \right\} + \lambda \|w\|_2^2
\]

Ridge Linear Regression

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\min_{w} \sum_{i=1}^{n} (w^T x_i - y_i)^2 + \lambda \|w\|_2^2
\]
Examples:

Soft-margin SVM:

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Ridge Linear Regression

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Lasso:

\[
\min_{w} \sum_{i=1}^{n} (w^T x_i - y_i)^2 + \lambda \|w\|_1
\]
Examples:

Soft-margin SVM:

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Returned solution is often sparse!
Examples:

Soft-margin SVM:

$$\min_{w,b} \sum_{i=1}^{n} \max \left\{ 0, 1 - y_i(w^T x_i + b) \right\} + \lambda \|w\|_2^2$$

Ridge Linear Regression

$$\min_{w} \sum_{i=1}^{n} (w^T x_i - y_i)^2 + \lambda \|w\|_2^2$$

Lasso:

$$\min_{w} \sum_{i=1}^{n} (w^T x_i - y_i)^2 + \lambda \|w\|_1$$

Returned solution is often sparse!

Good for feature selection!
Summary for today

1. Empirical risk minimization framework
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2. Need to restrict our hypothesis class:

Select hypothesis that is simple while can also explain the data reasonably well
Summary for today

1. Empirical risk minimization framework

2. Need to restrict our hypothesis class:
   Select hypothesis that is simple while can also explain the data reasonably well

3. Examples of loss functions & Regularizations