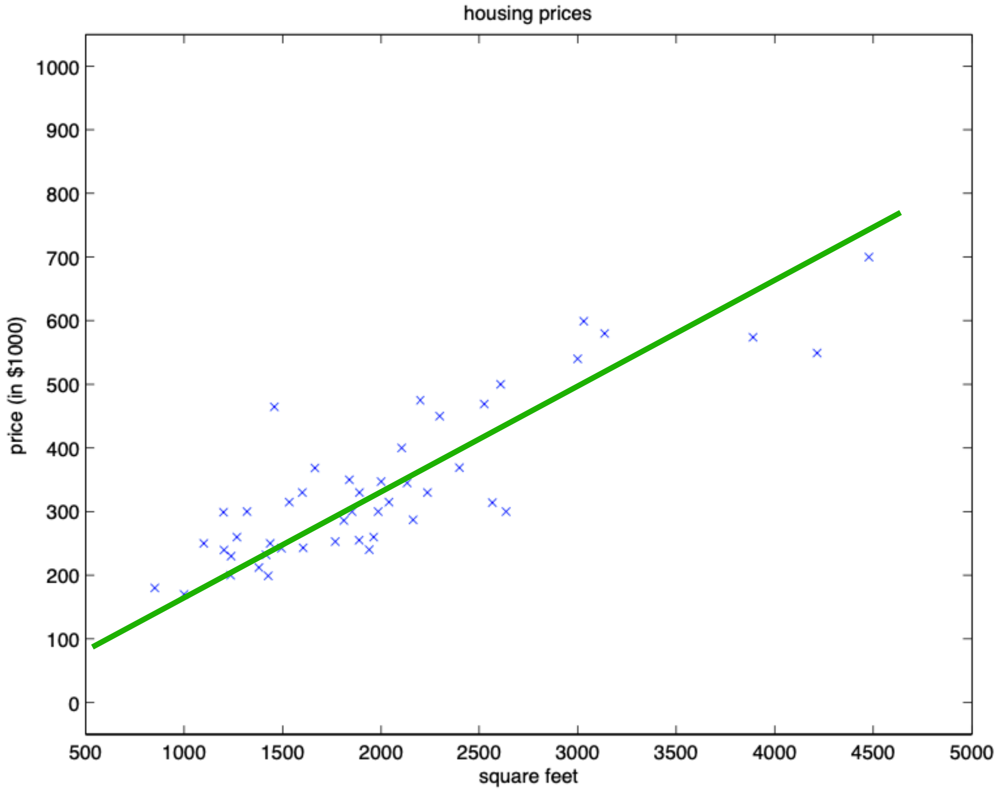
Empirical Risk Minimization

Announcements

Recap on Linear Regression

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



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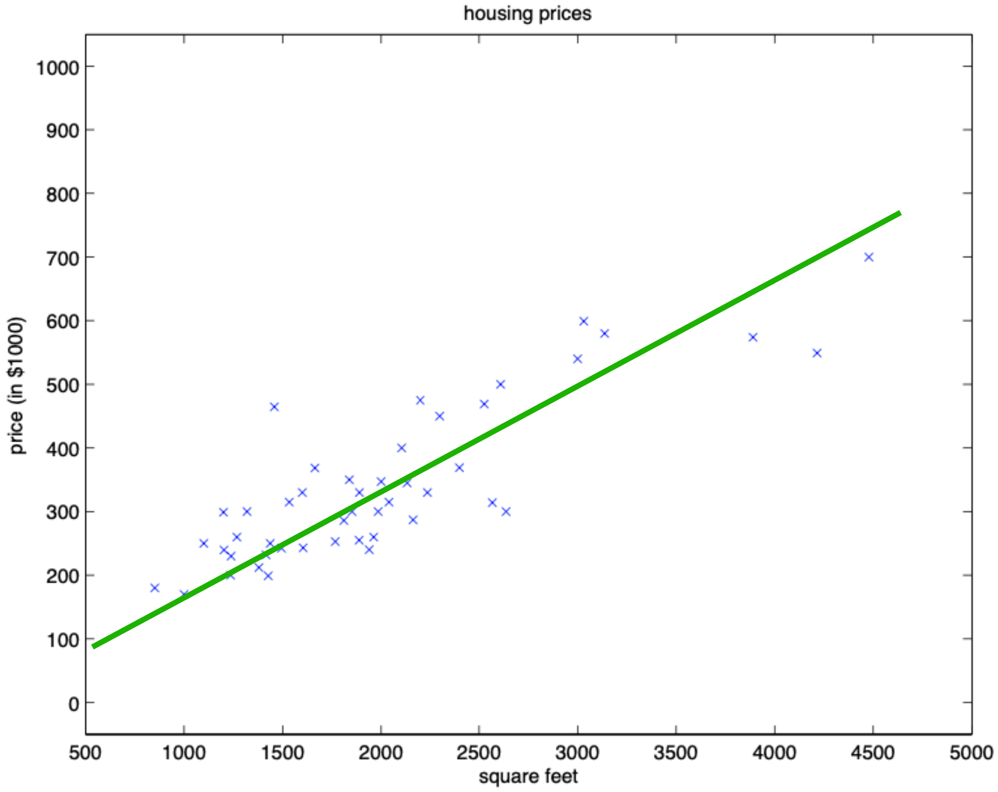

Least Regression with squared loss:

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

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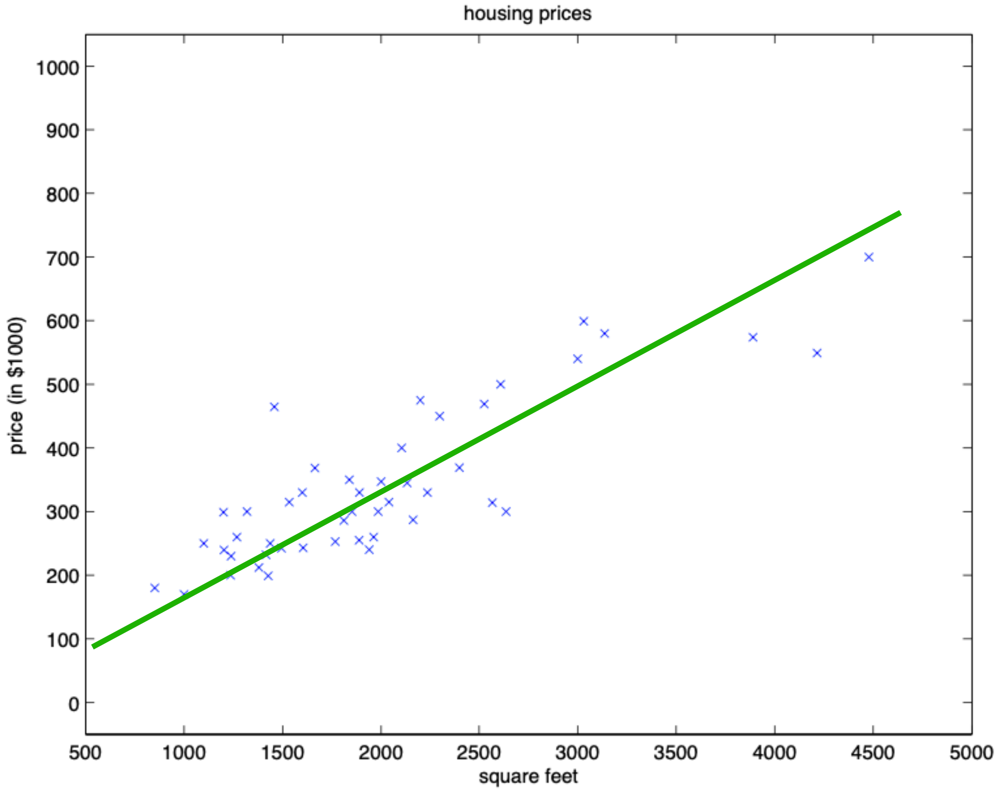

Derivation of Normal equation:

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

$$\nabla_w L(w) = XX^\top w - XY$$

$$X = \begin{bmatrix} | & | & & | \\ x_1 & x_2 & \cdots & x_n \\ | & | & & | \end{bmatrix} \quad Y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

Recap on SVM

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

Hard margin SVM:

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

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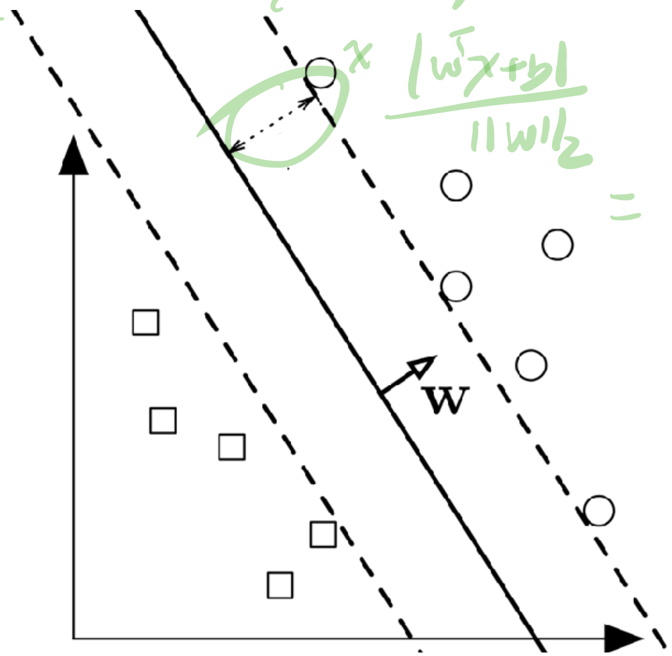

Width of the "street":

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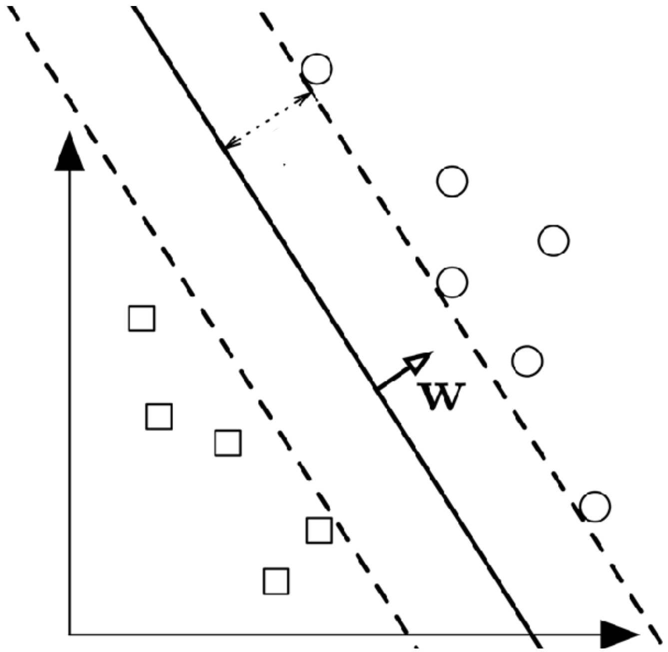

Width of the “street”:

$$2/\|w\|_2$$

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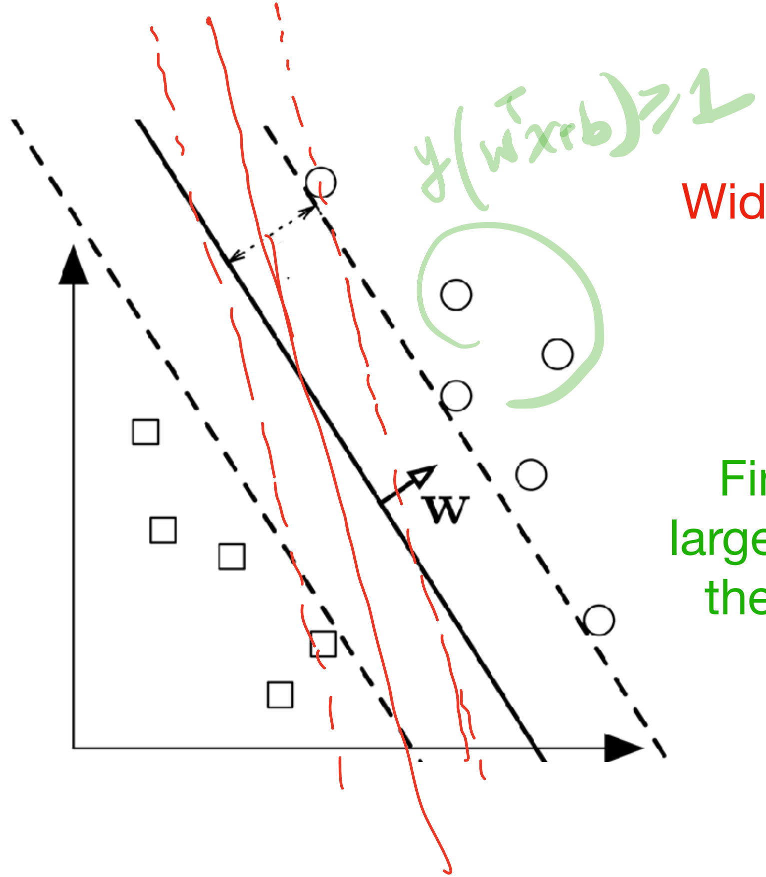

Width of the "street":

$$2/\|w\|_2$$

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

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

ERM

The ultimate objective function:

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

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Instead we have its **empirical** version

ERM

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$n \to \infty$

Instead we have its **empirical** version

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

ERM

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Empirical risk / Empirical error

The generalization error of ERM solution

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

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$$\mathbb{E}_{\mathcal{D}} \left[\mathbb{E}_{x,y \sim P} \ell(\hat{h}_{ERM}(x), y) \right]$$

↑

Training Data

The generalization error of ERM solution

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Test

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Note $\hat{h}_{ERM}$ is a random quantity as
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e.g., In LR: $\hat{w} = (XX^\top)^{-1} XY$.

The generalization error of ERM solution

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

$$\mathbb{E}_{\mathscr{D}}\left[\mathbb{E}_{x,y\sim P}\ell(\hat{h}_{ERM}(x), y)\right] \approx \min_{h\in\mathscr{H}} \mathbb{E}_{x,y\sim P}\ell(h(x), y)$$

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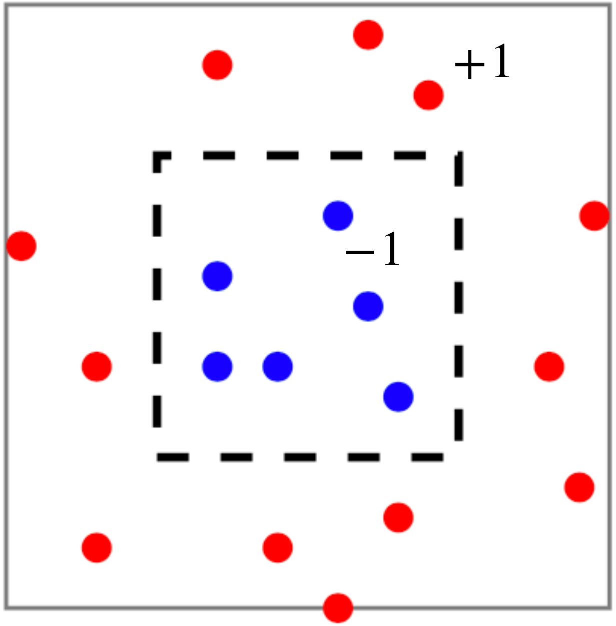
The Minimum expected loss we could get if we knew P

However, this may not hold if we are not careful about designing $\mathscr{H}$

Example:

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



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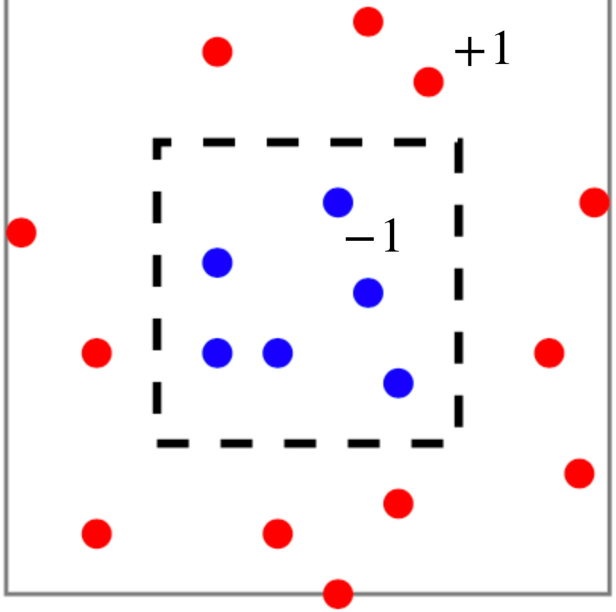

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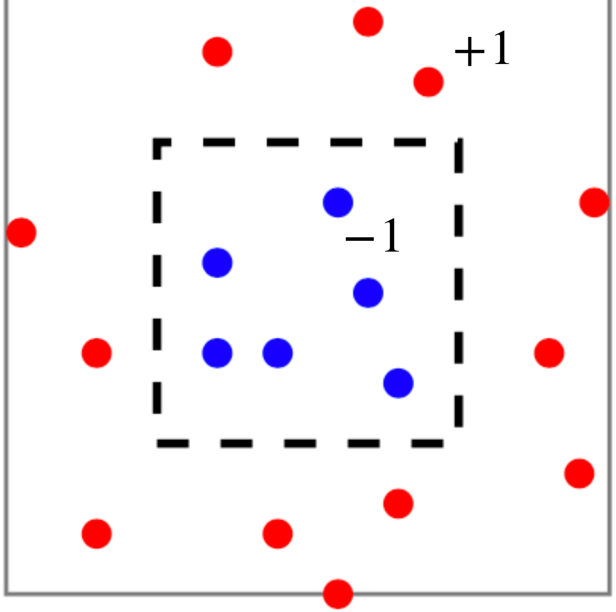

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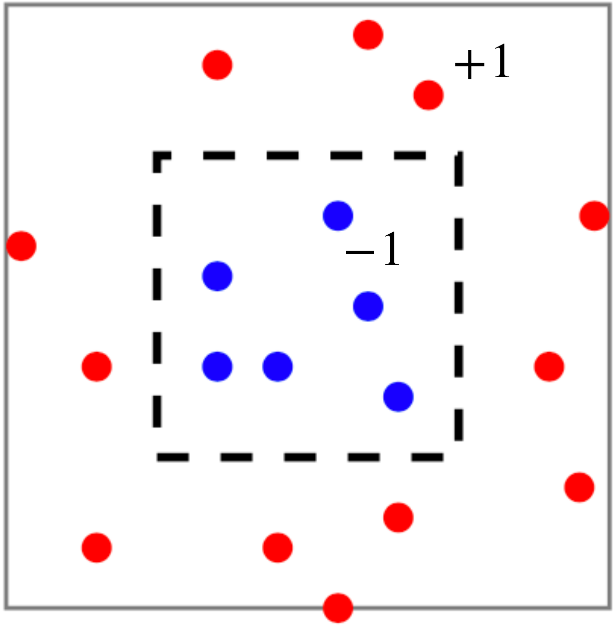

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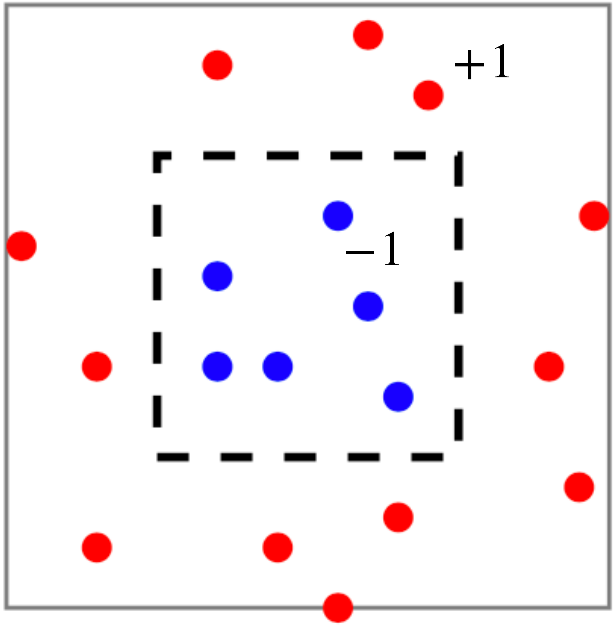

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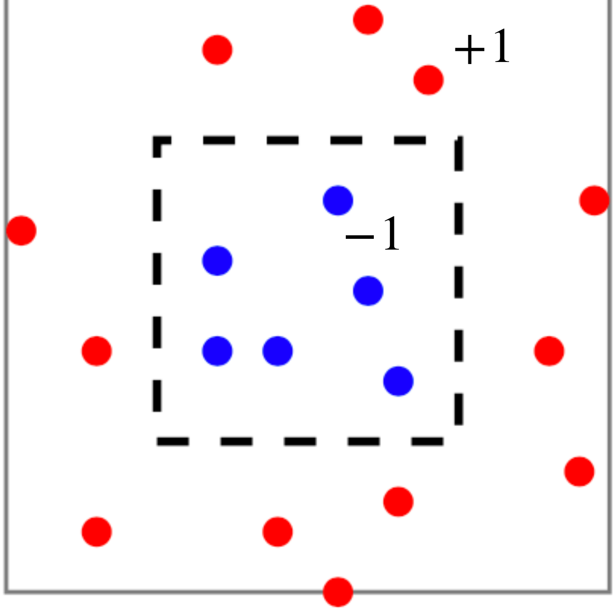

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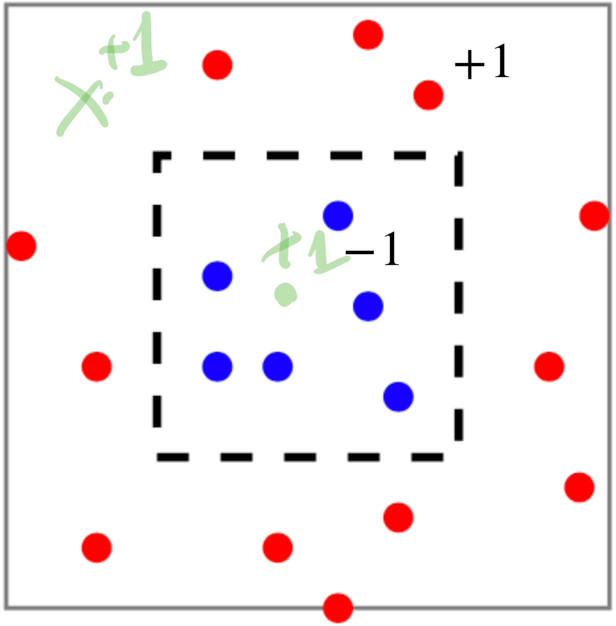

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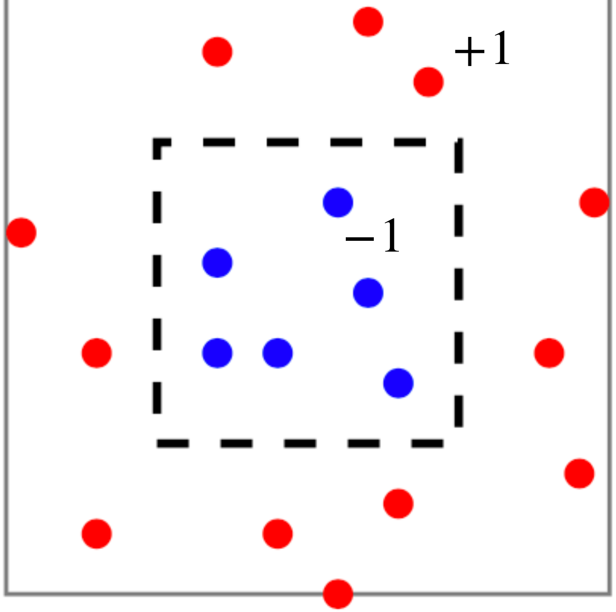

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A: area of smaller box / total area

ERM with inductive bias

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

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

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By restricting to $\mathcal{H}$, we bias towards solutions from $\mathcal{H}$

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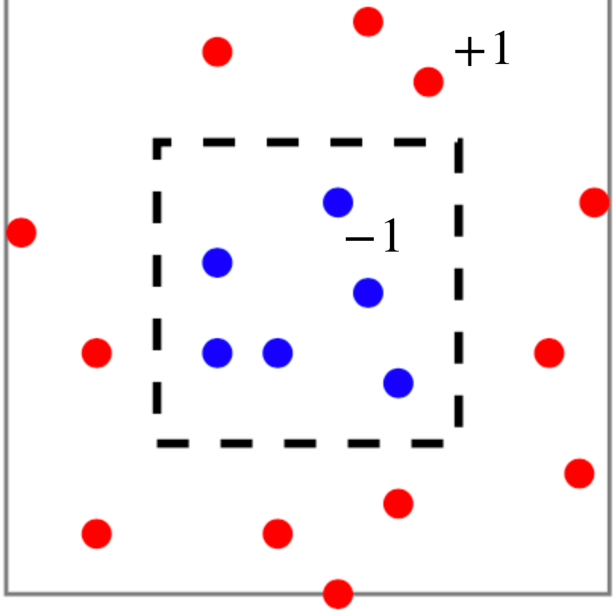

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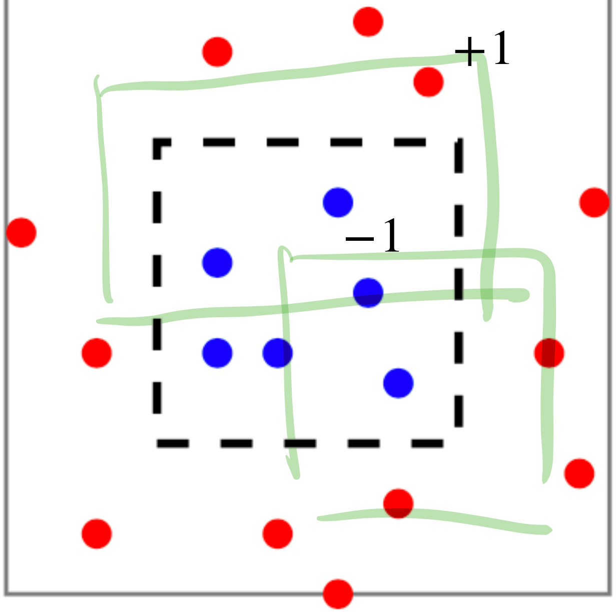

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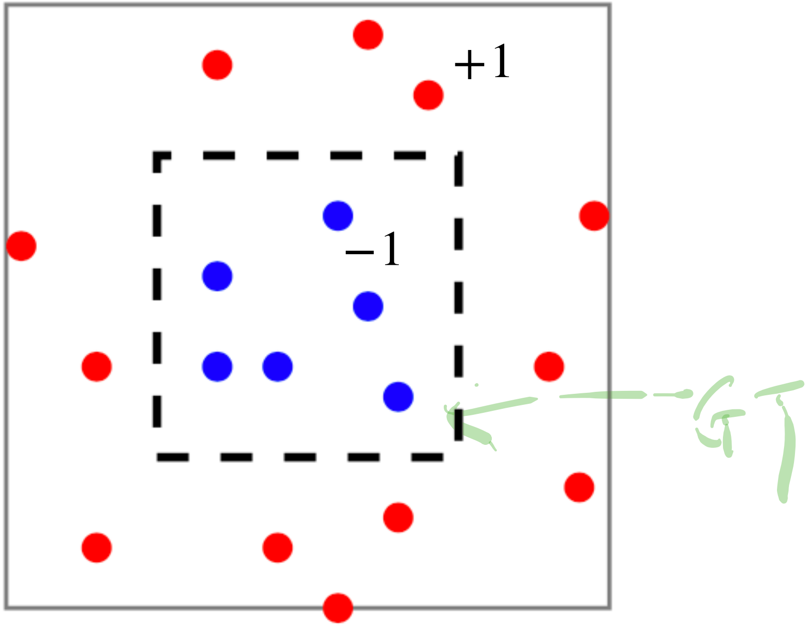

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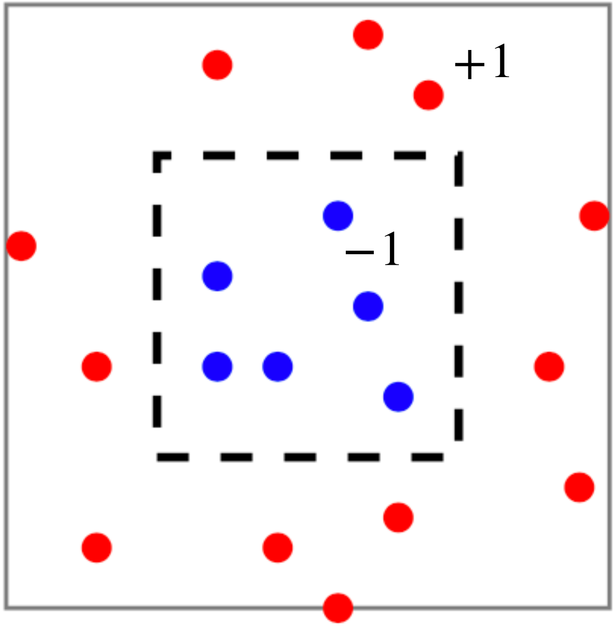

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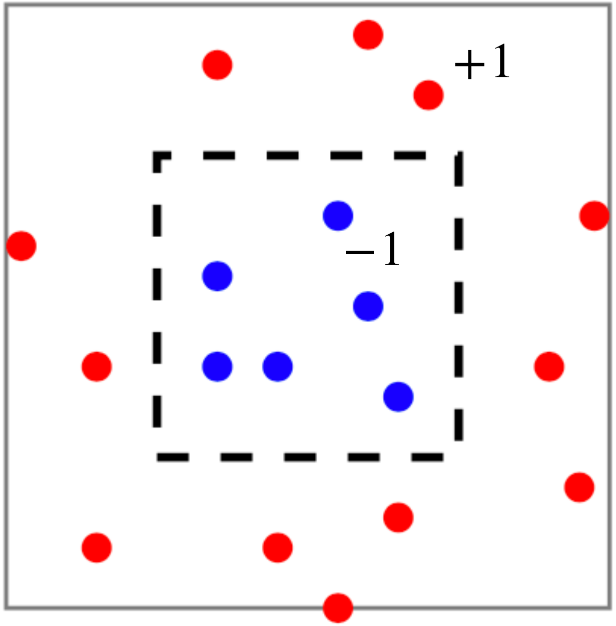

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(Exact proof out of the scope of this class — see CS 4783/5783)

Summary so far

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

To guarantee small test error, we need to restrict $\mathscr{H}$

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2. Examples on loss & hypothesis classes

3. Regularization

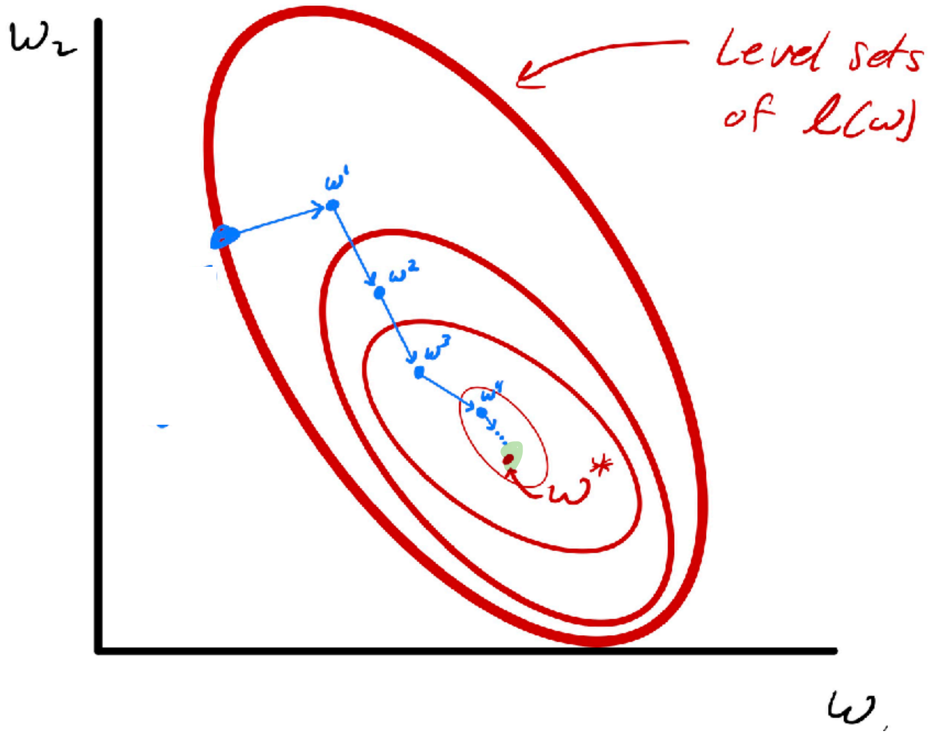
ERM with restricted hypothesis class

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

$$\text{s.t. } h \in \mathcal{H}$$

Let's go through several examples on Constraints under the linear regression context

Linear Regression: squared loss + ℓ_2 constraint



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

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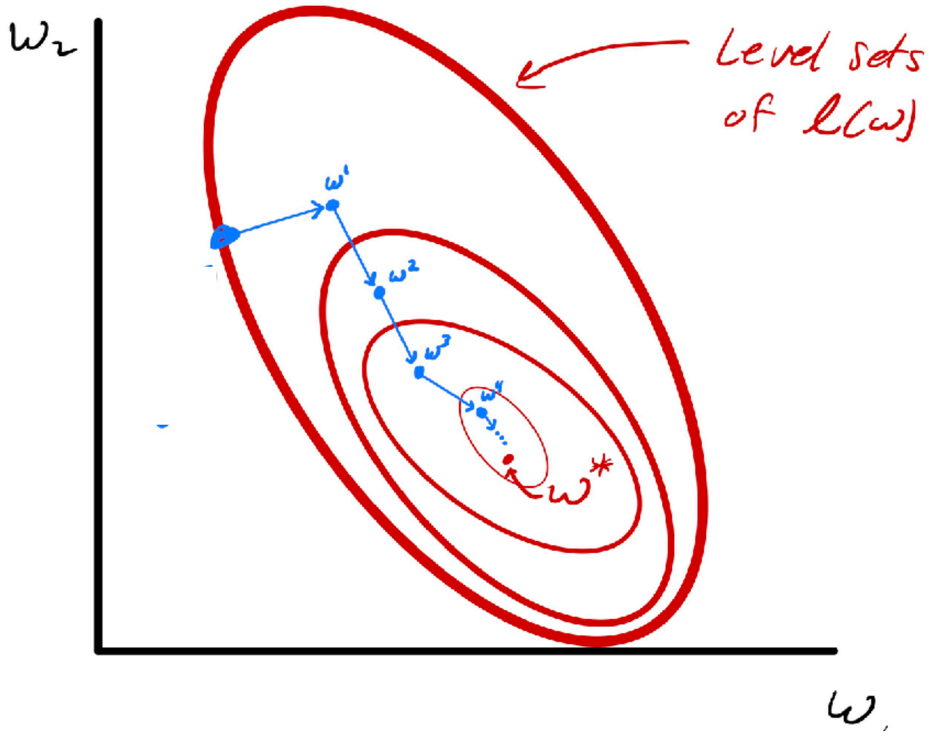

$$\min_w \frac{1}{n} \sum_{i=1}^{n} (w^\top x_i - y_i)^2$$

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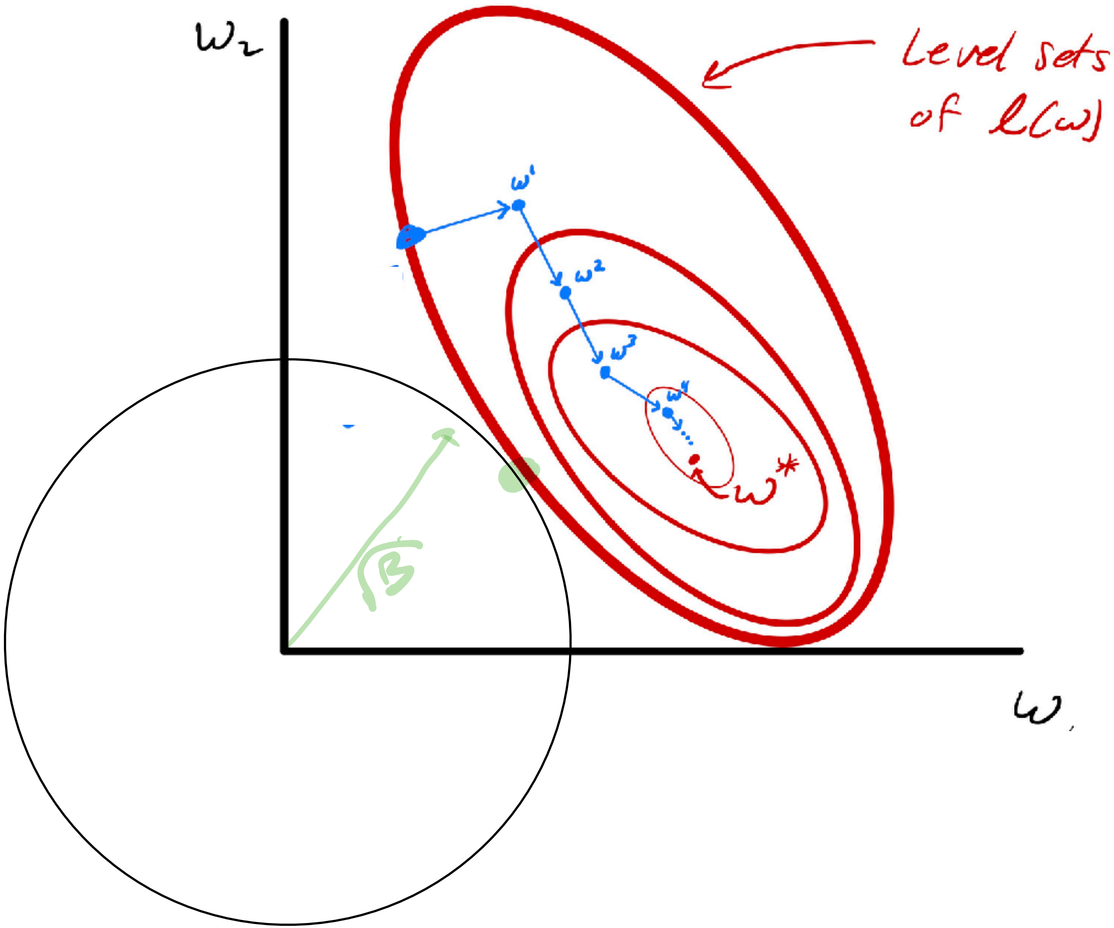

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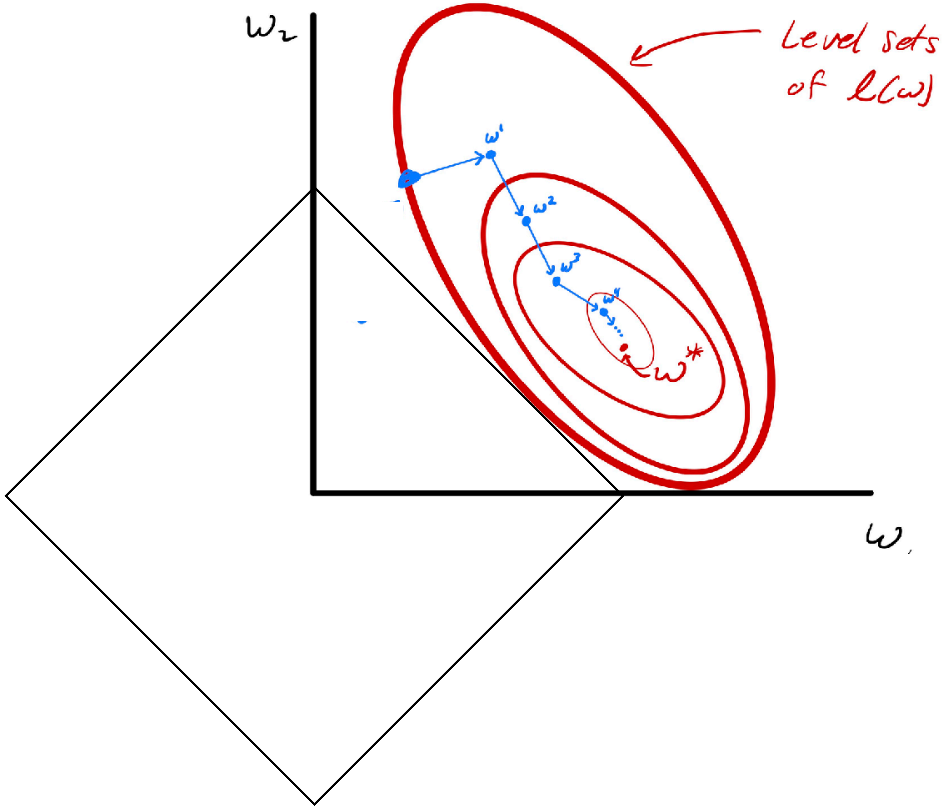
Linear Regression: squared loss + ℓ_1 constraint

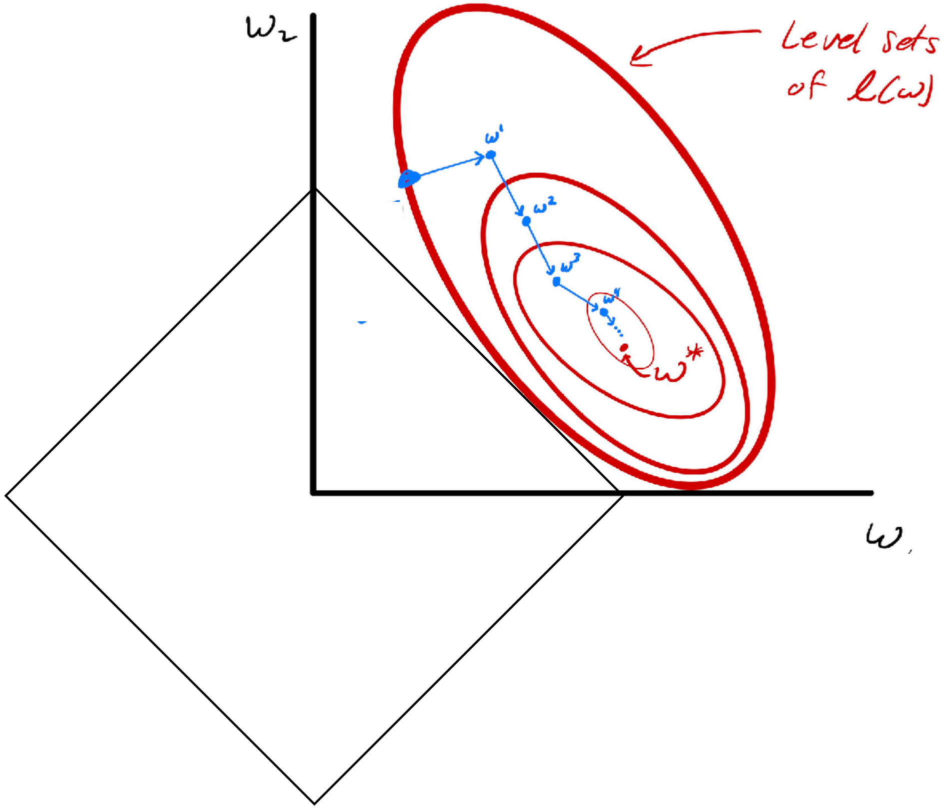


$$\min_w \frac{1}{n} \sum_{i=1}^{n} (w^\top x_i - y_i)^2$$

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

$\|w\|_1 = \sum_{i=1}^{d} |w_i|$

Linear Regression: squared loss + ℓ_1 constraint



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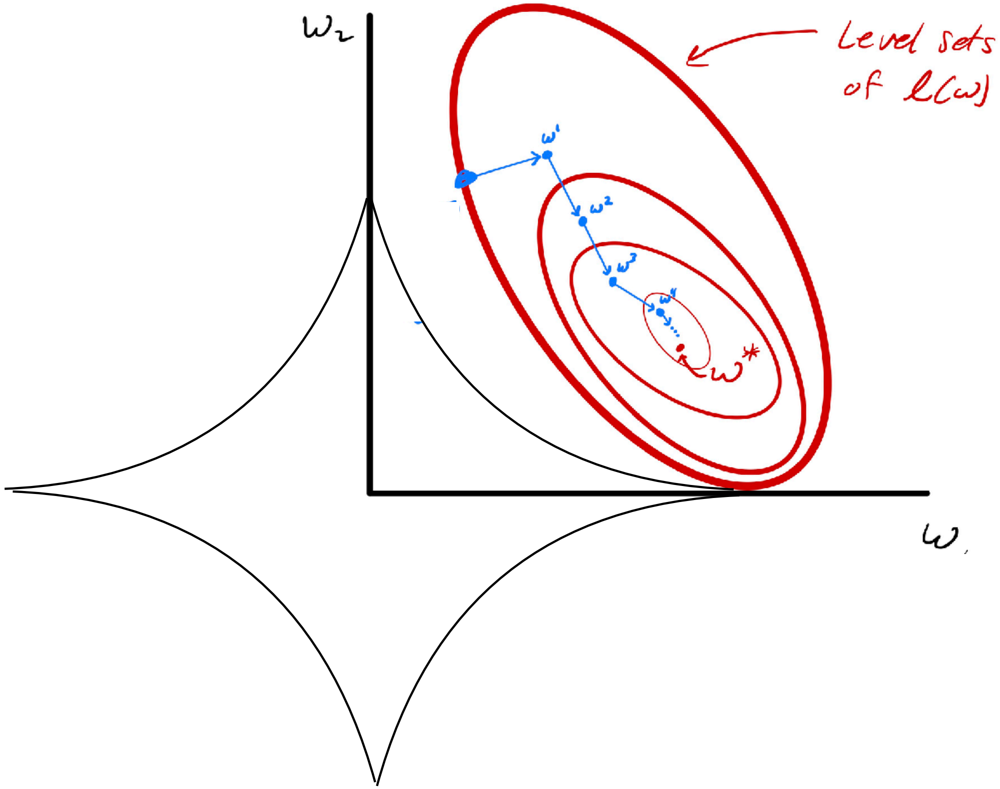
Advantage: give sparse solution

Linear Regression: squared loss + ℓ_p constraint



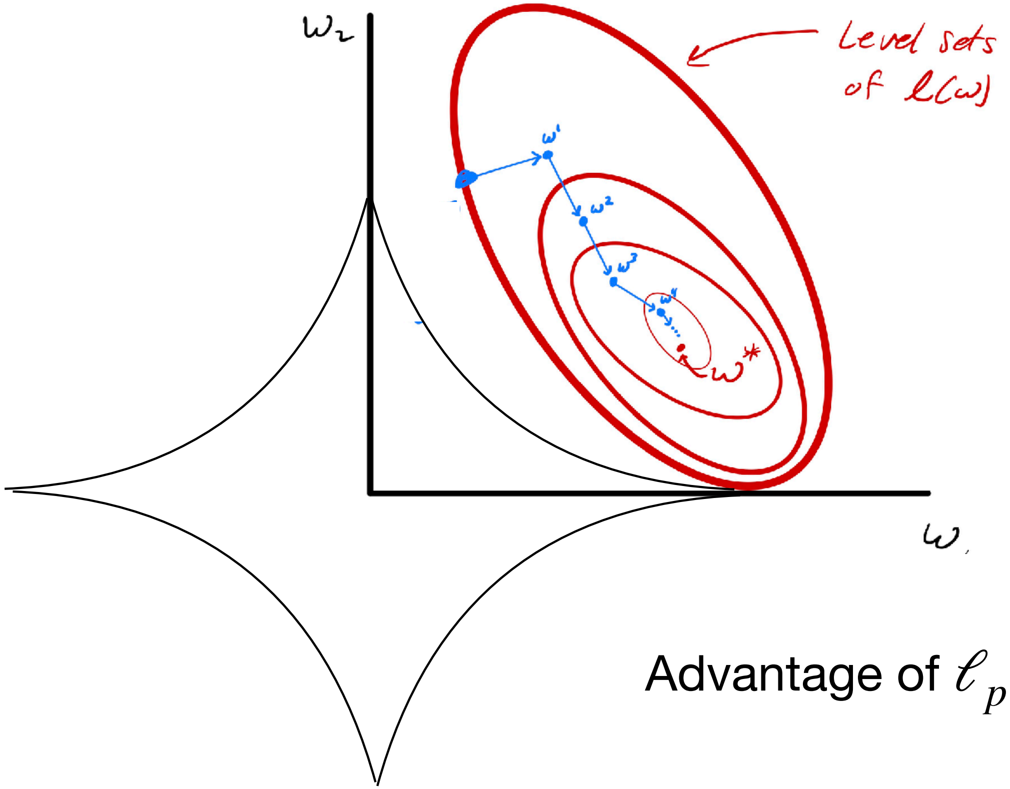
$$\min_w \frac{1}{n}\sum_{i=1}^{n}(w^\top x_i - y_i)^2$$

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

$0 < p < 1$

$$\|w\|_p = \left(\sum_{i=1}^{d} |w_i|^p\right)^{1/p}$$

Linear Regression: squared loss + ℓ_p constraint



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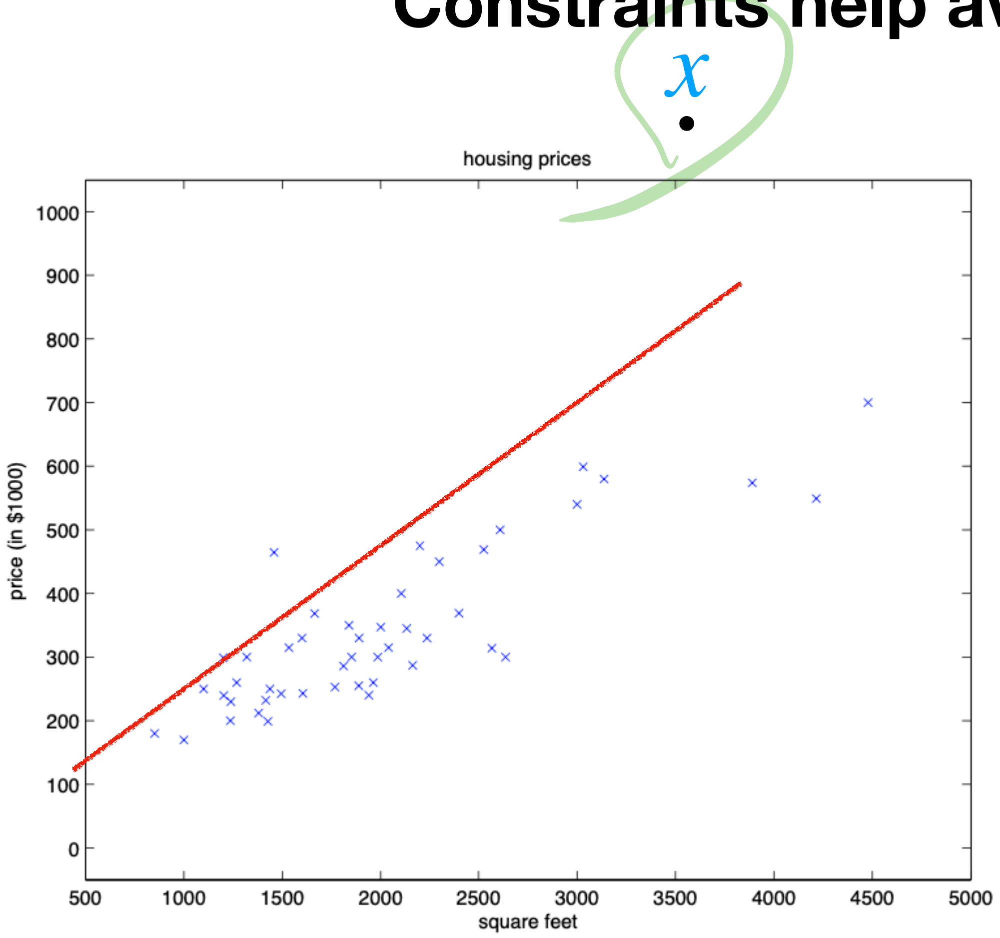
Advantage of ℓ_p constraint : very sparse solution

Disadvantage: Non-convex

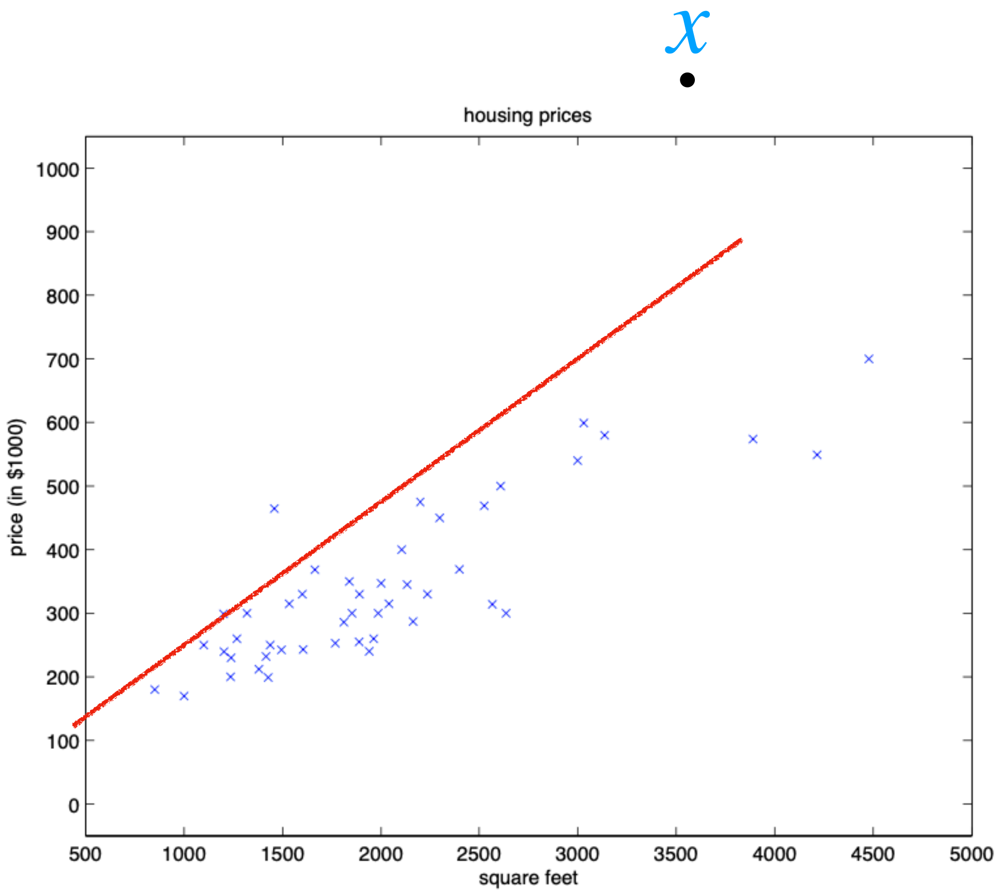
Constraints help avoid overfitting



Without constraint, we might overfit to an outlier

$(w^T x - y)^2$

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)

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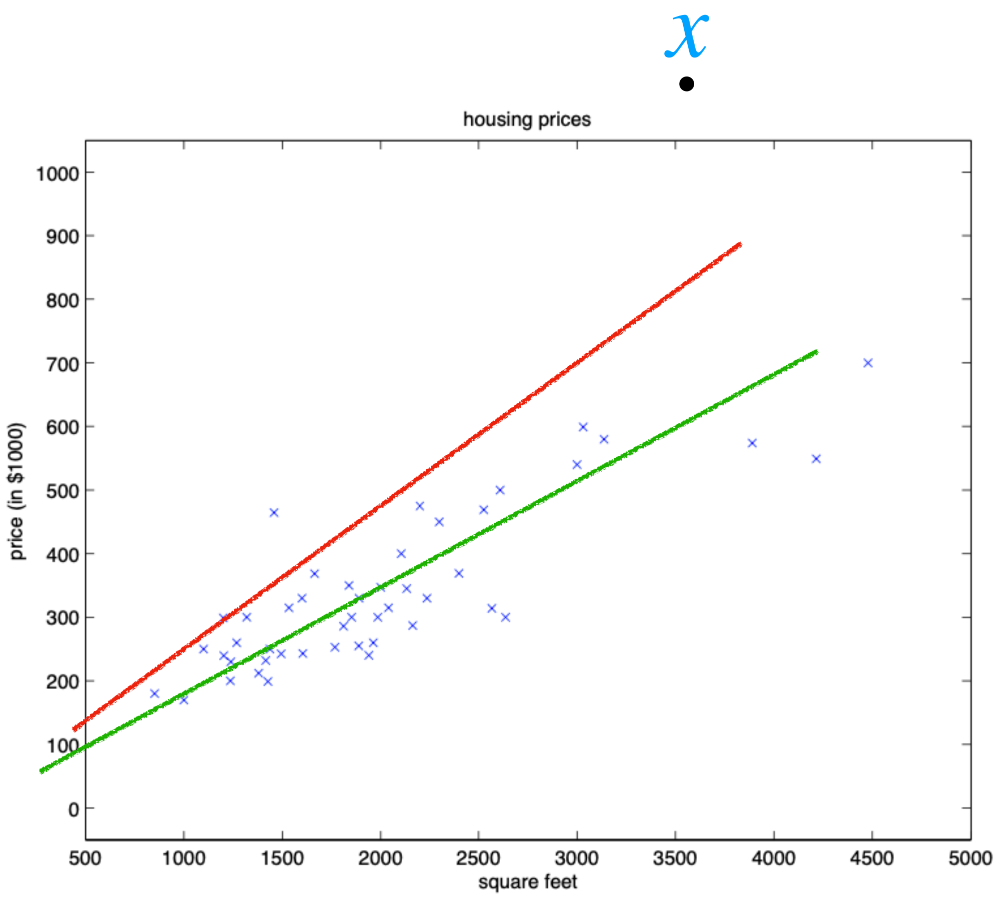

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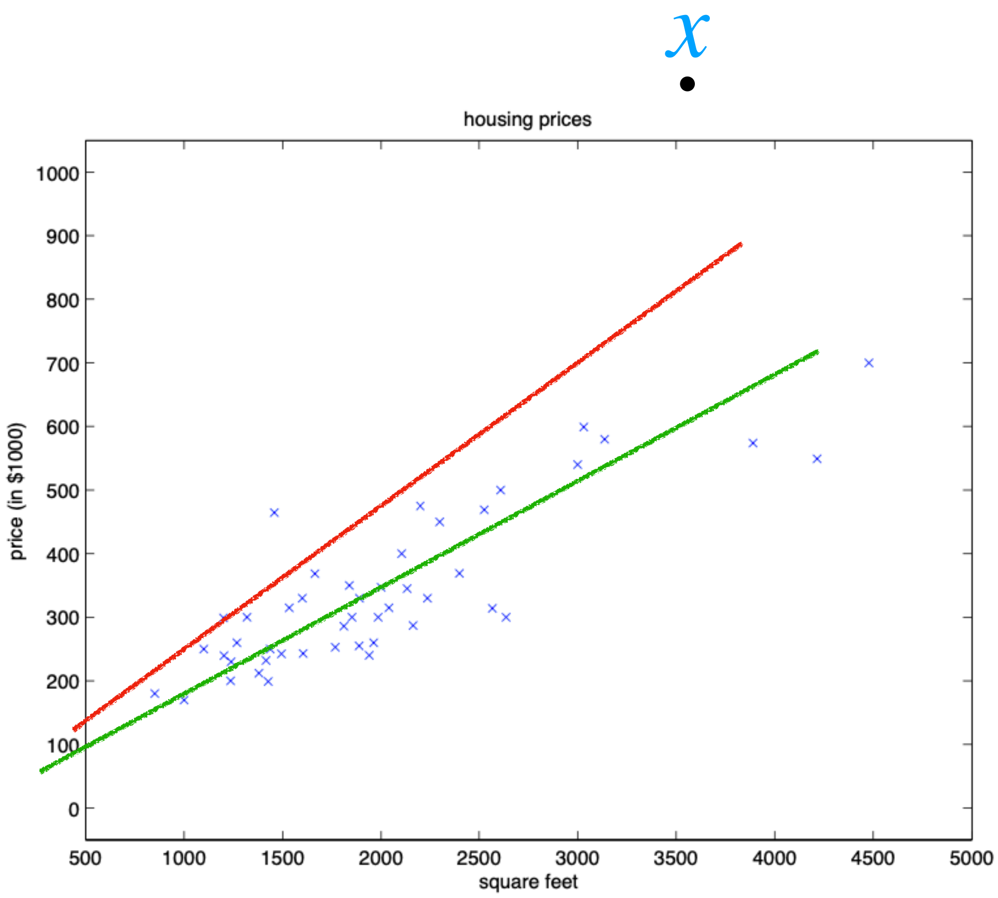


Without constraint, we might overfit to an outlier

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

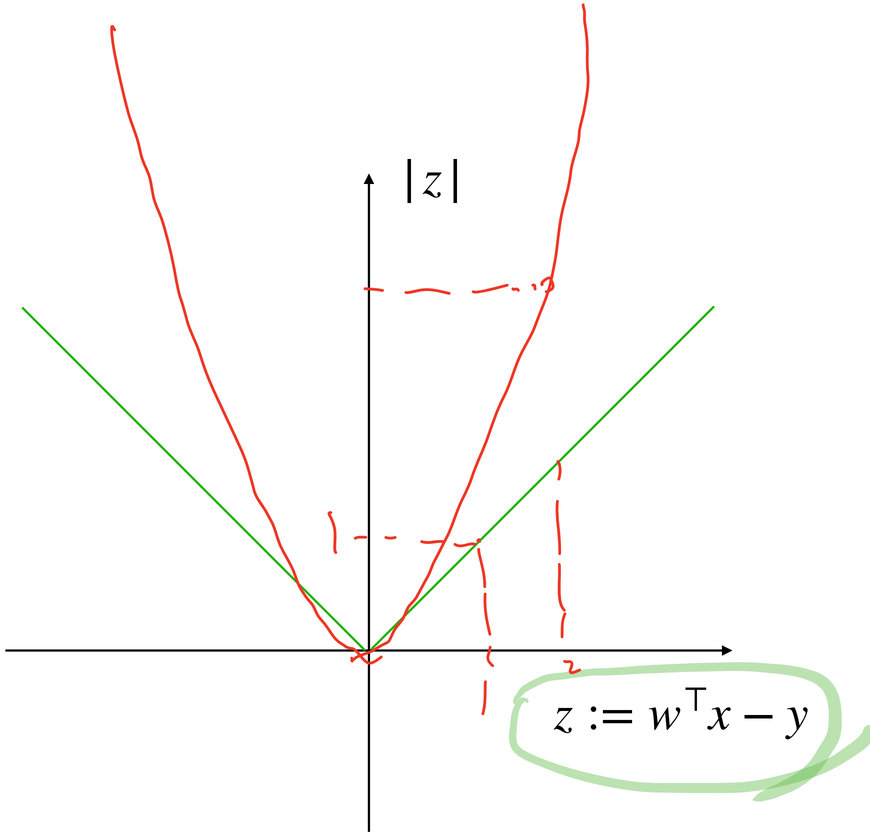
Absolute loss:

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

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

$R(w) = \|w\|_2^2$

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



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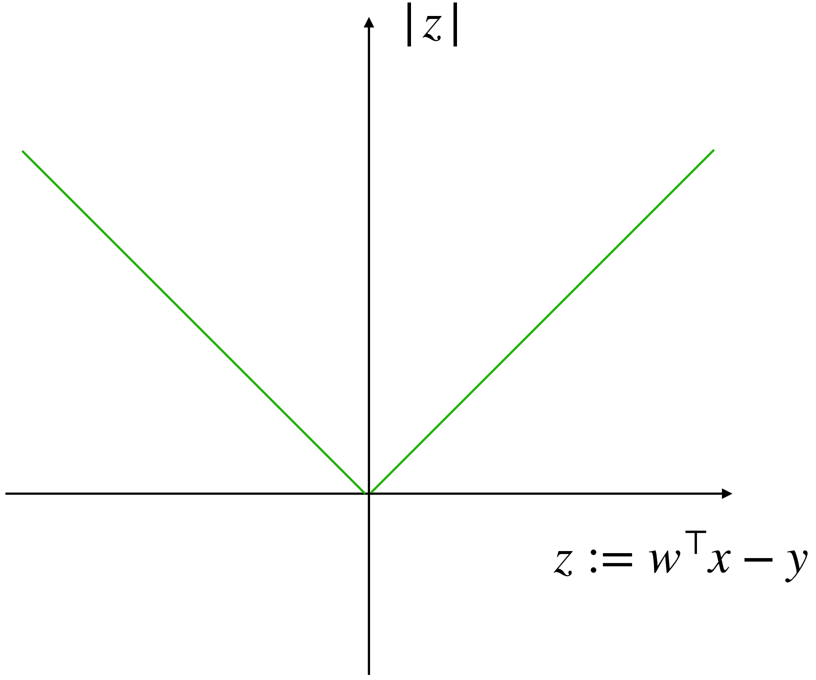

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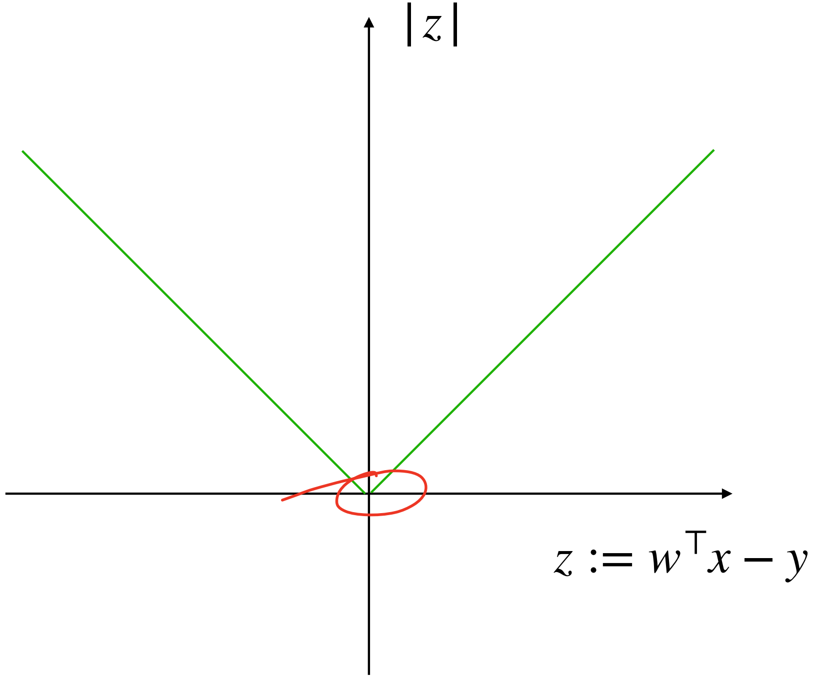
Disadvantage: no closed-form solution, non-differentiable at 0



Other loss functions with linear regression

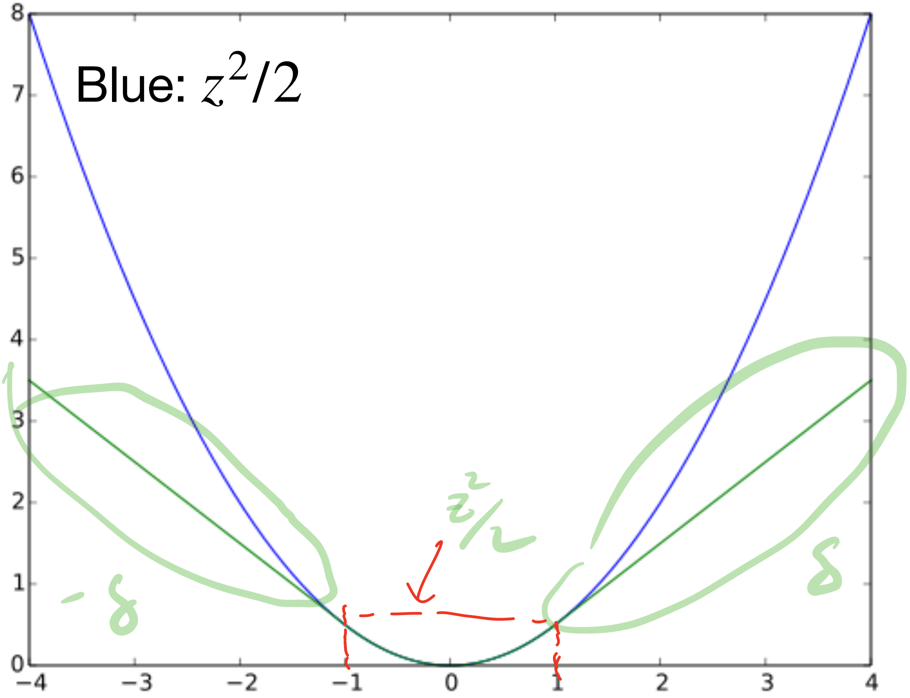
Huber loss:

$$\min_w \frac{1}{n} \sum_{i=1}^{n} L_\delta(w^\top x - y)$$

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

Where

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



Green: huber with $\delta = 1$

Other loss functions with linear regression

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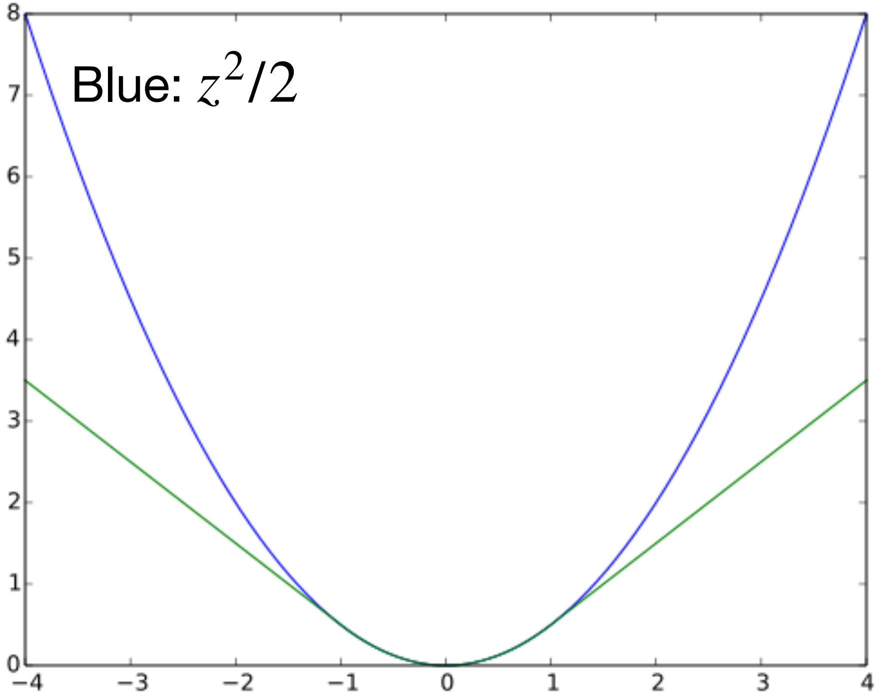

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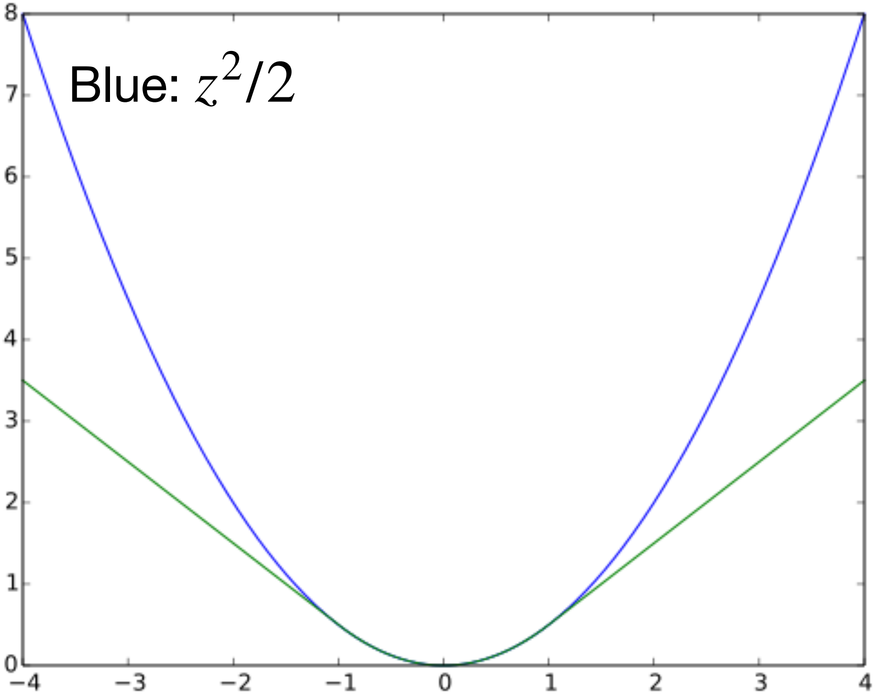
Advantage: best of both worlds

Disadvantage: additional parameter δ to tune



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Linear classification: Hinge loss + constraint

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

$$\text{s.t.} \quad \|w\|_2^2 \leq B$$

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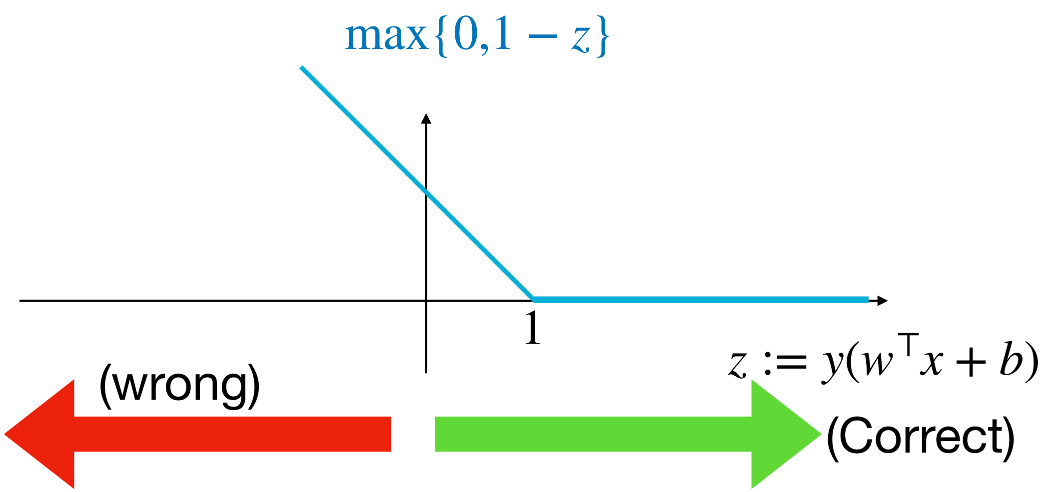

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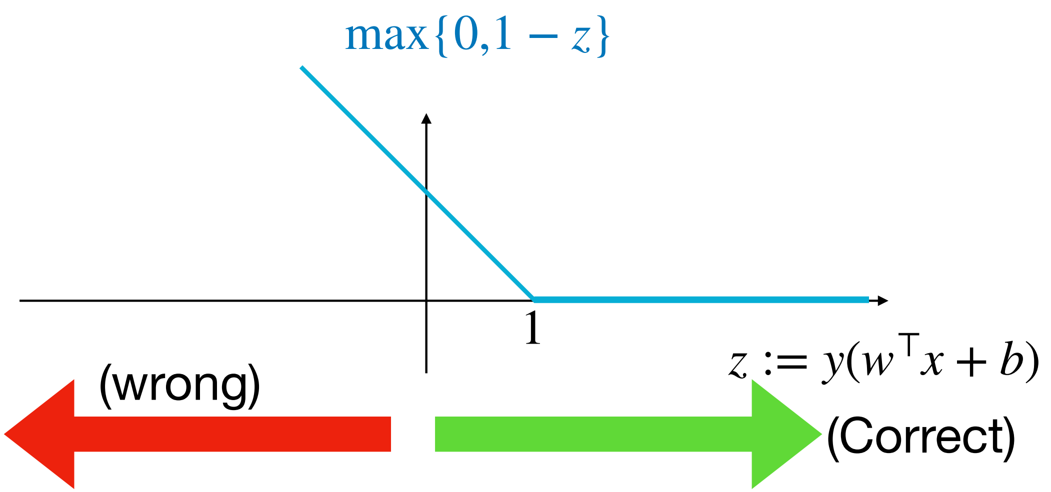
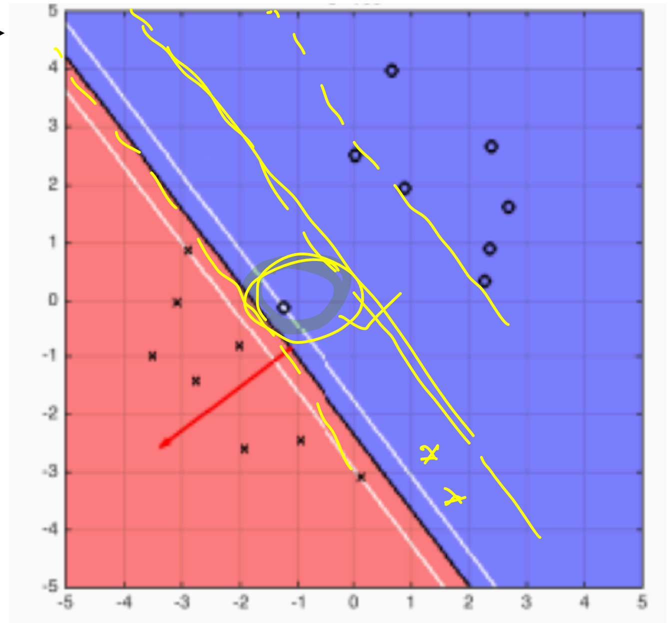
Constraint avoids overfit:
(Recall: small $\|w\|_2$ should have large street width)





Linear classification: Log-loss + constraints

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

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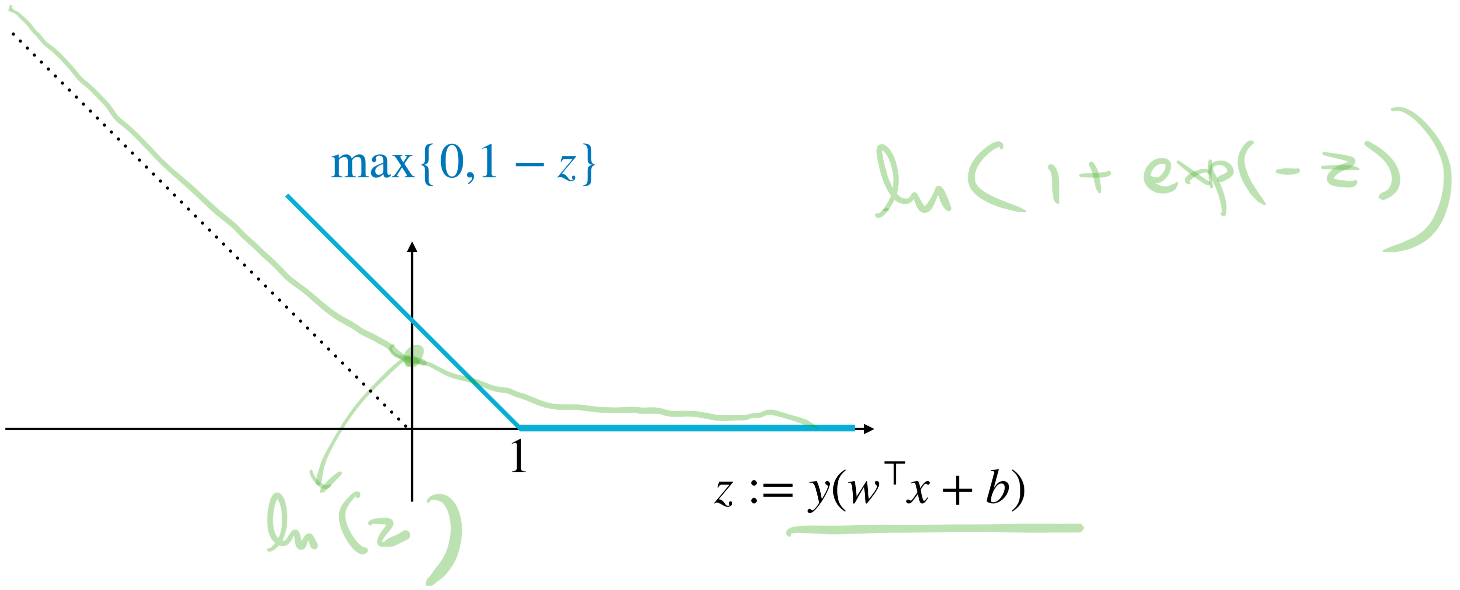

Linear classification: Exponential loss + constraints

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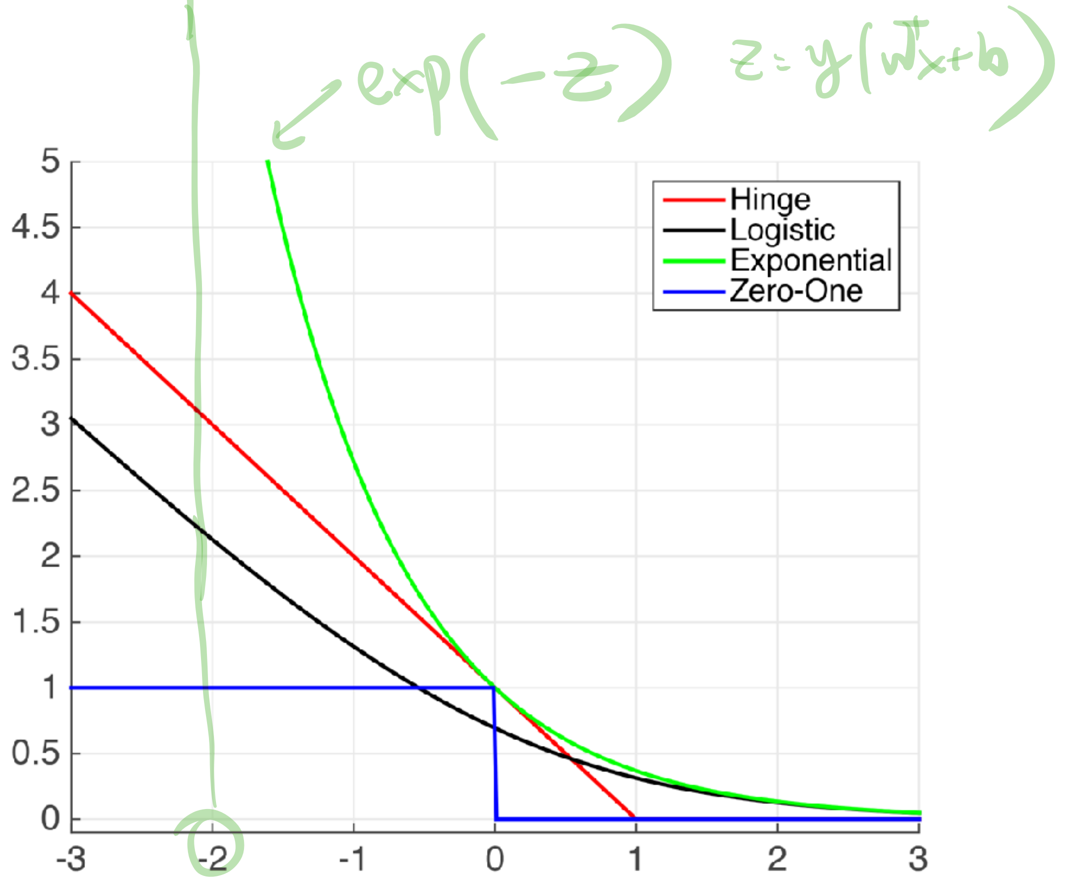

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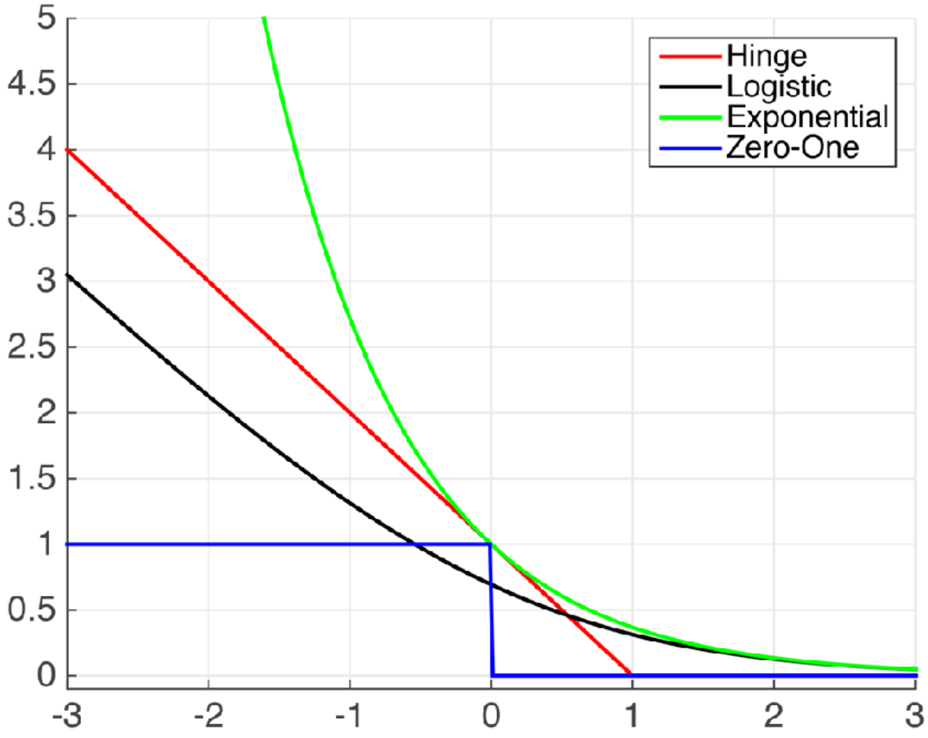
(Later, AdaBoost uses this loss)



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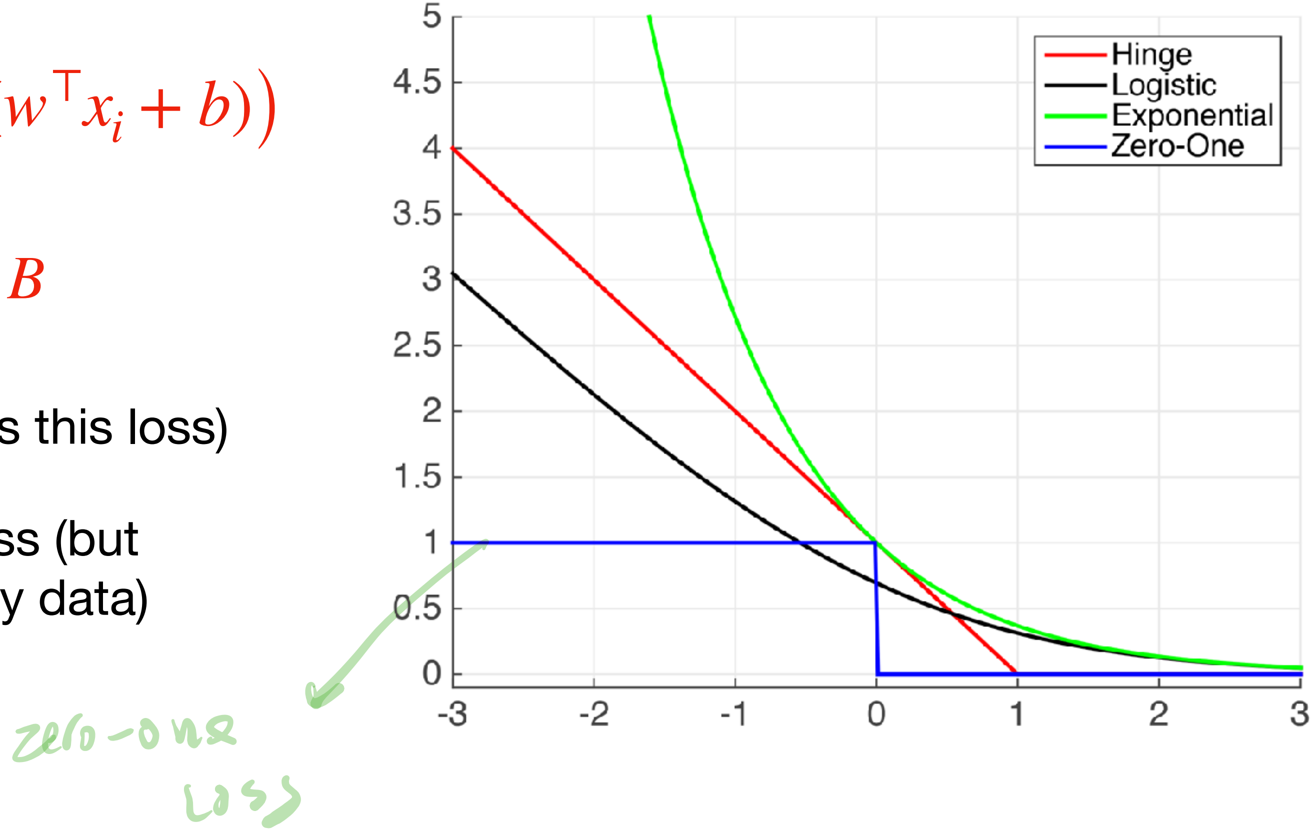
(Later, AdaBoost uses this loss)

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:

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

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

Regularization

We can turn constraint optimization problem into unconstrained using Lagrange multiplier

Example:

$$\min_w \frac{1}{n}\sum_{i=1}^{n}(w^\top x_i - y_i)^2 \quad \text{s.t. } \|w\|_1 \le B \quad \Longleftrightarrow \quad \min_w \frac{1}{n}\sum_{i=1}^{n}(w^\top x_i - y_i)^2 + \lambda\|w\|_2^2$$

Regularization

We can turn constraint optimization problem into unconstrained using Lagrange multiplier

Example:

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

$$\Longleftrightarrow$$

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$\lambda \|w\|_1$

(More details about Lagrange multiplier in Anil's optimization class CS4220)

Examples:

Soft-margin SVM:

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

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Ridge Linear Regression

$$\min_{w} \sum_{i=1}^{n} (w^\top x_i - y_i)^2 + \lambda \|w\|_2^2 \rightarrow (XX^\top + \lambda I)^{-1} XY$$

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Good for feature selection!

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2. Need to restrict our hypothesis class:

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

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

3. Examples of loss functions & Regularizations