Sparsity and the Lasso

CSE 446/546

Sewoong Oh & Pang Wei Koh

The story so far

- Regularization
  - Penalizes complex models towards simpler models
- One type of regularization: Ridge regression
  - Penalty on the L_2-norm of the model parameters
  - Shrinks model parameters w towards 0

- Today: A different form of regularization

Sparsity

- Definition: w is k-sparse if it has at most k non-zero entries
- Why sparsity?
  - Efficiency: If w is k-sparse, prediction depends only on k multiplies

$$\hat{y}_i = \hat{w}_{LS}^\top x_i = \sum_{j=1}^{d} x_i[j]\hat{w}_{LS}[j]$$

Sparsity

- Definition: w is k-sparse if it has at most k non-zero entries
- Why sparsity?
  - Efficiency: If w is k-sparse, prediction depends only on k multiplies
  - Interpretability: What are the relevant dimensions to make a prediction?

Lot size	Dishwasher
Single Family	Garbage disposal
Year built	Microwave
Last sold price	Range / Oven
Last sale price/sqft	Refrigerator
Finished sqft	Washer
Unfinished sqft	Dryer
Finished basement sqft	Laundry location
# floors	Heating type
Flooring types	Jetted Tub
Parking type	Deck
Parking amount	Fenced Yard
Cooling	Lawn
Heating	Garden
Exterior materials	Sprinkler System
Roof type	
Structure style	

Sparsity

- Definition: w is k-sparse if it has at most k non-zero entries
- Why sparsity?
  - Efficiency: If w is k-sparse, prediction depends only on k multiplies
  - Interpretability: What are the relevant dimensions to make a prediction?
  - Correctness: If you believe that the “true model” is sparse

Finding the best subset: Exhaustive search

$x \in \mathbb{R}^d$

- Try all subsets of size 1, 2, 3… and find one that minimizes validation error

X train $\Rightarrow$ size d

X test $\Rightarrow$ cheating

slow 2^d

Finding the best subset: Greedy search

Forward stepwise: start from simple model, iteratively add features

$T \leftarrow \emptyset$

For $j = 1, \ldots, k$ **do**

$$j^* \leftarrow \arg\min_{\ell} \min_{w} \sum_{i=1}^{n} \left(y_i - \sum_{j \in T \cup \{\ell\}} w[j] \times x_i[j] \right)^2$$

$T \leftarrow T \cup \{j^*\}$

Backward stepwise: start with full model, iteratively remove features

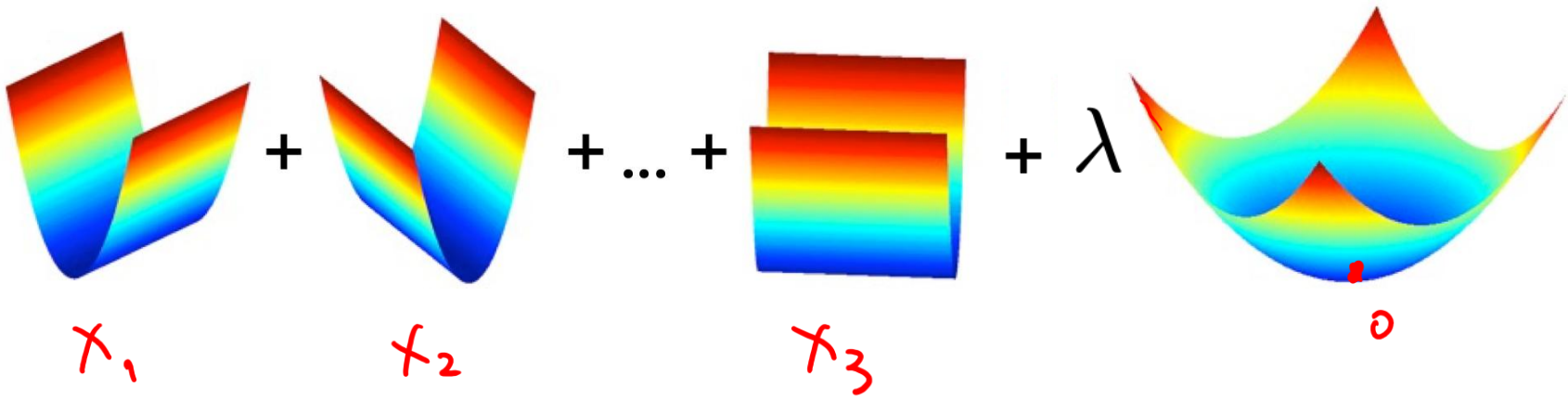
Forward + backward: do forward but remove features no longer important

(and many other variants)

Finding the best subset: Ridge regression

$$\hat{w}_{\text{ridge}} = \underset{w}{\text{argmin}} \sum_i \left(y_i - x_i^\top w\right)^2 + \lambda \|w\|_2^2$$

- Ridge regression makes coefficients small



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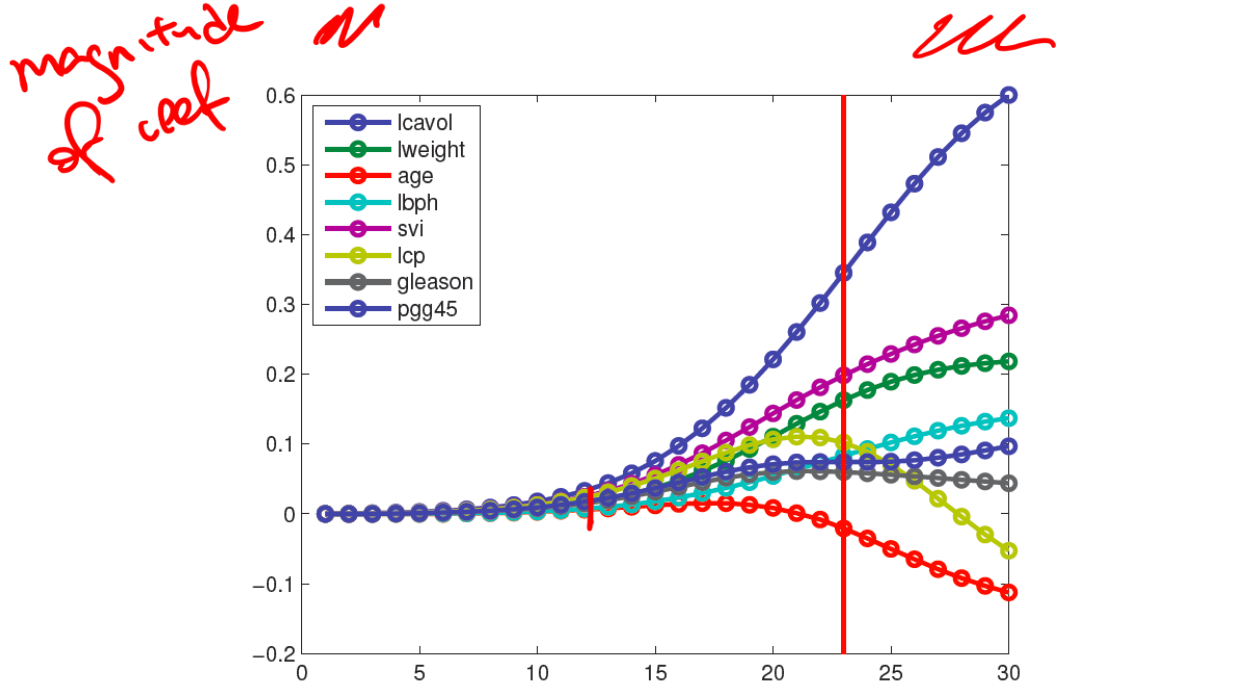
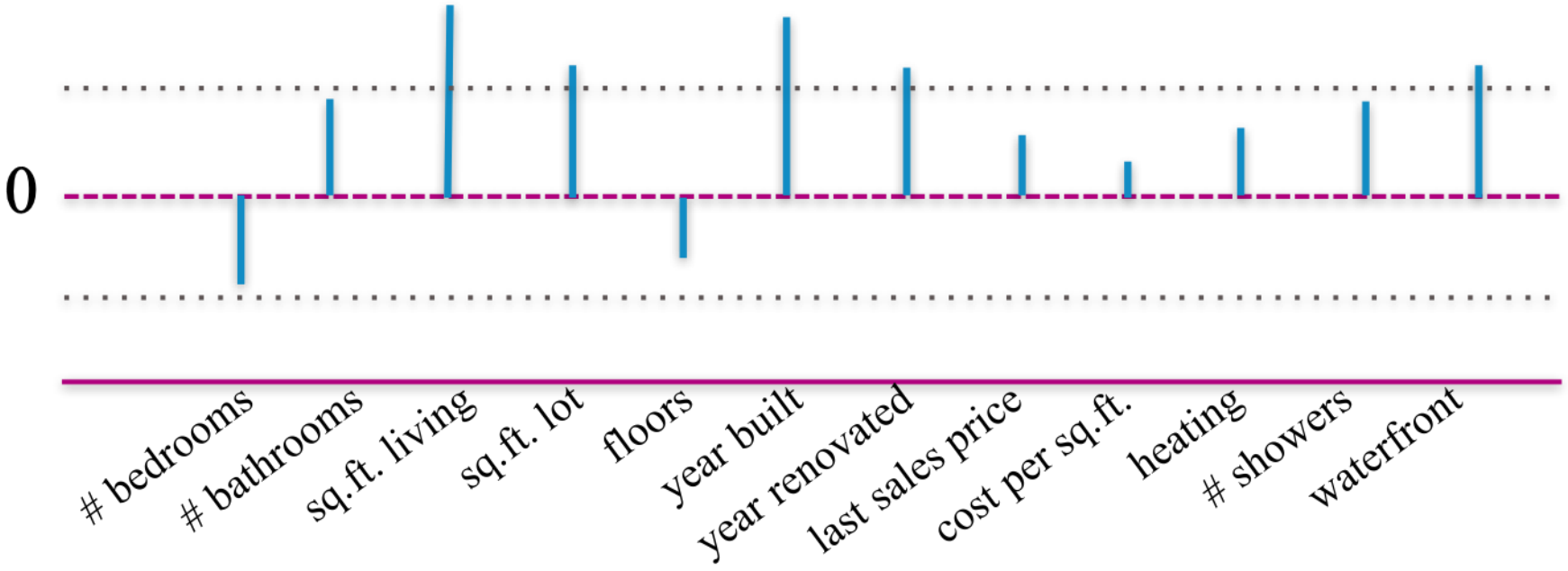


From Kevin Murphy's textbook

Finding the best subset: Ridge regression + threshold

$$\hat{w}_{\text{ridge}} = \underset{w}{\text{argmin}} \sum_i \left(y_i - x_i^\top w\right)^2 + \lambda \|w\|_2^2$$

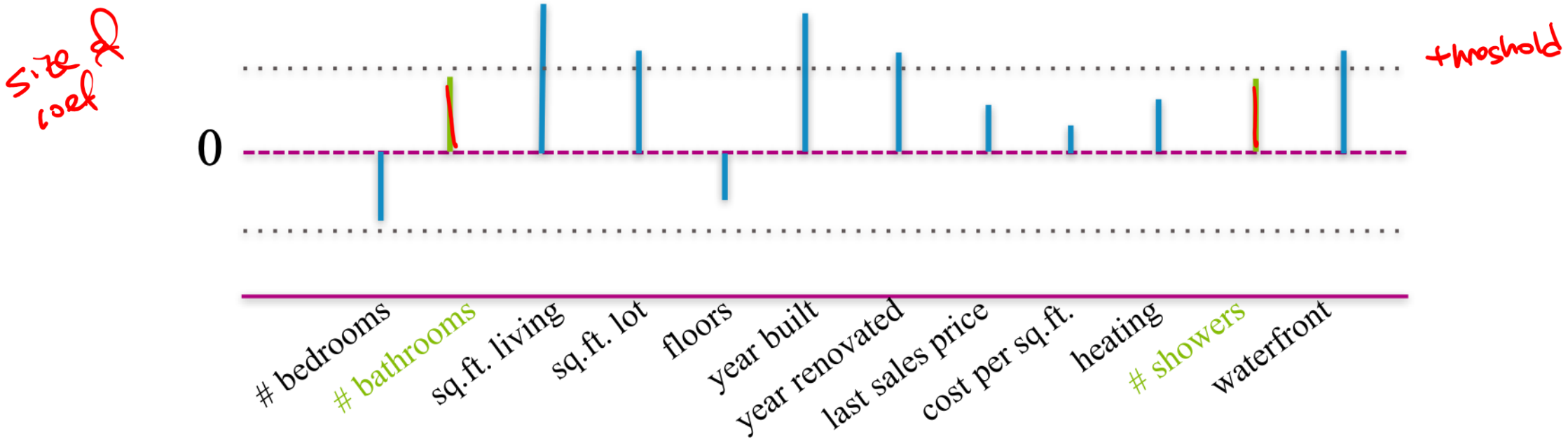
- Why don't we just set small ridge coefficients to 0?



Finding the best subset: Ridge regression + threshold

$$\hat{w}_{\text{ridge}} = \underset{w}{\text{argmin}} \sum_i \left(y_i - x_i^\top w\right)^2 + \lambda \|w\|_2^2$$

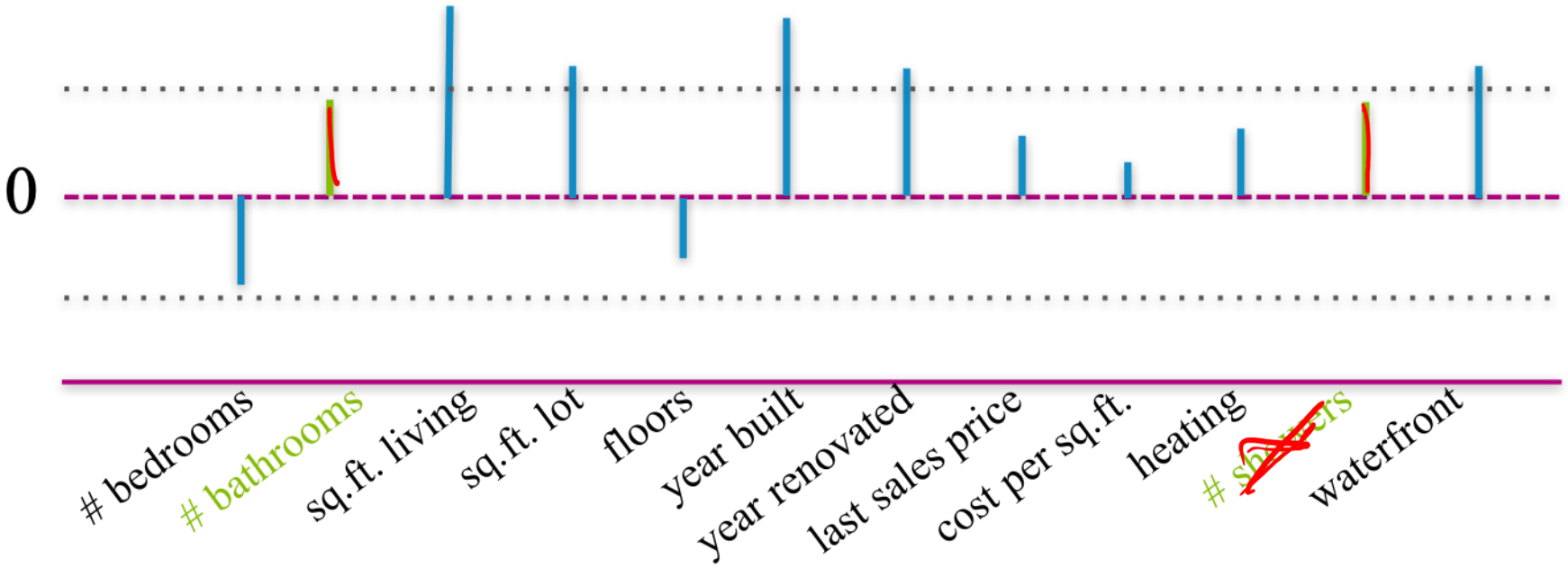
- Consider 2 related features (bathrooms, showers)



Finding the best subset: Ridge regression + threshold

$$\hat{w}_{\text{ridge}} = \underset{w}{\text{argmin}} \sum_i \left(y_i - x_i^\top w\right)^2 + \lambda \|w\|_2^2$$

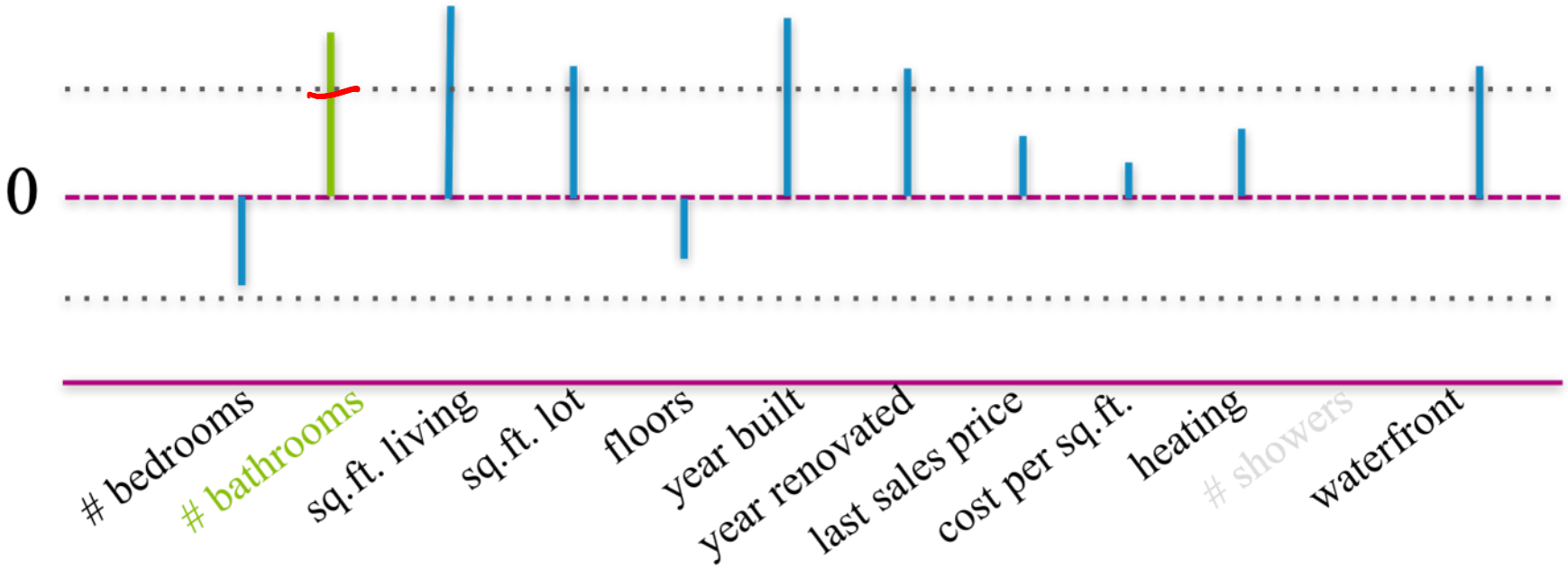
- What if we didn't include showers?



Finding the best subset: Ridge regression + threshold

$$\hat{w}_{\text{ridge}} = \underset{w}{\text{argmin}} \sum_i \left(y_i - x_i^\top w\right)^2 + \lambda \|w\|_2^2$$

- What if we didn't include showers? Weight on bathrooms increases!



Back to the drawing board

- We want to find parameters w that are sparse
- Ridge regression fails on correlated features
- Exhaustive search is too expensive
- Greedy search doesn't typically work well

Goal: Find a regularizer that gives us sparse solutions

$$\hat{w} = \underset{w}{\operatorname{argmin}} \sum_i \left(y_i - x_i^\top w\right)^2 + \lambda r(w)$$

$\|w\|_2^2$

ℓ_p norms

$$\hat{w}_{\text{ridge}} = \underset{w}{\text{argmin}} \sum_i (y_i - x_i^\top w)^2 + \lambda \|w\|_2^2$$

What if we used other norms? $\|w\|_p = \left(\sum_{k=1}^d |w_k|^p\right)^{1/p}$ for $0 < p < \infty$

$p=2$

$\|w\|_2 = \left(\sum_{k=1}^d |w_k|^2\right)^{1/2}$

$\|w\|_2^2 = \sum_{k=1}^d w_k^2$

$p=1$

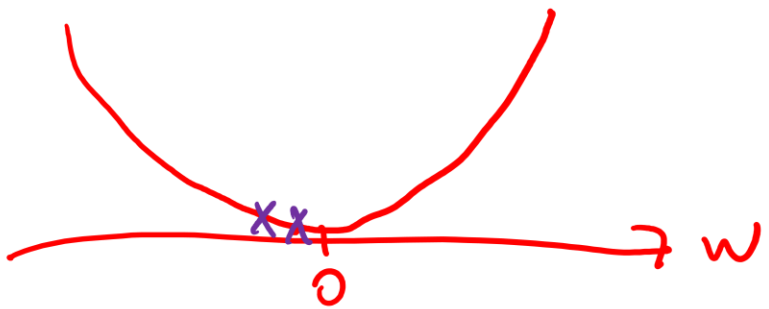
$\|w\|_1 = \sum_{k=1}^d |w_k|$

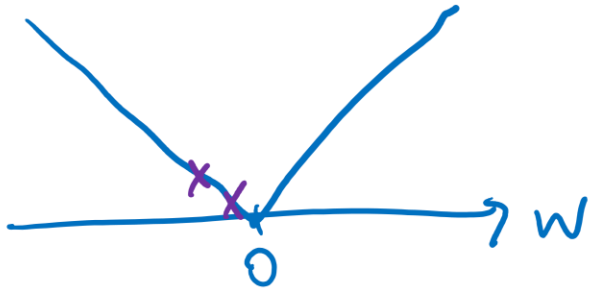
$p=\infty$

$\|w\|_\infty = \max_k (w_k)$

$p=0$

$\|w\|_0 = \text{card}(w)$





Lasso vs. ridge regression

$$\hat{w}_{\text{ridge}} = \underset{w}{\text{argmin}} \sum_i \left(y_i - x_i^\top w\right)^2 + \lambda \|w\|_2^2$$

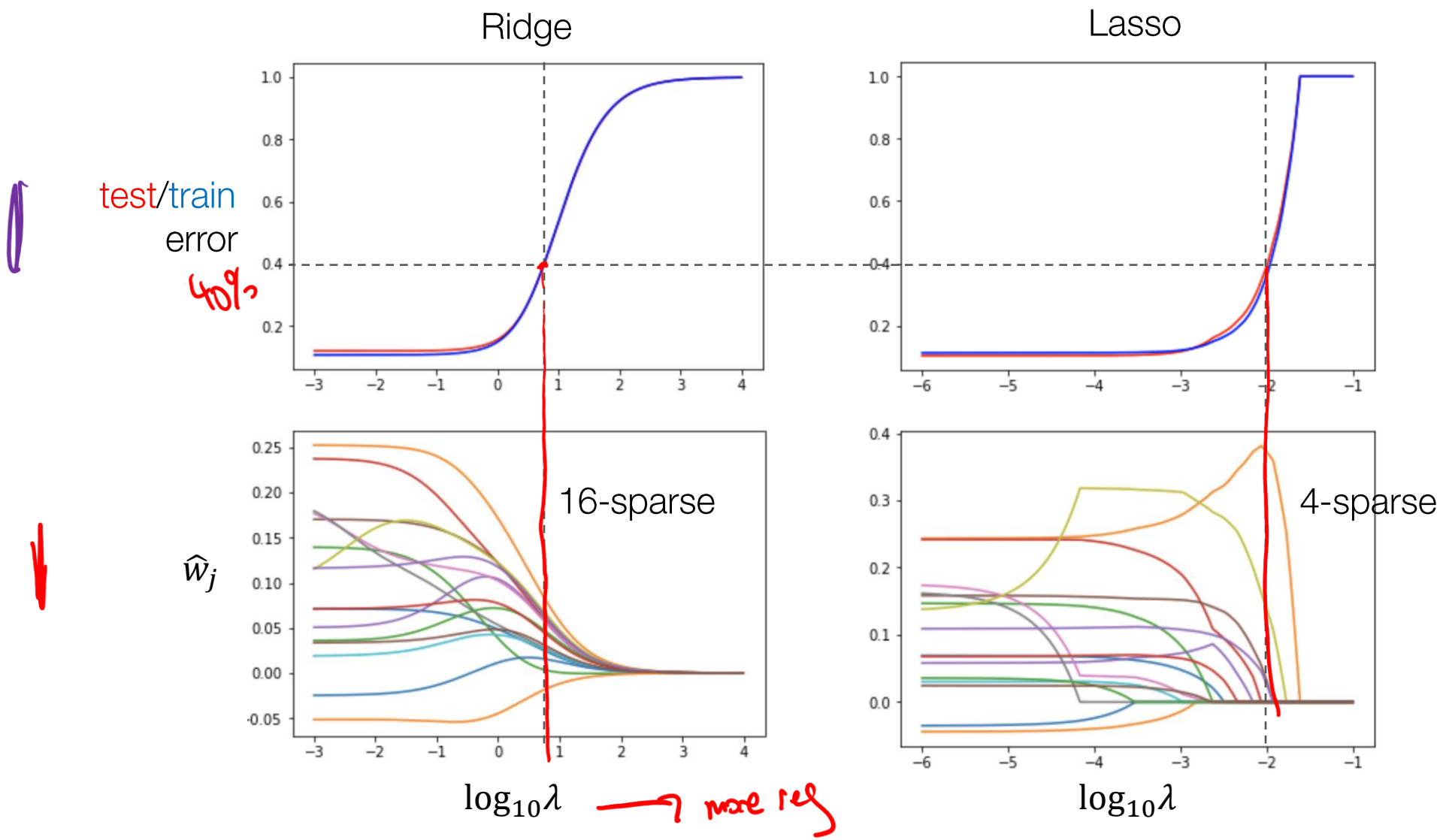
2

$$\hat{w}_{\text{lasso}} = \underset{w}{\text{argmin}} \sum_i \left(y_i - x_i^\top w\right)^2 + \lambda \|w\|_1$$

1

That's it! Somewhat magically, this generates sparse solutions.

Example: Housing price with 16 features



Algorithm: Lasso regression

1. **Model selection:** Choose λ based on cross-validation error, desired sparsity
2. **Feature selection:** Keep only features with non-zero (or not-too-small) weights in w at optimal λ
3. **(Optionally) Retrain** with the sparse model and $\lambda = 0$

Why is retraining helpful?

Example: Piecewise-linear fit

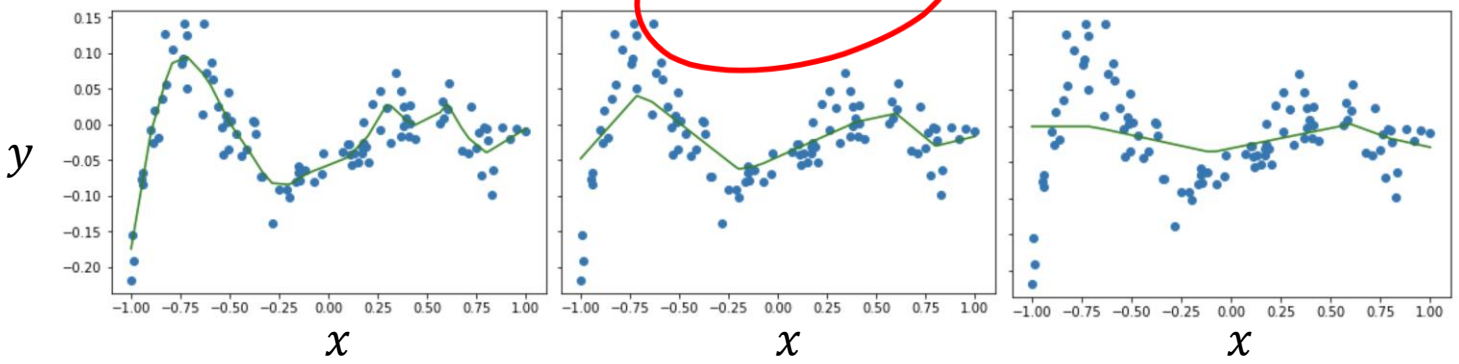
piecewise features

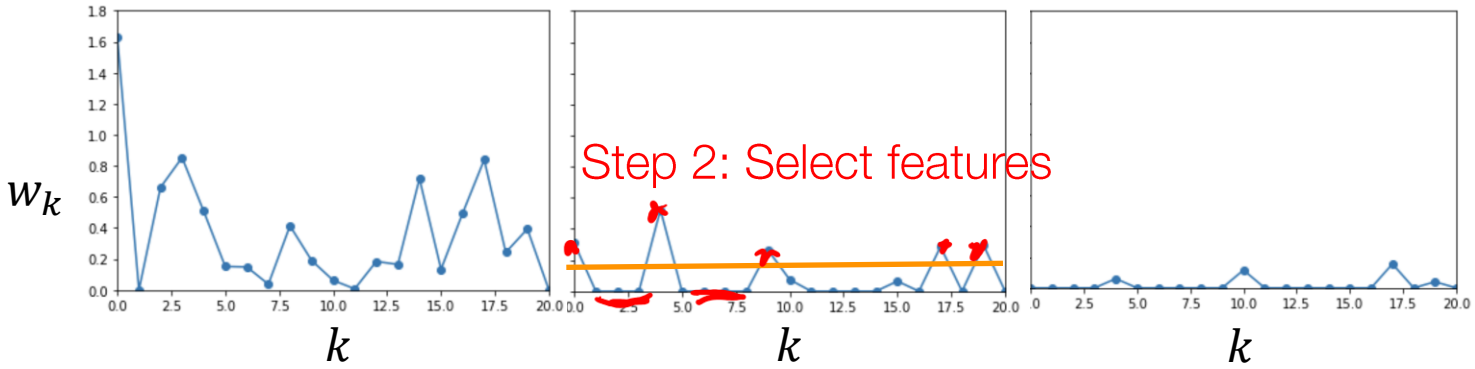
$$h_0(x) = 1$$
$$h_i(x) = [x + 1.1 - 0.1i]^+$$

$$\text{minimize}_w \sum_i \left(y_i - h(x_i)^T w\right)^2 + \lambda \|w\|_1$$

Step 1: Find optimal λ

$\lambda = 10^{-8}$ $\lambda = 10^{-4}$ $\lambda = 2 \times 10^{-4}$

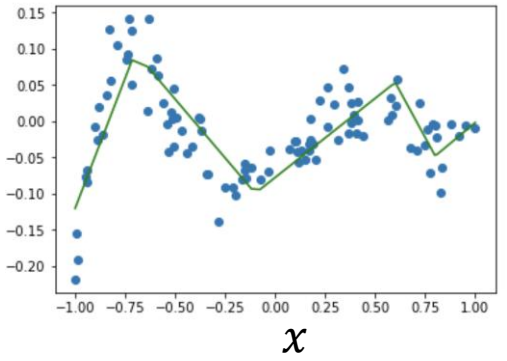


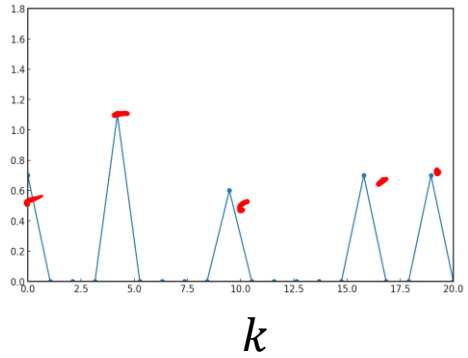


Step 2: Select features

Step 3: Retrain with selected features

$\lambda = 0$





Penalties vs. constraints

$$\hat{w}_{\mathrm{p}} = \underset{w}{\operatorname{argmin}} \sum_i \left(y_i - x_i^{\mathsf{T}} w\right)^2 + \lambda r(w)$$

$$\hat{w}_{\mathrm{c}} = \underset{w}{\operatorname{argmin}} \sum_i \left(y_i - x_i^{\mathsf{T}} w\right)^2 \quad \text{subject to} \quad r(w) \le \mu$$

These problems are equivalent in the following (informal) sense:

For any $\lambda \ge 0$, there exists μ such that $\hat{w}_{\mathrm{p}} = \hat{w}_{\mathrm{c}}$, and vice versa.

$$\hat{w}_{\mathbf{p}} = \underset{w}{\operatorname{argmin}} \sum_i \left(y_i - x_i^\top w\right)^2 + \lambda r(w)$$

$$\hat{w}_{\mathbf{c}} = \underset{w}{\operatorname{argmin}} \sum_i \left(y_i - x_i^\top w\right)^2 \quad \text{subject to} \quad r(w) \leq \mu$$

Note that $\hat{w}_{\mathbf{p}}$ is a function of λ and $\hat{w}_{\mathbf{c}}$ is a function of μ. We could have written $\hat{w}_p(\lambda)$ and $\hat{w}_{\mathbf{c}}(\mu)$ to make this explicit, but we'll leave it implicit to keep the notation cleaner.
Assume for convenience that the solutions to the above optimization problems are unique.
Then for any $\lambda \geq 0$, there exists μ such that $\hat{w}_{\mathbf{p}} = \hat{w}_{\mathbf{c}}$, and vice versa.

Proof:

Given λ, solve for $\hat{w}_{\mathbf{p}}$, then set $\mu = r\left(\hat{w}_{\mathbf{p}}\right)$. Denote $f(w) = \sum_i \left(y_i - x_i^\top w\right)^2$.
Assume for contradiction that $\hat{w}_{\mathbf{p}} \neq \hat{w}_{\mathbf{c}}$.
We know that $\hat{w}_{\mathbf{p}}$ is feasible (i.e., $r\left(\hat{w}_{\mathbf{p}}\right) \leq \mu$) because μ was set to exactly make $r\left(\hat{w}_p\right) = \mu$.
Since $\hat{w}_{\mathbf{c}}$ is the solution of the second optimization problem, we also know that:
(1) $r(\hat{w}_{\mathbf{c}}) \leq \mu = r\left(\hat{w}_{\mathbf{p}}\right)$ (because $\hat{w}_{\mathbf{c}}$ is feasible by definition)
(2) $\mathrm{f}(\hat{w}_{\mathbf{c}}) < \mathrm{f}\left(\hat{w}_{\mathbf{p}}\right)$ (because $\hat{w}_{\mathbf{c}}$ minimizes $f(w)$ out of all feasible points, and $\hat{w}_{\mathbf{p}}$ is feasible).
Putting these together, we get that $\mathrm{f}(\hat{w}_{\mathbf{c}}) + \lambda r(\hat{w}_{\mathbf{c}}) < \mathrm{f}\left(\hat{w}_{\mathbf{p}}\right) + \lambda r\left(\hat{w}_{\mathbf{p}}\right)$.
But this is a contradiction because by definition, $\hat{w}_{\mathbf{p}}$ is supposed to minimize $\mathrm{f}(w) + \lambda r(w)$.
Thus, $\hat{w}_{\mathbf{p}} = \hat{w}_{\mathbf{c}}$.

Feasible sets

$$\hat{w}_{\text{lasso}} = \underset{w}{\text{argmin}} \sum_i \left(y_i - x_i^\top w\right)^2 \quad \text{subject to} \quad \|w\|_1 \leq \mu$$

- Set of points that satisfy the constraints (of an optimization prob)

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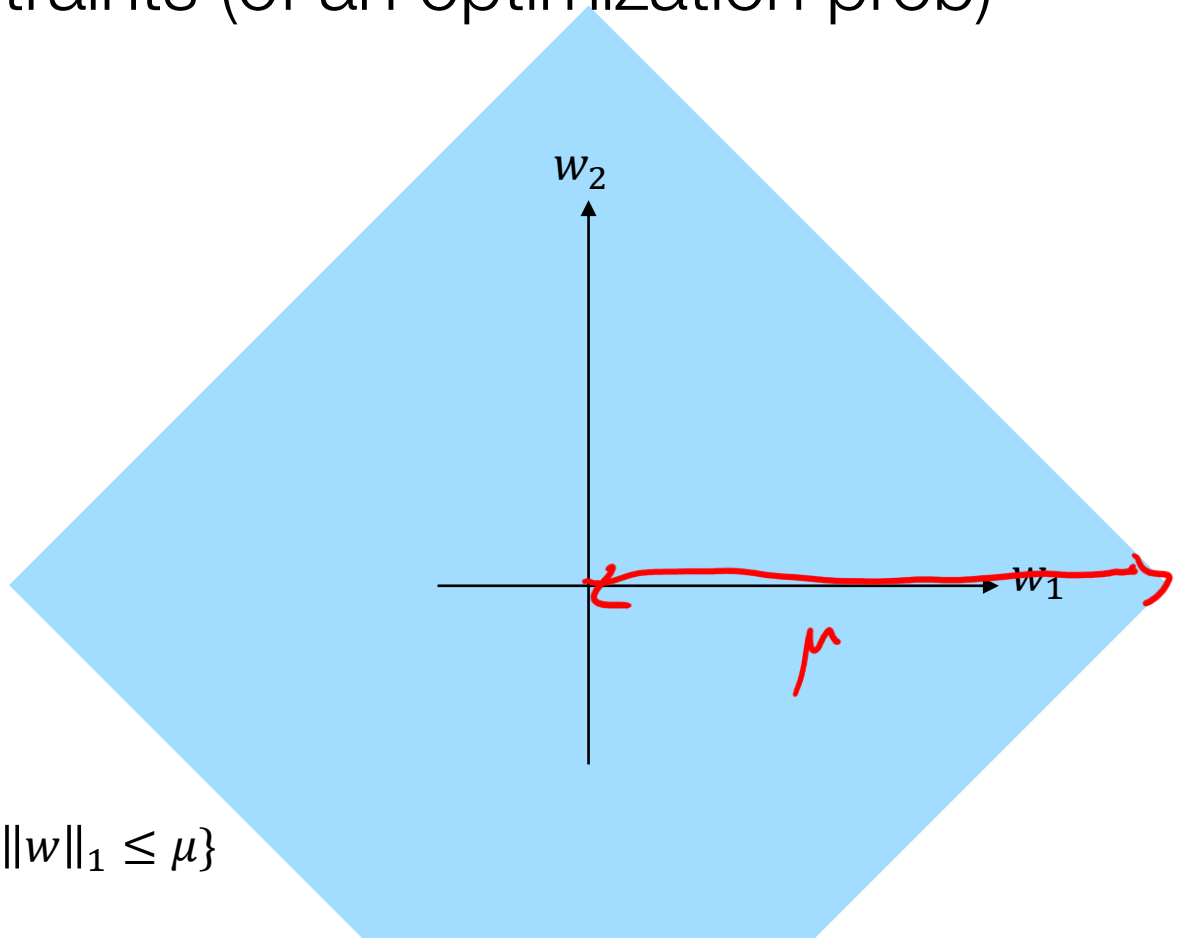
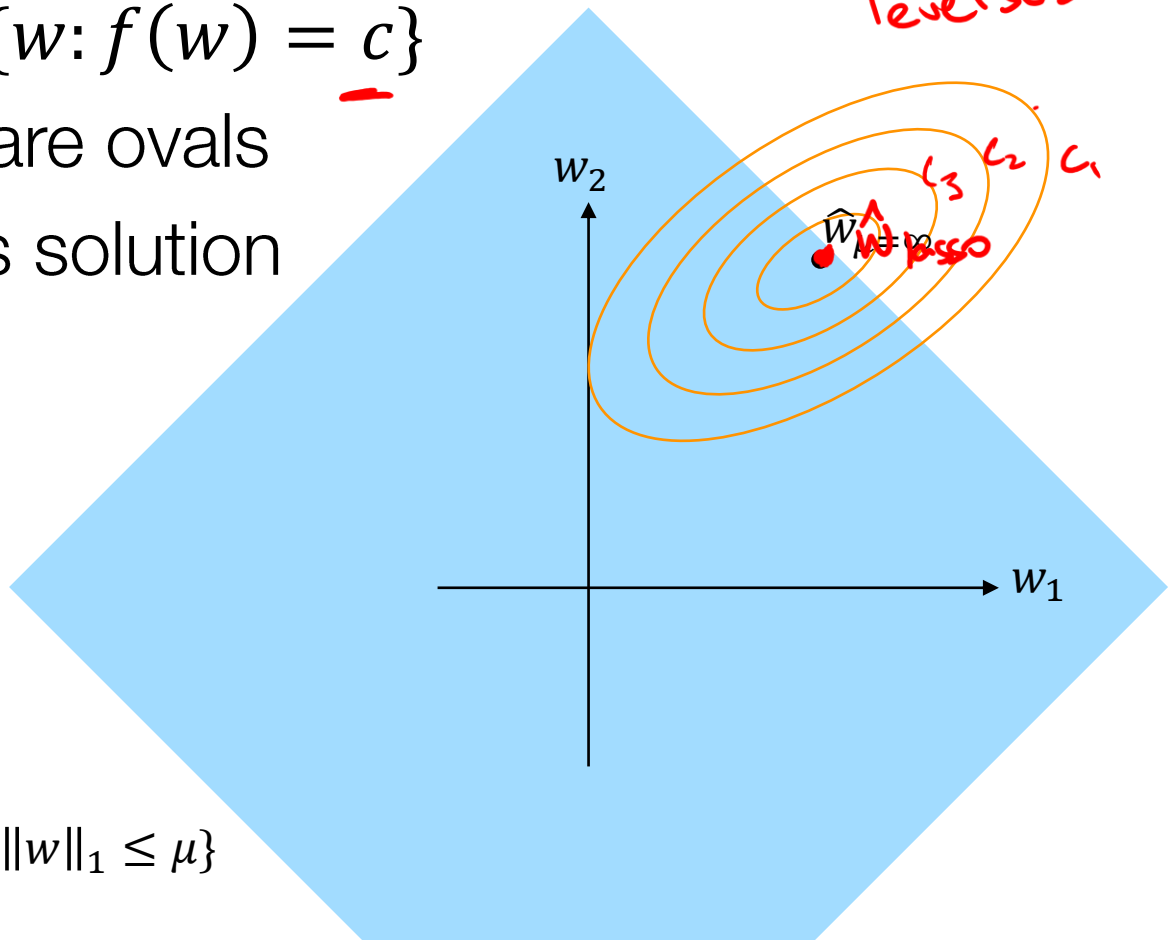


Feasible set $\{w \in \mathbb{R}^2 : \|w\|_1 \le \mu\}$

Level sets

$$\hat{w}_{\text{lasso}} = \underset{w}{\operatorname{argmin}} \sum_i (y_i - x_i^\top w)^2 \quad \text{subject to} \quad \|w\|_1 \leq \mu$$

- Level set $L_c(f)$ of a function f is $\{w: f(w) = c\}$
- Level sets of quadratic functions are ovals
- Center of oval is the least squares solution

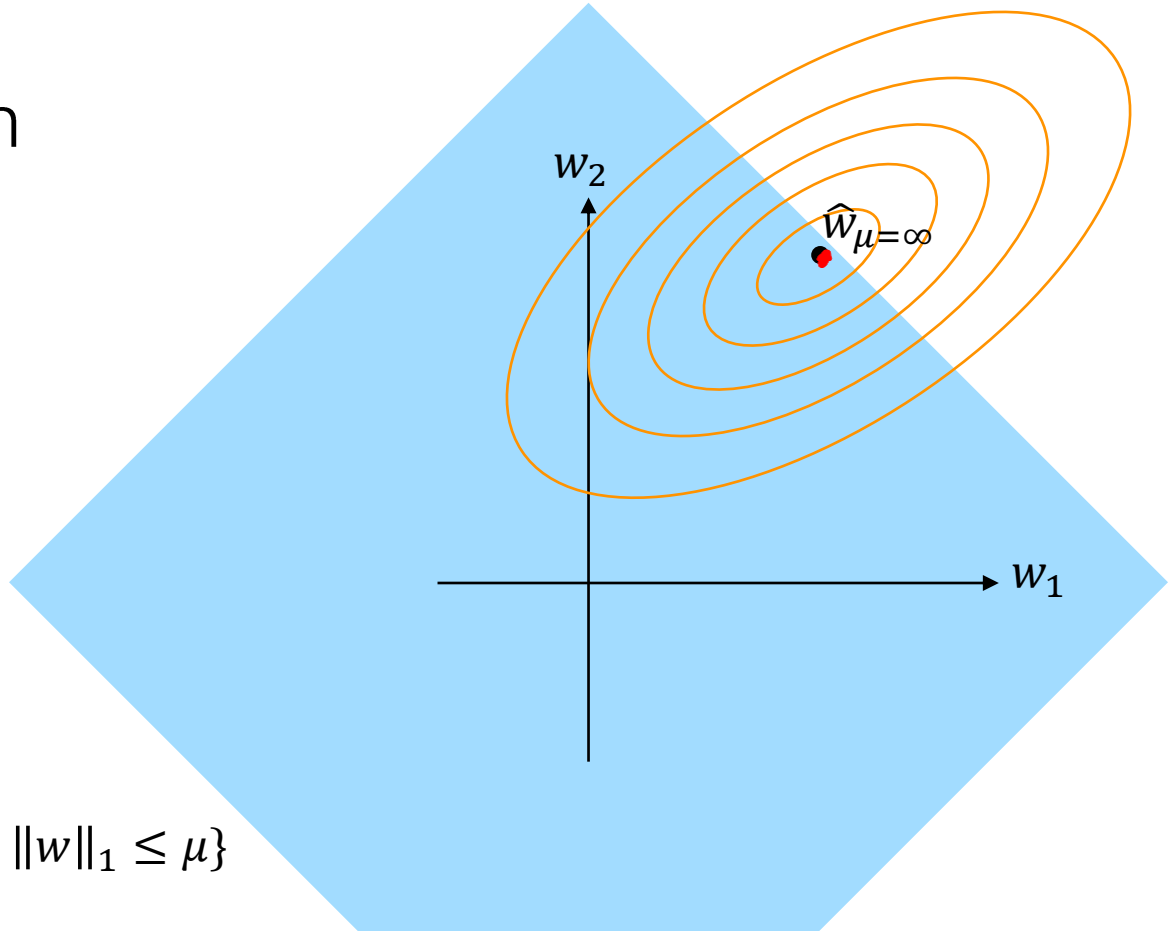


Feasible set $\{w \in \mathbb{R}^2: \|w\|_1 \leq \mu\}$

Why does Lasso give sparse solutions?

$$\hat{w}_{\text{lasso}} = \underset{w}{\operatorname{argmin}} \sum_i \left(y_i - x_i^\top w\right)^2 \quad \text{subject to} \quad \|w\|_1 \leq \mu$$

- For large μ, optimal solution doesn't change



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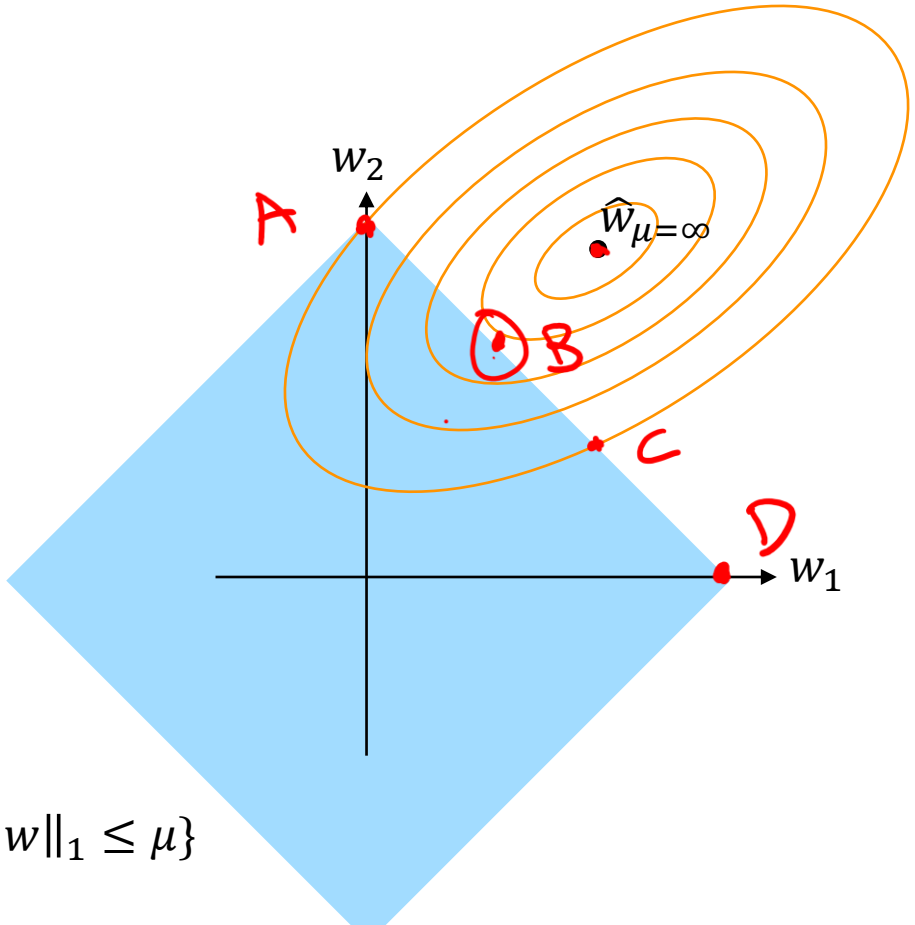
- As μ decreases, feasible set shrinks
- Equivalent to increasing regularization strength λ



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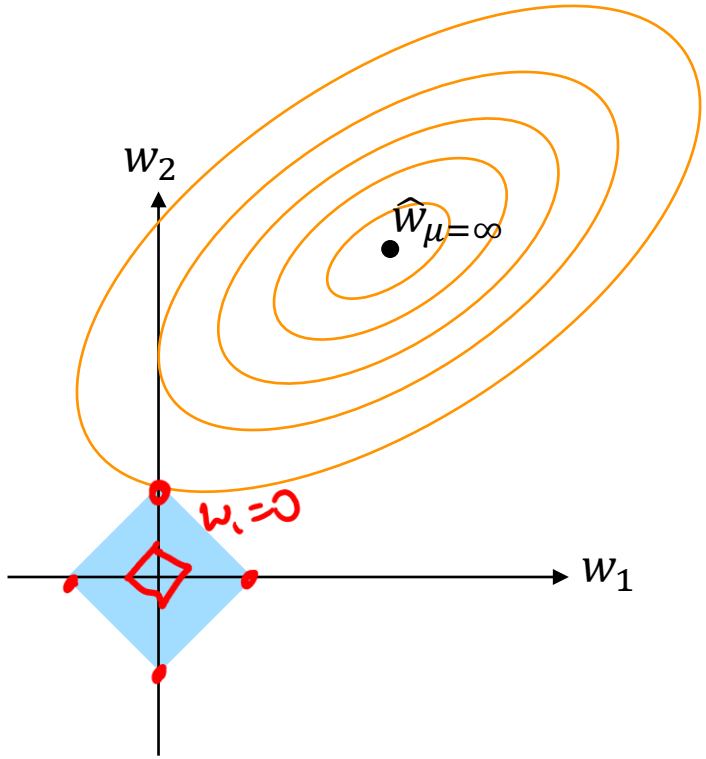
- For small enough μ, optimal solution becomes sparse!
- This is because ℓ_1 ball is pointy (sharp edges aligned with axes)



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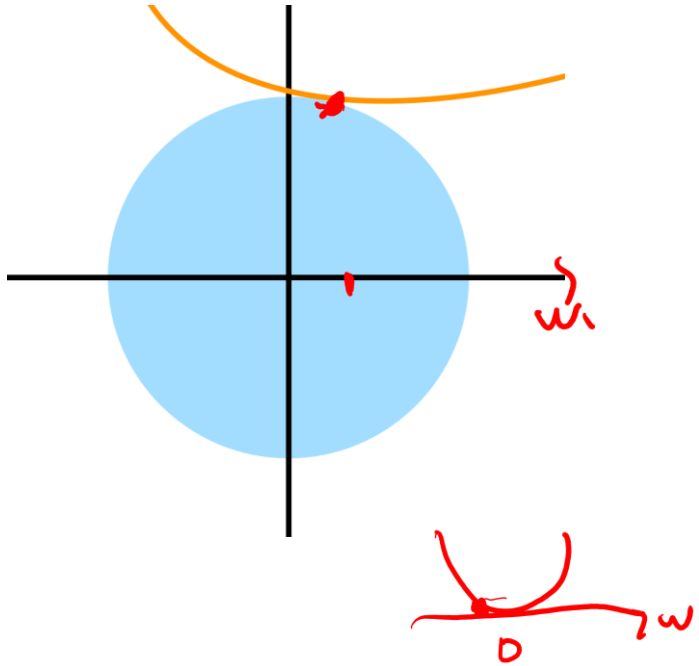
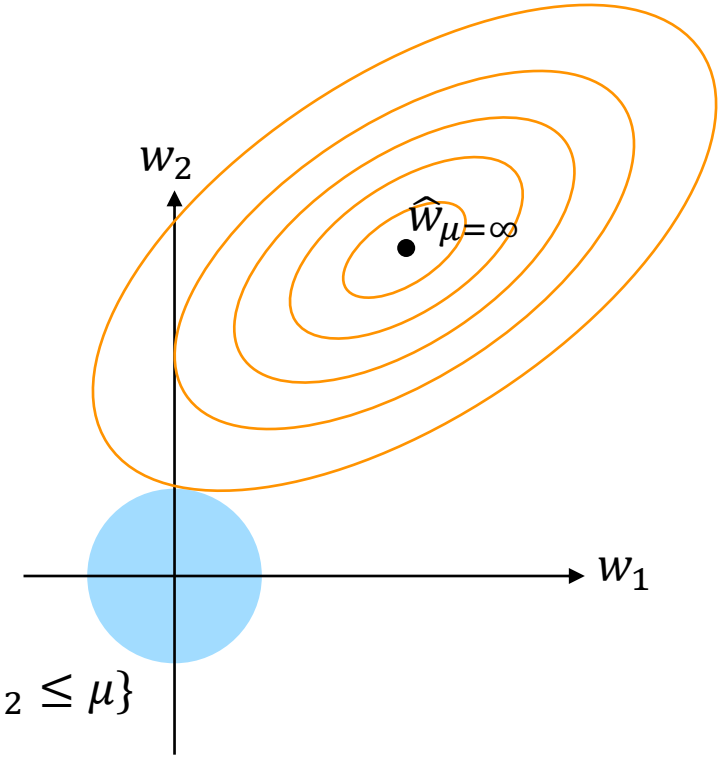
ℓ_2 ball instead finds dense solutions:



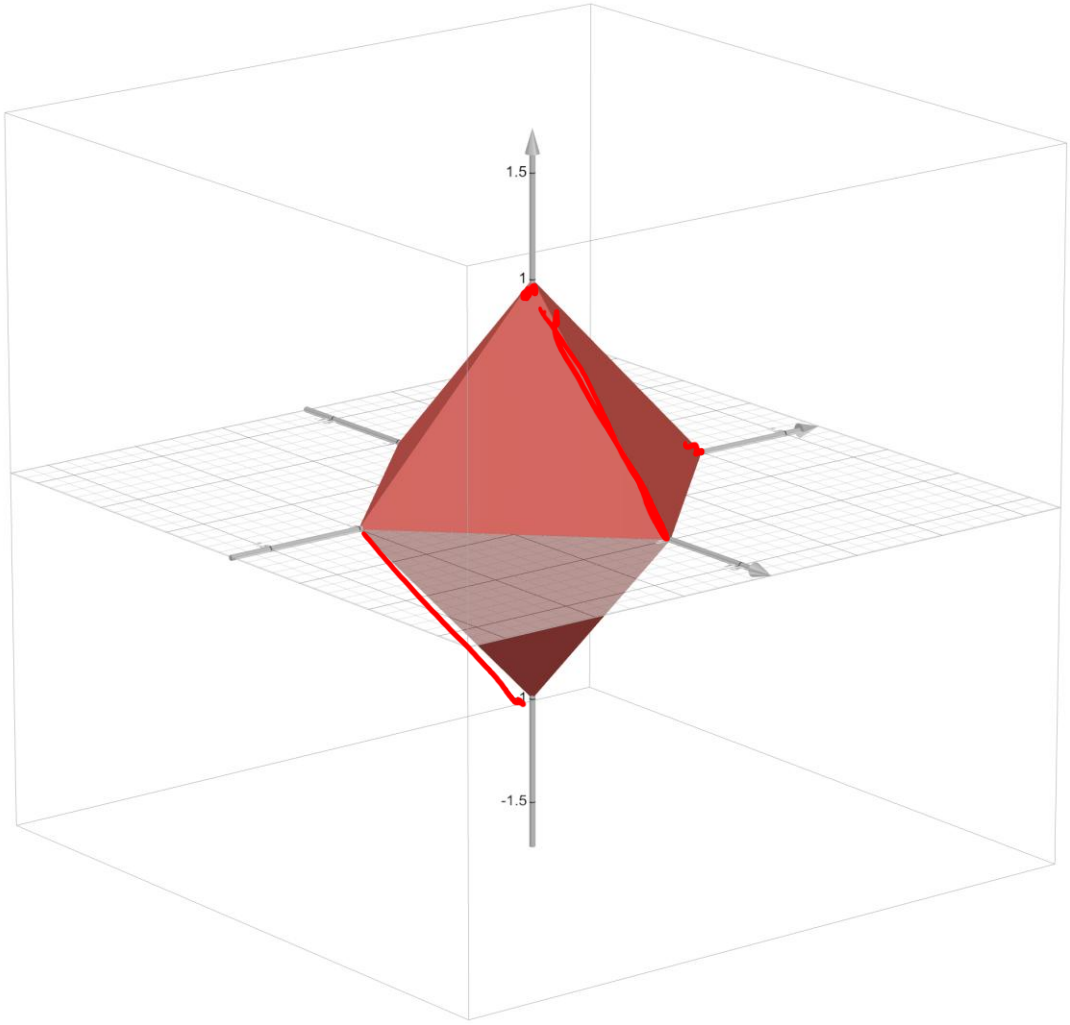


Feasible set $\{w \in \mathbb{R}^2 : \|w\|_2 \le \mu\}$

ℓ_1 ball in 3 dimensions

- Corners: 1-sparse
- Edges: 2-sparse

In higher dimensions, ℓ_1 ball is even “pointier”



Summary: Lasso regression (aka ℓ_1 regularization)

We can efficiently find sparse regression solutions by solving

$$\hat{w}_{\text{lasso}} = \underset{w}{\text{argmin}} \sum_i \left(y_i - x_i^\top w\right)^2 + \lambda \|w\|_1$$

It is equivalent to

$$\hat{w}_{\text{lasso}} = \underset{w}{\text{argmin}} \sum_i \left(y_i - x_i^\top w\right)^2 \quad \text{subject to} \quad \|w\|_1 \leq \mu$$

Next: How do we actually solve it?

Gradient Descent

CSE 446/546

Sewoong Oh & Pang Wei Koh

Why gradient descent?

$f(w) = \|y - Xw\|_2^2$

$\nabla f(w) = 2X^T(y - Xw) = 0$

$\Rightarrow \hat{w} = (X^TX)^{-1}X^Ty$

- Standard ML paradigm: Define loss, then optimize

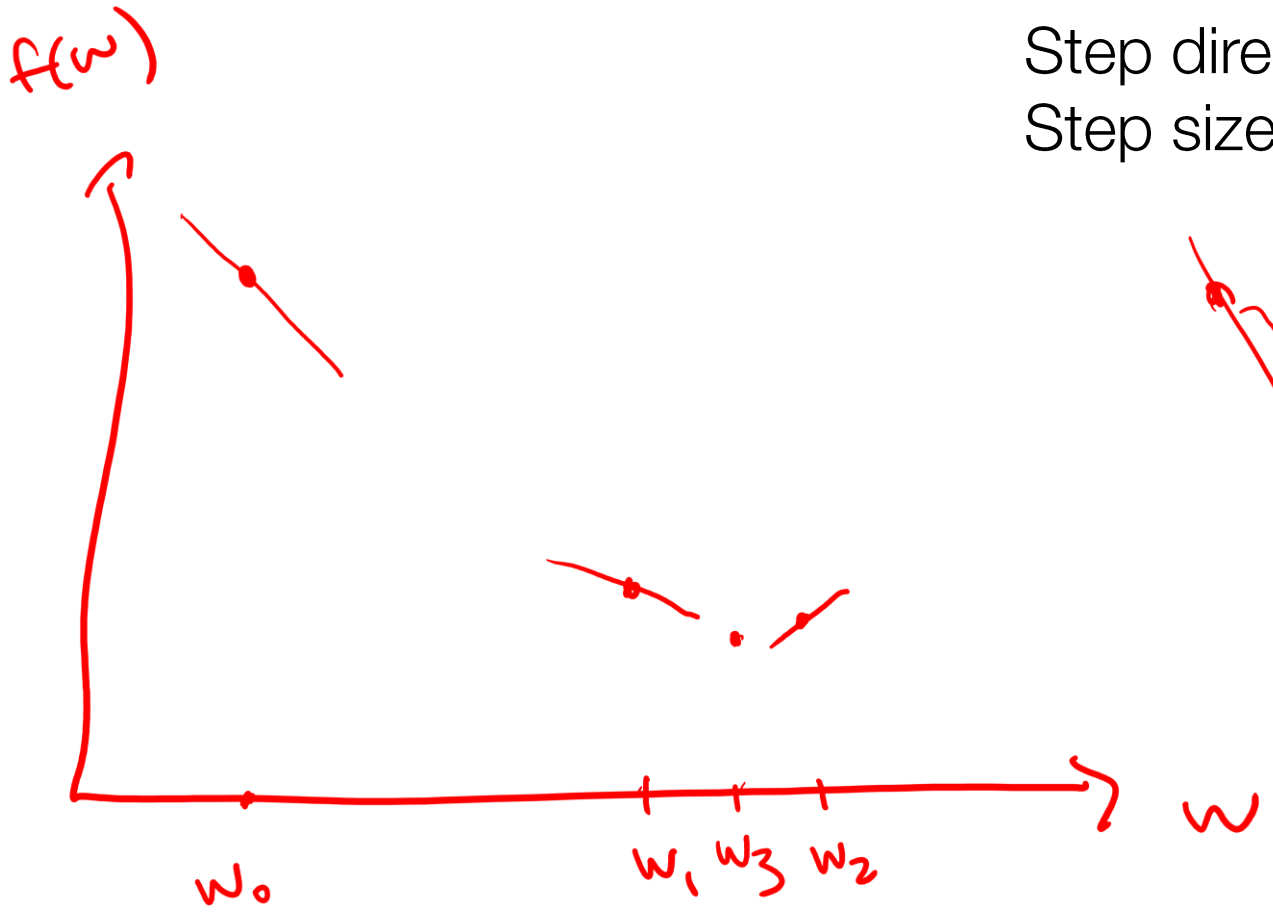
$$\widehat{w}_{LS} = \arg\min_w ||\mathbf{y} - \mathbf{X}w||_2^2 + \lambda\|w\|_1$$

$L(w)$

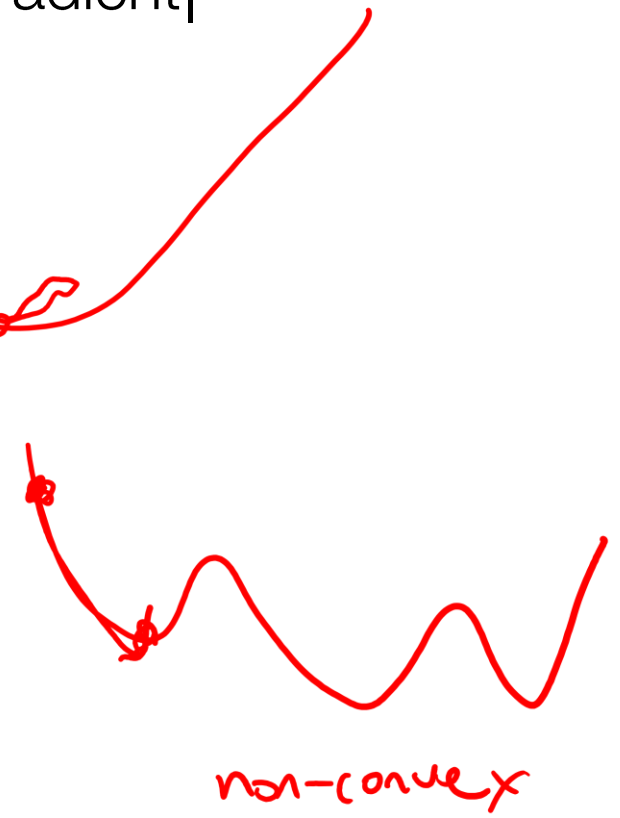
$= (X^TX)^{-1}X^Ty$

- But, no closed-form solutions for most losses we use in practice.
- Key idea: Iterative methods
- Used everywhere!

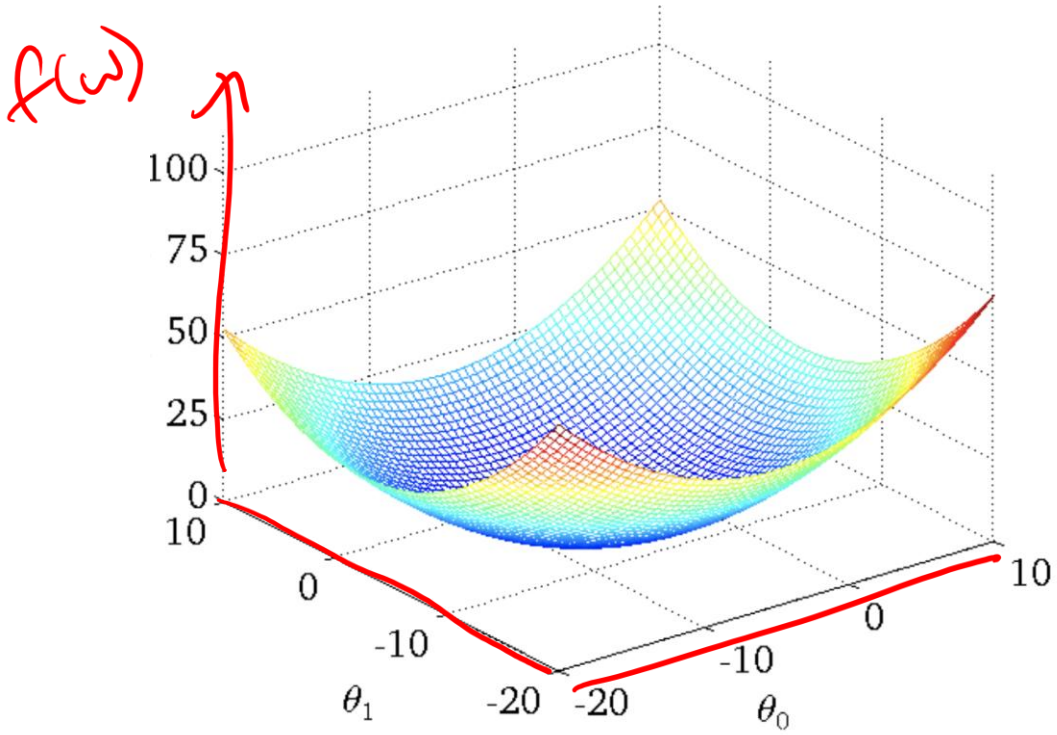
Gradient descent in one dimension

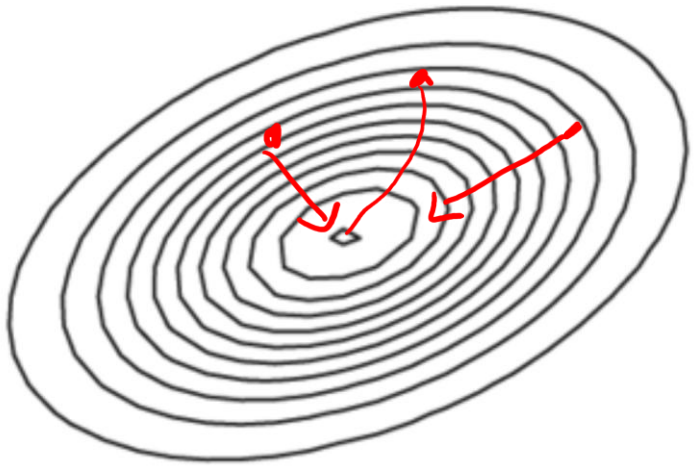


Step direction: −gradient
Step size: ∝ |gradient|



Gradient descent in multiple dimensions





Lecture plan

- Gradient descent algorithm + examples

- Theoretical analysis
  - When does it work?
  - How quickly does it converge?
  - How do we choose a step size?
  - Key idea: Convexity

- Not tested on proof details, but concepts are important & practical

Algorithm: Gradient descent

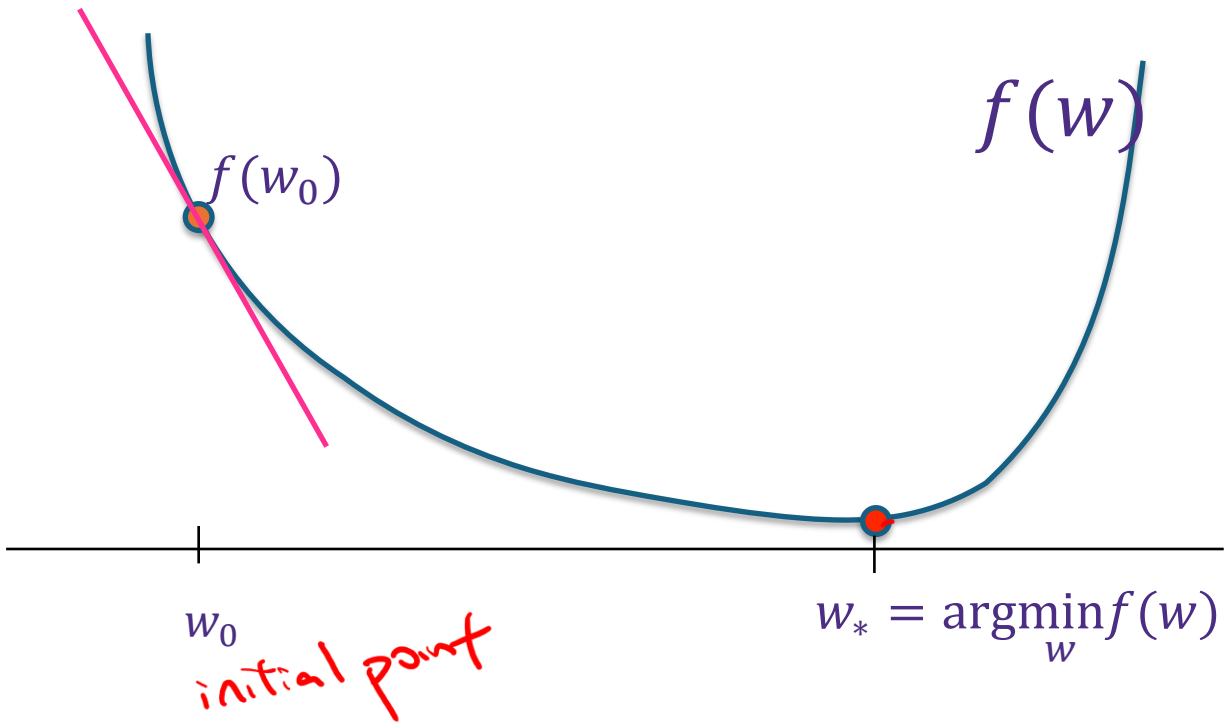
Algorithm

For t=0,1,2,3, …

$$w_{t+1} = w_t - \eta \frac{df(w)}{dw}\Big|_{w=w_t}$$

Hyperparameters:

- Initial point w_0
- Step size η



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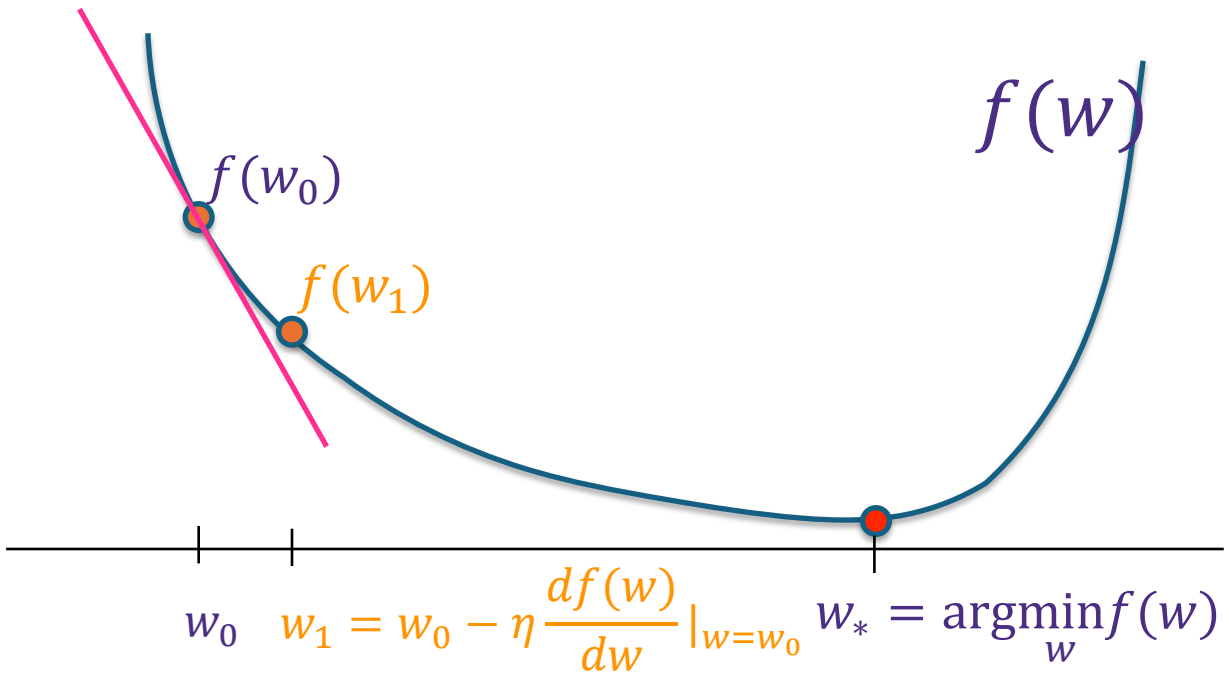

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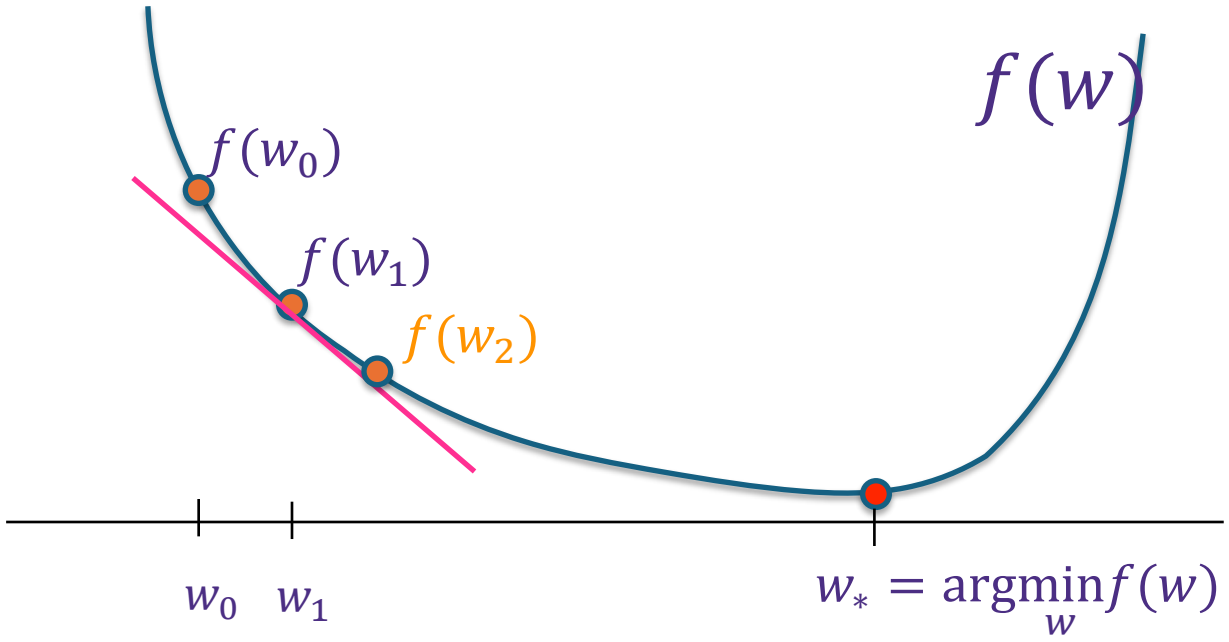

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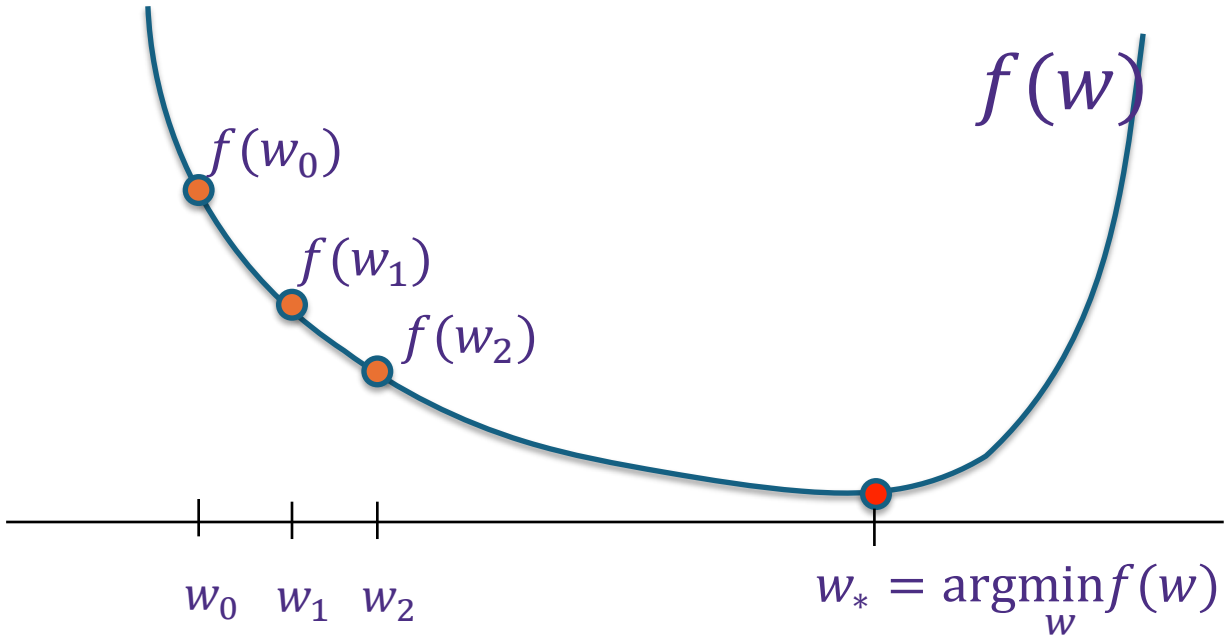
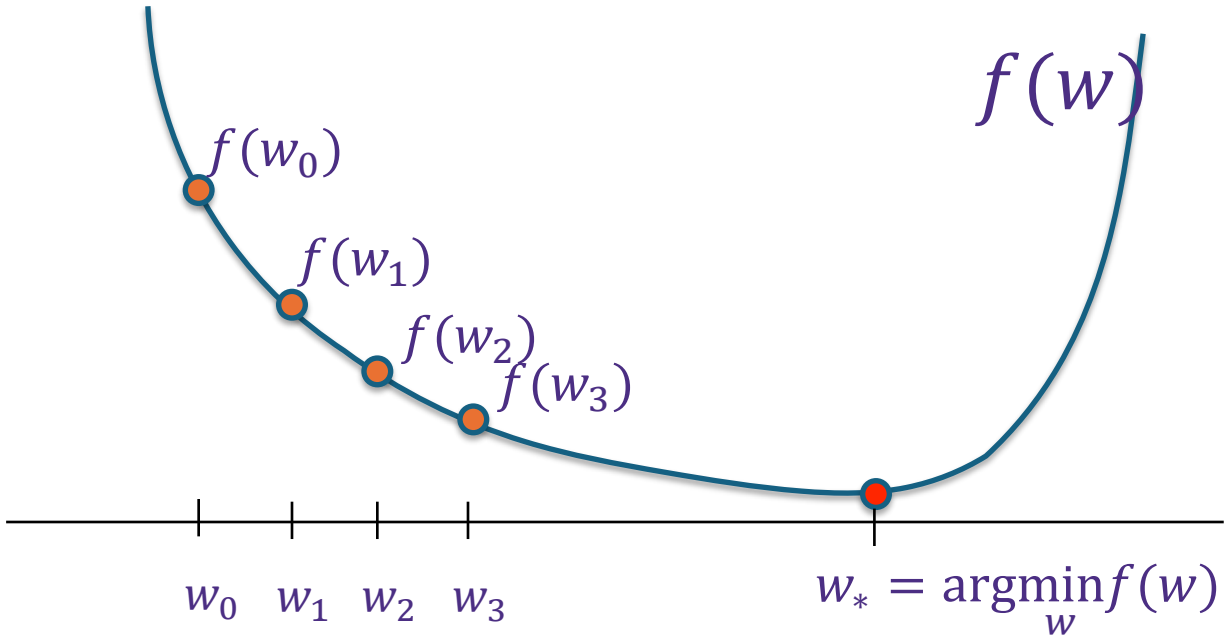


Algorithm: Gradient descent

Algorithm
For t=0,1,2,3, …

$$w_{t+1} = w_t - \eta \frac{df(w)}{dw}|_{w=w_t}$$

Hyperparameters:
- Initial point w_0
- Step size η



Algorithm: Gradient descent

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For t=0,1,2,3, …

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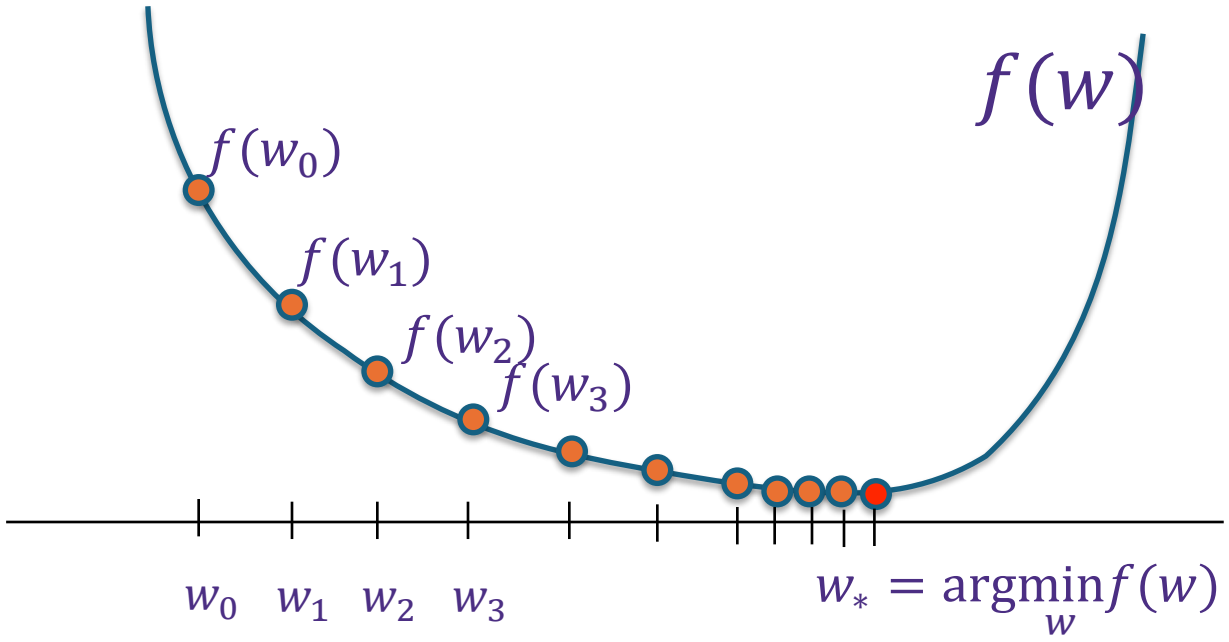
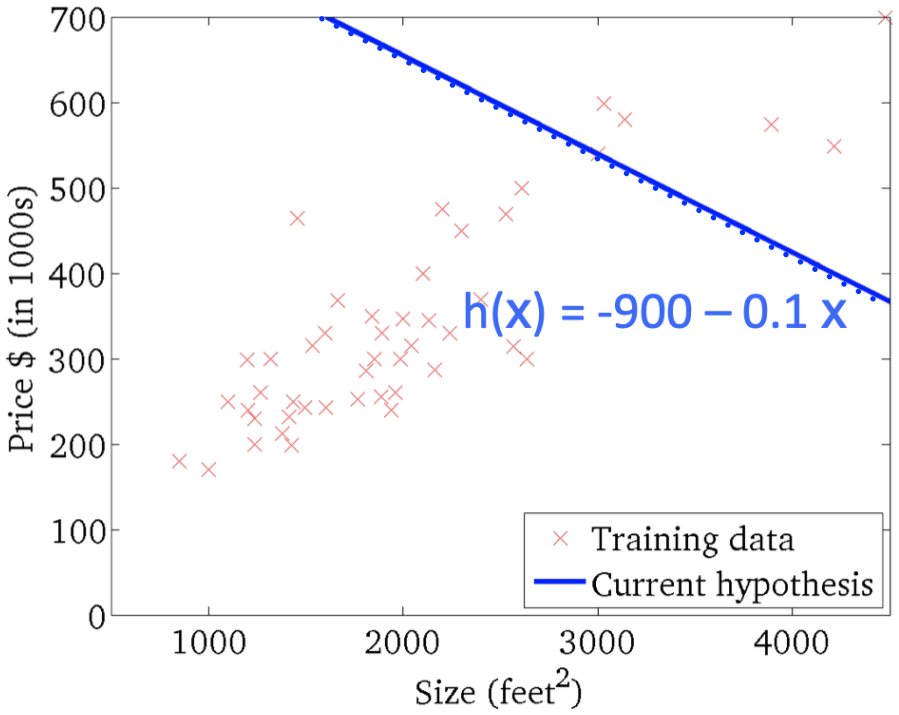


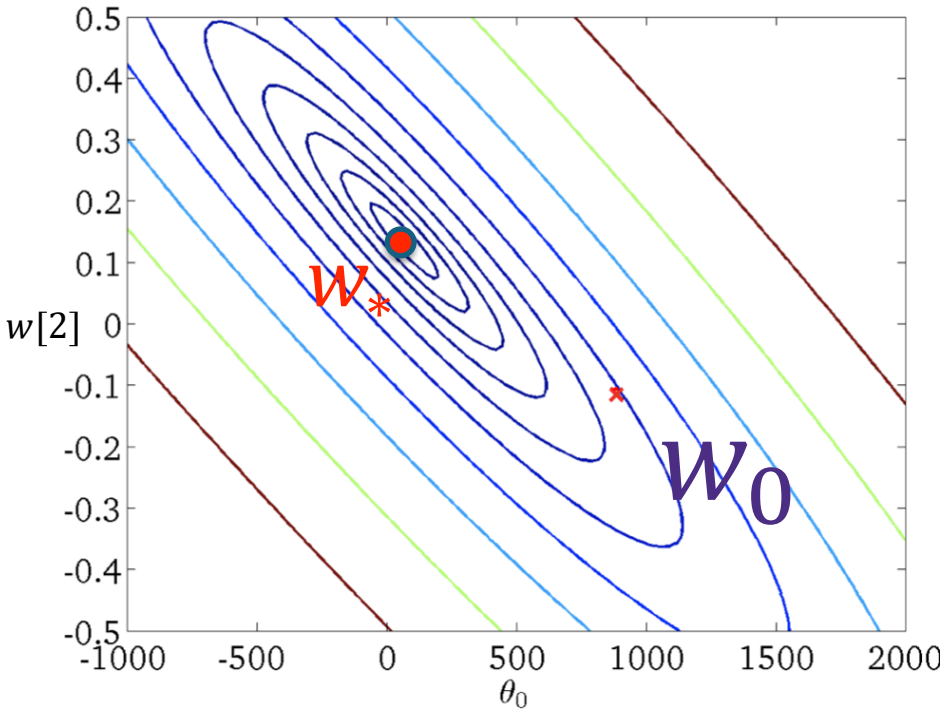
Note that as $t \to \infty$ we have $\frac{df(w)}{dw}|_{w=w_t} \to 0$

$$\{(x_i, y_i)\}_{i=1}^{n}$$

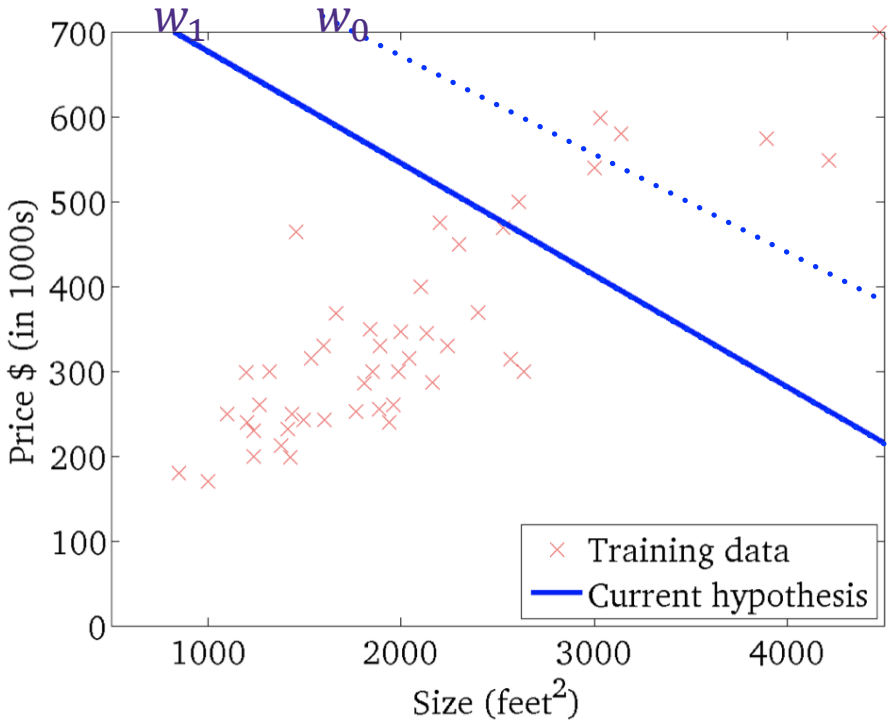


Evolution of the predictor

$$w_{t+1} \leftarrow w_t - \eta \cdot \nabla_w f(w_t)$$



GD dynamics in the parameter space



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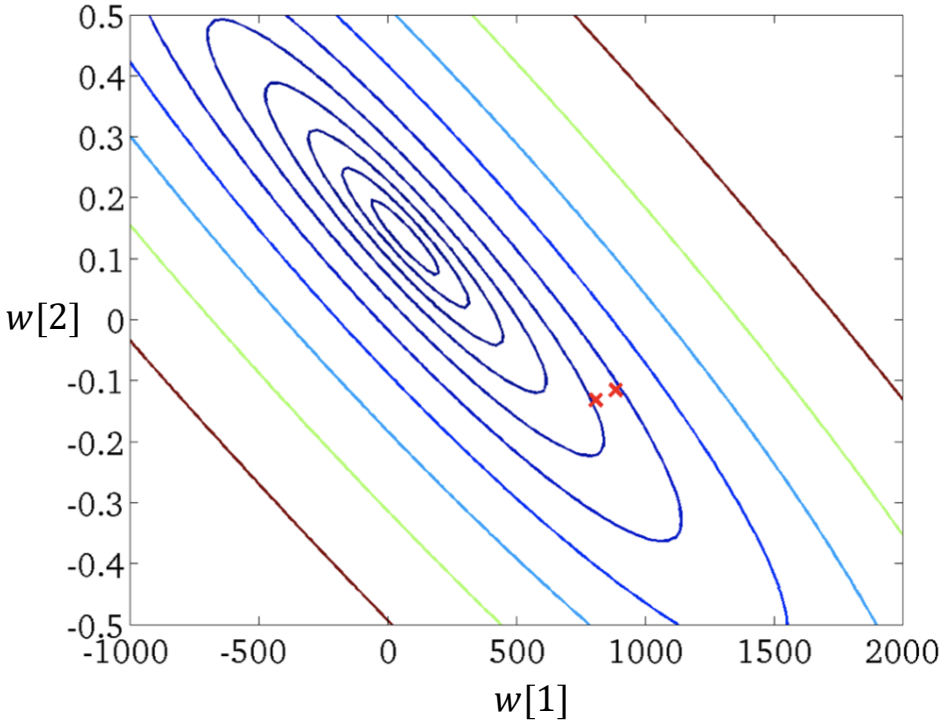
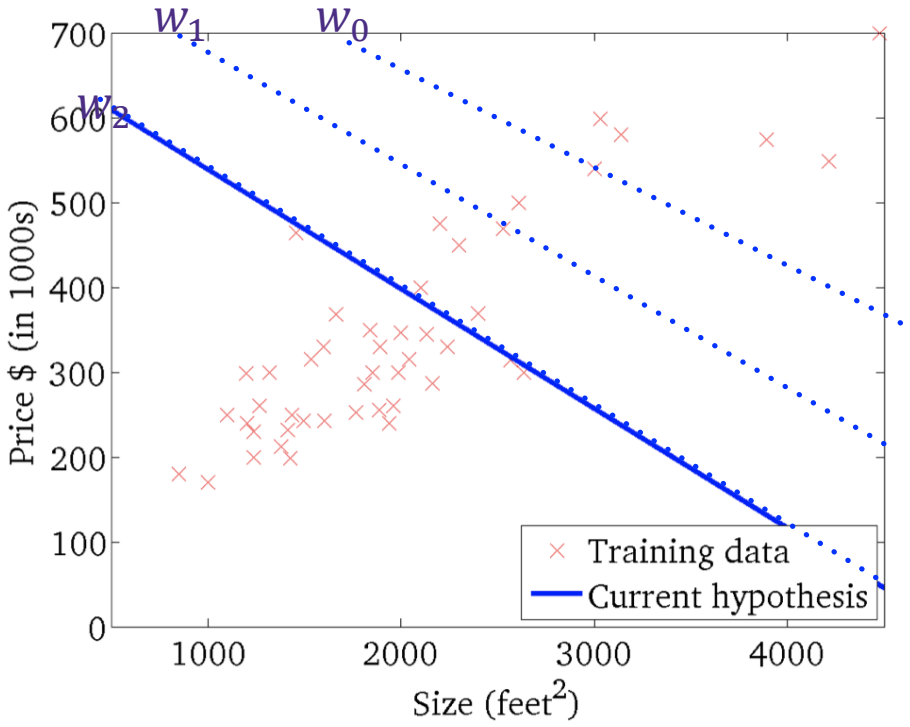
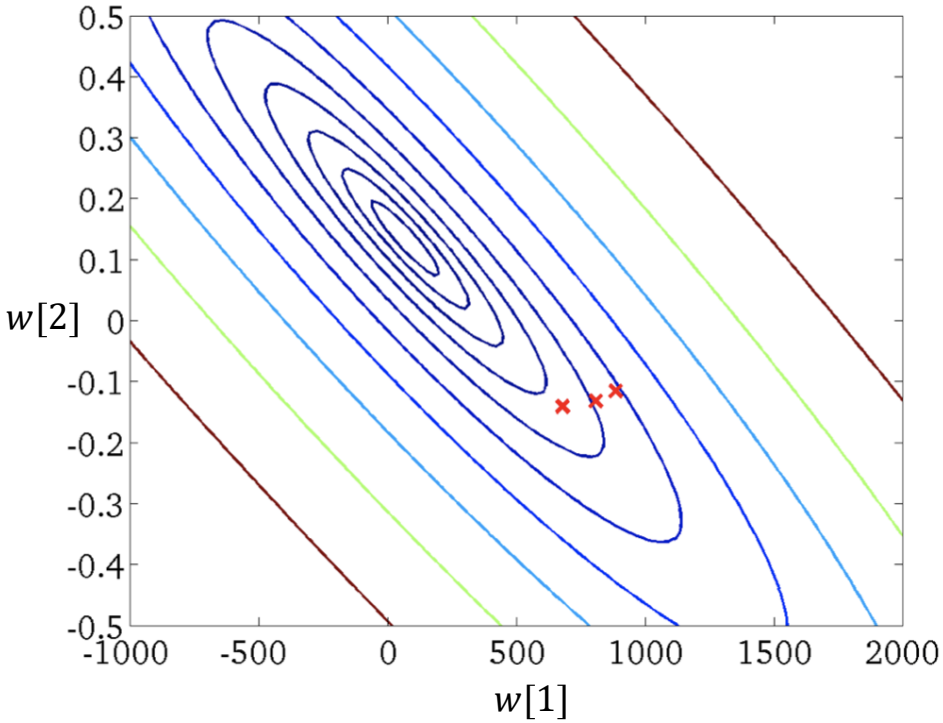


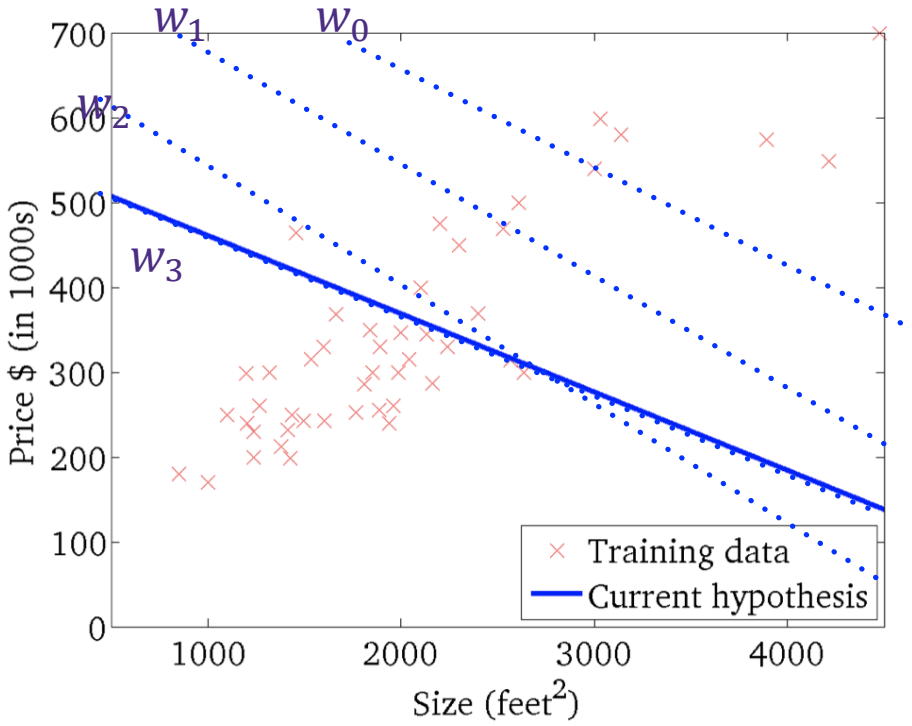
GD dynamics in the parameter space



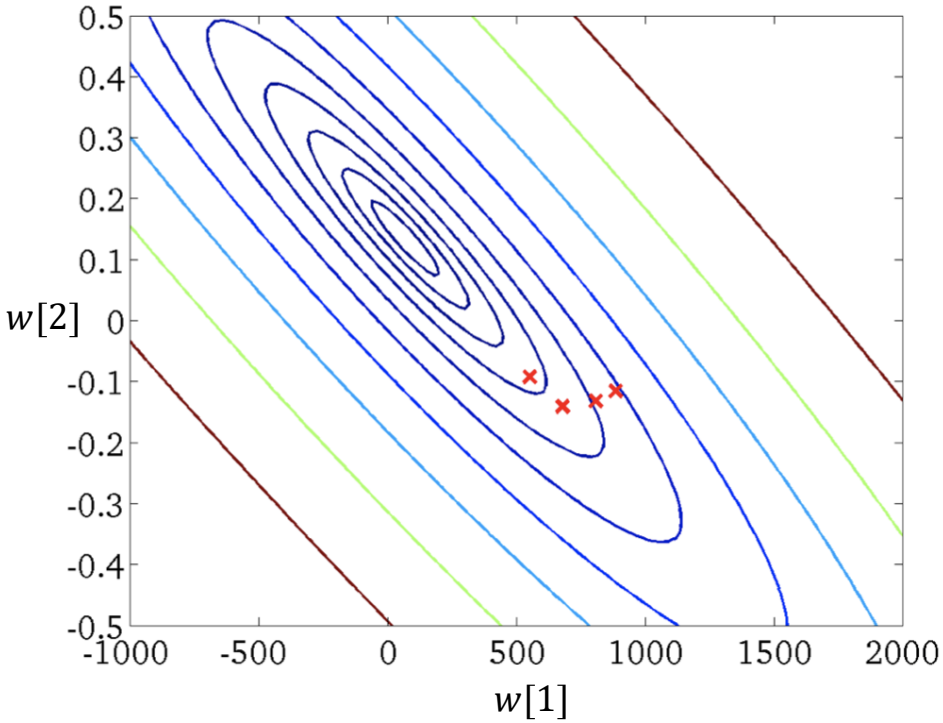
Evolution of the predictor



GD dynamics in the parameter space



Evolution of the predictor



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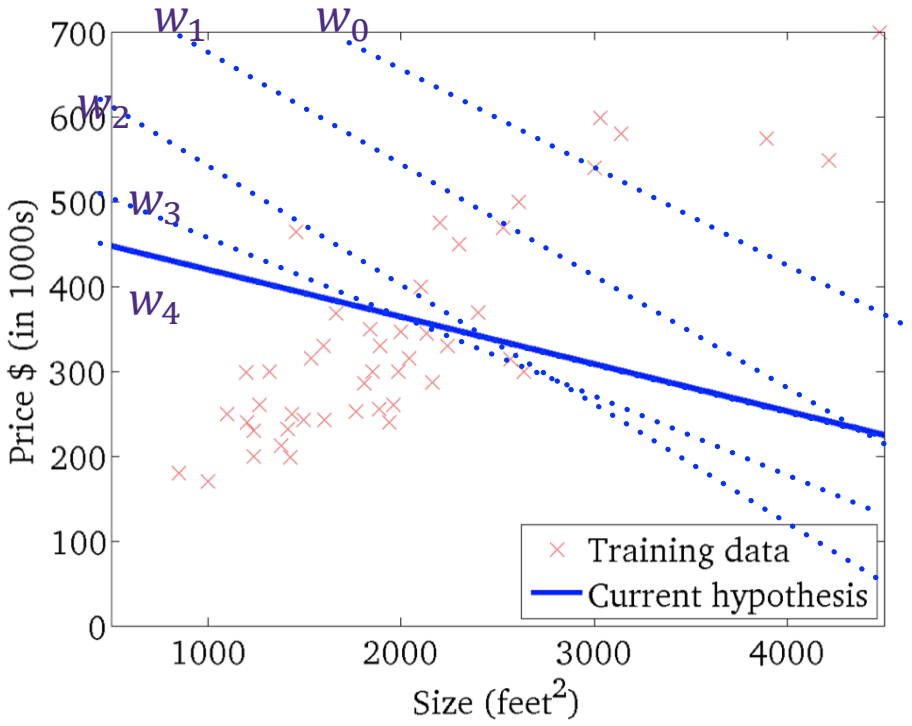

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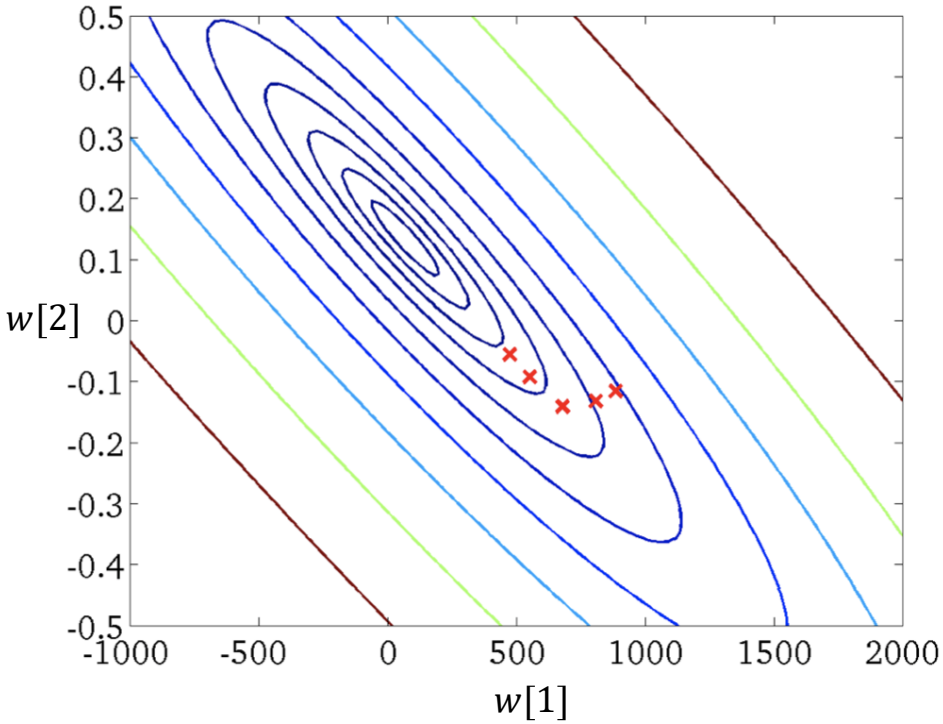
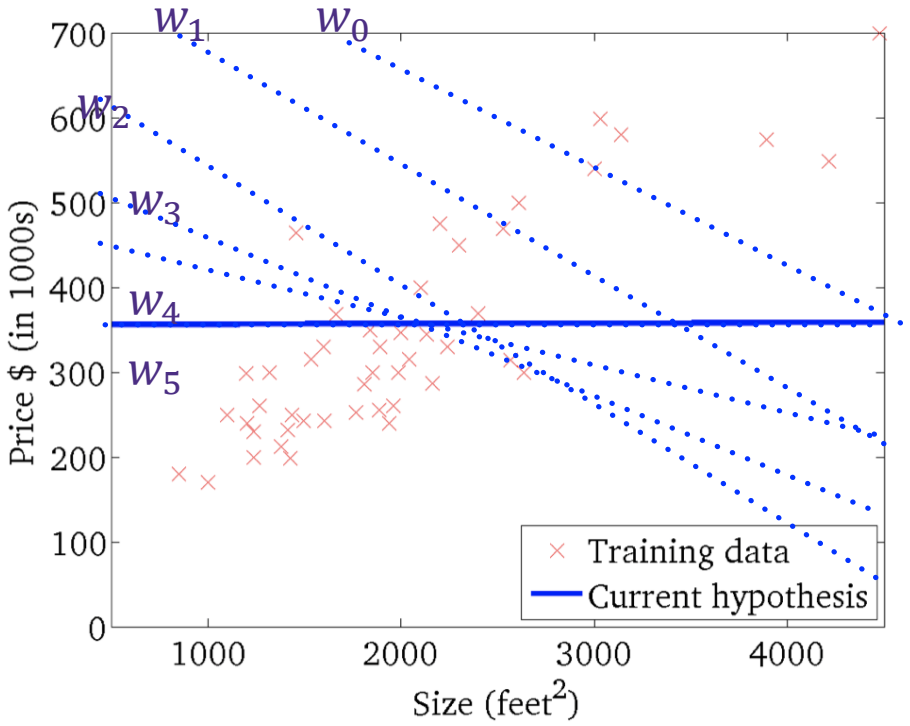


GD dynamics in the parameter space



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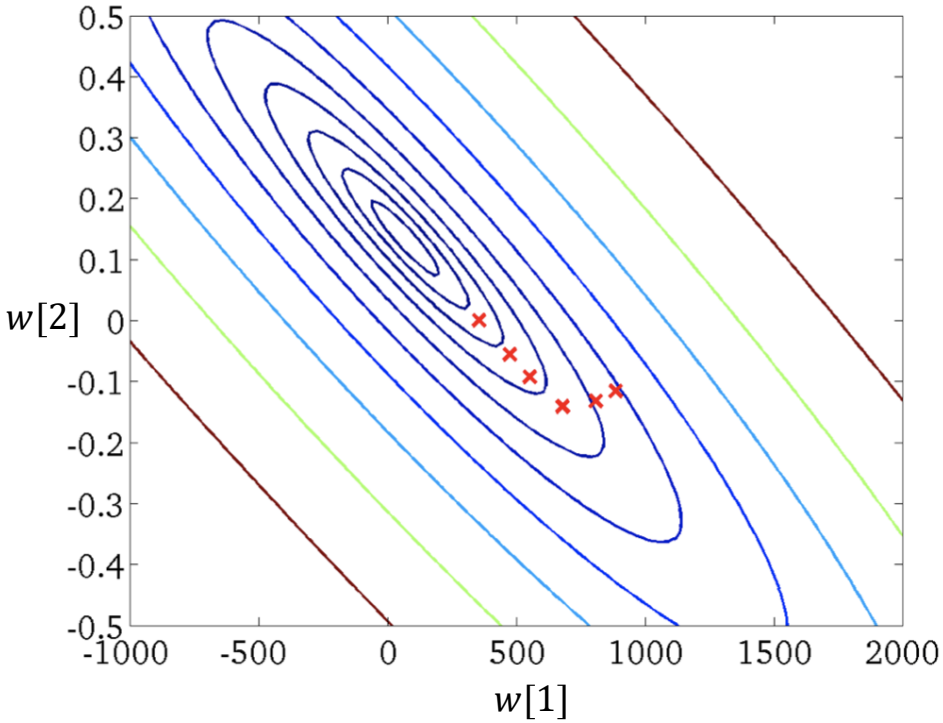
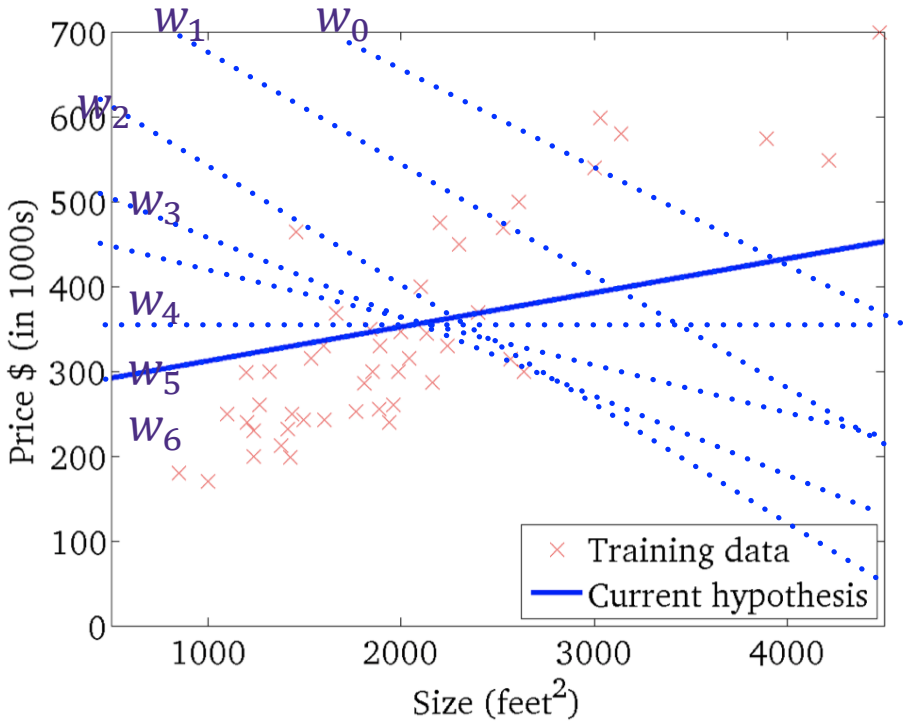


GD dynamics in the parameter space



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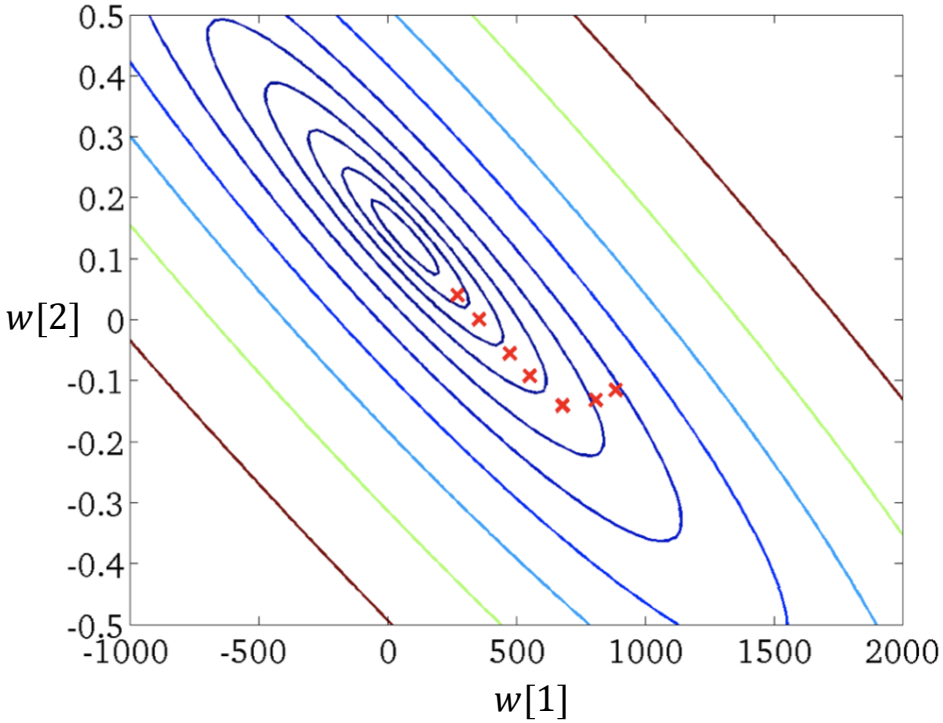

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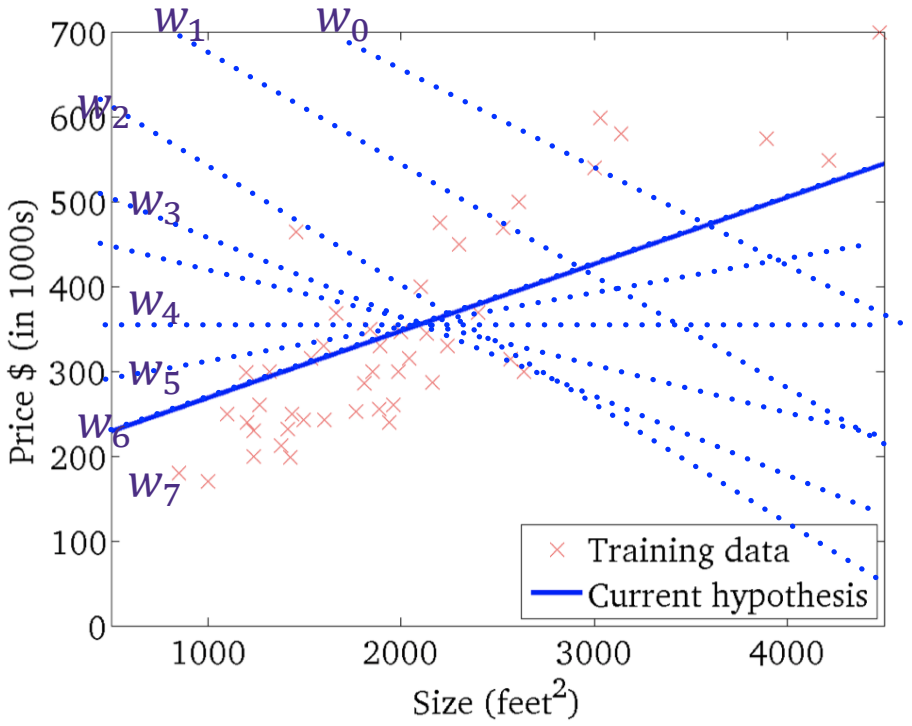

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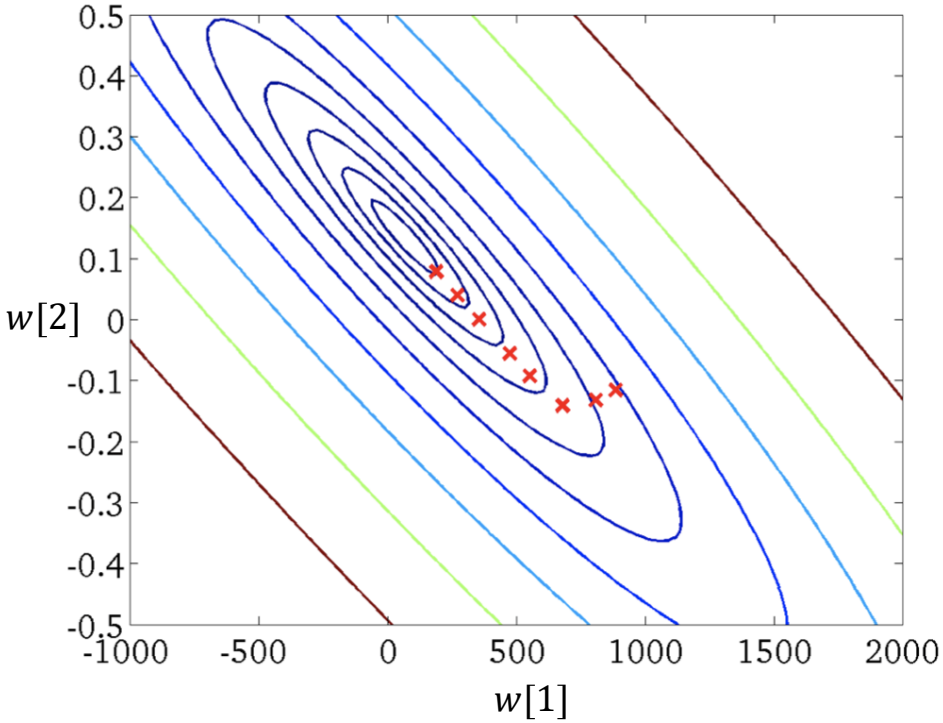
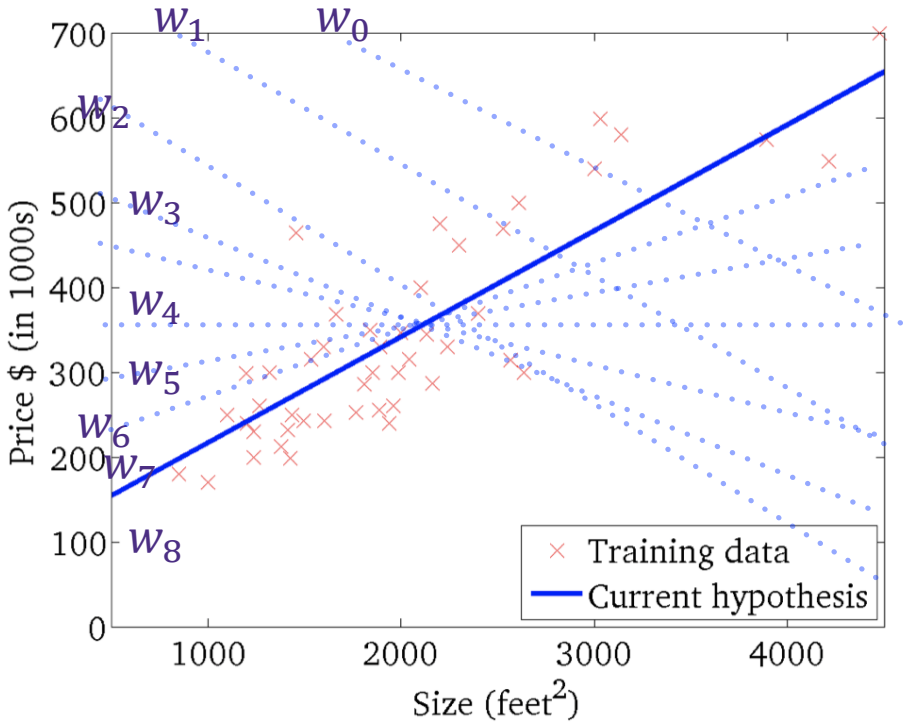
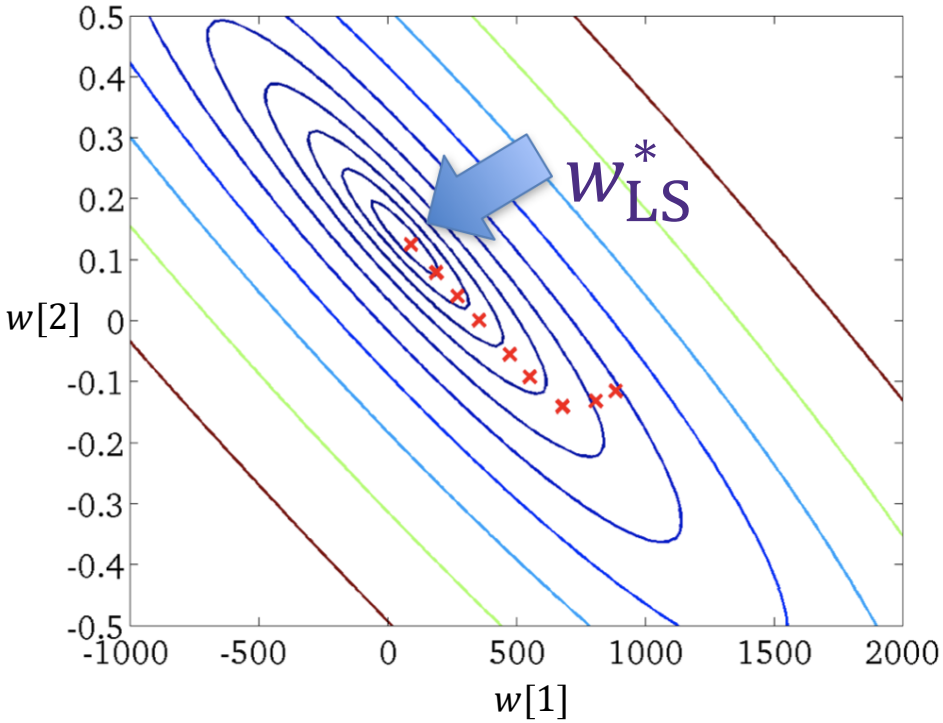


GD dynamics in the parameter space

See website for some gradient descent demo code



Evolution of the predictor



GD dynamics in the parameter space

Warmup: Quadratic functions

$$\hat{w} = \underset{w}{\operatorname{argmin}} \; \underbrace{aw^2 + bw + c}_{f(w)}$$

$$\frac{df}{dw} = 2aw + b$$

$$w_{t+1} := w_t - \eta \frac{df}{dw}\Big|_{w=w_t}$$

$$= w_t - \eta(2aw_t + b)$$

Example: Linear regression

$$\hat{w} = \underset{w}{\operatorname{argmin}} \underbrace{\frac{1}{2}\sum_i \left(y_i - x_i^\top w\right)^2}_{f(w)}$$

$$\nabla f(w) = -\sum_i (y_i - x_i^\top w)\, x_i$$

$$w_{t+1} = w_t - \eta \nabla f(w_t)$$

$$= w_t + \eta \sum_i (y_i - x_i^\top w_t)\, x_i$$

Example: Lasso

$$\hat{w} = \underset{w}{\operatorname{argmin}} \frac{1}{2} \|y - Xw\|_2^2 + \lambda \|w\|_1$$

How do you choose a step size?

- If η too small, converges very, very slowly.
- If η too big, does not converge!
- In practice: guess and check

Lecture plan

- Gradient descent algorithm + examples

- Theoretical analysis ← we are here
  - When does it work?
  - How quickly does it converge?
  - How do we choose a step size?
  - Key idea: Convexity

- Not tested on proof details, but concepts are important & practical

Convexity

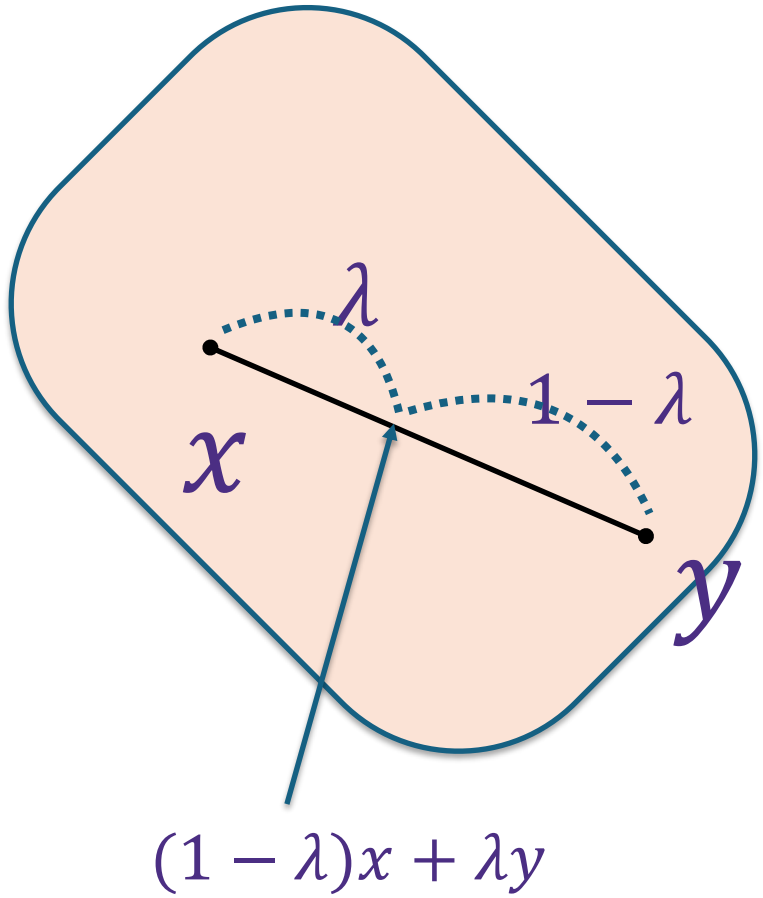
- Optimization problems are hard to solve in general
- The exception: convex optimization
  - Objective is a convex function
  - Constraints are convex sets

- Special class of problems that can be solved efficiently
- Surprisingly common in practice

What is a convex set?

What is a convex set?

A set $K \subset \mathbb{R}^d$ is convex if $(1-\lambda)x + \lambda y \in K$ for all $x, y \in K$ and $\lambda \in [0,1]$



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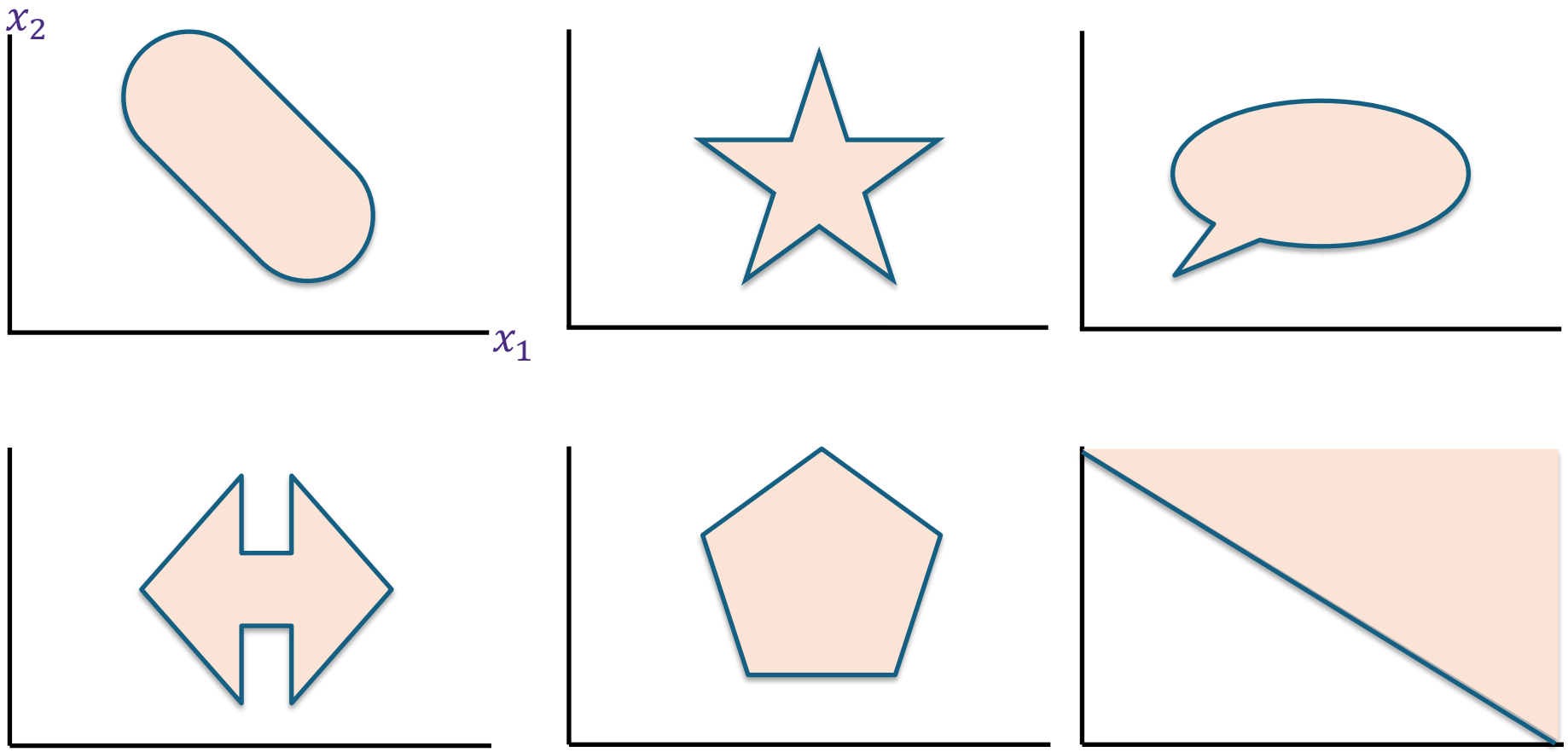
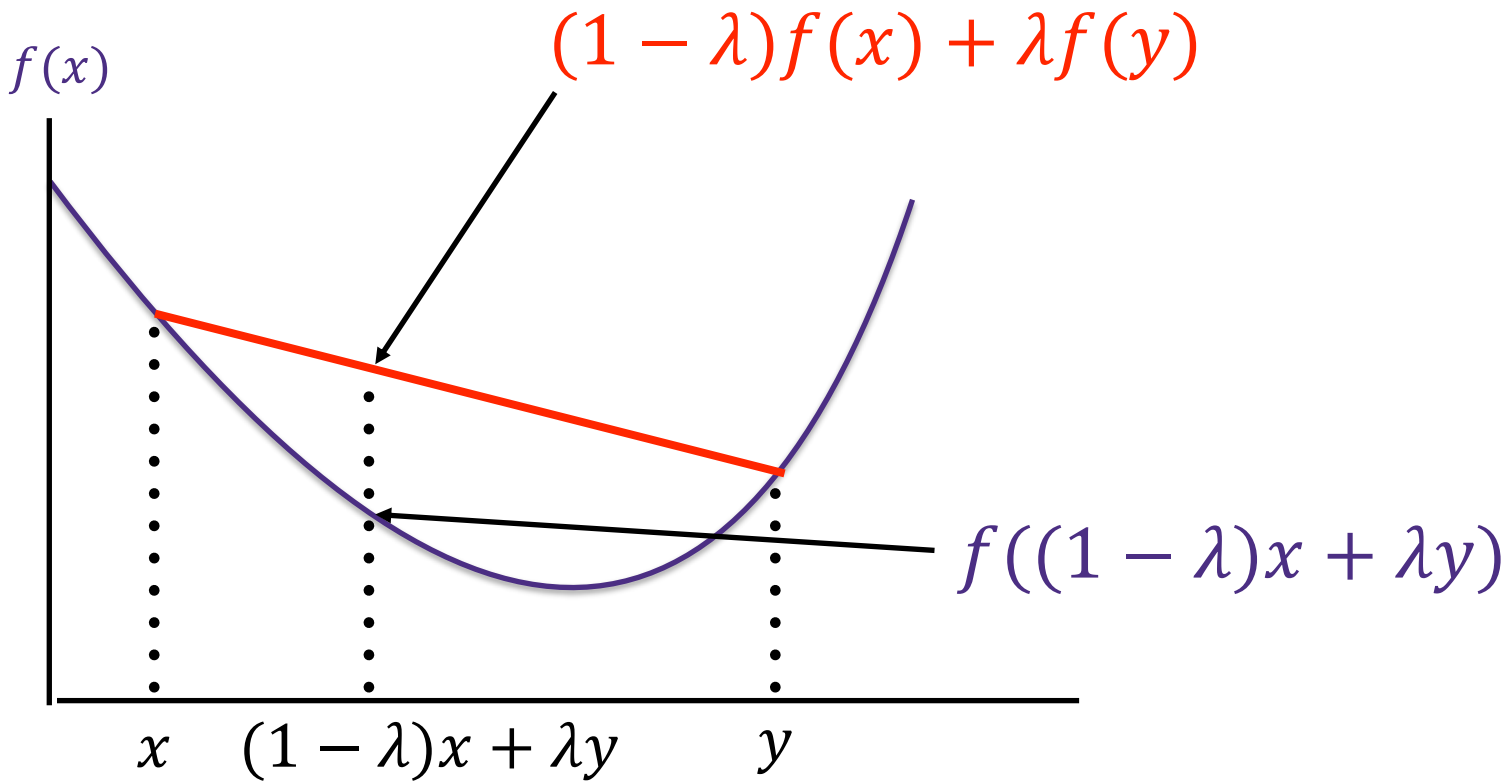


What is a convex function?

What is a convex function?

A function $f : \mathbb{R}^d \to \mathbb{R}$ is convex if $f((1-\lambda)x + \lambda y) \leq (1-\lambda)f(x) + \lambda f(y)$ for all $x, y \in \mathbb{R}^d$ and $\lambda \in [0, 1]$



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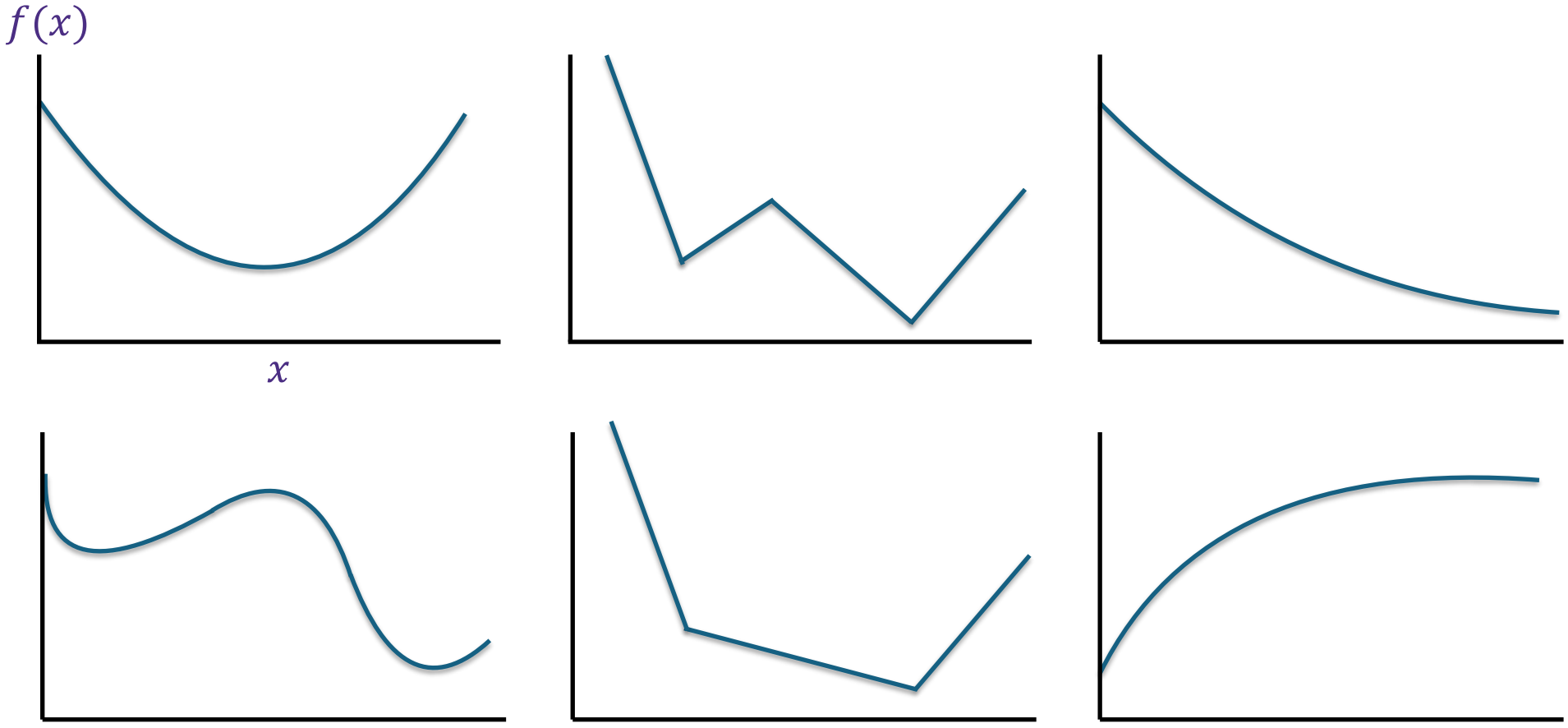

Convex functions and convex sets

Convex functions and convex sets

A set $K \subset \mathbb{R}^d$ is convex if $(1-\lambda)x + \lambda y \in K$ for all $x, y \in K$ and $\lambda \in [0,1]$

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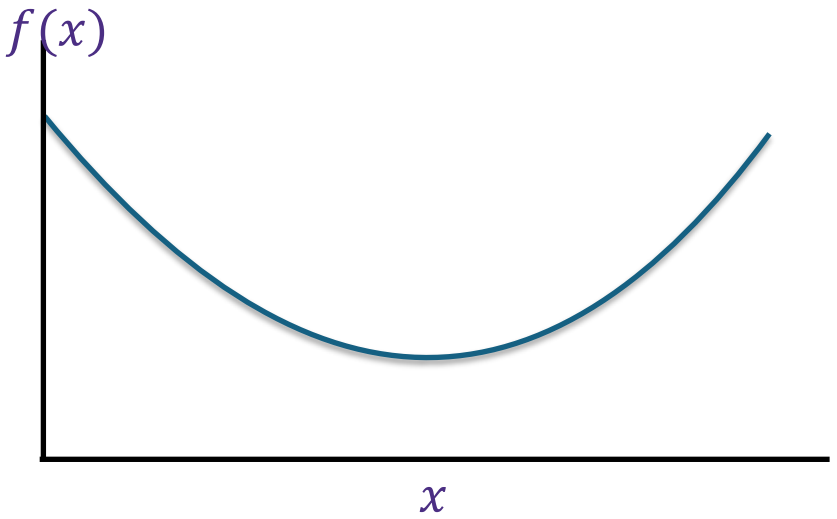
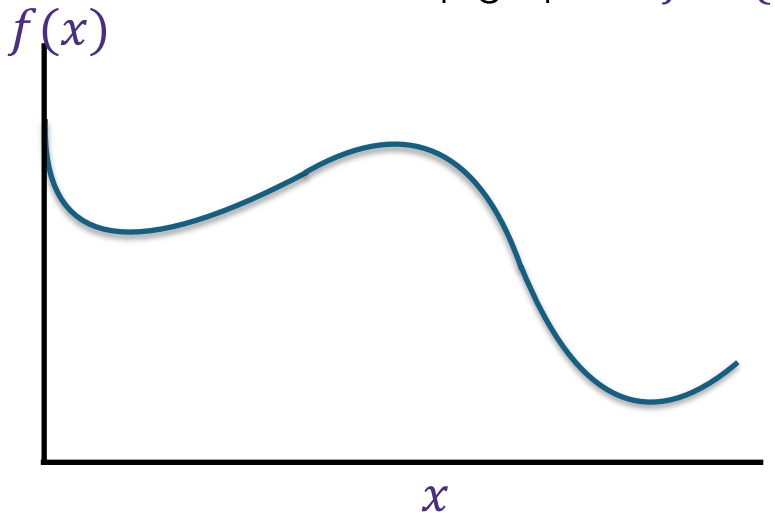
A function $f : \mathbb{R}^d \to \mathbb{R}$ is convex if the set $\{(x,t) \in \mathbb{R}^{d+1} : f(x) \leq t\}$ is convex

Graph of f is $\{(x,t): f(x) = t\}$
Epigraph of f is $\{(x,t): f(x) \leq t\}$



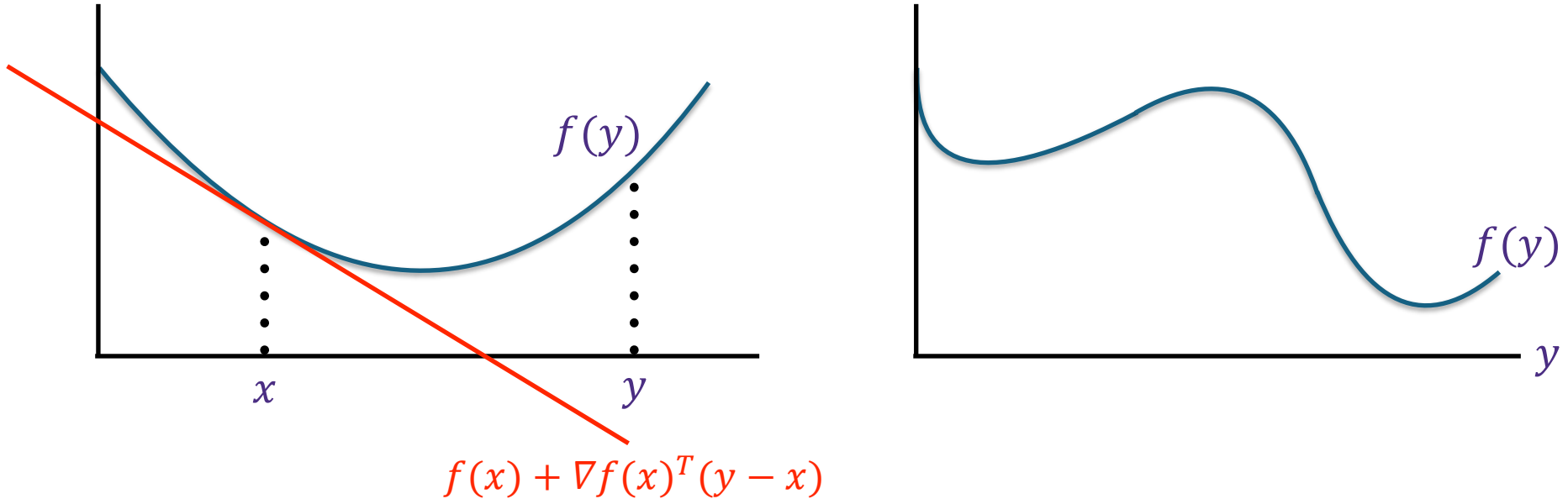


Convexity of differentiable functions

Convexity of differentiable functions

A function $f : \mathbb{R}^d \to \mathbb{R}$ is convex if the set $\{(x, t) \in \mathbb{R}^{d+1} : f(x) \leq t\}$ is convex

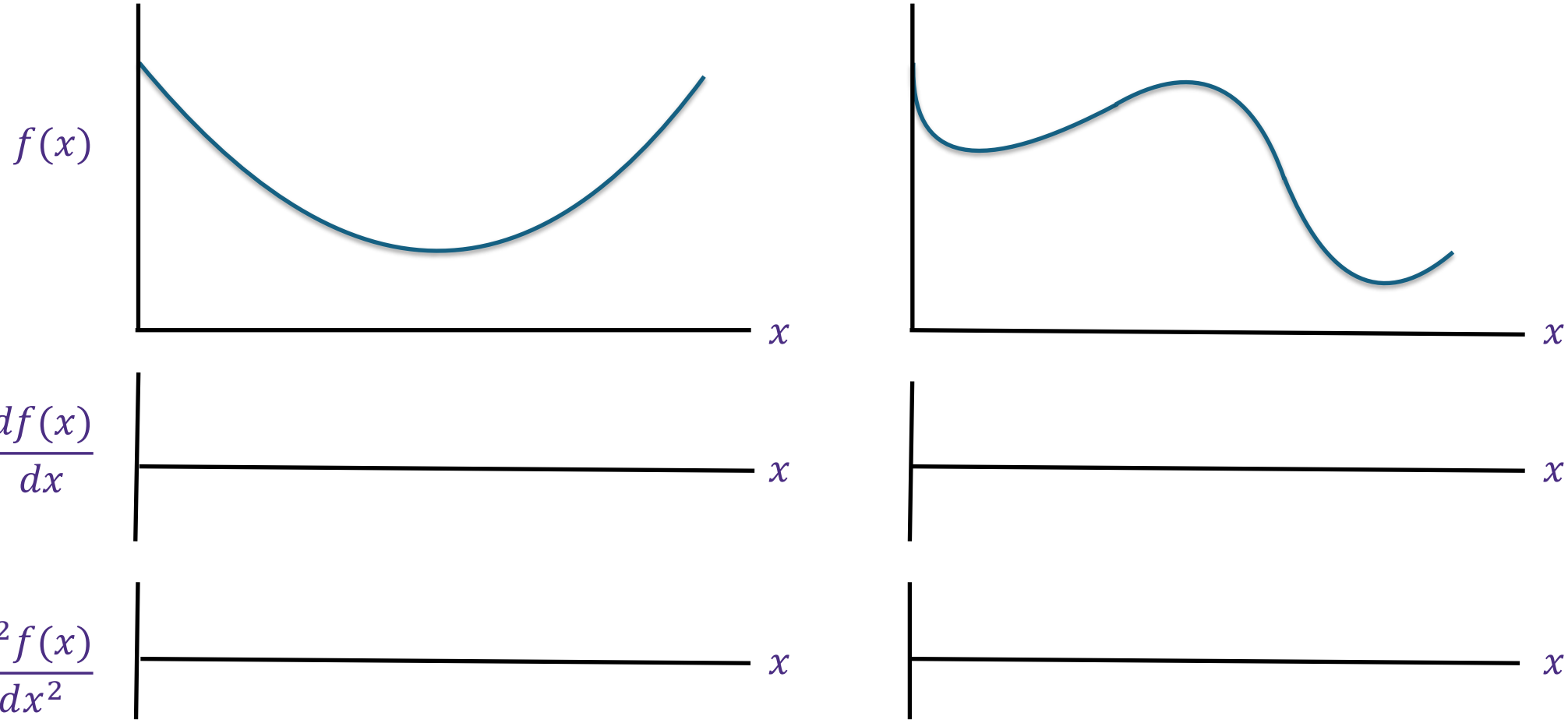
A function $f : \mathbb{R}^d \to \mathbb{R}$ that is differentiable everywhere is convex if $f(y) \geq f(x) + \nabla f(x)^\top (y - x)$ for all $x, y \in dom(f)$



Convexity of twice-differentiable functions

Convexity of twice-differentiable functions

A function $f : \mathbb{R}^d \to \mathbb{R}$ that is twice-differentiable everywhere is convex if $\nabla^2 f(x) \succeq 0$ for all $x \in dom(f)$



Convexity of twice-differentiable functions

A function $f : \mathbb{R}^d \to \mathbb{R}$ that is twice-differentiable everywhere is convex if $\nabla^2 f(x) \succeq 0$ for all $x \in dom(f)$

Recap: Definitions of convexity

A set $K \subset \mathbb{R}^d$ is convex if $(1-\lambda)x + \lambda y \in K$ for all $x, y \in K$ and $\lambda \in [0,1]$

A function $f : \mathbb{R}^d \to \mathbb{R}$ is convex if $f((1-\lambda)x + \lambda y) \leq (1-\lambda)f(x) + \lambda f(y)$ for all $x, y \in \mathbb{R}^d$ and $\lambda \in [0,1]$

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A function $f : \mathbb{R}^d \to \mathbb{R}$ that is twice-differentiable everywhere is convex if $\nabla^2 f(x) \succeq 0$ for all $x \in dom(f)$

Example: Ridge regression

$$\underset{w}{\operatorname{argmin}} \|y - Xw\|_2^2 + \lambda \|w\|_2^2$$

$$\underset{\|w\|_2^2 \leq \rho}{\operatorname{argmin}} \|y - Xw\|_2^2$$

Example: Lasso

$$\underset{w}{\operatorname{argmin}} \|y - Xw\|_2^2 + \lambda \|w\|_1$$

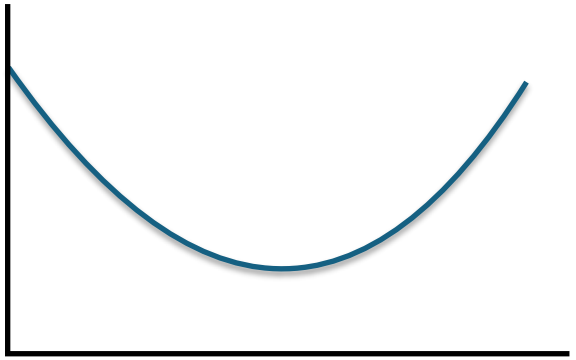
Why not directly solve $\underset{w}{\operatorname{argmin}} \|y - Xw\|_2^2 + \lambda \operatorname{card}(w)$?

Can interpret lasso as convex relaxation of cardinality objective

Convexity and gradient descent

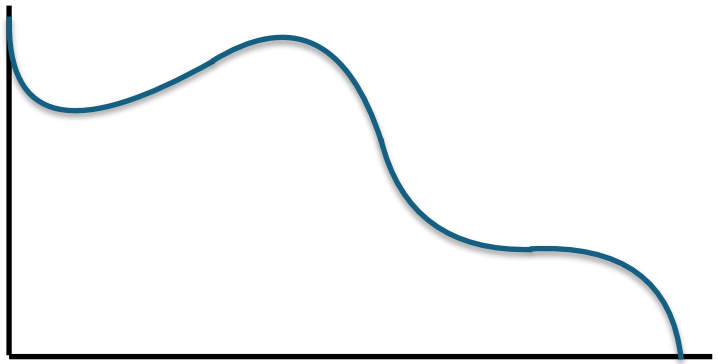
- All local minima are global minima

Convex function



Stationary points with $\nabla f(x) = 0$
are global minima

Non-convex function



Stationary points with $\nabla f(x) = 0$
could be a local minima,
a local maxima, or a saddle point

- Won't get stuck navigating the parameter constraints

Convexity and gradient descent

- Convexity => all local minima are global minima
- All local minima are global minima => ?

Convexity and gradient descent

- You can always run gradient descent whether $f(w)$ is convex or not!
- But if $f(w)$ is convex, we have guarantees on converging to the global minimum
- Linear regression, ridge regression, Lasso → all convex!

Lecture plan

- Gradient descent algorithm + examples

- Theoretical analysis
  - When does it work?
  - How quickly does it converge? ← we are here
  - How do we choose a step size?
  - Key idea: Convexity

- Not tested on proof details, but concepts are important & practical

Convergence analysis steps

1. Study single iteration: $f(w_{t+1})$ vs. $f(w_t)$
2. Piece iterations together to study how they converge

Single-iteration progress bound

Don't need convexity (yet).

Assume f is C^2, and gradient of f is Lipschitz continuous.

There exists L such that:

For all u, v, $\quad \|\nabla f(u) - \nabla f(v)\| \leq L\|u - v\|$.

For all w, $\quad \nabla^2 f(w) \preccurlyeq LI$.

For any u, v, $\quad v^T \nabla^2 f(u) v \leq L\|v\|^2$.

Single-iteration progress bound

For any $u, v,$ $\quad v^T \nabla^2 f(u) v \leq L\|v\|^2$.

Take Taylor expansion:

Single-iteration progress bound

$$w_{t+1} = w_t - \frac{1}{\mathrm{L}} \nabla f(w_t)$$

$$f(w_{t+1}) \leq f(w_t) + \nabla f(w_t)^{\top}(w_{t+1} - w_t) + \frac{L}{2}\|w_{t+1} - w_t\|_2^2$$

Single-iteration progress bound

When $\eta = \frac{1}{L}$,

$$f(w_{t+1}) \leq f(w_t) - \frac{1}{2L} \|\nabla f(w_t)\|_2^2$$

Same argument shows any $\eta < \frac{2}{L}$ will decrease f.

Convergence analysis steps

1. Study single iteration: $f(w_{t+1})$ vs. $f(w_t)$
2. Piece iterations together to study how they converge

Convergence rate of gradient descent

$$\|\nabla f(w_t)\| \to 0$$

$$f(w_t) - f(w^*) \to 0$$

Convergence rate of gradient descent

For some ϵ, how many iterations before $\|\nabla f(w_t)\|^2 \leq \epsilon$?

Assumptions:

- Gradient is Lipschitz continuous (as before)
- Step size is small enough (assume $1/L$)
- f is bounded below by $f(w^*)$

Proof sketch:

- Each iteration decreases f by at least $\frac{1}{2L}\|\nabla f(w_t)\|^2$
- Can't decrease below $f(w^*)$
- So $\|\nabla f(w_t)\|^2$ must be decaying fast enough

Convergence rate of gradient descent

$$f(w_{t+1}) \leq f(w_t) - \frac{1}{2L} \|\nabla f(w_t)\|_2^2$$

Convergence rate of gradient descent

$$T \geq \frac{2L\big(f(w_0) - f(w^*)\big)}{\epsilon}$$

Gradient descent requires

$T = O(1/\epsilon)$ iterations

to achieve $\|\nabla f(w_t)\|^2 \leq \epsilon$

Convergence rate of gradient descent

$$\|\nabla f(w_t)\| \leq \epsilon$$

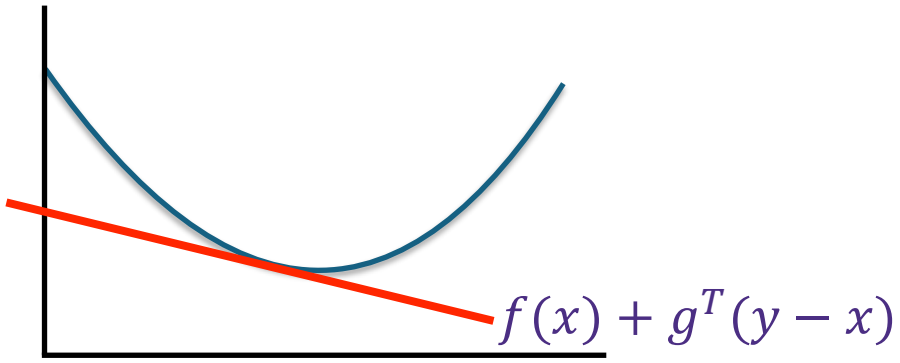
$$f(w_t) - f(w^*) \leq \epsilon$$

Lasso revisited

Subgradients

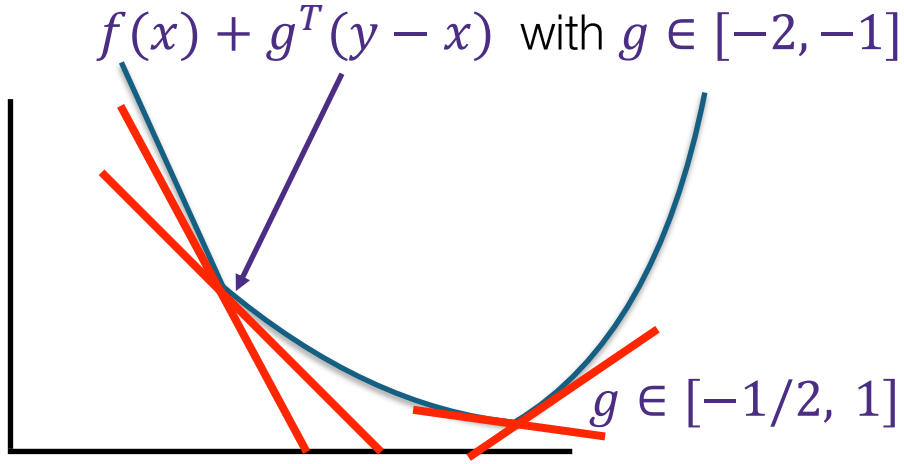
A vector $g \in \mathbb{R}^d$ is a **subgradient** at x if it satisfies
$f(y) \geq f(x) + g^T(y - x)$ for all $y \in \mathbb{R}^d$

Smooth convex function



Gradient is unique sub-gradient
Minimum at points where gradient is 0

Non-smooth convex function

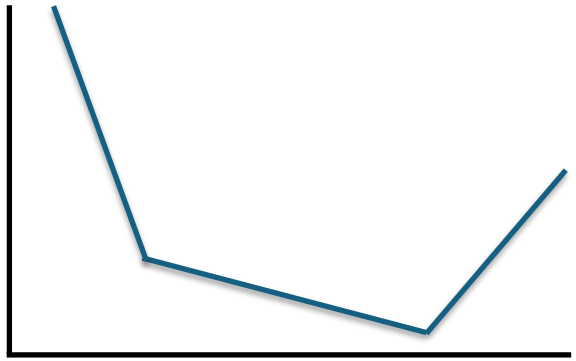


Minimum achieved at points where
subgradient set includes 0 vector

Subgradient descent for non-smooth functions

For each t,

Find any subgradient g_t, then set $w_{t+1} \leftarrow w_t - \eta_t g_t$



Works on non-smooth convex functions
Slower compared to smooth convex functions
Gradients don't get smaller near global minima

- Instead of last iterate w_t, keep track of best one
- Step size needs to decrease with t

Stochastic gradient descent (SGD)

$$\widehat{w} = \operatorname*{argmin}_{w} \frac{1}{n} \sum_{i=1}^{n} \ell_i(w)$$

Gradient descent: $w_{t+1} = w_t - \eta \nabla_w \left(\frac{1}{n} \sum_{i=1}^{n} \ell_i(w) \right) |_{w=w_t}$

Stochastic gradient descent: $w_{t+1} = w_t - \eta \nabla_w \ell_{I_t}(w) |_{w=w_t}$

I_t drawn uniformly at random from $\{1, \ldots, n\}$

n times faster per iteration!

And can even be better minimizer.

Minibatch stochastic gradient descent

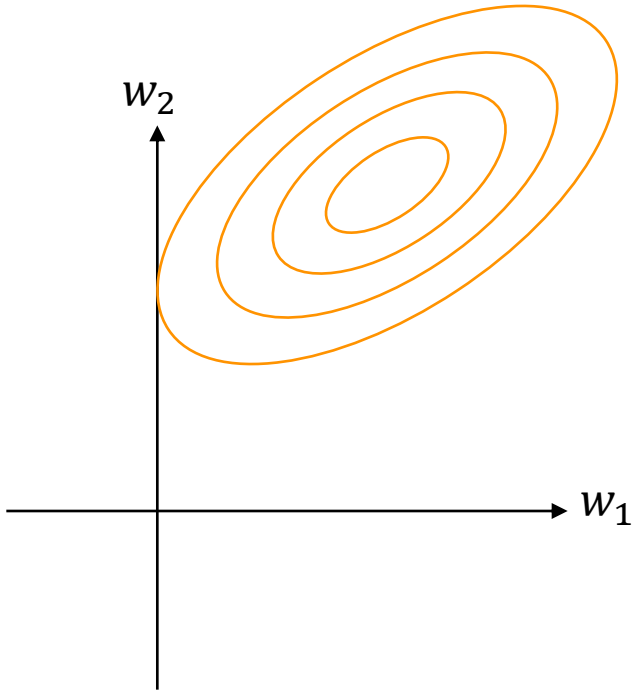
- Instead of one iterate, average B stochastic gradients together
- Advantages:
  - Smaller variance (by $1/B$)
  - Parallelization: Each gradient in the minibatch can be computed in parallel

- This is very widely used!

Summary

- Closed form -> iterative methods
- (Minibatch stochastic) gradient descent as a general-purpose optimizer
- Key theoretical tool: Convexity
- Many many variants. Highly active research area!
  - Schedulers
  - Adaptive step sizes
  - Momentum
  - Higher-order methods
  - Non-convex analysis
  - …

Bonus: Coordinate descent



Coordinate descent for lasso

$$\hat{w} = \underset{w}{\operatorname{argmin}} \ \frac{1}{2}\sum_{i=1}^{n}\left(y_i - x_i^\top w\right)^2 + \lambda\|w\|_1$$

$$\frac{d}{dw_k} f(w)$$
$$= \sum_{i=1}^{n}\left(x_i^\top w - y_i\right)x_{ik} + \lambda \operatorname{sign}(w_k)$$
$$= \sum_{i=1}^{n}\left(\sum_{j\neq k} x_{ij} w_j + x_{ik} w_k - y_i\right)x_{ik} + \lambda \operatorname{sign}(w_k)$$
$$= \sum_{i=1}^{n}\left(\sum_{j\neq k} x_{ij} w_j - y_i\right)x_{ik} + w_k \sum_{i=1}^{n} x_{ik} + \lambda \operatorname{sign}(w_k) \ni 0$$
...

Further reading

- Example gradient descent code on class website
- Boyd and Vandenberghe, Convex Optimization https://stanford.edu/~boyd/cvxbook/
- Mark Schmidt's CPSC 540 notes: https://www.cs.ubc.ca/~schmidtm/Courses/540-W18/L4.pdf
- 3Blue1Brown