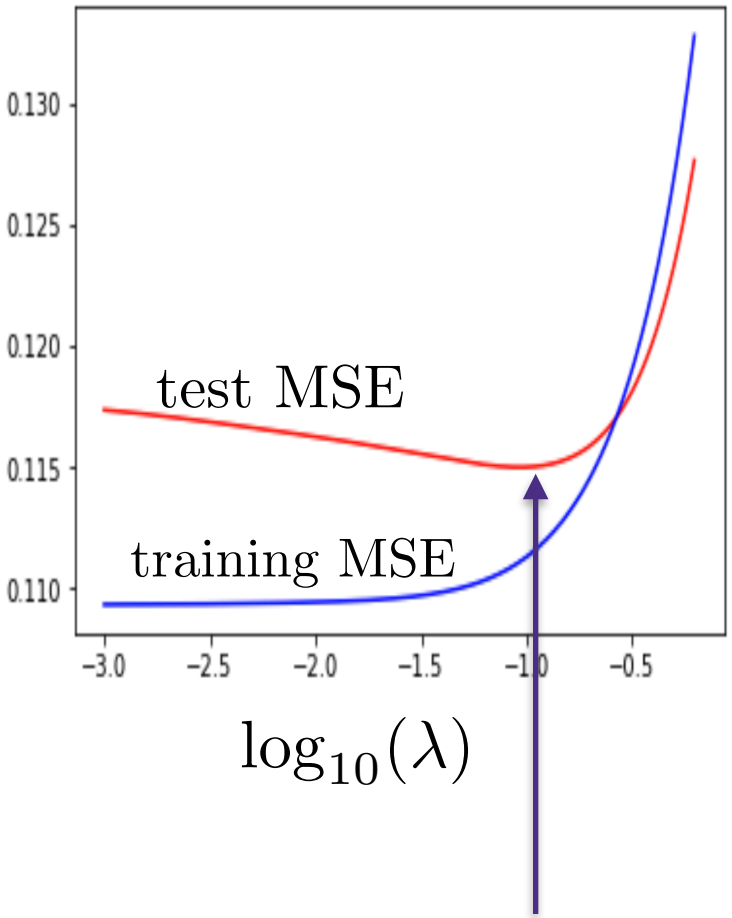
Finishing up bias-variance for Ridge

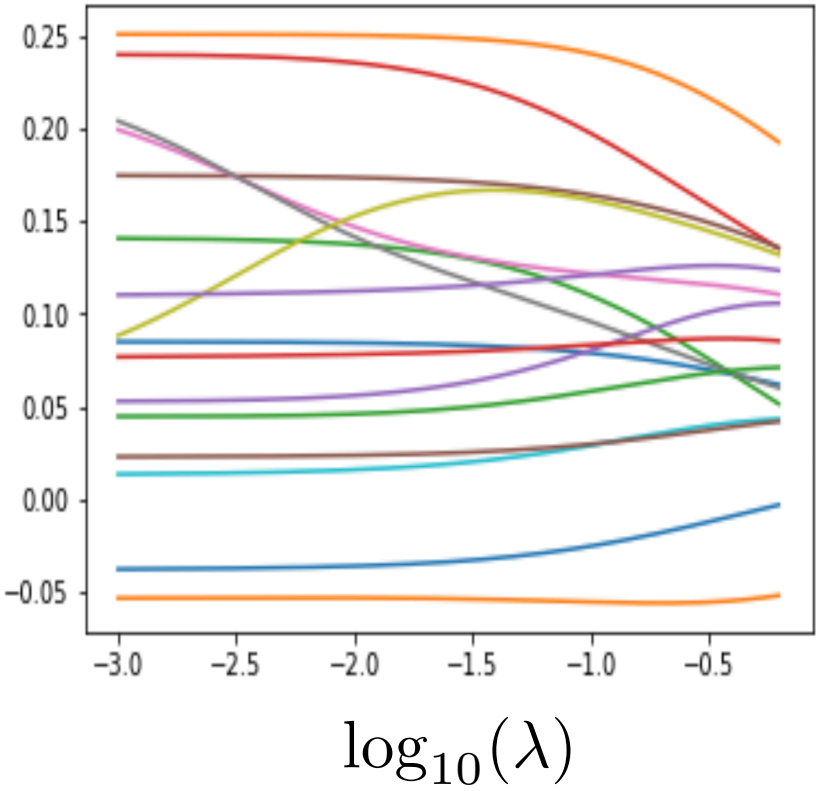


Ridge regression: $\text{minimize} \sum_{i=1}^{n} (w^T x_i - y_i)^2 + \lambda \|w\|_2^2$



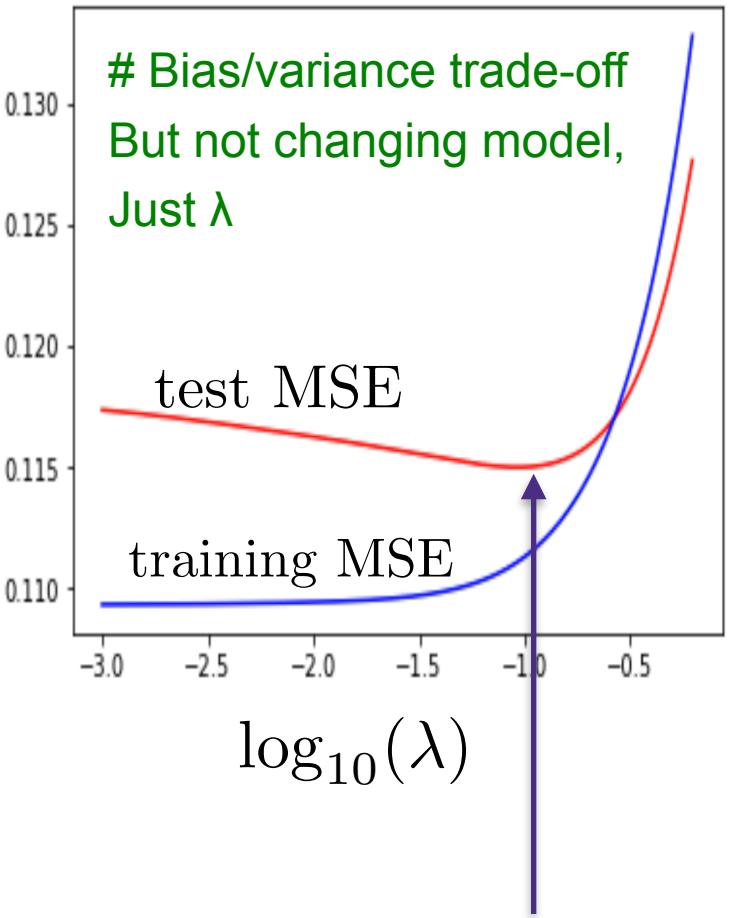
- this gain in test MSE comes from shrinking w's to get a less sensitive predictor
(which in turn reduces the variance)

Illustrative potato delivery: w_i

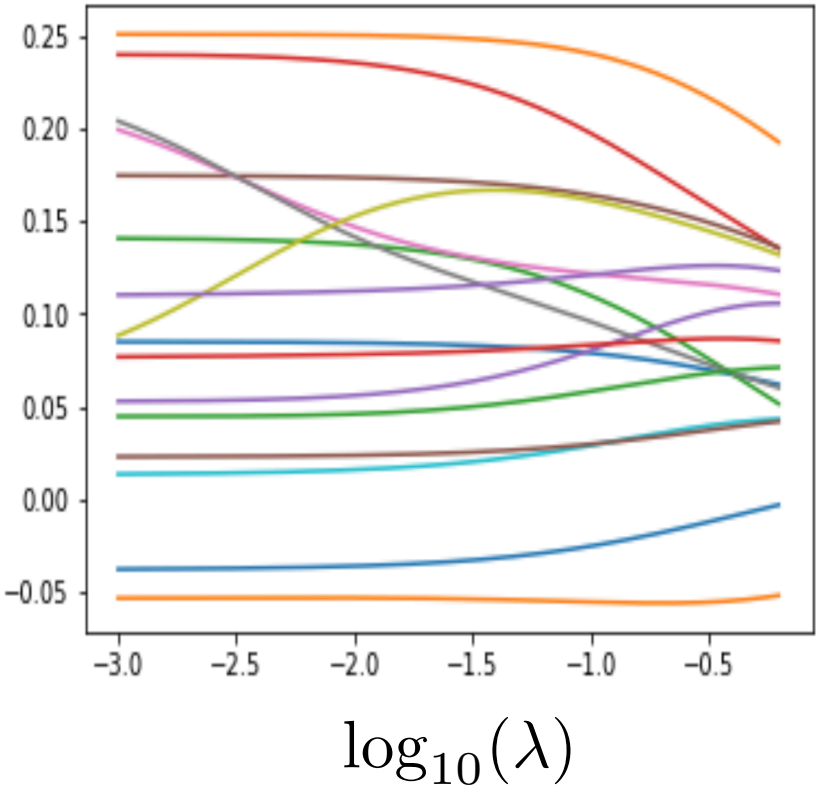


- this is the role of regularizer

Ridge regression: $\text{minimize} \sum_{i=1}^{n} (w^T x_i - y_i)^2 + \lambda \|w\|_2^2$



Illustrative potato delivery: w_i



- this gain in test MSE comes from shrinking w's to get a less sensitive predictor
  (which in turn reduces the variance)

- this is the role of regularizer

A quick trick/lemma for all of our pesky cross terms

Lemma:

$$\mathbb{E}[(A-B)^2] = \mathbb{E}[(A-C)^2] + \mathbb{E}[(B-C)^2]$$ [+ 2 E[(A-C)(B-C)]

When

(1) $(A-C)$ and $(B-C)$ have finite variance,

(2) There exists some information G which

(1) fixes $(A-C)$ and

(2) Makes $\mathbb{E}[B-C \mid G] = 0$

Bias-Variance Properties

- Recall: $\hat{w}_{\text{ridge}} = (\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I})^{-1}\mathbf{X}^T\mathbf{y}$
- To analyze bias-variance tradeoff, we need to assume probabilistic generative model: $x_i \sim P_X, \;\; \mathbf{y} = \mathbf{X}w + \epsilon, \;\; \epsilon \sim \mathcal{N}(0,\sigma^2\mathbf{I})$ for some ground truth model parameter w
- The true error at a sample with feature x is $\mathbb{E}_{y,\mathcal{D}_{\text{train}}|x}[(y - x^T\hat{w}_{\text{ridge}})^2 \,|\, x]$

Bias-Variance Properties

Plan: work through an example where we can directly put bias/ variance in terms of λ

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x is a test sample, $\hat{w}_{\text{ridge}}$ is fit to a dataset

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$$= \underbrace{\mathbb{E}_{y|x}[(y - \mathbb{E}[y\,|\,x])^2 \,|\, x]}_{\text{Irreducible Error}} + \underbrace{\mathbb{E}_{\mathcal{D}_{\text{train}}}[(\mathbb{E}[y\,|\,x] - x^T\hat{w}_{\text{ridge}})^2 \,|\, x]}_{\text{Learning Error}}$$

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Irreduc. Error — Bias-squared — Variance

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Suppose $\mathbf{X}^T\mathbf{X} = n\mathbf{I}$, then $\hat{w}_{\text{ridge}} = (\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I})^{-1}\mathbf{X}^T(\mathbf{X}w + \epsilon)$

$$= \frac{n}{n+\lambda}w + \frac{1}{n+\lambda}\mathbf{X}^T\epsilon$$

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Not realistic but pretend we're sampling independent Gaussians

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Not realistic but pretend we're sampling independent Gaussians

λ trades off weight on data vs. noise

Bias-Variance Properties

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\end{aligned}$$

(verify at home)

$$= \sigma^2 + \frac{\lambda^2}{(n+\lambda)^2}(w^Tx)^2 + \frac{\sigma^2 n}{(n+\lambda)^2}\|x\|_2^2$$

Irreduc. Error | Bias-squared | Variance

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Irreduc. Error | Bias-squared | Variance

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Irreduc. Error | Bias-squared | Variance

- λ trades off bias + variance
- Larger λ →

Bias-Variance Properties

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Irreduc. Error | Bias-squared | Variance

- λ trades off bias + variance
- Larger λ →
  - Bigger bias

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&\quad = \mathbb{E}_{y|x}[(y - x^Tw)^2 \,|\, x] + \mathbb{E}_{\mathcal{D}_{\text{train}}}[(x^Tw - x^T\hat{w}_{\text{ridge}})^2 \,|\, x]
\end{aligned}$$

$$= \sigma^2 + (x^Tw - \mathbb{E}_{\mathcal{D}_{\text{train}}}[x^T\hat{w}_{\text{ridge}}\,|\,x])^2 + \mathbb{E}_{\mathcal{D}_{\text{train}}}[(\mathbb{E}_{\tilde{\mathcal{D}}_{\text{train}}}[x^T\hat{w}_{\text{ridge}}\,|\,x] - x^T\hat{w}_{\text{ridge}})^2 \,|\, x]$$

(verify at home)

$$= \sigma^2 + \frac{\lambda^2}{(n+\lambda)^2}(w^Tx)^2 + \frac{\sigma^2 n}{(n+\lambda)^2}\|x\|_2^2$$

Irreduc. Error | Bias-squared | Variance

- λ trades off bias + variance
- Larger λ →
  - Bigger bias
  - Smaller variance

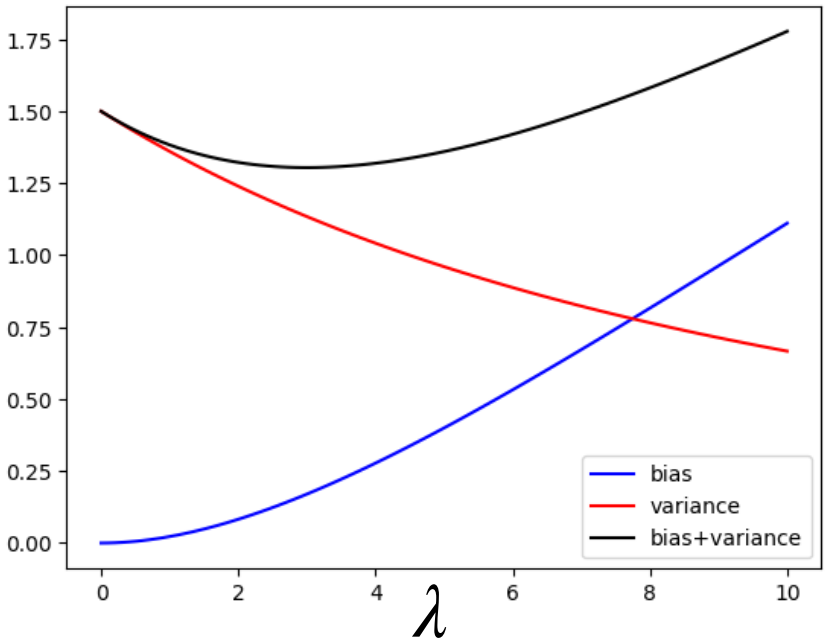
Bias-Variance Properties

Suppose $\mathbf{X}^T\mathbf{X} = n\mathbf{I}$,

- Ridge regressor: $\hat{w}_{ridge} = \arg\min_w \sum_{i=1}^{n} \left(y_i - x_i^T w\right)^2 + \lambda ||w||_2^2$
- True error

$$\mathbb{E}_{y,\mathcal{D}_{\text{train}}|x}[(y - x^T\hat{w}_{\text{ridge}})^2 \,|\, x] = \sigma^2 + \underbrace{\frac{\lambda^2}{(n+\lambda)^2}(w^T x)^2}_{\text{Bias-squared}} + \underbrace{\frac{\sigma^2 n}{(n+\lambda)^2}\|x\|_2^2}_{\text{Variance}}$$

d=10, n=20, $\sigma^2 = 3.0, \|w\|_2^2 = 10$



as λ →0,

$\hat{w}_{\text{ridge}} \to \hat{w}_{\text{LS}}$

as λ →∞

$\hat{w}_{\text{ridge}} \to 0$

What you need to know…

- Regularization
  - Penalizes complex models towards preferred, simpler models
- Ridge regression
  - L_2 penalized least-squares regression
  - Regularization parameter trades off model complexity with training error
  - Never regularize the offset!

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Simple Variable Selection
LASSO: Sparse Regression



Sparsity

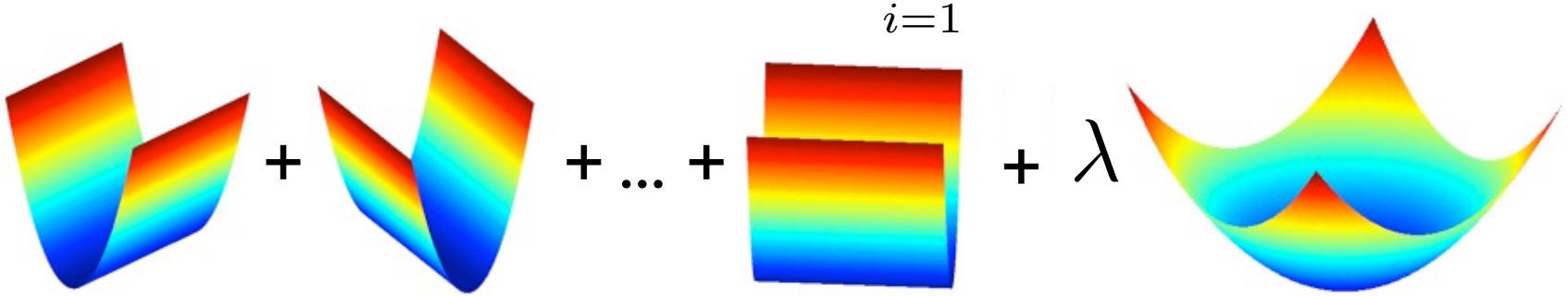
$$\widehat{w}_{LS} = \arg\min_{w} \sum_{i=1}^{n} \left(y_i - x_i^T w\right)^2$$

- **Vector w is sparse, if many entries are zero**

Ridge vs. Lasso Regression

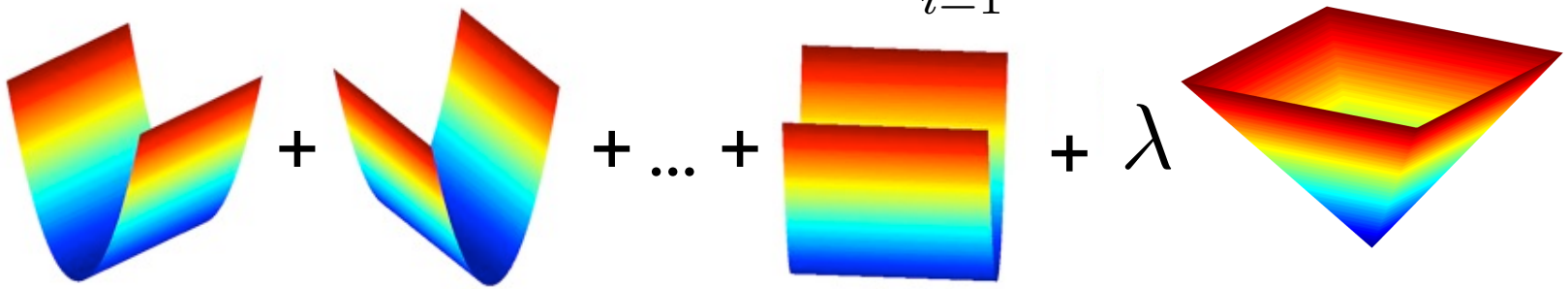
- Ridge Regression objective:

$$\widehat{w}_{ridge} = \arg\min_{w} \sum_{i=1}^{n} \left(y_i - x_i^T w\right)^2 + \lambda ||w||_2^2$$



- Lasso objective:

$$\widehat{w}_{lasso} = \arg\min_{w} \sum_{i=1}^{n} \left(y_i - x_i^T w\right)^2 + \lambda ||w||_1$$



Regularized/Penalized Least Squares

Regularized/Penalized Least Squares

$$\widehat{w}_r = \arg\min_w \sum_{i=1}^{n} \left(y_i - x_i^T w\right)^2 + \lambda r(w)$$

Regularized/Penalized Least Squares

$$\text{Ridge} : r(w) = ||w||_2^2$$

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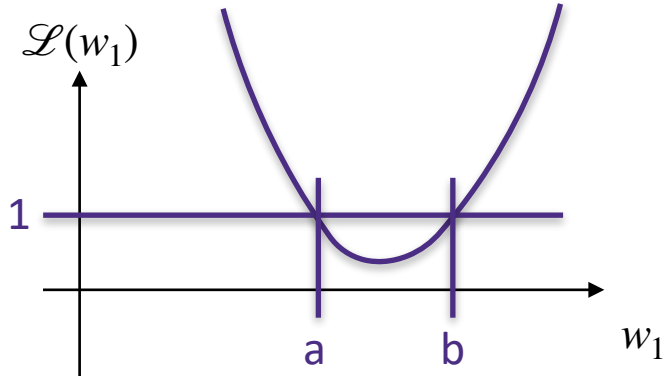
How does Lasso penalization affect solutions?

$$\text{minimize}_w \quad \sum_{i=1}^{n} (w^T x_i - y_i)^2$$

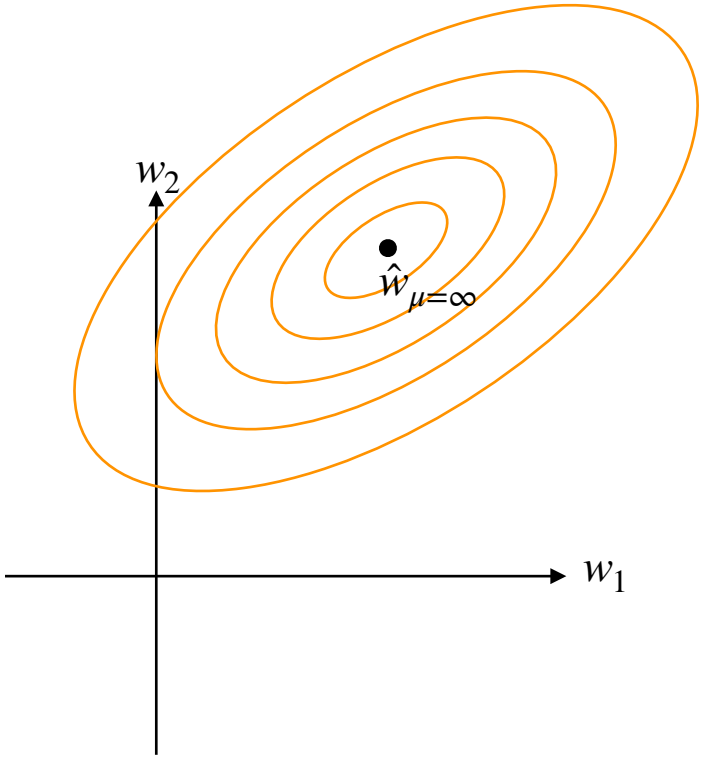
$$\text{subject to} \quad \|w\|_1 \leq \mu$$

- the ***level set*** of a function $\mathscr{L}(w_1, w_2)$ is defined as the set of points (w_1, w_2) that have the same function value (objective value)
- the level set of a quadratic function is an oval
- the center of the oval is the least squares solution $\hat{w}_{\mu=\infty} = \hat{w}_{\text{LS}}$

1-D example with quadratic loss



Level set of $\mathscr{L}(w_1)$ at value 1 is {a,b}



Why does Lasso give sparse solutions?

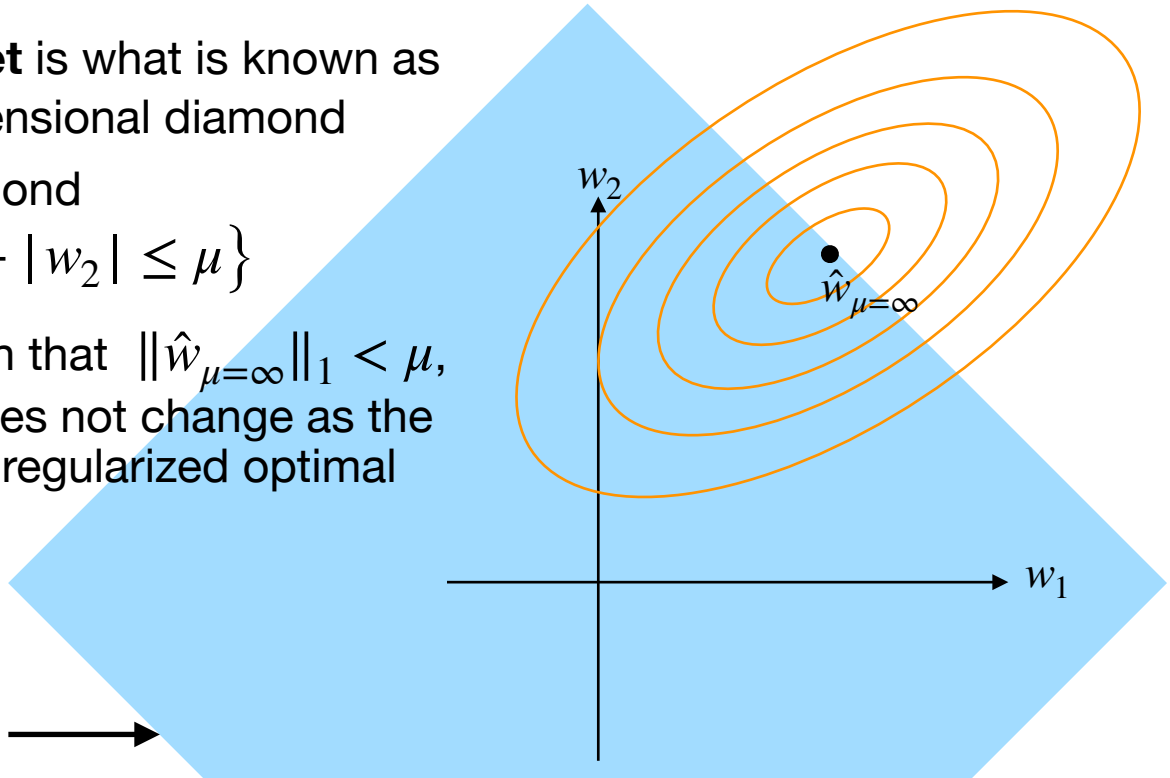
$$\text{minimize}_w \quad \sum_{i=1}^{n} (w^T x_i - y_i)^2$$

$$\text{subject to} \quad \|w\|_1 \leq \mu$$

- as we decrease μ from infinity, the feasible set becomes smaller
- the shape of the **feasible set** is what is known as L_1 ball, which is a high dimensional diamond
- In 2-dimensions, it is a diamond

$$\{(w_1, w_2) \mid |w_1| + |w_2| \leq \mu\}$$

- when μ is large enough such that $\|\hat{w}_{\mu=\infty}\|_1 < \mu$, then the optimal solution does not change as the feasible set includes the un-regularized optimal solution



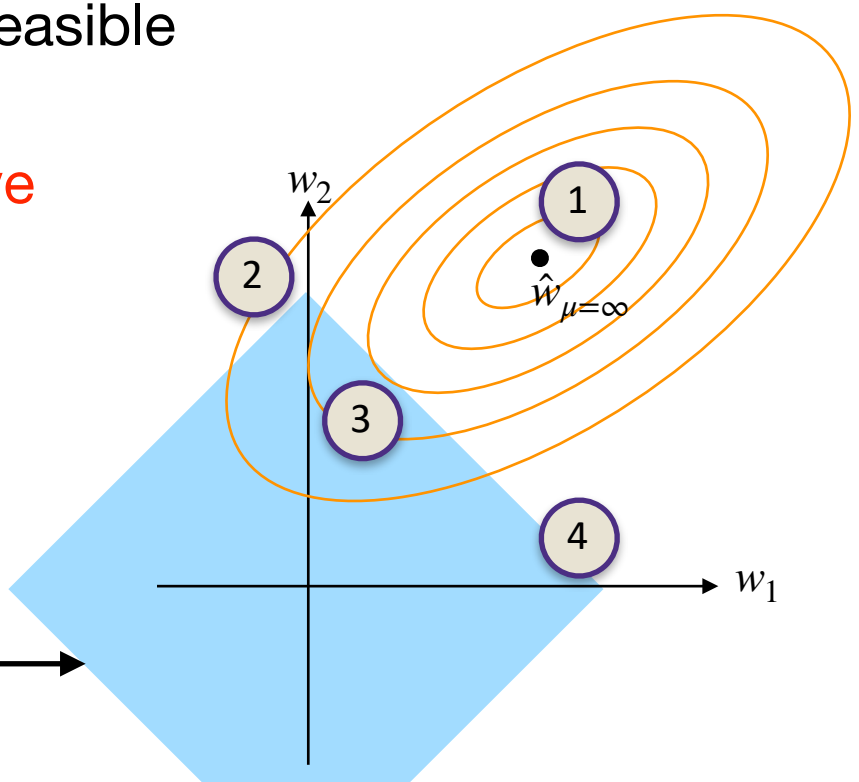
feasible set: $\{w \in \mathbb{R}^2 \mid \|w\|_1 \leq \mu\}$ ⟶

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- As μ decreases (which is equivalent to increasing regularization λ) the feasible set (blue diamond) shrinks
- The optimal solution of the above optimization is ?



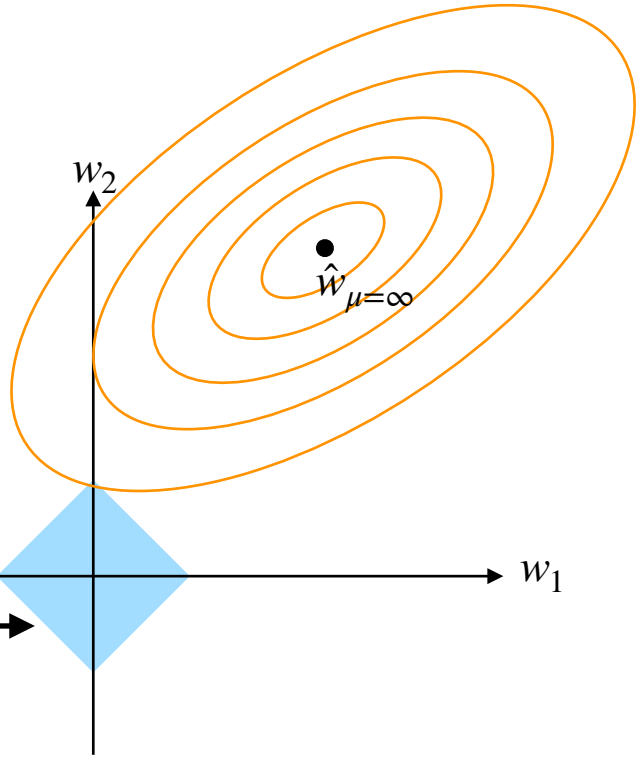
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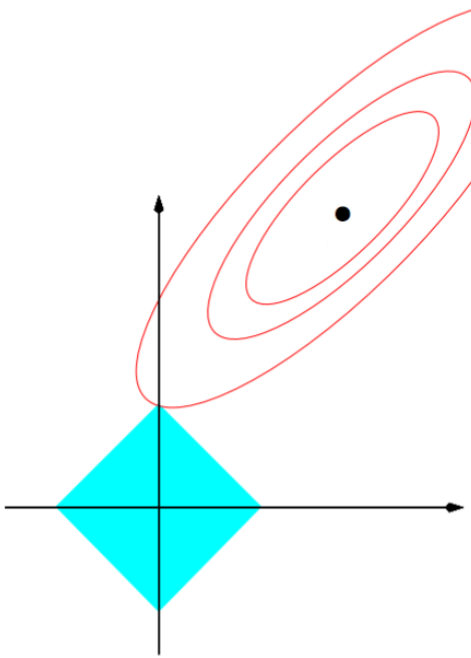
- For small enough μ, the optimal solution becomes **sparse**
- This is because the L_1-ball is "pointy",i.e., has sharp edges aligned with the axes

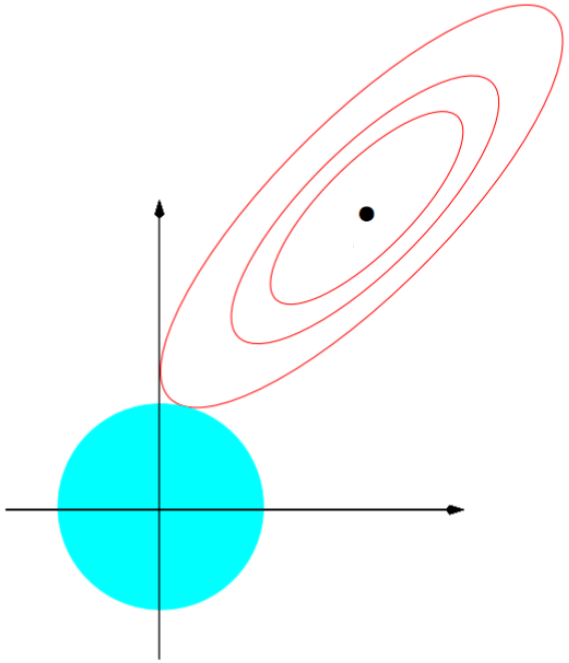


feasible set: $\{w \in \mathbb{R}^2 \mid \|w\|_1 \leq \mu\}$

Constrained Least Squares

- LASSO regression finds sparse solutions, as L_1-ball is "pointy"
- Ridge regression finds dense solutions, as L_2-ball is "smooth"



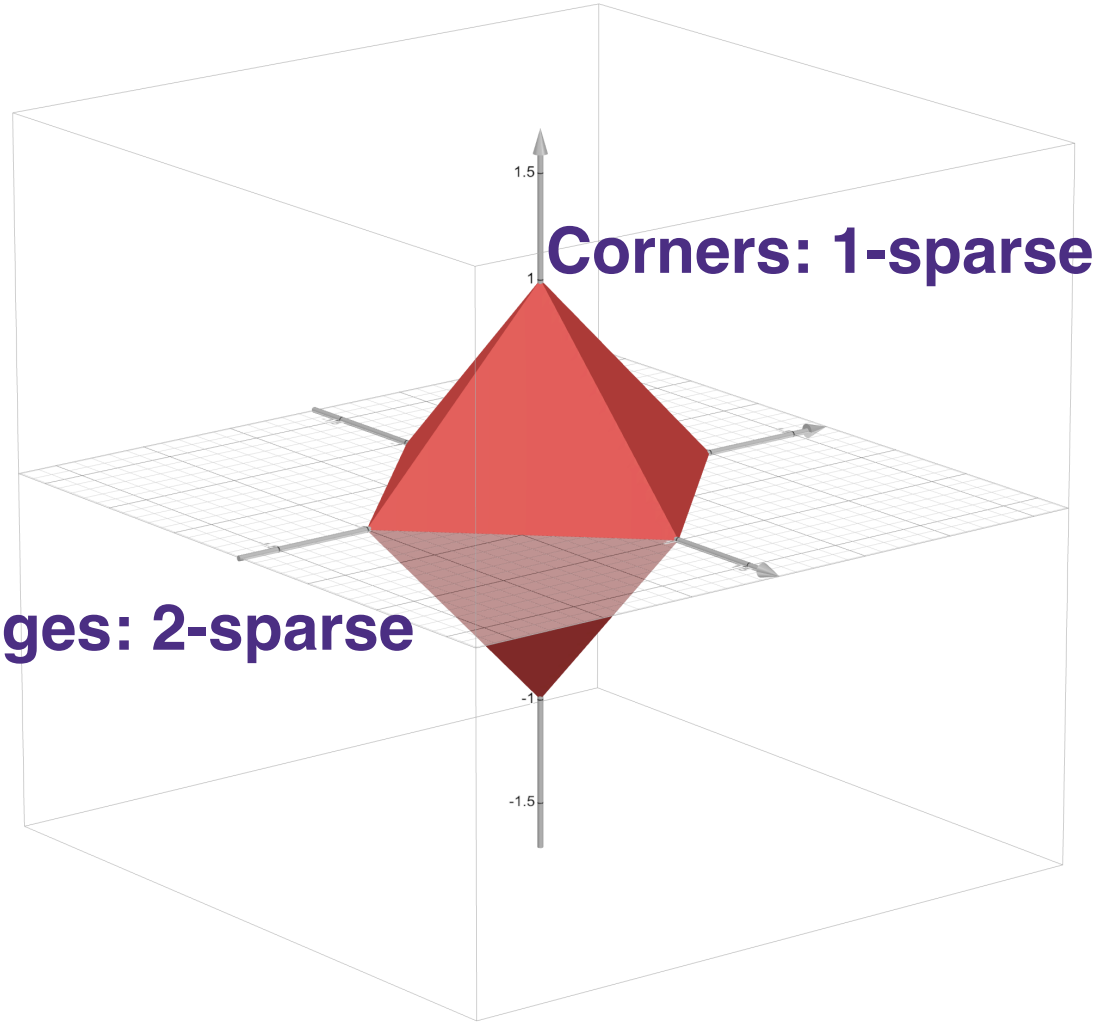


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L1 Ball in Higher Dimensions

> L1 ball 3 dimensions



CSE 546
Gradient Descent

UNIVERSITY of WASHINGTON



How do we find LASSO weights?

- This is related to some questions you might have so far in this course
  - Why do we use quadratic loss, $\sum_{i=1}^{n} (y_i - w^T x_i)^2$?
  - Why is Gaussian noise so popular?

$$f(z) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2}\frac{(z-\mu)^2}{\sigma^2}}$$

  - Why was Ridge Regression with L_2 regularizer, $\|w\|_2^2$, the first to be used?
  - When we want sparsity, why do we use L_1 regularizer, $\|w\|_1$, and not $L_{0.5}$ regularizer, $\|w\|_{0.5}$?

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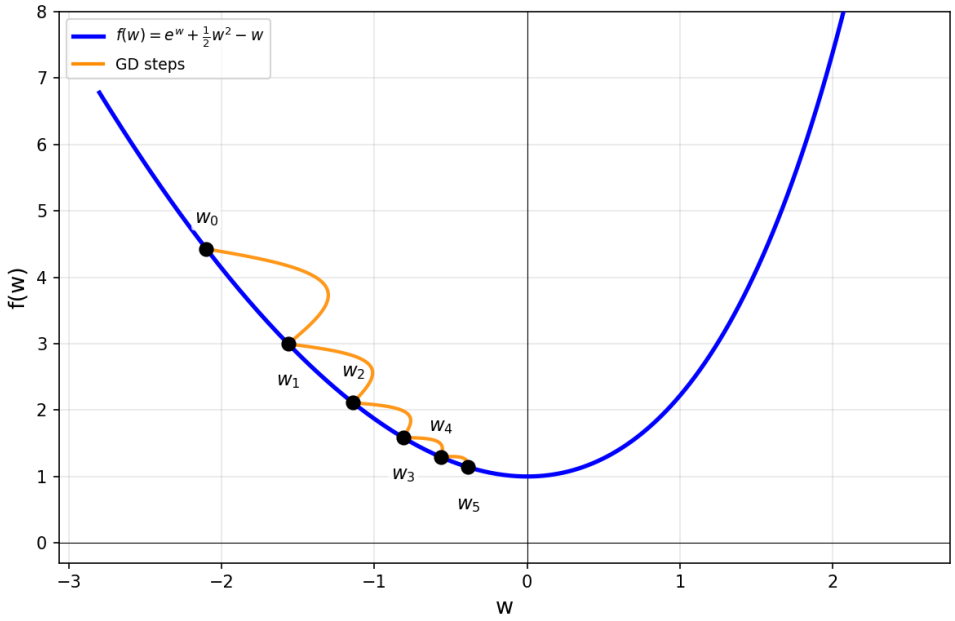
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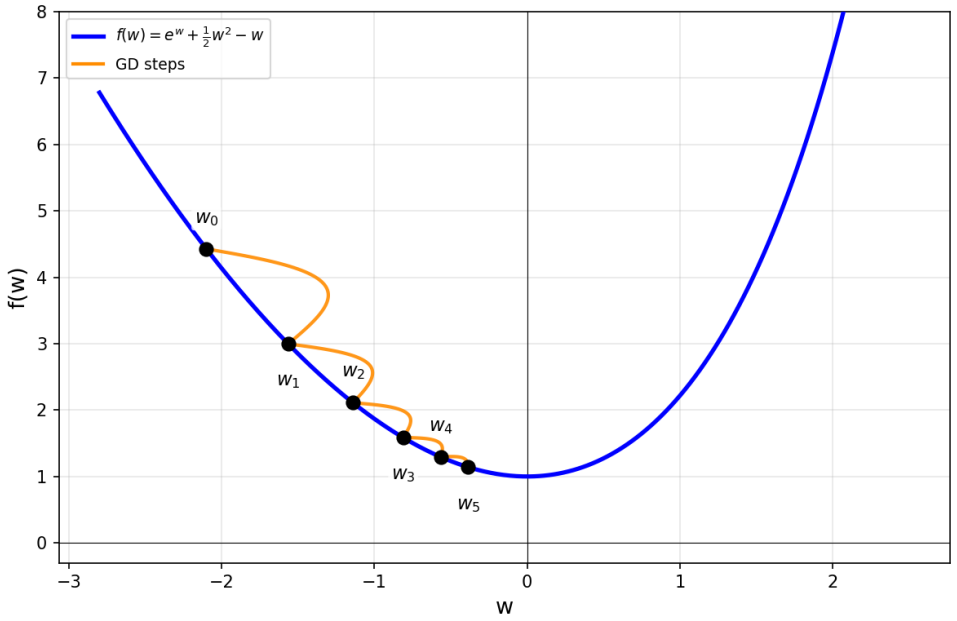
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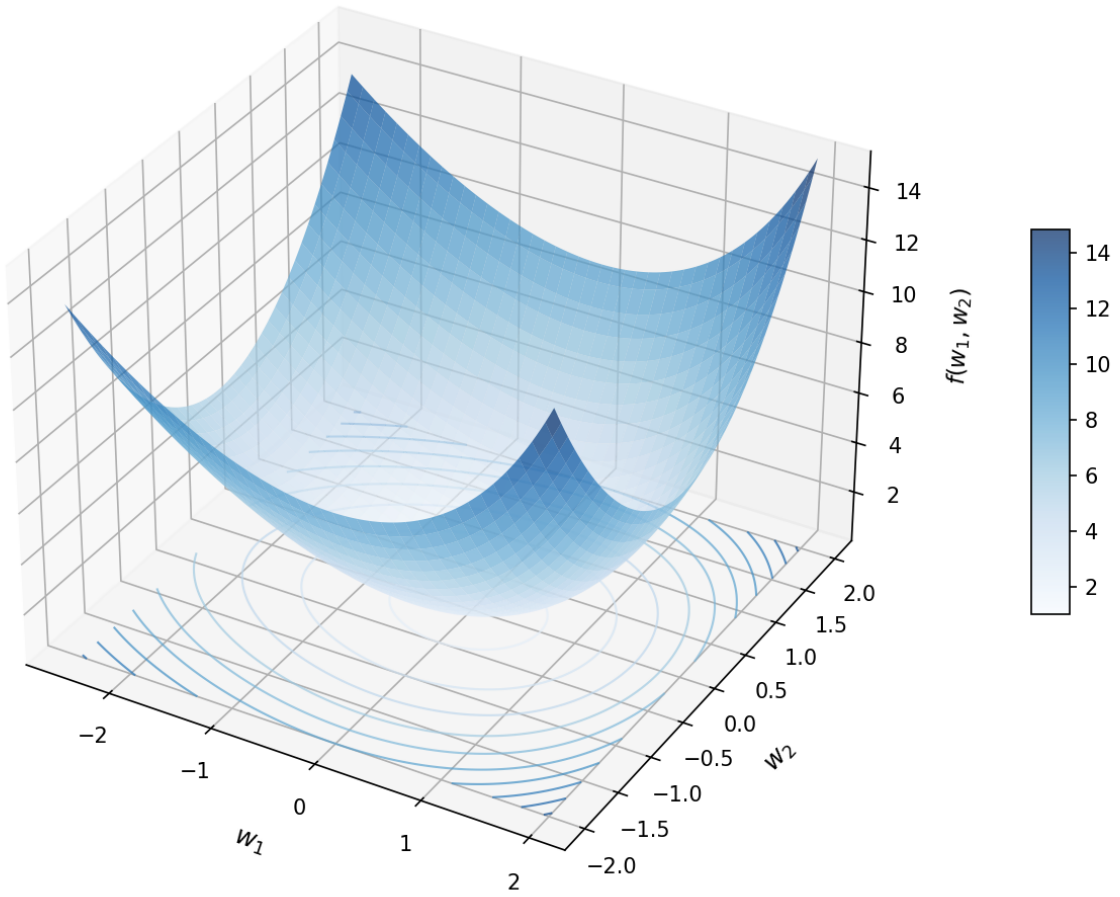
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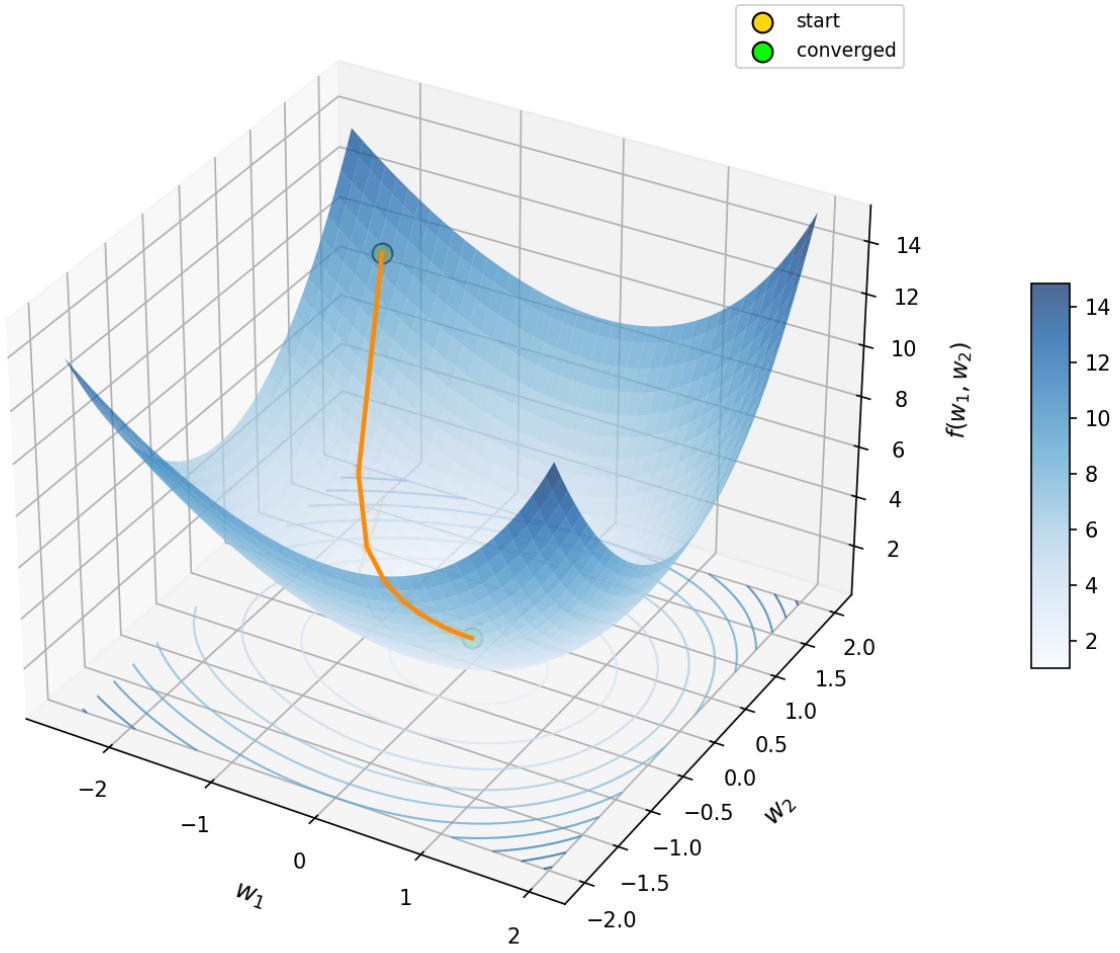
Step direction: $-\nabla_w f(w)$

Step size: $\eta \, | \nabla_w f(w) |$

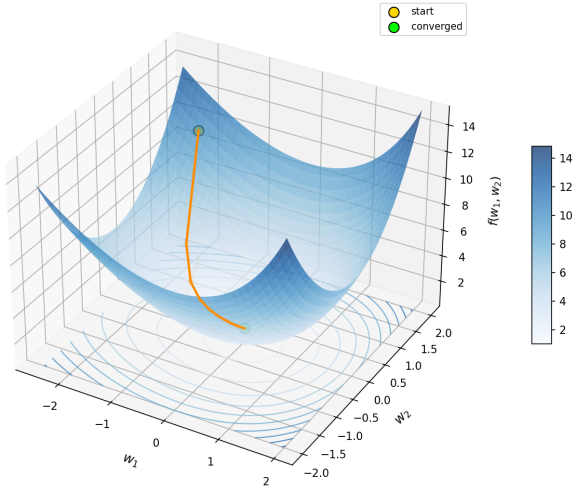
Gradient Descent in higher dimensions



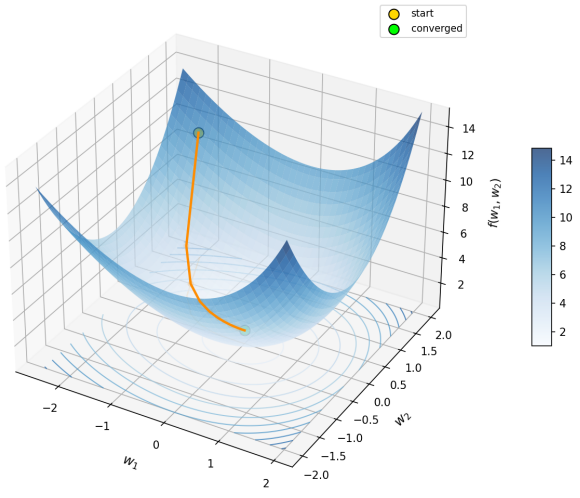
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Gradient Descent pseudocode

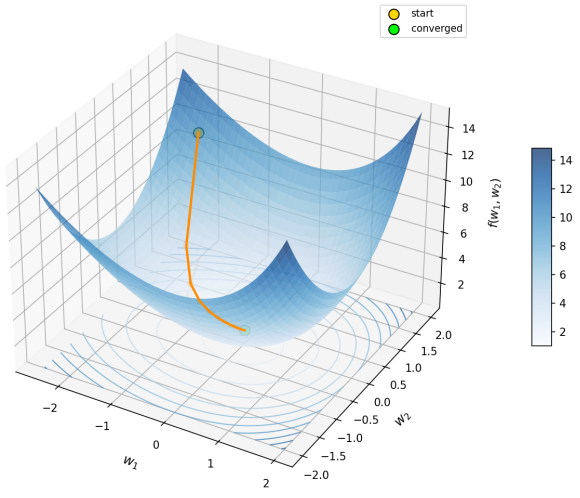


Gradient Descent pseudocode



GradientDescent(f, w_0, η, T) :

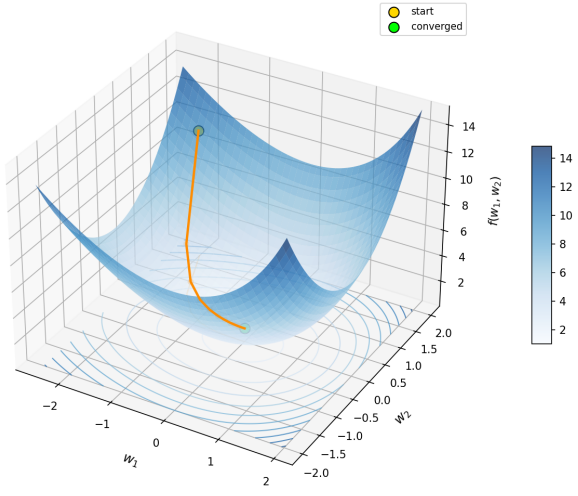
Gradient Descent pseudocode



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Gradient Descent pseudocode

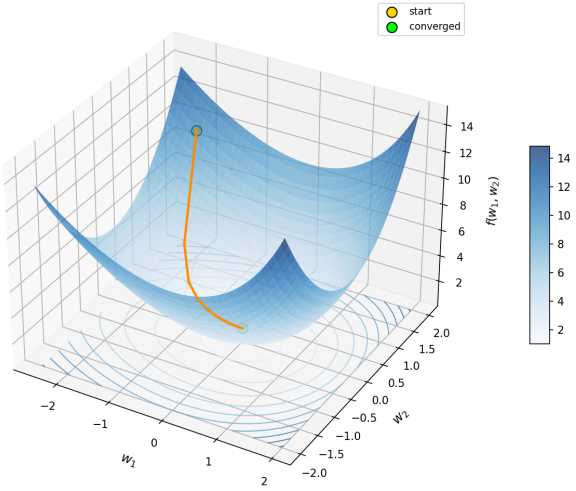


GradientDescent(f, w_0, η, T) :

For (t = 1 to T):

$$w_t = w_{t-1} - \eta \, | \, \nabla_{w_{t-1}} f(w_{t-1}) \, |$$

Gradient Descent pseudocode



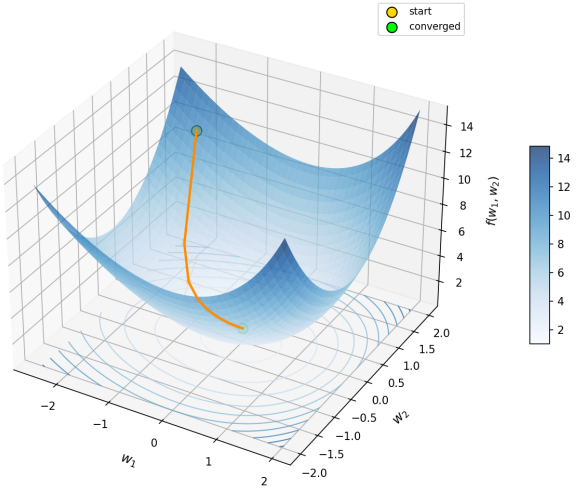
hyperparameters

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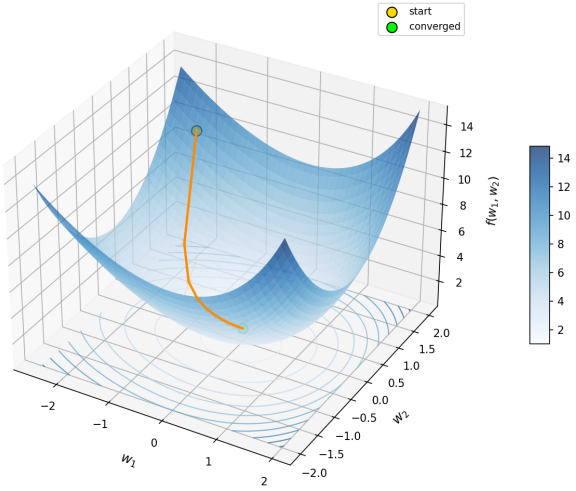
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Gradient Descent pseudocode



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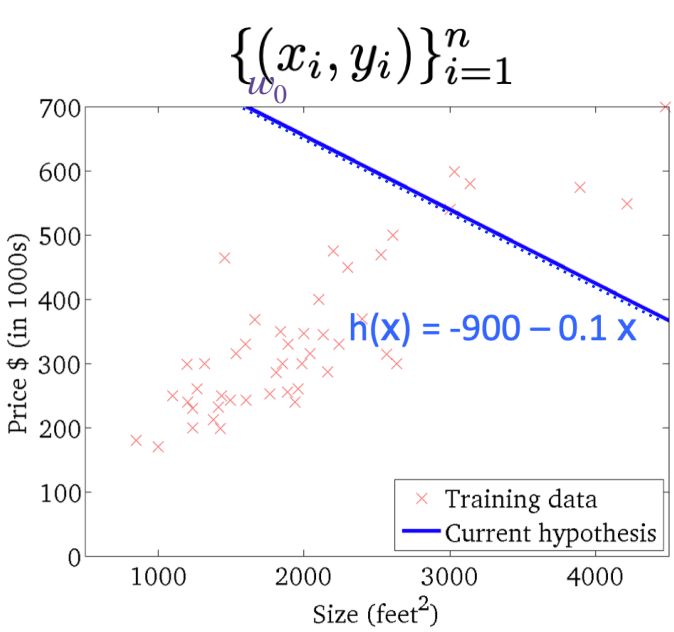
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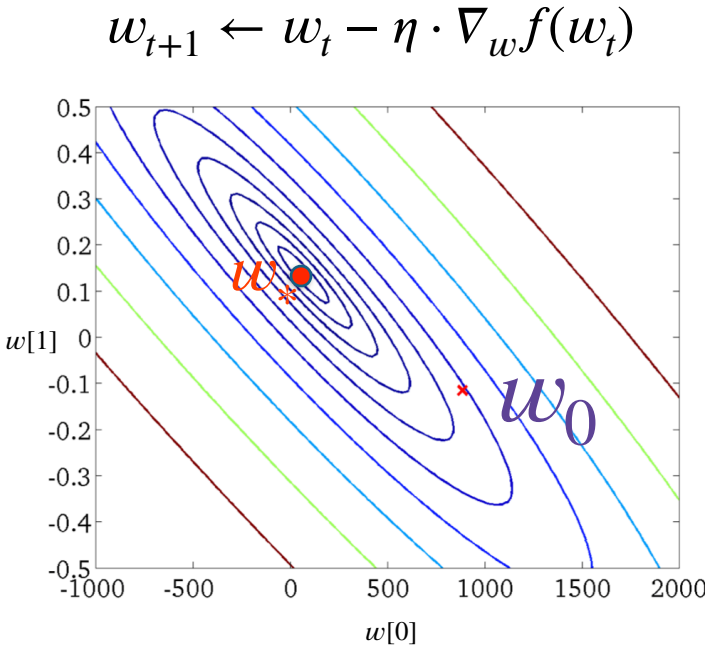
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To pick η? Trial and error…

GD for LS, offset + 1 feature, initialized w_0

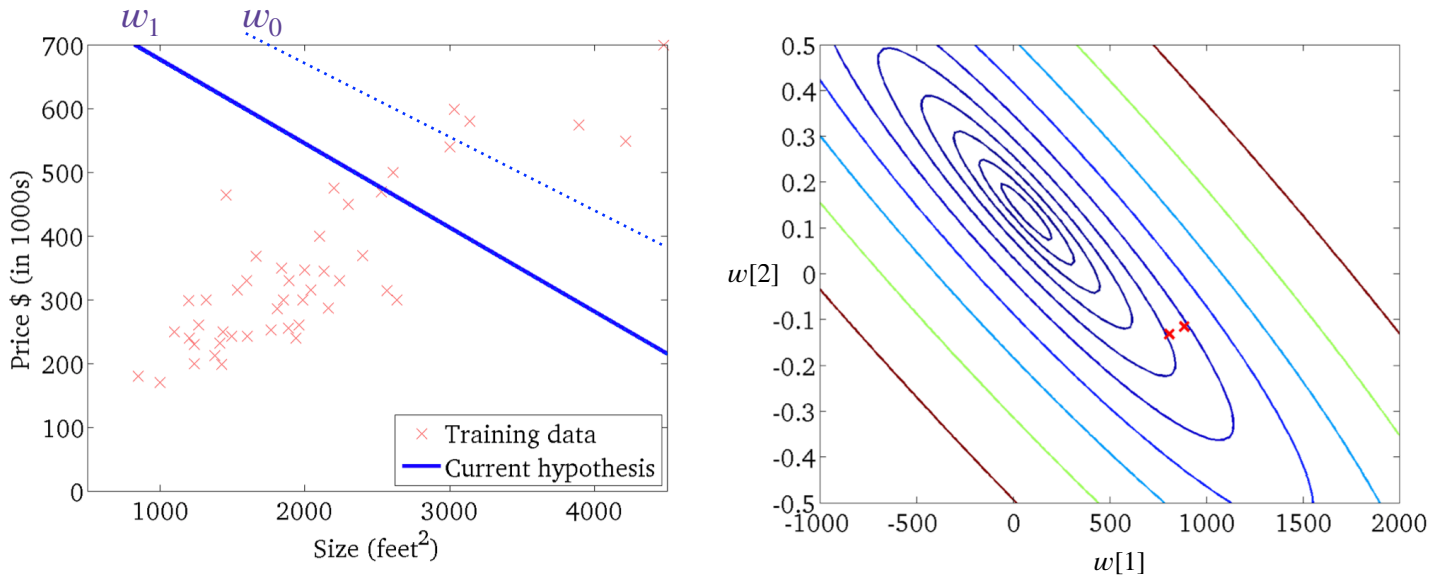




Evolution of the predictor y = w[0] + w[1]x

Gradient descent dynamics in the parameter space w
Ovals show the **level set** of the objective function

GD for LS, offset + 1 feature, w_1

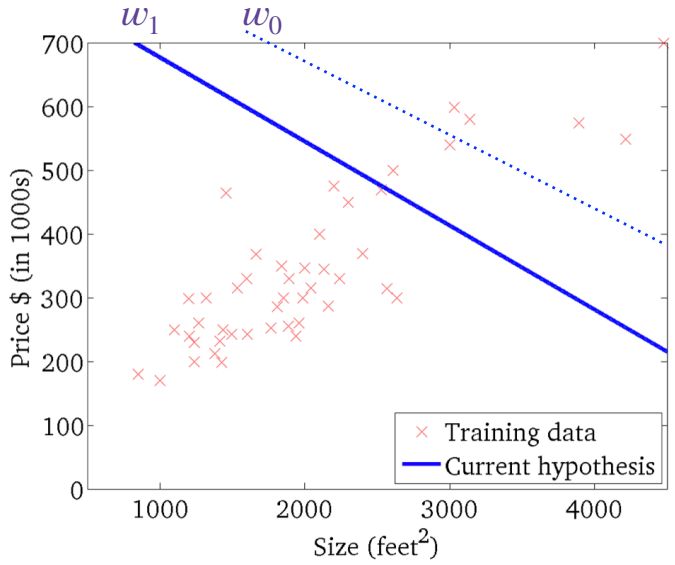


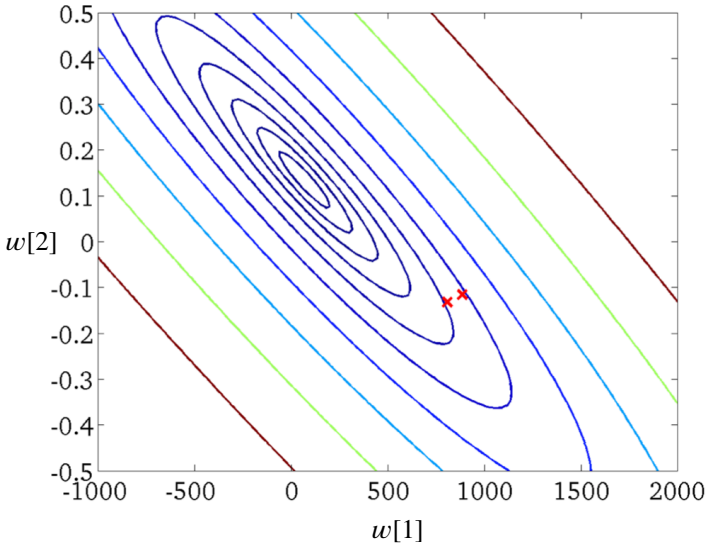
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current model

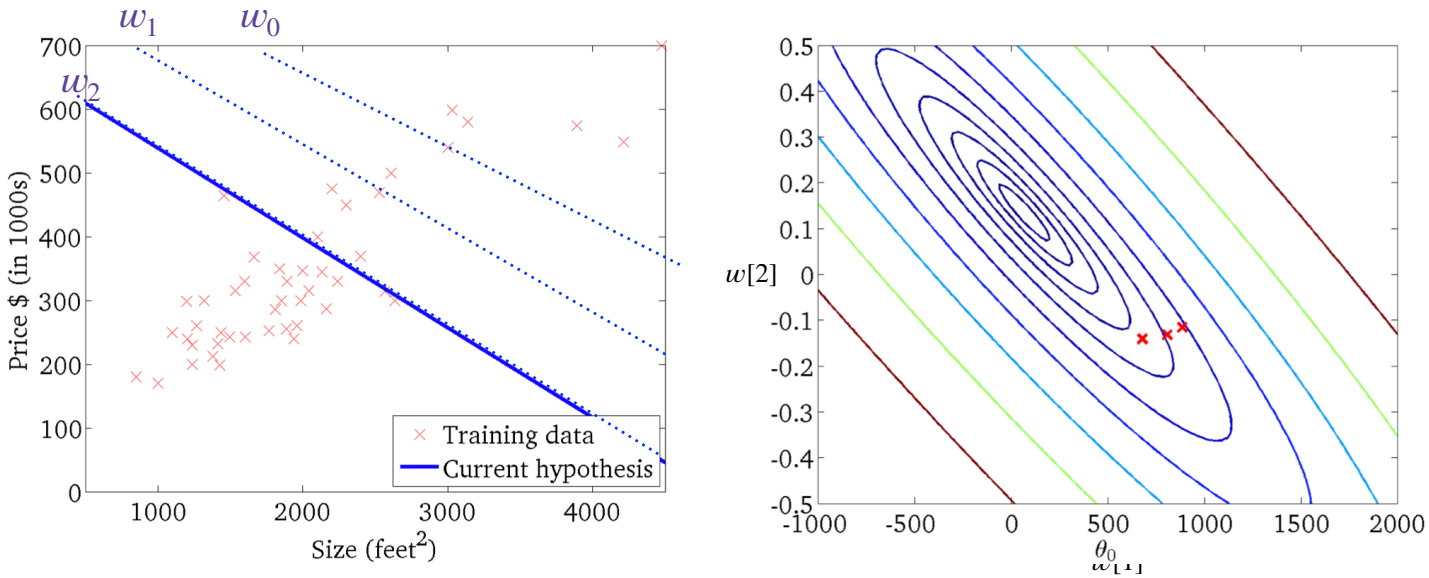




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GD for LS, offset + 1 feature, w_2

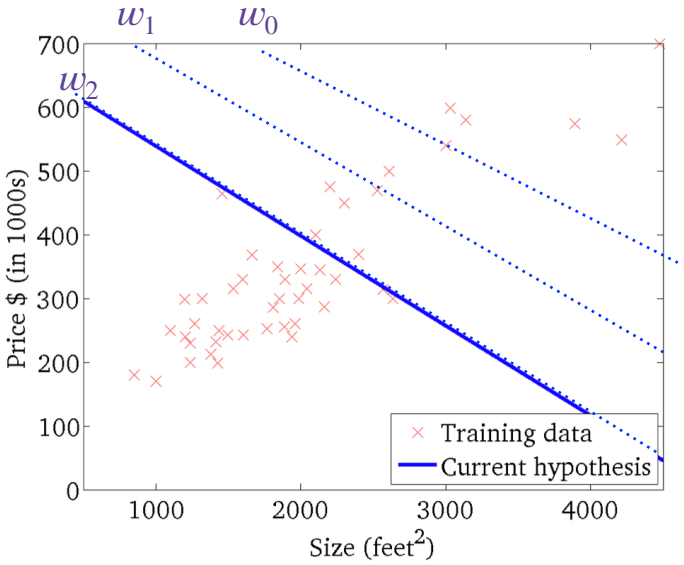


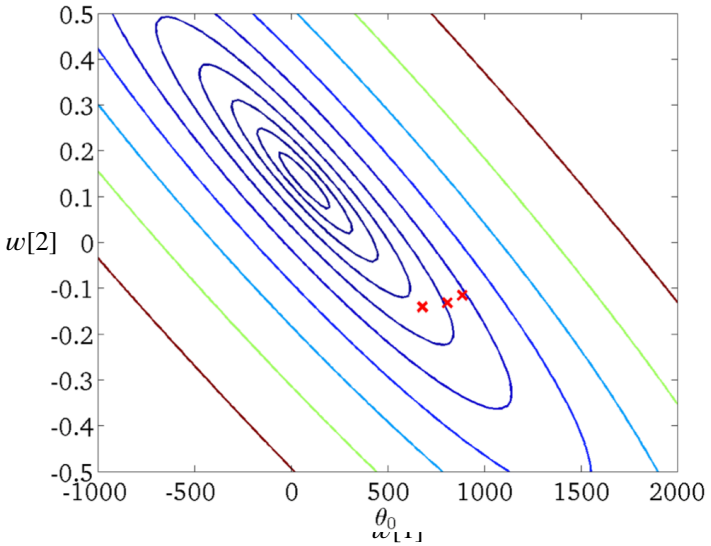
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current model

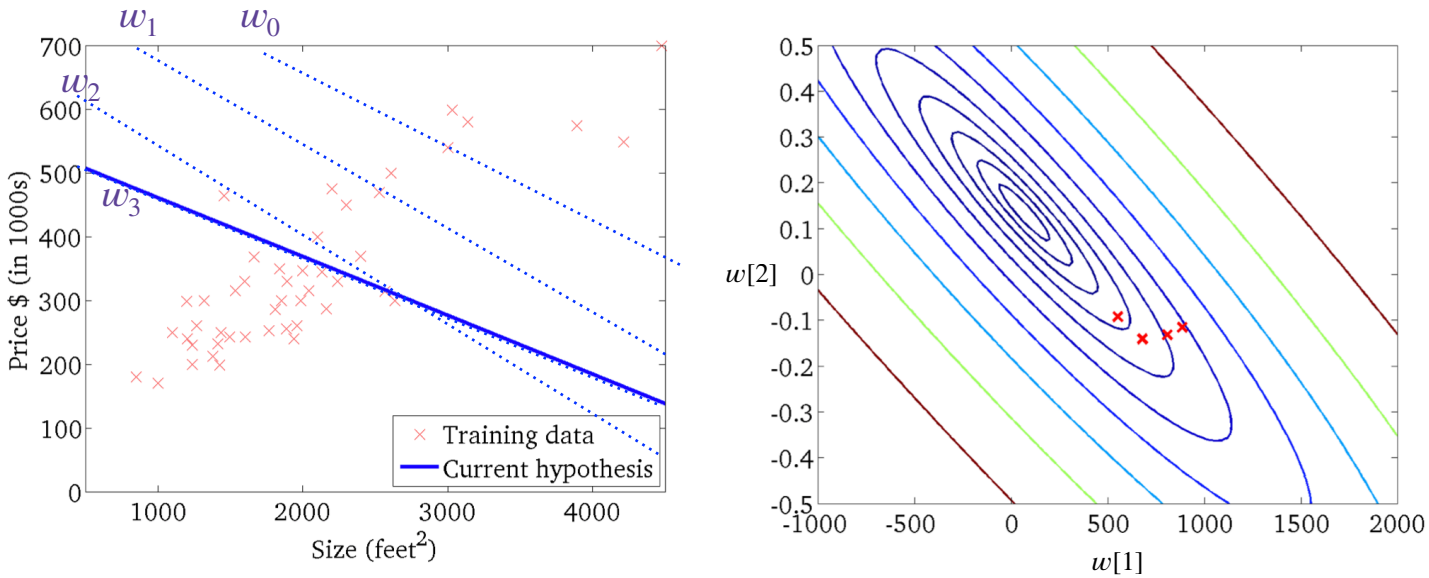




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GD for LS, offset + 1 feature, w_3

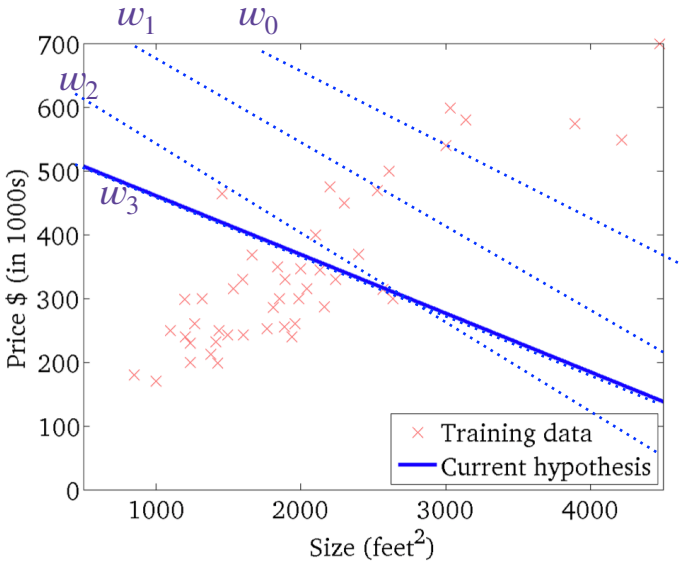


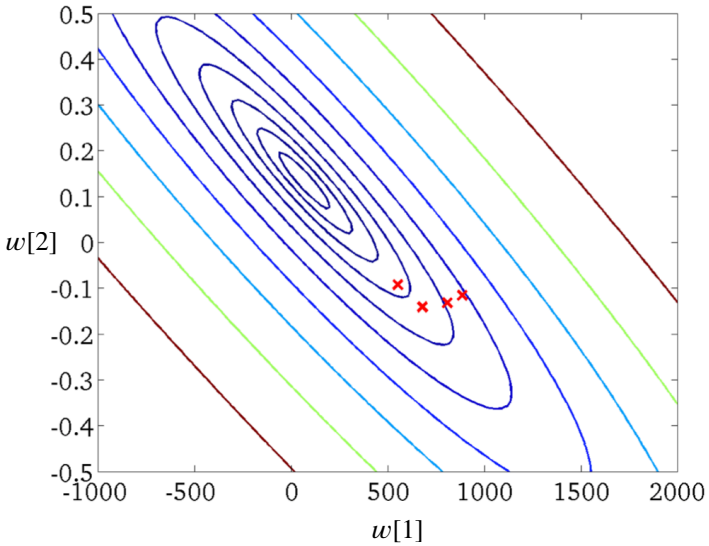
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current model

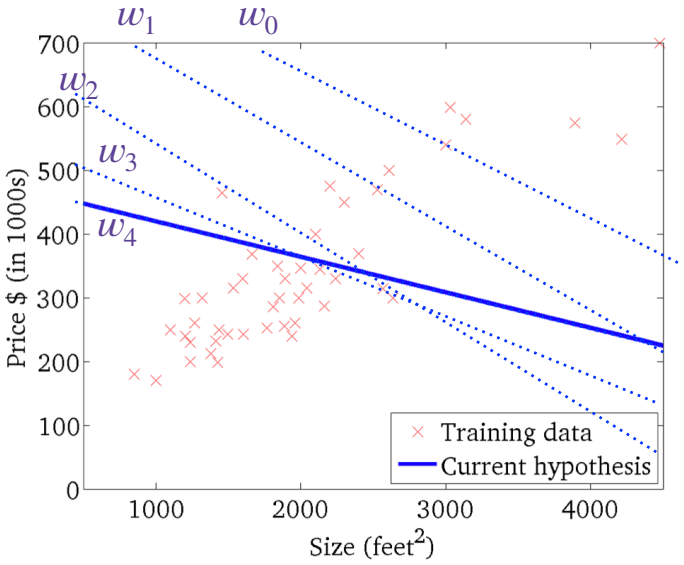


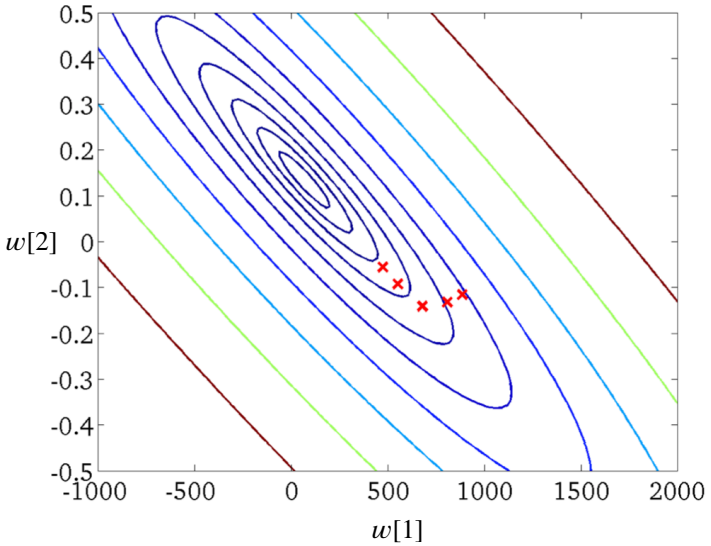


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GD for LS, offset + 1 feature, w_4…



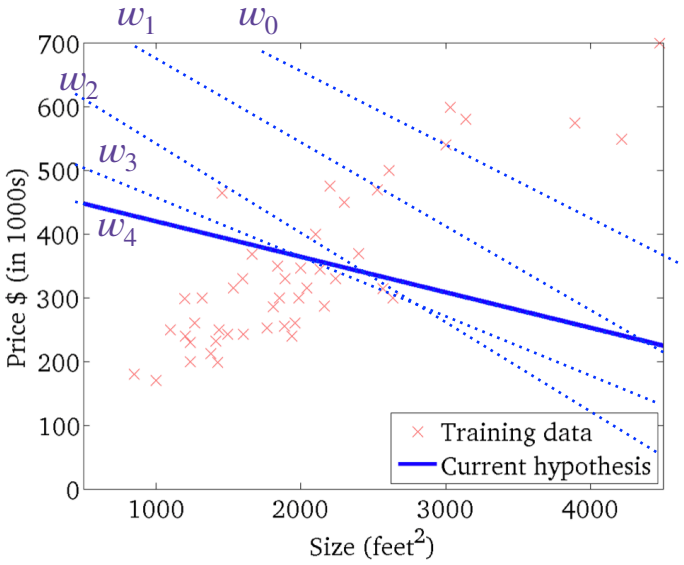


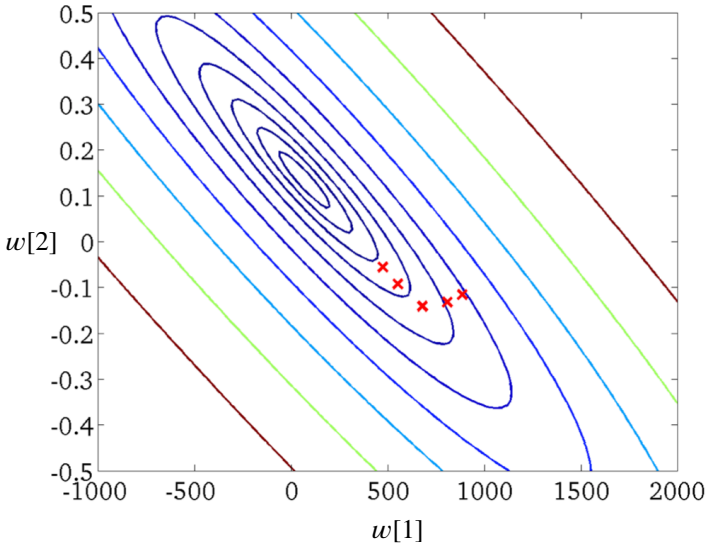
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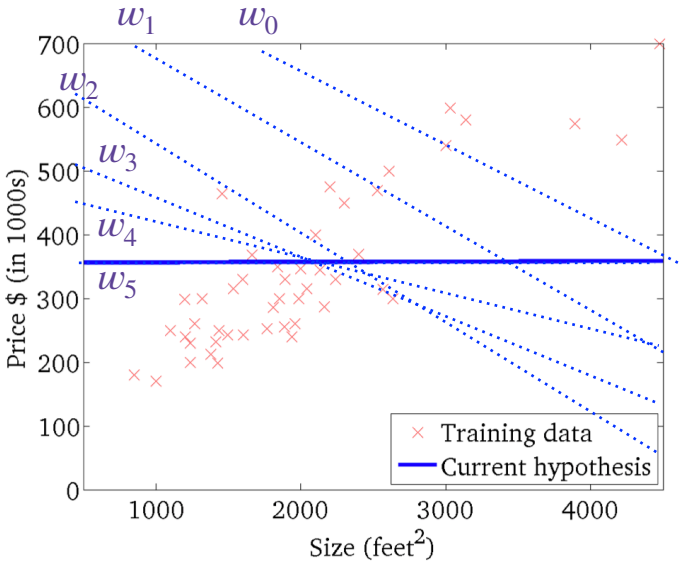


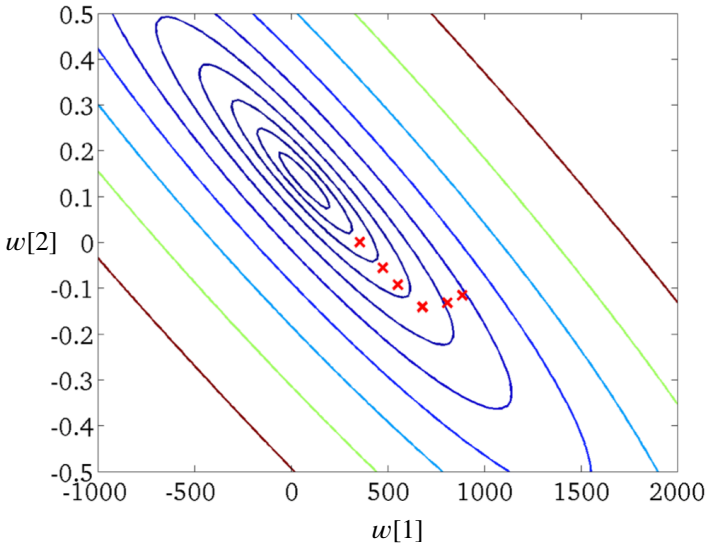
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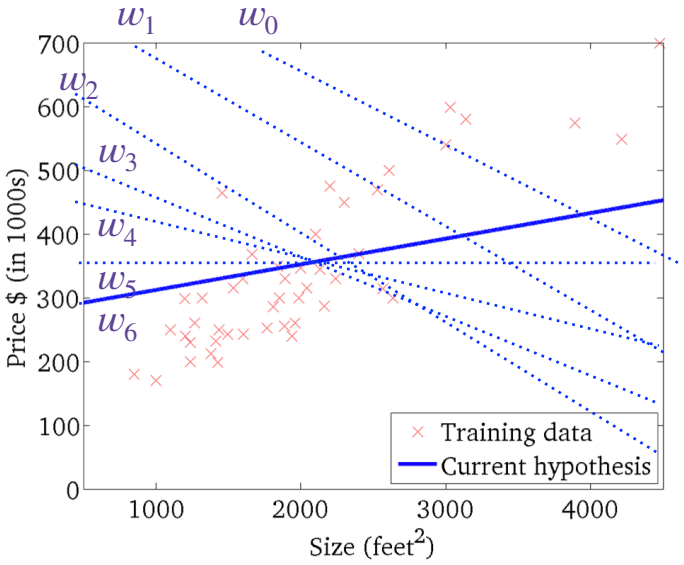


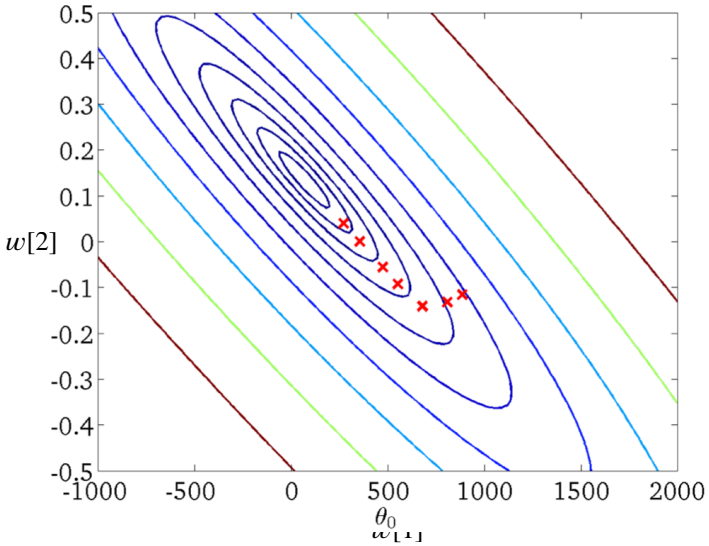
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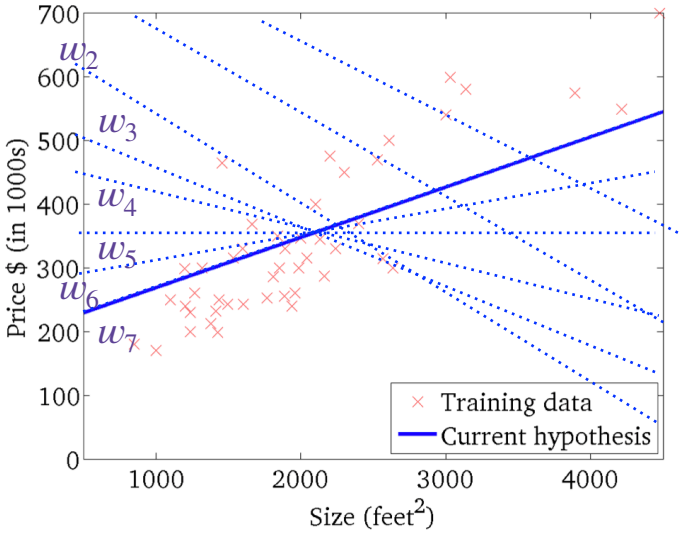


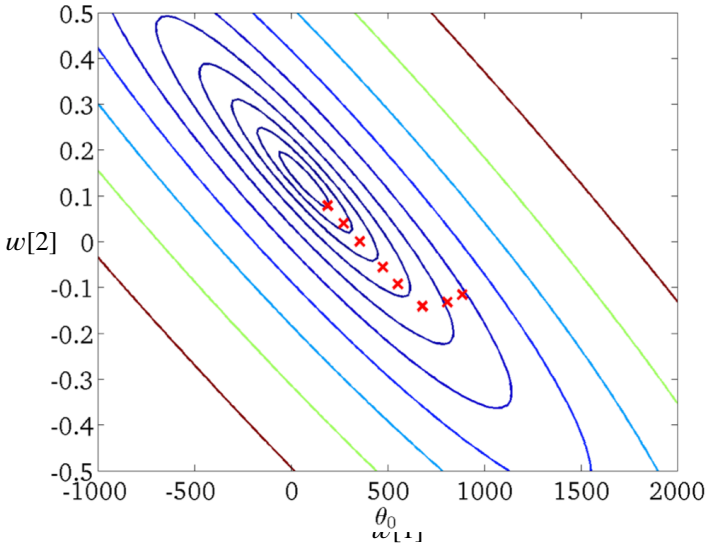
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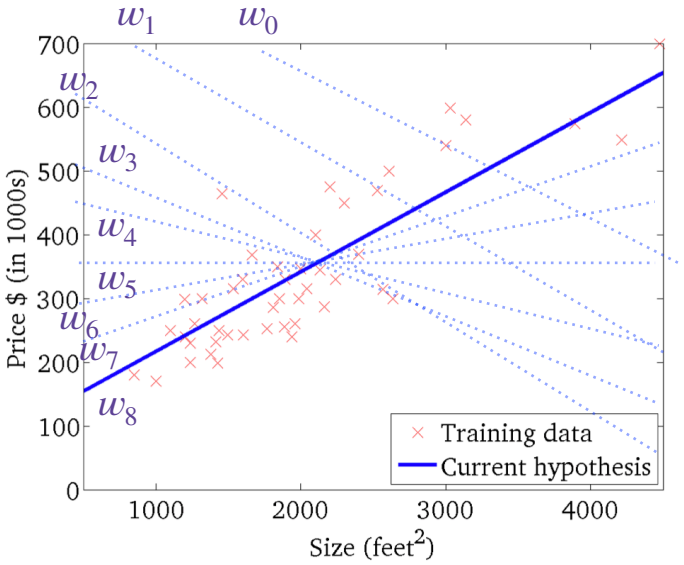


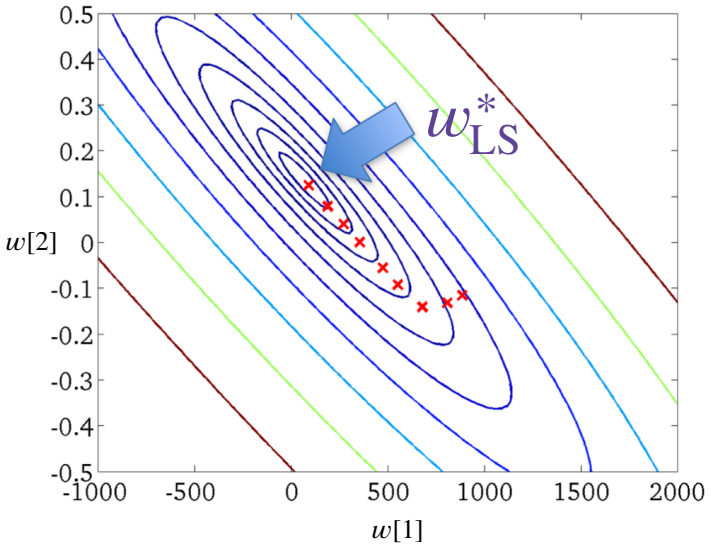
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GD for LS, analytically

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

f(w) or loss function

GD for LS, analytically

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

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from previous lectures

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from previous lectures

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how can we check if this is right?

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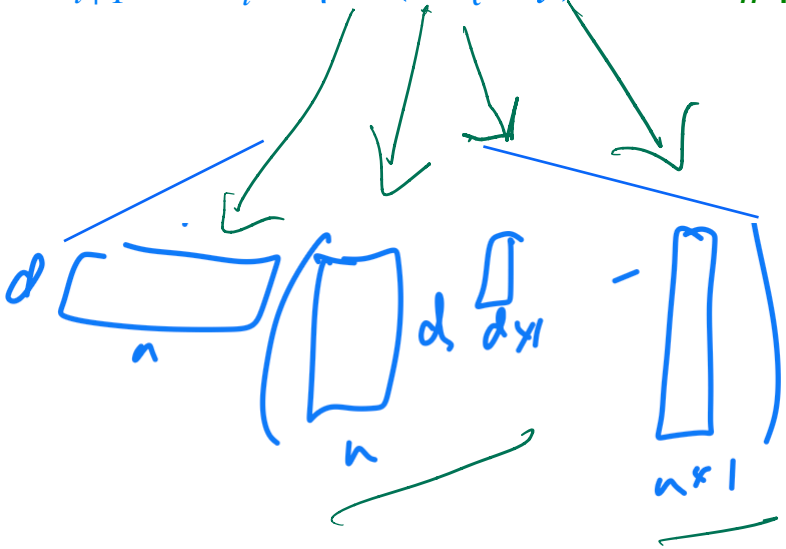
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$$\frac{d|w_i|}{dw_i} = \begin{cases} +1 & w_i > 0 \\ [-1, 1] & w_i = 0 \\ -1 & w_i < 0 \end{cases}$$

Gradient of absolute value is undefined at w=0, so define a sub gradient

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LASSO regularizer is convex. So?

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Local minima = global minimum

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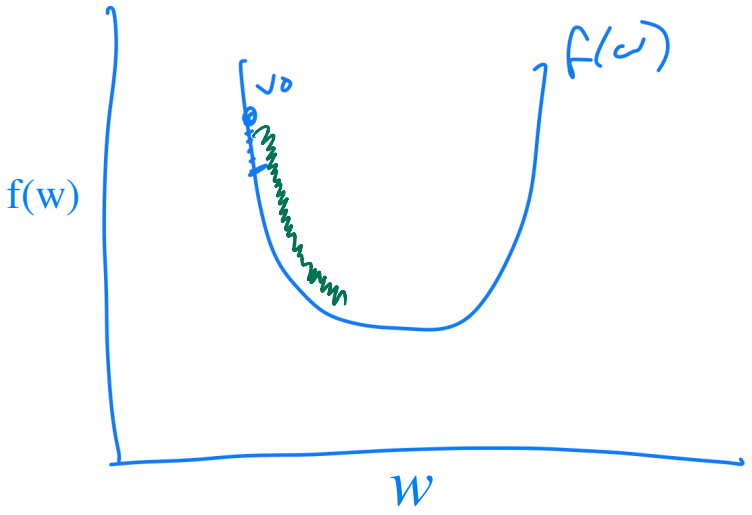
How do you choose a step size?

How do you choose a step size?

What can go wrong if η is too small?

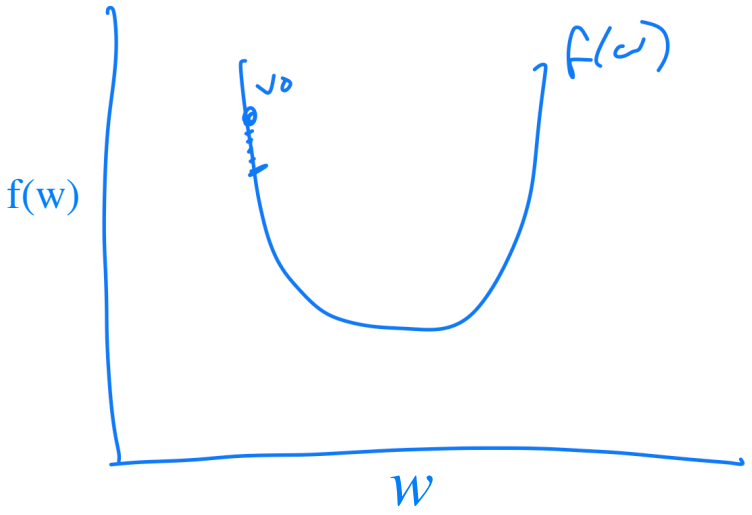
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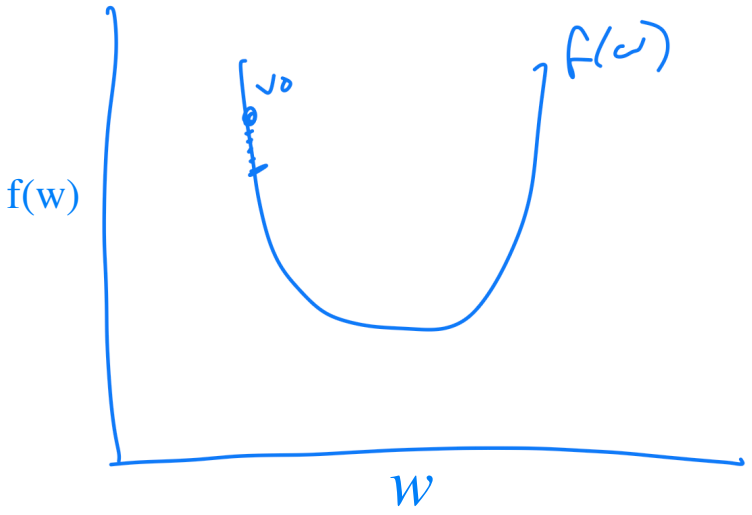
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Slow convergence

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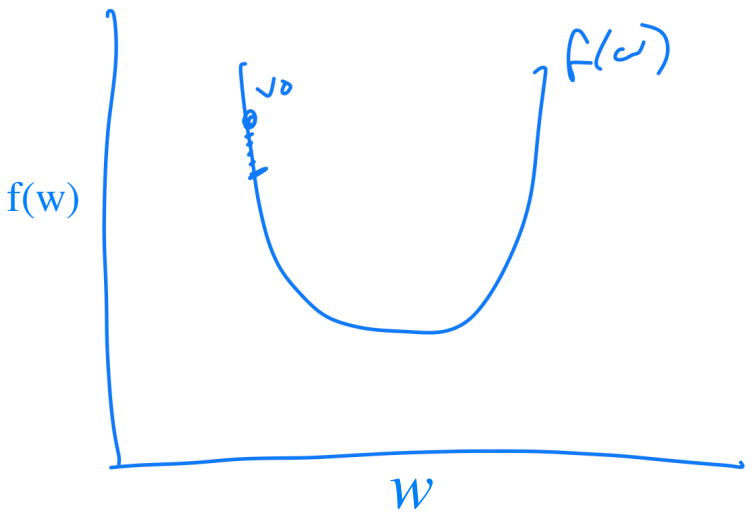


Slow convergence

What can go wrong if η is too large?

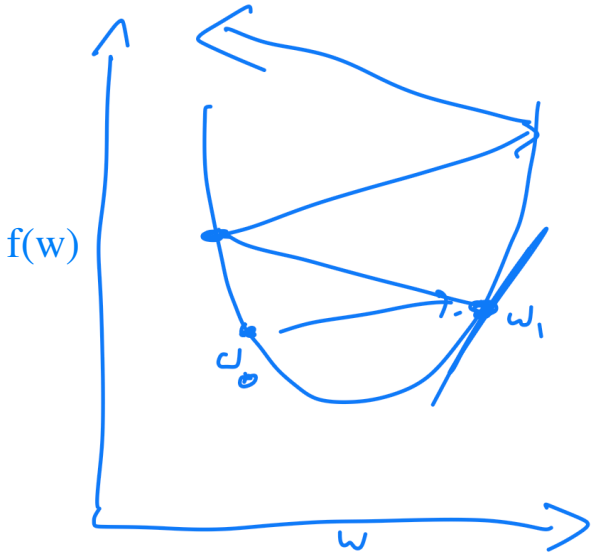
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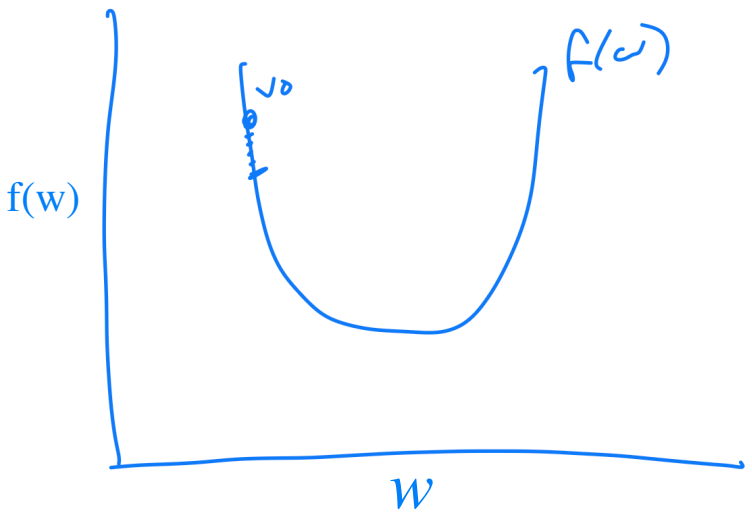
Slow convergence

What can go wrong if η is too large?



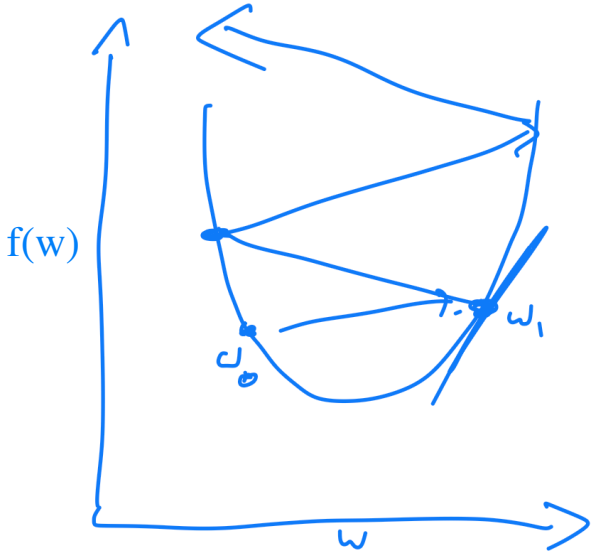
How do you choose a step size?

What can go wrong if η is too small?



Slow convergence

What can go wrong if η is too large?



Divergence!

How do you choose a step size?

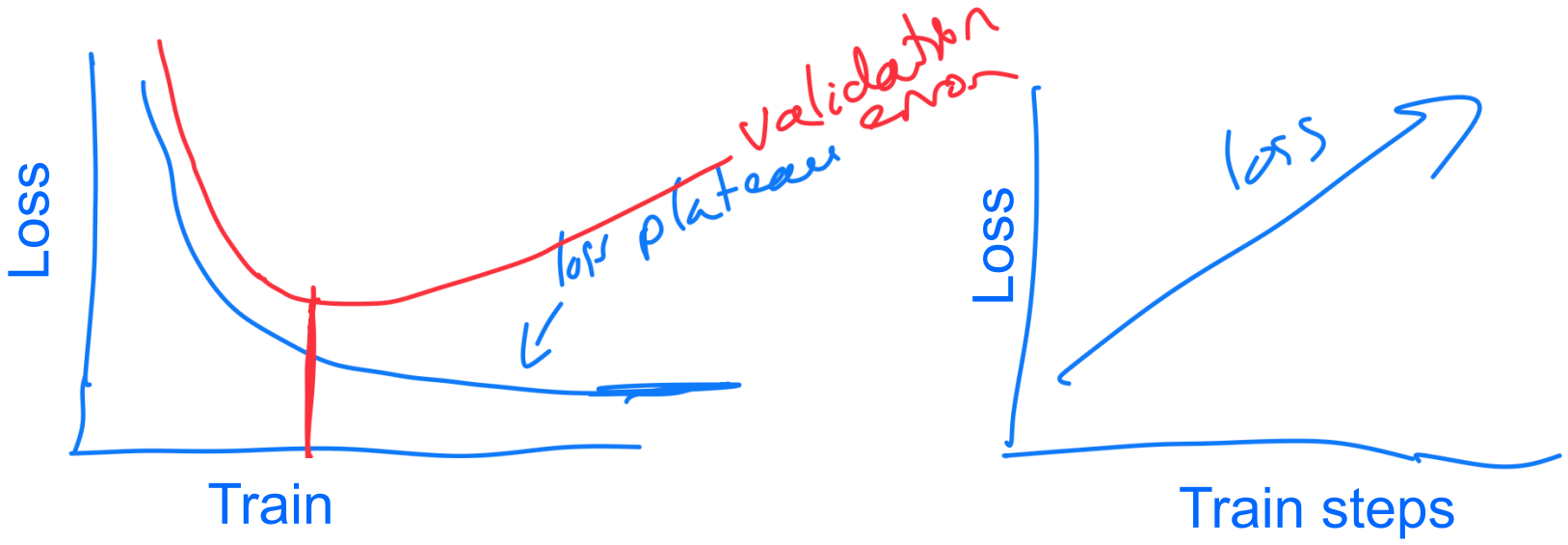
- In practice: guess and check

How do you choose a step size?

- In practice: guess and check # MAKE PLOTS

How do you choose a step size?

- In practice: guess and check # MAKE PLOTS



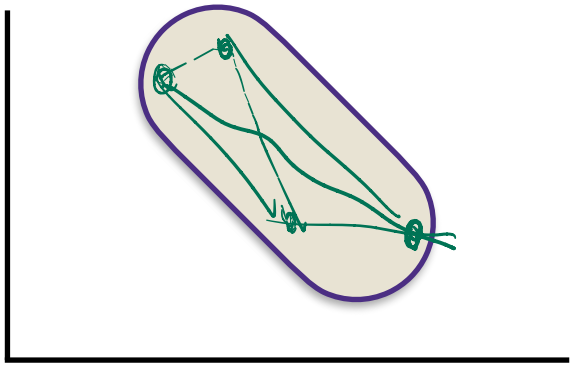
If I pick a learning rate η and observe the plot on the left, did I pick wrong?
What about the plot on the right?

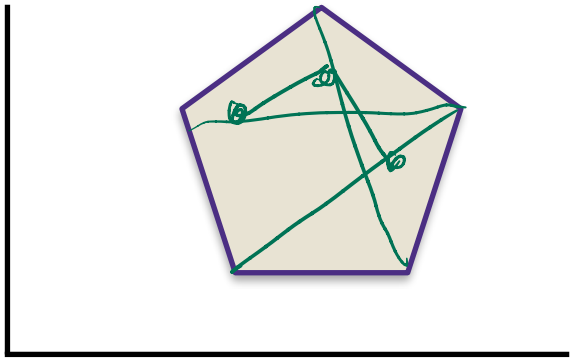
Convexity

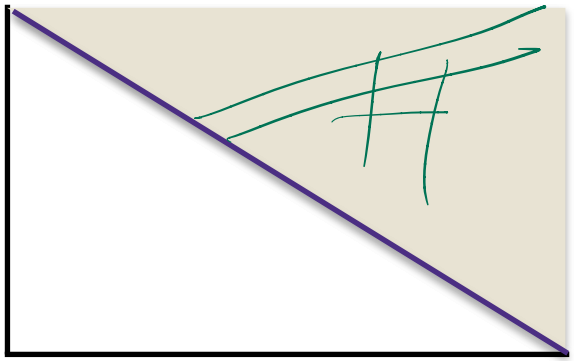
What is a convex set?

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

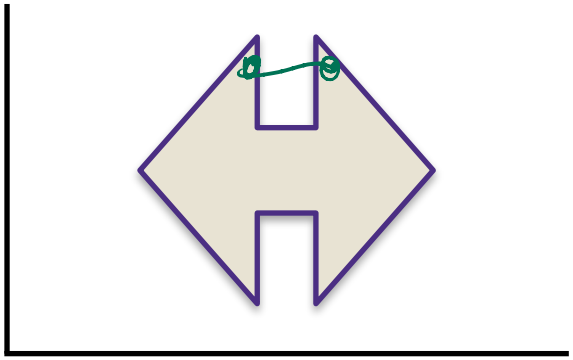
Examples of convex sets

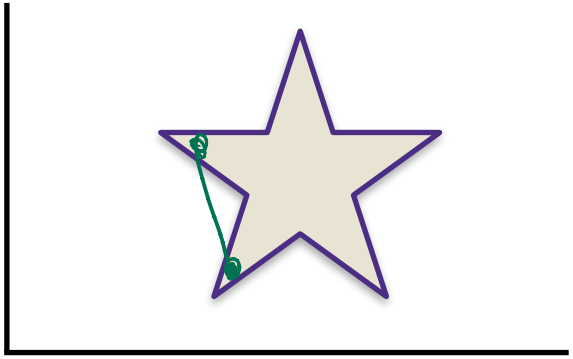


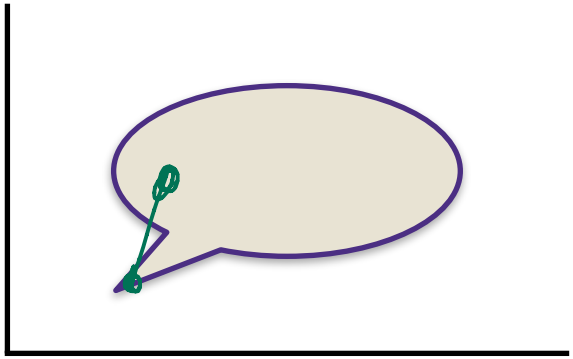




Examples of non-convex functions: anything else



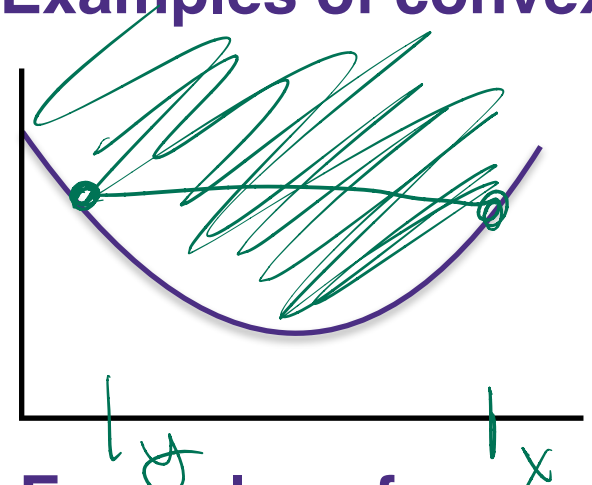


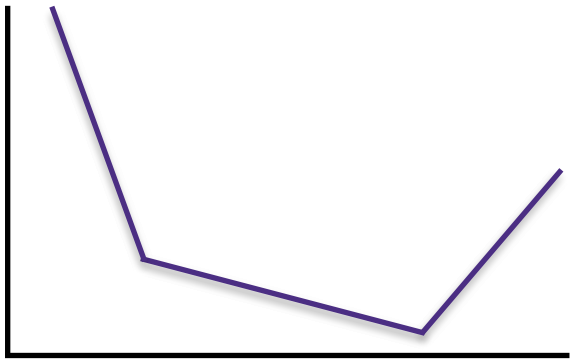


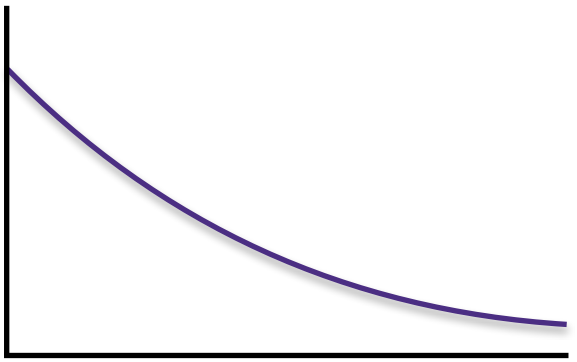
What is a convex function?

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 $x, y \in K$ and $\lambda \in [0, 1]$

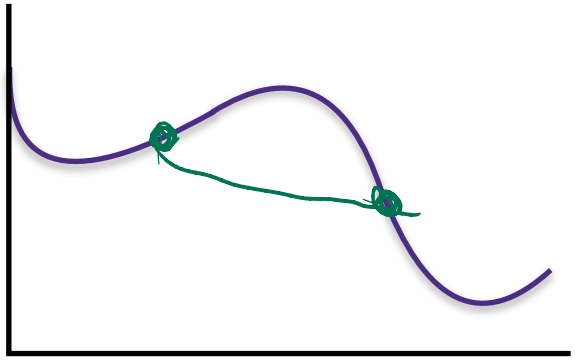
Examples of convex functions: "look like bowls"

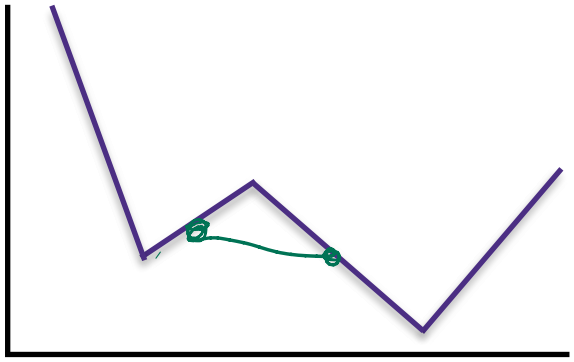


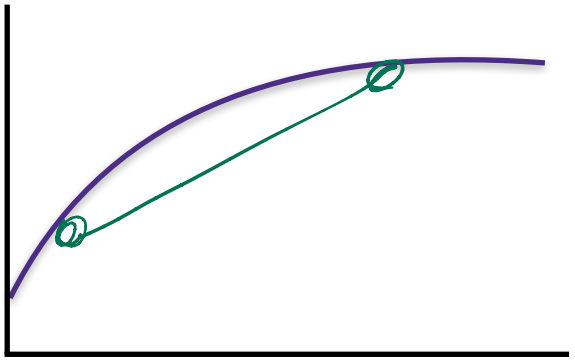




Examples of non-convex functions: anything else





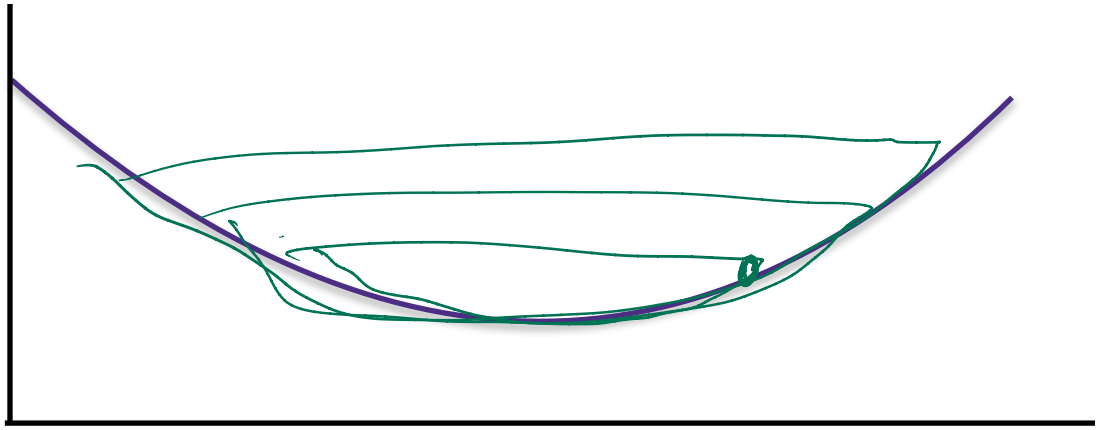


Convex functions and convex sets?

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

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 $x, y \in K$ and $\lambda \in [0,1]$

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

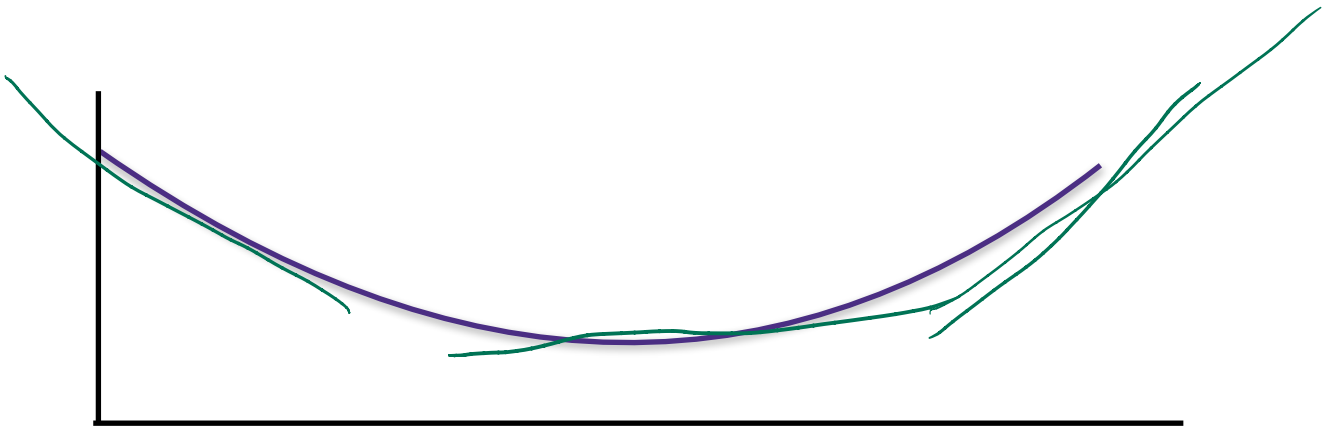


More definitions of convexity

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 $x, y \in K$ and $\lambda \in [0, 1]$

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 $x, y \in dom(f)$



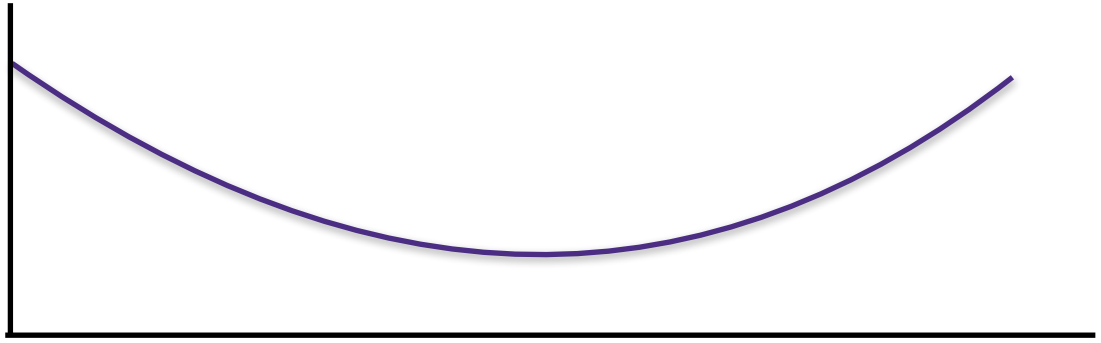
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A function $f : \mathbb{R}^d \to \mathbb{R}$ that is twice-differentiable everywhere is convex if $\nabla^2 f(x) \succeq 0$ for all $x \in dom(f)$

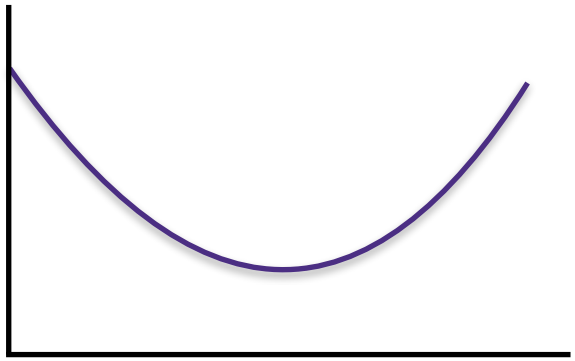


Why do we care about convexity?

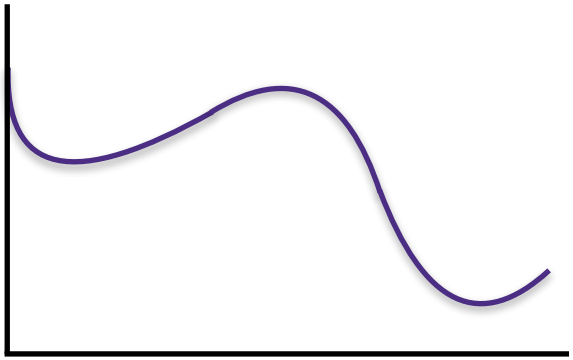
Convex functions

- All local minima are global minima
- Efficient to optimize (e.g., gradient descent)

Convex Function



Non-convex Function



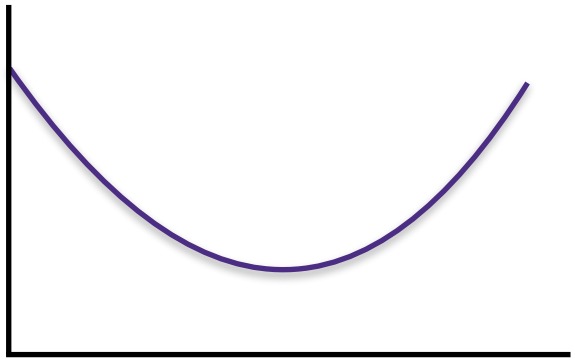
Gradient Descent

Initialize: $w_0 = 0$

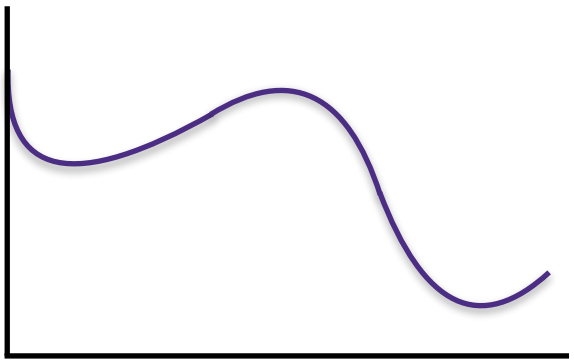
for $t = 1, 2, \ldots$

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

Convex Function



Non-convex Function



Sub-Gradient Descent

Initialize: $w_0 = 0$

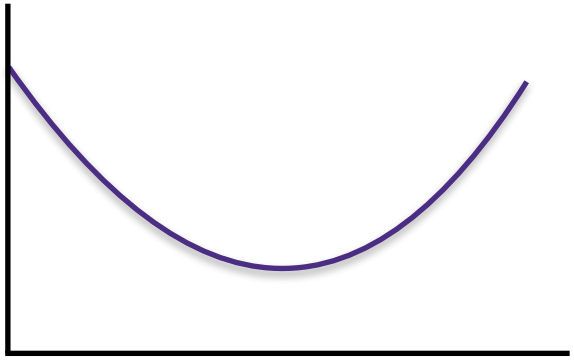
for $t = 1, 2, \ldots$

Find any g_t such that $f(y) \geq f(w_t) + g_t^\top (y - w_t)$

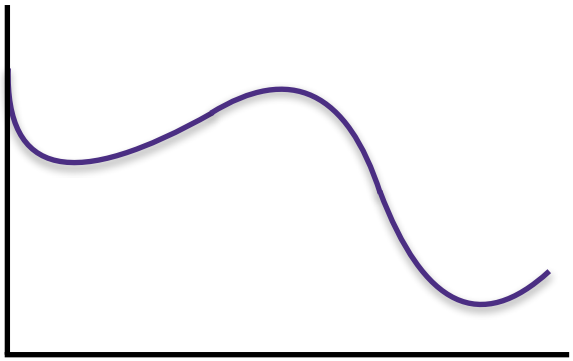
$w_{t+1} = w_t - \eta g_t$

g is a subgradient at x if $f(y) \geq f(x) + g^T (y - x)$

Convex Function



Non-convex Function



Coordinate descent

Initialize: $w_0 = 0$

for $t = 1, 2, \ldots$

Let $i_t = t \ \% \ n$

$$w_{t+1}^{(i_t)} = w_t^{(i_t)} - \eta_t \frac{\partial f(w)}{\partial w^{(i_t)}}\bigg|_{w=w_t}$$

Machine Learning Problems

- **Given data:**

$$\{(x_i, y_i)\}_{i=1}^{n} \qquad x_i \in \mathbb{R}^d \qquad y_i \in \mathbb{R}$$

- **Learning a model's parameters:** $\sum_{i=1}^{n} \ell_i(w)$

$$\text{Logistic Loss: } \ell_i(w) = \log(1 + \exp(-y_i\, x_i^T w))$$

$$\text{Squared error Loss: } \ell_i(w) = (y_i - x_i^T w)^2$$

Gradient Descent:

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

Optimization summary

- You can always run gradient descent whether f is convex or not. But you only have guarantees if f is convex
- Many bells and whistles can be added onto gradient descent such as momentum and dimension-specific step-sizes (Nesterov, Adagrad, ADAM, etc.)

Stochastic Gradient Descent

Gradient descent…

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Gradient descent… meet stochastic GD

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Stochastic Gradient Descent:

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

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

$$\mathbb{E}[\nabla \ell_{I_t}(w)] =$$

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E[Stochastic Gradient descent] = GD

- **Learning a model's parameters:** $\sum_{i=1}^{n} \ell_i(w)$

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

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- **How do we argue about GD/SGD's convergence?**

Stochastic Gradient Descent Convergence

Theorem: For Convex loss functions,

Let

Stochastic Gradient Descent Convergence

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If $\|w_1 - w_0\|_2^2 \leq R$

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If $\|w_1 - w_0\|_2^2 \le R$ and $\sup_w \max_i \|\nabla \ell_i(w)\|_2 \le G$ then

$$\mathbb{E}[\ell(\bar{w}) - \ell(w_*)] \le \frac{R}{2T\eta} + \frac{\eta G}{2} \le \sqrt{\frac{RG}{T}}$$

Stochastic Gradient Descent Convergence

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$$\eta = \sqrt{\frac{R}{GT}}$$

Averaging w_t

$$\bar{w} = \frac{1}{T}\sum_{t=1}^{T} w_t$$

(In practice use last iterate)

SGD convergence outline

SGD convergence outline

- Proof outline:
  - We'll argue that the gradient of the loss at time t is big if w_t's loss is big
  - Show that the weights at time t+1 are getting close to the optimum weights
    - By arguing about the update from time t to time t_+1

SGD Convergence: argue about update/gradients

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It’ll help to argue our update moves us towards OPT quickly if our loss is far from OPT

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Ignoring the second term and using our assmpt on how close we were to begin with

Stochastic Gradient Descent

Proof

Jensen's inequality:
For any random $Z \in \mathbb{R}^d$ and convex function $\phi : \mathbb{R}^d \to \mathbb{R}$, $\phi(\mathbb{E}[Z]) \leq \mathbb{E}[\phi(Z)]$

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Mini-batch SGD

Instead of one iterate, average B stochastic gradient together

Advantages:

- de-noises gradient
- Matrix computations
- Parallelization