Prediction pitfalls

Linear coefficients

Given data $\{(x_i, y_i)\}_{i=1}^n$ consider a linear model: $\widehat{\theta} = \arg\min_{\theta} \sum_{i=1}^{n} (y_i - \langle x_i, \theta \rangle)^2$

Claim: $\widehat{\theta}_j > \widehat{\theta}_1$ means feature i is more important than feature j to the model.

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False: if I rescaled jth dimension of data by some large constant (i.e., instead of square-feet, I change it to square-inches so that $x_{i,j} \rightarrow 144 x_{i,j}$) the magnitude of $\widehat{\theta}_j \rightarrow \widehat{\theta}_j / 144$ but the predictive power did not change!

This is why we frequently **normalize** our data by mean and variance:

$x_{i,j} \rightarrow (x_{i,j} - \mu_j)/\sigma_j$ where $\mu_j = \frac{1}{n} \sum_{i=1}^{n} x_{i,j}$ and $\sigma_j^2 = \frac{1}{n-1} \sum_{i=1}^{n} (x_{i,j} - \mu_j)^2$

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Claim: If $\widehat{\theta}_j = 0$ then the jth feature has no predictive power of target y

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Claim: If $\widehat{\theta}_j = 0$ then the *j*th feature has no predictive power of target y

False: Suppose feature 1 is #bathrooms and feature 2 is #toilets. Reasonable to assume these features extremely **correlated** so any choice of following gives same answer: $(\widehat{\theta}_1, \widehat{\theta}_2) = (\alpha, 0)$, $(\widehat{\theta}_1, \widehat{\theta}_2) = (0, \alpha)$, $(\widehat{\theta}_1, \widehat{\theta}_2) = (\frac{1}{3}\alpha, \frac{2}{3}\alpha)$

Correlation is not causation

Given data $\{(x_i, y_i)\}_{i=1}^n$ consider a linear model: $\widehat{\theta} = \arg\min_{\theta} \sum_{i=1}^{n} (y_i - \langle x_i, \theta \rangle)^2$

Claim: Suppose $\widehat{\theta}_j = 30{,}000$ and the jth feature represents #fireplaces. If I add m fireplaces in my house, I can expect to sell my house for $30{,}000m$ more!

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Claim: Suppose $\widehat{\theta}_j = 30{,}000$ and the jth feature represents #fireplaces. If I add m fireplaces in my house, I can expect to sell my house for $30{,}000m$ more!

False:

1) Correlation is not causation. If $\widehat{\theta}_j$ is large, it is correlated with the house price, but it is not necessarily the *cause* for the house price. More expensive houses are typically bigger and size correlates with more fireplaces.
Absurd example: fireman and fires seem to co-occur. Do fireman cause fire?

2) Train != Test dataset. A linear model may fit your data perfectly, but that doesn't mean it accurately extrapolates to data outside your training data. Moreover, this is impossible to know just using your training data.

How was the dataset collected?

Citizen reporting:
In the early 2010s, the city of Boston wanted to repair pot holes but wanted to allocate resources as efficiently as possible. So they released a smart phone app that automatically detects potholes via accelerometer data and sends back the GPS coordinates.

Claim: By fixing the potholes that are reported most frequently, resources are allocated to minimize the greatest number of total interactions with potholes

Crawford “The Hidden Biases in Big Data” https://hbr.org/2013/04/the-hidden-biases-in-big-data

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False. Counts are correlated with geographical areas with more smartphone ownership, which is correlated with wealthier areas versus those less wealthy or more elderly.

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ML automates bias of humans

Hiring example:
In an effort to avoid bias in its hiring practices, a company trains a machine learning model to predict Y from X where
X = resume
Y = whether applicant was hired, or job performance on the job

Claim: By using a data-driven process, any bias of the human resume screener is avoided.

https://www.reuters.com/article/us-amazon-com-jobs-automation-insight/amazon-scraps-secret-ai-recruiting-tool-that-showed-bias-against-women-idUSKCN1MK08G

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Claim: By using a data-driven process, any bias of the human resume screener is avoided.

False. The label Y (e.g., job performance) was evaluated by a human. If bias existed in these labels then all you've done is automated a system that is just as biased.

https://www.reuters.com/article/us-amazon-com-jobs-automation-insight/amazon-scraps-secret-ai-recruiting-tool-that-showed-bias-against-women-idUSKCN1MK08G

Further reading

Excellent textbook:
"*Fairness and Machine learning*" Solon Barocas, Moritz Hardt, Arvind Narayanan https://fairmlbook.org/

Relevant conferences:
ACM Conference on Fairness, Accountability, and Transparency https://facctconference.org/

Gradient Descent

- how are we going to find the solution for

$$\arg\min_{b,w} \sum_{i=1}^{n} \ell(b + w^T x_i, y_i)$$

- e.g., Lasso, Logistic Regression do not have closed form solution for

$$\nabla_{b,w} \mathcal{L}(b, w) = 0$$

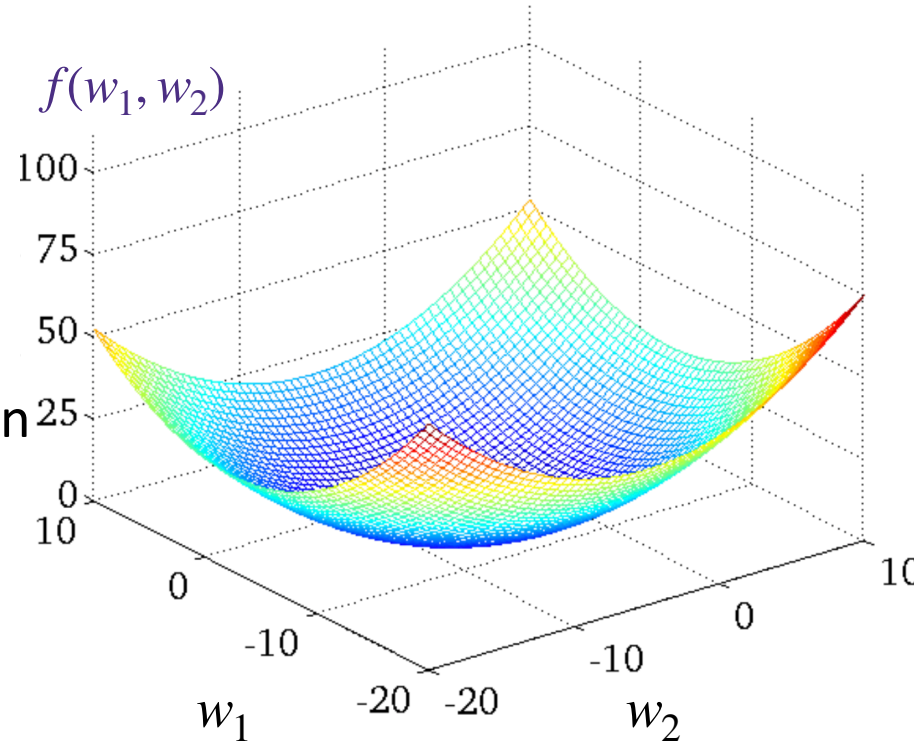
Running example: linear regression

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

- **Learning model parameters:**

$$\hat{w}_{\text{LS}} = \arg\min_{w \in \mathbb{R}^d} \underbrace{\|\mathbf{y} - \mathbf{X}w\|_2^2}_{f(w)}$$

- Although we know the optimal solution in a closed form, we will use this as a running example to understand GD



1-dimensional gradient descent

Let w_0 be an initial guess. How can we improve this solution?

Taylor series approximation:
For w very close to w_0 we have

$$f(w_0) + (w - w_0)\frac{df(w)}{dw}\Big|_{w=w_0}$$

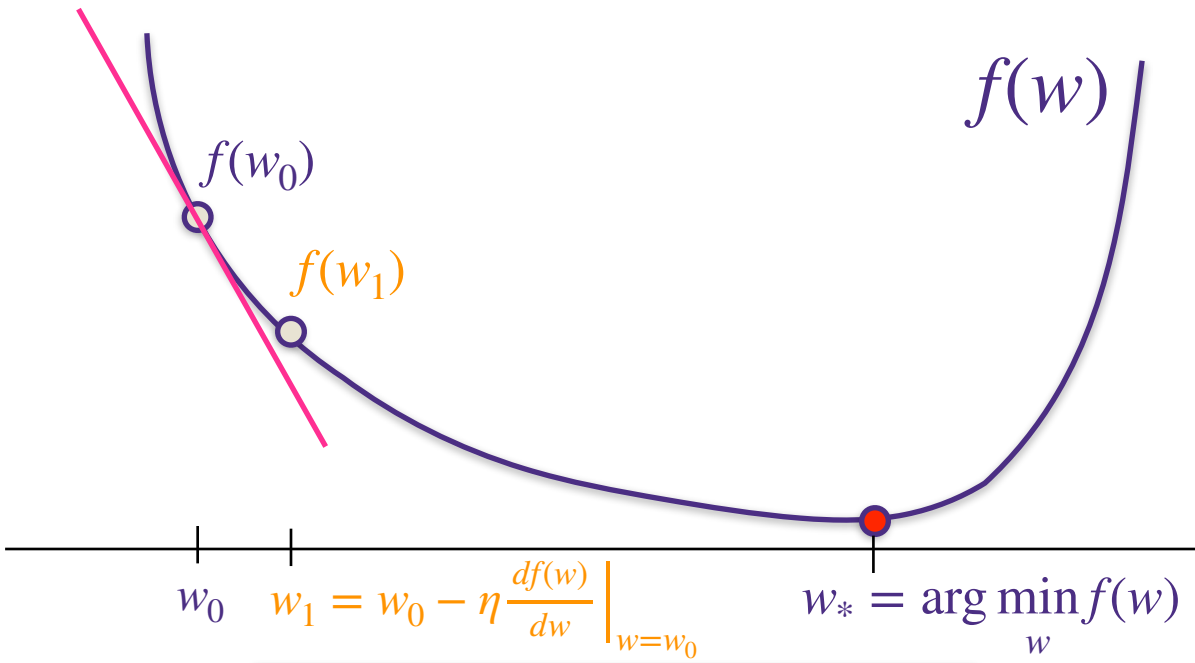
is very close to $f(w)$

Thus, for very small $\eta > 0$,

if $w_1 = w_0 - \eta \frac{df(w)}{dw}\Big|_{w=w_0}$ then

$$f(w_0) - \eta\left(\frac{df(w)}{dw}\Big|_{w=w_0}\right)^2$$

is very close to $f(w_1) < f(w_0)$



Gradient descent
For k=0,1,2,3,...

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

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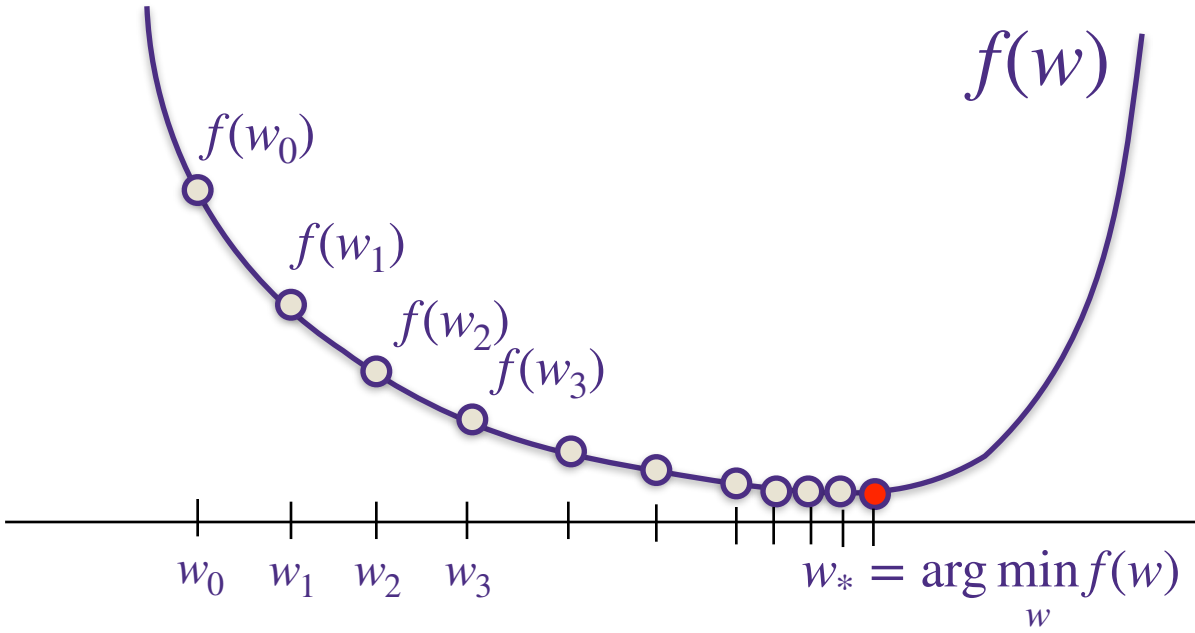


Gradient descent
For k=0,1,2,3,...

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

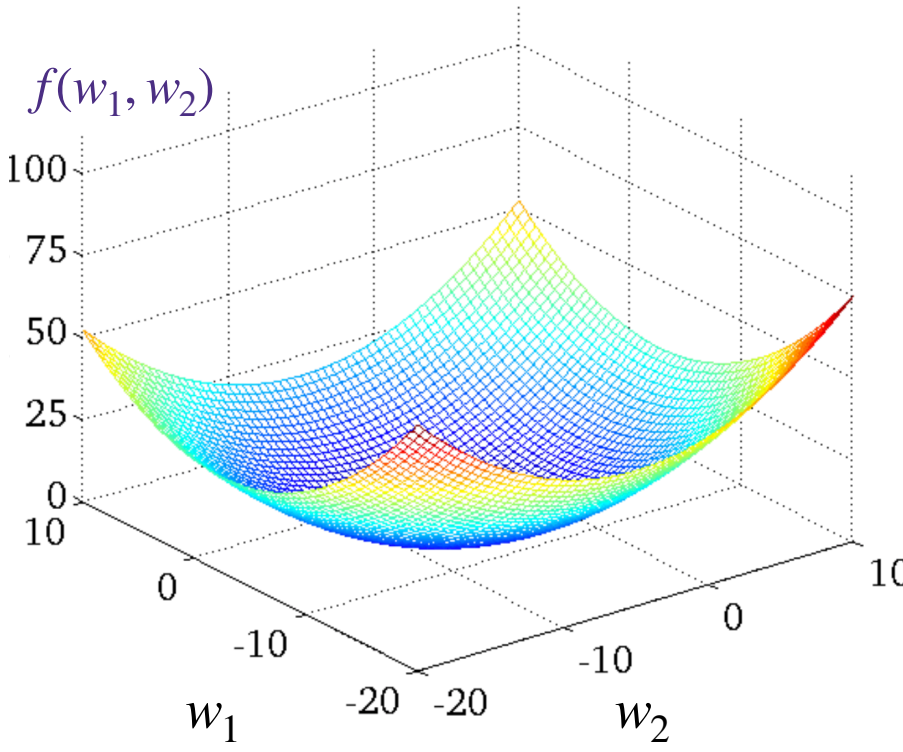
Note that as $k \to \infty$ we have $\frac{df(w)}{dw}\Big|_{w=w_k} \to 0$

Running example: linear regression

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

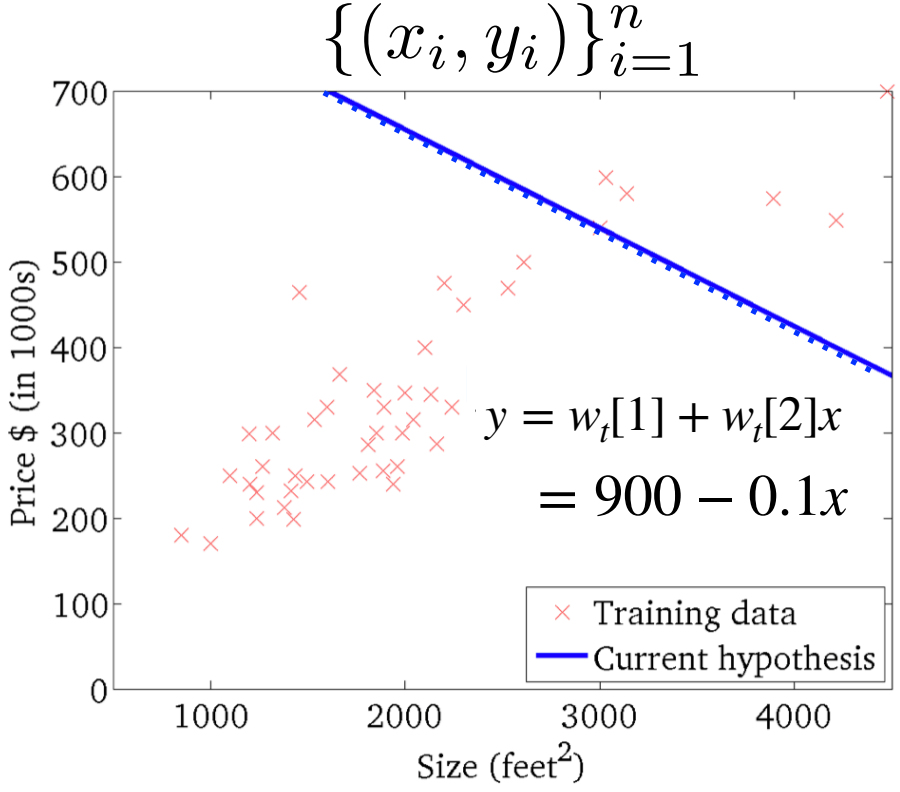
- **Learning model parameters:**

$$\hat{w}_{\text{LS}} = \arg\min_{w \in \mathbb{R}^d} \underbrace{\|\mathbf{y} - \mathbf{X}w\|_2^2}_{f(w)}$$

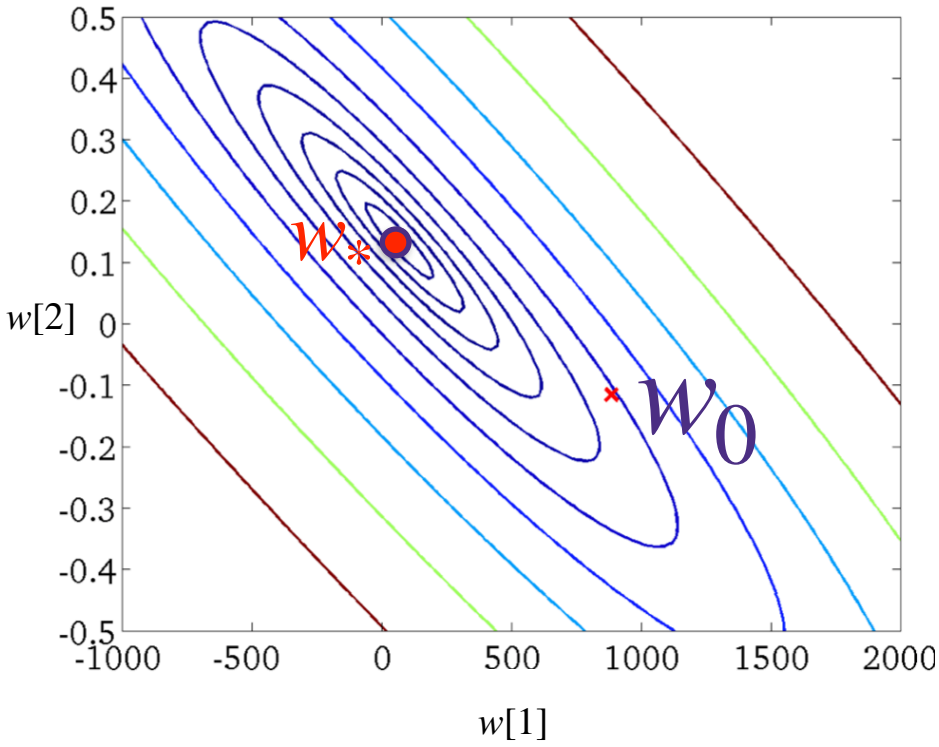


- **Gradient descent:**
  - Initialize: $w_0 = 0$
  - **For** t=0,1,2,…
    - $w_{t+1} \leftarrow w_t - \eta \cdot \nabla_w f(w_t)$

- $w_0 = (900, -0.1)$
- **For** t=0,1,2,…
  - $w_{t+1} \leftarrow w_t - \eta \cdot \nabla_w f(w_t)$



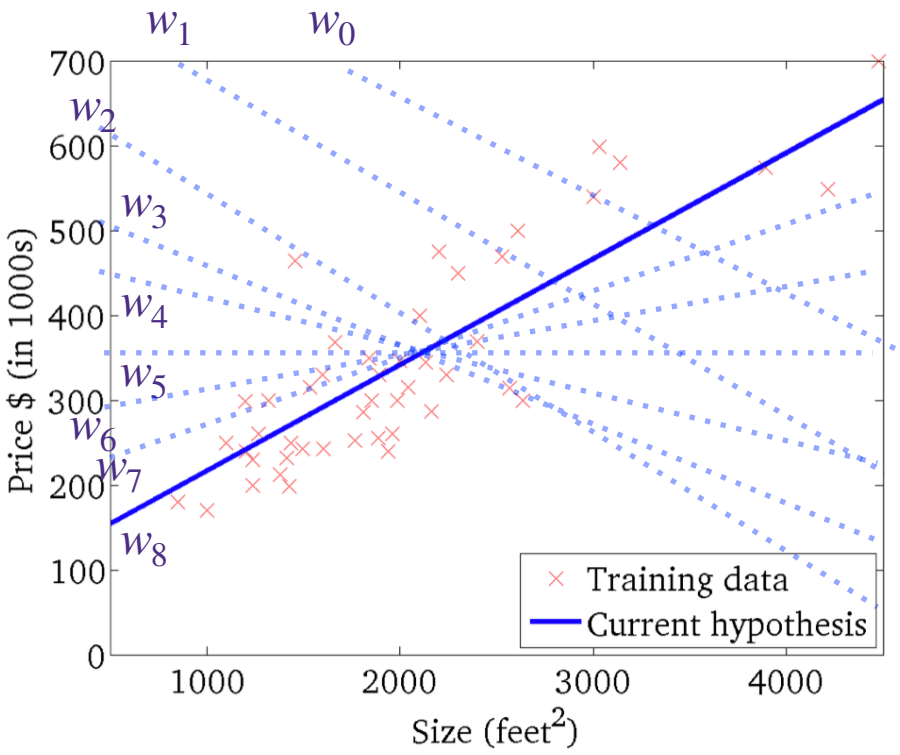
Evolution of the predictor



GD dynamics in the Parameter space

- Which direction will the GD move?

- $w_0 = (900, -0.1)$
- **For** t=0,1,2,…
  - $w_{t+1} \leftarrow w_t - \eta \cdot \nabla_w f(w_t)$



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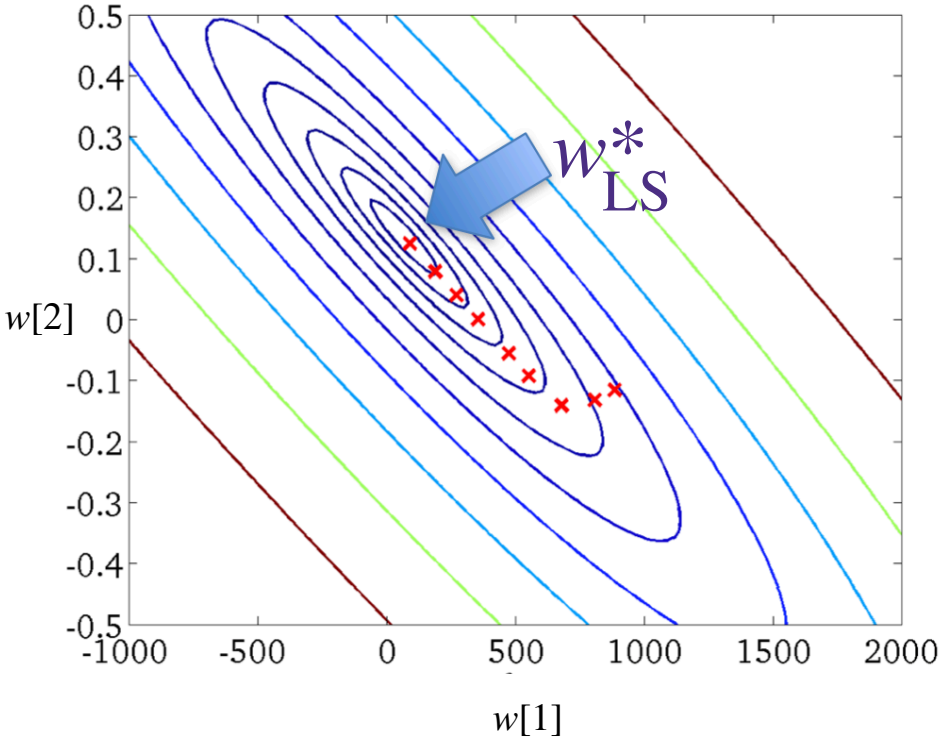

GD dynamics in the Parameter space

Gradient descent for linear regression

- In this example of linear regression, we can derive exactly the gradient descent trajectory
- Initialize: $w_0 = 0$
- **For** t=0,1,2,…
  - $w_{t+1} \leftarrow w_t - \eta \cdot \nabla_w f(w_t)$

For linear regression, we have

$$\hat{w}_{\text{LS}} = \arg\min_{w \in \mathbb{R}^d} \underbrace{\|\mathbf{y} - \mathbf{X}w\|_2^2}_{f(w)}$$

$$\nabla f(w_t) = -2\mathbf{X}^T(\mathbf{y} - \mathbf{X}w_t)$$

$$w_{t+1} = w_t + \eta 2\mathbf{X}^T(\mathbf{y} - \mathbf{X}w_t) = (\mathbf{I} - 2\eta\mathbf{X}^T\mathbf{X})w_t + 2\eta\mathbf{X}^T\mathbf{y}$$

Let the least-squares solution be $w^* = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$

$$\begin{aligned} w_{t+1} - w^* &= (\mathbf{I} - 2\eta\mathbf{X}^T\mathbf{X})w_t + 2\eta\mathbf{X}^T\mathbf{y} - w^* \\ &= (\mathbf{I} - 2\eta\mathbf{X}^T\mathbf{X})(w_t - w^*) + 2\eta\mathbf{X}^T\mathbf{y} - 2\eta\mathbf{X}^T\mathbf{X}w^* \\ &= (\mathbf{I} - 2\eta\mathbf{X}^T\mathbf{X})(w_t - w^*) \end{aligned}$$

How do you choose step size?

Let w_0 be an initial guess. How can we improve this solution?

Taylor series approximation:
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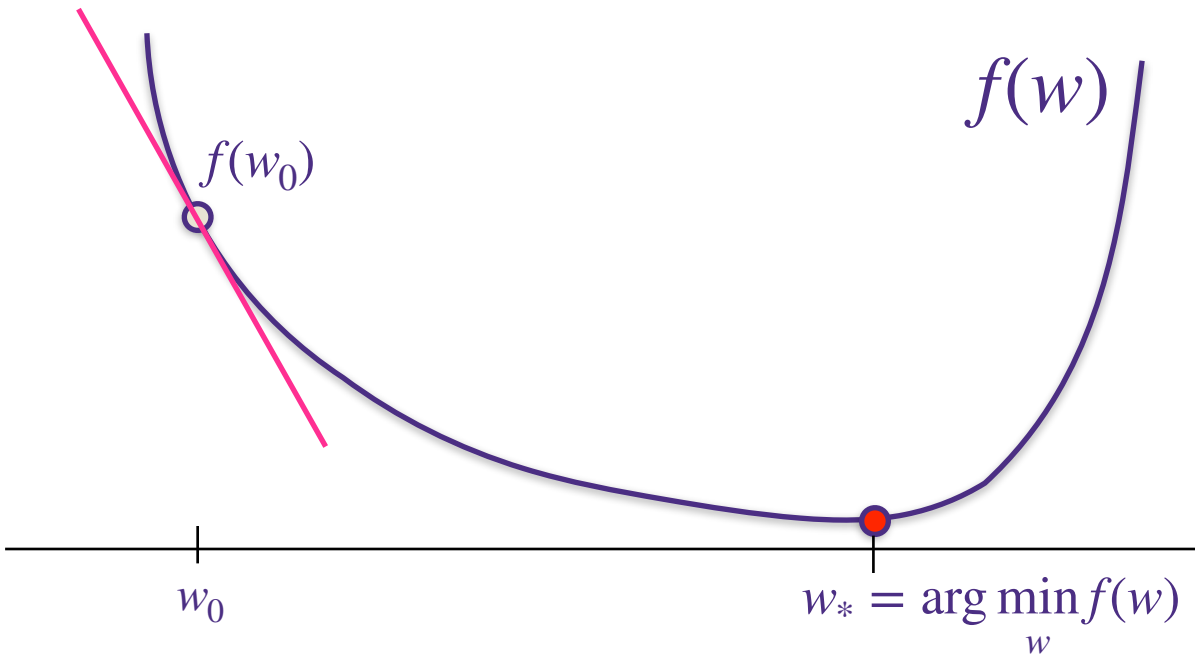

If η too big, does not converge!

If η too small, converges very, very slowly.

In practice: choose the largest value of η that converges (guess and check)

Gradient descent for Ridge regression

- Initialize: $w_0 = 0$
- **For** t=0,1,2,…
  - $w_{t+1} \leftarrow w_t - \eta \cdot \nabla_w f(w_t)$

For Ridge we have

$$\hat{w}_{\text{Ridge}} = \arg\min_{w \in \mathbb{R}^d} \underbrace{\frac{1}{2}\|\mathbf{y} - \mathbf{X}w\|_2^2 + \frac{\lambda}{2}\|w\|_2^2}_{f(w)}$$

$$\nabla f(w_t) = -\mathbf{X}^T(\mathbf{y} - \mathbf{X}w_t) + \lambda w_t$$

$$w_{t+1} = (1 - \lambda)w_t + \eta \mathbf{X}^T(\mathbf{y} - \mathbf{X}w_t)$$

Gradient descent for Lasso regression

- Initialize: $w_0 = 0$
- **For** t=0,1,2,…
  - $w_{t+1} \leftarrow w_t - \eta \cdot \nabla_w f(w_t)$

For Lasso we have

$$\hat{w}_{\text{Lasso}} = \arg\min_{w \in \mathbb{R}^d} \underbrace{\frac{1}{2}\|\mathbf{y} - \mathbf{X}w\|_2^2 + \lambda\|w\|_1}_{f(w)}$$

$$\nabla f(w_t) = -\mathbf{X}^T(\mathbf{y} - \mathbf{X}w_t) + \lambda \text{sign}(w_t)$$

$$w_{t+1} = w_t + \eta\mathbf{X}^T(\mathbf{y} - \mathbf{X}w_t) - \lambda \text{sign}(w_t)$$

Stochastic Gradient Descent

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:** $\sum_{i=1}^{n} \ell_i(w)$

Gradient Descent:

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

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

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

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

Stochastic Gradient Descent

Theorem

Let $w_{t+1} = w_t - \eta \nabla_w \ell_{I_t}(w)\Big|_{w=w_t}$ I_t drawn uniform at random from $\{1, \dots, n\}$ so that

$$\mathbb{E}\big[\nabla \ell_{I_t}(w)\big] = \frac{1}{n}\sum_{i=1}^{n} \nabla \ell_i(w) =: \nabla \ell(w)$$

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

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

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

(In practice use last iterate)

Stochastic Gradient Descent

Proof

$$\mathbb{E}[||w_{t+1} - w_*||_2^2] = \mathbb{E}[||w_t - \eta \nabla \ell_{I_t}(w_t) - w_*||_2^2]$$

Stochastic Gradient Descent

Proof

$$\mathbb{E}[||w_{t+1} - w_*||_2^2] = \mathbb{E}[||w_t - \eta \nabla \ell_{I_t}(w_t) - w_*||_2^2]$$

$$= \mathbb{E}[||w_t - w_*||_2^2] - 2\eta \mathbb{E}[\nabla \ell_{I_t}(w_t)^T (w_t - w_*)] + \eta^2 \mathbb{E}[||\nabla \ell_{I_t}(w_t)||_2^2]$$

$$\leq \mathbb{E}[||w_t - w_*||_2^2] - 2\eta \mathbb{E}[\ell(w_t) - \ell(w_*)] + \eta^2 G$$

$$\mathbb{E}[\nabla \ell_{I_t}(w_t)^T (w_t - w_*)] = \mathbb{E}\big[\mathbb{E}[\nabla \ell_{I_t}(w_t)^T (w_t - w_*) | I_1, w_1, \ldots, I_{t-1}, w_{t-1}]\big]$$

$$= \mathbb{E}\big[\nabla \ell(w_t)^T (w_t - w_*)\big]$$

$$\geq \mathbb{E}\big[\ell(w_t) - \ell(w_*)\big]$$

$$\sum_{t=1}^{T} \mathbb{E}[\ell(w_t) - \ell(w_*)] \leq \frac{1}{2\eta} \left(\mathbb{E}[||w_1 - w_*||_2^2] - \mathbb{E}[||w_{T+1} - w_*||_2^2] + T\eta^2 G\right)$$

$$\leq \frac{R}{2\eta} + \frac{T\eta G}{2}$$

Stochastic Gradient Descent

Proof

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

$$\mathbb{E}[\ell(\bar{w}) - \ell(w_*)] \leq \frac{1}{T} \sum_{t=1}^{T} \mathbb{E}[\ell(w_t) - \ell(w_*)] \qquad \bar{w} = \frac{1}{T} \sum_{t=1}^{T} w_t$$

Mini-batch SGD

- Instead of one iterate, average B stochastic gradient together

- Advantages:
  - Smaller variance: the variance of the stochastic gradient is smaller by a factor of $1/\sqrt{B}$
  - Parallelization: each gradient in the mini-batch can be computed in parallel

- If you have regularizer, $\frac{1}{n}\sum_{i=1}^{n} \ell_i(w) + r(w)$, then update with the stochastic gradient of the loss and gradient of the regularizer

Questions?

Memory vs compute

```
# generate some nonsense data for an example
X = np.random.randn(n,d)
y = np.random.randn(n)
```

```
# generate the random features
G = np.random.randn(p, d)*np.sqrt(.1)
b = np.random.rand(p)*2*np.pi
```

```
H = np.dot(X, G.T) + b.T
HTH = np.dot(H.T, H)
HTy = np.dot(H.T, y)
```

```
# construct HTH
HTH = np.zeros((p,p))
HTy = np.zeros(p)
for i in range(n):
    hi = np.dot(X[i,:], G.T)+b
    HTH += np.outer(hi, hi)
    HTy += y[i]*hi
    if i % 1000==0: print(i)
```

```
# construct HTH
HTH = np.zeros((p,p))
HTy = np.zeros(p)
block = p
for i in range(int(np.ceil(n/block))+1):
    Hi = np.dot(X[i*block:min(n,(i+1)*block),:], G.T)+b
    HTH += np.dot(Hi.T, Hi)
    HTy += np.dot(Hi.T, y[i*block:min(n,(i+1)*block)])
```

```
w = np.linalg.solve(HTH + lam*np.eye(p), HTy)
```

1 float in NumPy = 8 bytes

$10^6 \approx 2^{20}$ bytes = 1 MB

$10^9 \approx 2^{30}$ bytes = 1 GB

For each block compute the memory required in terms of n, p, d.

If d << p << n, what is the most memory efficient program (blue, green, red)?

If you have unlimited memory, what do you think is the fastest program?

Convexity

- When is an optimization (or learning) easy/fast to solve?

Recap: Ridge vs. Lasso

- **Ridge**

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

  - Very fast:
    - Closed form solution if used with linear models
    - Even with other loss functions, optimization is fast for squared ℓ_2 regularization, because $\|w\|_2^2$ is **convex and smooth**

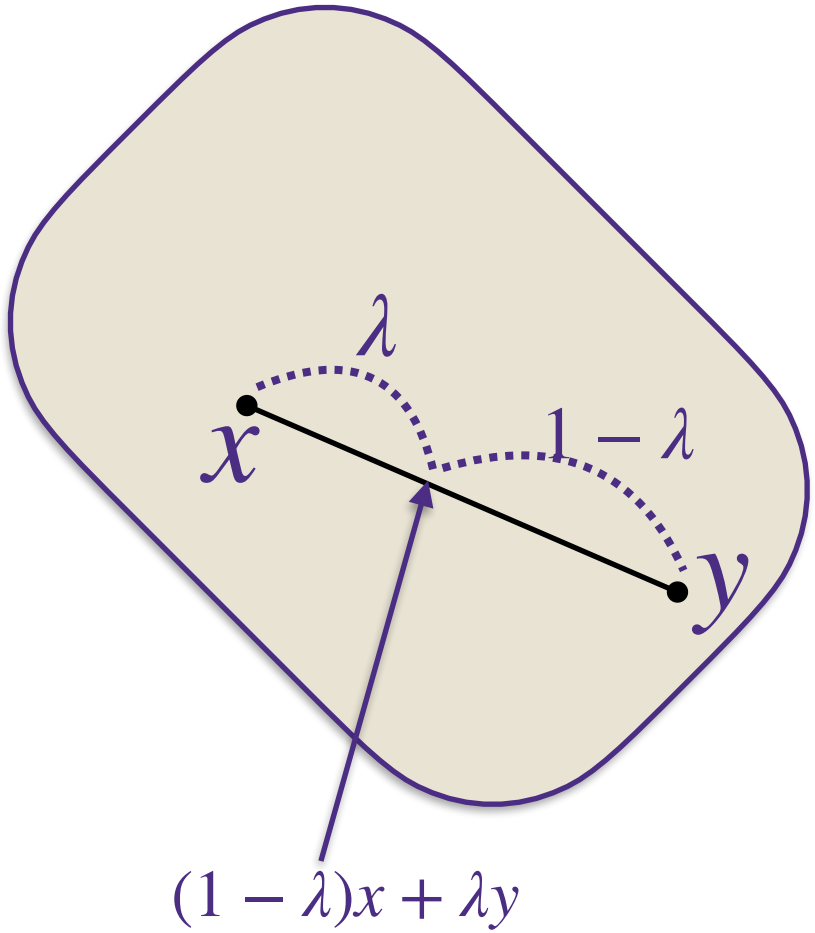
- **Lasso**

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

  - Slower than Ridge:
    - Requires iterative optimization algorithm like sub-gradient descent
    - In particular, it is slower because $\|w\|_1$ is **convex but non-smooth**

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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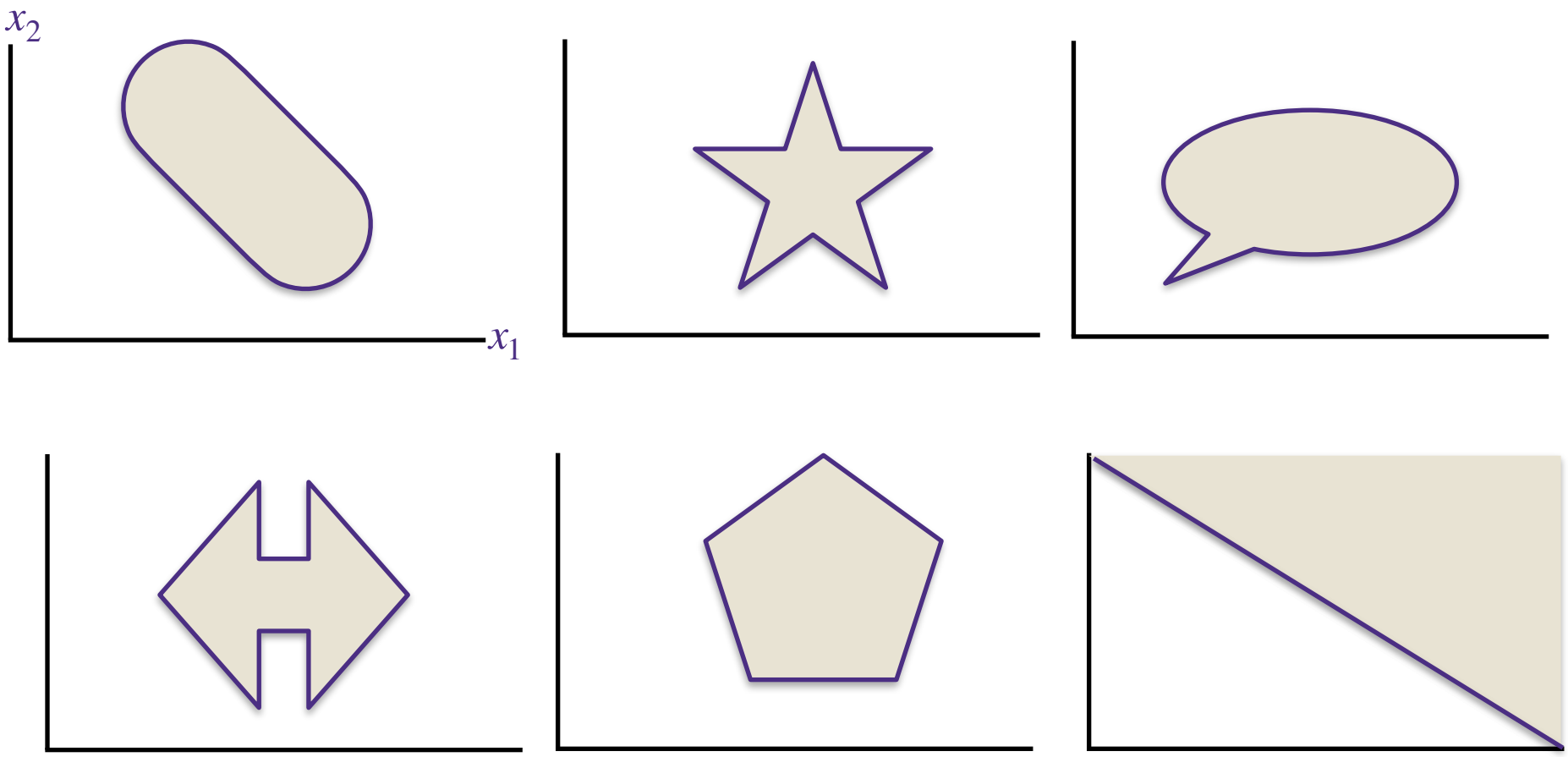
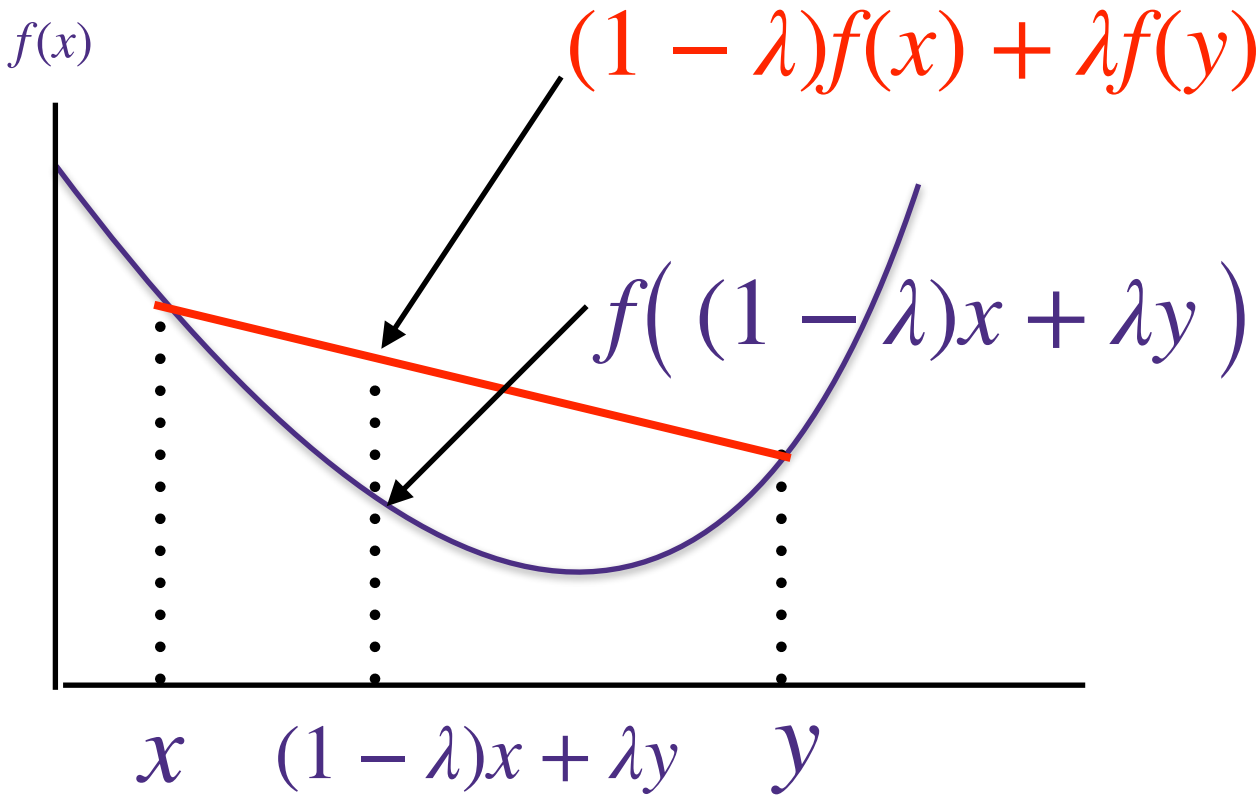


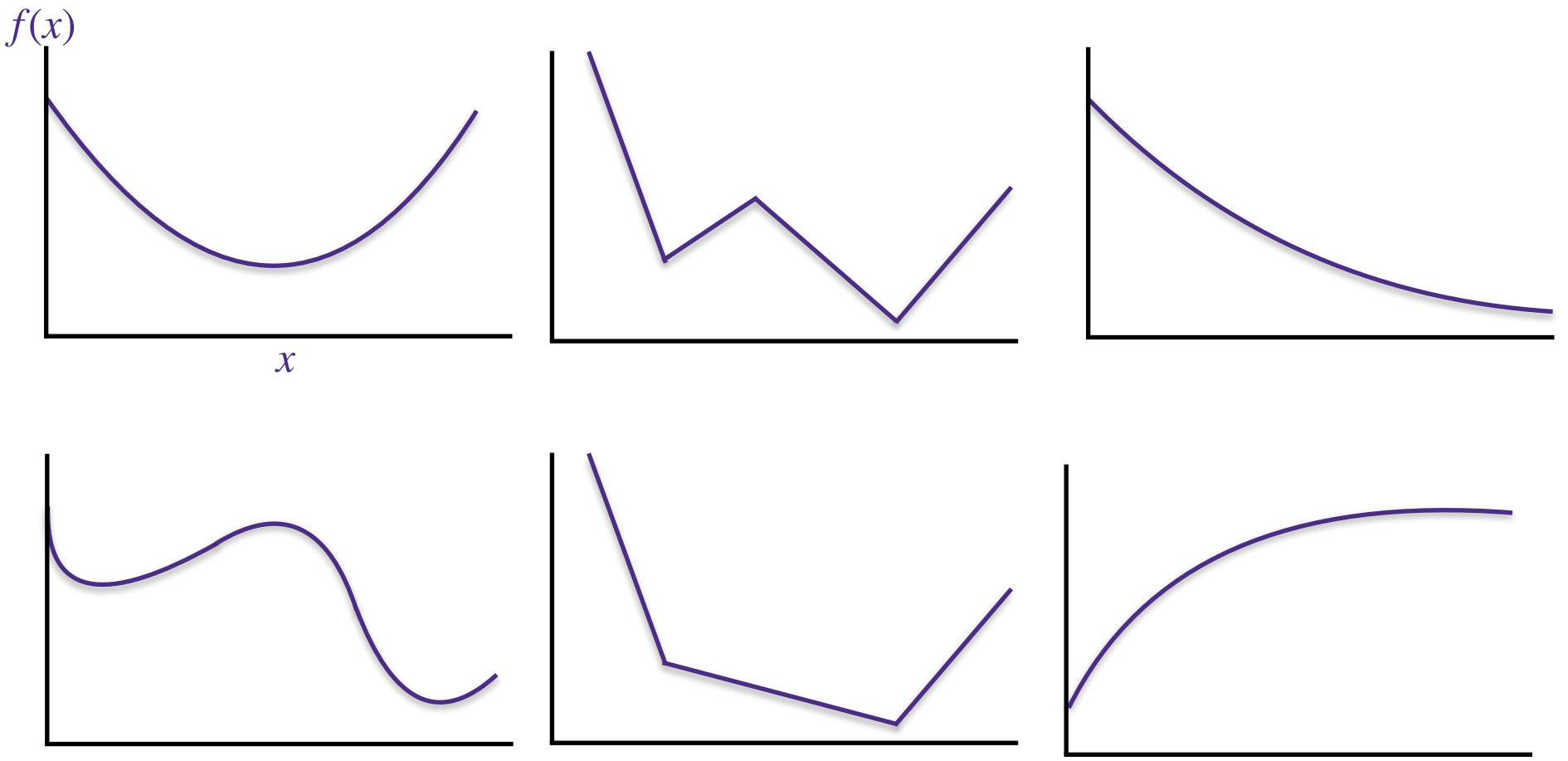
What is a convex function?

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 $\lambda \in [0, 1]$



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 $\lambda \in [0, 1]$



Convex functions and convex sets?

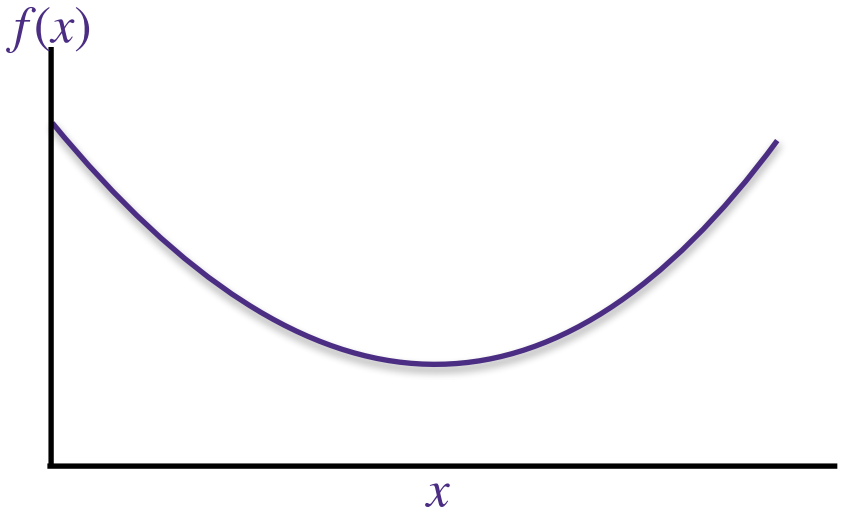
A set $K \subset \mathbb{R}^d$ is convex if $(1-\lambda)x + \lambda y \in K$ for all $x, y \in K$ and $\lambda \in [0,1]$

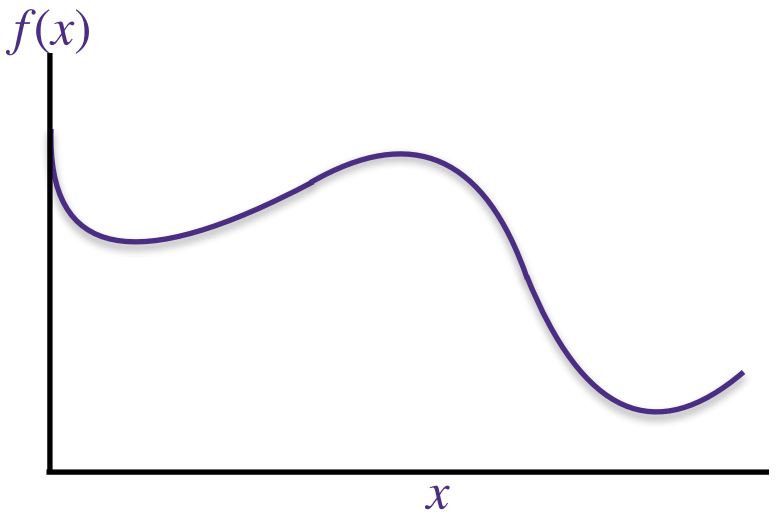
A function $f : \mathbb{R}^d \to \mathbb{R}$ is convex if $f((1-\lambda)x + \lambda y) \leq (1-\lambda)f(x) + \lambda f(y)$ for all $x, y \in \mathbb{R}^d$ and $\lambda \in [0,1]$

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

Graph of f id defined as $\{(x,t) \ : \ f(x) = t\}$

Epigraph of f is defined as $\{(x,t) \ : \ f(x) \leq t\}$





More definitions of convexity

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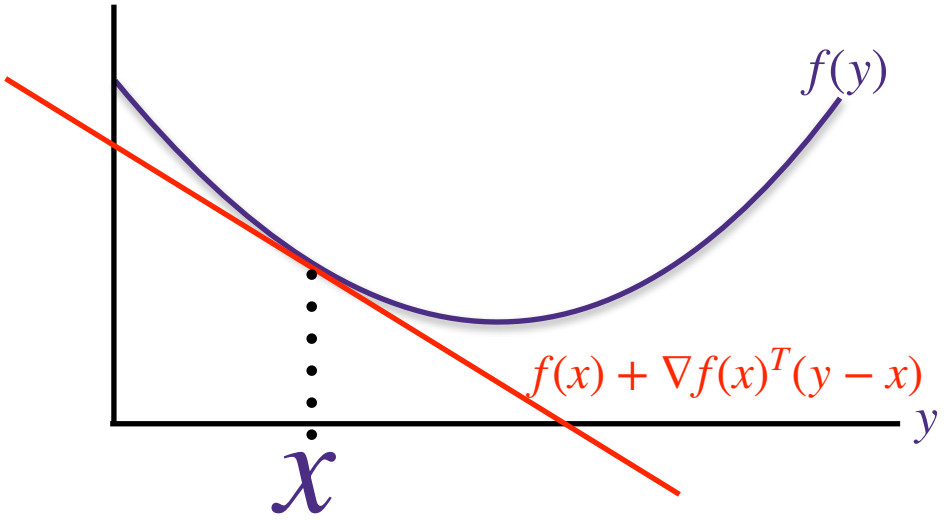
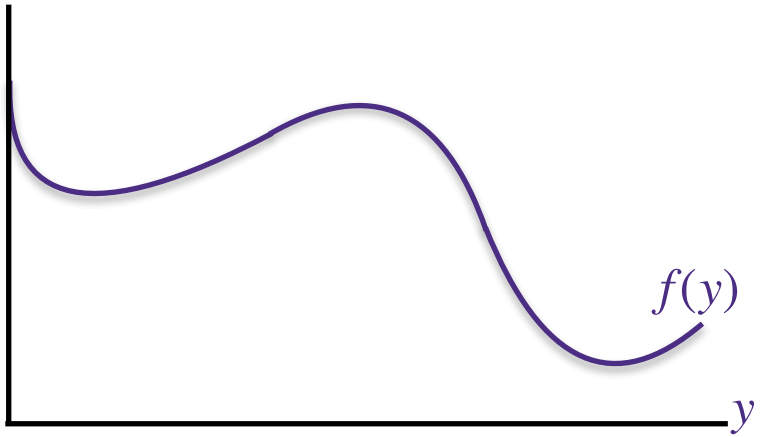
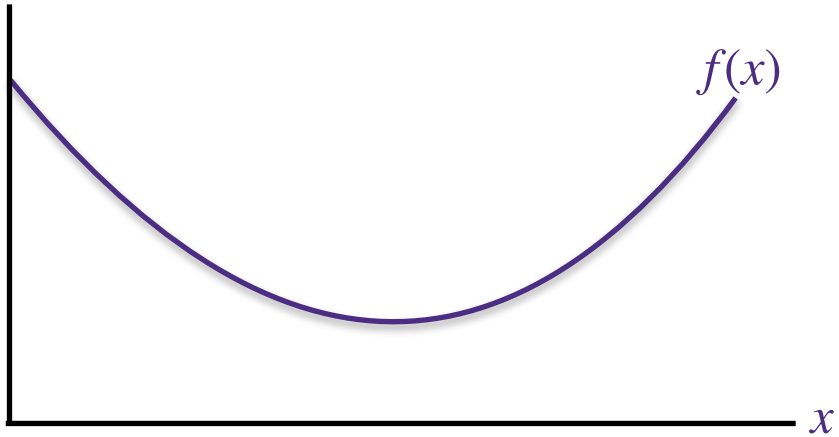
A function $f : \mathbb{R}^d \to \mathbb{R}$ that is differentiable everywhere is convex if $f(y) \geq f(x) + \nabla f(x)^\top (y - x)$ for all $x, y \in dom(f)$

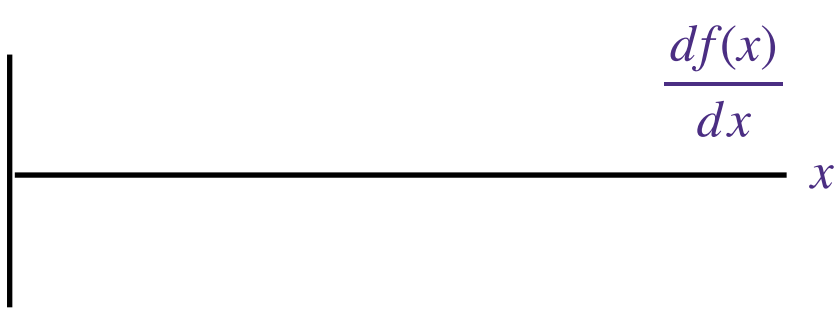


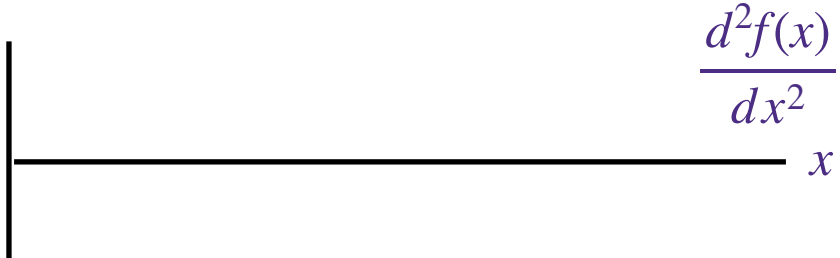


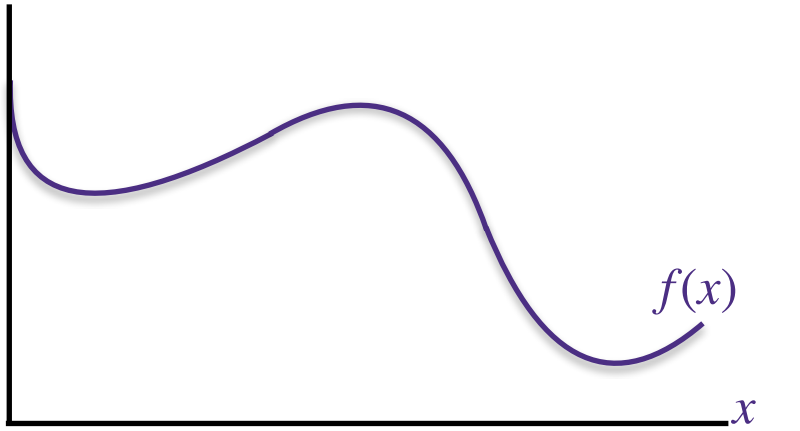
More definitions of convexity

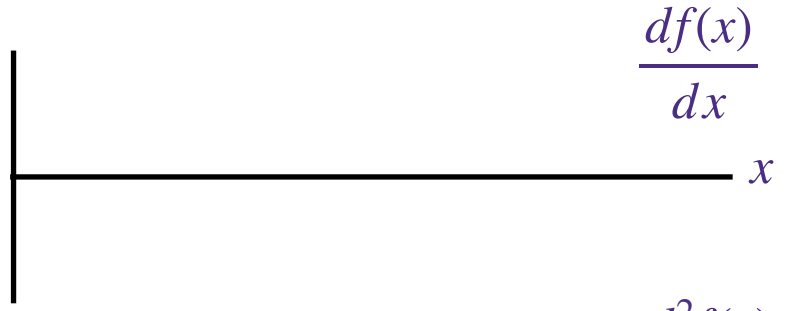
A function $f : \mathbb{R}^d \to \mathbb{R}$ that is twice-differentiable everywhere is convex if $\nabla^2 f(x) \succeq 0$ for all $x \in dom(f)$

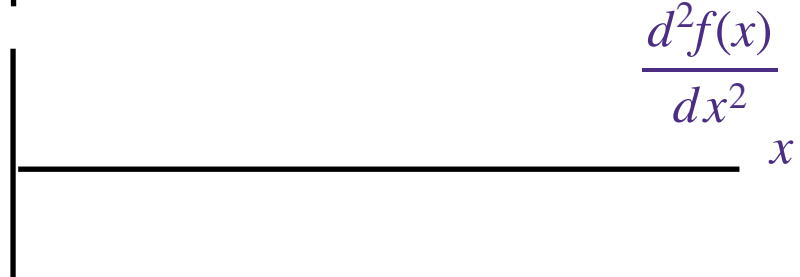












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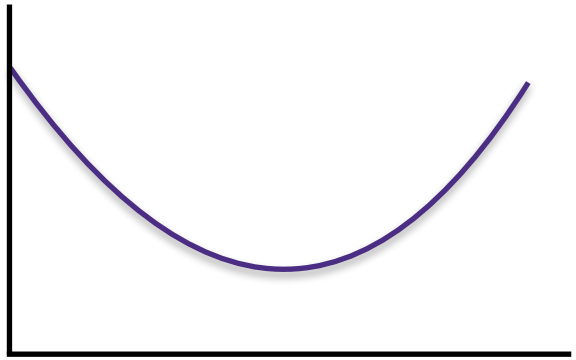
A function $f : \mathbb{R}^d \to \mathbb{R}$ that is twice-differentiable everywhere is convex if $\nabla^2 f(x) \succeq 0$ for all $x \in dom(f)$

Why do we care about convexity?

Convex functions

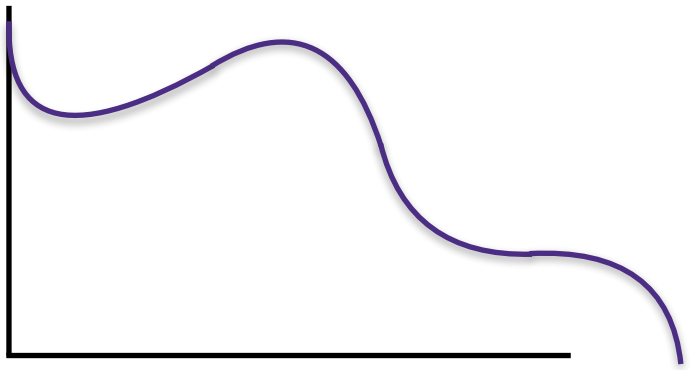
- All local minima are global minima
- Efficient to optimize (e.g., gradient descent)

Convex Function



We only need to find a point with $\nabla f(x) = 0$, which for convex functions implies that it is a local minima and a global minima

Non-convex Function



For non-convex functions, a stationary point with $\nabla f(x) = 0$ could be a local minima, a local maxima, or a saddle point

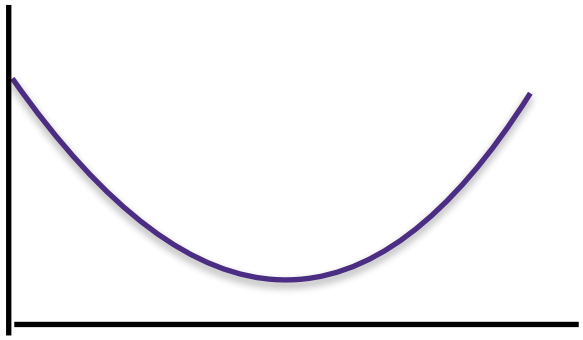
Gradient Descent on $\min_w f(w)$

Initialize: $w_0 = 0$

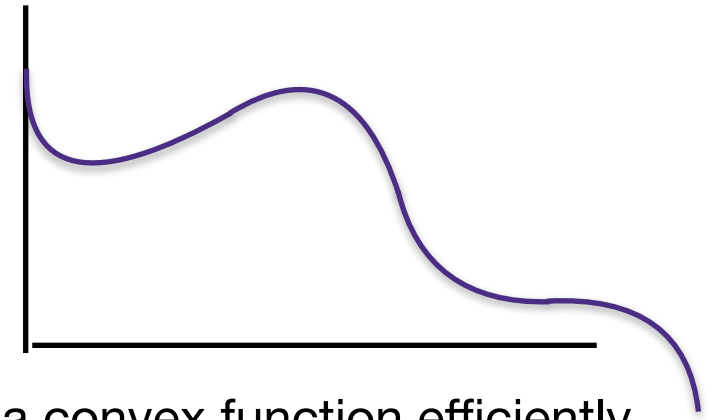
for $t = 1, 2, \ldots$

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

Convex Function



Non-convex Function



- Strength: Can find global minima of a convex function efficiently
- Weakness: Can only be applied to smooth functions
  - i.e., functions that is differentiable everywhere,
  - otherwise $\nabla f(x)$ is not defined and gradient descent cannot be applied

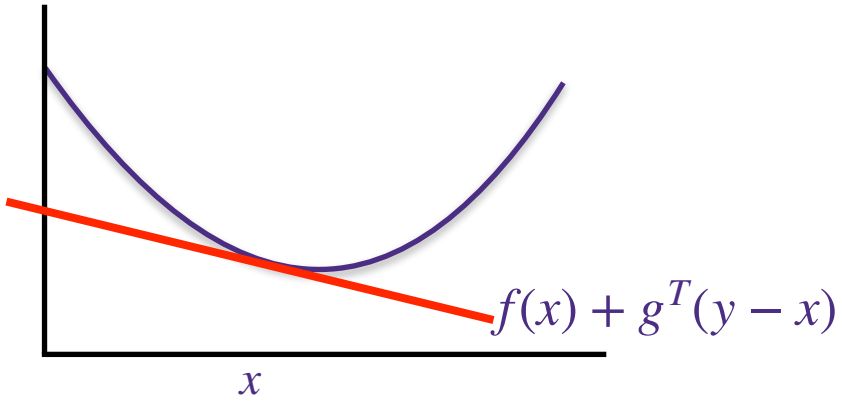
Sub-Gradient

Definition: a function is **non-smooth** if it is not differentiable everywhere

Definition: a vector $g \in \mathbb{R}^d$ is a **sub-gradient** at x if it satisfies

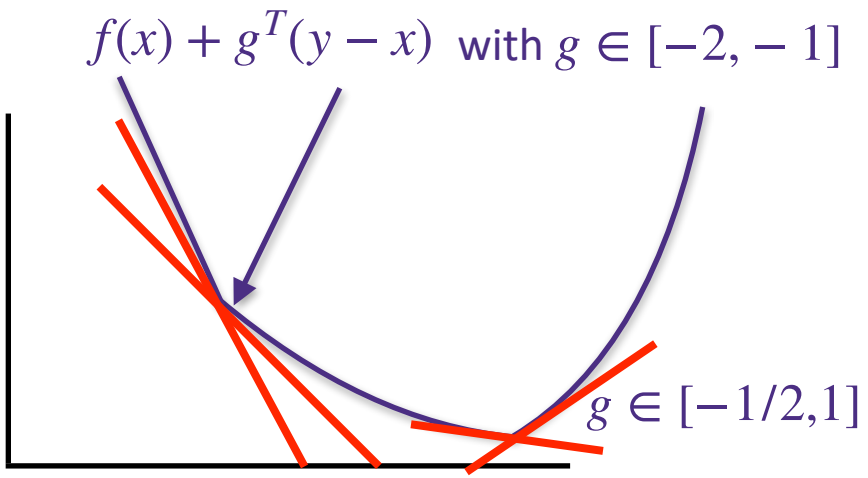
$$f(y) \geq f(x) + g^T(y - x) \text{ for all } y \in \mathbb{R}^d$$

Smooth Convex Function



- for smooth convex functions,
  - gradient is the unique sub-gradient, and
  - the global minimum is achieved at points where gradient is zero

Non-smooth Convex Function



- for non-smooth convex functions,
  - the minimum is achieved at points where sub-gradient set includes the zero vector

Sub-Gradient Descent for non-smooth functions

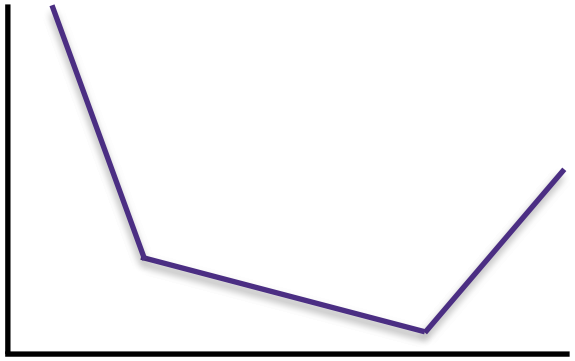
Initialize: $w_0 = 0$

for $t = 1, 2, \ldots$

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

$$w_{t+1} \leftarrow w_t - \eta_t g_t$$

Convex Function



Non-convex Function

- Strength: finds global minima for **non-smooth convex functions**
- Weakness: it is slower than gradient descent on convex smooth functions, because the gradient do not get smaller near the global minima
  - Instead of last iterate w_t, we use the best one we saw in all iterates
  - The stepsize needs to decrease with t

Optimization

- 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.)

Questions?