

Gradient descent and machine learning

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From linear regression ...

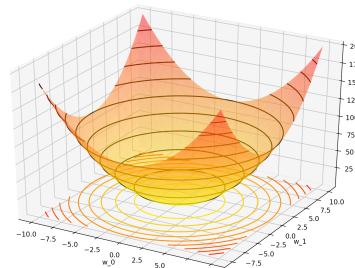
$$L(\mathbf{w}) = \frac{1}{n} \|\mathbf{X}\mathbf{w} - \mathbf{y}\|_2^2$$

continuous,
differentiable, convex

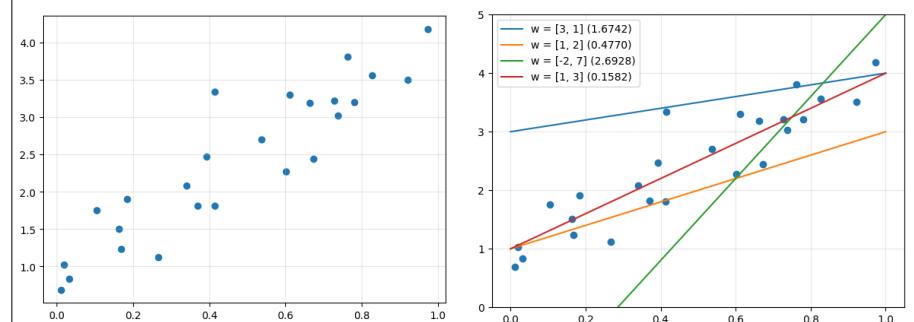
$$\mathbf{w}^* = \arg \min_{\mathbf{w}} L(\mathbf{w})$$

w

optimal
solution



Data space



Machine learning as optimization

Goal

- find parameters that minimize loss/error

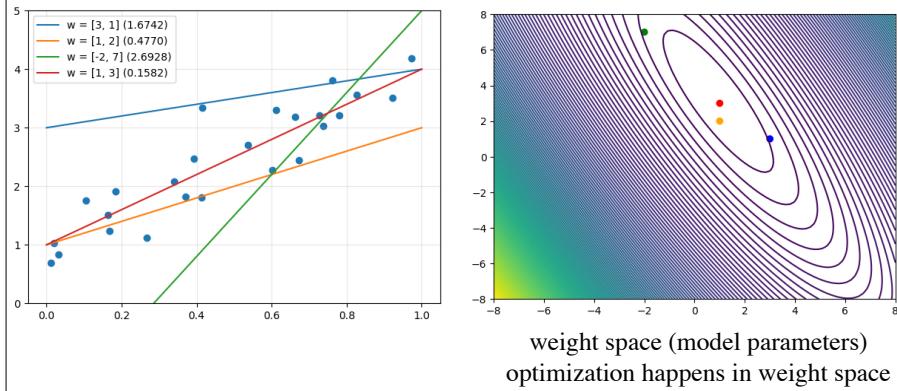
Challenge

- complex loss landscapes
- large-scale datasets

Solution

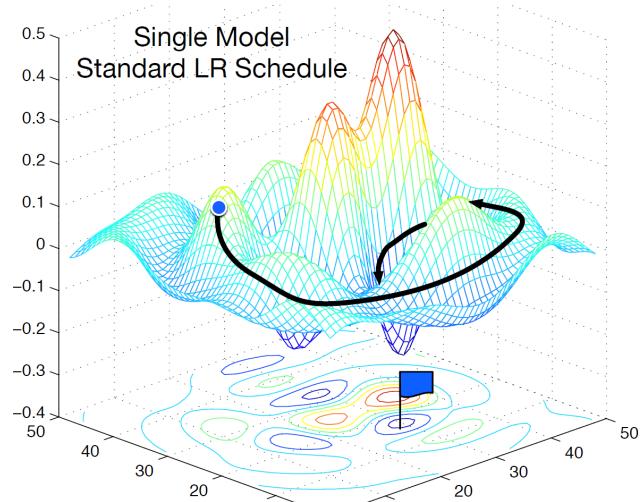
- gradient-based optimization methods

Data space vs parameter space



Gradient descent in ML

Gradient descent in ML



Gradient descent in ML

Want to **minimize** a loss function $L(\mathbf{w})$?

- use gradient descent:

- start with a guess $\mathbf{w}^{(0)}$
- use $\mathbf{w}^{(0)}$ to generate $\mathbf{w}^{(1)}$
- use $\mathbf{w}^{(1)}$ to generate $\mathbf{w}^{(2)}$
- ...

opposite direction
of the gradient

$$\mathbf{w}^{(t+1)} = \mathbf{w}^{(t)} - \eta \nabla_{\mathbf{w}} L (\mathbf{w}^{(t)})$$

Batch gradient descent

Batch gradient descent

$$w^{(t)} \rightarrow w^{(t+1)} \rightarrow w^{(t+2)} \rightarrow \dots$$

compute gradient
requires a full pass over
the training data

1 EPOCH refers to 1
pass over the data

Initialize vector \mathbf{w}

Repeat until convergence (or termination criteria)

$$w_j^{(t+1)} = w_j^{(t)} - \eta \frac{\partial L(\mathbf{w}^{(t)})}{\partial w_j^{(t)}}$$

simultaneously
update all w_j for
 $j = 0, \dots, d$

Gradient for linear regression

with respect to a single w_j

$$\begin{aligned}\frac{\partial L(\mathbf{w})}{\partial w_j} &= \frac{\partial}{\partial w_j} \left(\frac{1}{n} \sum_{i=1}^n (\mathbf{w}^T \mathbf{x}^{(i)} - y^{(i)})^2 \right) \\ &= \frac{2}{n} \sum_{i=1}^n (\mathbf{w}^T \mathbf{x}^{(i)} - y^{(i)}) \frac{\partial}{\partial w_j} (\mathbf{w}^T \mathbf{x}^{(i)} - y^{(i)}) \\ &= \frac{2}{n} \sum_{i=1}^n (\mathbf{w}^T \mathbf{x}^{(i)} - y^{(i)}) x_j^{(i)} \quad \text{partial derivative}\end{aligned}$$

Gradient for linear regression

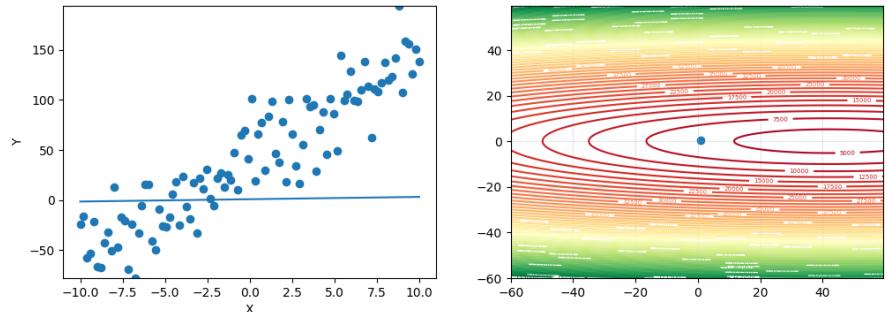
with respect to \mathbf{w}

$$\begin{aligned}\frac{\partial L(\mathbf{w})}{\partial \mathbf{w}} &= \frac{\partial}{\partial \mathbf{w}} \left(\frac{1}{n} \|\mathbf{X}\mathbf{w} - \mathbf{y}\|_2^2 \right) \\ &= \frac{2}{n} X^T(\mathbf{X}\mathbf{w} - \mathbf{y}) \quad \text{gradient vector}\end{aligned}$$

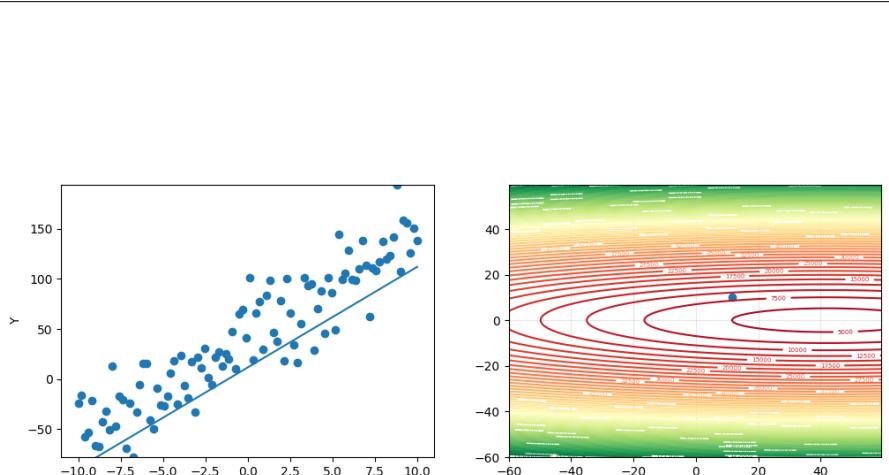
Show me the code

```
# initialize variables and weights
l_rate = 0.025
n_epochs = 10
w = np.zeros([2,1])

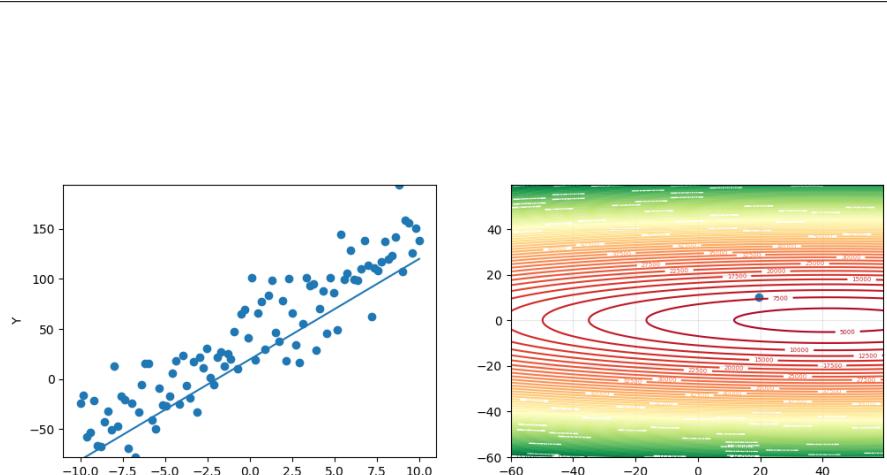
# apply gradient descent
for i in range(n_epochs):
    grad = 2 * (augX.T @ (augX @ w - Y) / n_points)
    w = w - l_rate * grad
```



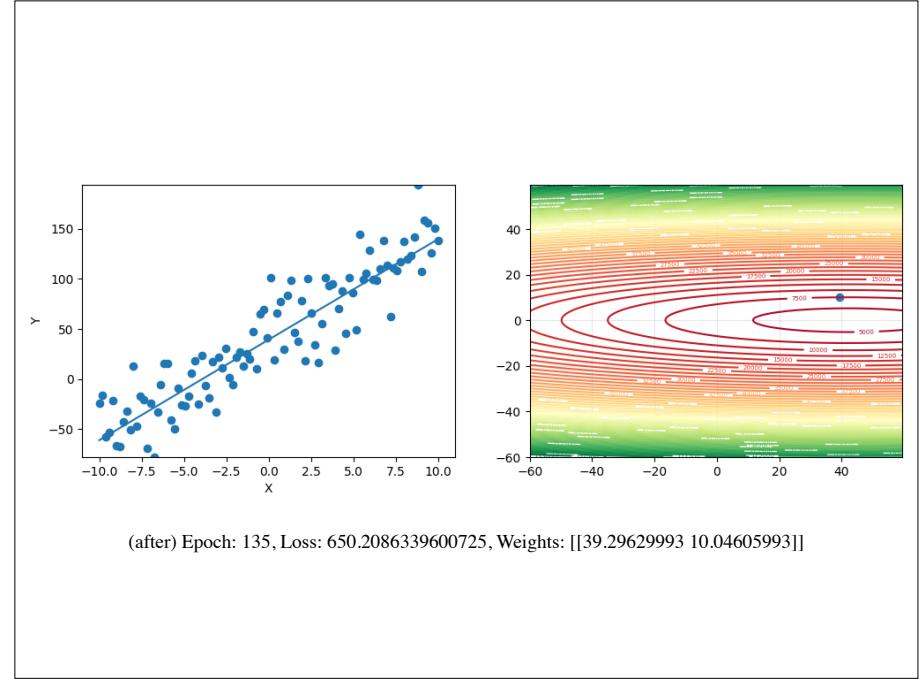
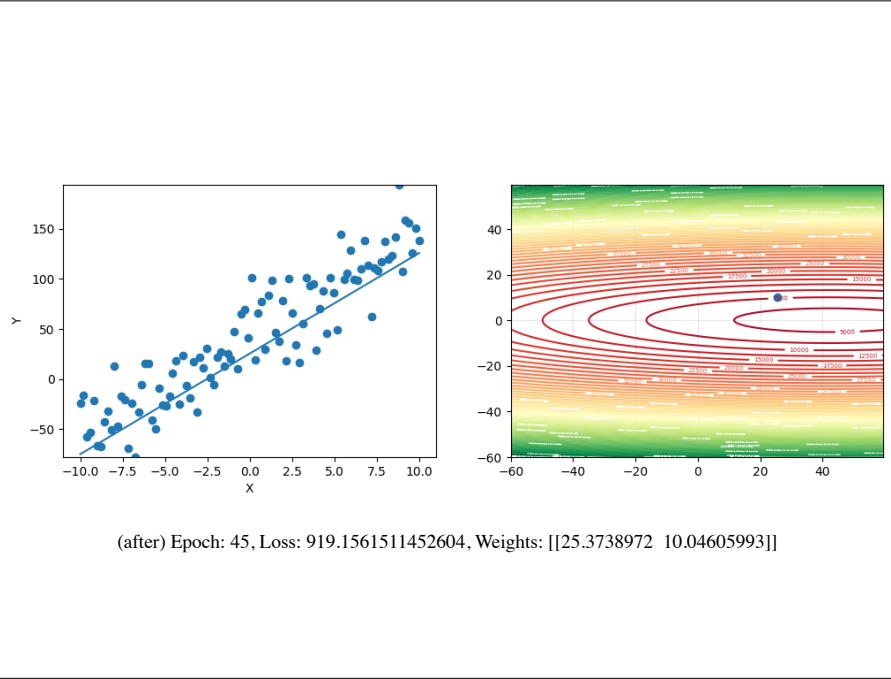
Before GD, Loss: 5620.634954793229, Weights: [[0.74069207 0.23126419]]



(after) Epoch: 15, Loss: 1571.2517204775763, Weights: [[11.5255559 10.04605956]]



(after) Epoch: 30, Loss: 1149.3156573586114, Weights: [[19.4909231 10.04605993]]

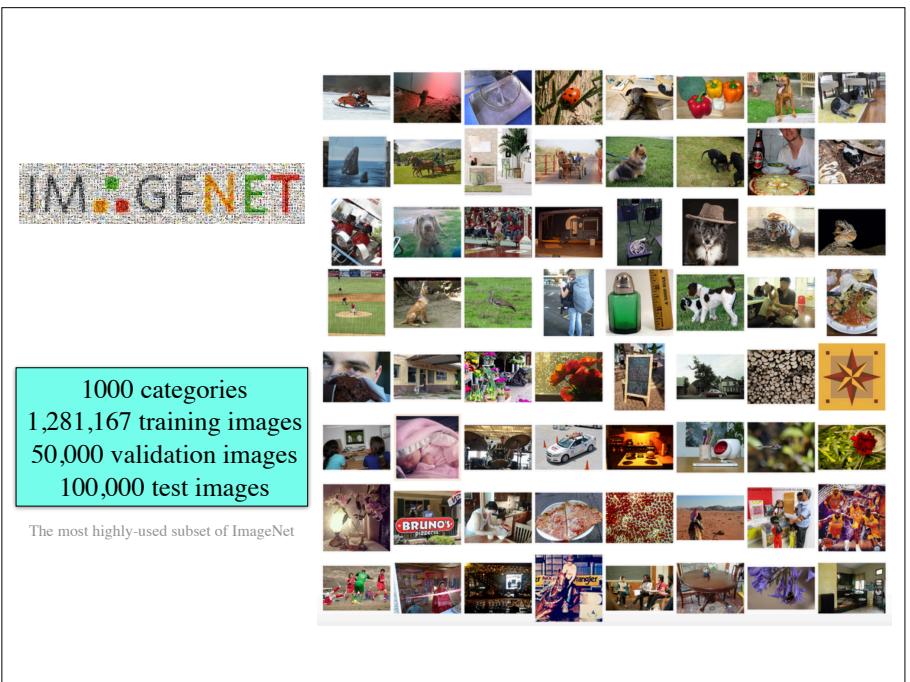


Performance

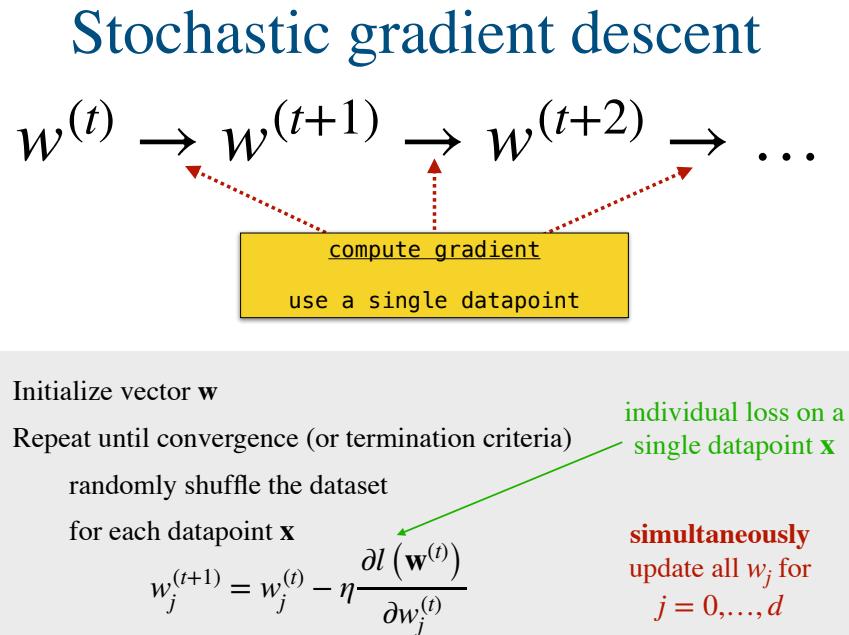
- Each iteration of batch gradient descent uses the entire training set
 - can be **slow** for big datasets

$$w_j^{(t+1)} = w_j^{(t)} - \eta \frac{2}{n} \sum_{i=1}^n \left(\mathbf{w}^{(t)T} \mathbf{x}^{(i)} - y^{(i)} \right) x_j^{(i)}$$

update for a single weight
sum over all instances in the training set



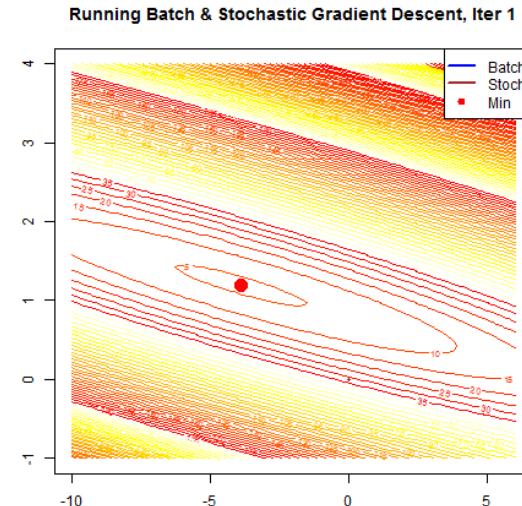
Stochastic and mini-batch gradient descent



Stochastic gradient descent

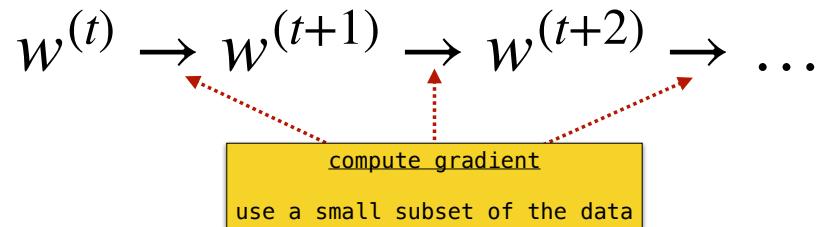
- ▶ Why not calculating an approximate gradient?
 - use a **single datapoint** at each update (stochastic sampling)
- ▶ Scalable method
 - huge impact on real-world applications
- ▶ Behavior
 - at some iterations loss may increase, but the algorithm can still make progress

Batch vs Stochastic



<https://sandipanweb.wordpress.com/2016/07/09/convergence-of-the-gradient-descent-algorithms-stochastic-and-batch-for-the-linear-logistic-regression-and-perceptron/>

Mini-batch gradient descent



Initialize vector \mathbf{w}

Repeat until convergence (or termination criteria)

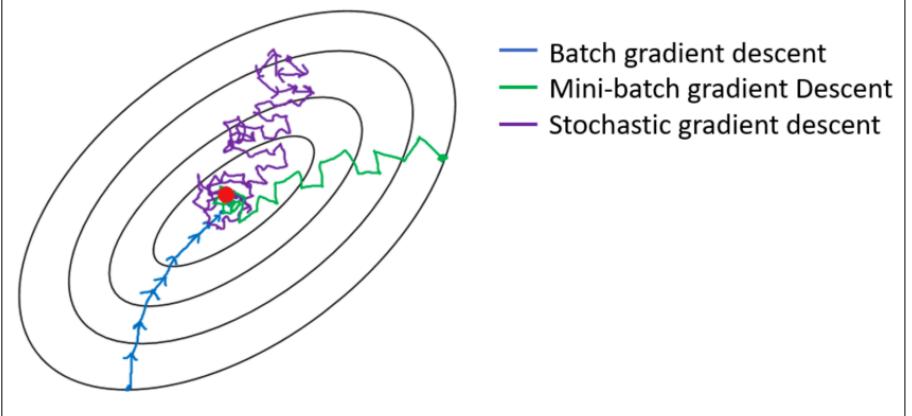
randomly split the dataset into batches of size m

for each batch

$$w_j^{(t+1)} = w_j^{(t)} - \eta \frac{\partial L(\mathbf{w}^{(t)})}{\partial w_j^{(t)}}$$

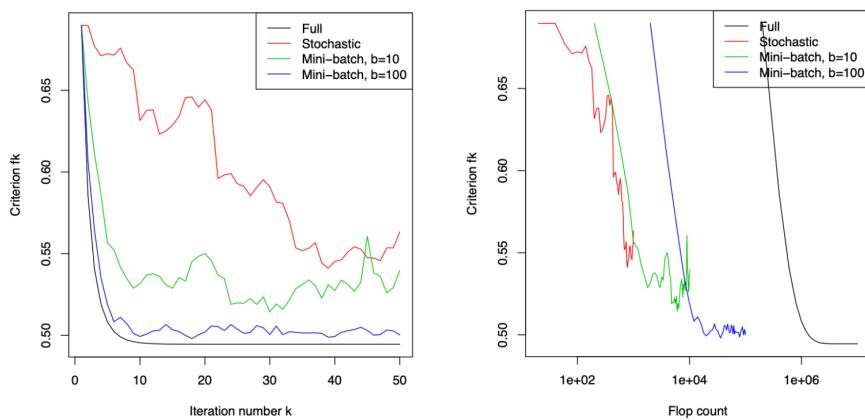
average loss over a
mini-batch

simultaneously
update all w_j for
 $j = 0, \dots, d$



<https://imaddabbura.github.io/post/gradient-descent-algorithm/>

Convergence comparison



Example from Ryan Tibshirani

Convergence Properties

Batch GD

- guaranteed convergence for convex functions
- slower but more stable

SGD

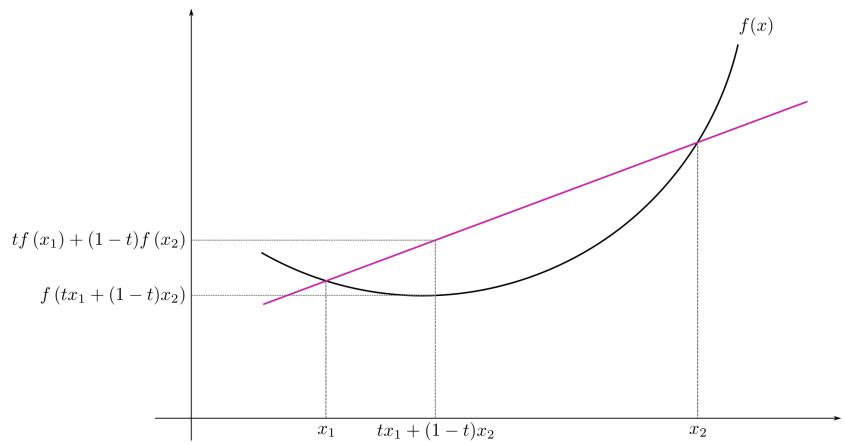
- faster iterations
- noisier path
- requires learning rate scheduling

Mini-batch GD

- better gradient estimation than SGD
- more efficient than batch GD
- popular in deep learning

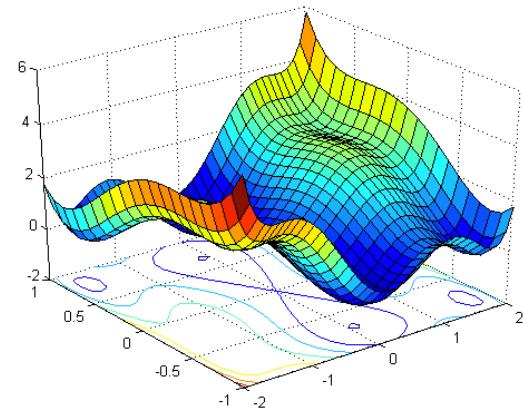
Convex function

A real-valued function is called convex if the line segment between any two points on the graph of the function lies above the graph between the two points.



Gradient descent and convexity

- If the function is **non-convex**, GD may not find the global minimum



Conclusion

- Gradient Descent
 - foundation of modern ML
- Multiple variants for different scenarios
- Modern techniques handle various challenges
- Critical for training deep neural networks