CS639:
Data Management for Data Science

Lecture 20: Optimization/Gradient Descent

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Today

1. Optimization

2. Gradient Descent

What is Optimization?

Find the minimum or maximum of an objective function given a set of constraints:

$$
\begin{aligned}
&\arg\min_x f_0(x) \\
&\quad \text{s.t.}\, f_i(x) \leq 0, i = \{1, \ldots, k\} \\
&\quad\quad h_j(x) = 0, j = \{1, \ldots l\}
\end{aligned}
$$

Why Do We Care?

Linear Classification

$$\arg\min_{w} \sum_{i=1}^{n} ||w||^2 + C \sum_{i=1}^{n} \xi_i$$

$$\text{s.t. } 1 - y_i x_i^T w \leq \xi_i$$

$$\xi_i \geq 0$$

Maximum Likelihood

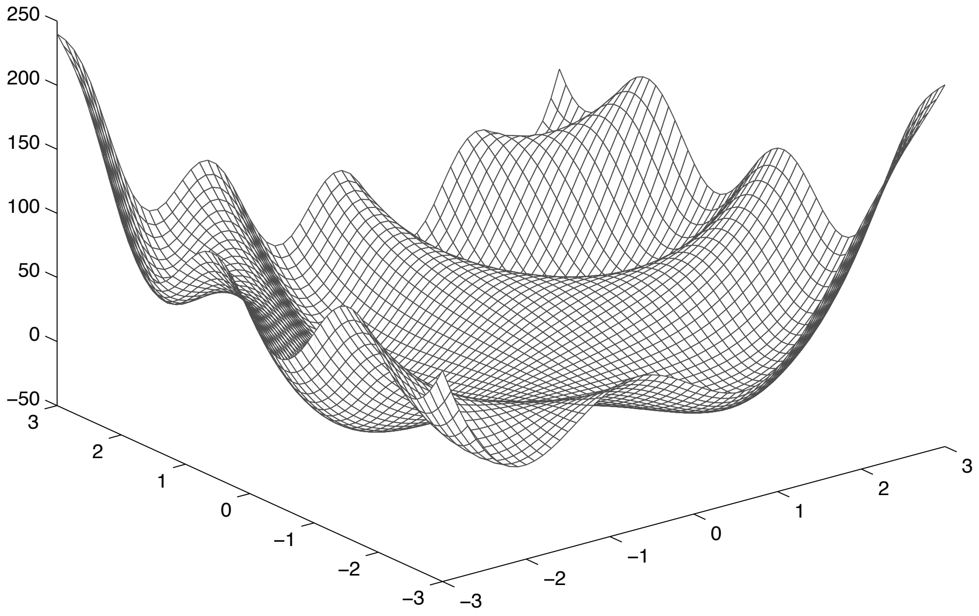
$$\arg\max_{\theta} \sum_{i=1}^{n} \log\, p_\theta(x_i)$$

K-Means

$$\arg \min_{\mu_1, \mu_2, \ldots, \mu_k} J(\mu) = \sum_{j=1}^{k} \sum_{i \in C_j} ||x_i - \mu_j||^2$$

Prefer Convex Problems

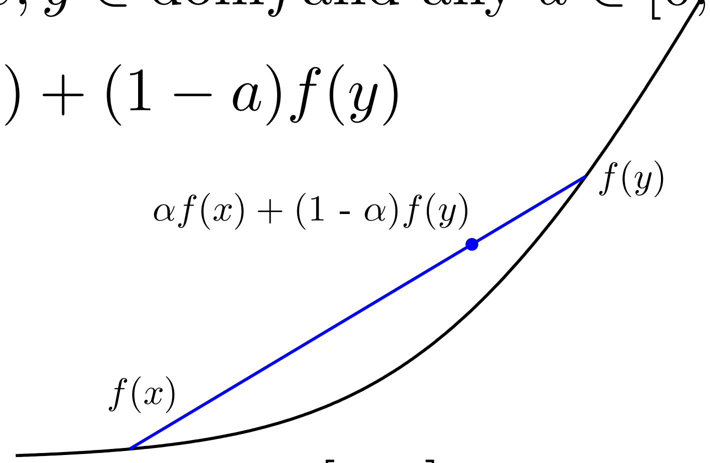
Local (non global) minima and maxima:



Convex Functions and Sets

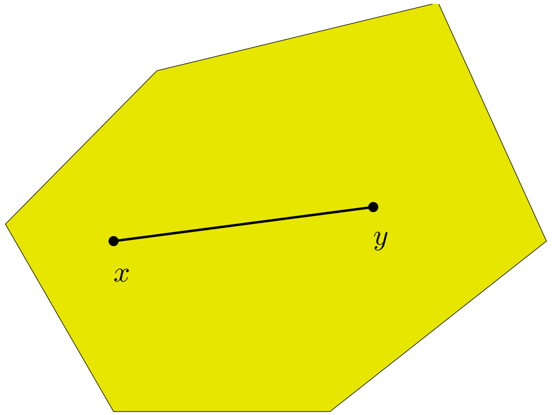
A function $f : \mathbb{R}^n \to \mathbb{R}$ is convex if for $x, y \in \mathrm{dom} f$and any $a \in [0, 1]$,

$$f(ax + (1 - a)y) \leq af(x) + (1 - a)f(y)$$



A set $C \subseteq \mathbb{R}^n$ is convex if for $x, y \in C$ and any $a \in [0, 1]$,

$$ax + (1 - a)y \in C$$



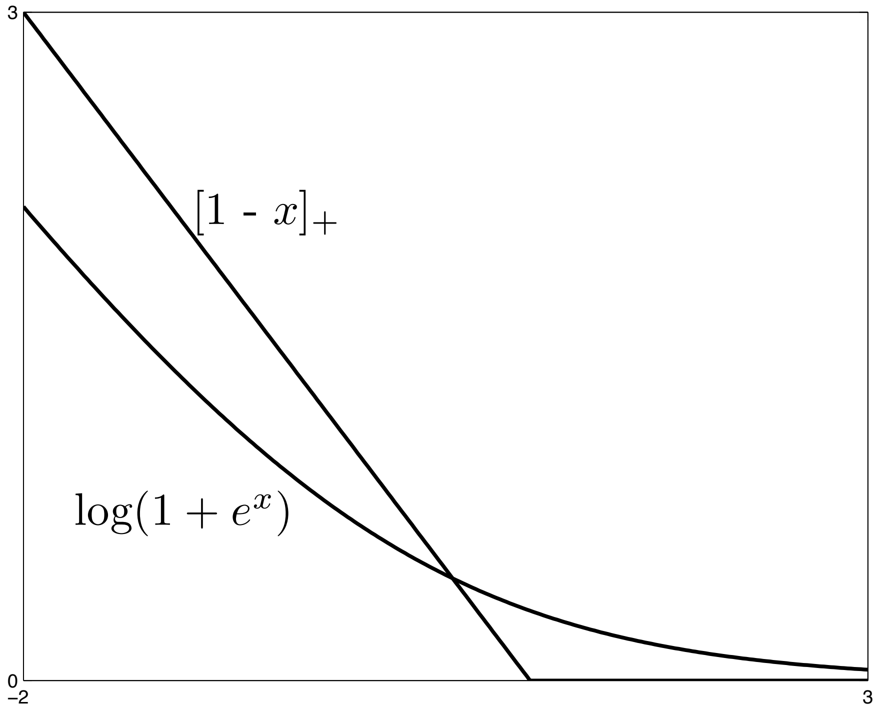
Important Convex Functions

SVM loss:

$$f(w) = \left[1 - y_i x_i^T w\right]_+$$

Binary logistic loss:

$$f(w) = \log\left(1 + \exp(-y_i x_i^T w)\right)$$



Convex Optimization Problem

$$
\begin{aligned}
\underset{x}{\text{minimize}}\ & f_0(x) && \text{(Convex function)} \\
\text{s.t.}\quad & f_i(x) \leq 0 && \text{(Convex sets)} \\
& h_j(x) = 0 && \text{(Affine)}
\end{aligned}
$$

Lagrangian Dual

Start with optimization problem:

$$\begin{aligned} \underset{x}{\text{minimize}} \;\; & f_0(x) \\ \text{s.t.} \;\; & f_i(x) \leq 0, \;\; i = \{1, \ldots, k\} \\ & h_j(x) = 0, \;\; j = \{1, \ldots, l\} \end{aligned}$$

Form *Lagrangian* using Lagrange multipliers $\lambda_i \geq 0$, $\nu_i \in \mathbb{R}$

$$\mathcal{L}(x, \lambda, \nu) = f_0(x) + \sum_{i=1}^{k} \lambda_i f_i(x) + \sum_{j=1}^{l} \nu_j h_j(x)$$

Form *dual function*

$$g(\lambda, \nu) = \inf_x \mathcal{L}(x, \lambda, \nu) = \inf_x \left\{ f_0(x) + \sum_{i=1}^{k} \lambda_i f_i(x) + \sum_{j=1}^{l} \nu_j h_j(x) \right\}$$

First Order Methods:

Gradient Descent

Newton’s Method

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Subgradient Descent

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Gradient Descent

The simplest algorithm in the world (almost). Goal:

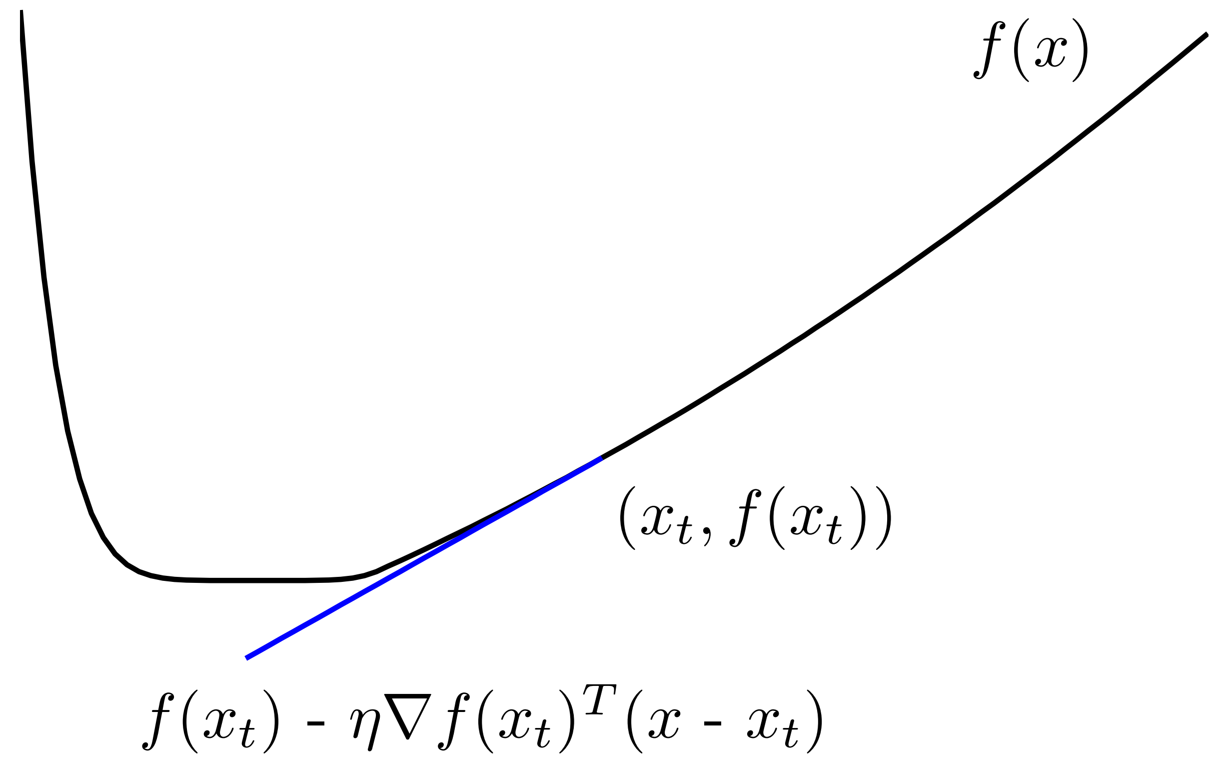
$$\underset{x}{\text{minimize}} \;\; f(x)$$

Just iterate

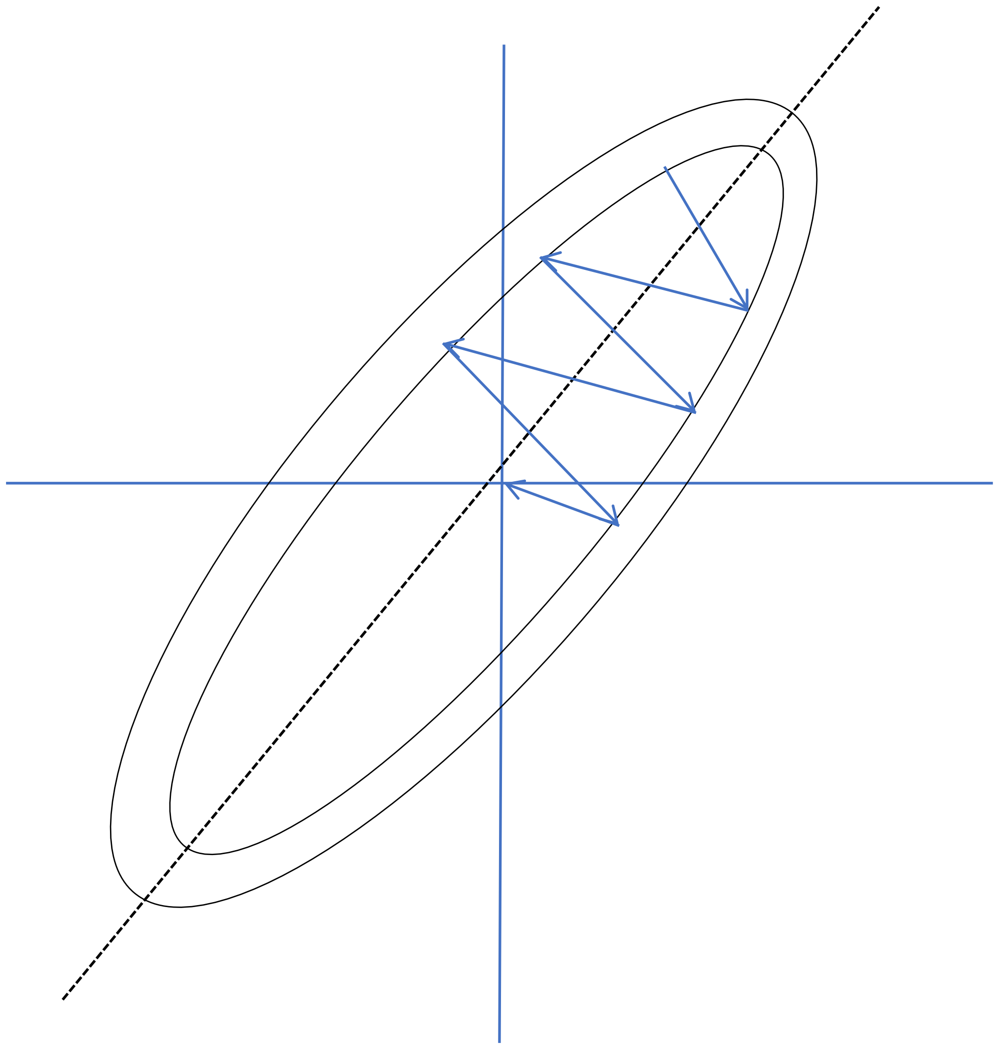
$$x_{t+1} = x_t - \eta_t \nabla f(x_t)$$

where η_t is stepsize.

Single Step Illustration



Full Gradient Descent Illustration



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Newton's Method

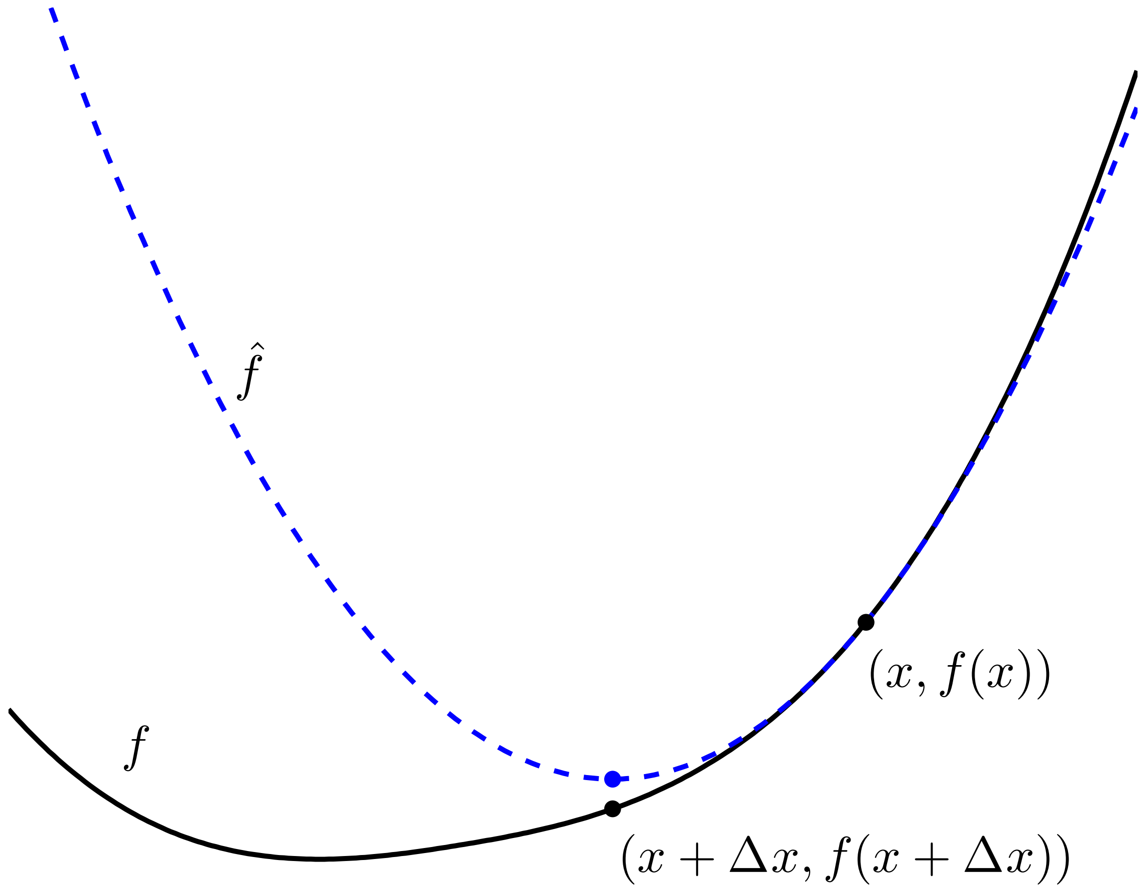
Idea: use a second-order approximation to function.

$$f(x+\Delta x) \approx f(x) + \nabla f(x)^T \Delta x + \frac{1}{2}\Delta x^T \nabla^2 f(x) \Delta x$$

Choose Δx to minimize above:

$$\Delta x = -\underbrace{\left[\nabla^2 f(x)\right]^{-1}}_{\text{Inverse Hessian}} \underbrace{\nabla f(x)}_{\text{Gradient}}$$

Newton's Method Picture



$\hat{f}$ is 2^{nd}-order approximation, f is true function.

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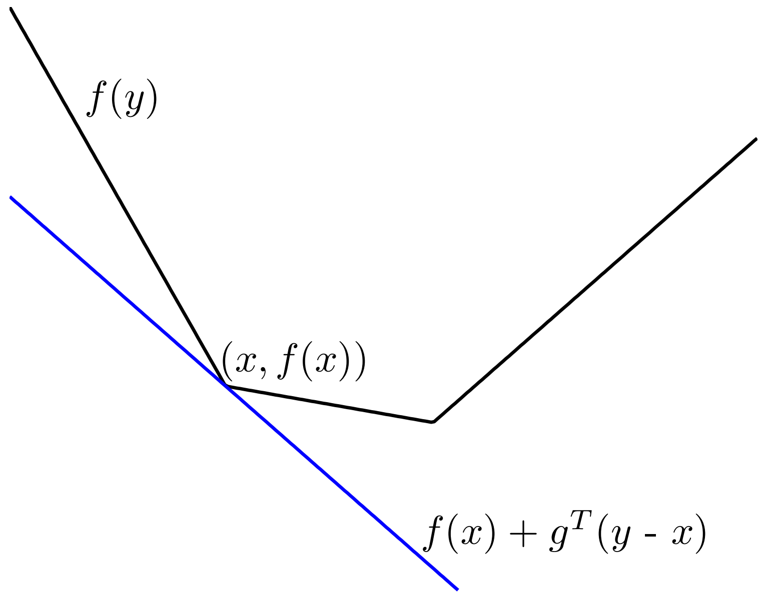
Subgradient Descent Motivation

Lots of non-differentiable convex functions used in machine learning:



The *subgradient set*, or subdifferential set, $\partial f(x)$ of f at x is

$$\partial f(x) = \left\{g : f(y) \geq f(x) + g^T(y - x) \;\; \text{for all } y\right\}.$$

Subgradient Descent – Algorithm

Really, the simplest algorithm in the world. Goal:

$$\underset{x}{\text{minimize}} \;\; f(x)$$

Just iterate

$$x_{t+1} = x_t - \eta_t g_t$$

where η_t is a stepsize, $g_t \in \partial f(x_t)$.

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Online learning and optimization

- Goal of machine learning :
  - Minimize expected loss

$$\min_h L(h) = \mathbf{E}\left[\text{loss}(h(x), y)\right]$$

given samples

$$(x_i, y_i) \;\; i = 1, 2 ... m$$

- This is Stochastic Optimization
  - Assume loss function is convex

Batch (sub)gradient descent for ML

- Process all examples together in each step

$$w^{(k+1)} \leftarrow w^{(k)} - \eta_t \left(\frac{1}{n} \sum_{i=1}^{n} \frac{\partial L(w, x_i, y_i)}{\partial w} \right)$$

$$\text{where } L \text{ is the regularized loss function}$$

- Entire training set examined at each step
- Very slow when *n* is very large

Stochastic (sub)gradient descent

- “Optimize” one example at a time
- Choose examples randomly (or reorder and choose in order)
  - Learning representative of example distribution

for $i = 1$ to n:

$$w^{(k+1)} \leftarrow w^{(k)} - \eta_t \frac{\partial L(w, x_i, y_i)}{\partial w}$$

where L is the regularized loss function

Stochastic (sub)gradient descent

for $i = 1$ to n:

$$w^{(k+1)} \leftarrow w^{(k)} - \eta_t \frac{\partial L(w, x_i, y_i)}{\partial w}$$

where L is the regularized loss function

- Equivalent to online learning (the weight vector *w* changes with every example)
- Convergence guaranteed for convex functions (to local minimum)

Hybrid!

- Stochastic – 1 example per iteration
- Batch – All the examples!
- Sample Average Approximation (SAA):
  - Sample *m* examples at each step and perform SGD on them
- Allows for parallelization, but choice of *m* based on heuristics

SGD - Issues

- Convergence very sensitive to learning rate
  - ( ) (oscillations near solution due to probabilistic nature of sampling) η_t
  - Might need to decrease with time to ensure the algorithm converges eventually
- Basically – SGD good for machine learning with large data sets!

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Statistical Learning Crash Course

Staggering amount of machine learning/stats can be written as:

$$\min_x \sum_{i=1}^{N} f(x, y_i)$$

N (number of y_i's, data) typically in the billions
Ex: Classification, Recommendation, Deep Learning.

De facto iteration to solve large-scale problems: **SGD**.

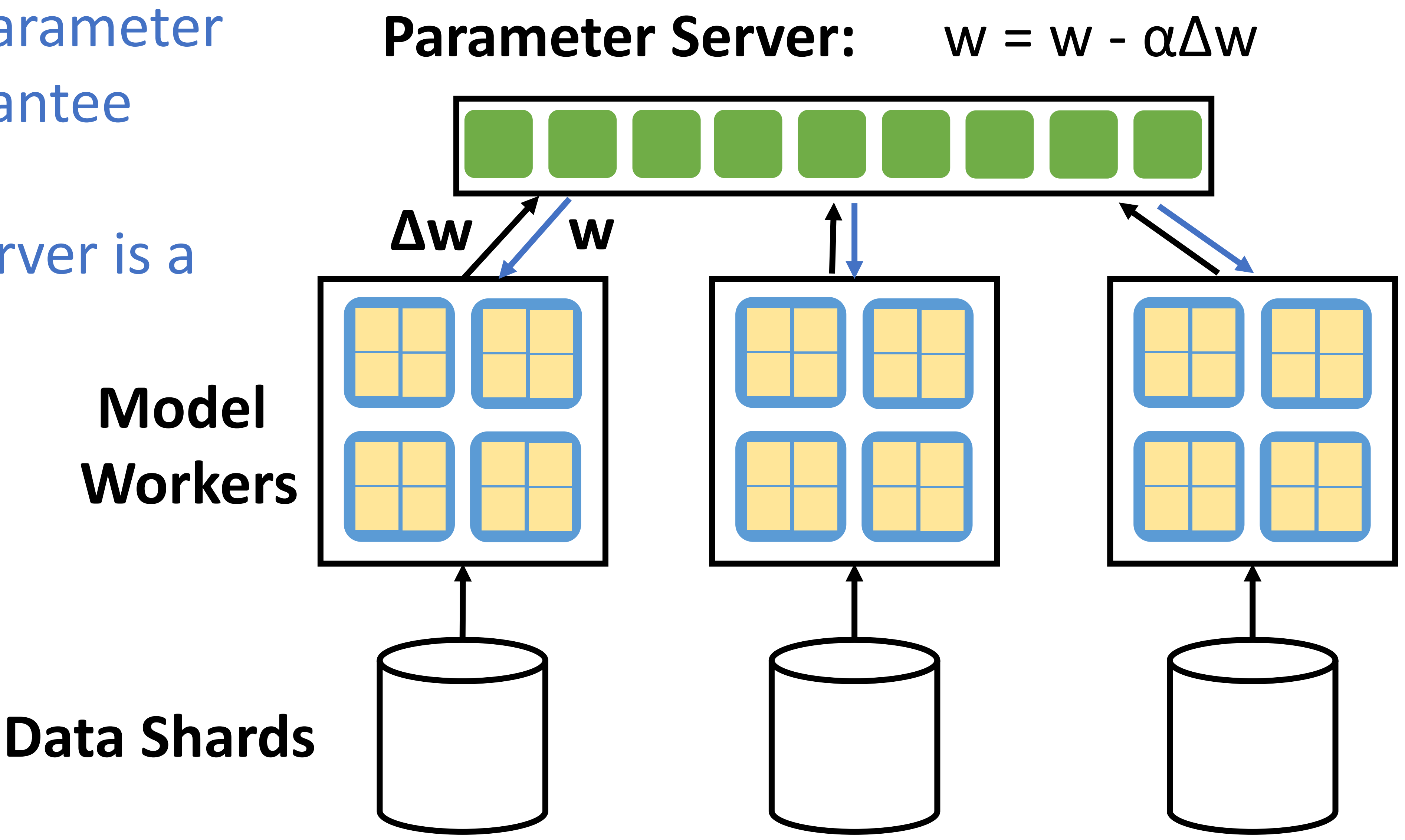
$$\boxed{x^{k+1} = x^k - \alpha N \nabla f(x^k, y_j)}$$

Billions of tiny iterations

Select one term, j, and estimate gradient.

Parallel SGD (Centralized)

- Centralized parameter updates guarantee convergence
- Parameter Server is a bottleneck



Parallel SGD (HogWild! - asynchronous)

Data Systems Perspective of SGD

$$x^{k+1} = x^k - \alpha N \nabla f(x^k, y_j)$$

Insane conflicts: Billions of tiny jobs (~100 instructions), RW conflicts on x

Multiple workers need to **communicate**!

HogWild!: For sparse convex models (e.g., logistic regression) run without locks; SGD still converges (answer is statistically correct)