

Gradient Descent

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Review: ERM

Our Setup from Statistical Learning Theory

The Spaces

- \mathcal{X} : input space
- \mathcal{Y} : outcome space
- \mathcal{A} : action space

Prediction Function (or “decision function”)

A **prediction function** (or **decision function**) gets input $x \in \mathcal{X}$ and produces an action $a \in \mathcal{A}$:

$$\begin{aligned} f: \mathcal{X} &\rightarrow \mathcal{A} \\ x &\mapsto f(x) \end{aligned}$$

Loss Function

A **loss function** evaluates an action in the context of the outcome y .

$$\begin{aligned} \ell: \mathcal{A} \times \mathcal{Y} &\rightarrow \mathbb{R} \\ (a, y) &\mapsto \ell(a, y) \end{aligned}$$

Risk and the Bayes Prediction Function

Definition

The **risk** of a prediction function $f : \mathcal{X} \rightarrow \mathcal{A}$ is

$$R(f) = \mathbb{E} \ell(f(x), y).$$

In words, it's the **expected loss** of f on a new example (x, y) drawn randomly from $P_{\mathcal{X} \times \mathcal{Y}}$.

Definition

A **Bayes prediction function** $f^* : \mathcal{X} \rightarrow \mathcal{A}$ is a function that achieves the *minimal risk* among all possible functions:

$$f^* \in \arg \min_f R(f),$$

where the minimum is taken over all functions from \mathcal{X} to \mathcal{A} .

- The risk of a Bayes prediction function is called the **Bayes risk**.

The Empirical Risk

Let $\mathcal{D}_n = ((x_1, y_1), \dots, (x_n, y_n))$ be drawn i.i.d. from $\mathcal{P}_{\mathcal{X} \times \mathcal{Y}}$.

Definition

The **empirical risk** of $f : \mathcal{X} \rightarrow \mathcal{A}$ with respect to \mathcal{D}_n is

$$\hat{R}_n(f) = \frac{1}{n} \sum_{i=1}^n \ell(f(x_i), y_i).$$

- But we saw that the **unconstrained** empirical risk minimizer overfits.
 - i.e. if we minimize $\hat{R}_n(f)$ over **all functions**, we overfit.

Constrained Empirical Risk Minimization

Definition

A **hypothesis space** \mathcal{F} is a set of functions mapping $\mathcal{X} \rightarrow \mathcal{A}$.

- It is the collection of prediction functions we are choosing from.

- **Empirical risk minimizer** (ERM) in \mathcal{F} is

$$\hat{f}_n \in \arg \min_{f \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^n \ell(f(x_i), y_i).$$

- From now on “ERM” always means “constrained ERM”.
- So we should always specify the hypothesis space when we’re doing ERM.

Example: Linear Least Squares Regression

Setup

- Input space $\mathcal{X} = \mathbb{R}^d$
- Output space $\mathcal{Y} = \mathbb{R}$
- Action space $\mathcal{Y} = \mathbb{R}$
- Loss: $\ell(\hat{y}, y) = (y - \hat{y})^2$
- **Hypothesis space:** $\mathcal{F} = \{f : \mathbb{R}^d \rightarrow \mathbb{R} \mid f(x) = w^T x, w \in \mathbb{R}^d\}$
- Given data set $\mathcal{D}_n = \{(x_1, y_1), \dots, (x_n, y_n)\}$,
 - Let's find the ERM $\hat{f} \in \mathcal{F}$.

Example: Linear Least Squares Regression

Objective Function: Empirical Risk

The function we want to minimize is the empirical risk:

$$\hat{R}_n(w) = \frac{1}{n} \sum_{i=1}^n (w^T x_i - y_i)^2,$$

where $w \in \mathbb{R}^d$ parameterizes the hypothesis space \mathcal{F} .

- Now, we have ended up with an optimization problem:

$$\min_{w \in \mathbb{R}^d} \hat{R}_n(w).$$

Gradient Descent

Unconstrained Optimization

Setting

Objective function $f : \mathbb{R}^d \rightarrow \mathbb{R}$ is *differentiable*.

Want to find

$$x^* = \arg \min_{x \in \mathbb{R}^d} f(x)$$

The Gradient

- Let $f : \mathbb{R}^d \rightarrow \mathbb{R}$ be differentiable at $x_0 \in \mathbb{R}^d$.
- The **gradient** of f at the point x_0 , denoted $\nabla_x f(x_0)$, is the direction to move in for the **fastest increase** in $f(x)$, when starting from x_0 .

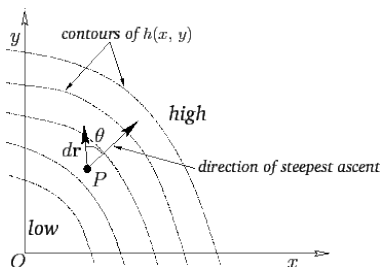


Figure A.111 from Newtonian Dynamics, by Richard Fitzpatrick.

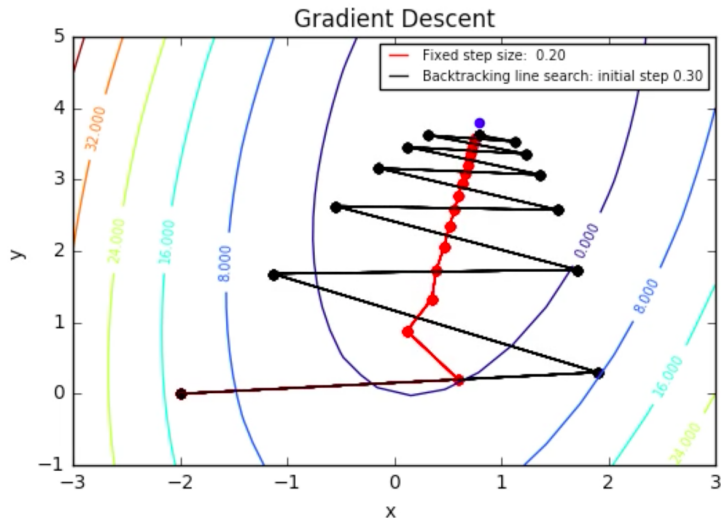
Gradient Descent

Gradient Descent

- Initialize $x = 0$
- repeat
 - $x \leftarrow x - \underbrace{\eta}_{\text{step size}} \nabla f(x)$
- until stopping criterion satisfied

Choosing the step size is the key in gradient descent.

Gradient Descent Path



Gradient Descent: Step Size

- A fixed step size will work, eventually, as long as it's small enough (roughly - details to come)
 - Too fast, may diverge
 - In practice, try several fixed step sizes
- Intuition on when to take big steps and when to take small steps?

Convergence Theorem for Fixed Step Size

Theorem

Suppose $f : \mathbb{R}^d \rightarrow \mathbb{R}$ is convex and differentiable, and ∇f is **Lipschitz continuous** with constant $L > 0$, i.e.

$$\|\nabla f(x) - \nabla f(x')\| \leq L\|x - x'\|$$

for any $x, x' \in \mathbb{R}^d$. Then gradient descent with fixed step size $\eta \leq 1/L$ **converges**. In particular,

$$f(x^{(k)}) - f(x^*) \leq \frac{\|x^{(0)} - x^*\|^2}{2\eta k}.$$

This says that gradient descent is guaranteed to converge and that it converges with rate $O(1/k)$.

Gradient Descent: When to Stop?

- Wait until $\|\nabla f(x)\|_2 \leq \varepsilon$, for some ε of your choosing.
 - (Recall $\nabla f(x) = 0$ at minimum.)
- For learning setting,
 - evaluate performance on validation data as you go
 - stop when not improving, or getting worse