Gradient Descent and Loss Functions

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NYU

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Homework 1

- Homework 1 will be released on course website today (Sept 12). You have until Oct 3 noon (12pm) to finish.
- Submit PDF to Gradescope.
- Course website: `https://cs.nyu.edu/courses/fall23/CSCI-GA.2565-001/`

Review: ERM

Our Machine Learning Setup

Prediction Function

A **prediction function** gets input x and produces an output $\hat{y} = f(x)$.

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Loss Function

A **loss function** $\ell(\hat{y}, y)$ evaluates an action in the context of the outcome y.

Risk and the Bayes Prediction Function

Definition

The **risk** of a prediction function $f : \mathcal{X} \to \mathcal{Y}$ 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 $P_{\mathcal{X}\times\mathcal{Y}}$.

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Definition

A **Bayes prediction function** f^* is a function that achieves the *minimal risk* among all possible functions:

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

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

The Empirical Risk

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

Definition

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

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

- The **unconstrained** empirical risk minimizer can overfit.
  - 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 $\mathcal{X} \to \mathcal{Y}$.

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- An **empirical risk minimizer** (ERM) in $\mathcal{F}$ is

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

- 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

- Loss: $\ell(\hat{y}, y) = (y - \hat{y})^2$

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- Loss: $\ell(\hat{y}, y) = (y - \hat{y})^2$
- **Hypothesis space:** $\mathcal{F} = \left\{ f : \mathrm{R}^d \to \mathrm{R} \mid f(x) = w^T x,\, w \in \mathrm{R}^d \right\}$

- Given a data set $\mathcal{D}_n = \{(x_1, y_1), \ldots, (x_n, y_n)\}$,
  - Our goal is to find the ERM $\hat{f} \in \mathcal{F}$.

Example: Linear Least Squares Regression

Objective Function: Empirical Risk

We want to find the function in $\mathcal{F}$, parametrized by $w \in \mathrm{R}^d$, that minimizes the empirical risk:

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

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- How do we solve this optimization problem?

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

- (For OLS there's a closed form solution, but in general there isn't.)

Gradient Descent

Unconstrained Optimization

Setting

We assume that the objective function $f : \mathbb{R}^d \rightarrow \mathbb{R}$ is *differentiable.*
We want to find

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

The Gradient

- Let $f : \mathrm{R}^d \to \mathrm{R}$ be differentiable at $x_0 \in \mathrm{R}^d$.
- The **gradient** of f at the point x_0, denoted $\nabla_x f(x_0)$, is the direction in which $f(x)$ **increases fastest**, if we start from x_0.
- The **gradient** of f is the partial derivatives of all dimensions: $\nabla f(x) = [\partial f / \partial x_1(x), ..., \partial f / \partial x_d(x)]$.

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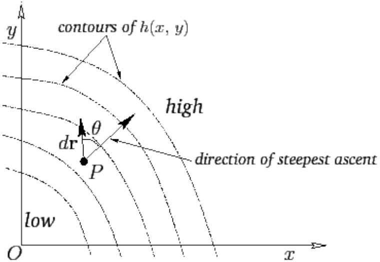

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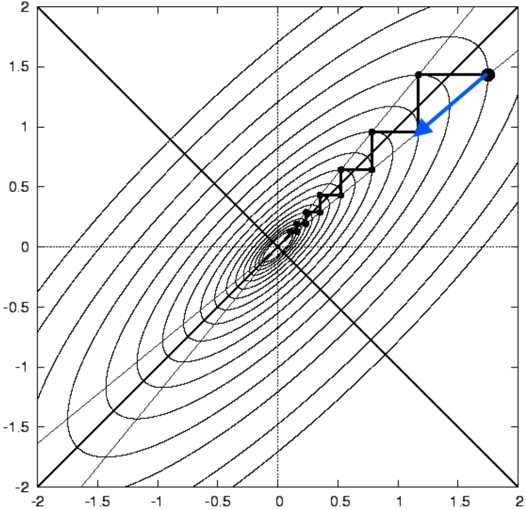
- The "step size" η is not the amount by which we update x!
- "Step size" is also referred to as "learning rate" in neural networks literature.

Gradient Descent Path



Gradient Descent: Step Size

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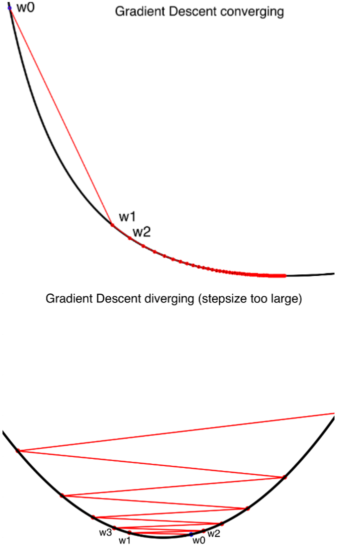
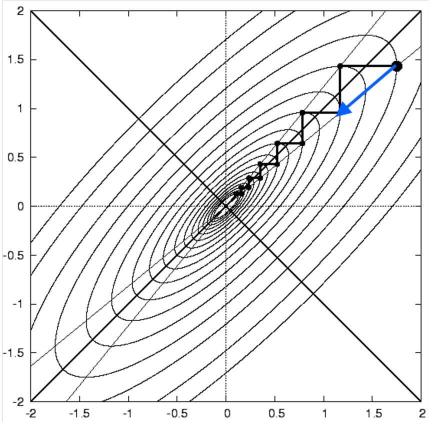
A fixed step size will work, eventually, as long as it's small enough

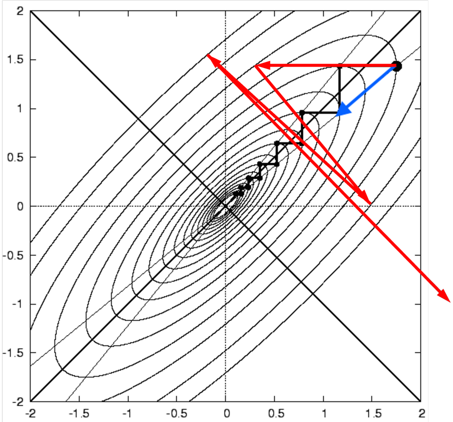
- If η is too large, the optimization process might diverge
- In practice, it often makes sense to try several fixed step sizes
- Intuition on when to take big steps and when to take small steps?



2D Divergence example



Small Step Size



Large Step Size

Notes on Convergence

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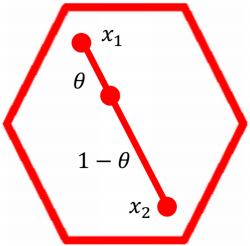
- Gradient descent with an appropriate step size converges to stationary point (derivative = 0) for differentiable functions.
- Stationary points can be (local) minima, (local) maxima, saddle points, etc.
- Gradient descent can converge to global minimum for **convex functions**.

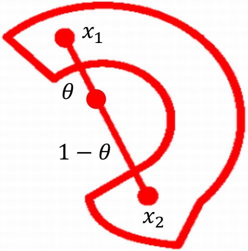
Convex Sets

Definition

A set C is **convex** if for any $x_1, x_2 \in C$ and any θ with $0 \leqslant \theta \leqslant 1$ we have

$$\theta x_1 + (1 - \theta) x_2 \in C.$$





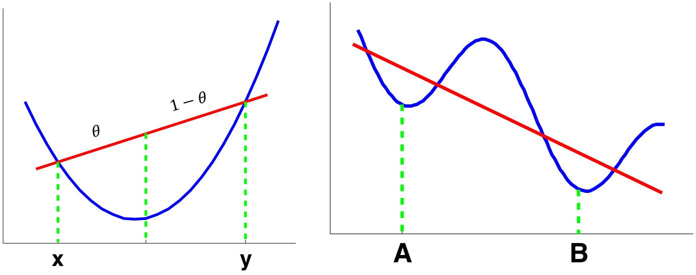
KPM Fig. 7.4

Convex Functions

Definition

A function $f : \mathbb{R}^n \to \mathbb{R}$ is **convex** if $\mathbf{dom}\, f$ is a convex set and if for all $x, y \in \mathbf{dom}\, f$, and $0 \leqslant \theta \leqslant 1$, we have

$$f(\theta x + (1-\theta)y) \leqslant \theta f(x) + (1-\theta) f(y).$$



KPM Fig. 7.5

Convergence Theorem for Fixed Step Size

Theorem

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

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

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

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

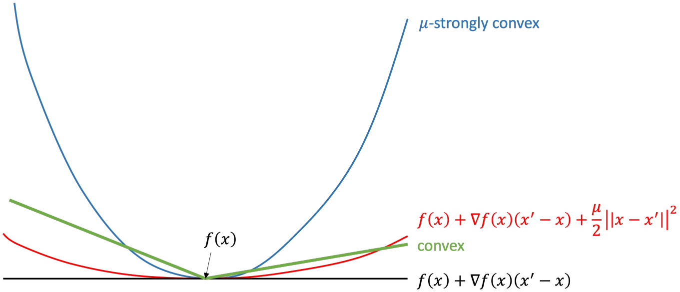
This says that gradient descent is guaranteed to converge and that it converges with rate $O(1/k)$.

Strongly Convex Functions

Definition

A function f is μ-strongly convex if

$$f(x') \geqslant f(x) + \nabla f(x) \cdot (x' - x) + \frac{\mu}{2}\|x - x'\|^2$$



Convergence Theorem for Strongly Convex Functions

Theorem

If f is L-smooth and μ-strongly convex, and step size $0 < \eta \leqslant \frac{1}{L}$, then gradient descent converges with the following inequality:

$$\|x^{(k)} - x^*\|^2 \leqslant (1 - \eta\mu)^k \|x^{(0)} - x^*\|^2$$

This means we can get linear convergence, but it depends on μ. If the estimate of μ is bad then the rate is not great.

Gradient Descent: When to Stop?

- Wait until $\|\nabla f(x)\|_2 \leqslant \varepsilon$, for some ε of your choosing.
  - (Recall $\nabla f(x) = 0$ at a local minimum.)

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    - (Recall $\nabla f(x) = 0$ at a local minimum.)
- **Early stopping:**
    - evalute loss on validation data (unseen held out data) after each iteration;
    - stop when the loss does not improve (or gets worse).

Gradient Descent for Empirical Risk - Scaling Issues

Quick recap: Gradient Descent for ERM

- We have a hypothesis space of functions $\mathcal{F} = \left\{ f_w : \mathcal{X} \to \mathcal{Y} \mid w \in \mathrm{R}^d \right\}$
  - Parameterized by $w \in \mathrm{R}^d$.

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

- Suppose $\ell(f_w(x_i), y_i)$ is differentiable as a function of w.
- Then we can do gradient descent on $\hat{R}_n(w)$

Gradient Descent: Scalability

- At every iteration, we compute the gradient at the current w:

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- We have to iterate over all n training points to take a single step. $[O(n)]$
- Can we make progress without looking at all the data before updating w?

Stochastic Gradient Descent

"Noisy" Gradient Descent

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- Turns out this can work just fine!
- **Intuition**:
  - Gradient descent is an iterative procedure anyway.
  - At every step, we have a chance to recover from previous missteps.

Minibatch Gradient

- The **full gradient** is

$$\nabla \hat{R}_n(w) = \frac{1}{n} \sum_{i=1}^{n} \nabla_w \ell(f_w(x_i), y_i)$$

- It's an average over the **full batch** of data $\mathcal{D}_n = \{(x_1, y_1), \ldots, (x_n, y_n)\}$.

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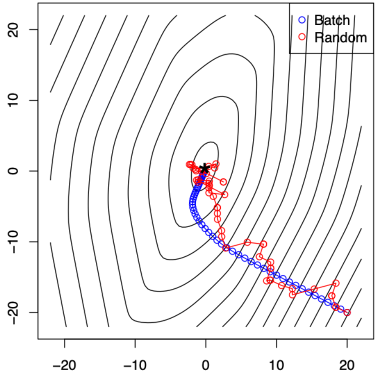
Batch vs Stochastic Methods



(Slide adapted from Ryan Tibshirani)

Rule of thumb for stochastic methods:

- Stochastic methods work well far from the optimum
- But struggle close the the optimum

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$$\mathbb{E}\left[\nabla \hat{R}_N(w)\right] = \nabla \hat{R}_n(w)$$

- The bigger the minibatch, the better the estimate.

$$\mathrm{Var}\left[\nabla \hat{R}_N(w)\right] = \mathrm{Var}\left[\frac{1}{N}\sum_i \nabla \hat{R}_i(w)\right] = \frac{1}{N^2}\mathrm{Var}\left[\sum_i \nabla \hat{R}_i(w)\right] = \frac{1}{N}\mathrm{Var}\left[\nabla \hat{R}_i(w)\right]$$

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- Because of vectorization, the computation cost of minibatches is sublinear

Convergence of SGD

- For convergence guarantee, use **diminishing step sizes**, e.g. $\eta_k = 1/k$
- Theoretically, GD is much faster than SGD in terms of convergence rate and number of steps:
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  - but most of that advantage comes into play once we're already pretty close to the minimum
  - in many ML problems we don't care about optimizing to high accuracy (why?)

Step Sizes in Minibatch Gradient Descent

Minibatch Gradient Descent (minibatch size N)

- initialize $w = 0$
- repeat
  - randomly choose N points $\{(x_i, y_i)\}_{i=1}^{N} \subset \mathcal{D}_n$
  - $w \leftarrow w - \eta \left[\frac{1}{N}\sum_{i=1}^{N} \nabla_w \ell(f_w(x_i), y_i)\right]$

- For SGD, fixed step size can work well in practice.

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- For SGD, fixed step size can work well in practice.
- Typical approach: Fixed step size reduced by constant factor whenever validation performance stops improving (staircase decay).
- Other schedules: inverse time decay (1/t) etc.

Convergence of SGD Theorem (Optional)

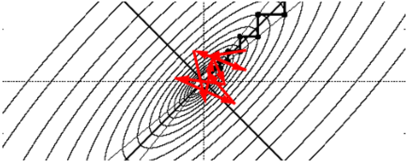
More on why we need a diminishing step size.

Theorem

If f is L-smooth and convex, and SGD has bounded variance $Var(\nabla f(x^{(k)})) \leqslant \sigma^2$ for all k, then SGD with step size $\eta \leqslant \frac{1}{L}$ satisifies:

$$\min_k \mathbb{E}[\|f(x^{(k)}\|^2] \leqslant \frac{f(x^{(0)} - f(x^*))}{\sum_k \eta_k} + \frac{L\sigma^2}{2}\frac{\sum_k \eta_k^2}{\sum_k \eta_k}$$

The extra term of variance will dominate if the step size does not decrease. [1]



[1] https://www.cs.ubc.ca/~schmidtm/Courses/540-W19/L11.pdf

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- If $\eta_k = \eta$, then $\sum_k \eta_k = k\eta, \sum_k \eta_k^2 = k\eta^2$, error$= O(1/k) + O(\eta)$.

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- If $\eta_k = \eta$, then $\sum_k \eta_k = k\eta, \sum_k \eta_k^2 = k\eta^2$, error$= O(1/k) + O(\eta)$.
- If $\eta_k = \eta/k$, then $\sum_k \eta_k = O(log(k)), \sum_k \eta_k^2 = O(1)$, error$= O(1/\log(k))$.

Convergence of SGD Theorem (Optional)

Theorem

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- If $\eta_k = \eta/k$, then $\sum_k \eta_k = O(log(k)), \sum_k \eta_k^2 = O(1)$, error$=O(1/\log(k))$.
- If $\eta_k = \eta/\sqrt{k}$, then $\sum_k \eta_k = O(\sqrt{k}), \sum_k \eta_k^2 = O(\log(k))$, error$=O(log(k)/\sqrt{k}) = \tilde{O}(1/\sqrt{k})$.

Summary

- **Gradient descent** or **"full-batch" gradient descent**
  - Use full data set of size n to determine step direction

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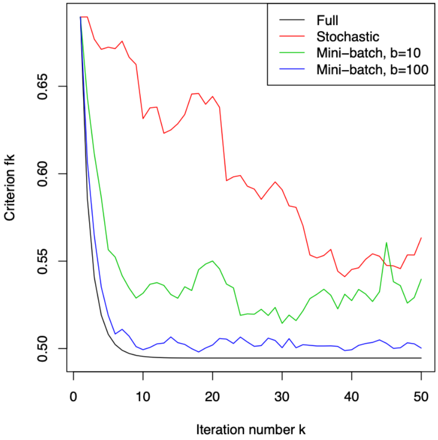
These days terminology isn't used so consistently, so when referring to SGD, always clarify the [mini]batch size.

SGD is much more efficient in time and memory cost and has been quite successful in large-scale ML.

Example: Logistic regression with ℓ_2 regularization

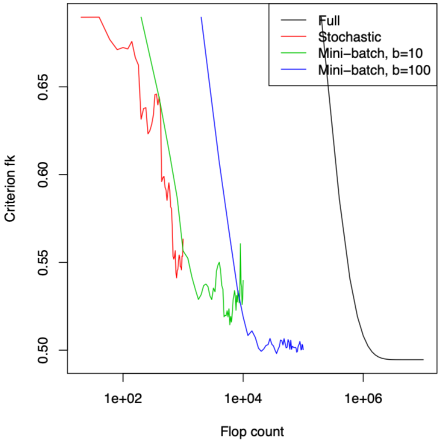
Batch methods converge faster :



(Example from Ryan Tibshirani)

Example: Logistic regression with ℓ_2 regularization

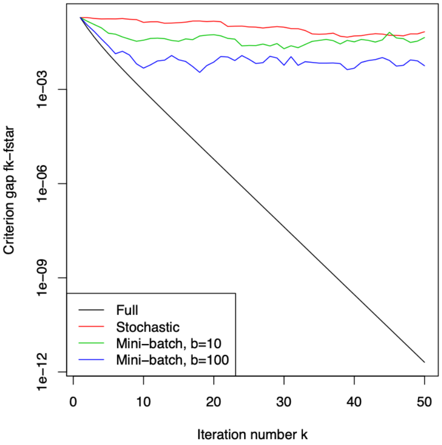
Stochastic methods are computationally more efficient:



(Example from Ryan Tibshirani)

Example: Logistic regression with ℓ_2 regularization

Batch methods are much faster close to the optimum:



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Loss Functions: Regression

Regression Problems

- Examples:
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- Notation:
  - $\hat{y}$ is the predicted value (the action)
  - y is the actual observed value (the outcome)

Loss Functions for Regression

- A loss function in general:

$$(\hat{y}, y) \mapsto \ell(\hat{y}, y) \in \mathrm{R}$$

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    - what you have to add to your prediction to get the correct answer.
- A loss $\ell(\hat{y}, y)$ is called **distance-based** if:
    1. It only depends on the residual:

$$\ell(\hat{y}, y) = \psi(y - \hat{y}) \quad \text{for some } \psi : \mathbf{R} \to \mathbf{R}$$

    2. It is zero when the residual is 0:

$$\psi(0) = 0$$

Distance-Based Losses are Translation Invariant

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- Sometimes the relative error $\frac{\hat{y}-y}{y}$ is a more natural loss (but not translation-invariant)
- Often you can transform response y so it's translation-invariant (e.g. log transform)

Some Losses for Regression

- **Residual:** $r = y - \hat{y}$
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y	$\hat{y}$	$\lvert r\rvert = \lvert y - \hat{y}\rvert$	$r^2 = (y - \hat{y})^2$
1	0	1	1
5	0	5	25
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- An outlier is a data point that differs significantly from other observations.

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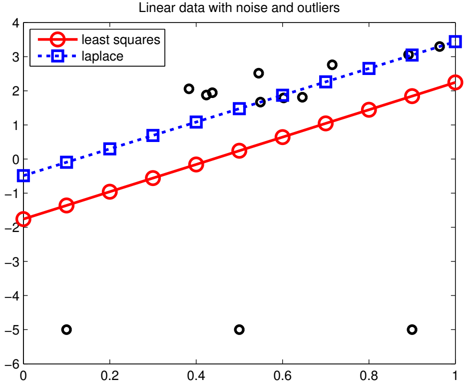
- Outliers typically have large residuals.
- Square loss much more affected by outliers than absolute loss.

Loss Function Robustness

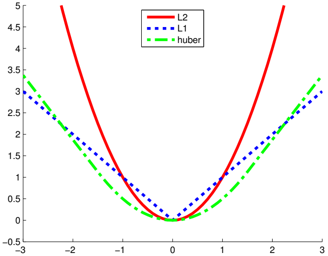
- **Robustness** refers to how affected a learning algorithm is by outliers.



KPM Figure 7.6

Some Losses for Regression

- **Square** or ℓ_2 Loss: $\ell(r) = r^2$ (*not robust*)
- **Absolute** or **Laplace** Loss: $\ell(r) = |r|$ (*not differentiable*)
  - gives **median regression**
- **Huber** Loss: Quadratic for $|r| \leqslant \delta$ and linear for $|r| > \delta$ (*robust and differentiable*)
  - Equal values and slopes at $r = \delta$



KPM Figure 7.6

Classification Loss Functions

The Classification Problem

- Examples:
  - Predict whether the image contains a cat
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How can we optimize the model output?

The Score Function

- Output space $\mathcal{Y} = \{-1, 1\}$
- **Real-valued prediction function** $f : \mathcal{X} \to R$

Definition

The value $f(x)$ is called the **score** for the input x.

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Definition

The value $f(x)$ is called the **score** for the input x.

- In this context, f may be called a **score function**.
- The magnitude of the score can be interpreted as our **confidence of our prediction**.

The Margin

Definition

The **margin** (or **functional margin**) for a predicted score $\hat{y}$ and the true class $y \in \{-1, 1\}$ is $y\hat{y}$.

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- The margin is a measure of how **correct** we are:
  - If y and $\hat{y}$ are the same sign, prediction is **correct** and margin is **positive**.
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- We want to **maximize the margin**.
- Most classification losses depend only on the margin (they are **margin-based losses**).

Classification Losses: $0-1$ Loss

- If $\tilde{f}$ is the inference function (1 if $f(x) > 0$ and -1 otherwise), then
- The **0-1 loss** for $f : \mathcal{X} \to \{-1, 1\}$:

$$\ell(f(x), y) = 1(\tilde{f}(x) \neq y)$$

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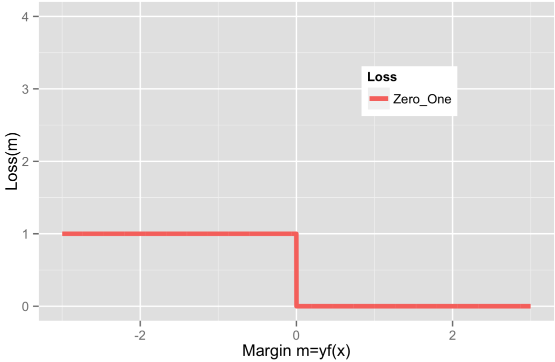
Minimizing empirical $0-1$ risk not computationally feasible.

$\hat{R}_n(f)$ is non-convex, not differentiable, and even discontinuous.

Classification Losses

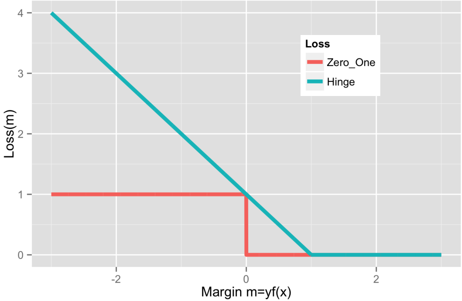
Zero-One loss: $\ell_{0\text{-}1} = 1(m \leqslant 0)$



- x-axis is **margin**: $m > 0 \iff$ correct classification

Hinge Loss

SVM/Hinge loss: $\ell_{\text{Hinge}} = \max(1 - m, 0)$



Hinge is a **convex**, **upper bound** on $0-1$ loss. Not differentiable at $m = 1$.

We will cover SVM and Hinge loss in more details in future lectures.

Logistic Regression

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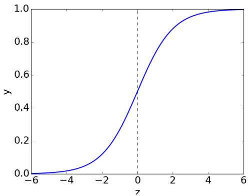
- Two equivalent types of logistic regression losses, depending on the labels.
- If the label is 0 or 1:
- $\hat{y} = \sigma(z)$, where σ is the sigmoid function, and $z = f(x) = w^\top x$.

$$\sigma(z) = \frac{1}{1 + \exp(-z)}$$



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- Remember the negative sign!

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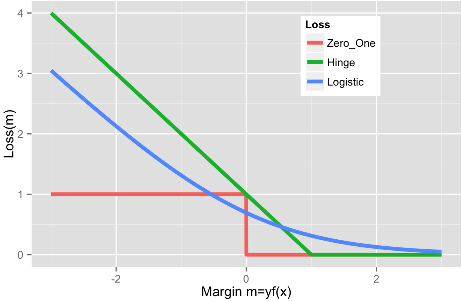
Logistic Regression

- If the label is -1 o 1:
- Note: $1 - \sigma(z) = \sigma(-z)$
- Now we can derive an equivalent loss form:

$$
\begin{aligned}
\ell_{\text{Logistic}} &= \begin{cases} -\log(\sigma(z)) & \text{if} \quad y = 1 \\ -\log(\sigma(-z)) & \text{if} \quad y = -1 \end{cases} \\
&= -\log(\sigma(yz)) \\
&= -\log\left(\frac{1}{1 + e^{-yz}}\right) \\
&= \log(1 + e^{-m}).
\end{aligned}
$$

Logistic Loss

Logistic/Log loss: $\ell_{\text{Logistic}} = \log\left(1 + e^{-m}\right)$



Logistic loss is differentiable. Logistic loss always rewards a larger margin (the loss is never 0).

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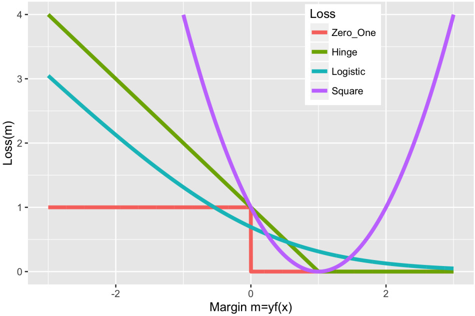
- Loss $\ell(f(x), y) = (f(x) - y)^2$.
- Turns out, can write this in terms of margin $m = f(x)y$:
- Using fact that $y^2 = 1$, since $y \in \{-1, 1\}$.

$$
\begin{aligned}
\ell(f(x), y) &= (f(x) - y)^2 \\
&= f^2(x) - 2f(x)y + y^2 \\
&= f^2(x)y^2 - 2f(x)y + 1 \\
&= (1 - f(x)y)^2 \\
&= (1 - m)^2
\end{aligned}
$$

What About Square Loss for Classification?



Heavily penalizes outliers (e.g. mislabeled examples).

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