CS 480/680
Introduction to Machine Learning

Lecture 2
Linear Regression and Loss Function Design

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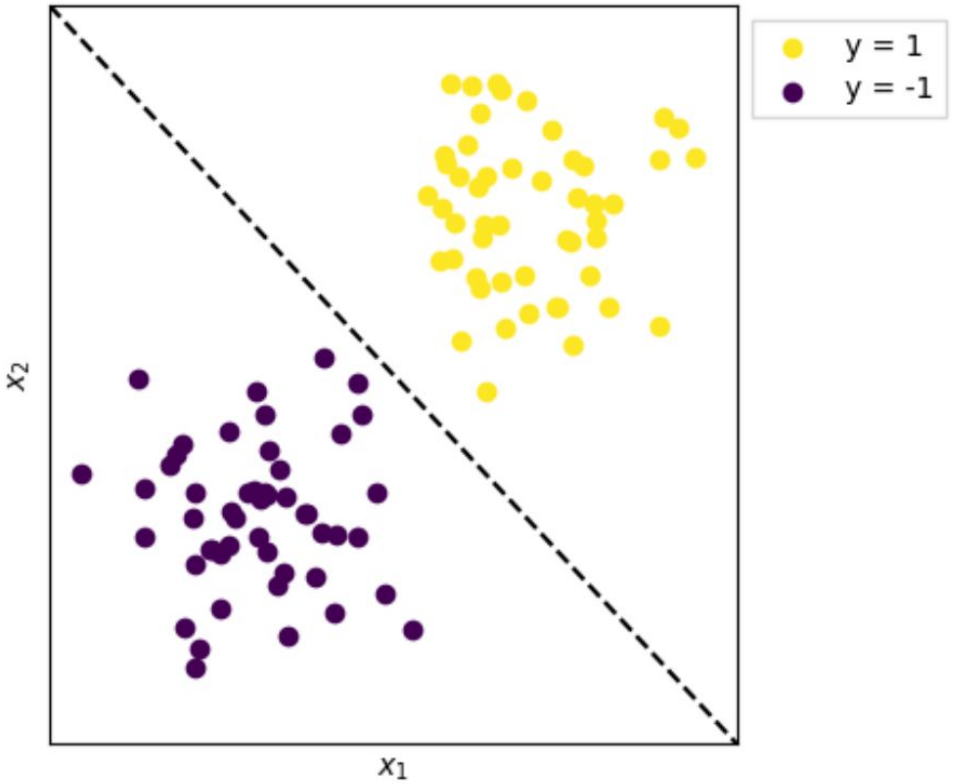
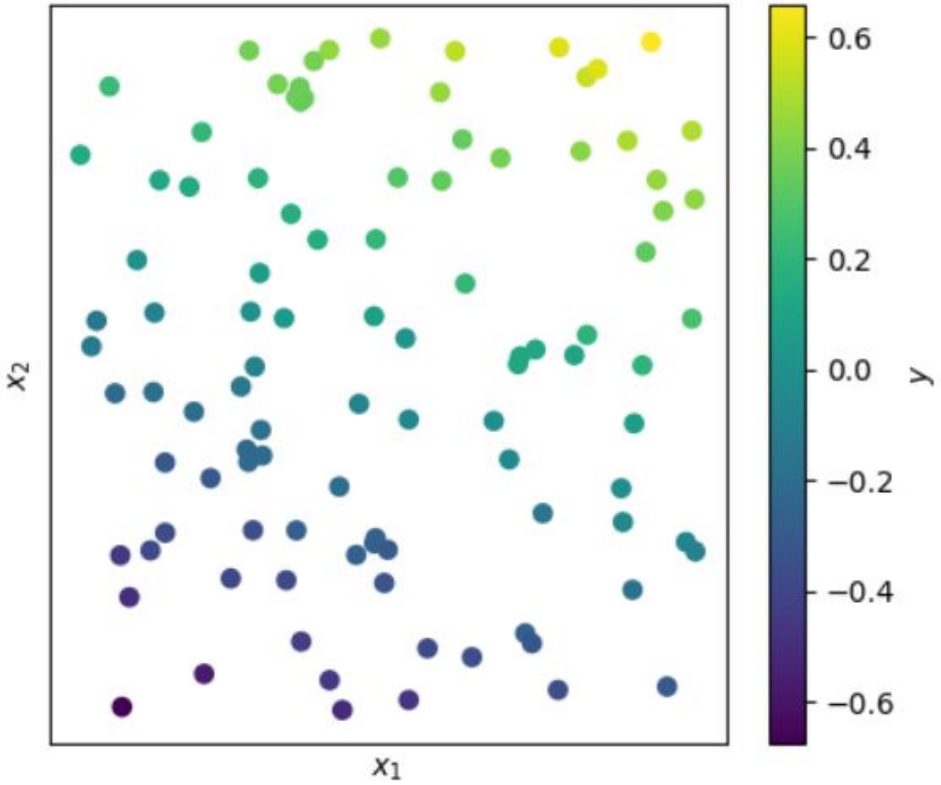
UNIVERSITY OF WATERLOO | FACULTY OF MATHEMATICS

Last lecture: The perceptron algorithm learns a hyperplane to classify linearly separable data



In regression, the goal is to predict continuous values



How can we learn in this setting?

1. Expand on our idea of “mistake” to deviation from ideal behavior
2. Select or design a loss *function*
3. Find the parameters that minimize the loss function

Lecture Aims

At the end of the lecture, we should be able to:

- ★ Write code to solve a simple regression problem numerically, given a dataset.
- ★ Characterize and design loss functions using correct terminology and sound mathematical principles.
- ★ Adhere to best practices for model evaluation and iterative improvement.

Lecture Outline

I. **What's the basic process for solving regression?**

   Models, loss functions, and empirical risk minimization

II. **What should one consider in loss function design?**

   Designing for optimization, stability, and generalization

III. **How do you evaluate model performance iteratively?**

   Overfitting, data splits, and cross validation

IV. **Summary + Housekeeping**

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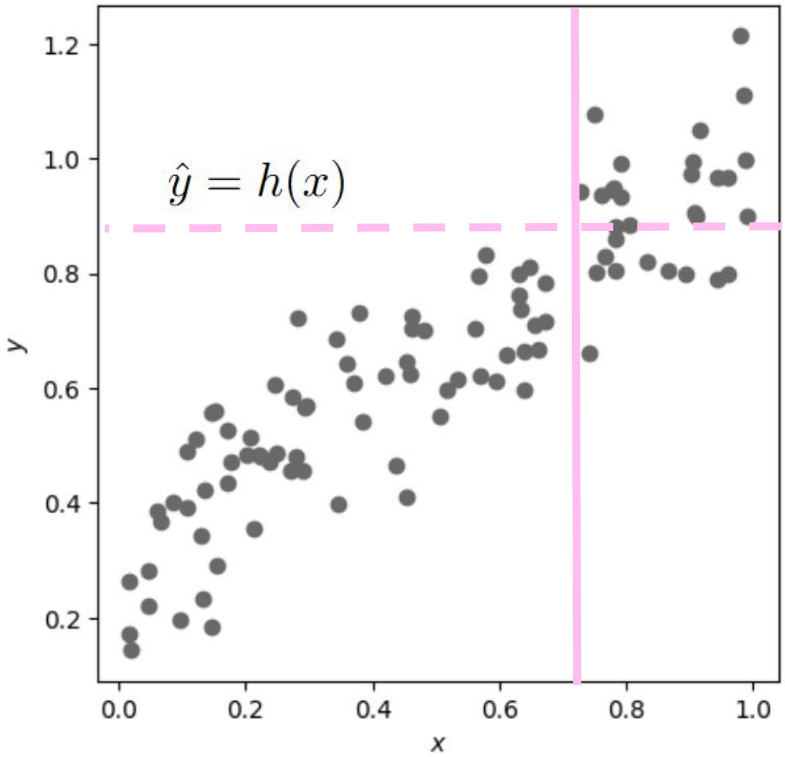
The Regression Problem



Given: $(\vec{x}_1, y_1), ...(\vec{x}_k, y_k), \vec{x}_i \in \mathbb{R}^d, y \in \mathbb{R}$
Goal: Learn $h : \mathbb{R}^d \to \mathbb{R}$ that best approximates relationship between variables.

From last lecture: Statistical (Batch) vs. Online Learning

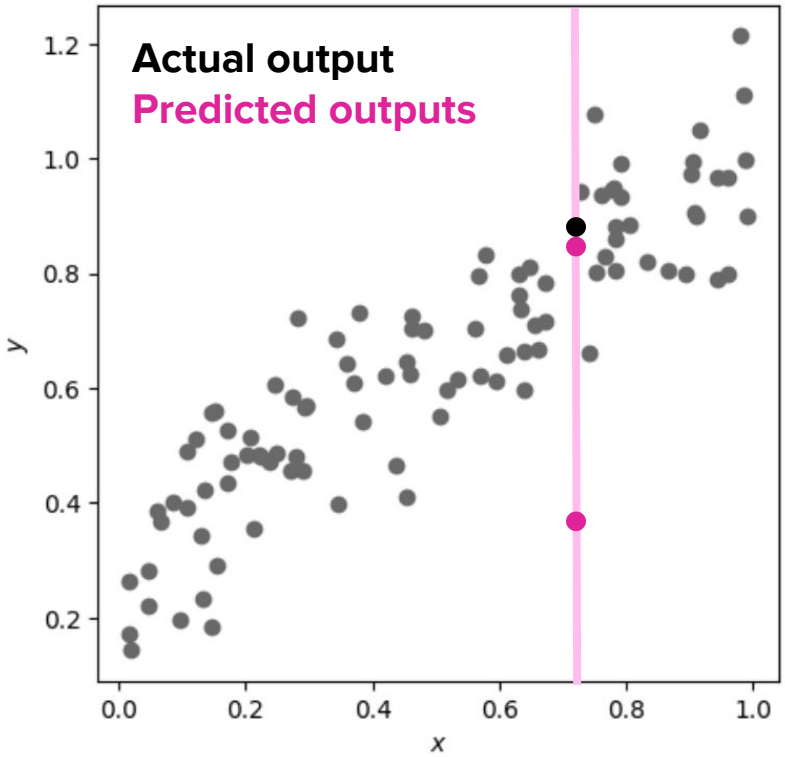
Online Learning:

- Learner has access to a data *stream*
- Prediction is made before knowing its true value
- Interested in minimizing the number of errors

Batch Learning:

- Given a training set $(\vec{x_1}, y_1), (\vec{x_2}, y_2), ...(\vec{x_k}, y_k) \sim_{i.i.d} P$, where
  - $i.i.d$: independently and identically distributed
  - P: some unknown distribution
- Goal: learn $h : \mathbb{R}^d \to \{\pm 1\}$ such that $\Pr_{(x,y)\sim P}[h(x) = y]$ to be large.

Restating the regression problem



Batch Learning:

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  - ~~(Classification) learn $h : \mathbb{R}^d \to \{\pm 1\}$~~
  - (Regression) learn $h : \mathbb{R}^d \to \mathbb{R}$

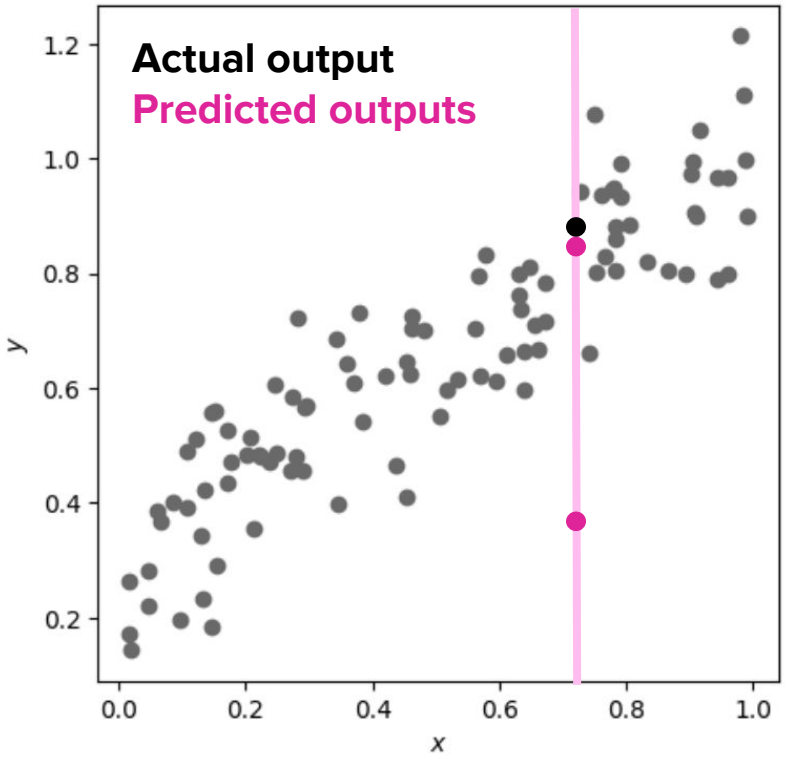
$E_{(x,y)\sim P}[l_w(x, y)]$ is small

Empirical Risk Minimization:

$$\text{argmin}_w \frac{1}{n} \sum_{i=1}^{n} l_w(\vec{x}_i, y_i)$$

$$\lim_{n\to\infty} \frac{1}{n} \sum_{i=1}^{n} l_w(\vec{x}_i, y_i) = \text{argmin}_w E_{(x,y)\sim P}[l_w(\boldsymbol{X}, \boldsymbol{y})]$$

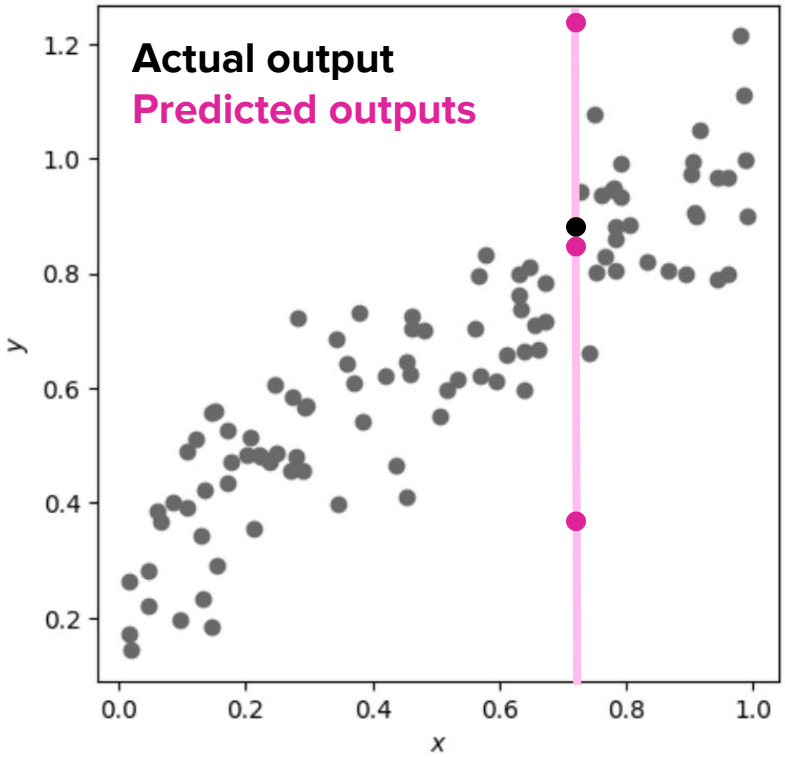
Restating the regression problem



Batch Learning, Restated:

- Given: A training set $(\vec{x_1}, y_1), (\vec{x_2}, y_2), ...(\vec{x_k}, y_k) \sim_{i.i.d} P$, **and loss function** $l_w(x, y)$
- Goal: $\text{argmin}_w \frac{1}{n} \sum_{i=1}^{n} l_w(\vec{x}_i, y_i)$

The loss function defines your performance objective



Select loss function of

$$l_w(x_i, y_i) = (h(x_i) - y_i)^2$$

Where:

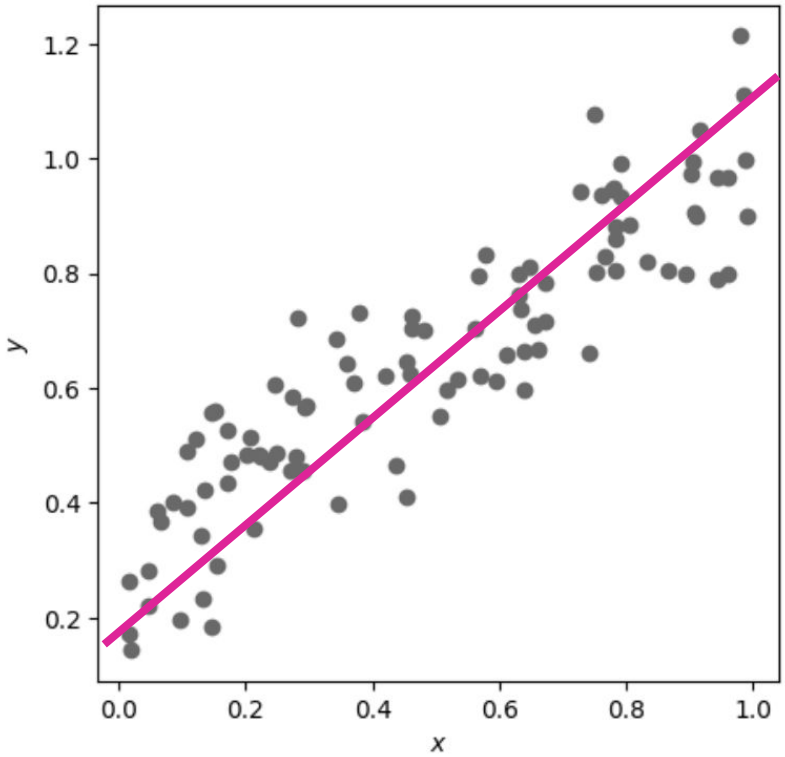
$h(x_i)$: output predicted by the model given the feature vector x_i, and
yi : is the true output

Then the expected loss is given by:

$$E[l_w] = \frac{1}{n}\sum_{i=1}^{n}\gamma_i^2$$

Where $\gamma_i = h(x_i) - y_i$ is the residual for sample (x_i, y_i)

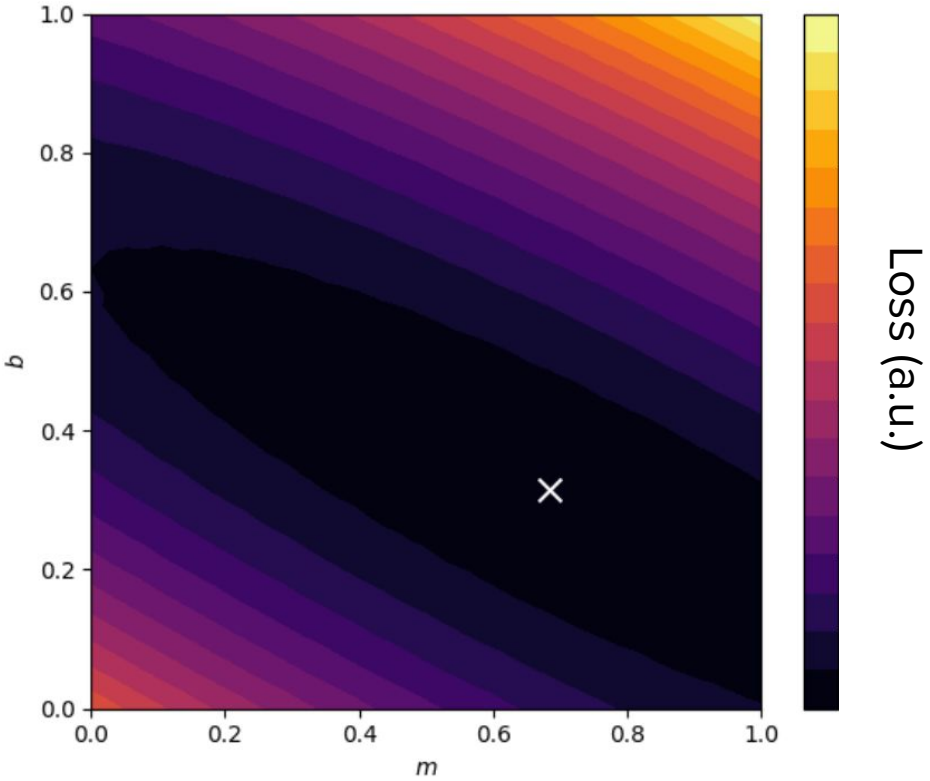
The linear regression predictor hypothesis class



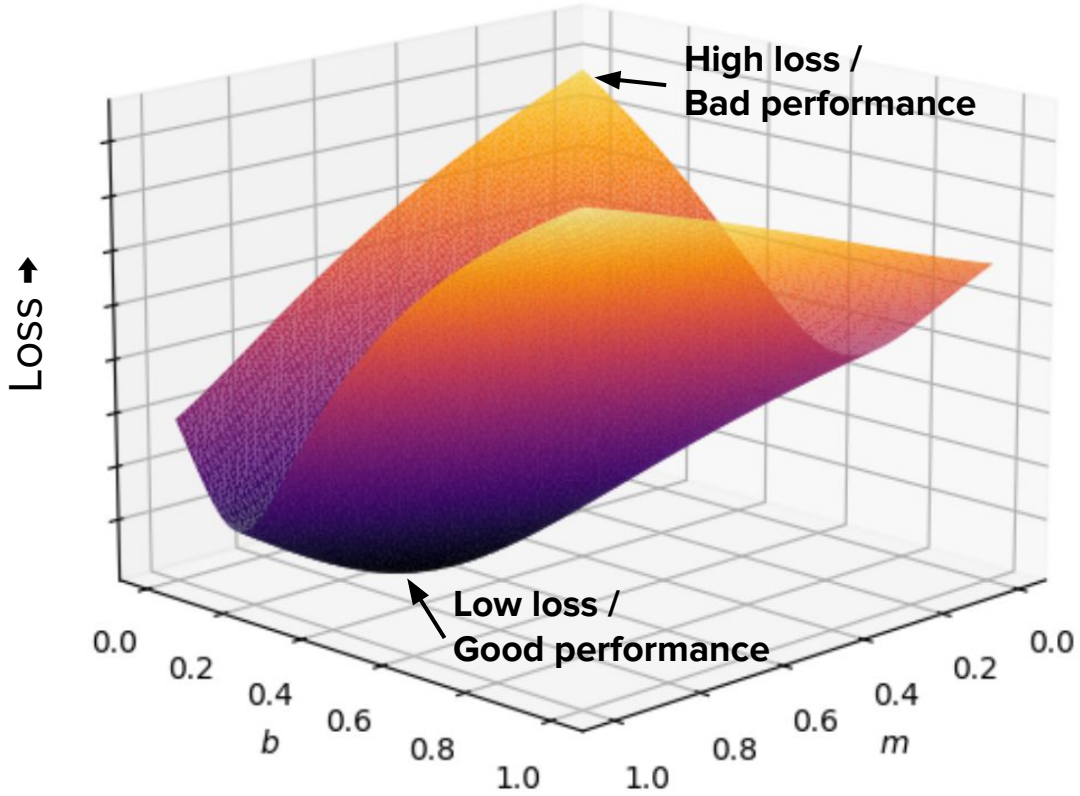
If we assume a model of the form $y = mx + b$, where m, b are parameters. Then

$$
\begin{aligned}
E[l_w] &= \sum_{i=1}^{n} \gamma_i^2 \\
&= \sum_{i=1}^{n} (h(x_i) - y_i)^2 \\
&= \sum_{i=1}^{n} (\langle (m, b), (x_i, 1) \rangle - y_i)^2 \\
&= \sum_{i=1}^{n} (\langle w, x_i' \rangle - y_i)^2
\end{aligned}
$$

How to minimize the loss?
Brute force search suggests a unique set of parameters



The loss function surface and the gradient



Interlude: Calculus Review

Derivative:

Let $f(x) : \mathbb{R} \to \mathbb{R}$ be a scalar-valued function of one variable. Then

$f'(x) = \frac{df}{dx} : \mathbb{R} \to \mathbb{R}$, is the derivative of $f(x)$

Example: $f(x) = x^2 + 3x + 5$, then $f'(x) = 2x + 3$

Gradient:

Let $f(\vec{x}) : \mathbb{R}^d \to \mathbb{R}$ be a scalar-valued function of a d-vector. Then

$\nabla f(\vec{x}) = (\frac{\partial f}{\partial x_1}, \ldots \frac{\partial f}{\partial x_d}) : \mathbb{R}^d \to \mathbb{R}^d$, is the gradient of $f(\vec{x})$

Example: $f(\vec{x}) = 2x_1 + 3x_2 + 5x_3$, then $\nabla f(\vec{x}) = (2, 3, 5)$

Adapted from Gautam Kamath's lecture notes

Interlude: Calculus Review (Continued)

Hessian:

Let $f(\vec{x}) : \mathbb{R}^d \to \mathbb{R}$ be a a scalar-valued function of a d-vector. Then

$\nabla^2 f(\vec{x}) : \mathbb{R}^d \to \mathbb{R}^{d \times d}$, is the Hessian of $f(\vec{x})$

$$\nabla^2 f(\vec{x}) = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_d} \\ \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_d \partial x_1} & \cdots & \frac{\partial^2 f}{\partial x_d^2} \end{bmatrix}$$

Example: $f(x) = 3x_1^2 + 2x_1x_2 + 5x_2^2$, then $\nabla^2 f(\vec{x}) = \begin{pmatrix} 6 & 2 \\ 2 & 10 \end{pmatrix}$

Adapted from Gautam Kamath's lecture notes

Equivalent notation of loss to leverage the gradient

Let A, $\mathbb{R}^{n\times(d+1)}$, be a matrix of the padded feature vectors in the training dataset,

$$A = \begin{bmatrix} — & x_1' & — \\ — & x_2' & — \\ & \vdots & \\ — & x_n' & — \end{bmatrix}$$

and z, $\mathbb{R}^{n\times 1}$, be a matrix of the outputs of the training dataset,

$$z = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

then we can write the total loss L as:

$$\begin{aligned} L &= \sum_{i=1}^{n} (\langle w, x_i' \rangle - y_i)^2 \\ &= \|Aw - z\|_2^2 \end{aligned}$$

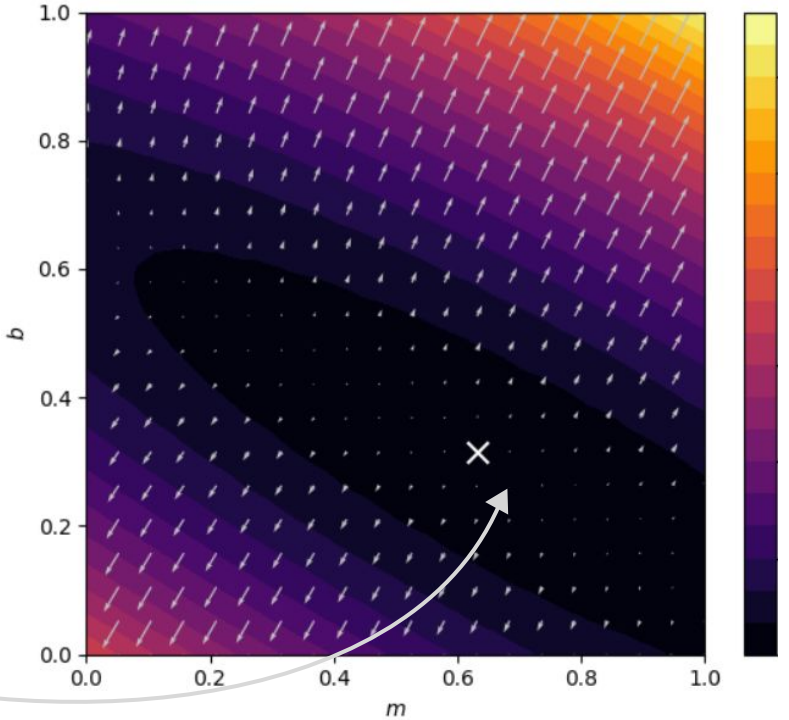
How to find the solution?
Leveraging the gradient of the loss function

We are interested in the gradient of the loss with respect to the parameters w, that is $\nabla_w L$

$$\begin{aligned}\nabla_w L &= \nabla_w \|Aw - z\|_2^2 \\ &= \nabla_w (Aw - z)^T (Aw - z) \\ &= \nabla_w \left[w^T A^T A w - 2 z^T A w + z^T z \right] \\ &= 2A^T A w - 2A^T z\end{aligned}$$

The expression for the loss can be rearranged to solve for the parameters where the gradient is zero:

$$\begin{aligned}2A^T A w - 2A^T z &= 0 \\ 2A^T A w &= 2A^T z \\ w &= (A^T A)^{-1} A^T z\end{aligned}$$



Practical issues with minimizing the loss function

- A^TA might not be invertible
- A^TA can be computationally intensive
- Could be imprecise if ill-conditioned
- Could also solve system of linear equations with gaussian elimination

Summary of our process to solve a regression problem

Define Performance	Select a Model	Estimate Parameters
Specified a loss function in the statistical learning setting using empirical risk minimization.	Linear: $y = mx + b$ Rewrite as: $y = < (m,b) , (x,1) >$ $y = < w , x' >$	✘ Used brute force to find a high-performing solution (low loss) ✔ Computed gradient and determined parameters where it is zero.

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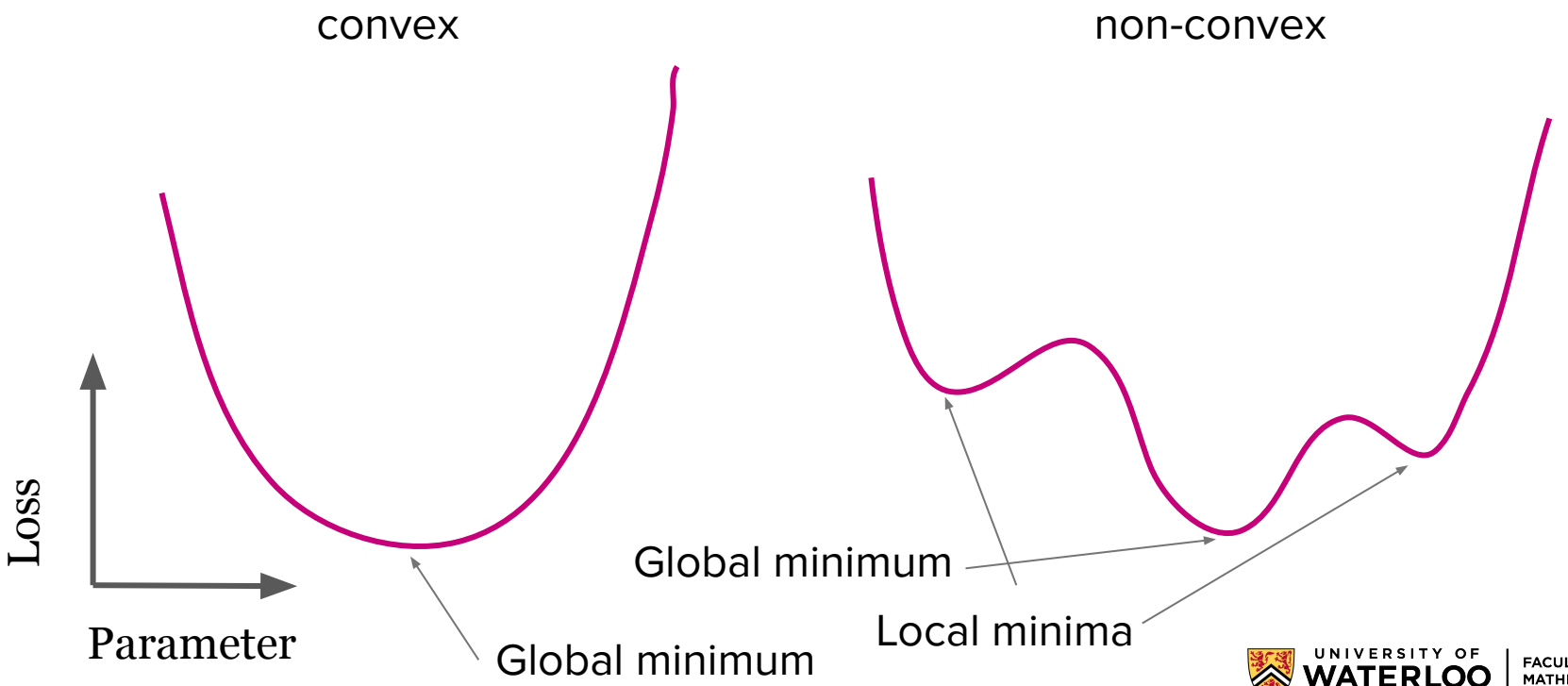
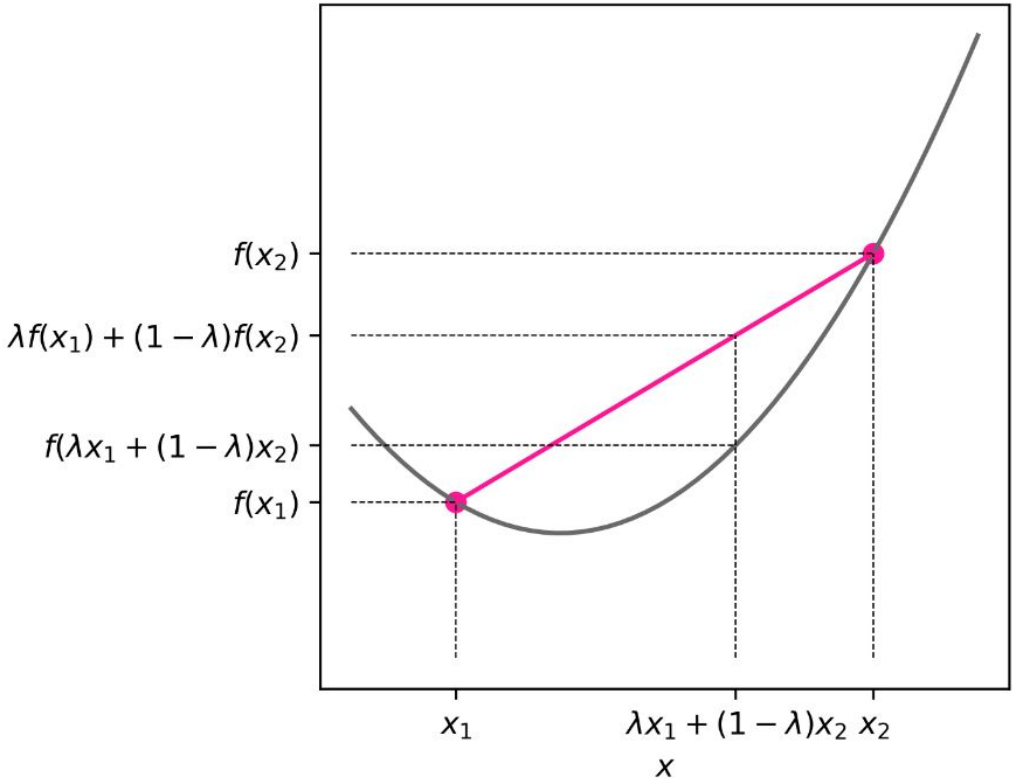
Can we be sure that the minimum is a global minimum?



A function is convex iff it satisfies Jensen's Inequality

Jensen's Inequality:

$$f(\lambda x_1 + (1-\lambda)x_2) \leq \lambda f(x_1) + (1-\lambda) f(x_2)$$

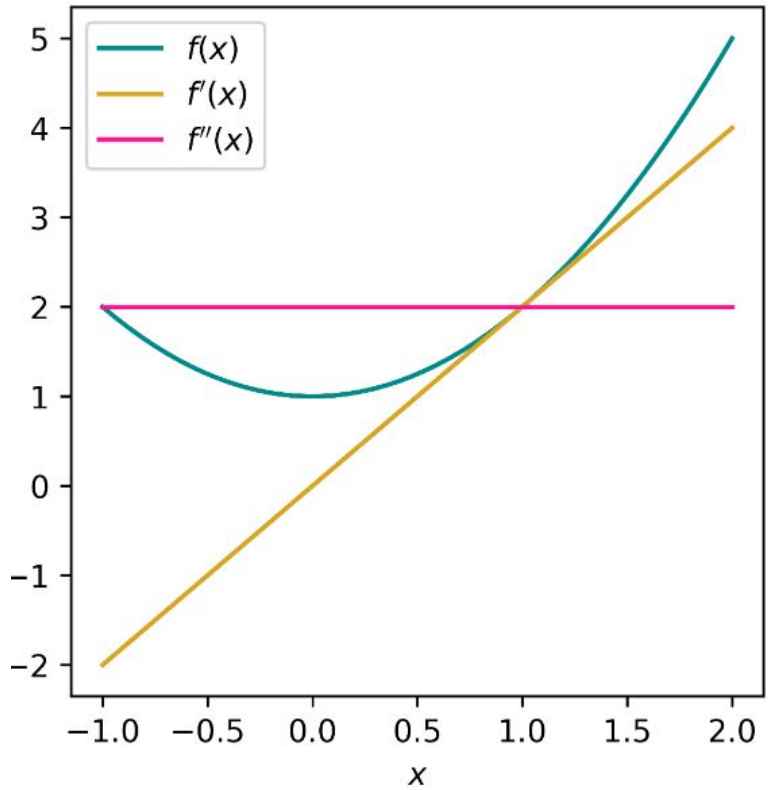


A twice-differentiable function is convex iff its Hessian is everywhere positive semidefinite

For a function $f : \mathbb{R} \to \mathbb{R}$:
$f''(x) \geq 0 \, \forall x$
$\implies$ Function is convex

For a function $f : \mathbb{R}^d \to \mathbb{R}$:
Hessian $\nabla^2 f(x)$ is Positive Semidefinite (PSD) for all x
$\implies$ Function is convex

Positive Semidefinite (PSD)
Notation: $M \succcurlyeq 0$
A matrix $M \in \mathbb{R}^{d \times d}$ is PSD iff $v^T M v \geq 0 \, \forall v, v \in \mathbb{R}^d$



Convex functions are straightforward to optimize

Fermat's condition:

If x is a local extremum of f, then $\nabla f(x) = 0$

If f is convex, the converse is also true:
$\nabla f(x) = 0 \implies$ global extremum

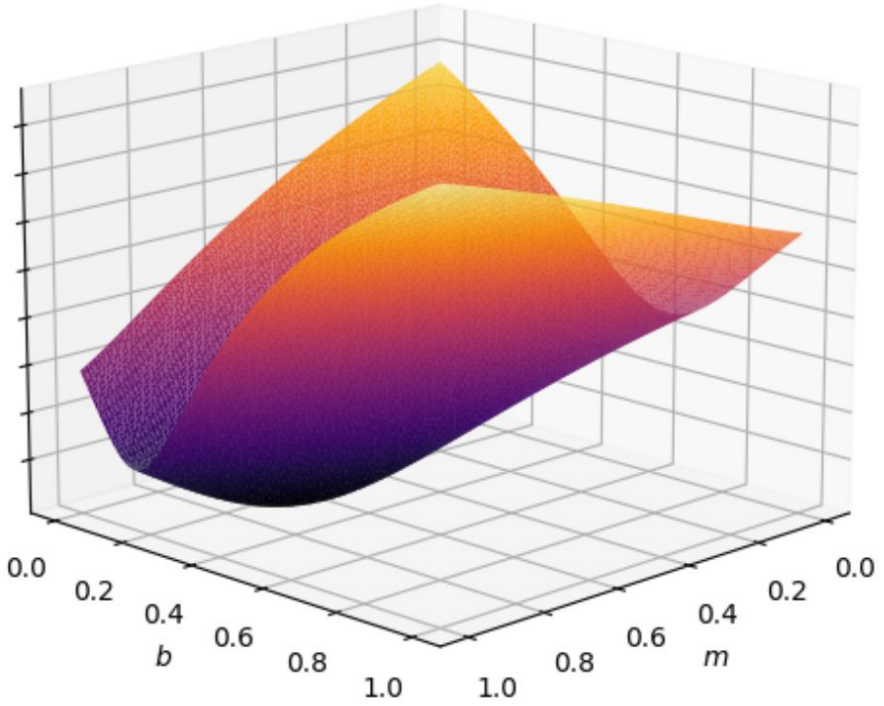
Is the least-squares loss convex?

Recall that the least-squares loss was defined as:

$$L = \|Aw - z\|_2^2$$
$$\nabla_w L = 2A^T Aw - 2A^T z$$
$$\nabla_w^2 L = 2A^T A$$

Is the Hessian positive semidefinite?

$$2v^T A^T Av \geq 0 \, \forall v$$
$$2\|Av\|_2^2 \geq 0 \, \forall v$$



Visualizing the Loss Landscape of Neural Nets

Hao Li[1], **Zheng Xu**[1], **Gavin Taylor**[2], **Christoph Studer**[3], **Tom Goldstein**[1]
[1]University of Maryland, College Park [2]United States Naval Academy [3]Cornell University
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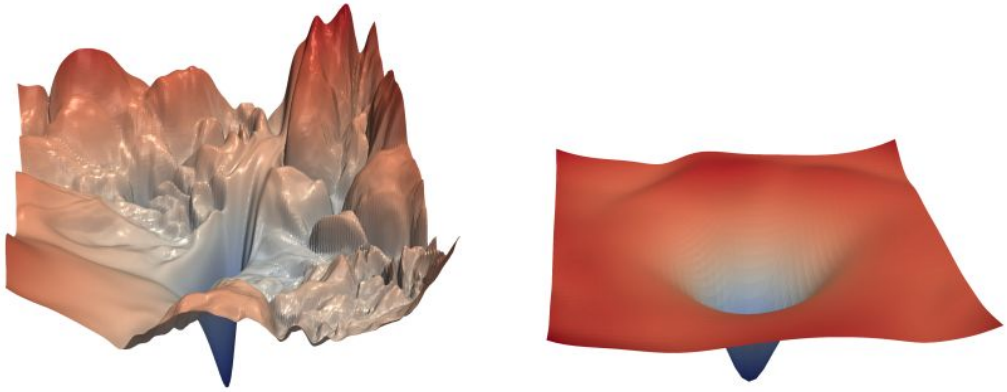
Abstract

Neural network training relies on our ability to f
non-convex loss functions. It is well-known t
designs (e.g., skip connections) produce loss fur
chosen training parameters (batch size, learning
ers that generalize better. However, the reason
effect on the underlying loss landscape, are not v
explore the structure of neural loss functions, an
generalization, using a range of visualization met
"filter normalization" method that helps us visu
make meaningful side-by-side comparisons betv
a variety of visualizations, we explore how netv
landscape, and how training parameters affect th



(a) without skip connections (b) with skip connections

Figure 1: The loss surfaces of ResNet-56 with/without skip connections. The proposed filter normalization scheme is used to enable comparisons of sharpness/flatness between the two figures.

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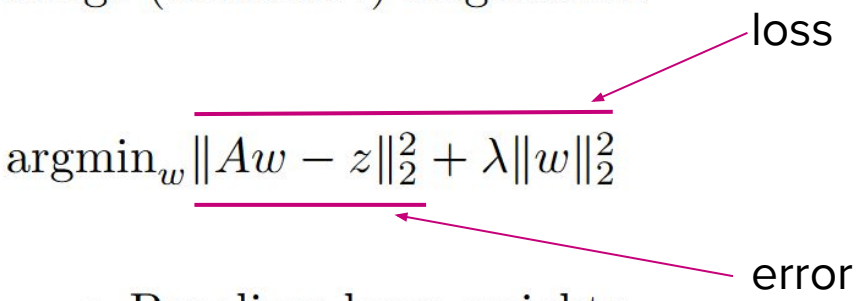
Stabilize the weights with L_2 Regularization

Ridge (Tikhonov) Regression:



- Penalizes large weights
- Stabilizes the weights

Sparsify the weights with L_1 Regularization

Lasso Regression:

$$\text{argmin}_w \|Aw - z\|_2^2 + \lambda \|w\|_1$$

- Penalizes non-zero weights
- Sparsifies the weights (many will be zero)
- Will cause many features to be ignored

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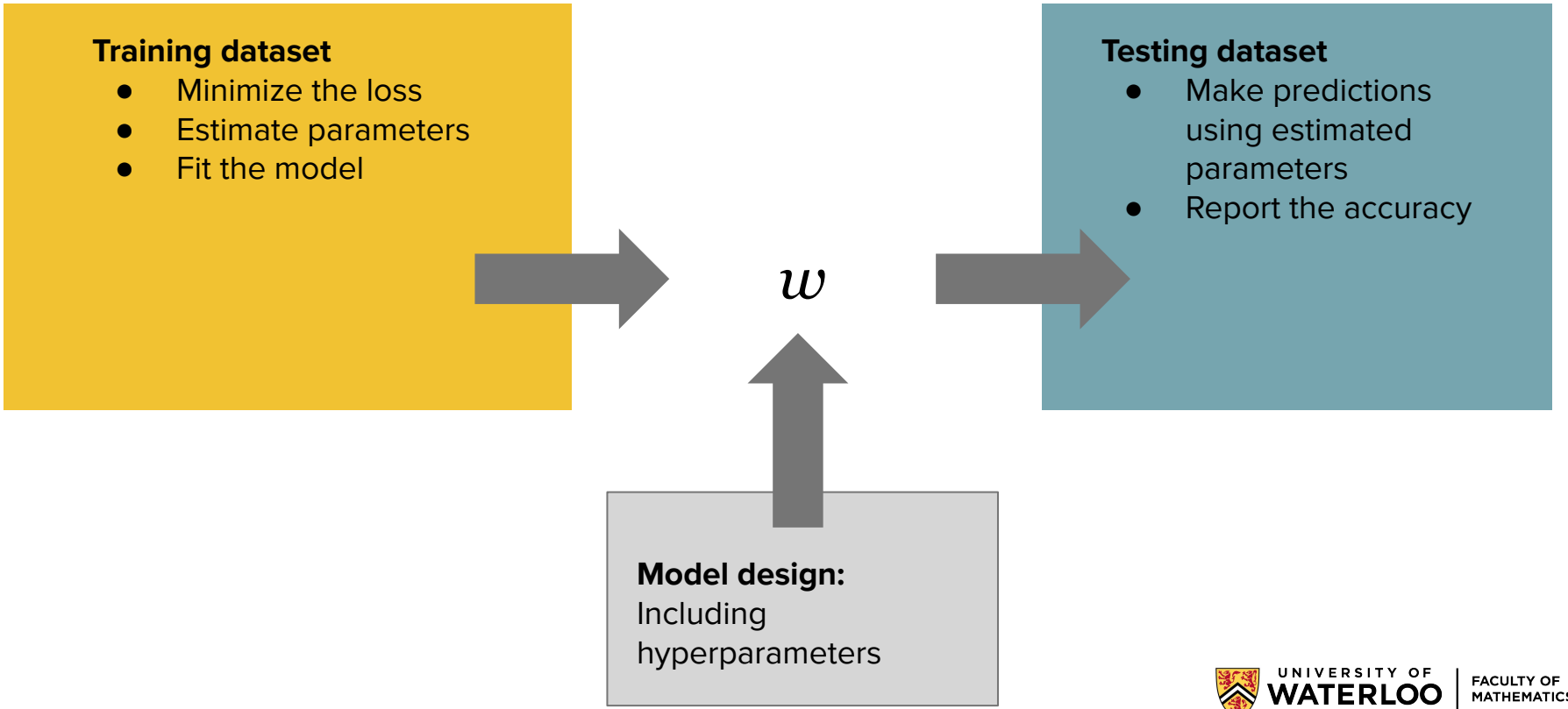
Correct use of training and testing datasets



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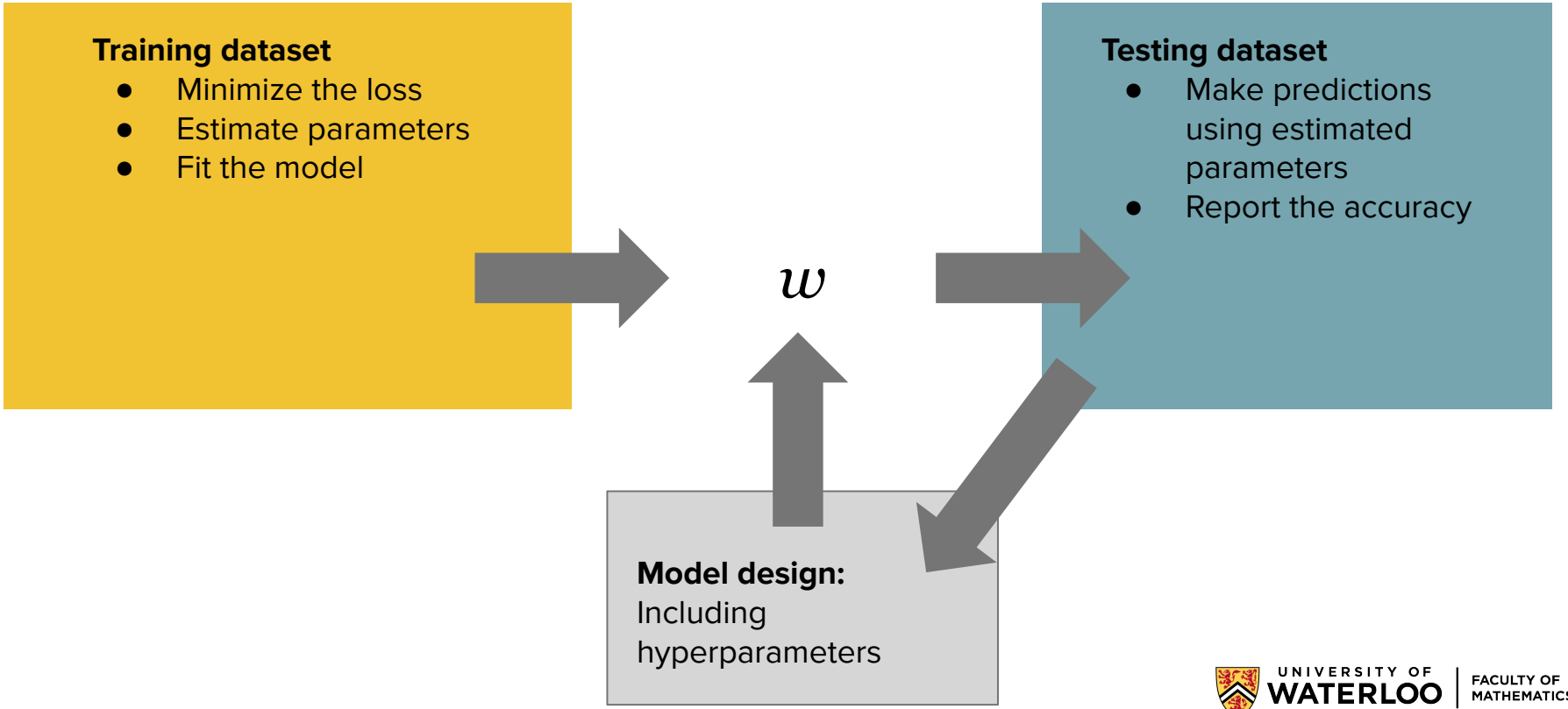
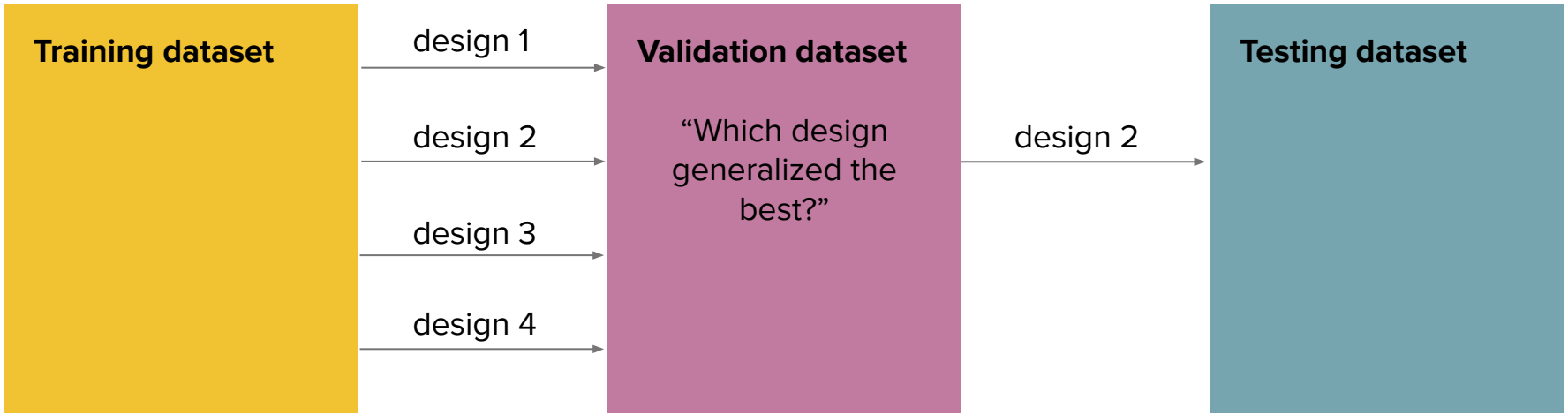
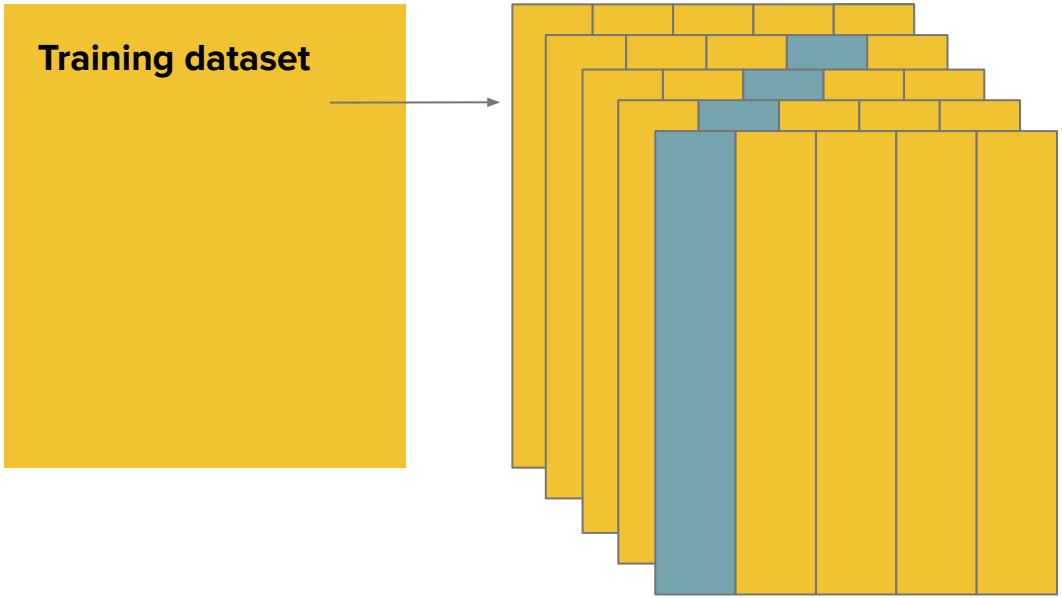


Introducing a validation dataset



Cross-validation for small datasets



Algorithm 1 Cross-Validation.

Input:
1: Dataset $D = \{(x_i, y_i) \in \mathbb{R}^{d+1}\}$,
2: number of folds k
Output: Optimal hyperparameter λ
3: **for** $\lambda = \lambda_1, \lambda_2, \ldots$ **do**
4: **for** $i = 1,2,\ldots,k$ **do**
$w_{\lambda,i} = \text{train}(\cup_{j \neq i}^{k} D_j)$
$\text{Perf}_{\lambda,i} = \text{Acc}(D_i)$
5: **end for**
$\text{Perf}_\lambda = \frac{1}{k} \sum_{i=1}^{k} \text{Perf}_{\lambda,i}$
6: **end for**
7: **return** $\text{argmax}_\lambda \text{Perf}_\lambda$

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- Write code to solve a simple regression problem numerically, given a dataset.
- Characterize and design loss functions using correct terminology and sound mathematical principles.
- Adhere to best practices for model evaluation and iterative improvement.

Errata

- On the slide titled, "Equivalent notation of loss to leverage the gradient" a reference was made to constructing a loss *matrix*. This has been corrected to "We can write the total loss, L as ...".

- A previous version of the slide deck had a slide titled "If a function is convex, its second derivative is positive." This statement was incorrect because a convex function requires the second derivative to be non-negative (≥ 0, not strictly positive, > 0). Additionally, a function may be convex but not necessarily everywhere twice differentiable. The corrected statement reads: "A twice-differentiable function of more than one variable is convex *if and only if* its Hessian is everywhere positive semidefinite," emphasizing that this condition must hold for all points in the function's domain. This clarification highlights that having a positive semidefinite Hessian matrix everywhere in the domain is a sufficient and necessary condition for convexity in the context of twice-differentiable functions. However, convexity as a broader property does not inherently require the function to be twice differentiable or the Hessian to be defined everywhere.