CS 480/680
Introduction to Machine Learning

Lecture 2
Linear Regression and Loss Function Design

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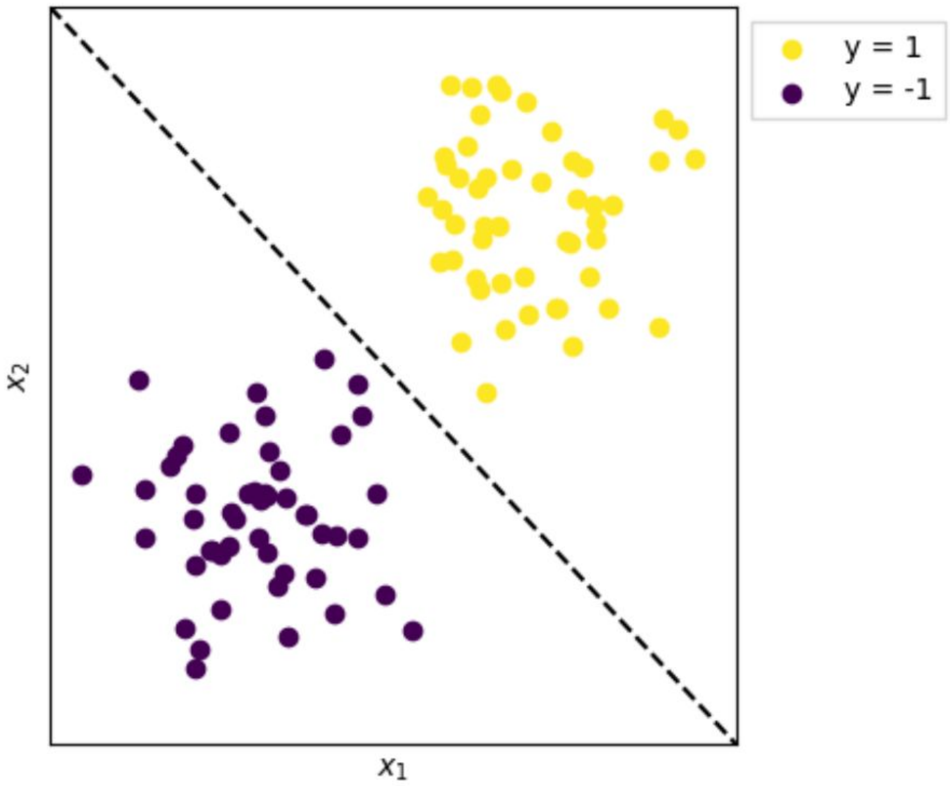
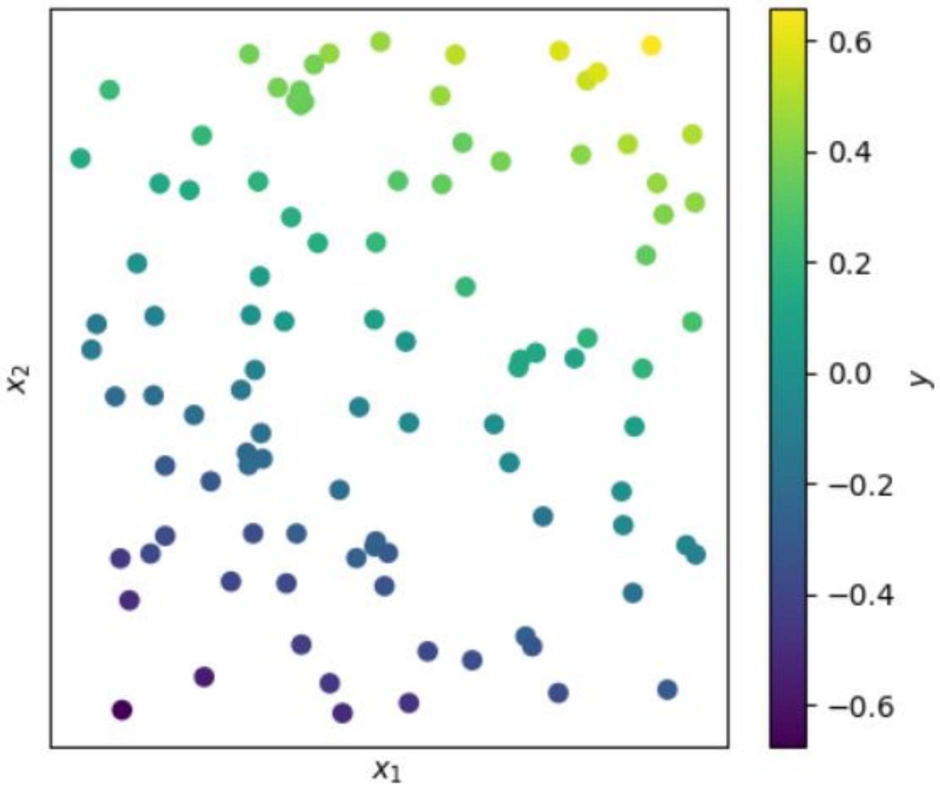
Last lecture: The perceptron algorithm learns a hyperplane to classify linearly separable data



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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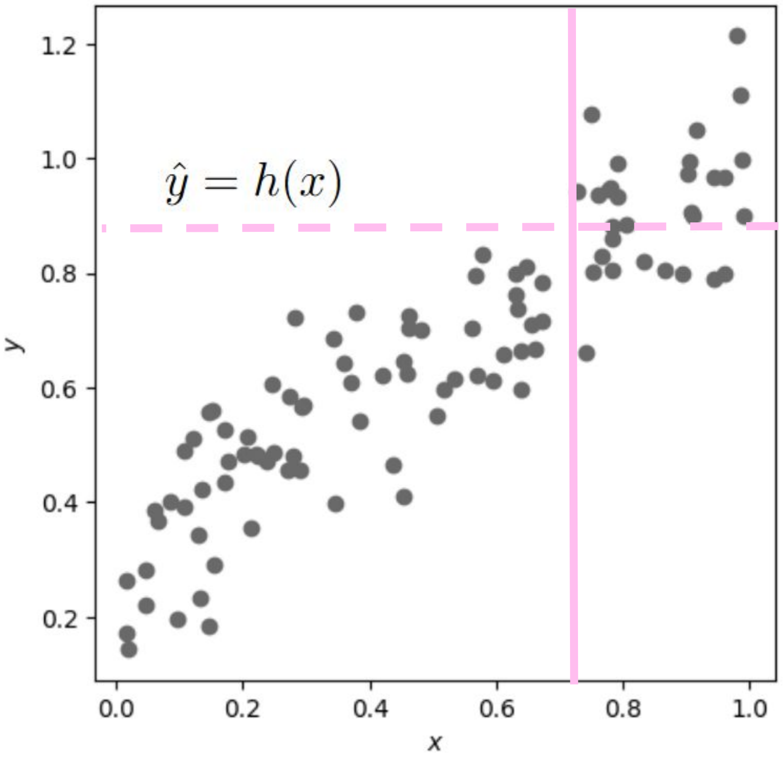
The Regression Problem



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

Statistical (Batch) vs. Online Learning

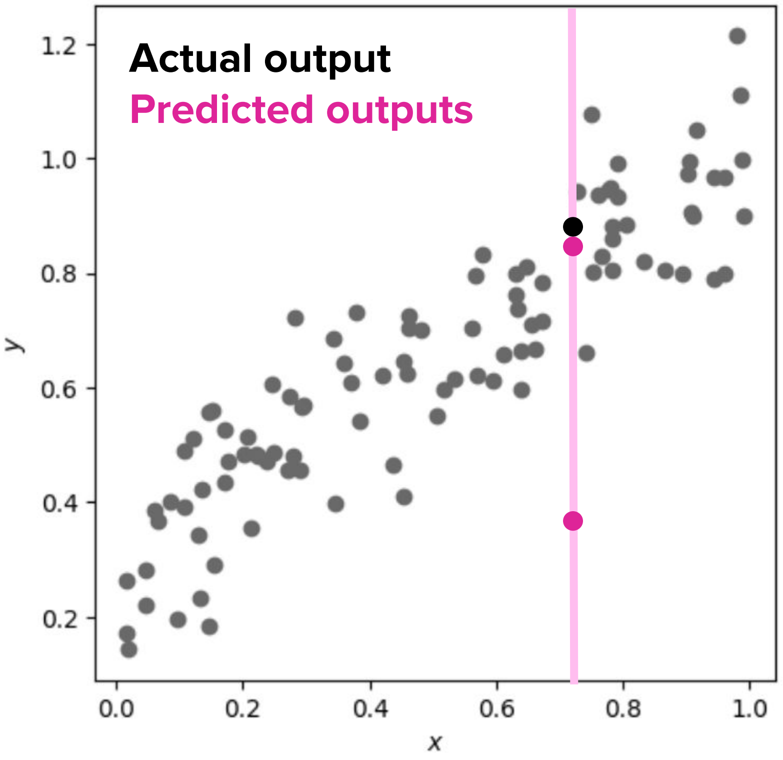
Online Learning:

- 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 $h : \mathbb{R}^{\mathrm{d}} \to \{\pm 1\}$ such that $\Pr_{(x,y)\sim P}[h(x) = y]$ to be large.

Restating the regression problem



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 $h : \boxed{\mathbb{R}^d \rightarrow \{\pm 1\}}$ such that $\boxed{\Pr_{(x,y)\sim P}[h(x) = y] \text{ to be large.}}$

– ~~(Classification) learn $h : \mathbb{R}^d \rightarrow \{\pm 1\}$~~

– (Regression) learn $h : \mathbb{R}^d \rightarrow \mathbb{R}$

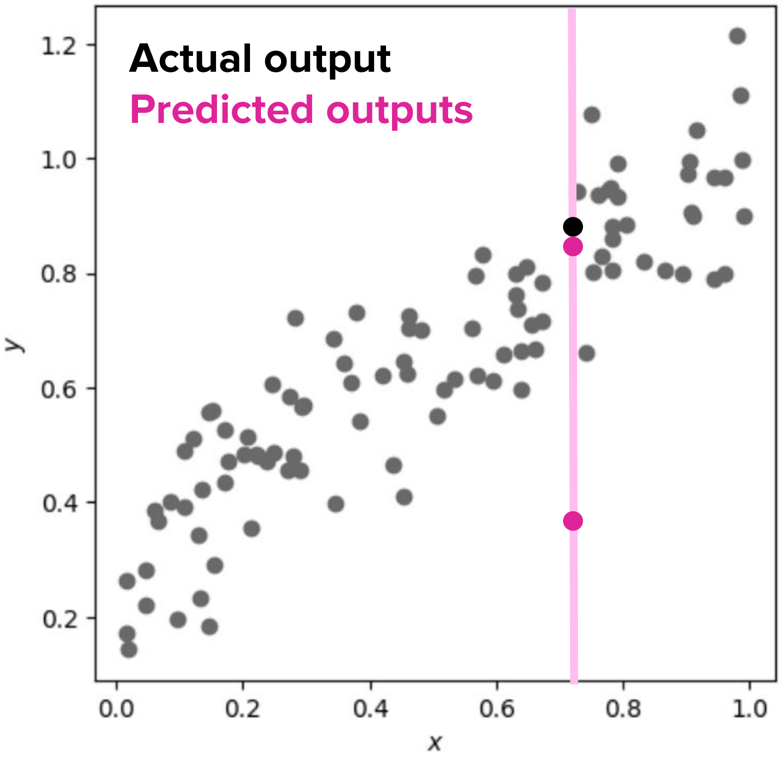
$\boxed{E_{(x,y)\sim P}[l_w(x, y)] \text{ is small}}$

Empirical Risk Minimization:

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

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

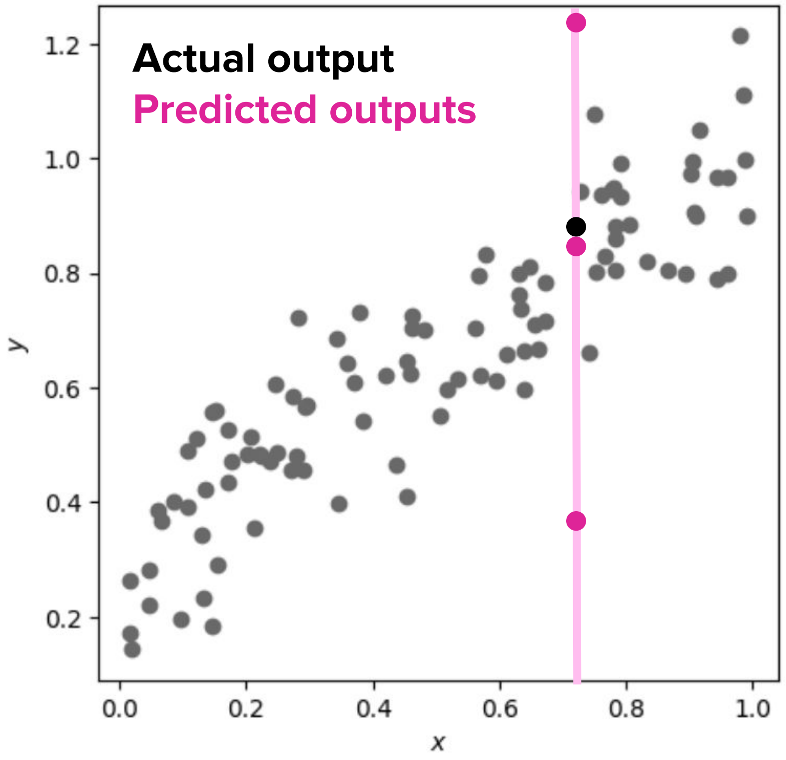
Restating the regression problem



Batch Learning, Restated:

- Given: A training set $(\vec{x_1}, y_1), (\vec{x_2}, y_2), \ldots(\vec{x_k}, y_k) \sim_{i.i.d} P$, **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

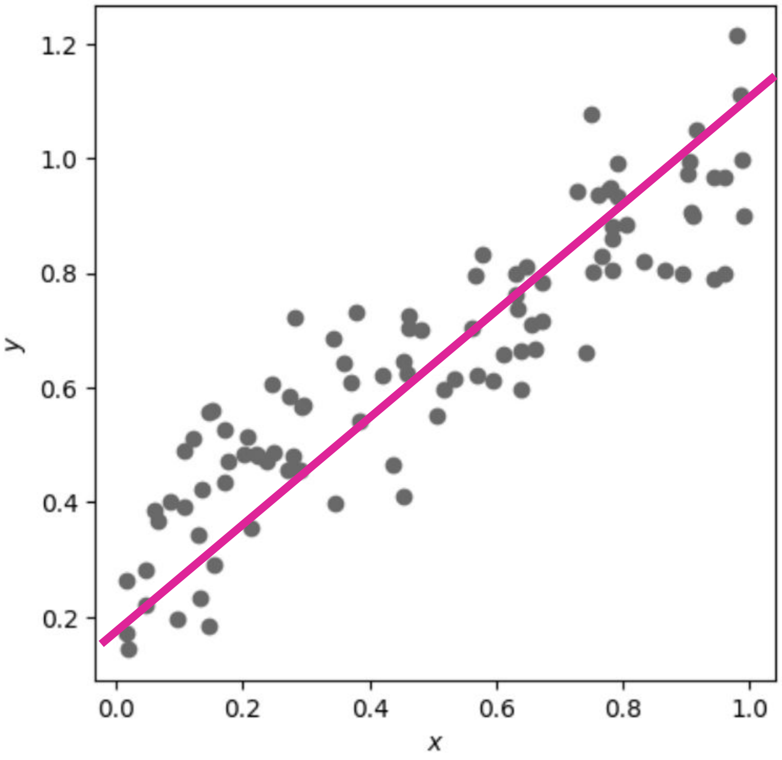
yi : is the true output

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)

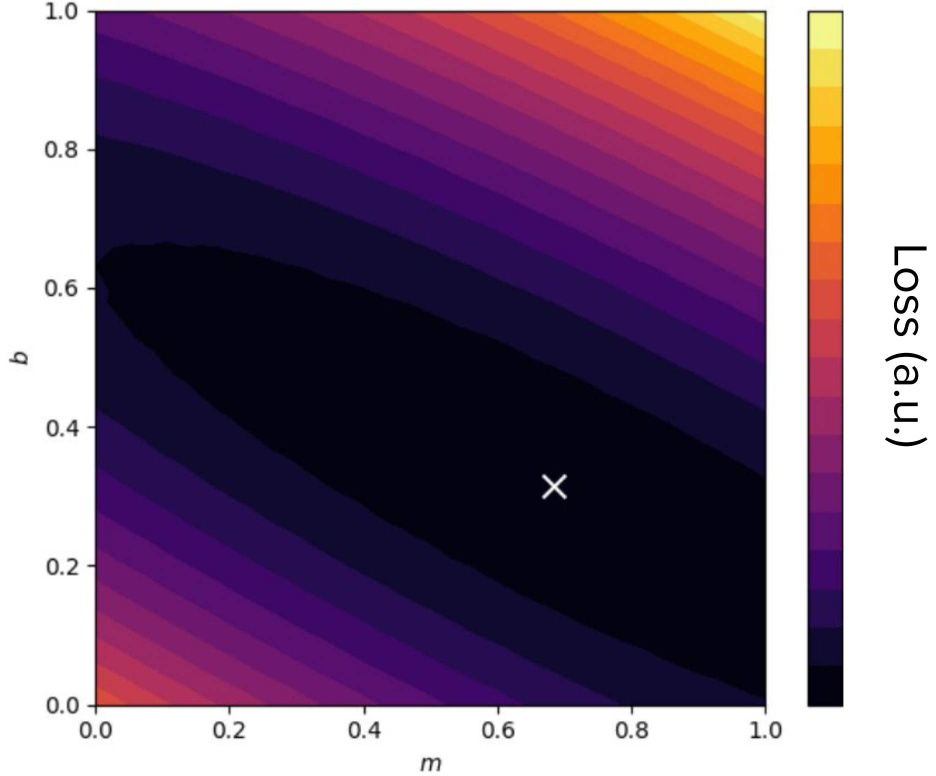
The linear regression predictor hypothesis class



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



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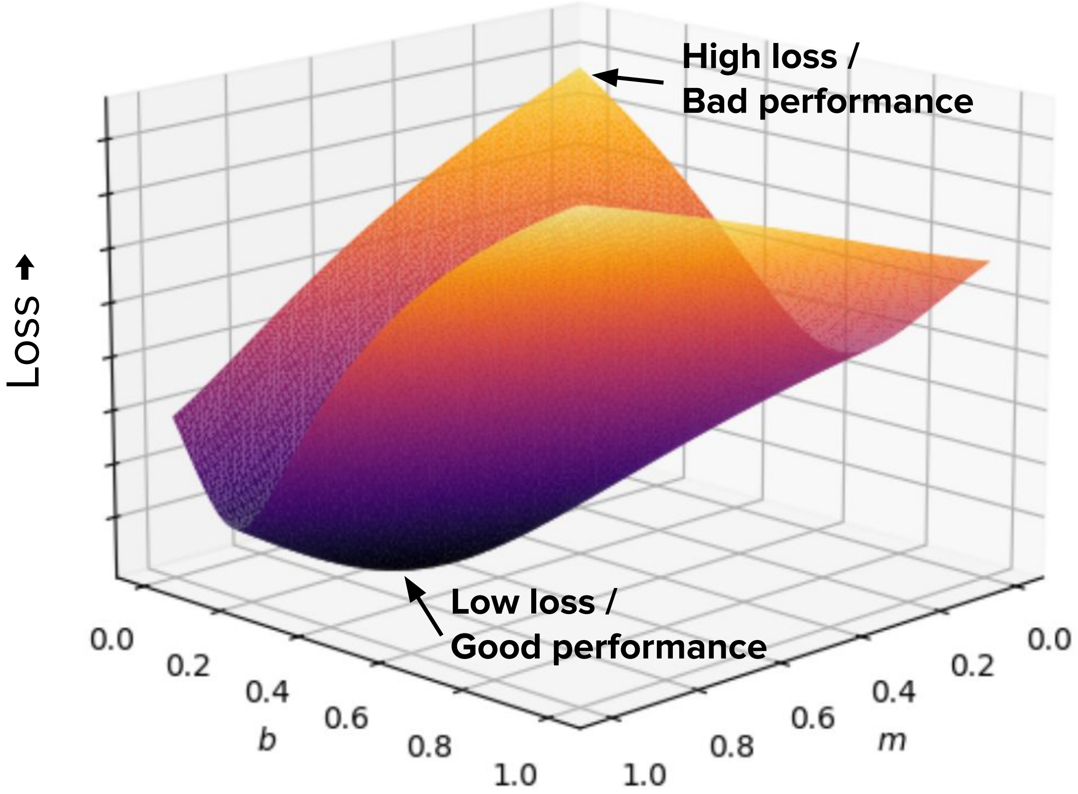
The loss function surface and the gradient



Interlude: Calculus Review

Derivative:

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

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

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

Gradient:

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

$\nabla f(\vec{x}) = (\frac{\partial f}{\partial x_1}, \ldots \frac{\partial f}{\partial x_d}) : \mathbb{R}^{\mathrm{d}} \rightarrow \mathbb{R}^{\mathrm{d}}$, 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: $f(x) = 3x_1^2 + 2x_1 x_2 + 5x_2^2$, then $\nabla^2 f(\vec{x}) = \begin{pmatrix} 6 & 2 \\ 2 & 10 \end{pmatrix}$

Equivalent notation for loss

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 construct a loss matrix, L, $\mathbb{R}^{n\times 1}$ as

$$L = \|Aw - z\|_2^2$$

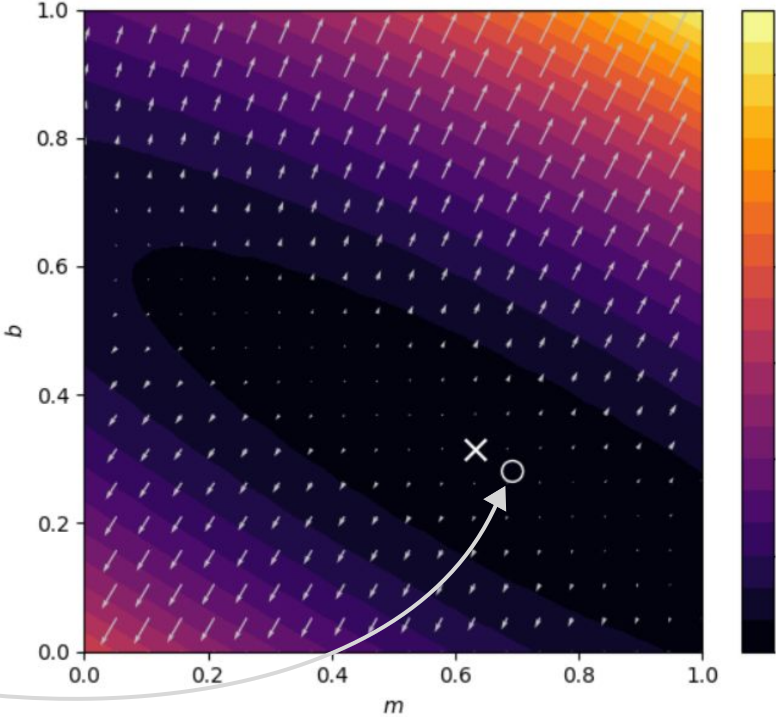
How to find the solution?
Leveraging the gradient of the loss function

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:

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



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 the regression problem

Define Performance | Select a Model | Estimate Parameters

Specified a loss function in the statistical learning setting using empirical risk minimization.

Linear:
$y = mx + b$

Generalizes to:
$y = < (m,b) , (x,1) >$

✘ Used brute force to find a high-performing solution (low loss)

✔ Computed gradient and determined parameters where it is zero.

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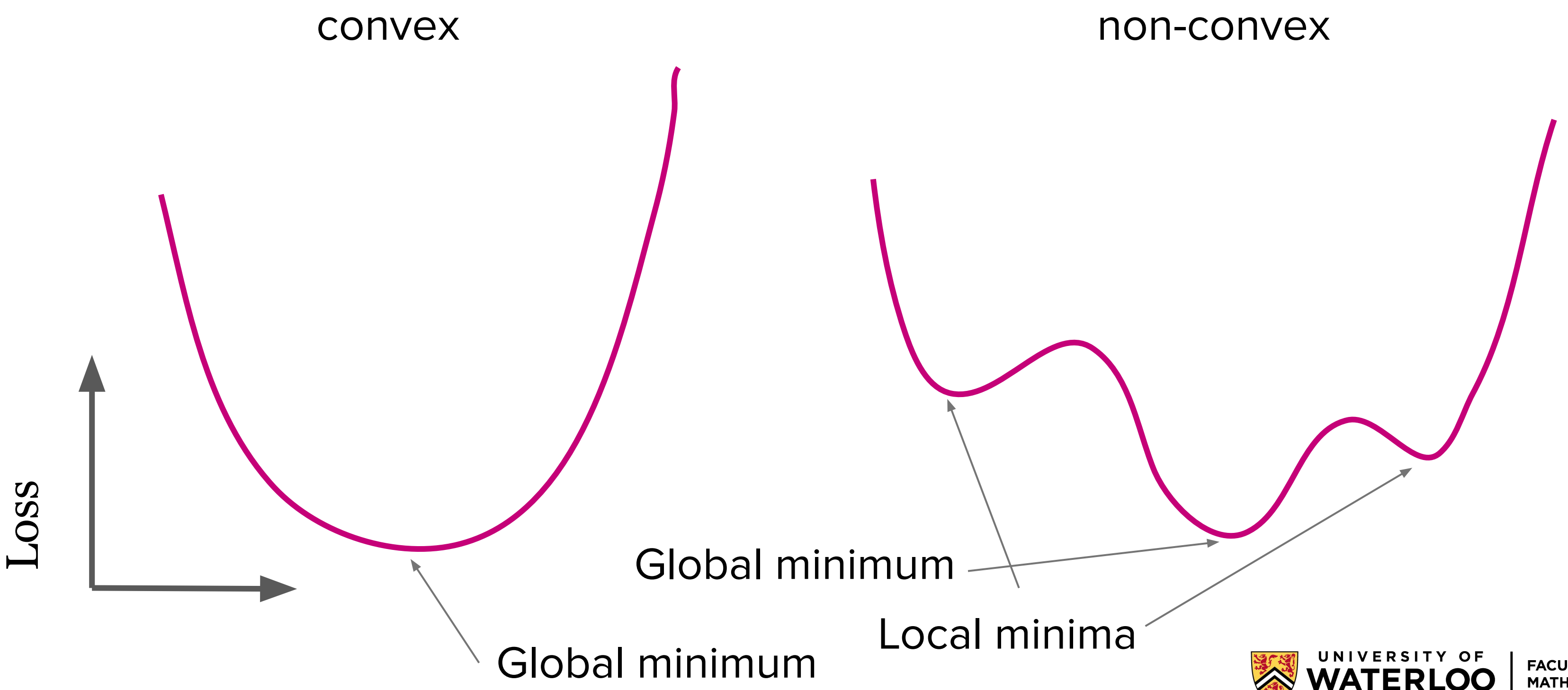
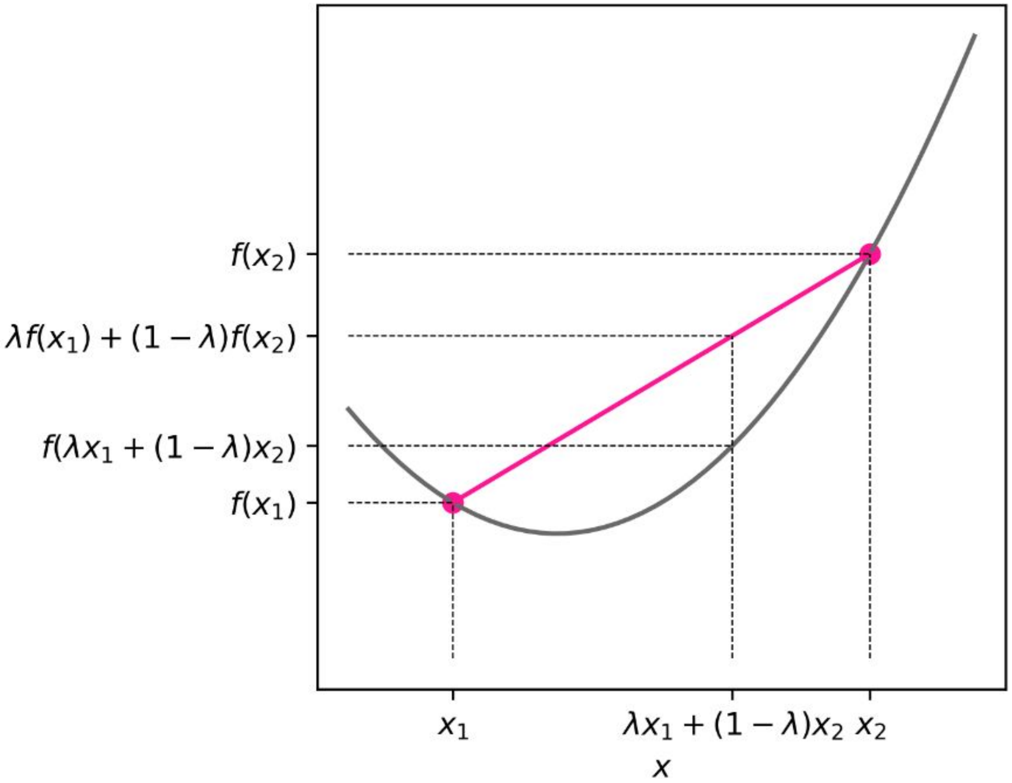
Can we be sure that the minimum is a global minimum?



Definition:
A function is convex <u>**iff**</u> it satisfies Jensen's Inequality

Jensen's Inequality:
$f(\lambda x_1 + (1-\lambda)x_2) \leq \lambda f(x_1) + (1-\lambda) f(x_2)$



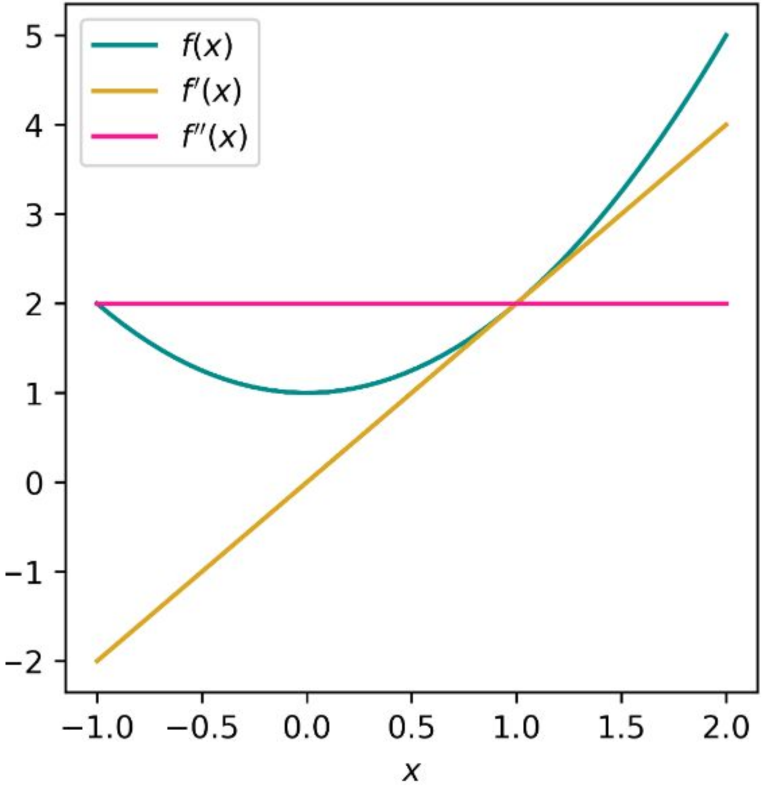
If a function is convex, its second derivative is strictly positive

$$\text{For } x \in \mathbb{R} : f''(x) \geq 0 \, \forall x$$

$$\text{For } x \in \mathbb{R}^{\mathrm{d}} : \nabla^2 f(x) \geq 0$$

$$\implies v^T H v \geq 0$$

(Hessian is positive semidefinite)



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

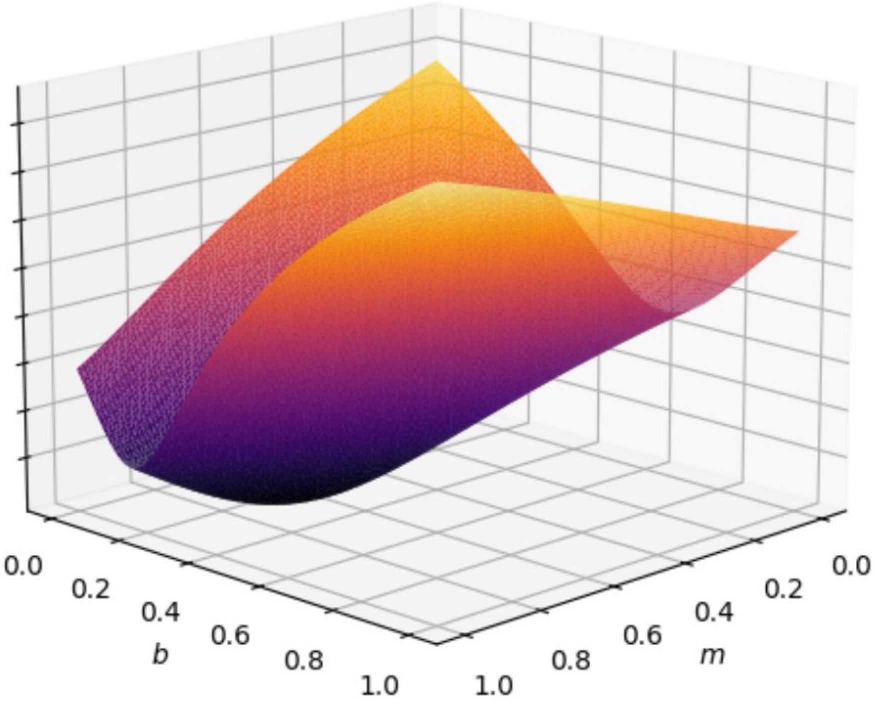
Is the least-squares loss convex?

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?

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



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Stabilize the weights with L_2 Regularization

Ridge (Tikhonov) Regression:

$$\operatorname{argmin}_w \overbrace{\underbrace{\|Aw - z\|_2^2}_{\text{error}} + \lambda \|w\|_2^2}^{\text{loss}}$$

- 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

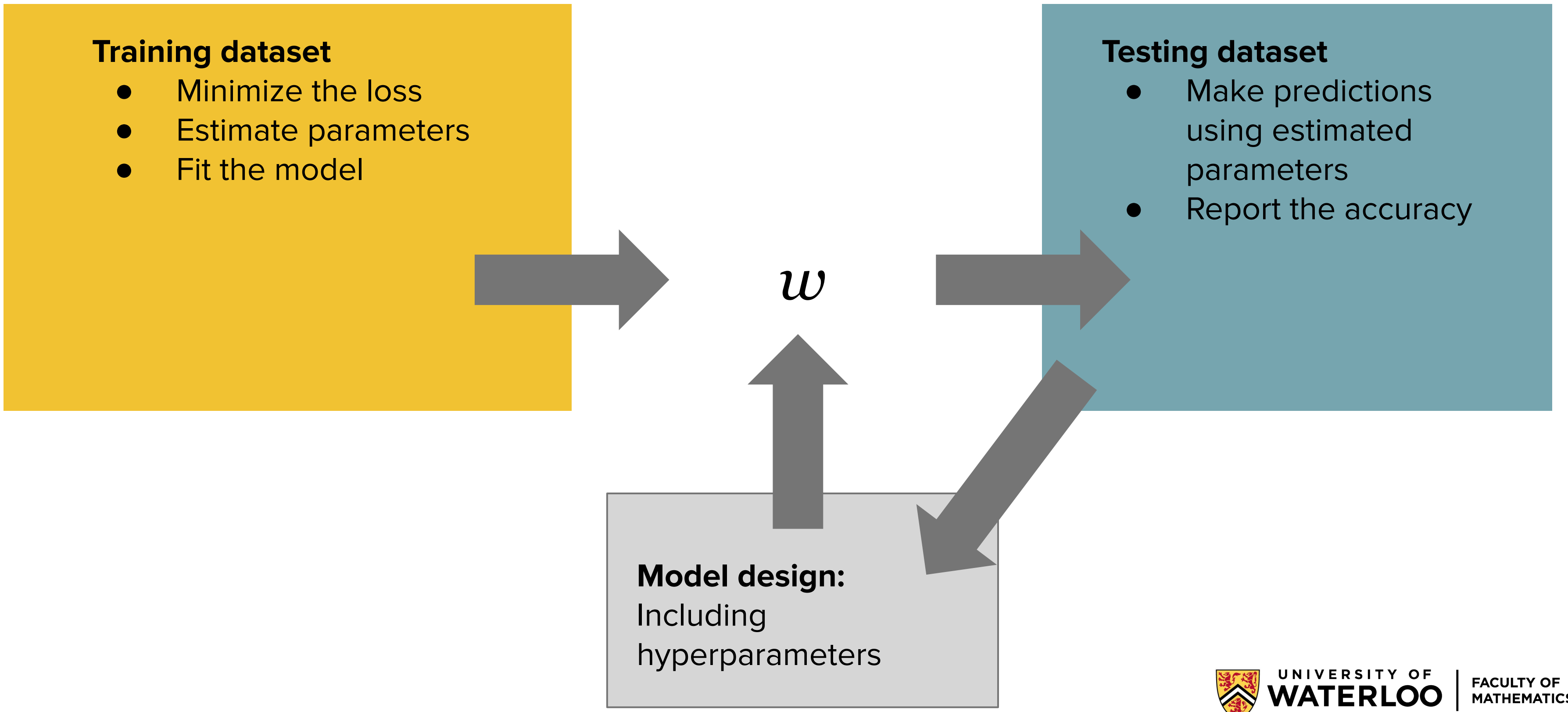
Training dataset
- Minimize the loss
- Estimate parameters
- Fit the model

w

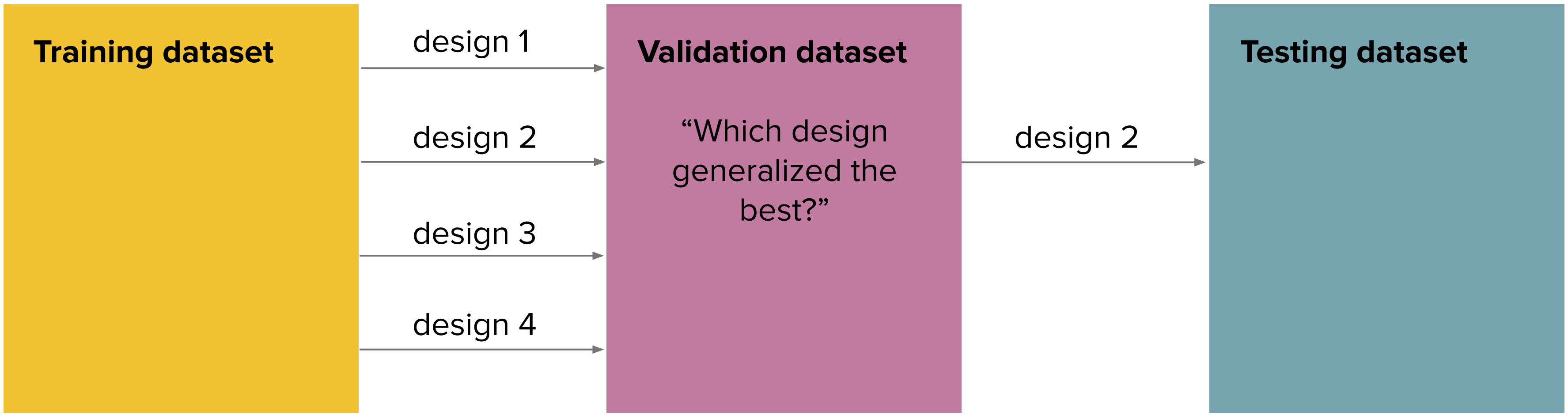
Testing dataset
- Make predictions using estimated parameters
- Report the accuracy

Model design:
Including hyperparameters

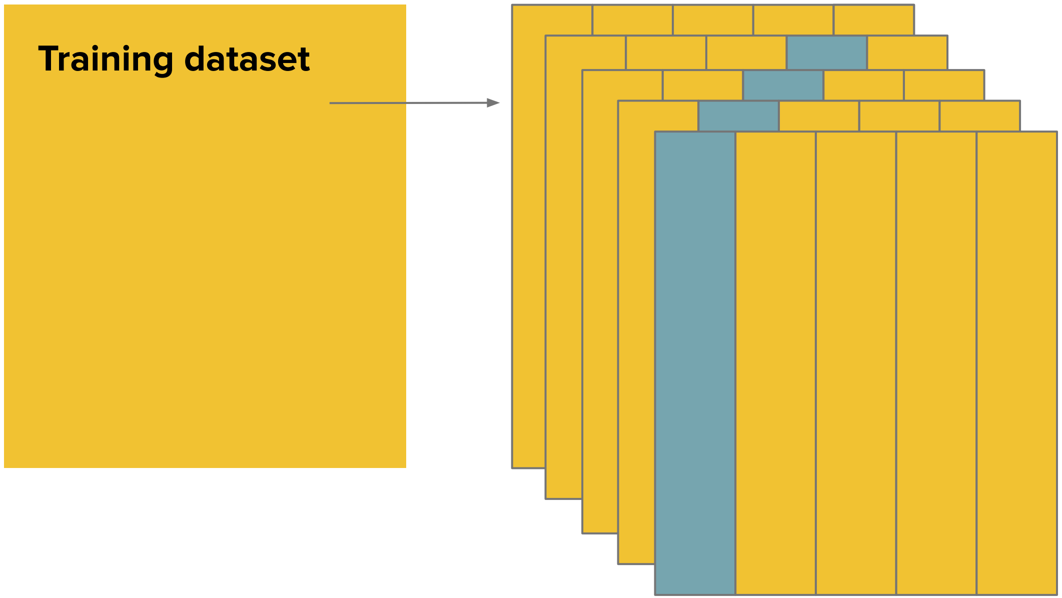
Incorrect use of training and testing datasets



Introducing a validation dataset



Cross-validation for small datasets



Algorithm 1 Cross-Validation.

Input:

Dataset $D = \{(x_i, y_i) \in \mathbb{R}^{d+1}\}$,

number of folds k

Output: Optimal hyperparameter λ

for $\lambda = \lambda_1, \lambda_2, \ldots$ **do**

  for i = 1,2,...,k **do**

    $w_{\lambda,i} = \text{train}(\cup_{j \neq i}^{k} D_j)$

    $\text{Perf}_{\lambda,i} = \text{Acc}(D_i)$

  end for

  $\text{Perf}_\lambda = \frac{1}{k} \sum_{i=1}^{k} \text{Perf}_{\lambda,i}$

end for

return $\text{argmax}_\lambda \text{Perf}_\lambda$

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Lecture	Date	Topics
~~0~~	~~05/09/2024~~	~~Introduction + Administrative Remarks~~
~~1~~	~~10/09/2024~~	~~Halfspaces the Perceptron Algorithm~~
~~2~~	~~12/09/2024~~	~~Linear Regression and Convexity~~
3	17/09/2024	Maximum Likelihood Estimation
4	19/09/2024	k-means Clustering
5	24/09/2024	k-NN Classification and Logistic Regression
6	26/09/2024	Hard-margin SVM
7	01/10/2024	Soft-margin SVM
8	03/10/2024	Kernel methods
9	08/10/2024	Decision Trees
10	10/10/2024	Bagging and Boosting
	15/10/2024	NO LECTURE - MIDTERM BREAK
	17/10/2024	NO LECTURE- MIDTERM BREAK
11	22/10/2024	Expectation Maximization Algorithm
12	24/10/2024	MLPs and Fully-Connected NNs
	29/10/2024	NO LECTURE - MIDTERM EXAM
13	31/10/2024	Convolutional Neural Networks
14	05/11/2024	Recurrent Neural Networks
15	07/11/2024	Attention and Transformers
16	12/11/2024	Graph Neural Networks (Time permitting)
17	14/11/2024	VAEs and GANs
18	19/11/2024	Flows
19	21/11/2024	Contrastive Learning (Time permitting)
20	26/11/2024	Robustness
21	28/11/2024	Privacy (Saber Malekmohammadi)
22	03/12/2024	Fairness

Visualizing the Loss Landscape of Neural Nets

Hao Li[1], Zheng Xu[1], Gavin Taylor[2], Christoph Studer[3], Tom Goldstein[1]
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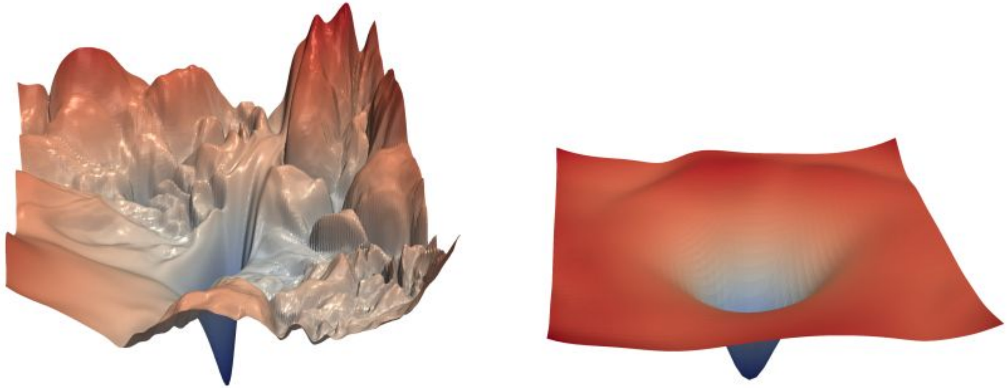
Abstract

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 fu
chosen training parameters (batch size, learning
ers that generalize better. However, the reason
effect on the underlying loss landscape, are not
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 bet
a variety of visualizations, we explore how net
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.