CS498: Algorithmic Engineering

Lecture 21: The Learning Problem & Stochastic Gradient Descent

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Week 12

Outline

1. Where We Are
2. The Learning Problem
3. Stochastic Gradient Descent
4. Adam, AdamW & Learning Rate Schedules
5. Putting It All Together: Lasso Regression
6. Summary

1 Where We Are

2 The Learning Problem

3 Stochastic Gradient Descent

4 Adam, AdamW & Learning Rate Schedules

5 Putting It All Together: Lasso Regression

6 Summary

Where We Are in the Course

Part I: Discrete Optimization (L1–9)
LP, IP, branch-and-bound, ...

Philosophy: structured discrete problems $\rightarrow$ exact solvers.

Part II: Continuous Opt & Metaheuristics (L10–16)
GD, convex optimization, Lagrangian, KKT, GA.

Philosophy: convexity gives guarantees; metaheuristics when it doesn't.

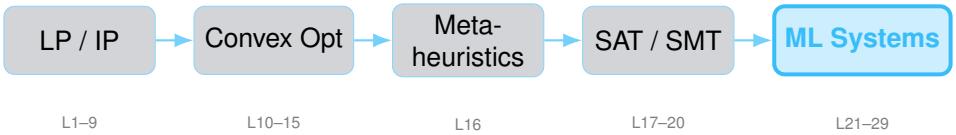
Part III: SAT/SMT (L17–20)
SAT, CDCL, SMT, Z3, formal verification.

Philosophy: encode constraints, let the solver search.

Part IV:Machine Learning Systems (L21–29)
Starts today.

Philosophy: what happens when the objective itself is **unknown**?

The Course Arc



Every tool we've built solves a **known** objective.
In ML, the objective **comes from data**.

What Changes Today?

Before: you are given $f(\mathbf{x})$ explicitly. Minimize it or satisfy constraints.

Now: you have **data** $\{(x_i, y_i)\}_{i=1}^n$, and we don't know the true relationship $y = g(x)$.

You **choose** two things:

- A **model** f_θ: a parameterized function that maps inputs to predictions.
  Examples: linear model $f_\theta(x) = \theta^\top \mathbf{x}$, polynomial, or (later) a neural network.
- A **loss function** L: measures how bad a prediction is for one θ.
  Examples: squared error $L(\hat{y}, y) = (\hat{y} - y)^2$, absolute error $|\hat{y} - y|$.

Then optimize:

$$\min_\theta \ \frac{1}{n} \sum_{i=1}^{n} L\big(f_\theta(x_i),\ y_i\big)$$

The question is... how do you choose f_θ? How do you optimize when n is enormous? And why does any of it generalize?

1 Where We Are

2 The Learning Problem

3 Stochastic Gradient Descent

4 Adam, AdamW & Learning Rate Schedules

5 Putting It All Together: Lasso Regression

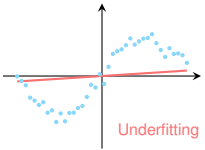
6 Summary

A Concrete Problem

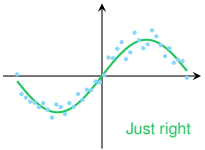
You measure $n = 100$ noisy data points from $y = \sin(x) + \varepsilon$.

Goal: fit a polynomial $\hat{y} = a_0 + a_1 x + a_2 x^2 + \cdots + a_d x^d$. Which degree d?

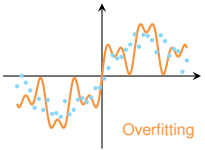
Degree 1



Degree 4



Degree 20



Which Model is Better?

Degree 1 (straight line):

- Low complexity, poor fit.
- **High bias**: the model can't capture the curve at all.

Degree 20 (wiggly polynomial):

- Perfect fit on training data (near-zero training loss).
- **High variance**: terrible on new data. Memorized the noise.

Key insight

We care about performance on **unseen** data: this is called **generalization**. A model that memorizes training data is useless.

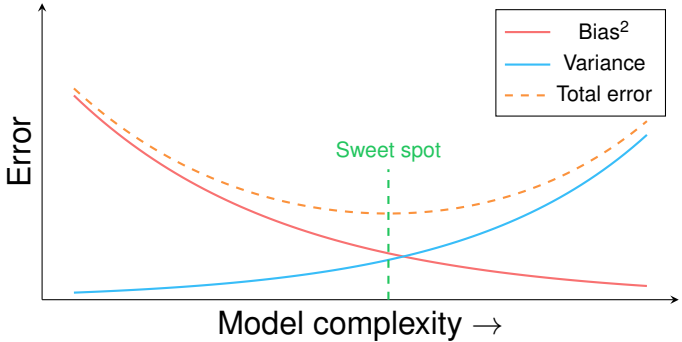
The Bias–Variance Decomposition

For any model, the **expected test error** decomposes as:

$$\underbrace{\mathbb{E}\left[(y - \hat{y})^2\right]}_{\text{Expected test error}} = \underbrace{\text{Bias}^2}_{\substack{\text{error from wrong} \\ \text{assumptions}}} + \underbrace{\text{Variance}}_{\substack{\text{sensitivity to} \\ \text{training set}}} + \underbrace{\sigma^2}_{\substack{\text{irreducible} \\ \text{noise}}}$$

- **Bias**: a degree-1 polynomial can never capture $\sin(x)$, no matter how much data.
- **Variance**: a degree-20 polynomial changes wildly depending on which data points you sample.
- **Noise** σ^2: no model can do better than this (the data is inherently noisy).

The Bias–Variance Tradeoff



The deal: too simple → high bias; too complex → high variance. The sweet spot minimizes total error.

Empirical Risk Minimization

How do we formalize “fit the data”?

Choose:

- A model family f_θ (e.g., degree-d polynomial, neural net).
- A loss function L (e.g., squared error $L(\hat{y}, y) = (\hat{y} - y)^2$).

Solve:

$$\min_\theta \underbrace{\frac{1}{n}\sum_{i=1}^{n} L\big(f_\theta(x_i),\ y_i\big)}_{\text{Empirical Risk } \hat{R}(\theta)}$$

In words: pick the parameters θ that minimize average loss on training data.

But. . .

Minimizing training loss perfectly gives us degree 20. We need something more.

Train / Test Split

The question is... how do we measure generalization without deploying the model?

Simple answer: split the data.

- **Training set** (80%): optimize θ on this.
- **Test set** (20%): evaluate final performance here. **Never** train on it.

The test set is a **proxy** for real-world performance.

But: what about **hyperparameters**? These are choices you make *before* training:

- Learning rate η, regularization strength λ, model architecture (number of layers, etc.).
- If you tune hyperparameters on the test set, it's no longer a fair evaluation.
- Solution: **validation set**, a third split used for tuning.
- Train on train, tune on validation, report on test.

Regularization = Constrained Optimization

Previously, we added constraints to optimization problems to penalize complexity: **Regularization**.

L2 regularization (ridge regression):

$$\min_{\theta} \frac{1}{n} \sum_{i=1}^{n} L\big(f_\theta(x_i), y_i\big) \; + \; \lambda \|\theta\|^2$$

- λ large $\rightarrow$ strong penalty on big weights $\rightarrow$ simpler model.
- $\lambda = 0$ $\rightarrow$ no penalty $\rightarrow$ back to plain ERM.

The deal: accept slightly worse training loss for **much better generalization**.

Classification and Cross-Entropy

So far our running example is regression ($y \in \mathbb{R}$). But what about **classification** ($y \in \{0, 1\}$)?

Idea: output a **probability** $\hat{y} = p(y = 1 \mid x) \in [0, 1]$.

Squared error $(\hat{y} - y)^2$ works, but does not penalize confident wrong predictions as sharply cross-entropy. We want a loss that **heavily penalizes confident wrong predictions**.

Cross-entropy loss (binary):

$$L(\hat{y}, y) \;=\; -\big[y \log \hat{y} + (1 - y) \log(1 - \hat{y})\big]$$

- If $y = 1$ and $\hat{y} \to 0$: $L \to +\infty$. Confident and wrong $\Rightarrow$ huge penalty.
- If $y = 1$ and $\hat{y} = 0.99$: $L \approx 0.01$. Confident and right $\Rightarrow$ tiny penalty.

Key insight: cross-entropy comes from information theory. It measures how "surprised" the model is by the true label.

Common Loss Functions

Task	Loss	Formula
Regression	Squared error	$L = (\hat{y} - y)^2$
Regression	Absolute error	$L = \lvert\hat{y} - y\rvert$
Classification	Cross-entropy	$L = -y \log \hat{y} - (1-y) \log(1-\hat{y})$
Classification	Hinge (SVM)	$L = \max(0,\ 1 - y\hat{y})$

Key insight: the loss function encodes what "good" means. Squared error penalizes big mistakes quadratically; absolute error is more robust to outliers.

The Learning Problem:Summary

The Learning Problem

1. **Given:** training data $\{(x_i, y_i)\}_{i=1}^n$
2. **Choose:** model family f_θ, loss function L
3. **Solve:** Minimize $\min_\theta \frac{1}{n} \sum_{i=1}^{n} L\big(f_\theta(x_i), y_i\big) + \lambda$ regularization on training data.
4. **Evaluate:** on held-out test data, fine tune hyperparameters on validation data.

This is **just optimization**.

The question is... how do we optimize when n is enormous?

1 Where We Are

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6 Summary

The Scale Problem

Modern datasets

- ImageNet: **1.2 million** images
- Common Crawl (LLM training): **3 trillion** tokens
- Spotify recommendations: **600 million+** users $\times$ 100 million tracks

Recall: gradient descent computes

$$\nabla_\theta \hat{R}(\theta) = \frac{1}{n} \sum_{i=1}^{n} \nabla_\theta \, L\big(f_\theta(x_i), y_i\big)$$

For $n = 10^9$, **one gradient step** touches every data point. That's absurd.

The question is... can we get a useful gradient without touching all the data?

SGD: The Key Idea

Stochastic Gradient Descent:

Sample a random **mini-batch** $B \subset \{1, \ldots, n\}$, $|B| = b$.

Compute the **stochastic gradient**:

$$g_B \;=\; \frac{1}{b} \sum_{i \in B} \nabla_\theta \, L\big(f_\theta(x_i), y_i\big)$$

Update: $\theta \;\leftarrow\; \theta - \eta \, g_B$

Key insight

$\mathbb{E}[g_B] = \nabla_\theta \hat{R}(\theta)$. The mini-batch gradient is an **unbiased estimate** of the full gradient.

Cost per step: $O(b)$ instead of $O(n)$.
If $b = 64$ and $n = 10^9$, that's a **15-million-fold speedup** per step.

Why Is the Estimate Unbiased?

Each $i \in B$ is sampled uniformly from $\{1, \ldots, n\}$.

For a single sample i:

$$\mathbb{E}_i\left[\nabla_\theta L(f_\theta(x_i), y_i)\right] = \frac{1}{n}\sum_{j=1}^{n} \nabla_\theta L(f_\theta(x_j), y_j) = \nabla_\theta \hat{R}(\theta)$$

Averaging b samples doesn't change the expectation:

$$\mathbb{E}[g_B] = \nabla_\theta \hat{R}(\theta)$$

But: the estimate has **variance**. Larger $b \to$ lower variance, higher cost.

Full-Batch GD vs. SGD

	Full-Batch GD	**SGD (mini-batch)**
Gradient	Exact $\nabla \hat{R}(\theta)$	Estimate g_B
Cost / step	$O(n)$	$O(b)$
Path	Smooth, deterministic	Noisy, stochastic
Memory	All data in memory	Only batch in memory

SGD Convergence

The mini-batch gradient g_B is unbiased, but it has **variance**:

$$\sigma^2 \;=\; \mathbb{E}\big[\|g_B - \nabla \hat{R}(\theta)\|^2\big]$$

In words: σ^2 measures how much the mini-batch gradient *fluctuates* around the true gradient. Smaller batch $\rightarrow$ larger σ^2.

For **convex** f with step size $\eta_t = c/\sqrt{T}$:

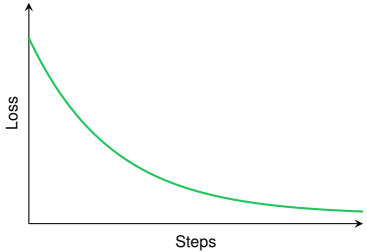
$$\mathbb{E}\big[f(\theta_T)\big] - f(\theta^*) \;\leq\; O\!\left(\frac{\|\theta_0 - \theta^*\|^2 + \sigma^2}{\sqrt{T}}\right)$$

SGD converges at rate $O(1/\sqrt{T})$, slower than GD's $O(1/T)$, but each step is **massively** cheaper.

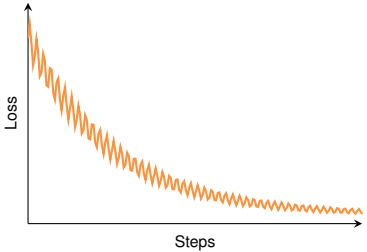
The deal: for the same wall-clock time, SGD typically makes far more progress because it takes many more (cheaper) steps.

The Variance–Computation Tradeoff

Large batch ($b = 512$)



Small batch ($b = 16$)



- **Larger batch** $\rightarrow$ lower variance $\rightarrow$ smoother curve, but more expensive per step.
- **Smaller batch** $\rightarrow$ higher variance $\rightarrow$ noisier, but cheaper and often converges to same final loss.
- **Rule of thumb:** batch sizes of 32–512 work well in practice.

An Epoch of SGD

Each batch $\rightarrow$ one gradient step $\rightarrow$ one θ update

1 epoch = 3 updates (if $b = 4$, $n = 12$)

SGD in Python

```python
import numpy as np

def sgd(X, y, theta, lr=0.01, batch_size=32, epochs=100):
    n = len(y)
    for epoch in range(epochs):
        # Shuffle data each epoch
        perm = np.random.permutation(n)
        X, y = X[perm], y[perm]
        for i in range(0, n, batch_size):
            X_b = X[i:i+batch_size]
            y_b = y[i:i+batch_size]
            grad = compute_gradient(theta, X_b, y_b)
            theta = theta - lr * grad
    return theta
```

Key points: shuffle each epoch (avoid cycles), process in mini-batches, update after each batch.

Why Does SGD Work for Neural Nets?

The elephant in the room

Neural networks define **non-convex** loss landscapes.
SGD convergence theory requires convexity.

Why does this work at all?

Three insights from the last decade of research:

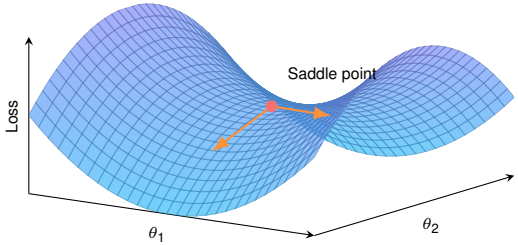
1. Benign loss landscapes
2. SGD noise helps escape bad regions
3. Implicit regularization

Insight 1: Benign Loss Landscapes

Overparameterized networks: more parameters than data points.

Key conjecture: in high dimensions, local minima have loss values **very close** to the global minimum.

The real obstacles are **saddle points**, not local minima.

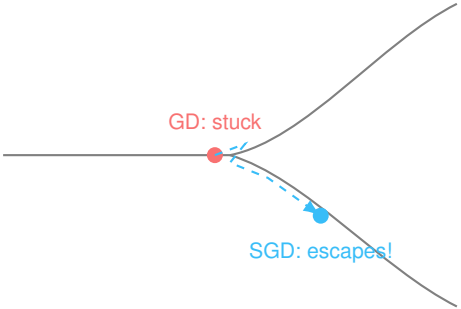


Insight 2: SGD Noise Helps

At a saddle point, the true gradient is zero (or near zero).

Full-batch GD: gets stuck. The gradient really is near zero.

SGD: the stochastic noise “kicks” the iterate away from saddle points.

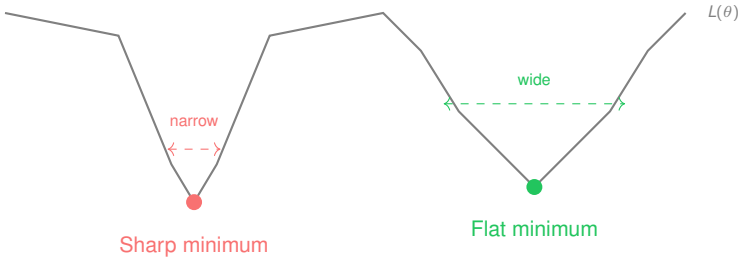


Noise breaks the symmetry at saddle points

The noise in SGD is a **feature**, not a bug.

Insight 3: Implicit Regularization

SGD with small batch sizes tends to converge to **flat** minima.



Both minima have similar training loss, but flat minima **generalize better**:

small perturbations to θ don't change the loss much.

Takeaway: SGD's noise acts as a natural regularizer, steering toward solutions that generalize well.

SGD for Non-Convex Problems:Summary

Why SGD works in practice

1. **Benign landscapes:** in overparameterized models, most local minima are nearly as good as the global minimum.
2. **Noise helps:** stochastic gradients escape saddle points that trap full-batch GD.
3. **Implicit regularization:** SGD noise biases the solution toward flat minima that generalize.

Key insight: theory for convex problems gives us the foundation. Practice shows SGD works far beyond what theory can prove.

1 Where We Are

2 The Learning Problem

3 Stochastic Gradient Descent

4 Adam, AdamW & Learning Rate Schedules

5 Putting It All Together: Lasso Regression

6 Summary

Can We Do Better Than Vanilla SGD?

Problem: vanilla SGD uses the **same** learning rate η for all parameters.

But parameters behave very differently:

- Some gradients are **large** and consistent, well-determined direction.
- Some gradients are **small** and noisy, uncertain direction.
- Some dimensions have steep curvature, others are flat.

The question is... can we **adapt** the learning rate per parameter?

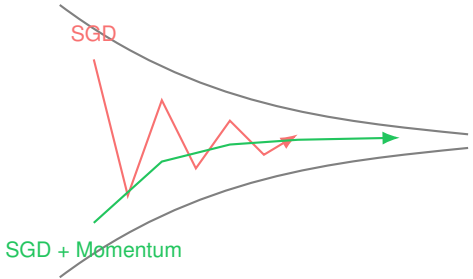
Momentum: Smoothing the Gradient

Before Adam, a key idea: **momentum**.

Instead of using g_t directly, maintain a running average:

$$m_t = \beta\, m_{t-1} + (1 - \beta)\, g_t$$

Update: $\theta \leftarrow \theta - \eta\, m_t$



Adam: Adaptive Moment Estimation

Adam combines **momentum** and **adaptive learning rates**:

First moment (smoothed gradient direction):

$$m_t = \beta_1 \, m_{t-1} + (1 - \beta_1) \, g_t$$

Second moment (smoothed gradient magnitude):

$$v_t = \beta_2 \, v_{t-1} + (1 - \beta_2) \, g_t^2$$

Bias correction: $\hat{m}_t = m_t / (1 - \beta_1^t), \quad \hat{v}_t = v_t / (1 - \beta_2^t)$

Update:

$$\theta \leftarrow \theta - \eta \cdot \frac{\hat{m}_t}{\sqrt{\hat{v}_t} + \varepsilon}$$

In words: move in the smoothed gradient direction, but **slow down** in dimensions with large gradients. Defaults: $\beta_1 = 0.9$, $\beta_2 = 0.999$, $\varepsilon = 10^{-8}$.

AdamW: The Weight Decay Fix

L2 regularization in Adam is NOT the same as weight decay

Adam + L2: the gradient of the penalty term $\lambda\theta$ gets scaled by the adaptive learning rate $1/\sqrt{\hat{v}_t}$.

This means the regularization strength **varies per parameter**. Not what we intended.

AdamW: apply weight decay **directly** to parameters, *separate* from the gradient:

$$\theta \leftarrow \theta - \eta \left(\frac{\hat{m}_t}{\sqrt{\hat{v}_t} + \varepsilon} + \lambda \theta \right)$$

The deal: AdamW **decouples** weight decay from the gradient update.

This is the standard optimizer choice for many modern large-scale neural network training runs.

Adam vs. AdamW: The Difference

Adam + L2

$g_t \leftarrow \nabla L(\theta) + \lambda\theta$

m_t, v_t from g_t

$\theta \leftarrow \theta - \eta\, \hat{m}_t / (\sqrt{\hat{v}_t} + \varepsilon)$

Regularization gets scaled by $1/\sqrt{\hat{v}_t}$

Coupling problem

AdamW

$g_t \leftarrow \nabla L(\theta)$

m_t, v_t from g_t

$\theta \leftarrow \theta - \eta\big(\hat{m}_t / (\sqrt{\hat{v}_t} + \varepsilon) + \lambda\theta\big)$

Weight decay applied uniformly

Decoupled, correct

Loshchilov & Hutter (2019): this seemingly small fix **consistently improves generalization**.

Learning Rate Schedules

Problem: a constant learning rate is suboptimal.

- Too high $\rightarrow$ diverge or oscillate.
- Too low $\rightarrow$ converge painfully slowly.

Cosine decay:

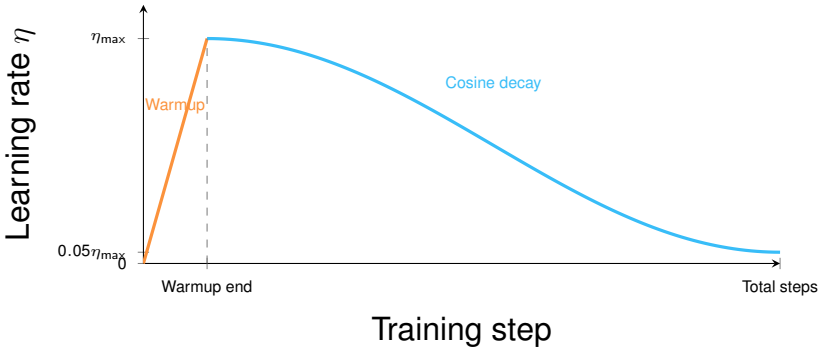
$$\eta_t = \eta_{\min} + \frac{1}{2}(\eta_{\max} - \eta_{\min})\left(1 + \cos\left(\frac{t - T_w}{T - T_w} \cdot \pi\right)\right)$$

In words: start carefully, take larger steps after warmup, then decay smoothly for fine-tuning.

Why warmup? Early gradients are unreliable; small initial steps let Adam's moments stabilize.

Learning Rate Schedule: Visual

Linear warmup followed by cosine decay:



Learning Rate Warmup: Intuition

At initialization, the model weights are **random**.

- Gradients in the first few steps point in essentially **random** directions.
- Adam's running averages m_t, v_t have no history yet.
- A large LR + unreliable gradients = **destructive updates**.

Warmup (typically 1–5% of total training):

- Start with tiny LR, ramp up linearly.
- By the time LR reaches its peak, Adam's moments are well-calibrated.

Key insight: warmup is the "calibration phase" for adaptive optimizers.

Optimizers: Comparison

	SGD	Adam	AdamW
Adaptive LR	×	✓	✓
Momentum	Optional	Built-in	Built-in
Weight decay	Correct	Coupled	Decoupled
Hyperparams	η	η, β_1, β_2	$\eta, \beta_1, \beta_2, \lambda$
Used for LLMs	Rarely	Sometimes	**Almost always**

Takeaway: AdamW with warmup + cosine decay is the standard recipe for training large neural networks.

Putting It All Together

```
import math
import torch
optimizer = torch.optim.AdamW(
    model.parameters(),
    lr=1e-3,
    weight_decay=0.01
)
def lr_lambda(step, warmup=2000, total=100000):
    if step < warmup:
        return step / warmup
    progress = (step - warmup) / (total - warmup)
    progress = min(progress, 1.0)
    return 0.5 * (1 + math.cos(math.pi * progress))

scheduler = torch.optim.lr_scheduler.LambdaLR(
    optimizer,
    lr_lambda=lr_lambda)

...
optimizer.step()   # update weights
scheduler.step()   # update learning rate for future steps
```

1 Where We Are

2 The Learning Problem

3 Stochastic Gradient Descent

4 Adam, AdamW & Learning Rate Schedules

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6 Summary

Everything in Action

We now have all the pieces. Let's use them on a real problem.

Problem: predict California housing prices from 8 features, with $n = 20{,}640$ houses.

Model: linear regression $\hat{y} = \mathbf{w}^\top \mathbf{x} + b$ with **L1 regularization** (Lasso):

$$\min_{\mathbf{w},\, b} \; \frac{1}{n} \sum_{i=1}^{n} \left(\mathbf{w}^\top \mathbf{x}_i + b - y_i \right)^2 + \lambda \|\mathbf{w}\|_1$$

Why Lasso?

- **ERM:** squared loss.
- **Regularization:** $\lambda \|\mathbf{w}\|_1$ encourages **sparse** solutions.
- **Feature selection:** Lasso tells you which features *matter*.

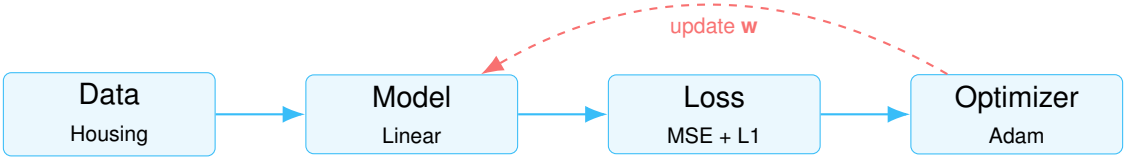
Lasso with SGD:The Code

```
import torch
from sklearn.datasets import fetch_california_housing
from torch.utils.data import DataLoader, TensorDataset
# Load data
X, y = fetch_california_housing(return_X_y=True)
X = torch.tensor(X, dtype=torch.float32)
y = torch.tensor(y, dtype=torch.float32)

# Train/test split (80/20)
X_train, X_test = X[:16512], X[16512:]
y_train, y_test = y[:16512], y[16512:]

# Normalize using training mean/std only
mean = X_train.mean(dim=0)
std = X_train.std(dim=0)

X_train = (X_train - mean) / std
X_test = (X_test - mean) / std

loader = DataLoader(TensorDataset(X_train, y_train), batch_size=256, shuffle=True)
```

Lasso with SGD:Training

```
w = torch.randn(8, requires_grad=True)
b = torch.zeros(1, requires_grad=True)
optimizer = torch.optim.Adam([w, b], lr=0.01)
lam = 0.1  # L1 regularization strength

for epoch in range(100):
    for X_batch, y_batch in loader:
        y_hat = X_batch @ w + b
        mse = ((y_hat - y_batch)**2).mean()       # ERM
        l1 = lam * w.abs().sum()                   # regularization
        loss = mse + l1
        optimizer.zero_grad()
        loss.backward()
        optimizer.step()
```

What Just Happened?



Everything from this lecture:

- **ERM:** minimize MSE on training data.
- **Regularization:** L1 penalty drives unimportant weights to zero.
- **Mini-batch SGD + Adam:** scalable optimization on 20K data points.
- **Train/test split:** verify generalization on held-out data.

But: this model is **linear**. It can only capture linear relationships.

Can we do better? $\Rightarrow$ Next lecture: neural networks, nonlinear function approximators.

1 Where We Are

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6 Summary

Key Takeaways

1. **ML is optimization under uncertainty:** the objective comes from data, not a formula.
2. **Generalization is everything:** train/test split, regularization, and the bias-variance tradeoff.
3. **SGD makes scale possible:** unbiased gradient estimates at a fraction of the cost.
4. **Adam/AdamW is the standard:** adaptive LR + decoupled weight decay.
5. **The noise in SGD is a feature:** it escapes saddle points and regularizes implicitly.